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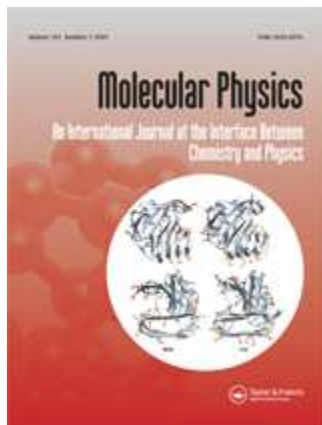
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Conformers of gaseous threonine

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Conformers of Gaseous Threonine

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Abstract

Following an extensive search on the potential energy surfaces (PES) of the natural amino acid L-threonine (Thr) and its allotropic form L-allo-threonine (aThr), 56 and 61 conformers of Thr and aThr, respectively, have been located with the help of density functional theory (DFT). Accurate structures, relative energies, rotational as well as quartic and sextic centrifugal distortion constants, dipole moments, ^{14}N nuclear quadrupole coupling constants, anharmonic vibrational frequencies and double-harmonic infrared intensities have been determined from *ab initio* electronic structure calculations for the five most stable Thr and aThr conformers. The global minimum, **Thr-I**, has a cyclic triple H-bond motif with strong $\text{OH}\cdots\text{N}$, $\text{C}=\text{O}\cdots\text{HO}$, and a weaker $\text{NH}\cdots\text{OH}$ H-bond, where the latter two involves the side chain OH, and an energetically unfavorable trans $-\text{COOH}$ arrangement. The best relative energies of the conformers, accurate within $\pm 1 \text{ kJ mol}^{-1}$, have been determined through the first-principles composite focal-point analysis (FPA) approach. There are four and three conformers of Thr and aThr, respectively, within a relative energy of 5 kJ mol^{-1} . Similarly to other amino acids investigated, lower levels of electronic structure theory, especially the Hartree–Fock level, are unable to determine the correct relative energies of the conformers. The rotational, the quartic and sextic centrifugal distortion, and the ^{14}N nuclear quadrupole coupling constants as well as the anharmonic vibrational fundamentals and double-harmonic infrared intensities, all determined using DFT, should aid identification and characterization of the conformers of threonine and allo-threonine by rotational and vibrational spectroscopies, respectively.

Keywords: neutral L-threonine • neutral L-allo-threonine • amino acids • *ab initio* calculations • conformational analysis • structure elucidation

This paper is dedicated to Professor Fritz Schaefer on the occasion of his 65th birthday.

I. INTRODUCTION

During the last decades, determination and characterization of the structures of biomolecules, in particular those of proteins and peptides, have been in the focal point of experimental and theoretical research. Since amino acids (AA) are the building blocks of these biopolymers, the structural investigation of AAs, extending from solids to the gas phase, also received considerable attention. Experimental and theoretical structural investigations related to AAs, executed prior to 1999, have been reviewed in ref. 1. During the last decade a considerable number of novel experimental and first-principles computational investigations have been performed on different aspects of the structures of amino acids [2-4], peptides [5,6], and their various complexes [7]. The review of all these studies is out of the scope of the present study and thus only a small number of high-level computational studies originating from our own group are mentioned.

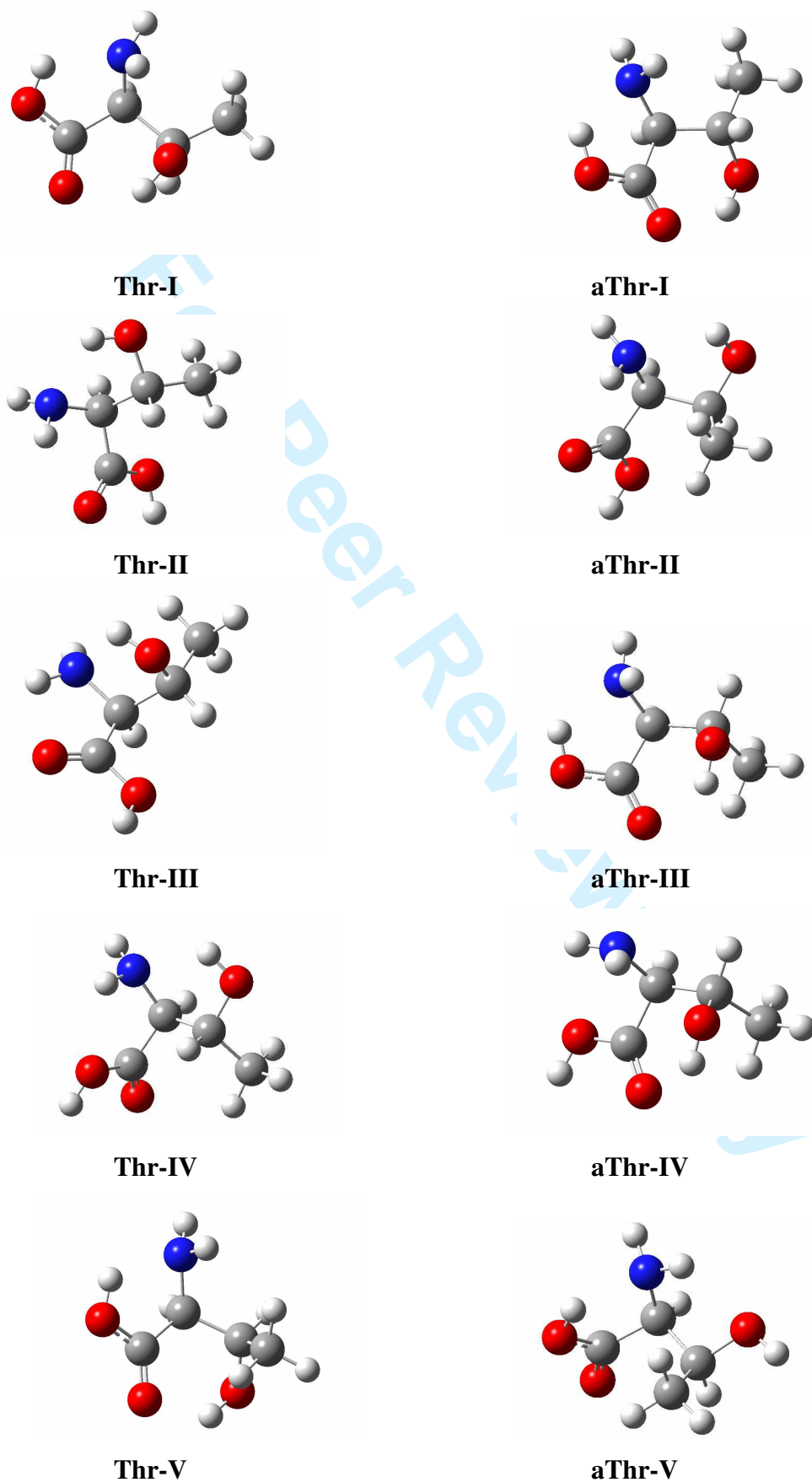
There is only a limited number of natural amino acids and the relatively small size of these molecules allows the application of highly sophisticated experimental and computational techniques during studies related to their equilibrium and dynamical structures usually investigated through their rotational-vibrational spectra. Consequently, we have a detailed understanding of the basics of the structural characteristics of AAs. AAs are chiral, with the sole exception of glycine. In solution and in the solid state, AAs are found in different zwitterionic forms. In the gas phase, however, AAs exist in their neutral form. Furthermore, as AAs are very flexible molecules, all of them exhibit a large number of low-energy conformers and a complex, highly structured potential energy surface (PES). Due partially to the low volatility of AAs and their tendency to decomposition when heated, most of these conformers are not amenable to experimental scrutiny but they can be subjected to detailed quantum chemical investigations. Characterization of the complex PESs of amino acids should precede and supplement related experimental structural studies.

Chiral AAs can play a role in chirally selective organocatalysis, the most important amino acid in this respect appears to be proline (Pro) [8]. As to other applications of AAs in chemistry, one may mention functionalization of fullerenes, carbon nanotubes and semiconductor quantum dots with amino acids [9]. Search for signs of life in the universe is also based principally on structural and spectroscopic characterization of AAs [10]. As of today, it seems that none of the AAs have been found outside of our own planet. Threonine, being an essential amino acid is involved in many studies with biochemical importance, for which the present conformational results could prove useful. As examples, we mention the

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3 studies of metallic complexes of threonine [11-13] and the possible use of Thr and its
4 derivatives in organocatalysis [14].
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7 The number of local minima on the respective PESs and the structural properties of the
8 related conformers, including accurate relative energy estimates, are available for a number of
9 amino acids [1]. The most accurate relative energies, mostly obtained within the focal-point
10 analysis (FPA) approach [15,16], are available for the amino acids glycine (Gly) [4,17-19],
11 alanine (Ala) [18,20], and proline (Pro) [1-3]. The present computational study expands the
12 list of structurally particularly well characterized amino acids by establishing all of the lower-
13 energy and almost all of the higher-energy conformers of L-threonine (see Figure 1), one of
14 the two amino acids, the other one being isoleucine, exhibiting two chirality centers. This
15 feature of threonine was one of the reasons for performing this study. The two diastereomers
16 need to be examined separately during conformational and spectroscopic studies as for all
17 practical purposes they appear as two distinct molecules. Obviously, both L-threonine and L-
18 allo-threonine has an enantiomer pair, D-threonine and D-allo-threonine, respectively. In what
19 follows, L-threonine and L-allo-threonine will be abbreviated as Thr and aThr, respectively. In
20 the biosphere only Thr is abundant. Detailed structural characterization of the lowest-energy
21 conformers of these diastereomers was another important aim of the present study. The
22 present study yielded, as primary information, equilibrium structures, relative energies, and a
23 large number of spectroscopic molecular parameters related to the vibrational and rotational
24 spectra of the most important conformers of the two forms of threonine, Thr and aThr. The
25 computational results obtained should help identification of at least some of the conformers of
26 threonine by means of rotational and vibrational spectroscopies.
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Figure 1. Pictorial representation of the five lowest-energy conformers of L-threonine (Thr) and L-allo-threonine (aThr)



II. COMPUTATIONAL DETAILS

Most of the atom-centered Gaussian basis sets selected for the electronic structure computations of this study contain both polarization and diffuse functions, as they are both needed for the determination of accurate structures and relative energies for H-bonded systems [21]. The subcompact 3-21G basis [22] lacks these functions and thus it has been used only for pre-screening the conformers at the Hartree–Fock [23] level of electronic structure theory. The 6-31G* [24] and 6-311++G** [25] bases, used in this study extensively for geometry optimizations and subsequent force field determinations, contain 260 and 369 contracted Gaussian functions (CGFs), respectively, for threonine. The correlation-consistent, polarized-valence (aug)-cc-p(C)VnZ, $n = 2$ (D), 3 (T), 4 (Q) basis sets of Dunning and coworkers [26,27] have been employed extensively for single-point energy calculations within the FPA approach. (Note that only the augmented (aug) basis set contains diffuse functions, while tight functions, necessary for calculation of core correlation [28] and relativistic effects [29] are only part of core-polarized (C) basis sets.) For Thr, the aug-cc-pVDZ, cc-pVTZ, cc-pCVTZ, aug-cc-pVTZ, and aug-cc-pVQZ basis sets contain 265, 366, 470, 575, and 1054 CGFs, respectively. Only the pure spherical harmonics have been employed in the cc basis sets used in this study.

Electronic wave functions have been determined in this study by the single-configuration, self-consistent-field, restricted Hartree–Fock (RHF) method [23,30,31], by second-order Møller–Plesset perturbation theory, *i.e.*, MP2 [32], by coupled cluster (CC) methods [33] including all single and double excitations (CCSD) [34] and in cases, additionally, a perturbative correction for contributions from connected triple excitations [CCSD(T)] [35], and by a hybrid density functional theory (DFT) approach usually abbreviated as B3LYP [36]. The T_1 diagnostic values of coupled cluster theory [37] are around 0.013 for the different conformers of Thr, suggesting that they can adequately be described by single-reference-based electron correlation methods. The eight lowest 1s-like core orbitals were kept frozen in all post-Hartree–Fock treatments unless otherwise noted.

Rotation barriers corresponding to the methyl group were computed via restricted optimizations [38-40], fixing the methyl torsional coordinate, at the MP2/cc-pVDZ level.

The electronic structure program packages Gaussian03 [41] and MOLPRO [42] have been used extensively during this study. The package MAB-ACESII [43] was employed for the methyl rotational barrier computations.

II.1. Geometry optimizations

Similarly to a scheme first employed for glycine [17], the conformers of Thr and aThr determined in this study are numbered by Roman numerals (see Figure 1) and reflect the energy order of the conformers determined at the B3LYP/6-311++G** level.

Initial structures for the geometry optimizations of the conformers of Thr and aThr were generated by replacing the appropriate H atom of the global minimum of serine with a CH₃ group followed by an optimization at the HF/3-21G level. Then, 5 of the 6 torsional angles characterizing threonine, CCOH (carboxyl), CCC=O, CCNH, CCC-O, and CCOH (side chain), were modified systematically by 60 degrees. This resulted in $6^5 = 7776$ initial structures for one diastereomer. Initial geometry optimizations on the 7776 structures were performed for each diastereomer at the inexpensive RHF/3-21G level. This simple level of electronic structure theory was chosen for the prescreening of the conformers as it was widely assumed [1] that the RHF/3-21G PESs of amino acids and peptides are more structured than their counterparts determined at more sophisticated, and thus computationally more demanding levels of electronic structure theory. Further optimizations were executed at the more reliable B3LYP/6-31G*, B3LYP/6-311++G**, and MP2/aug-cc-pVTZ levels. Initial structures for the latter optimizations were the local minima found on the RHF/3-21G PES of Thr and aThr.

Relative energies of the lowest-energy conformers of Thr and aThr, obtained by geometry optimizations at the HF/3-21G, DFT(B3LYP)/6-31G*, DFT(B3LYP)/6-311++G**, and MP2/aug-cc-pVTZ levels, are given in Table 1. Cartesian coordinates of the optimized structures and energies of all the conformers found in this study are provided as Supplementary Material.

Table 1. Relative energies (kJ mol^{-1}) of the most stable L-threonine and L-allo-threonine conformers obtained from geometry optimizations performed at the MP2/aug-cc-pVTZ, DFT(B3LYP)/6-311++G**, DFT(B3LYP)/6-31G*, and RHF/3-21G levels^[a]

Conformer	MP2/ aug-cc-pVTZ	DFT(B3LYP)/ 6-311++G**	DFT(B3LYP)/ 6-31G*	RHF/ 3-21G
Thr-I	0.00	0.00	0.00	0.00
Thr-II	2.54	1.34	3.18	4.24
Thr-III	4.29	4.33	7.15	-0.96
Thr-IV	4.41	4.80	1.38	3.54
Thr-V	6.77	5.34	9.07	7.69
Thr-VI		7.30		2.68
Thr-VII		7.86		9.95
Thr-VIII		8.06		11.16
Thr-IX		10.82		24.21
Thr-X		11.34		-0.71
Thr-XI		11.47		4.49
Thr-XII		11.91		14.07
aThr-I	0.00	0.00	0.00	0.00
aThr-II	-1.13	0.64	5.48	-0.30
aThr-III	3.18	4.13	4.27	1.39
aThr-IV	5.79	6.43	8.77	1.87
aThr-V	3.50	7.08	13.65	12.53
aThr-VI		7.23		13.02
aThr-VII		7.30		8.32
aThr-VIII		7.42		14.56
aThr-IX		8.11		7.36
aThr-X		8.21		5.62
aThr-XI		10.01		7.81
aThr-XII		10.10		19.49
aThr-XIII		10.13		0.34

^[a] The relative energies of conformer **aThr-I** with respect to conformer **Thr-I** at the MP2, B3LYP/6-311++G**, B3LYP/6-31G*, and RHF levels is 3.67, 2.20, -1.06, and 2.37 kJ mol^{-1} , respectively.

II.2. Focal-point analysis (FPA)

In order to obtain accurate estimates of the relative energies of the conformers of Thr and aThr with corresponding uncertainties, the FPA approach [15,16] was utilized for both diastereomers. The five lowest-energy structures of Thr and aThr (Figure 1), obtained at the B3LYP/6-311++G** level, were included in this investigation.

Extrapolation of the energies to the complete basis set (CBS) limit at the RHF and MP2 levels was performed, as part of the FPA approach, using the formulas $E_n = E_{\text{CBS}} + A(n+1)\exp(-9\sqrt{n})$ [44] and $\varepsilon_n = \varepsilon_{\text{CBS}} + Bn^{-3}$ [45], respectively. In these formulas n is the cardinal number of the augmented, correlation-consistent basis sets aug-cc-pVnZ ($n \in \{3,4\}$), A and B are parameters, E_n is the RHF energy, and ε_n is the MP2 correlation energy increment, and CBS refers to the complete basis set limit. Energy corrections were treated additively, taking advantage of the fact that the contribution of higher-level electron correlation to the requested relative energies does not change significantly with the size of the basis set. CCSD and CCSD(T) correlation energy increments were calculated using the cc-pVTZ basis set.

From the auxiliary corrections needed to be determined within the FPA approach, the core correction was obtained at the MP2/cc-pCVTZ level as the difference between explicit frozen-core (fc) and all-electron (ae) energy computations. The relativistic contributions to the relative energies were estimated within the Douglas-Kroll (DK) formalism [46], as implemented in MOLPRO, at the MP2(ae)/cc-pCVTZ level. After deemed to be unimportant even at the level of precision of this study, the diagonal Born–Oppenheimer corrections (DBOC) [47] were not computed and thus were completely neglected. Zero-point vibrational energies (ZPVE) were obtained as harmonic and anharmonic correction values at the B3LYP/6-311++G** and B3LYP/6-31G* levels, respectively.

The resulting composite single-point relative energies are shown in Tables 2 and 3 for Thr and aThr, respectively.

Table 2. FPA relative energies and energy increments (δ), all in kJ mol^{-1} , for the 5 lowest-energy conformers of L-threonine^[a]

Energy term	Basis	Thr-I	Thr-II	Thr-III	Thr-IV	Thr-V
RHF	aug-cc-pVDZ	0.00	-3.14	-2.01	7.52	0.42
	aug-cc-pVTZ	0.00	-3.01	-2.11	7.80	0.72
	aug-cc-pVQZ	0.00	-2.99	-2.20	7.80	0.77
	CBS	0.00	-2.99	-2.21	7.79	0.78
δ [MP2]	aug-cc-pVDZ	0.00	4.60	6.25	-2.48	5.05
	aug-cc-pVTZ	0.00	5.36	6.47	-3.43	5.90
	aug-cc-pVQZ	0.00	5.36	6.43	-3.47	5.94
	CBS	0.00	5.36	6.39	-3.49	5.98
δ [CCSD]	cc-pVTZ	0.00	-0.74	-1.38	0.66	-0.93
δ [CCSD(T)]	cc-pVTZ	0.00	0.93	1.35	-1.08	1.19
MP2(ae) – MP2(fc)	cc-pCVTZ	0.00	0.08	0.00	0.04	0.08
Relativistic	cc-pCVTZ	0.00	-0.05	0.00	0.03	-0.04
ZPVE(harm)		0.00	-0.41	-1.05	0.68	-0.72
ZPVE(anharm) – ZPVE(harm)		0.00	0.14	0.20	-0.21	0.44
FPA relative energies		0.00	2.32	3.30	4.42	6.77

^[a] All the FPA energy computations were performed employing the fully optimized B3LYP/6-311++G** structures as references. Energy increments (δ) refer to the previous level of theory, MP2 to RHF, CCSD to MP2, and CCSD(T) to CCSD. The abbreviations (fc) and (ae) show that the correlated-level electronic structure computations were done with the frozen core approximation or with all electrons, respectively. The ZPVE(harm)s (harmonic zero-point vibrational energies) correspond to B3LYP/6-311++G** harmonic frequencies. The ZPVE(anharm)s (anharmonic zero-point vibrational energies) were obtained at the B3LYP/6-31G* level based on quartic normal coordinate force fields and second-order vibrational perturbation theory (VPT2).

Table 3. FPA relative energies and energy increments (δ), all in kJ mol^{-1} , for the 5 lowest-energy conformers of L-allo-threonine.^[a]

Energy term	Basis	aThr-I	aThr-II	aThr-III	aThr-IV	aThr-V
RHF	aug-cc-pVDZ	0.00	-8.53	2.19	-3.63	4.70
	aug-cc-pVTZ	0.00	-8.55	2.22	-3.17	4.66
	aug-cc-pVQZ	0.00	-8.42	2.40	-2.98	4.88
	CBS	0.00	-8.41	2.43	-2.95	4.91
δ [MP2]	aug-cc-pVDZ	0.00	6.46	0.47	7.56	-1.77
	aug-cc-pVTZ	0.00	7.94	1.18	9.11	-0.66
	aug-cc-pVQZ	0.00	8.25	1.41	9.39	-0.29
	CBS	0.00	8.48	1.57	9.60	-0.01
δ [CCSD]	cc-pVTZ	0.00	-1.54	-0.68	-2.32	0.26
δ [CCSD(T)]	cc-pVTZ	0.00	2.14	0.53	1.89	0.89
MP2(ae) – MP2(fc)	cc-pCVTZ	0.00	-0.01	0.04	0.08	-0.04
Relativistic	cc-pCVTZ	0.00	-0.05	-0.03	-0.06	-0.02
ZPVE(harm)		0.00	-1.40	-0.53	-0.85	-0.91
ZPVE(anharm) – ZPVE(harm)		0.00	-0.01	0.09	-0.02	0.13
FPA rel. energies		0.00	-0.80	3.42	5.37	5.21

^[a] See footnote [a] to Table 2. The relative energy of conformer **aThr-I** with respect to conformer **Thr-I** is 3.07 kJ mol^{-1} .

II.3. Spectroscopic parameters

For all local minima, quadratic force constants were computed at the B3LYP/6-311++G** level using the B3LYP/6-311++G** optimized structures, thus avoiding the nonzero-force dilemma [48]. For the five lowest-energy conformers of Thr and aThr quartic force fields in normal coordinate space have been determined at the B3LYP/6-31G* level, again at the fully optimized B3LYP/6-31G* structure. The related harmonic and anharmonic vibrational fundamentals of Thr and aThr are reported in Tables 4 and 5, respectively. No scaling of the force fields or of the resulting vibrational wavenumbers has been attempted. The anharmonic vibrational fundamentals were obtained through second-order vibrational perturbation theory (VPT2) [49].

The optimized structures determine the equilibrium rotational constants, while the quadratic and cubic force fields yield the equilibrium quartic and sextic centrifugal distortion constants in the *A*-reduced representation. The anharmonic force fields determined also allow the calculation of vibrationally averaged ground-state rotational constants. For the five lowest-energy Thr and aThr conformers these spectroscopic constants are reported in Tables 6 and 7, respectively.

The ^{14}N nuclear quadruple coupling constants, resulting from the non-spherical distribution of the nuclear charge, have been determined at the B3LYP/6-311++G** level.

Table 4. Harmonic vibrational fundamentals (ω), their VPT2 anharmonic corrections ($\Delta\nu$), and double-harmonic vibrational intensities (I) of the 5 lowest energy conformers of L-threonine^[a]

number	Thr-I			Thr-II			Thr-III			Thr-IV			Thr-V		
	ω	$\Delta\nu$	I	ω	$\Delta\nu$	I	ω	$\Delta\nu$	I	ω	$\Delta\nu$	I	ω	$\Delta\nu$	I
1	3819	-177	46.8	3742	-186	64.9	3762	-188	84.1	3705	-195	131.3	3758	-187	78.7
2	3595	-181	15.3	3708	-199	91.8	3713	-196	60.9	3600	-182	16.1	3718	-198	84.5
3	3495	-108	11.1	3582	-181	12.1	3612	-183	21.9	3518	-129	1.1	3592	-181	11.8
4	3455	-262	277.5	3497	-191	6.2	3516	-142	18.8	3467	-259	264.4	3511	-105	4.8
5	3114	-142	18.4	3115	-142	18.9	3109	-148	23.5	3114	-143	15.6	3113	-143	18.3
6	3098	-141	28.9	3109	-143	24.4	3095	-135	35.2	3086	-113	26.6	3107	-143	24.9
7	3055	-131	9.9	3085	-139	8.3	3078	-130	2.0	3055	-138	5.1	3092	-141	5.7
8	3041	-119	7.7	3040	-133	13.2	3023	-160	23.0	3034	-144	29.1	3038	-134	11.9
9	3033	-132	13.5	2959	-106	38.3	3000	-137	19.8	3021	-165	21.4	2964	-109	39.5
10	1824	-31	324.4	1800	-31	296.8	1808	-33	304.2	1808	-31	287.4	1811	-29	321.0
11	1651	-50	32.9	1662	-31	39.5	1642	-58	77.4	1658	-48	38.1	1659	-57	36.8
12	1503	-42	4.4	1502	-36	3.2	1501	-73	4.8	1502	-51	9.7	1502	-39	4.0
13	1484	-9	6.7	1484	-20	6.0	1489	-39	6.0	1491	-48	5.5	1483	-19	3.6
14	1430	-34	6.3	1441	-46	54.3	1431	-30	55.5	1445	-39	16.5	1439	-47	44.4
15	1418	-40	427.2	1425	-32	4.4	1416	-44	23.4	1419	-45	232.8	1409	-32	29.7
16	1409	-34	9.6	1404	-34	23.6	1401	-17	5.6	1409	-33	215.9	1400	-36	0.9
17	1387	-36	4.9	1375	-5	20.3	1370	-34	11.6	1394	-39	21.4	1377	-5	3.6
18	1359	-35	8.0	1339	-19	31.8	1337	-4	24.0	1371	-33	41.7	1333	-14	53.6
19	1280	-32	57.0	1311	-11	81.1	1302	-30	3.1	1311	-30	18.0	1309	-26	59.6
20	1276	-37	0.4	1265	-39	7.5	1258	-31	21.0	1270	-23	2.5	1289	-29	14.8
21	1209	-40	21.5	1226	-33	20.0	1221	-35	49.2	1220	-46	23.6	1229	-18	17.5
22	1197	-37	9.7	1158	-34	75.1	1162	-33	112.9	1192	-36	9.6	1163	-37	213.1
23	1151	-29	24.6	1136	-31	167.6	1136	-32	154.5	1140	-32	8.9	1138	-31	43.8
24	1084	-24	14.4	1113	-40	54.7	1104	-28	27.3	1106	-31	50.5	1110	-37	7.7
25	1052	-18	55.9	1074	-29	12.9	1076	-30	52.8	1090	-31	79.6	1072	-31	14.8
26	1017	-24	11.5	1052	-21	35.6	1026	-22	25.2	1045	-21	5.2	1050	-19	31.7
27	984	-35	88.3	958	-41	46.6	937	-28	0.7	968	-32	23.1	932	-41	16.9
28	909	-24	54.3	925	-22	35.3	892	-45	77.0	903	-41	84.1	921	-23	88.3
29	878	-47	103.5	872	-29	38.8	869	-24	23.9	872	-40	83.5	868	-20	36.4
30	854	-26	51.0	854	-14	98.7	830	-27	75.8	837	-52	61.4	831	-21	92.2
31	822	-18	13.7	742	-19	37.1	728	-14	28.6	799	-18	26.7	752	-16	24.0
32	751	-15	6.7	666	-16	17.3	659	-3	34.0	754	-10	3.1	643	-20	58.8
33	650	-11	8.9	610	-41	108.9	630	-31	58.1	609	-29	18.0	595	-46	56.3
34	559	-12	9.3	601	-18	125.4	575	-41	163.9	575	-19	117.5	586	-19	160.0
35	532	-23	3.9	543	-11	1.0	545	-12	22.0	549	-11	3.8	548	-11	6.9
36	453	-50	7.9	469	-1	8.8	476	-10	28.5	491	-5	7.3	467	0	10.6
37	403	-11	88.0	385	-6	21.8	450	-3	4.6	456	-6	3.1	396	-8	6.7
38	368	-17	34.8	366	-3	6.3	349	-4	3.3	377	-5	7.8	365	-3	9.4
39	356	-7	24.7	307	-7	4.1	301	-3	0.5	337	-11	18.2	309	-8	8.3
40	310	-2	3.7	290	-21	7.4	270	-8	6.0	298	-29	13.0	291	-2	2.3
41	251	-2	12.6	267	-3	3.2	240	-12	0.9	251	-16	3.5	260	-1	1.5
42	225	-19	1.2	230	5	0.5	215	-23	11.8	245	-12	3.6	221	-4	0.6
43	179	-1	5.4	171	-1	1.0	181	-1	0.5	203	-11	8.0	162	-1	0.7
44	86	-3	3.1	84	0	5.3	81	2	1.2	111	-9	3.0	86	-2	3.5
45	51	-4	5.7	47	-2	0.9	69	7	2.2	67	-9	1.2	41	-3	1.6

^[a] Harmonic frequencies and intensities were calculated at the B3LYP/6-311++G** level, while anharmonic corrections correspond to the B3LYP/6-31G* level of theory. Frequencies and intensities are given in cm^{-1} and in $\text{km} \cdot \text{mol}^{-1}$, respectively.

Table 5. Harmonic vibrational fundamentals (ω), their VPT2 anharmonic corrections ($\Delta\nu$), and double-harmonic vibrational intensities (I) of the 5 lowest energy conformers of L-allo-threonine^[a]

number	aThr-I			aThr-II			aThr-III			aThr-IV			aThr-V		
	ω	$\Delta\nu$	I	ω	$\Delta\nu$	I	ω	$\Delta\nu$	I	ω	$\Delta\nu$	I	ω	$\Delta\nu$	I
1	3690	-197	191.6	3751	-186	70.1	3789	-182	38.5	3752	-190	56.6	3837	-175	35.5
2	3596	-180	12.5	3718	-196	67.3	3586	-182	14.0	3740	-186	85.5	3574	-182	19.3
3	3506	-125	1.6	3589	-182	13.4	3493	-103	9.8	3595	-182	12.3	3507	-100	1.4
4	3464	-263	268.4	3512	-188	6.8	3455	-265	279.7	3505	-131	4.9	3453	-251	273.3
5	3114	-142	16.0	3111	-142	20.3	3128	-141	7.0	3110	-142	20.6	3112	-143	15.5
6	3101	-141	27.5	3096	-137	36.5	3095	-137	25.1	3094	-128	32.1	3092	-137	22.6
7	3041	-140	7.3	3076	-138	9.1	3043	-106	19.6	3066	-133	7.3	3049	-132	20.6
8	3034	-117	15.4	3068	-130	1.6	3035	-116	24.0	3059	-136	13.2	3037	-128	5.6
9	2937	-85	50.2	3029	-101	13.8	3032	-128	14.0	3028	-151	13.8	3031	-121	15.2
10	1808	-21	307.4	1804	-33	299.0	1821	-28	305.2	1780	-34	279.2	1834	-30	338.2
11	1660	-45	32.5	1672	-8	40.7	1653	-45	35.2	1643	-80	39.6	1668	-33	45.6
12	1501	-37	5.5	1503	-100	5.0	1507	-69	3.5	1505	-68	5.9	1501	-42	10.3
13	1488	-6	4.0	1489	17	5.1	1490	11	13.0	1493	-40	10.4	1497	-43	3.5
14	1446	-54	11.0	1429	-30	45.2	1429	-46	174.6	1444	-39	31.2	1426	-58	128.5
15	1416	-52	435.3	1425	-35	26.8	1415	-41	158.8	1412	-14	14.9	1417	-20	232.0
16	1405	-30	61.4	1412	-19	13.8	1408	-30	107.8	1395	-54	19.3	1405	-46	30.6
17	1385	-38	12.3	1377	-40	7.6	1400	-36	42.5	1394	-41	31.4	1384	-33	5.3
18	1369	-5	0.3	1330	-28	36.2	1352	-34	14.5	1343	-32	12.7	1364	-39	14.6
19	1315	-1	76.0	1295	-27	16.1	1316	-34	7.6	1317	-34	9.3	1317	-41	1.5
20	1269	-32	4.4	1263	-33	9.6	1267	-39	4.5	1285	-35	2.9	1260	-34	11.6
21	1216	-42	36.9	1215	-36	31.0	1204	-41	27.4	1212	-34	10.7	1228	-36	14.4
22	1189	-28	4.8	1173	-35	14.3	1194	-32	19.2	1147	-37	243.0	1192	-34	25.8
23	1152	-31	15.1	1130	-34	250.5	1141	-30	33.6	1143	-30	129.4	1125	-30	34.9
24	1111	-31	26.0	1111	-28	98.6	1091	-27	34.9	1090	-26	11.2	1109	-28	79.0
25	1084	-32	57.0	1072	-29	18.5	1074	-25	8.9	1080	-34	19.9	1063	-27	4.7
26	1056	-30	10.9	1027	-28	17.7	1035	-21	42.3	1045	-22	32.6	1021	-29	37.4
27	975	-28	26.3	958	-39	30.9	973	-36	106.9	943	-23	7.8	964	-34	109.8
28	919	-34	78.2	921	-20	48.2	915	-26	46.6	901	-42	32.5	930	-26	42.1
29	884	-29	63.6	850	-41	131.1	880	-45	110.3	829	-52	136.2	883	-56	72.8
30	847	-62	18.9	828	-18	4.7	860	-23	38.2	816	-23	25.2	867	-25	25.9
31	840	-14	102.8	723	-21	19.4	813	-17	8.7	771	-17	34.4	829	-15	8.9
32	736	-12	5.8	650	-13	15.8	754	-14	8.2	709	-9	9.6	731	-10	17.0
33	631	-20	126.3	644	-8	78.3	607	-9	0.6	629	-30	99.3	648	-13	16.6
34	591	-9	3.9	570	-64	20.4	552	-34	11.0	569	-49	207.7	623	-10	8.5
35	571	-8	5.7	549	-21	152.0	524	-27	11.6	531	-9	19.6	495	-7	0.6
36	485	-1	15.6	457	-5	25.9	476	-15	20.1	498	-5	6.9	424	-5	11.7
37	406	-10	1.6	414	-2	4.0	437	-9	102.2	391	-2	0.9	362	-10	12.1
38	357	-10	10.2	362	-5	7.2	366	-18	31.0	358	-6	26.1	325	-32	5.6
39	347	-32	25.7	302	-10	5.1	349	-6	9.7	324	-3	14.7	306	-7	38.7
40	331	-7	3.7	255	-19	1.7	331	-3	8.0	269	-4	3.7	280	3	73.4
41	302	-13	10.6	249	-2	3.2	241	-1	3.0	241	-7	0.2	272	1	25.4
42	235	-18	6.2	228	-18	8.6	229	-1	5.1	230	-6	3.6	248	-11	0.3
43	208	-7	6.7	166	0	1.9	199	0	5.5	187	-5	3.6	174	-1	10.5
44	94	-2	0.9	82	-1	6.0	86	-2	4.1	120	-6	3.5	86	-7	3.9
45	71	-8	2.0	62	1	0.9	47	-4	5.1	45	-5	0.6	80	-4	2.2

^[a] See footnote [a] to table 4.

III. CONFORMATIONAL ANALYSIS

III.1. Preliminary tests

The method described in section II.1 for studying the conformational space of Thr and aThr systematically was tested on the neutral amino acids glycine (Gly) and L-alanine (Ala), where the number of conformers are well established as a result of previous high-level first-principles studies [17-20].

At the RHF/3-21G level, only 6 of the 8 and 11 of the 13 conformers were found for Gly and Ala, respectively. The RHF/3-21G optimizations failed to yield the high-energy conformers **Gly-VIIp** and **Gly-VIIIIn** for Gly. The most stable conformers {**Gly-Ip,Gly-IIIn**} [4] were obtained {28,49} times out of a total of 216 initial structures. Using the same conformational search but this time at the RHF/6-31G** level, all Gly conformers were found. These observations show the possible dangers of using RHF/3-21G optimizations for prescreening the possible conformers of amino acids (and most likely peptides). It is comforting, nevertheless, that RHF/3-21G optimizations always missed only the highest-energy conformers.

The discrepancies obtained for the amino acids Gly and Ala based on the initial prescreening of the conformers at the RHF/3-21G level led us to an extended study of the role of initial geometry optimizations. Taking the Thr conformers determined at the B3LYP/6-311++G** level, preliminary optimizations at the RHF/3-21G, RHF/3-21G**, and RHF/3-21+G** levels were done, continued by B3LYP/6-311++G** level optimizations. It was found that the final B3LYP/6-311++G** structures were often different from the initial B3LYP/6-311++G** structures when using the different basis sets for the preoptimizations at the RHF level. Thus, the conformers found on the PES corresponding to the final optimization level depend somewhat on the level of the initial optimizations. Since the conformers found by only one of the methods were of high relative energy (above 15 kJ mol⁻¹ in all cases), it is safely concluded that this effect is due to the fine structure of the high-energy regions of the different PESs. While this observation is certainly somewhat disturbing, it seems to be not relevant for the low-energy conformers, of highest relevance for practical applications.

III.2. Initial optimizations

Using the inexpensive RHF/3-21G method, 68 and 66 conformers were found for L-threonine and L-allo-threonine, respectively. When B3LYP/6-311++G** geometry optimizations were performed, using the RHF/3-21G conformers as initial structures, some of the higher-energy RHF/3-21G conformers disappeared, thus finally 56 and 61 conformers were found this way for Thr and aThr, respectively. Of the 7776 initial structures for each diastereomer, {202, 455, 328, 78, 146} and {220, 422, 534, 336, 131} ended up as {**Thr-I, Thr-II, Thr-III, Thr-IV, Thr-V**} and {**aThr-I, aThr-II, aThr-III, aThr-IV, aThr-V**}, respectively. This clearly shows that these lowest-energy conformers have substantial catchment regions. The smallest region corresponds to **Thr-XV** with only 12 initial structures ending up at that conformer.

III.3. Comparison with the study of Zhang and Lin [50]

The recent investigation of Zhang and Lin [50] is similar to our work in many respects. An important distinction is that in that paper only the L-threonine diastereomer was considered. For L-Thr, Zhang and Lin found 71 conformers at the B3LYP/6-311++G** level, while, as stated above, we found only 56 conformers. This result is the more curious as their grid for the initial optimization was somewhat less systematic, it was based partially on chemical intuition, and they included much less (only 1296) initial points than the grid corresponding to the present study contains (7776). The difference is due to the different theoretical levels used for the initial optimizations, and in this case show that the RHF/3-21G PES is less structured (68 conformers found) than the PES obtained at the B3LYP/6-311++G** level (71 conformers found). Overall, Zhang and Lin obtained 16 conformers which were not found and missed one conformer which was found in the present study. Since the dependence of the results of the conformational search on the method of initial optimization seems to be only relevant for higher-energy conformers, it is important to stress that all conformers of L-Thr up to a relative energy of 19 kJ mol^{-1} agree in the two studies.

IV. STRUCTURES

The MP2 and DFT(B3LYP) levels of electronic structure theory yield equilibrium structures which may suffer from different problems. It is the intramolecular basis set superposition error (BSSE) that can be quite significant at the MP2 level, especially when smaller basis sets are used, hindering the determination of truly accurate equilibrium structures. By design, this is much less of a problem at the DFT levels. The usual functionals of DFT theory, like B3LYP, suffer, however, from the inability to describe dispersion effects. Therefore, it is comforting to note that the RHF, DFT(B3LYP), and MP2 levels produce the same minima for the five lowest-energy conformers of Thr and aThr. This means that the structures predicted for the lowest-energy conformers are as dependable as can be expected at these levels of electronic structure theory.

It is of fundamental interest to investigate which intramolecular factors (electronic effects including exchange, electrostatic, and hyperconjugative interactions, steric repulsion, H-bonding capabilities, and dispersive interactions) lead to stabilization of the many possible conformers of Thr and aThr. Most of these effects are operative in stabilizing the configurations resulting from rotations around the appropriate single bonds of these molecules.

Threonine is a representative of the three hydroxyamino acids whereby the OH group in the side chain is capable of strong intramolecular H-bonds. The subsequent increase in the number of low-energy conformations has been proved in this study. The presence of NH, carboxylic OH, and side-chain OH H-bond donors and N, C=O, carboxylic OH, and side-chain OH H-bond acceptors allow for the existence of the following types of H-bonds: (a) bifurcated H-bonds between NH₂ and C=O, similar to that found in the most stable conformers of glycine [4,17] and alanine [18,20]; (b) simple H-bonds, like N-H to side-chain OH, carboxylic O-H, and C=O; (c) carboxylic O-H to C=O, side-chain O-H, and NH₂; and (d) side-chain O-H to carbonyl oxygen, nitrogen, and carboxylic OH.

The structure of the global minimum, **Thr-I**, is stabilized by strong OH \cdots N, OH \cdots O=C and weaker NH \cdots O H-bonds, whereby the COOH, NH₂, and the side-chain OH functional groups are interconnected via the three intramolecular H-bonds, while the -COOH group is in an energetically unfavorable trans conformation. In the case of **Thr-II**, although the -COOH group is now in the favorable cis conformation, this substantial energy gain, on the order of 20 kJ mol⁻¹, is not able to compensate for the energy difference between the H-bonds in **Thr-I** and **Thr-II**. **Thr-II** exhibits weaker NH \cdots O=C and OH \cdots N H-bonds. The H-bond arrangements in the most stable conformers of Thr are completely different from those for

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3 glycine and α -alanine, where the global minima have a cis $-\text{COOH}$ arrangement with a
4 bifurcated (and thus less strong) $\text{NH}\cdots\text{O}=\text{C}$ H-bonds, while the second lowest energy
5 conformers have a trans $-\text{COOH}$ arrangement and strong $\text{OH}\cdots\text{N}$ H-bonds. This shows, and
6 this conclusion is similar to that obtained in a MW study on the conformers of cysteine [51],
7 that the presence of a polar side chain has a major effect on the conformational preferences of
8 amino acids.
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14 In the case of L-allo-threonine, the global minimum, **aThr-I**, is stabilized, very similarly
15 to **Thr-I**, by strong $\text{OH}\cdots\text{O}=\text{C}$ and $\text{OH}\cdots\text{N}$ H-bonds, while the $-\text{COOH}$ group is again in the
16 less favorable trans conformation. As to **aThr-II**, the $-\text{COOH}$ group is in a cis conformation,
17 while $\text{OH}\cdots\text{N}$ and $\text{NH}\cdots\text{O}=\text{C}$ H-bonds can be found.
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21 A number of different secondary structural effects characterize the other conformers.
22 Among them one can find the $\text{OH}\cdots\text{NH}\cdots\text{O}=\text{C}$ structural motif in **Thr-III** whereby the same
23 NH group is included in a H-bond chain. In **Thr-IV**, the stability is due to the $\text{OH}\cdots\text{O}=\text{C}$ and
24 $\text{OH}\cdots\text{N}$ bonds. While **aThr-III** has the same H-bonds as **Thr-I**, the change in chirality causes
25 the methyl group to be in a highly unfavorable position. Furthermore, **aThr-IV** is stabilized
26 by a sequential $\text{NH}\cdots\text{OH}\cdots\text{O}=\text{C}$ H-bond arrangement involving $\text{NH}\cdots\text{OH}$ and $\text{OH}\cdots\text{O}=\text{C}$ H-
27 bond, including the same side-chain OH group.
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33 In all five low-energy Thr and aThr conformers, the methyl group is found in a
34 staggered position with respect to the β -carbon atom. One can compute straightforwardly the
35 pure (vibrationless) internal rotation barrier of the CH_3 group in Thr and aThr. This was done
36 in the present study at the MP2(fc)/cc-pVDZ level. The rotation barriers determined for the
37 methyl group in Thr and aThr are between 1100 and 1300 cm^{-1} . Furthermore, note that for
38 the three lowest-energy conformers of alanine [20], the methyl rotation barrier is also about
39 1200 cm^{-1} , computed, as part of this study, at the same level of theory. The characteristic
40 increase of the rotation barrier in these natural amino acids with respect to ethane, where the
41 barrier is 1140 cm^{-1} at this level [16], originates most probably from increased
42 hyperconjugation, due to the presence of CC and CX (X = O, N) bonds. Note also that the
43 internal rotation barrier of the methyl group can be substantially smaller than the barriers
44 reported; for example, it is only about 400 cm^{-1} in acetaldehyde [40] and much smaller in
45 toluene. Observation of transitions between the energy levels under the slightly different
46 barriers, aimed compounded by different reduced masses due to the structural differences of
47 the conformers, should help identification of the low-energy conformers of Thr and Ala, as
48 well.
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Note, finally, that the only threonine conformer considered by Lakard [52] in a study of the vibrational fundamentals of hydroxyamino acids at the harmonic level, though the figure included in that paper is not particularly instructive, is definitely not the global minimum and it is not even among the five most stable conformers.

V. RELATIVE ENERGIES

As observed repeatedly for amino acids, the introductory Hartree–Fock level of electronic structure theory, independently of the basis set used, is unable to yield the correct relative energies of the conformers of Thr and aThr (see Tables 2 and 3). At the extrapolated RHF/CBS level, **Thr-II** and **Thr-III** both have lower energies than **Thr-I**, while **Thr-IV** has a very high relative energy. These RHF/CBS results clearly show the inadequacy of this level of theory in predicting relative conformational energies for this class of compounds due to its inadequacy in describing fine electrostatic and H-bonding effects. The MP2 level of theory stabilizes **Thr-IV** substantially, while it destabilizes all the other conformers considered. For Thr, the explicit MP2/aug-cc-pVQZ and the extrapolated MP2/CBS relative energies deviate at most by 0.04 kJ mol^{-1} , an excellent agreement indeed, contributing greatly to the overall accuracy of the FPA relative conformational energies. For aThr, the extrapolation contributions are larger by almost an order of magnitude but they are still surprisingly small on an absolute scale; consequently, the error due to MP2 extrapolation remains a small factor of the overall estimated precision of the FPA relative energies. Compared to $\delta[\text{MP2}]$, the $\delta[\text{CCSD}]$ and $\delta[\text{CCSD(T)}]$ energy increments are relatively small though can affect relative energies by at most 2 kJ mol^{-1} . Overall, it seems safe to attribute about 0.7 kJ mol^{-1} accuracy to the CCSD(T)/CBS limit FPA relative energies. Based on the CCSD – HF and CCSD(T) – CCSD increments, the relative energy corrections due to electron correlation effects beyond CCSD(T) are estimated to be considerably less than 0.5 kJ mol^{-1} , thus these missing corrections should not affect significantly the CCSD(T)/CBS limit FPA relative energies and their uncertainty estimates.

The DFT(B3LYP) level performs reasonably well, the FPA relative energies, including the ZPVE corrections, are quite similar to the B3LYP/6-311++G** relative energies. This shows again the utility of the DFT approach for conformational energy studies.

Interestingly, but again in line with our study on the conformers of Pro [2], the relative energies are barely affected by consideration of the core-core and core-valence correlation

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3 and the relativistic effects. Even the largest change is smaller than 0.1 kJ mol^{-1} . This is
4 comforting and makes accurate relative energy predictions for the conformers of the building
5 blocks of biopolymers considerably less expensive.
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9 ZPVE corrections are substantial and can affect relative energies on the order of 2
10 kJ mol^{-1} . It is also of general interest to compare harmonic and anharmonic ZPVE corrections
11 to the relative energies. The anharmonic contributions to relative energies of the Thr
12 conformers are on the order of 0.5 kJ mol^{-1} . This is significant but not substantial given the
13 other sources of error in the present computations contributing to the final FPA relative
14 energy estimates.
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18 The above statements nearly stand for aThr, as well. The RHF level of theory gives
19 relative energies with considerable error, underestimating the relative energies of **aThr-II** and
20 **aThr-IV**. The MP2 increment compensates most of this error by destabilizing these
21 conformers. Compared to MP2, $\delta[\text{CCSD}]$ and $\delta[\text{CCSD(T)}]$ energy corrections are fairly
22 small yet can affect relative energies by over 2 kJ mol^{-1} . Core correlation and relativistic
23 effects are on the order of 0.01 kJ mol^{-1} , while ZPVE corrections can reach nearly 1.5
24 kJ mol^{-1} .
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28 In the case of aThr, the B3LYP/6-311++G** level gives a different relative energy order
29 than the FPA approach. In the cases of **aThr-I** and **aThr-II**, this is due to the ZPVE
30 corrections, which shows the importance of including ZPVE for conformational studies. It is
31 interesting to find that the FPA relative energies give the same relative energy order as the
32 MP2/aug-cc-pVTZ level for the optimized structures.
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36 Since the FPA energy difference between **aThr-I** and **aThr-II** is only 0.8 kJ mol^{-1} and
37 the assumed uncertainty of the present FPA relative energies is $\pm 1 \text{ kJ mol}^{-1}$, even the present
38 extensive computations are insufficient to determine the lowest-energy conformer of aThr.
39 Similarly, the small FPA energy difference between **aThr-IV** and **aThr-V** does not allow an
40 unambiguous determination of their energy order.
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44 In order to estimate the uncertainty on the FPA energies resulting from the choice of
45 reference structures, MP2/aug-cc-pVTZ//B3LYP/6-311++G** relative energies were
46 compared to MP2/aug-cc-pVTZ//MP2/aug-cc-pVTZ energies. The average effect is 0.1 and
47 0.3 kJ mol^{-1} for Thr and aThr, respectively, suggesting that the DFT reference structures
48 chosen are appropriate for the purposes of the present study.
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VI. VIBRATIONAL FUNDAMENTALS

Many vibrational fundamentals are found to be characteristic for some of the conformers of Thr and aThr (*cf.* Tables 4 and 5). One of the most useful fundamentals characterizing the conformers is the intense stretching vibrational motion of the carboxyl group, ω_{10} , at about 1800 cm^{-1} . The spread in ω_{10} is substantial, from 1780 (**aThr-IV**) to 1834 cm^{-1} (**aThr-V**). The anharmonic corrections alter this picture only slightly as all the VPT2 corrections are between 28 and 34 cm^{-1} . When the C=O group is not involved in H-bonding, *e.g.*, for **Thr-V**, the fundamental is at a high wavenumber, while a strong H-bond between C=O and the side-chain OH results in a substantially lower wavenumber, as for **aThr-IV**. The exact wavenumber of this fundamental should also depend on the *cis vs trans* arrangement of the carboxylic group, though this effect cannot be seen clearly from the data of Tables 4 and 5.

Other simple nuclear motions, such as OH stretching (ω_1, ω_2) and NH stretching (ω_3, ω_4), should also be discussed. The OH stretching motion characterizes conformers by intensity ratios (I_1/I_2) varying from 0.7 to 15.3 , and by frequency differences ($\omega_1 - \omega_2$) varying between 12 and 263 cm^{-1} , with anharmonic corrections altering only slightly these differences. Correlation between the H-bond structure and the OH band origins cannot be so easily used for identification purposes as ω_{10} . Nearly the same stands for the NH stretching motion. The NH stretches also characterize conformers by their relative intensities (I_3/I_4) and frequency differences ($\omega_3 - \omega_4$). Interestingly, in most cases the $\omega_3 - \omega_4$ frequency differences are considerably modified by the anharmonic corrections.

Various other fundamentals, including $\omega_{14}, \omega_{15}, \omega_{18}, \omega_{21}, \omega_{22}, \omega_{24}$, and ω_{26} , can also be found where the intensities or the wavenumbers are characteristic of the different conformers. Nevertheless, in these cases the use of this information to identify conformers based on the availability of the infrared spectrum, for example in a matrix isolation study, is not straightforward due to the presence of nearby fundamentals of similar energies.

VII. ROTATIONAL SPECTRA

There are three possible routes to identify conformers via rotational spectroscopy if results from related electronic structure computations are available. The most obvious route is based on the comparison of measured effective rotational constants with equilibrium or vibrationally averaged computed rotational constants. The second route uses the information contained in computed dipole moments and selection rules and thus allows interpretation of measured relative intensities of rotational lines. In the case of amino acids a third route is also open, namely one can use computed ^{14}N nuclear quadruple coupling constants for the identification of a conformer.

At the B3LYP/6-311++G** level, the rotational constants corresponding to the optimized equilibrium structures are accurate enough to be useful to deduce the presence of most of the conformers when evaluating experimental data of microwave and millimeterwave spectroscopic studies. Furthermore, some of the conformers (*e.g.*, **Thr-I** and **Thr-IV**, as well as **aThr-I**) have substantial dipole moments thus helping the observation of the related rotational transitions. Nevertheless, given the limited accuracy of the rotational constants obtained at the B3LYP and MP2 levels, in certain cases it might be quite difficult to distinguish the conformers of Thr and aThr based on this information alone. This holds, for example, for **Thr-II** and **Thr-V**. Unfortunately, in this case the ^{14}N nuclear quadruple coupling constants are also rather similar, hindering further the unequivocal identification of these conformers. In contrast, while the rotational constants of **Thr-I** and **Thr-III** are rather similar, in this case the ^{14}N nuclear quadruple coupling constants allow for an easy distinction between the measured spectroscopic data of the two conformers.

The relatively accurate rotational and quartic centrifugal distortion (QCD) constants determined should facilitate the observation of the low-energy conformers of L-Thr and L-aThr, especially **Thr-I** and **aThr-I**. The sextic centrifugal distortion constants are so small (they are given in mHz units in Tables 6 and 7) that it is unlikely that they could be determined experimentally with any reasonable certainty. Their smallness also means that the experimental spectrum could straightforwardly be fitted with just the effective rotational and quartic centrifugal distortion constants.

Table 6. Equilibrium rotational constants (A_e , B_e , C_e), their vibrational corrections (ΔA , ΔB , ΔC) leading to ground-state rotational constants A_0 , B_0 , and C_0 , A -reduced quartic (ΔJ , ΔK , Δ_{JK} , δ_J , δ_K) and sextic (Φ_J , Φ_K , Φ_{JK} , Φ_{KJ} , ϕ_j , ϕ_k , ϕ_{jk}) centrifugal distortion constants, ^{14}N nuclear quadrupole coupling tensor elements (χ_{aa} , χ_{bb} , χ_{cc}), and total dipole moments (μ_{total}) of the five lowest-energy conformers of L-threonine^[a]

	Thr-I	Thr-II	Thr-III	Thr-IV	Thr-V
A_e	3 201.77	2 865.57	3 128.28	2 679.22	2 882.14
ΔA	-32.91	-24.61	-38.07	-27.82	-25.09
B_e	1 498.69	1 587.52	1 476.30	1 749.67	1 549.45
ΔB	-25.80	-13.55	-14.75	-17.45	-17.18
C_e	1 256.81	1 194.30	1 294.91	1 354.93	1 222.85
ΔC	-8.64	-10.49	-9.29	-10.67	-6.24
ΔJ	0.258	0.270	0.172	0.211	0.300
ΔK	-0.017	-0.142	-0.118	0.192	-0.526
Δ_{JK}	0.404	0.269	0.723	0.006	0.697
δ_J	0.065	0.052	0.020	0.035	0.069
δ_K	0.155	0.620	-1.217	-0.028	-0.727
Φ_J	-0.15	-0.10	0.08	-0.02	-0.15
Φ_K	20.45	13.57	-1.49	-0.20	61.88
Φ_{JK}	6.61	4.77	-4.70	0.10	26.28
Φ_{KJ}	-27.18	-18.09	5.05	-0.47	-87.56
ϕ_j	-0.08	-0.04	0.02	0.00	-0.04
ϕ_k	70.70	27.48	-59.03	1.89	138.08
ϕ_{jk}	-0.36	-1.23	2.03	-0.06	-1.54
χ_{aa}	-4.08	-4.83	-0.94	-4.51	-4.80
χ_{bb}	2.12	2.92	3.24	2.66	2.84
χ_{cc}	1.96	1.90	-2.30	1.85	1.95
μ_{total}	4.37	2.36	3.02	5.14	3.00

Table 6. cont.

[a] The equilibrium rotational and quartic centrifugal distortion constants, given in MHz and kHz, respectively, correspond to the parent isotopologue, and were determined at the B3LYP/6-311++G** level. Vibrational corrections and sextic centrifugal distortion constants, given in MHz and mHz, respectively, were determined from anharmonic force fields obtained at the B3LYP/6-31G* level. The nuclear quadrupole coupling tensor elements given correspond to the ^{14}N nucleus (in MHz). Dipole moments are given in debye.

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Table 7. Equilibrium (A_e , B_e , C_e) rotational constants, their vibrational corrections (ΔA , ΔB , ΔC) leading to ground-state rotational constants A_0 , B_0 , and C_0 , A -reduced quartic (Δ_J , Δ_K , Δ_{JK} , δ_J , δ_K) and sextic (Φ_J , Φ_K , Φ_{JK} , Φ_{KJ} , ϕ_j , ϕ_k , ϕ_{jk}) centrifugal distortion constants, ^{14}N nuclear quadrupole coupling constants (χ_{aa} , χ_{bb} , χ_{cc}), and total dipole moments (μ_{total}) of the five lowest-energy conformers of L-allo-threonine^[a]

	aThr-I	aThr-II	aThr-III	aThr-IV	aThr-V
A_e	3 076.01	3 019.18	2 773.73	2 738.22	3 059.09
ΔA	-25.24	-29.23	-29.65	-24.31	-28.66
B_e	1 639.65	1 464.42	1 702.83	1 627.34	1 483.53
ΔB	-15.83	-9.65	-15.32	-17.21	-14.60
C_e	1 117.74	1 316.22	1 341.31	1 417.04	1 336.00
ΔC	-9.71	-16.16	-13.67	-15.98	-14.96
Δ_J	0.102	0.278	0.250	0.277	0.244
Δ_K	0.248	0.084	0.157	0.909	0.055
Δ_{JK}	0.027	0.170	0.438	0.226	0.190
δ_J	0.032	0.048	0.060	0.016	0.030
δ_K	0.170	2.004	-1.337	-0.661	1.386
Φ_J	0.00	-0.13	0.03	-0.11	0.01
Φ_K	-0.37	28.67	1.20	7.30	18.87
Φ_{JK}	-0.06	11.43	-0.45	4.46	6.76
Φ_{KJ}	0.10	-40.04	-1.50	-16.01	-25.65
ϕ_j	0.00	0.01	0.04	0.03	0.04
ϕ_k	0.00	117.36	-1.27	20.51	89.59
ϕ_{jk}	0.00	-5.55	1.60	-6.23	-1.09
χ_{aa}	-4.64	-5.02	-4.65	-0.34	-0.21
χ_{bb}	2.67	3.02	2.75	0.67	2.86
χ_{cc}	1.97	2.00	1.90	-0.33	-2.65
μ_{total}	5.31	1.85	4.41	2.75	4.57

^[a] See footnote [a] to Table 6.

VIII. SUMMARY

Following an extensive search utilizing $6^5 = 7776$ initial structures for each diastereomer, 68 and 66 conformers (local minima on their related PESs) were found for L-threonine and L-allo-threonine, respectively, at the RHF/3-21G level of electronic structure theory. After geometry optimizations at the B3LYP/6-311++G** level, 56 and 61 conformers remained for L-threonine and L-allo-threonine, respectively, within an energy range of 51 and 52 kJ mol⁻¹, respectively. The PESs of the Thr and aThr molecules clearly depend on the level of theory used for their determination. Lacking high-level definitive computational studies, only conformers obtained at several medium theoretical levels should be considered as ones whose likely existence is confirmed by theory. Fortunately, the results obtained show that the conformers found in the lower-energy regions of the PESs have the same bonding arrangements at the HF, DFT(B3LYP), and MP2 levels of theory, thus these conformers should in fact exist.

Following the FPA approach, relative energy predictions with an accuracy of ± 1 kJ mol⁻¹ were determined for the five lowest-energy conformers of both diastereomers of Thr. The computations clearly predict the global minimum for Thr, called **Thr-I**. However, for aThr the relative energies of two conformers, **aThr-I** and **aThr-II** are the same within the uncertainty of the FPA approach. In contrast to the global minimum of Gly and Ala, **Thr-I** contains an energetically unfavorable trans carboxylic group, and it is stabilized by strong OH \cdots N, OH \cdots O=C and weaker NH \cdots O H-bonds, whereby the COOH, NH₂, and the side-chain OH functional groups are interconnected via three intramolecular H-bonds. **aThr-I** is stabilized, very similarly to **Thr-I**, by strong OH \cdots O=C and OH \cdots N H-bonds, while the COOH group, to allow for these bonds, is again in the less favorable trans conformation. **Thr-II** and **aThr-II** also have similar structures, with energetically favorable cis carboxylic groups, but weaker H-bonds, NH \cdots O=C and OH \cdots N for both **Thr-II** and **aThr-II**. The structural differences between the most stable conformers of Gly and Ala and those of Thr and aThr are clearly due to the presence of the polar side chain. The side chain's significant effect on conformer stability was already observed for cysteine [51]. In the notation of Alonso et al., the presence of OH and SH polar side chains favor type-**III** conformers over type-**I** conformers known as global minima for Gly and Ala. As expected, the methyl group is in a staggered conformation for all the low-energy conformers of Thr and aThr, with rotational barriers varying between 1100 and 1300 cm⁻¹.

Spectroscopic parameters (harmonic and anharmonic frequencies, double-harmonic vibrational intensities, rotational constants with corresponding vibrational corrections, A-

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3 reduced quartic and sextic centrifugal distortion constants, dipole moments and nuclear
4 quadrupole coupling constants) were calculated for the conformers of Thr and aThr. Several
5 of these parameters show the possibility for the experimental distinction of the conformers.
6 Most important are the characteristic stretching C=O (ω_{10}), NH (ω_3, ω_4) and OH (ω_1, ω_2)
7 vibrational fundamentals if the vibrational spectra of the conformers were available.
8 Assignment of the conformers based on pure rotational spectra can be based on rotational
9 constant (equilibrium, $A_e, B_e,$ and $C_e,$ as well as vibrationally averaged $A_0, B_0,$ and C_0
10 constants are provided), A -reduced quartic centrifugal distortion constants ($\Delta_J, \Delta_K, \Delta_{JK}, \delta_J,$ and
11 δ_K) and nuclear quadrupole coupling constants ($\chi_{aa}, \chi_{bb},$ and χ_{cc}) corresponding to the ^{14}N
12 nucleus. It seems feasible that conformers of Thr (and similarly those of Ala) could be
13 identified if transitions between the energy levels corresponding to internal rotation
14 characterized by slightly different methyl rotation barriers became available.
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REFERENCES

- [1] A. G. Császár, A. Perczel, *Progr. Biophys. Mol. Biol.* **71**, 243 (1999).
- [2] E. Czinki, A. G. Császár, *Chem. Eur. J.* **9**, 1008 (2003).
- [3] W. D. Allen, E. Czinki, A. G. Császár, *Chem. Eur. J.* **10**, 4512 (2004).
- [4] V. Kasalová, W. D. Allen, H. F. Schaefer III, E. Czinki, A. G. Császár, *J. Comp. Chem.* **28**, 1373 (2007).
- [5] P. Hudáky, I. Jákli, A. G. Császár, A. Perczel, *J. Comp. Chem.* **22**, 732 (2001).
- [6] I. Jákli, A. Perczel, Ö. Farkas, A. G. Császár, C. Sosa, I. G. Csizmadia, *J. Comp. Chem.* **21**, 626 (2000).
- [7] F. Pollreisz, Á. Gömöröy, G. Schlosser, K. Vékey, I. Solt, A. G. Császár, *Chem. Eur. J.* **11**, 5908 (2005).
- [8] (a) G. Guillea, D. T. Ramon, *Tetrahedron-Asymmetry* **17**, 1675 (2006). (b) B. List, *Synlett* **11**, 1675 (2001).
- [9] (a) X. Michalat, F. F. Pinaud, L. A. Bentolila, J. M. Tsay, S. Doose, G. Sundaresan, S. S. Wu, S. S. Gambhir, S. Weiss, *Science* **307**, 538 (2005). (b) A. Mavrandonakis, S. C. Farantos, G. E. Froudakis, *J. Phys. Chem. B* **110**, 6048 (2006).
- [10] F. Combes, Q. R. Nguyeu, G. Wlodarczak, *Astron. Astrophys.* **308**, 618 (1996).
- [11] S. Daydé, D. Champmartin, P. Rubini, G. Berthon, *Inorg. Chim. Acta* **339**, 513 (2002).
- [12] Y. Inomata, T. Takeuchi, T. Moriwaki, *Spectrochim. Acta* **40A**, 179 (1984).
- [13] S. Boudesocque, Z. Damaj, L. Dupont, J.-B. Behr, E. Guillon, *J. Inorg. Biochem.* **102**, 1514 (2008).
- [14] (a) S. S. V. Ramasastry, H. Zhang, F. Tanaka, C. F. Barbes III, *J. Am. Chem. Soc.* **129**, 288 (2007). (b) N. Utsumi, M. Imai, F. Tanaka, S. S. V. Ramasastry, C. F. Barbes III, *Org. Lett.* **17**, 3445 (2007).
- [15] W. D. Allen, A. L. L. East, A. G. Császár, *Structures and Conformations of Non-Rigid Molecules*, eds. J. Laane, M. Dakkori, B. van der Veken, H. Oberhammer, Kluwer: Dordrecht, 1993, p.343.
- [16] A. G. Császár, W. D. Allen, H. F. Schaefer III, *J. Chem. Phys.* **108**, 9751 (1998).
- [17] A. G. Császár, *J. Am. Chem. Soc.* **114**, 9568 (1992).
- [18] C. H. Hu, M. Z. Shen, H. F. Schaefer, *J. Am. Chem. Soc.* **115**, 2923 (1993).
- [19] A. G. Császár, *J. Mol. Struct.* **346**, 141 (1995).
- [20] A. G. Császár, *J. Phys. Chem.* **100**, 3541 (1996).
- [21] M. J. Frisch, J. A. Pople, J. E. Del Bene, *J. Phys. Chem.* **89**, 3664 (1985).

- 1
2
3
4
5 [22] J. S. Binkley, J. A. Pople, W. J. Hehre, J. Am. Chem. Soc. **102**, 939 (1980).
6 [23] C. C. J. Roothaan, Rev. Mod. Phys. **23**, 69 (1951); Ibid. **32**, 179 (1960).
7 [24] R. Ditchfield, W. J. Hehre, J. A. Pople, J. Chem. Phys. **54**, 724 (1971).
8 [25] (a) R. Krishnan, J. S. Binkley, R. Seeger, J. A. Pople, J. Chem. Phys. **72**, 650 (1980). (b)
9 T. Clark, J. Chandrasekhar, G. W. Spitznagel, P. v. R. Schleyer, J. Comp. Chem. **4**, 294
10 (1983). (c) M. J. Frisch, J. A. Pople, J. S. Binkley, J. Chem. Phys. **80**, 3265 (1984).
11 [26] T. H. Dunning Jr., J. Chem. Phys. **90**, 1007 (1989).
12 [27] R. A. Kendall, T. H., Dunning, Jr., R. J. Harrison, J. Chem. Phys. **96**, 6796 (1992).
13 [28] A. G. Császár, W. D. Allen, J. Chem. Phys. **104**, 2746 (1996).
14 [29] G. Tarczay, A. G. Császár, W. Klopper, H. M. Quiney, Mol. Phys. **99**, 1769 (2001).
15 [30] P. Pulay, Mol. Phys. **17**, 197 (1969).
16 [31] W. J. Hehre, L. Radom, P. v. R. Schleyer, J. A. Pople, *Ab Initio Molecular Orbital*
17 *Theory*, Wiley-Interscience, New York, **1986**.
18 [32] (a) C. Møller, M. S. Plesset, Phys. Rev. **46**, 618 (1934). (b) R. Krishnan, M. J. Frisch, J.
19 A. Pople, J. Chem. Phys. **72**, 4244 (1980).
20 [33] (a) J. Čížek, J. Chem. Phys. **45**, 4256 (1966). (b) J. Čížek, J. Paldus, Physica Scripta **21**,
21 251 (1980).
22 [34] R. J. Bartlett, C. E. Dykstra, J. Paldus, in *Advanced Theories and Computational*
23 *Approaches to the Electronic Structure of Molecules*, ed. C. E. Dykstra, Reidel,
24 Dordrecht, **1984**, p. 127.
25 [35] K. Raghavachari, G. W. Trucks, J. A. Pople, M. Head-Gordon, Chem. Phys. Lett. **157**,
26 479 (1989).
27 [36] (a) P. A. M. Dirac, Proc. Cambridge Philos. Soc. **26**, 376 (1930). (b) A. D. Becke, Phys.
28 Rev. B **38**, 3098 (1988). (c) A. D. Becke, J. Chem. Phys. **98**, 5648 (1993). (d) C. Lee, W.
29 Yang, R. G. Parr, Phys. Rev. B **37**, 785 (1988). (e) S. H. Vosko, L. Wilk, M. Nusair, Can.
30 J. Phys. **58**, 1200 (1980).
31 [37] T. J. Lee, P. R. Taylor, Int. J. Quantum Chem. Symp. **23**, 199 (1989).
32 [38] V. Szalay, A. G. Császár, M. L. Senent, J. Chem. Phys. **117**, 6489 (2002).
33 [39] W. D. Allen, A. Bódi, V. Szalay, A. G. Császár, J. Chem. Phys. **124**, 224310 (2006).
34 [40] A. G. Császár, V. Szalay, M. L. Senent, J. Chem. Phys. **120**, 1203 (2004).
35 [41] Gaussian 03, Revision C.02, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria,
36 M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C.
37 Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G.

Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komáromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, J. A. Pople, Gaussian, Inc., Wallingford CT, 2004.

[42] MOLPRO is a package of *ab initio* programs written by H.-J. Werner, P. J. Knowles, R. Lindh, F. R. Manby, M. Schütz, P. Celani, T. Korona, G. Rauhut, R. D. Amos, A. Bernhardsson, A. Berning, D. L. Cooper, M. J. O. Deegan, A. J. Dobbyn, F. Eckert, C. Hampel, G. Hetzer, A. W. Lloyd, S. J. McNicholas, W. Meyer, M. E. Mura, A. Nicklaß, P. Palmieri, R. Pitzer, U. Schumann, H. Stoll, A. J. Stone, R. Tarroni, T. Thorsteinsson.

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[44] (a) W. Klopper, W. Kutzelnigg, *J. Mol. Struct. (THEOCHEM)* **135**, 339 (1986); (b) A. Karton, J. M. L. Martin, *Theor. Chem. Acc.* **115**, 330 (2006); (c) G. Tasi, A. G. Császár, *Chem. Phys. Lett.* **438**, 139 (2007).

[45] W. M. Klopper, K. L. Bak, P. Jørgensen, J. Olsen, T. Helgaker, *J. Phys. B* **32**, 103 (1999).

[46] M. Douglas, N. M. Kroll, *Ann. Phys.* **82**, 89 (1974).

[47] N. C. Handy, Y. Yamaguchi, H. F. Schaefer, *J. Chem. Phys.* **84**, 4481 (1986).

[48] W. D. Allen, A. G. Császár, *J. Chem. Phys.* **98**, 2983 (1993).

[49] (a) D. A. Clabo Jr., W. D. Allen, R. B. Remington, Y. Yamaguchi, H. F. Schaefer, *Chem. Phys.* **123**, 187 (1988). (c) W. D. Allen, Y. Yamaguchi, A. G. Császár, D. A. Clabo Jr., R.

1
2
3
4
5 B. Remington, H. F. Schaefer, Chem. Phys. **145**, 427 (1990). (d) H. H. Nielsen, Rev.
6 Mod. Phys. **23**, 90 (1951). (e) D. Papousek, M. R. Aliev, *Molecular Vibrational-*
7 *Rotational Spectra*, Elsevier: Amsterdam, 1982. (e) J. K. G. Watson, In *Vibrational*
8 *Spectra and Structure*, Vol. 6; J. R. Durig, Ed., Elsevier: Amsterdam, 1997; p. 1.

9
10
11 [50] M. Zhang, Z. Lin, J. Mol. Struct. (THEOCHEM) **760**, 159 (2006).

12
13 [51] M. E. Sanz, S. Blanco, J. C. López, J. L. Alonso, Angew. Chem. Int. Ed. **47**, 6216 (2008).

14
15 [52] B. Lakard, J. Mol. Struct. (THEOCHEM) **681**, 183 (2004).
16
17
18
19
20
21
22
23
24
25
26
27
28
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Supplementary material to

Conformers of Gaseous Threonine

**Tamás Szidarovszky, Gábor Czakó,
and Attila G. Császár***

*Laboratory of Molecular Spectroscopy, Institute of Chemistry, Eötvös University,
H-1518 Budapest 112, P.O. Box 32, Hungary*

Coordinates and energies are given in angstroms and Hartrees, respectively.

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3 B3LYP/6-311++G** geometry and energy of conformer: Thr-I
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5	N	-0.0533470	1.7038990	0.2314590
6	H	0.3590150	1.5838260	1.1539310
7	C	-0.0442190	0.4246410	-0.4896880
8	H	-0.0363780	0.6334110	-1.5655940
9	C	1.1430510	-0.5037890	-0.1593510
10	C	-1.3815210	-0.3070190	-0.2275860
11	H	0.9807530	-1.4445550	-0.6929990
12	O	1.1738110	-0.7476170	1.2544990
13	O	-1.5379430	-1.4843320	-0.4334870
14	H	0.5281650	-1.4335760	1.4592670
15	O	-2.3522510	0.4880920	0.2309000
16	H	-1.9233980	1.3640610	0.3658960
17	H	0.4619530	2.4261160	-0.2564510
18	C	2.4888610	0.0865890	-0.5502360
19	H	2.6921460	1.0080080	0.0020550
20	H	3.2850080	-0.6229850	-0.3194590
21	H	2.5202000	0.3067220	-1.6209910

22 Energy: -438.426915844
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24 MP2/aug-cc-pVTZ geometry and energy of conformer: Thr-I
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26	N	-0.0228480	1.6903810	0.2688530
27	H	0.3571380	1.5014330	1.1926450
28	C	-0.0325080	0.4464470	-0.4999460
29	H	-0.0298410	0.6933330	-1.5652570
30	C	1.1266340	-0.5049620	-0.2019770
31	C	-1.3566840	-0.2788850	-0.2338380
32	H	0.9942280	-1.3951460	-0.8198310
33	O	1.0926700	-0.8586950	1.1824380
34	O	-1.5115450	-1.4644300	-0.4282970
35	H	0.3890420	-1.5121760	1.2899200
36	O	-2.3254110	0.5169110	0.2285460
37	H	-1.8749420	1.3828820	0.3633260
38	H	0.5611700	2.3913320	-0.1672090
39	C	2.4747650	0.1241160	-0.4701750
40	H	2.6378010	0.9763930	0.1888130
41	H	3.2640720	-0.6010270	-0.2850380
42	H	2.5423180	0.4597270	-1.5052230

43 Energy: -437.569506052
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B3LYP/6-311++G** geometry and energy of conformer: Thr-II

N	0.1698080	1.9023870	-0.2684410
H	-0.2646530	2.2031330	0.6005130
C	0.0095320	0.4556970	-0.4335040
H	0.1436610	0.2014940	-1.4869980
C	1.1509880	-0.2394760	0.3675790
C	-1.3579540	-0.0283770	0.0303600
H	0.9800490	-0.0154010	1.4325370
O	2.3843380	0.3221540	-0.0481070
O	-1.9633040	0.4334080	0.9670390
H	2.2258460	1.2762680	-0.1233500
O	-1.8319130	-1.0523370	-0.7148490
H	-2.6858660	-1.3164590	-0.3376500
H	-0.2736900	2.4134800	-1.0233540
C	1.2294720	-1.7442590	0.1711070
H	2.0924090	-2.1322730	0.7155260
H	0.3336330	-2.2460040	0.5428480
H	1.3547640	-1.9882530	-0.8868970

Energy: -438.426405842

MP2/aug-cc-pVTZ geometry and energy of conformer: Thr-II

N	0.2150230	1.8995500	-0.2575850
H	-0.1945680	2.1704510	0.6322350
C	0.0255610	0.4647260	-0.4423400
H	0.1655710	0.2119030	-1.4929450
C	1.1255050	-0.2468140	0.3655030
C	-1.3322570	-0.0060160	0.0244210
H	0.9583930	0.0023120	1.4228040
O	2.3791580	0.2520800	-0.0617590
O	-1.9065580	0.4302560	0.9989700
H	2.2461020	1.2094890	-0.1537030
O	-1.8337900	-0.9937040	-0.7499910
H	-2.6799650	-1.2499270	-0.3476670
H	-0.2729080	2.4221520	-0.9748690
C	1.1348810	-1.7470710	0.1852070
H	1.9852550	-2.1657050	0.7198930
H	0.2231230	-2.1980880	0.5736040
H	1.2312190	-1.9974390	-0.8707660

Energy: -437.568537183

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3 B3LYP/6-311++G** geometry and energy of conformer: Thr-III
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5	N	0.2094330	1.7152330	-0.1760860
6	H	-0.6680670	2.1553750	0.0824120
7	C	-0.0118720	0.3237980	-0.5681810
8	H	0.0155870	0.1764700	-1.6565370
9	C	1.0858580	-0.5745470	0.0705780
10	C	-1.4037190	-0.1054630	-0.1245350
11	H	0.7987080	-1.6203050	-0.0509580
12	O	1.1203250	-0.3330130	1.4690640
13	O	-2.2215460	0.6197410	0.3847900
14	H	1.1141340	0.6321260	1.5671760
15	O	-1.6434660	-1.4057260	-0.3949310
16	H	-2.5376390	-1.6066530	-0.0800330
17	H	0.6467190	2.2569870	-0.9096480
18	C	2.4509340	-0.3415200	-0.5768270
19	H	3.1999520	-0.9598210	-0.0783840
20	H	2.4364200	-0.6061270	-1.6392160
21	H	2.7584420	0.7036820	-0.4798050

22 Energy: -438.425267222
23

24 MP2/aug-cc-pVTZ geometry and energy of conformer: Thr-III
25

26	N	0.2492490	1.7005400	-0.0943430
27	H	-0.6354210	2.1587430	0.0954840
28	C	0.0053990	0.3490860	-0.5806540
29	H	0.0293140	0.2596820	-1.6725250
30	C	1.0622810	-0.5943080	0.0167490
31	C	-1.3768040	-0.0776380	-0.1403450
32	H	0.7963960	-1.6228230	-0.2230430
33	O	1.0116590	-0.4870430	1.4301680
34	O	-2.1809450	0.6371420	0.4151040
35	H	0.9905650	0.4688270	1.6009130
36	O	-1.6271430	-1.3628440	-0.4648840
37	H	-2.5218930	-1.5520120	-0.1410080
38	H	0.7611310	2.2526500	-0.7679740
39	C	2.4464370	-0.2736420	-0.5189330
40	H	3.1775120	-0.9316470	-0.0533970
41	H	2.4894600	-0.4120260	-1.6005470
42	H	2.7157510	0.7557890	-0.2815170

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44 Energy: -437.567871617
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B3LYP/6-311++G** geometry and energy of conformer: Thr-IV

N	-0.8186040	1.7821470	-0.3309400
H	-0.4205930	2.2264530	0.4902180
C	-0.1907550	0.4827140	-0.6154870
H	-0.2403160	0.3129490	-1.6958070
C	1.3049830	0.3558530	-0.2214000
C	-1.0409900	-0.6447280	0.0052240
H	1.8278280	1.1798690	-0.7182750
O	1.8587050	-0.8277410	-0.7734890
O	-0.6466930	-1.7830180	0.1086290
H	1.2999960	-1.5654680	-0.4817550
O	-2.2578630	-0.2671330	0.3987980
H	-2.2986430	0.7001230	0.2224650
H	-0.7310480	2.4259210	-1.1077820
C	1.5543040	0.4490370	1.2868790
H	2.6267670	0.3784660	1.4762780
H	1.2076150	1.3994270	1.7078940
H	1.0601870	-0.3668810	1.8205460

Energy: -438.425087806

MP2/aug-cc-pVTZ geometry and energy of conformer: Thr-IV

N	-0.8469700	1.7575370	-0.3515190
H	-0.4202520	2.2160600	0.4449560
C	-0.1880080	0.4816160	-0.6407020
H	-0.2058270	0.3118280	-1.7189970
C	1.2812450	0.3921050	-0.1960970
C	-0.9985460	-0.6609140	-0.0233860
H	1.8031190	1.2381650	-0.6495230
O	1.8855410	-0.7690010	-0.7349080
O	-0.5854010	-1.8013960	0.0445680
H	1.3019170	-1.5067420	-0.4896980
O	-2.1993670	-0.3017450	0.4305310
H	-2.2366340	0.6681460	0.2544960
H	-0.7843440	2.3915280	-1.1365740
C	1.4380670	0.4501610	1.3170880
H	2.4963730	0.4107630	1.5663950
H	1.0286300	1.3685400	1.7429320
H	0.9430750	-0.4017230	1.7837030

Energy: -437.568109398

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3 B3LYP/6-311++G** geometry and energy of conformer: Thr-V
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5	N	0.0878610	1.8845440	-0.2474540
6	H	-0.3917680	2.3981650	-0.9779090
7	C	0.0107380	0.4342910	-0.4629700
8	H	0.1992680	0.2340690	-1.5192340
9	C	1.1514520	-0.2329730	0.3539300
10	C	-1.3471450	-0.1754040	-0.1421140
11	H	0.9439590	-0.0532130	1.4202630
12	O	2.3757110	0.3865930	-0.0067480
13	O	-1.9674510	-0.9263050	-0.8509510
14	H	2.1852190	1.3350420	-0.0707650
15	O	-1.8030990	0.2224500	1.0760170
16	H	-2.6616110	-0.2041570	1.2184690
17	H	-0.3257800	2.1450650	0.6425700
18	C	1.2860290	-1.7265050	0.1067550
19	H	0.3901020	-2.2680380	0.4198280
20	H	1.4616040	-1.9248700	-0.9535260
21	H	2.1362480	-2.1122220	0.6723260

22 Energy: -438.424882619
23

24 MP2/aug-cc-pVTZ geometry and energy of conformer: Thr-V
25

26	N	0.1323170	1.8850100	-0.2398030
27	H	-0.3851820	2.4055810	-0.9373440
28	C	0.0255380	0.4460660	-0.4714850
29	H	0.2234190	0.2429400	-1.5234790
30	C	1.1249650	-0.2390800	0.3539410
31	C	-1.3254930	-0.1491490	-0.1490500
32	H	0.9202350	-0.0342170	1.4133990
33	O	2.3721180	0.3200200	-0.0177380
34	O	-1.9554290	-0.9057310	-0.8526960
35	H	2.2067270	1.2729040	-0.0975950
36	O	-1.7604520	0.2515710	1.0750780
37	H	-2.6155270	-0.1864530	1.2124170
38	H	-0.2621800	2.1194620	0.6649800
39	C	1.1905960	-1.7306230	0.1205030
40	H	0.2719570	-2.2211660	0.4408860
41	H	1.3476350	-1.9355180	-0.9379430
42	H	2.0231640	-2.1487700	0.6826920

43 Energy: -437.566928008
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B3LYP/6-311++G** geometry and energy of conformer: Thr-VI

N	-0.1205910	-1.3994510	0.9934550
H	0.6843540	-1.9870540	1.1766820
C	0.0453620	-0.6034940	-0.2238470
H	0.1076370	-1.2881030	-1.0755180
C	-1.1634380	0.3346920	-0.4254480
C	1.3463630	0.2005650	-0.1861960
H	-0.9657120	0.9360790	-1.3234400
O	-1.3228340	1.1989520	0.7008040
O	1.4524000	1.3773840	0.0802880
H	-0.5447420	1.7724370	0.7281070
O	2.4247430	-0.5770420	-0.4372330
H	3.2153660	-0.0241560	-0.3365820
H	-0.2848060	-0.7932050	1.7912620
C	-2.4662010	-0.4274630	-0.6119270
H	-2.4117260	-1.0770210	-1.4898120
H	-2.6786830	-1.0439070	0.2621090
H	-3.2845380	0.2809320	-0.7533560

Energy: -438.424133922

B3LYP/6-311++G** geometry and energy of conformer: Thr-VII

N	-0.2126490	-1.8206810	0.2695310
H	0.6963680	-2.2371360	0.0915470
C	-0.0588590	-0.3743060	0.4934350
H	0.1337270	-0.1187090	1.5409580
C	1.1198260	0.1563020	-0.3520380
C	-1.3643260	0.3376500	0.0770720
H	0.8613840	0.0300670	-1.4131850
O	2.2224130	-0.7126690	-0.0397190
O	-1.6463270	1.4582080	0.4133890
H	2.9926440	-0.4272070	-0.5413650
O	-2.1464320	-0.4043400	-0.7179290
H	-1.6964710	-1.2791270	-0.7789300
H	-0.6015280	-2.2763270	1.0887040
C	1.4670790	1.6123580	-0.0711460
H	0.6175860	2.2674990	-0.2664390
H	1.7673000	1.7364090	0.9722120
H	2.2979840	1.9276830	-0.7100800

Energy: -438.423921028

B3LYP/6-311++G** geometry and energy of conformer: Thr-VIII

N	-0.2084540	-1.8209760	0.2747170
H	-0.5884260	-2.2874110	1.0915720
C	-0.0611780	-0.3761680	0.4970470
H	0.1300150	-0.1147640	1.5449710
C	1.1216980	0.1503630	-0.3647410
C	-1.3683130	0.3333540	0.0879310
H	0.8590060	0.0084350	-1.4175870

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3	O	2.2620890	-0.6977210	-0.1707490
4	O	-1.6539280	1.4500480	0.4350620
5	H	2.7424990	-0.3963070	0.6088270
6	O	-2.1450690	-0.4006600	-0.7198480
7	H	-1.6980480	-1.2759530	-0.7845350
8	H	0.6994060	-2.2316040	0.0752000
9	C	1.4647860	1.6096880	-0.1035720
10	H	0.6032420	2.2577260	-0.2648960
11	H	1.7896870	1.7492970	0.9339650
12	H	2.2751070	1.9206650	-0.7662380

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14 Energy: -438.423845140

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19 B3LYP/6-311++G** geometry and energy of conformer: Thr-IX

21	N	-0.0413720	-1.2438400	1.2151860
22	H	-0.4512880	-0.5827480	1.8688640
23	C	0.0489910	-0.6334050	-0.1137760
24	H	0.1221530	-1.4314140	-0.8563140
25	C	-1.1244190	0.3107930	-0.4859690
26	C	1.3669610	0.1376410	-0.1436700
27	H	-0.8688630	0.8061800	-1.4346770
28	O	-1.3193560	1.2905110	0.5314350
29	O	1.5026810	1.2866770	0.2175540
30	H	-0.4926710	1.7887950	0.6097410
31	O	2.3929550	-0.5994420	-0.6046390
32	H	3.1961640	-0.0599000	-0.5337760
33	H	-0.6188080	-2.0753080	1.1987160
34	C	-2.4390040	-0.4345690	-0.6583710
35	H	-3.2299950	0.2721390	-0.9154470
36	H	-2.3656490	-1.1788380	-1.4561210
37	H	-2.7268480	-0.9367590	0.2686250

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39 Energy: -438.422793907

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44 B3LYP/6-311++G** geometry and energy of conformer: Thr-X

47	N	-0.7159900	1.8667120	-0.3779960
48	H	-1.6256120	1.8132780	0.0724060
49	C	-0.2274210	0.5196140	-0.6370400
50	H	-0.2443500	0.2711770	-1.7078130
51	C	1.2519180	0.4003020	-0.1951320
52	C	-1.1431430	-0.5226050	0.0383960
53	H	1.7960570	1.1940310	-0.7177100
54	O	1.7132030	-0.8796130	-0.6972480
55	O	-2.2010150	-0.2314190	0.5339270
56	H	2.5869850	-1.0707420	-0.3407960
57	O	-0.7044020	-1.7898210	0.0132530
58	H	0.2085550	-1.8088900	-0.3413880
59	H	-0.8149610	2.4009910	-1.2315750
60	C	1.4653320	0.5363510	1.3051990
	H	2.5324730	0.5170550	1.5479870
	H	1.0589610	1.4912200	1.6428960

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3 H 0.9714170 -0.2702470 1.8539750
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11 Energy: -438.422596879
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13 B3LYP/6-311++G** geometry and energy of conformer: Thr-XI
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15 N 0.2721470 1.7740430 -0.1393730
16 H -0.4706620 2.3967660 -0.4377880
17 C -0.0160480 0.4107210 -0.5430580
18 H -0.0100170 0.3536420 -1.6383150
19 C 1.0771350 -0.5531780 -0.0418440
20 C -1.4075120 -0.0760430 -0.1107240
21 H 0.8021700 -1.5640000 -0.3625790
22 O 1.0197440 -0.4778630 1.3906870
23 O -2.2209430 0.5799150 0.4862410
24 H 1.7380740 -0.9988080 1.7621040
25 O -1.6549650 -1.3431230 -0.5296150
26 H -2.5487490 -1.5733900 -0.2340880
27 H 0.3044390 1.8222300 0.8747980
28 C 2.4625120 -0.2056670 -0.5753600
29 H 3.2066290 -0.9019880 -0.1746780
30 H 2.4863000 -0.2915600 -1.6655790
31 H 2.7395710 0.8123810 -0.3008560

32 Energy: -438.422545547
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36 B3LYP/6-311++G** geometry and energy of conformer: Thr-XII
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38 N -0.3918680 -1.8080200 0.0591660
39 H 0.2072020 -2.4092460 0.6133980
40 C -0.0940770 -0.3946940 0.3435790
41 H 0.0322280 -0.3089030 1.4295700
42 C 1.1925940 0.1328910 -0.3226840
43 C -1.3475190 0.4463280 0.0038290
44 H 1.0098690 0.2263680 -1.4036040
45 O 2.1675350 -0.9003230 -0.0999060
46 O -1.3404290 1.6372420 -0.1713370
47 H 3.0300670 -0.5665560 -0.3662960
48 O -2.4704220 -0.2815410 -0.0416310
49 H -2.1822440 -1.2144770 0.0855630
50 H -0.1835860 -2.0259460 -0.9124850
51 C 1.6762110 1.4681240 0.2313580
52 H 0.9374760 2.2493880 0.0579500
53 H 1.8636890 1.3864030 1.3060920
54 H 2.6116440 1.7601980 -0.2578590

55 Energy: -438.422381394
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B3LYP/6-311++G** geometry and energy of conformer: Thr-XIII

4	N	0.1393900	1.6827480	-0.1833630
5	H	-0.7556280	2.1431390	-0.0768630
6	C	-0.0061670	0.2798290	-0.5857260
7	H	0.0586770	0.1388500	-1.6733230
8	C	1.1242110	-0.5572270	0.0774390
9	C	-1.3538260	-0.3194580	-0.2039090
10	H	0.8804760	-1.6138220	-0.0470670
11	O	1.1221560	-0.3064010	1.4749940
12	O	-1.6529560	-1.4685890	-0.4001350
13	H	1.0374890	0.6556750	1.5669090
14	O	-2.2069690	0.5721520	0.3554310
15	H	-3.0252280	0.0955100	0.5619860
16	H	0.6947530	2.2056200	-0.8488730
17	C	2.4892440	-0.2671130	-0.5466740
18	H	3.2540710	-0.8530160	-0.0335630
19	H	2.5046460	-0.5340110	-1.6083410
20	H	2.7563950	0.7893370	-0.4464240

21 Energy: -438.422193322

26 B3LYP/6-311++G** geometry and energy of conformer: Thr-XIV

28	N	-0.4677310	1.9484360	-0.5428900
29	H	-0.7951780	2.1586770	0.3949690
30	C	-0.1411500	0.5362040	-0.6702830
31	H	-0.1310180	0.2699140	-1.7313490
32	C	1.3092720	0.2621520	-0.1624140
33	C	-1.1642830	-0.3732770	0.0134630
34	H	1.9153790	1.0352330	-0.6370180
35	O	1.8202810	-0.9690960	-0.6604630
36	O	-2.0967840	-0.0082680	0.6809700
37	H	1.2333110	-1.6835630	-0.3847850
38	O	-0.8992500	-1.6951330	-0.1933110
39	H	-1.5737260	-2.2049340	0.2825270
40	H	-1.2235650	2.1996050	-1.1702620
41	C	1.4548000	0.3706860	1.3545110
42	H	0.8641450	-0.3922640	1.8726270
43	H	2.5015340	0.2302420	1.6303540
44	H	1.1374230	1.3534360	1.7139430

46 Energy: -438.421670064

51 B3LYP/6-311++G** geometry and energy of conformer: Thr-XV

53	N	-0.5212800	1.9195560	-0.3539110
54	H	-1.4085510	2.1468730	-0.7876350
55	C	-0.1467790	0.5362390	-0.6136420
56	H	-0.1970690	0.3730820	-1.6967470
57	C	1.3370160	0.2839400	-0.2277290
58	C	-1.0622550	-0.5410210	-0.0179100
59	H	1.9017020	1.0668540	-0.7374530
60	O	1.8064530	-0.9417070	-0.7728690
	O	-0.7584980	-1.7042820	0.1308880
	H	1.2328330	-1.6470070	-0.4412700

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O	-2.2863880	-0.0781620	0.3159760
H	-2.7965040	-0.8339630	0.6471060
H	-0.6232490	2.0984370	0.6392250
C	1.6039220	0.3789600	1.2759790
H	1.0468580	-0.3812500	1.8317710
H	2.6675240	0.2186430	1.4617960
H	1.3414620	1.3659440	1.6684320

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11 Energy: -438.421541581
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16 B3LYP/6-311++G** geometry and energy of conformer: Thr-XVI

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N	-0.5784370	1.9273800	-0.3001630
H	-1.5639310	1.9610530	-0.0624250
C	-0.1618670	0.5658300	-0.6153250
H	-0.1575770	0.3509260	-1.6947020
C	1.3032400	0.3231520	-0.1345260
C	-1.1604060	-0.4132230	-0.0195820
H	1.8698550	1.1737450	-0.5220660
O	1.8822860	-0.8134290	-0.7654910
O	-2.2139900	-0.1214550	0.4850880
H	1.3800660	-1.5932590	-0.5006030
O	-0.7477020	-1.7048750	-0.1311570
H	-1.4365850	-2.2635080	0.2607090
H	-0.4038050	2.5579800	-1.0721420
C	1.4435010	0.2902270	1.3847650
H	0.9465270	-0.5871630	1.8114230
H	2.4995740	0.2429680	1.6573180
H	1.0033700	1.1877580	1.8241070

35 Energy: -438.421498297
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40 B3LYP/6-311++G** geometry and energy of conformer: Thr-XVII

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N	0.1925480	1.7437770	-0.1447390
H	-0.5504030	2.3440600	-0.4826600
C	-0.0084330	0.3694890	-0.5689890
H	0.0439780	0.3267250	-1.6628590
C	1.1174410	-0.5363630	-0.0338600
C	-1.3566760	-0.2851970	-0.2228820
H	0.8860490	-1.5606770	-0.3458350
O	1.0254870	-0.4406310	1.3969590
O	-1.6657180	-1.4048070	-0.5485520
H	1.7152420	-0.9816570	1.7928540
O	-2.1919900	0.5317220	0.4580840
H	-3.0037250	0.0282580	0.6235180
H	0.1913940	1.7957730	0.8687470
C	2.4967900	-0.1348560	-0.5426870
H	3.2632900	-0.7851120	-0.1088520
H	2.5510850	-0.2432930	-1.6298490
H	2.7183000	0.9007690	-0.2833100

59 Energy: -438.421395397
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5 B3LYP/6-311++G** geometry and energy of conformer: Thr-XVIII
6

7	N	-0.2129830	-1.0623770	1.3729630
8	H	0.5188070	-1.6573580	1.7433640
9	C	0.0265030	-0.6918630	-0.0182400
10	H	0.0102800	-1.5990650	-0.6270800
11	C	-1.0985340	0.2484450	-0.5228210
12	C	1.4190500	-0.1000950	-0.2463730
13	H	-0.8162340	0.5952760	-1.5273860
14	O	-1.2696890	1.3717290	0.3430670
15	O	2.3385430	-0.6609470	-0.7850040
16	H	-0.4479210	1.8772640	0.3501910
17	O	1.5504410	1.1615820	0.2656620
18	H	2.4644810	1.4448560	0.1089310
19	H	-0.3111580	-0.2398700	1.9584330
20	C	-2.4403560	-0.4649240	-0.6019200
21	H	-2.7207720	-0.8558160	0.3767910
22	H	-3.2060500	0.2376930	-0.9358340
23	H	-2.3948850	-1.2946280	-1.3118270

24 Energy: -438.421382922
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29 B3LYP/6-311++G** geometry and energy of conformer: Thr-XIX
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31	N	-0.5696310	1.8862950	-0.1508650
32	H	-1.5710780	2.0111070	-0.2426360
33	C	-0.1522570	0.5515110	-0.5758770
34	H	-0.2093940	0.4004490	-1.6680100
35	C	1.3336840	0.2989270	-0.1978800
36	C	-1.0591820	-0.5347480	-0.0200670
37	H	1.8968610	1.1266370	-0.6414560
38	O	1.8244570	-0.8656270	-0.8487910
39	O	-0.7348240	-1.6908140	0.1298040
40	H	1.2963020	-1.6117610	-0.5327560
41	O	-2.3110320	-0.1028440	0.2416540
42	H	-2.8232490	-0.8662890	0.5502290
43	H	-0.1119810	2.5931520	-0.7162030
44	C	1.5928720	0.2824840	1.3075740
45	H	1.1042200	-0.5727850	1.7822870
46	H	2.6663120	0.2023140	1.4900590
47	H	1.2199140	1.1983370	1.7707060

48 Energy: -438.421129086
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53 B3LYP/6-311++G** geometry and energy of conformer: Thr-XX
54

55	N	-0.7308580	1.8669150	-0.3601330
56	H	-1.6534570	1.8017010	0.0615410
57	C	-0.2256480	0.5281620	-0.6279700
58	H	-0.2417900	0.2921640	-1.7038690
59	C	1.2540160	0.4061920	-0.1696320
60	C	-1.1396460	-0.5302060	0.0254530
	H	1.8113110	1.2031620	-0.6714560

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3	O	1.7894760	-0.8786780	-0.5895420
4	O	-2.2222220	-0.2589620	0.4762090
5	H	2.0945190	-0.8200270	-1.5009370
6	O	-0.6704930	-1.7866820	0.0312010
7	H	0.2600400	-1.7900010	-0.2772600
8	H	-0.8053110	2.4195510	-1.2044330
9	C	1.4446210	0.5224260	1.3319580
10	H	2.5077960	0.5170690	1.5785010
11	H	1.0000950	1.4547610	1.6825500
12	H	0.9686570	-0.3116490	1.8544930

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14 Energy: -438.421075307

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18 B3LYP/6-311++G** geometry and energy of conformer: Thr-XXI

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21	N	-0.1193650	-1.2422280	1.1368790
22	H	-0.7776110	-2.0136960	1.1012910
23	C	0.0657780	-0.6525800	-0.2053300
24	H	0.0930950	-1.4052590	-1.0012280
25	C	-1.0959750	0.3286130	-0.4698970
26	C	1.4563490	0.0192130	-0.2394780
27	H	-0.8754030	0.9044240	-1.3728620
28	O	-1.1315500	1.2969050	0.5950170
29	O	2.4368950	-0.5963240	-0.5696990
30	H	-1.1403550	0.7782500	1.4164830
31	O	1.5240350	1.3032300	0.1397980
32	H	0.6327720	1.6133520	0.4136110
33	H	0.7547210	-1.6216240	1.4865990
34	C	-2.4455210	-0.3617540	-0.6339720
35	H	-3.2215390	0.3827010	-0.8204340
36	H	-2.4251390	-1.0579320	-1.4775960
37	H	-2.7238110	-0.9160590	0.2671200

38 Energy: -438.420967528

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42 B3LYP/6-311++G** geometry and energy of conformer: Thr-XXII

43				
44				
45	N	0.1782550	1.7228290	0.2842200
46	H	-0.6668530	2.2807450	0.3206010
47	C	-0.0392250	0.4883760	-0.4518520
48	H	-0.0672370	0.6306060	-1.5468320
49	C	1.1089650	-0.5127620	-0.2017160
50	C	-1.4107930	-0.0678890	-0.1098930
51	H	0.8946880	-1.4207490	-0.7753650
52	O	2.2625080	0.1367780	-0.7610310
53	O	-2.2905550	0.5491840	0.4347260
54	H	3.0496880	-0.3488870	-0.4963900
55	O	-1.5753610	-1.3417690	-0.5425510
56	H	-2.4864820	-1.5973140	-0.3326620
57	H	0.9279740	2.2566180	-0.1373290
58	C	1.3134620	-0.8632360	1.2677040
59	H	0.4443980	-1.3956850	1.6643090
60	H	2.1782030	-1.5253940	1.3813450
	H	1.4706580	0.0397710	1.8581780

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3 Energy: -438.420596988
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8 B3LYP/6-311++G** geometry and energy of conformer: Thr-XXIII
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10	N	0.0120870	1.9356770	-0.3341160
11	H	-0.3803690	2.2146210	0.5608410
12	C	0.0014210	0.4814200	-0.4447510
13	H	0.1248570	0.2008000	-1.4964290
14	C	1.1377810	-0.2121200	0.3696660
15	C	-1.3554650	-0.0168880	0.0213570
16	H	1.0035400	0.0601490	1.4204530
17	O	2.3872280	0.3820180	0.0007360
18	O	-1.9293540	0.3867380	1.0022350
19	H	2.6817810	-0.0087930	-0.8301520
20	O	-1.8542620	-0.9951490	-0.7680010
21	H	-2.7049560	-1.2656010	-0.3882800
22	H	0.9723890	2.2634540	-0.3721110
23	C	1.1824480	-1.7285930	0.2222510
24	H	0.2711830	-2.1973010	0.6001650
25	H	1.2910510	-2.0191660	-0.8287740
26	H	2.0299150	-2.1296730	0.7821950

27 Energy: -438.420534409
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32 B3LYP/6-311++G** geometry and energy of conformer: Thr-XXIV
33

34	N	0.0119250	1.9373550	-0.3075720
35	H	-0.2756370	2.2039380	0.6298530
36	C	0.0074290	0.4839820	-0.4356370
37	H	0.1266720	0.2233540	-1.4904560
38	C	1.1383400	-0.2289210	0.3504060
39	C	-1.3473670	-0.0157720	0.0411010
40	H	1.0170610	0.0255590	1.4123780
41	O	2.3440630	0.3653650	-0.1502420
42	O	-1.8764470	0.3305740	1.0681020
43	H	3.0886180	0.0467400	0.3691960
44	O	-1.9031380	-0.9129260	-0.8025300
45	H	-2.7533580	-1.1802360	-0.4193160
46	H	0.9543590	2.2806180	-0.4612160
47	C	1.1577340	-1.7445970	0.1751410
48	H	0.2548410	-2.2063460	0.5830840
49	H	1.2380620	-2.0100760	-0.8819350
50	H	2.0132750	-2.1772930	0.7027090

51 Energy: -438.420532603
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56 B3LYP/6-311++G** geometry and energy of conformer: Thr-XXV
57

58	N	-0.0982090	-0.9222640	1.5056010
59	H	-0.4033540	-0.0727720	1.9712700
60	C	0.0241960	-0.6964720	0.0660630
	H	-0.0069430	-1.6612420	-0.4428670

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3	C	-1.0699750	0.2239260	-0.5571600
4	C	1.4178810	-0.1519790	-0.2274710
5	H	-0.7621570	0.4686480	-1.5845570
6	O	-1.2291980	1.4238350	0.1999730
7	O	2.2628330	-0.6897130	-0.8921060
8	H	-0.3823340	1.8864730	0.2251450
9	O	1.6133590	1.0745110	0.3401930
10	H	2.5212570	1.3481780	0.1375670
11	H	-0.7767400	-1.6484490	1.7007460
12	C	-2.4306990	-0.4553140	-0.5986290
13	H	-2.7618690	-0.7198500	0.4087850
14	H	-3.1688490	0.2253430	-1.0263690
15	H	-2.3959110	-1.3605100	-1.2102240

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17 Energy: -438.420255853

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21 B3LYP/6-311++G** geometry and energy of conformer: Thr-XXVI

22				
23	N	0.0633420	1.8760450	-0.8002950
24	H	-0.6911350	2.2811890	-1.3437440
25	C	-0.0618980	0.4246150	-0.7404920
26	H	-0.2839710	0.0592170	-1.7473250
27	C	1.2982590	-0.2071300	-0.3158400
28	C	-1.1897900	-0.0476620	0.1774590
29	H	2.0078960	0.0821460	-1.1011540
30	O	1.2036510	-1.6294900	-0.2295240
31	O	-1.5031670	0.4832820	1.2141990
32	H	0.8956790	-1.9844830	-1.0702380
33	O	-1.8235030	-1.1400740	-0.3082810
34	H	-2.4854800	-1.4087570	0.3478570
35	H	0.0023140	2.2714150	0.1334010
36	C	1.8210300	0.2769900	1.0274330
37	H	2.7765770	-0.2096730	1.2322450
38	H	1.9845790	1.3559740	1.0136360
39	H	1.1286850	0.0300450	1.8348720

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41 Energy: -438.419934224

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45 B3LYP/6-311++G** geometry and energy of conformer: Thr-XXVII

46				
47				
48	N	-0.1477480	-1.2451090	1.2118140
49	H	0.5851420	-1.9075620	1.4414960
50	C	0.0718540	-0.6750820	-0.1209180
51	H	0.0987670	-1.4998220	-0.8359600
52	C	-1.0995360	0.2391890	-0.5135570
53	C	1.4566250	0.0029070	-0.2447220
54	H	-0.8773570	0.6694560	-1.4987920
55	O	-1.1125680	1.3122150	0.4627730
56	O	2.4141490	-0.5827170	-0.6802200
57	H	-1.8417980	1.9129960	0.2790870
58	O	1.5649110	1.2627530	0.2257370
59	H	0.6808940	1.5922380	0.4806670
60	H	-0.1570900	-0.5225230	1.9244680
	C	-2.4393920	-0.4807500	-0.5560590
	H	-2.6576680	-0.9415590	0.4072180

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3 H -3.2413630 0.2181820 -0.8141730
4 H -2.4245310 -1.2612310 -1.3214940
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6 Energy: -438.419811701
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11 B3LYP/6-311++G** geometry and energy of conformer: Thr-XXVIII

12
13 N -0.6588050 1.8625360 -0.5595770
14 H -0.8737180 2.1075010 0.4000050
15 C -0.1266380 0.5143400 -0.6877920
16 H -0.0600670 0.2732550 -1.7542180
17 C 1.3184760 0.2840640 -0.1258770
18 C -1.0548320 -0.5348160 -0.1000970
19 H 1.9287600 1.0845780 -0.5567530
20 O 1.8753450 -0.9201020 -0.6324910
21 O -0.8413310 -1.7259050 -0.1781570
22 H 1.2382390 -1.6322210 -0.4753670
23 O -2.1114040 -0.0377660 0.5676020
24 H -2.6090450 -0.7930570 0.9182420
25 H -0.0077870 2.5449210 -0.9316010
26 C 1.4101950 0.3578180 1.3984430
27 H 0.8479970 -0.4538100 1.8703310
28 H 2.4534480 0.2621220 1.7046720
29 H 1.0297100 1.3107010 1.7780340

30 Energy: -438.419618259
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35 B3LYP/6-311++G** geometry and energy of conformer: Thr-XXIX

36
37 N -0.0871570 1.9085340 -0.3383170
38 H 0.8440900 2.3005820 -0.4424250
39 C -0.0019850 0.4566440 -0.4779060
40 H 0.1923090 0.2206870 -1.5288930
41 C 1.1339210 -0.1940040 0.3705940
42 C -1.3450910 -0.1778920 -0.1611230
43 H 0.9463610 0.0433070 1.4218420
44 O 2.3638060 0.4730740 0.0648070
45 O -1.8944520 -1.0257130 -0.8164930
46 H 2.7266250 0.0944400 -0.7443420
47 O -1.8615880 0.2943260 1.0021790
48 H -2.7138580 -0.1457640 1.1410130
49 H -0.4192310 2.1558790 0.5889780
50 C 1.2605670 -1.7019010 0.1872100
51 H 0.3531380 -2.2245160 0.4975750
52 H 1.4391160 -1.9549470 -0.8639970
53 H 2.0949480 -2.0799850 0.7818750

54 Energy: -438.419484049
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59 B3LYP/6-311++G** geometry and energy of conformer: Thr-XXX

60 N -0.0859000 1.9079330 -0.3251160

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3	H	-0.3394860	2.1550230	0.6266150
4	C	0.0020860	0.4569830	-0.4730680
5	H	0.1949150	0.2311420	-1.5244370
6	C	1.1319070	-0.2085120	0.3550460
7	C	-1.3445060	-0.1710060	-0.1495830
8	H	0.9485110	0.0075140	1.4169540
9	O	2.3226510	0.4689490	-0.0699170
10	O	-1.9255980	-0.9801220	-0.8250050
11	H	3.0684270	0.1400290	0.4412950
12	O	-1.8296330	0.2700200	1.0397620
13	H	-2.6914500	-0.1521820	1.1750310
14	H	0.8253190	2.3116030	-0.5171120
15	C	1.2462170	-1.7147260	0.1400390
16	H	0.3470720	-2.2376420	0.4754280
17	H	1.4024770	-1.9410030	-0.9175840
18	H	2.0919340	-2.1172240	0.7062960

19 Energy: -438.419445973

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24 B3LYP/6-311++G** geometry and energy of conformer: Thr-XXXI

25				
26	N	0.0226880	1.8829110	-0.7477320
27	H	-0.0475930	2.2518860	0.1961090
28	C	-0.0780880	0.4250940	-0.7315620
29	H	-0.3173430	0.0781800	-1.7377690
30	C	1.2917580	-0.1916710	-0.3632020
31	C	-1.1765330	-0.0745510	0.2105690
32	H	1.9746650	0.1220520	-1.1627080
33	O	1.1024600	-1.6101060	-0.4094690
34	O	-1.3502240	0.3354120	1.3341080
35	H	1.9148880	-2.0402240	-0.1257220
36	O	-1.9709380	-1.0041770	-0.3579820
37	H	-2.6198160	-1.2768510	0.3094590
38	H	-0.7344130	2.2887150	-1.2864540
39	C	1.8584040	0.2592780	0.9793800
40	H	1.1961620	-0.0108780	1.8036750
41	H	2.8334410	-0.2111340	1.1445750
42	H	2.0175620	1.3399410	0.9885940

43 Energy: -438.419177858

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49 B3LYP/6-311++G** geometry and energy of conformer: Thr-XXXII

50				
51	N	0.2123150	1.7949590	-0.3540140
52	H	-0.6767870	2.2832420	-0.3203950
53	C	0.0569650	0.4803330	0.2767830
54	H	-0.0193580	0.5335320	1.3775230
55	C	-1.2174430	-0.1968910	-0.2613670
56	C	1.3191750	-0.3137730	-0.0449410
57	H	-1.1067690	-0.3137230	-1.3410020
58	O	-2.3212590	0.7096960	-0.0993030
59	O	1.4054250	-1.2877890	-0.7470460
60	H	-2.6666440	0.6159610	0.7955320
	O	2.3952080	0.2415500	0.5669980
	H	3.1774180	-0.2592300	0.2892040

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2
3 H 0.9145200 2.3493500 0.1220400
4 C -1.5167480 -1.5426150 0.3866820
5 H -0.7189440 -2.2590610 0.1894470
6 H -1.6275550 -1.4392730 1.4731840
7 H -2.4487760 -1.9454950 -0.0155640
8

9 Energy: -438.418743997
10
11

12 B3LYP/6-311++G** geometry and energy of conformer: Thr-XXXIII
13

14
15 N 0.1397450 1.8101650 -0.2514790
16 H -0.0758470 1.9704100 0.7270110
17 C -0.0141670 0.4038760 -0.5759280
18 H 0.0054740 0.2835100 -1.6651870
19 C 1.0553640 -0.5714780 -0.0099780
20 C -1.3937160 -0.0493330 -0.1107970
21 H 0.7677450 -1.5828450 -0.3236360
22 O 0.9793940 -0.4663570 1.4144760
23 O -2.1132080 0.5439400 0.6462270
24 H 1.6144900 -1.0712790 1.8097940
25 O -1.7279690 -1.2479100 -0.6563910
26 H -2.5939090 -1.4910480 -0.2961730
27 H 1.0828410 2.1319050 -0.4321430
28 C 2.4603480 -0.2720870 -0.5254650
29 H 2.7932880 0.7235320 -0.2209950
30 H 3.1748030 -0.9969400 -0.1233010
31 H 2.5001960 -0.3416580 -1.6164960
32

33 Energy: -438.418617731
34
35

36 B3LYP/6-311++G** geometry and energy of conformer: Thr-XXXIV
37

38 N -0.0864220 1.8827520 -0.3881530
39 H -0.2161500 2.1985570 0.5669810
40 C -0.0010770 0.4273660 -0.4907660
41 H 0.1749660 0.1758490 -1.5384330
42 C 1.1311440 -0.2344060 0.3526040
43 C -1.3535260 -0.1684670 -0.1313090
44 H 0.9098310 -0.0636140 1.4151150
45 O 2.3847960 0.3704120 0.0237010
46 O -1.9740550 -0.9640620 -0.7870780
47 H 2.4158190 1.2504100 0.4118210
48 O -1.7894910 0.2860150 1.0726780
49 H -2.6553420 -0.1165290 1.2386080
50 H 0.7242920 2.3317870 -0.7964030
51 C 1.2769300 -1.7244850 0.0857050
52 H 1.5242280 -1.8972410 -0.9649690
53 H 2.0815620 -2.1339670 0.6989200
54 H 0.3549300 -2.2634800 0.3136280
55

56 Energy: -438.418555341
57
58

59 B3LYP/6-311++G** geometry and energy of conformer: Thr-XXXV
60

N 0.0917630 1.6853540 -0.2798000

1				
2				
3	H	-0.4573790	2.2698680	-0.9028850
4	C	-0.0286220	0.2636940	-0.6443290
5	H	0.0338930	0.0834860	-1.7237960
6	C	1.0799940	-0.5797020	0.0323560
7	C	-1.4007230	-0.2774530	-0.2038580
8	H	0.8497840	-1.6226300	-0.1935980
9	O	1.0101390	-0.4903110	1.4529150
10	O	-1.8562380	-1.2992030	-0.6415960
11	H	1.1248270	0.4298200	1.7167150
12	O	-2.0433920	0.4716800	0.7065130
13	H	-1.4565220	1.2216190	0.9216580
14	H	1.0504170	2.0097190	-0.3530370
15	C	2.4818140	-0.2565940	-0.4865930
16	H	3.2025490	-0.9315590	-0.0218990
17	H	2.5402450	-0.3805410	-1.5715970
18	H	2.7909960	0.7657420	-0.2410720

19 Energy: -438.418544325

22
23 B3LYP/6-311++G** geometry and energy of conformer: Thr-XXXVI

25	N	0.0708310	1.7809980	-0.1976800
26	H	0.0381060	1.8727830	0.8122810
27	C	-0.0054870	0.3829930	-0.5890670
28	H	0.0662670	0.3254570	-1.6797750
29	C	1.0896840	-0.5581780	-0.0195660
30	C	-1.3608240	-0.2378110	-0.2528200
31	H	0.8456220	-1.5733960	-0.3543720
32	O	0.9684250	-0.4745010	1.4062670
33	O	-1.7204550	-1.3074780	-0.6828650
34	H	1.5656060	-1.1104280	1.8115760
35	O	-2.1098740	0.5017770	0.5853340
36	H	-2.9204380	-0.0015630	0.7557710
37	H	0.9318380	2.2026780	-0.5260350
38	C	2.4941150	-0.1908780	-0.4875280
39	H	3.2286470	-0.8853190	-0.0687510
40	H	2.5702870	-0.2492170	-1.5774300
41	H	2.7685560	0.8168790	-0.1655030

42 Energy: -438.418434988

45
46
47 B3LYP/6-311++G** geometry and energy of conformer: Thr-XXXVII

49	N	0.1090110	1.9085680	-0.2778820
50	H	-0.3578410	2.1975030	0.5789480
51	C	-0.0143240	0.4593990	-0.4314020
52	H	0.1500950	0.2129880	-1.4866650
53	C	1.1425100	-0.1986680	0.3784840
54	C	-1.3823120	-0.0619370	0.0293890
55	H	0.9671800	0.0404480	1.4388440
56	O	2.3633750	0.3772310	-0.0516370
57	O	-2.0275380	0.4690960	0.8914280
58	H	2.1914600	1.3290880	-0.1272750
59	O	-1.8428990	-1.1886880	-0.5711610
60	H	-1.2186910	-1.4986880	-1.2390940
	H	-0.3412570	2.4005820	-1.0417190
	C	1.2544310	-1.7061750	0.2142150

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2
3 H 0.3869450 -2.2252250 0.6278000
4 H 1.3719730 -1.9740750 -0.8411230
5 H 2.1417280 -2.0594170 0.7423000
6

7 Energy: -438.418268937
8
9

10
11 B3LYP/6-311++G** geometry and energy of conformer: Thr-XXXVIII

12
13 N -0.0445150 1.8411230 -0.8161040
14 H -0.0854710 2.2370770 0.1167920
15 C -0.0751130 0.3824500 -0.7732460
16 H -0.2465950 0.0247420 -1.7923700
17 C 1.3084440 -0.1752870 -0.3296780
18 C -1.2177640 -0.2315310 0.0386100
19 H 2.0057670 0.1160630 -1.1257520
20 O 1.2658630 -1.5965570 -0.2013670
21 O -1.9137270 -1.1417590 -0.3353580
22 H 0.9285230 -1.9878970 -1.0146650
23 O -1.3906670 0.3723350 1.2411960
24 H -2.1212720 -0.0818210 1.6879910
25 H -0.8311320 2.2083060 -1.3400340
26 C 1.8274690 0.3648290 0.9943180
27 H 1.1554670 0.1140490 1.8169030
28 H 2.8026100 -0.0815240 1.1987580
29 H 1.9537470 1.4482280 0.9493130

30 Energy: -438.418218677
31
32

33
34 B3LYP/6-311++G** geometry and energy of conformer: Thr-XXXIX

35
36 N -0.0830810 1.8518360 0.3146390
37 H -0.7244710 2.4595480 -0.1843000
38 C -0.0226530 0.5332950 -0.3298020
39 H 0.1033300 0.5918830 -1.4199590
40 C 1.1584090 -0.2637270 0.2390910
41 C -1.3827400 -0.1201750 -0.1003520
42 H 1.0219930 -0.3505930 1.3222030
43 O 2.3102310 0.5542040 -0.0344630
44 O -2.3156460 -0.0052540 -0.8557080
45 H 3.0688680 0.1872910 0.4293310
46 O -1.4680440 -0.8050750 1.0623800
47 H -2.3826060 -1.1161140 1.1440460
48 H 0.8412870 2.2700580 0.2776170
49 C 1.3094350 -1.6443720 -0.3930080
50 H 0.4419370 -2.2737740 -0.1816120
51 H 1.4348690 -1.5600170 -1.4755450
52 H 2.1893350 -2.1522550 0.0125080

53 Energy: -438.418020902
54
55

56 B3LYP/6-311++G** geometry and energy of conformer: Thr-XL

57
58 N -0.1612090 1.8585250 -0.8496080
59 H -0.2908270 2.2675740 0.0700790
60 C -0.0719470 0.4070660 -0.7559960
H -0.2420690 -0.0169090 -1.7519930

1				
2				
3	C	1.3092720	-0.1388770	-0.2645430
4	C	-1.1976090	-0.0803980	0.1421810
5	H	2.0437980	0.2427830	-0.9914770
6	O	1.3369470	-1.5651060	-0.2603410
7	O	-1.5739050	0.4855770	1.1379730
8	H	1.0143320	-1.8980920	-1.1048840
9	O	-1.7295370	-1.2433400	-0.2904530
10	H	-2.3948350	-1.5177750	0.3596680
11	H	0.6710300	2.2549010	-1.2724080
12	C	1.7203040	0.3100540	1.1293340
13	H	1.0170000	-0.0498200	1.8826770
14	H	2.7078920	-0.0951210	1.3579690
15	H	1.7739890	1.3986790	1.1943340

Energy: -438.417869111

B3LYP/6-311++G** geometry and energy of conformer: Thr-XLI

22	N	-0.0324190	1.8809760	0.2178140
23	H	0.9174830	2.2371620	0.2617440
24	C	-0.0102640	0.5346410	-0.3572560
25	H	0.1228490	0.5293260	-1.4499360
26	C	1.1478610	-0.2671260	0.2737380
27	C	-1.3777240	-0.1002820	-0.1168230
28	H	1.0090450	-0.2649770	1.3560960
29	O	2.3755060	0.4448480	0.0638300
30	O	-2.2342510	-0.2074120	-0.9598840
31	H	2.6717170	0.2893440	-0.8405110
32	O	-1.5506410	-0.5192870	1.1561710
33	H	-2.4564920	-0.8566440	1.2268390
34	H	-0.5859150	2.5130440	-0.3499110
35	C	1.2422390	-1.6966610	-0.2461360
36	H	1.3817710	-1.7127060	-1.3331180
37	H	2.0902380	-2.2044780	0.2175360
38	H	0.3386540	-2.2655300	-0.0155120

Energy: -438.417733846

B3LYP/6-311++G** geometry and energy of conformer: Thr-XLII

46	N	-0.1222980	1.8873060	-0.6396680
47	H	-0.9207210	2.2735960	-1.1306130
48	C	-0.1057810	0.4266650	-0.7363740
49	H	-0.3007800	0.1536900	-1.7742100
50	C	1.2991960	-0.1167110	-0.3963820
51	C	-1.2320710	-0.2469870	0.0532940
52	H	1.9536850	0.2695470	-1.1885170
53	O	1.1888910	-1.5395840	-0.5044280
54	O	-2.1162890	-0.9078920	-0.4258930
55	H	2.0349580	-1.9367710	-0.2766300
56	O	-1.1830250	0.0428670	1.3828920
57	H	-1.9451560	-0.3911980	1.7953530
58	H	-0.1740100	2.1940600	0.3259880
59	C	1.8713840	0.3069440	0.9536610
59	H	1.2604830	-0.0579250	1.7798680
60	H	2.8845130	-0.0937390	1.0639980
	H	1.9501240	1.3950000	1.0166830

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4 Energy: -438.416965250
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8 B3LYP/6-311++G** geometry and energy of conformer: Thr-XLIII
9

10	N	-0.1884010	1.8592180	-0.8039330
11	H	-0.1763880	2.2626160	0.1269550
12	C	-0.0866920	0.4043140	-0.7457610
13	H	-0.2827200	-0.0034590	-1.7391440
14	C	1.3024700	-0.1417190	-0.3132850
15	C	-1.1871910	-0.0894740	0.1855540
16	H	2.0128020	0.2516140	-1.0572480
17	O	1.2184370	-1.5635710	-0.4432620
18	O	-1.3958530	0.3624570	1.2860100
19	H	2.0395800	-1.9559420	-0.1303880
20	O	-1.9183050	-1.0843050	-0.3492670
21	H	-2.5748520	-1.3471760	0.3144420
22	H	0.5650520	2.2627820	-1.3494770
23	C	1.7707250	0.2713900	1.0785380
24	H	1.0997700	-0.1051910	1.8520370
25	H	2.7758950	-0.1222930	1.2622740
26	H	1.8295590	1.3588160	1.1699600

27 Energy: -438.416792867
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31 B3LYP/6-311++G** geometry and energy of conformer: Thr-XLIV
32

33	N	-0.2539740	1.8118220	-0.8630330
34	H	-0.2459270	2.2387700	0.0565390
35	C	-0.0767670	0.3649860	-0.7832200
36	H	-0.1973930	-0.0377650	-1.7938440
37	C	1.3197120	-0.1199840	-0.2759520
38	C	-1.2101560	-0.2684040	0.0115920
39	H	2.0404690	0.2451540	-1.0250510
40	O	1.3789220	-1.5431340	-0.2061510
41	O	-1.7867480	-1.2773090	-0.3034450
42	H	0.9824640	-1.9282970	-0.9956810
43	O	-1.4976270	0.4183110	1.1431320
44	H	-2.2231820	-0.0470650	1.5866210
45	H	0.4770620	2.2372970	-1.4232810
46	C	1.7377930	0.3991930	1.0918970
47	H	1.0432690	0.0726830	1.8678610
48	H	2.7288430	0.0087860	1.3312460
49	H	1.7923410	1.4899920	1.1026350

50 Energy: -438.416053844
51
52

53 B3LYP/6-311++G** geometry and energy of conformer: Thr-XLV
54

55	N	0.1630950	1.7075640	-0.0322460
56	H	0.6465600	2.2990720	-0.6956160
57	C	-0.0323770	0.3508990	-0.5364590
58	H	-0.0172260	0.2965400	-1.6365640
59	C	1.1050810	-0.5521540	0.0129250
60	C	-1.4378860	-0.1215240	-0.1233730
	H	0.9027210	-1.6052370	-0.2222720

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2				
3	O	1.1227050	-0.4729230	1.4261710
4	O	-2.2778080	0.6232810	0.3020840
5	H	1.0406050	0.4712750	1.6354030
6	O	-1.7249500	-1.4252630	-0.3255160
7	H	-0.9362300	-1.9165780	-0.5858770
8	H	-0.7359660	2.1251710	0.1899360
9	C	2.4618020	-0.1940790	-0.5961350
10	H	3.2345380	-0.8329170	-0.1648700
11	H	2.4612040	-0.3342800	-1.6819950
12	H	2.7228330	0.8443880	-0.3760850

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14 Energy: -438.415737637

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18 B3LYP/6-311++G** geometry and energy of conformer: Thr-XLVI

19				
20	N	-0.0508300	-1.1284500	1.3522490
21	H	-0.6861400	-1.9103200	1.4493350
22	C	0.0711170	-0.6923310	-0.0389100
23	H	0.0900770	-1.5796180	-0.6728010
24	C	-1.0662360	0.2298520	-0.5392520
25	C	1.4626880	-0.0503900	-0.2307850
26	H	-0.7933010	0.6024960	-1.5352830
27	O	-1.0968310	1.3452070	0.3845800
28	O	2.3657060	-0.6138380	-0.7865340
29	H	-1.7358810	2.0007760	0.0876010
30	O	1.6209510	1.1885430	0.2828700
31	H	0.7556060	1.5358060	0.5672710
32	H	-0.3629500	-0.3778700	1.9583500
33	C	-2.4219130	-0.4597790	-0.6051170
34	H	-3.1953000	0.2378440	-0.9401650
35	H	-2.3951920	-1.2888550	-1.3176150
36	H	-2.7136560	-0.8445110	0.3746140

37 Energy: -438.415355600

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41 B3LYP/6-311++G** geometry and energy of conformer: Thr-XLVII

42				
43	N	-0.1393770	-1.2392960	1.1878900
44	H	-0.3759920	-0.5238630	1.8692910
45	C	0.0673120	-0.6225140	-0.1232850
46	H	0.1245600	-1.4196460	-0.8763400
47	C	-1.1396880	0.2800330	-0.4790320
48	C	1.3687840	0.1981300	-0.1669470
49	H	-0.9078410	0.7730600	-1.4337810
50	O	-1.3412220	1.2622190	0.5326770
51	O	1.4511120	1.3587170	0.1476190
52	H	-0.5372540	1.8011280	0.5688900
53	O	2.4918700	-0.4744940	-0.5292080
54	H	2.2734510	-1.3720590	-0.8091390
55	H	0.6729020	-1.7485960	1.5174310
56	C	-2.4327160	-0.5075230	-0.6253210
57	H	-3.2466560	0.1773170	-0.8700350
58	H	-2.3487600	-1.2473270	-1.4261320
59	H	-2.6749960	-1.0252380	0.3033930

60 Energy: -438.414630711

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5 B3LYP/6-311++G** geometry and energy of conformer: Thr-XLVIII
6

7	N	-0.3093120	1.8173620	-0.7919380
8	H	-0.2057330	2.2298510	0.1281830
9	C	-0.0999250	0.3707870	-0.7688310
10	H	-0.2361820	-0.0079360	-1.7828960
11	C	1.3125220	-0.0918840	-0.3201590
12	C	-1.2294770	-0.2713500	0.0324150
13	H	2.0031750	0.3357620	-1.0639610
14	O	1.3047620	-1.5160080	-0.4408370
15	O	-1.9866440	-1.1099910	-0.3741840
16	H	2.1526800	-1.8621870	-0.1453820
17	O	-1.3149460	0.2418950	1.2901770
18	H	-2.0754660	-0.1803350	1.7176260
19	H	0.3338500	2.2725790	-1.4301000
20	C	1.7646010	0.3529890	1.0682660
21	H	1.1241500	-0.0610000	1.8476480
22	H	2.7923170	0.0187060	1.2443580
23	H	1.7646980	1.4425990	1.1567000

24 Energy: -438.414283769
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29 B3LYP/6-311++G** geometry and energy of conformer: Thr-XLIX
30

31	N	0.0188040	1.8879400	0.0602360
32	H	-0.5314530	2.4781900	-0.5539310
33	C	-0.0264390	0.4795030	-0.3705270
34	H	0.1084390	0.4689370	-1.4534090
35	C	1.1736440	-0.2618220	0.2594430
36	C	-1.3957570	-0.1640140	-0.1133930
37	H	1.0365350	-0.2901230	1.3597310
38	O	2.3587350	0.4569650	-0.0276790
39	O	-2.2322540	-0.3006710	-0.9614520
40	H	2.1259980	1.3965790	0.0348010
41	O	-1.6698960	-0.5232730	1.1736700
42	H	-0.8831860	-0.4457880	1.7293170
43	H	-0.3321940	2.0166600	1.0051110
44	C	1.3369480	-1.6842380	-0.2537480
45	H	1.4735680	-1.6795700	-1.3377740
46	H	2.2195680	-2.1392410	0.1990630
47	H	0.4680530	-2.3019720	-0.0115240

48 Energy: -438.413726133
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52 B3LYP/6-311++G** geometry and energy of conformer: Thr-L
53

54	N	-0.0193390	1.9348650	-0.3129230
55	H	-0.3476760	2.2004530	0.6114240
56	C	-0.0090690	0.4826610	-0.4315110
57	H	0.1272900	0.2295700	-1.4911420
58	C	1.1328590	-0.2189090	0.3460590
59	C	-1.3600240	-0.0349790	0.0716030
60	H	1.0153220	0.0412290	1.4059820
	O	2.3318790	0.3744670	-0.1702150

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3	O	-1.8122780	0.2717380	1.1399960
4	H	3.0780050	0.0978320	0.3706940
5	O	-2.0288580	-0.8953150	-0.7341780
6	H	-1.5665320	-0.9928420	-1.5754600
7	H	0.9246910	2.2878880	-0.4322790
8	C	1.1505470	-1.7360270	0.1795160
9	H	0.2485640	-2.1954970	0.5927880
10	H	1.2375320	-2.0083120	-0.8766420
11	H	2.0063500	-2.1679780	0.7062730

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13 Energy: -438.412787935

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16
17 B3LYP/6-311++G** geometry and energy of conformer: Thr-LI

18				
19	N	-0.5499040	1.8495380	0.1823190
20	H	-0.0445280	2.6264980	-0.2302400
21	C	-0.1538490	0.5868590	-0.4496230
22	H	-0.2720030	0.6103460	-1.5498140
23	C	1.3446910	0.3140810	-0.1723850
24	C	-1.1011110	-0.5257980	-0.0040250
25	H	1.8557720	1.2563750	-0.4261020
26	O	1.8486280	-0.7301690	-1.0040560
27	O	-0.8150630	-1.6338890	0.3571310
28	H	1.7896270	-0.4590360	-1.9259660
29	O	-2.3956750	-0.1113140	-0.1141420
30	H	-2.9562530	-0.8505220	0.1658840
31	H	-1.5415740	2.0209590	0.0618960
32	C	1.6794420	-0.0382060	1.2687200
33	H	1.2878900	-1.0241720	1.5170040
34	H	2.7633910	-0.0489780	1.3990150
35	H	1.2488460	0.7031260	1.9445180

36 Energy: -438.412520745

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39
40 B3LYP/6-311++G** geometry and energy of conformer: Thr-LII

41				
42	N	0.2369850	1.7669510	-0.1157790
43	H	0.2444820	1.8058290	0.8996530
44	C	-0.0356190	0.4048080	-0.5330590
45	H	-0.0339100	0.3710630	-1.6310630
46	C	1.0887910	-0.5364620	-0.0545660
47	C	-1.4372410	-0.0943320	-0.0974050
48	H	0.8829370	-1.5551740	-0.4236540
49	O	1.0122230	-0.5341990	1.3717490
50	O	-2.2380670	0.5957790	0.4653890
51	H	1.7946760	-0.9600330	1.7355520
52	O	-1.7673000	-1.3651360	-0.4534940
53	H	-1.0163640	-1.8135060	-0.8609330
54	H	-0.5136290	2.3788050	-0.4179000
55	C	2.4664660	-0.1225380	-0.5617240
56	H	3.2306520	-0.8089680	-0.1825880
57	H	2.5021720	-0.1599360	-1.6541430
58	H	2.7008570	0.8928550	-0.2430900

59 Energy: -438.412327313

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3
4 B3LYP/6-311++G** geometry and energy of conformer: Thr-LIII

5
6 N -0.0157450 1.9284530 -0.3551070
7 H 0.9425150 2.2644440 -0.3771390
8 C -0.0158390 0.4747840 -0.4465130
9 H 0.1186900 0.1948500 -1.5023330
10 C 1.1299630 -0.2047700 0.3631430
11 C -1.3684510 -0.0339030 0.0573790
12 H 0.9882930 0.0659390 1.4127010
13 O 2.3744590 0.3975370 -0.0057140
14 O -1.8472690 0.3249370 1.0974490
15 H 2.6899450 -0.0091940 -0.8209040
16 O -2.0025540 -0.9595760 -0.7047700
17 H -1.5308170 -1.0890570 -1.5363530
18 H -0.4294060 2.2119870 0.5289950
19 C 1.1782850 -1.7214480 0.2168190
20 H 0.2673790 -2.1918950 0.5950210
21 H 1.2992960 -2.0137530 -0.8338880
22 H 2.0234900 -2.1236540 0.7789650

23 Energy: -438.411988888

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26
27 B3LYP/6-311++G** geometry and energy of conformer: Thr-LIV

28
29 N 0.0406680 1.9300640 -0.1267260
30 H 0.8995460 2.3176010 -0.4983940
31 C -0.0186320 0.5051050 -0.3983340
32 H 0.1265710 0.2537380 -1.4657010
33 C 1.1322660 -0.1816700 0.3724040
34 C -1.3863840 -0.0457010 0.0328150
35 H 1.0330280 0.1279170 1.4188160
36 O 2.3222680 0.3924520 -0.1922470
37 O -2.0734610 0.4245080 0.8916290
38 H 3.0523630 0.2677310 0.4216880
39 O -1.8035300 -1.1529370 -0.6434010
40 H -1.1673720 -1.3880820 -1.3302720
41 H -0.7545930 2.4290070 -0.5067970
42 C 1.1693010 -1.7035160 0.2692830
43 H 0.2937940 -2.1644340 0.7324840
44 H 1.2368310 -2.0247000 -0.7749220
45 H 2.0536300 -2.0867110 0.7853140

46 Energy: -438.408744171

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49
50 B3LYP/6-311++G** geometry and energy of conformer: Thr-LV

51
52 N 0.1042250 1.7712250 -0.4127240
53 H -0.2829180 2.0351080 0.4878570
54 C -0.0332940 0.3410080 -0.6030150
55 H -0.0080720 0.1205260 -1.6806800
56 C 1.0600600 -0.5563650 0.0447560
57 C -1.4157890 -0.0784180 -0.0789080
58 H 0.7997590 -1.6055380 -0.1687220
59 O 0.9984480 -0.3258250 1.4481010
60 O -2.0775670 0.5768820 0.6709500
H 1.6653060 -0.8613930 1.8890180

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2				
3	O	-1.8655080	-1.2888320	-0.5103240
4	H	-1.2568720	-1.6726490	-1.1530050
5	H	1.0706490	2.0700050	-0.4541640
6	C	2.4547590	-0.2890290	-0.5180950
7	H	3.1844500	-0.9626690	-0.0587450
8	H	2.4836260	-0.4576530	-1.5985310
9	H	2.7771010	0.7347090	-0.3122020

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11 Energy: -438.407983479

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14
15 B3LYP/6-311++G** geometry and energy of conformer: Thr-LVI

16				
17	N	0.0930600	1.9231390	-0.0296460
18	H	1.0479800	2.2371380	-0.1661680
19	C	-0.0137050	0.5165040	-0.3755210
20	H	0.0834070	0.3232590	-1.4628520
21	C	1.1342270	-0.2502140	0.3279310
22	C	-1.3654200	-0.0382280	0.1110090
23	H	1.0294650	-0.0553320	1.3968950
24	O	2.3859230	0.3411080	-0.0395730
25	O	-1.7407760	0.0029640	1.2455530
26	H	2.6739060	-0.0359060	-0.8786200
27	O	-2.1348580	-0.6361750	-0.8438090
28	H	-1.7035400	-0.5759120	-1.7048350
29	H	-0.5335310	2.5085680	-0.5689720
30	C	1.1251160	-1.7493860	0.0570910
31	H	1.2180240	-1.9604610	-1.0153740
32	H	1.9642800	-2.2220950	0.5710840
33	H	0.2049640	-2.2164690	0.4159390

34 Energy: -438.407467696

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3 B3LYP/6-311++G** geometry and energy of conformer: aThr-I
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5	N	0.2923440	1.8515520	0.0058230
6	H	0.0289510	2.0580980	-0.9537200
7	C	0.0568290	0.4377930	0.3400420
8	H	-0.0800310	0.3642720	1.4251160
9	C	-1.1837500	-0.2176340	-0.3222290
10	C	1.3458670	-0.3568710	0.0329220
11	H	-1.0098190	-0.2383200	-1.4117690
12	O	-1.3712230	-1.5348850	0.1653400
13	O	1.3762730	-1.5610510	-0.0738490
14	H	-0.5259760	-2.0018520	0.0657870
15	O	2.4389950	0.3972740	-0.0854610
16	H	2.1233100	1.3260630	-0.0065920
17	H	-0.2275260	2.4764410	0.6096490
18	C	-2.4695860	0.5477090	-0.0373330
19	H	-2.6399370	0.6192240	1.0409560
20	H	-2.4542010	1.5531140	-0.4640690
21	H	-3.3096980	0.0054080	-0.4747620

22 Energy: -438.426076096
23

24 MP2/aug-cc-pVTZ geometry and energy of conformer: aThr-I
25

26	N	0.2779100	1.8412290	0.0116870
27	H	0.0219000	2.0222540	-0.9537360
28	C	0.0504700	0.4334780	0.3478070
29	H	-0.0983050	0.3549570	1.4284760
30	C	-1.1651990	-0.2188160	-0.3265250
31	C	1.3314440	-0.3491660	0.0377150
32	H	-0.9799290	-0.2326860	-1.4114700
33	O	-1.3534250	-1.5333810	0.1594760
34	O	1.3699800	-1.5584090	-0.0706310
35	H	-0.4906890	-1.9749690	0.0787340
36	O	2.4182540	0.4132350	-0.0918330
37	H	2.0755600	1.3332470	-0.0058470
38	H	-0.2853630	2.4505600	0.5896710
39	C	-2.4433220	0.5407600	-0.0398110
40	H	-2.5984810	0.6093950	1.0375240
41	H	-2.4271300	1.5425680	-0.4658640
42	H	-3.2817580	-0.0030290	-0.4705160

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44 Energy: -435.933243196
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B3LYP/6-311++G** geometry and energy of conformer: aThr-II

N	0.3845910	1.7459650	0.1091240
H	-0.0076120	1.8208290	1.0430750
C	-0.0023820	0.4823340	-0.5098950
H	-0.0121850	0.6105720	-1.5953050
C	1.0913670	-0.5924520	-0.2199330
C	-1.3845200	0.0038690	-0.0869770
H	0.8795460	-1.4680330	-0.8372570
O	2.3333930	-0.0789570	-0.6746890
O	-2.0387470	0.4683270	0.8134310
H	2.3787120	0.8301190	-0.3403510
O	-1.8044800	-1.0422640	-0.8358020
H	-2.6737640	-1.3113630	-0.5009800
H	0.0344840	2.5356120	-0.4203560
C	1.1635060	-1.0059530	1.2505090
H	1.9840080	-1.7134110	1.3829300
H	1.3567510	-0.1432830	1.8944120
H	0.2387730	-1.4864350	1.5842230

Energy: -438.425833825

MP2/aug-cc-pVTZ geometry and energy of conformer: aThr-II

N	0.4252700	1.7279270	0.0802170
H	0.0052150	1.8007140	1.0015020
C	0.0140320	0.4777880	-0.5389850
H	0.0133340	0.5931430	-1.6230830
C	1.0628600	-0.6080150	-0.2122960
C	-1.3582370	0.0215490	-0.1021900
H	0.8484860	-1.4893660	-0.8162380
O	2.3283540	-0.1285860	-0.6299060
O	-2.0001310	0.5004240	0.8064990
H	2.3531660	0.7904650	-0.3172260
O	-1.7805750	-1.0365590	-0.8313230
H	-2.6448750	-1.2891150	-0.4685780
H	0.0771310	2.5161590	-0.4503700
C	1.0708360	-0.9743800	1.2627500
H	1.8646780	-1.6953590	1.4465340
H	1.2658770	-0.0925510	1.8739110
H	0.1219680	-1.4134730	1.5741970

Energy: -437.568540604

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3 B3LYP/6-311++G** geometry and energy of conformer: aThr-III
4

5	N	-0.9006290	1.7481870	-0.2100110
6	H	-0.6137430	2.0552030	0.7168340
7	C	-0.1875900	0.5111930	-0.5698130
8	H	-0.1835870	0.4335630	-1.6630430
9	C	1.2722380	0.4666440	-0.0591800
10	C	-1.0282340	-0.6883160	-0.0699370
11	H	1.7022080	1.4472520	-0.2879700
12	O	1.2802490	0.4061520	1.3696180
13	O	-0.5803840	-1.7937070	0.1077570
14	H	1.0651210	-0.4986610	1.6300760
15	O	-2.3148780	-0.3914370	0.1338070
16	H	-2.3802580	0.5818950	0.0004750
17	H	-0.7090630	2.4992030	-0.8627630
18	C	2.1481710	-0.6083830	-0.6969090
19	H	3.1679950	-0.5168610	-0.3163470
20	H	1.7698160	-1.6072410	-0.4775380
21	H	2.1785030	-0.4865580	-1.7840710

22 Energy: -438.424501996
23

24 MP2/aug-cc-pVTZ geometry and energy of conformer: aThr-III
25

26	N	-0.9211890	1.7352070	-0.1692450
27	H	-0.6547970	1.9815240	0.7804080
28	C	-0.1861370	0.5300810	-0.5660090
29	H	-0.1727840	0.4844290	-1.6583880
30	C	1.2509350	0.4858440	-0.0337820
31	C	-0.9952070	-0.6850570	-0.0925070
32	H	1.6698990	1.4823170	-0.1922880
33	O	1.2223290	0.3330430	1.3840800
34	O	-0.5186200	-1.7837330	0.0919080
35	H	0.9784000	-0.5877200	1.5545360
36	O	-2.2918140	-0.4223490	0.0948870
37	H	-2.3581610	0.5531170	-0.0294690
38	H	-0.6841900	2.5181670	-0.7647840
39	C	2.1425890	-0.5374470	-0.7122100
40	H	3.1506690	-0.4583060	-0.3087350
41	H	1.7656160	-1.5444030	-0.5502960
42	H	2.1854330	-0.3517910	-1.7862180

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44 Energy: -437.566898070
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B3LYP/6-311++G** geometry and energy of conformer: aThr-IV

N	-0.3892980	1.9484780	-0.1407350
H	-1.3630650	2.2121010	-0.2407070
C	-0.1382820	0.5713100	-0.5719860
H	-0.3208970	0.5120350	-1.6485280
C	1.3359430	0.2164080	-0.2936370
C	-1.0971610	-0.3984880	0.1209660
H	1.9254210	1.0006590	-0.7751470
O	1.6341190	0.3370720	1.0967300
O	-0.8841980	-1.0018660	1.1498550
H	1.0848210	-0.3093910	1.5626510
O	-2.2873330	-0.4716000	-0.5179610
H	-2.8675950	-1.0442020	0.0082530
H	-0.1034020	2.0691190	0.8262380
C	1.7475030	-1.1443130	-0.8542200
H	1.1907290	-1.9588570	-0.3827620
H	1.5802620	-1.1908490	-1.9347820
H	2.8100860	-1.3083240	-0.6658000

Energy: -438.423629378

MP2/aug-cc-pVTZ geometry and energy of conformer: aThr-IV

N	-0.3790920	1.9401160	-0.1350980
H	-1.3619210	2.1786020	-0.1948500
C	-0.1361750	0.5698900	-0.5795430
H	-0.3283600	0.5140030	-1.6518560
C	1.3248370	0.2154370	-0.3096790
C	-1.0760710	-0.3933950	0.1202200
H	1.9206620	0.9816240	-0.8071580
O	1.6271250	0.3510920	1.0752350
O	-0.8475650	-1.0032430	1.1478020
H	1.0600390	-0.2873130	1.5333150
O	-2.2743230	-0.4559280	-0.5027490
H	-2.8354310	-1.0309440	0.0432130
H	-0.0834380	2.0268120	0.8320320
C	1.6964820	-1.1580140	-0.8407310
H	1.1271970	-1.9375410	-0.3339980
H	1.5036750	-1.2242780	-1.9123370
H	2.7548810	-1.3406460	-0.6665720

Energy: -437.565902301

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3 B3LYP/6-311++G** geometry and energy of conformer: aThr-V
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5	N	0.1053490	1.7111100	0.1581730
6	H	1.0854160	1.8783950	0.3668560
7	C	-0.0393510	0.4423970	-0.5739110
8	H	-0.0127820	0.5804690	-1.6593570
9	C	1.0977130	-0.5395250	-0.2258400
10	C	-1.3942710	-0.2099300	-0.2411520
11	H	0.9531240	-1.4190970	-0.8614810
12	O	2.3017990	0.1453140	-0.6037880
13	O	-1.8242730	-1.1610560	-0.8398760
14	H	3.0564300	-0.4151700	-0.3967810
15	O	-2.0341380	0.3603780	0.7885420
16	H	-1.4518760	1.1001040	1.0774480
17	H	-0.2076160	2.4909730	-0.4107310
18	C	1.1397260	-0.9718500	1.2393900
19	H	0.2342920	-1.5187110	1.5132360
20	H	1.9877770	-1.6432220	1.4051720
21	H	1.2477870	-0.1151550	1.9084820

22 Energy: -438.423380829
23

24 MP2/aug-cc-pVTZ geometry and energy of conformer: aThr-V
25

26	N	0.1575090	1.6961910	0.1338620
27	H	1.1507150	1.8483260	0.2787810
28	C	-0.0267150	0.4433150	-0.6005700
29	H	0.0049130	0.5677780	-1.6845700
30	C	1.0655250	-0.5594850	-0.2244650
31	C	-1.3735630	-0.1825210	-0.2475020
32	H	0.9077530	-1.4438650	-0.8462870
33	O	2.2921070	0.0872120	-0.5783160
34	O	-1.8372570	-1.1236860	-0.8481290
35	H	3.0186070	-0.4872490	-0.3119620
36	O	-1.9674870	0.3778160	0.8156470
37	H	-1.3507070	1.1005680	1.0784340
38	H	-0.1774380	2.4784930	-0.4160750
39	C	1.0498910	-0.9506280	1.2428630
40	H	0.1217560	-1.4618460	1.4974000
41	H	1.8734260	-1.6350450	1.4502990
42	H	1.1586800	-0.0753150	1.8813740

43 Energy: -437.566777895
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B3LYP/6-311++G** geometry and energy of conformer: aThr-VI

N	-0.0955450	1.7052140	0.3193320
H	0.4774690	2.4074860	-0.1340140
C	-0.0726050	0.4494920	-0.4424550
H	-0.0935300	0.7230100	-1.5029350
C	1.1660500	-0.4430630	-0.2519370
C	-1.3814260	-0.3300020	-0.2062950
H	1.0391450	-1.3050670	-0.9143420
O	2.2670620	0.3635170	-0.6976100
O	-1.5236910	-1.4897210	-0.4952410
H	3.0725230	-0.1617450	-0.6601850
O	-2.3635310	0.4165420	0.3158280
H	-1.9670610	1.3036330	0.4661020
H	0.2796840	1.5796930	1.2549450
C	1.3732850	-0.9397380	1.1771510
H	0.5289080	-1.5519480	1.5021080
H	2.2705950	-1.5630170	1.2320000
H	1.5105320	-0.1113850	1.8784040

Energy: -438.423320511

B3LYP/6-311++G** geometry and energy of conformer: aThr-VII

N	0.3060560	1.7244680	0.1537380
H	-0.1197550	2.5140820	-0.3165110
C	0.0042770	0.4681200	-0.5281790
H	0.0490430	0.6474130	-1.6051200
C	1.1338870	-0.5646780	-0.2303070
C	-1.3627410	-0.1561850	-0.2693680
H	0.9785260	-1.4255290	-0.8836850
O	2.3685730	0.0158680	-0.6187760
O	-1.8233390	-1.0663460	-0.9112650
H	2.3554670	0.9213590	-0.2726940
O	-2.0152340	0.3964180	0.7843780
H	-2.8531700	-0.0812000	0.8831160
H	-0.0324240	1.7235720	1.1093950
C	1.1692200	-1.0283630	1.2269030
H	0.2530000	-1.5574210	1.5061570
H	2.0108700	-1.7094250	1.3645110
H	1.3081970	-0.1850180	1.9096770

Energy: -438.423294504

B3LYP/6-311++G** geometry and energy of conformer: aThr-VIII

N	0.1061950	1.7130560	0.1089890
H	-0.1991930	2.4812620	-0.4789130
C	-0.0383150	0.4234250	-0.5794570
H	-0.0144500	0.5241650	-1.6712780
C	1.1022820	-0.5531840	-0.1850540
C	-1.3976000	-0.2148360	-0.2416990
H	0.9465960	-1.4692210	-0.7630410
O	2.3680850	0.0337640	-0.5154930
O	-1.8281630	-1.1729800	-0.8291910

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3 H 2.4833750 0.0216670 -1.4715890
4 O -2.0386790 0.3711110 0.7783210
5 H -1.4611440 1.1180690 1.0548850
6 H 1.0816620 1.8813750 0.3382470
7 C 1.1502810 -0.8954490 1.2981160
8 H 0.2271110 -1.3841240 1.6161150
9 H 1.9825600 -1.5764890 1.4822410
10 H 1.3002780 -0.0029870 1.9098790

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12 Energy: -438.423250569
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19 B3LYP/6-311++G** geometry and energy of conformer: aThr-IX

20
21 N -0.4700340 1.8581390 -0.5036360
22 H -1.4462760 1.9687400 -0.2517430
23 C -0.1257190 0.4457680 -0.6907120
24 H -0.1321780 0.1326500 -1.7441580
25 C 1.3210010 0.2523440 -0.1432150
26 C -1.1790270 -0.3999110 0.0137780
27 H 1.9279470 0.9503350 -0.7419440
28 O 1.3624510 0.6402260 1.2200270
29 O -2.1056740 0.0418210 0.6466070
30 H 0.9028030 1.4924160 1.2653450
31 O -0.9978990 -1.7232300 -0.1820470
32 H -1.7060930 -2.1812740 0.2962030
33 H -0.2695600 2.4092260 -1.3285370
34 C 1.9286460 -1.1343720 -0.2701480
35 H 1.4156750 -1.8533090 0.3676070
36 H 1.8801800 -1.4887520 -1.3033210
37 l 2.9773190 -1.0905170 0.0310880

38 Energy: -438.422988926
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42 B3LYP/6-311++G** geometry and energy of conformer: aThr-X

43
44 N -0.0706400 1.8513750 0.4304850
45 H -0.8015610 2.4343720 0.0385110
46 C -0.0101110 0.5454640 -0.2349080
47 H 0.0760400 0.7191310 -1.3115900
48 C 1.2292760 -0.2438020 0.2365980
49 C -1.2956410 -0.2494770 -0.0007820
50 H 1.1981220 -0.2971060 1.3346710
51 O 1.2224710 -1.5620190 -0.3071070
52 O -1.4205870 -1.2122340 0.7220080
53 H 0.5050680 -2.0484850 0.1173620
54 O -2.3426980 0.2900380 -0.6666500
55 H -3.1317400 -0.2263660 -0.4407460
56 H -0.2479070 1.7503990 1.4255420
57 C 2.5238650 0.4218880 -0.2028810
58 H 2.5651170 1.4547350 0.1438520
59 H 3.3764300 -0.1287220 0.1989890
60 H 2.5970890 0.4116940 -1.2941580

Energy: -438.422948728

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B3LYP/6-311++G** geometry and energy of conformer: aThr-XI

N	0.1469390	1.8441480	-0.2188930
H	1.0444240	2.2507980	0.0186950
C	0.0351320	0.4793590	0.3014670
H	-0.0666100	0.4326210	1.4009690
C	-1.1978290	-0.2503050	-0.2873520
C	1.3115900	-0.2963660	0.0005650
H	-1.0387560	-0.3553120	-1.3687040
O	-1.3557960	-1.5292520	0.3169630
O	1.3707050	-1.4626870	-0.3127690
H	-0.5713950	-2.0479690	0.0936400
O	2.4222800	0.4552640	0.1637220
H	3.1873610	-0.1094880	-0.0254090
H	-0.5749010	2.4347970	0.1768420
C	-2.4894680	0.5163650	-0.0415430
H	-2.4908480	1.4749640	-0.5638340
H	-3.3296370	-0.0738430	-0.4114660
H	-2.6422690	0.6834710	1.0293620

Energy: -438.422264697

B3LYP/6-311++G** geometry and energy of conformer: aThr-XII

N	-0.0891570	1.7228900	0.2217640
H	0.3490020	1.6604070	1.1358180
C	-0.0683190	0.4272240	-0.4702970
H	-0.0849100	0.6348470	-1.5464650
C	1.1644080	-0.4688090	-0.1974050
C	-1.3859740	-0.3326680	-0.2056250
H	1.0185890	-1.3940950	-0.7617110
O	2.3541240	0.2023690	-0.6368980
O	-1.5480790	-1.4878790	-0.5032730
H	2.4512550	0.0833850	-1.5868230
O	-2.3423230	0.4190980	0.3532350
H	-1.9349630	1.3055260	0.4803420
H	0.4217430	2.4252430	-0.2994180
C	1.3607160	-0.8135510	1.2725730
H	0.4789450	-1.3142930	1.6782660
H	2.2164130	-1.4819000	1.3784580
H	1.5732560	0.0787700	1.8691920

Energy: -438.422230945

B3LYP/6-311++G** geometry and energy of conformer: aThr-XIII

N	0.1158580	1.9111030	0.0026970
H	1.0805230	2.1701190	-0.1850590
C	0.0641450	0.4990990	0.3560990
H	-0.0762030	0.3375390	1.4366790
C	-1.1334750	-0.1856550	-0.3450930
C	1.4228810	-0.1587480	0.0152710
H	-0.9381290	-0.2058440	-1.4241570
O	-1.1676360	-1.5454070	0.1603980

3	O	2.4008870	0.4959440	-0.2412560
4	H	-1.8436190	-2.0486490	-0.3050580
5	O	1.4683700	-1.4957880	0.0562940
6	H	0.5635150	-1.8470890	0.1931630
7	H	-0.2344520	2.4998300	0.7473510
8	C	-2.4552460	0.5147660	-0.0707120
9	H	-2.4264030	1.5341060	-0.4572570
10	H	-3.2774300	-0.0122920	-0.5647450
11	H	-2.6615990	0.5397900	1.0033220

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13 Energy: -438.422218686

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18 B3LYP/6-311++G** geometry and energy of conformer: aThr-XIV

19	N	0.7751260	-1.7248190	-0.4758970
20	H	0.3038300	-2.2180650	0.2770570
21	C	0.1719150	-0.3943200	-0.6706380
22	H	0.1789760	-0.1529840	-1.7376480
23	C	-1.2909930	-0.3575850	-0.1876570
24	C	1.0742560	0.6783180	-0.0042650
25	H	-1.2372330	-0.7751200	1.1853570
26	O	0.8024680	1.8510420	0.0140900
27	O	-2.1070570	-0.6731630	1.5834840
28	H	2.2102410	0.1884310	0.4995500
29	O	2.1805470	-0.7773710	0.3073910
30	H	0.7408280	-2.2929180	-1.3129930
31	H	-2.0291190	0.9633640	-0.3637190
32	C	-1.5644350	1.7582940	0.2168870
33	H	-2.0313080	1.2653700	-1.4147540
34	H	-3.0729760	0.8433870	-0.0537440
35	H	-1.8144520	-1.1323040	-0.7687000

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37 Energy: -438.422129382

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41 B3LYP/6-311++G** geometry and energy of conformer: aThr-XV

42	N	-0.3833390	1.9501280	-0.2376000
43	H	0.0990310	2.1654390	0.6307180
44	C	-0.1203530	0.5557770	-0.6070070
45	H	-0.3389180	0.4368510	-1.6703970
46	C	1.3293600	0.0862610	-0.3259530
47	C	-1.1302340	-0.2856700	0.1698980
48	H	1.9831030	0.7405290	-0.9123140
49	O	1.6866600	0.3380700	1.0309350
50	O	-0.9880250	-0.6435880	1.3188490
51	H	1.0558260	-0.1410600	1.5883970
52	O	-2.2269680	-0.5845690	-0.5492320
53	H	-2.8373550	-1.0631780	0.0338280
54	H	-0.0366960	2.5801960	-0.9520110
55	C	1.5882770	-1.3652690	-0.7310060
56	H	1.3713220	-1.5223760	-1.7923260
57	H	2.6363210	-1.6146280	-0.5545420
58	H	0.9750950	-2.0585680	-0.1481520

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60 Energy: -438.422021799

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B3LYP/6-311++G** geometry and energy of conformer: aThr-XVI

N	-0.4278870	1.9034380	-0.0420630
H	-0.0323130	2.6176180	-0.6469940
C	-0.1849850	0.5620140	-0.6134030
H	-0.3578330	0.5204760	-1.6948000
C	1.2850930	0.2017140	-0.3222380
C	-1.2172610	-0.4082460	0.0015880
H	1.9082510	0.9677570	-0.8042200
O	1.5089420	0.2606320	1.0997010
O	-2.2611460	-0.6424840	-0.5497270
H	1.2070720	1.1403910	1.3766870
O	-0.9146800	-0.9439810	1.1935370
H	-0.0204370	-0.6463270	1.4688160
H	-1.4222640	2.0964830	0.0275360
C	1.7123820	-1.1684240	-0.8211510
H	1.5809770	-1.2343430	-1.9041250
H	2.7658190	-1.3357760	-0.5906460
H	1.1296390	-1.9660320	-0.3546830

Energy: -438.421535885

B3LYP/6-311++G** geometry and energy of conformer: aThr-XVII

N	-0.2297340	1.9470650	-0.4745560
H	-1.1646910	2.2910160	-0.6614080
C	-0.1088510	0.5104460	-0.7039720
H	-0.2467870	0.3173010	-1.7706480
C	1.3174410	0.0555880	-0.3161510
C	-1.2106510	-0.2979920	-0.0140570
H	1.6468340	0.4338870	1.0201920
O	-2.1376670	-0.8320280	-0.5668760
O	1.0524110	-0.0328280	1.6211000
H	-1.0722580	-0.3295370	1.3460660
O	-1.8286000	-0.8212050	1.7019970
H	0.0360520	2.1838420	0.4755720
H	1.5644250	-1.4303980	-0.5677110
C	0.9216780	-2.0586030	0.0574810
H	1.3760510	-1.6899050	-1.6134420
H	2.6023200	-1.6734370	-0.3333070
H	1.9902490	0.6499230	-0.9391650

Energy: -438.421431774

B3LYP/6-311++G** geometry and energy of conformer: aThr-XVIII

N	0.1367420	1.9111710	-0.0195110
H	1.1092390	2.1729220	-0.1564180
C	0.0685810	0.5042900	0.3503230
H	-0.0690430	0.3585950	1.4360650
C	-1.1321920	-0.1829680	-0.3512630
C	1.4246690	-0.1664190	0.0236070

3	H	-0.9404890	-0.2019300	-1.4268040
4	O	-1.2010840	-1.5780670	0.0407520
5	O	2.4198160	0.4811200	-0.1788630
6	H	-1.7302420	-1.6579050	0.8426370
7	O	1.4462850	-1.5042150	0.0141820
8	H	0.5319020	-1.8473900	0.1104770
9	H	-0.2606610	2.5112030	0.6918150
10	C	-2.4541690	0.5153590	-0.0788160
11	H	-2.4182110	1.5435650	-0.4396280
12	H	-3.2678850	-0.0044110	-0.5895460
13	H	-2.6732730	0.5348780	0.9963060

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15 Energy: -438.421364331

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19 B3LYP/6-311++G** geometry and energy of conformer: aThr-XIX

21	N	0.1671450	1.9561490	-0.1718390
22	H	-0.3723320	2.4885980	-0.8459240
23	C	0.0342680	0.5218640	-0.4094280
24	H	0.1674140	0.3279530	-1.4779020
25	C	1.1390660	-0.2372620	0.3747630
26	C	-1.3327830	-0.0205040	0.0104540
27	H	1.0692050	0.0804310	1.4194270
28	O	0.8723870	-1.6394320	0.4137580
29	O	-1.9223610	0.3189850	1.0059460
30	H	1.0153240	-2.0108990	-0.4642360
31	O	-1.8300440	-0.9182520	-0.8702630
32	H	-2.6680760	-1.2460920	-0.5079580
33	H	-0.1966740	2.1851100	0.7495690
34	C	2.5301180	0.0657240	-0.1669890
35	H	2.7120540	1.1411190	-0.1758400
36	H	3.2861900	-0.4228710	0.4511410
37	H	2.6330140	-0.3057310	-1.1937160

38 Energy: -438.421204845

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43 B3LYP/6-311++G** geometry and energy of conformer: aThr-XX

45	N	-0.4951630	1.8015490	-0.5771520
46	H	-1.5005070	1.9208360	-0.5652420
47	C	-0.0938610	0.3975930	-0.7380120
48	H	-0.0341500	0.0748980	-1.7856670
49	C	1.3288430	0.2623880	-0.1160000
50	C	-1.0782190	-0.5614060	-0.0851940
51	H	1.9502370	0.9697670	-0.6898680
52	O	1.2897060	0.6617970	1.2443070
53	O	-1.0718660	-1.7535550	-0.2596650
54	H	0.7689090	1.4788490	1.2666600
55	O	-1.9855560	0.0526560	0.7102510
56	H	-2.5499500	-0.6417760	1.0831530
57	H	-0.1096510	2.3741530	-1.3195130
58	C	1.9603920	-1.1157170	-0.2012190
59	H	2.0137860	-1.4552020	-1.2388610
60	H	2.9742960	-1.0679840	0.2013200
	H	1.3919620	-1.8487140	0.3714800

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3 Energy: -438.421165644
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8 B3LYP/6-311++G** geometry and energy of conformer: aThr-XXI
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10	N	0.1550590	1.9403860	-0.1050090
11	H	-0.1862400	2.1358790	0.8323630
12	C	0.0300920	0.5121720	-0.3937590
13	H	0.1395260	0.3546680	-1.4686200
14	C	1.1462050	-0.2640180	0.3308230
15	C	-1.3260100	-0.0425950	0.0496940
16	H	1.0597460	-0.0335880	1.4019900
17	O	0.8543870	-1.6499770	0.1152550
18	O	-1.7922750	0.1196250	1.1517150
19	H	1.4723300	-2.1816090	0.6258860
20	O	-1.9773990	-0.6946550	-0.9352320
21	H	-2.8111690	-1.0219750	-0.5629610
22	H	-0.3995170	2.4908820	-0.7513510
23	C	2.5351150	0.1079310	-0.1713640
24	H	2.7059130	1.1797390	-0.0606470
25	H	3.3028570	-0.4255870	0.3979590
26	H	2.6410210	-0.1620040	-1.2258180

27 Energy: -438.421106779
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31 B3LYP/6-311++G** geometry and energy of conformer: aThr-XXII
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33	N	-0.1124730	1.9266840	0.2569850
34	H	0.2871330	2.2110180	-0.6328570
35	C	-0.0008280	0.4857490	0.4222260
36	H	-0.1516610	0.2316800	1.4761780
37	C	-1.1208590	-0.2676600	-0.3698590
38	C	1.3827810	-0.0286220	0.0087170
39	H	-0.8929340	-0.1798850	-1.4443190
40	O	-1.1885150	-1.6423510	-0.0013230
41	O	2.2193330	0.6104530	-0.5747550
42	H	-0.3046750	-2.0272800	-0.0214280
43	O	1.5837780	-1.3349320	0.3472720
44	H	2.4655530	-1.5860110	0.0292480
45	H	0.4189510	2.4093410	0.9731870
46	C	-2.4987920	0.3171920	-0.1027020
47	H	-2.5527210	1.3587760	-0.4145730
48	H	-3.2416440	-0.2685830	-0.6482270
49	H	-2.7312760	0.2588410	0.9640520

50 Energy: -438.420944975
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54 B3LYP/6-311++G** geometry and energy of conformer: aThr-XXIII
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56	N	0.2097500	1.8057310	-0.1676450
57	H	-0.1877190	1.9895030	0.7473180
58	C	-0.0217050	0.4297000	-0.5665910
59	H	-0.0423750	0.3713030	-1.6627930
60	C	1.0714630	-0.5912140	-0.1048360
	C	-1.3885330	-0.0185340	-0.0863530

3	H	0.8179830	-1.5692990	-0.5311040
4	O	2.3414320	-0.1580460	-0.6080570
5	O	-2.0218220	0.4941680	0.8010970
6	H	2.3556710	-0.2694490	-1.5647710
7	O	-1.8192840	-1.1148880	-0.7564950
8	H	-2.6757500	-1.3657910	-0.3780900
9	H	1.2041230	2.0049380	-0.1519620
10	C	1.2175380	-0.7105330	1.4035170
11	H	0.2901000	-1.0572990	1.8651450
12	H	2.0103750	-1.4227020	1.6383170
13	H	1.4841610	0.2522940	1.8446700

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15 Energy: -438.420921096

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19 B3LYP/6-311++G** geometry and energy of conformer: aThr-XXIV

21	N	0.1990200	1.8121770	-0.1094000
22	H	-0.0969370	1.9402520	0.8520420
23	C	-0.0254920	0.4496320	-0.5552190
24	H	-0.0384780	0.4320180	-1.6496890
25	C	1.0619570	-0.5854300	-0.1404790
26	C	-1.3873510	-0.0188260	-0.0773540
27	H	0.7965950	-1.5458740	-0.5997710
28	O	2.2631170	-0.0846300	-0.7432940
29	O	-1.9996800	0.4452380	0.8507490
30	H	3.0049420	-0.6274440	-0.4584330
31	O	-1.8409650	-1.0700160	-0.8016230
32	H	-2.6942080	-1.3324490	-0.4236850
33	H	1.1788750	2.0541600	-0.2034550
34	C	1.2265880	-0.7611090	1.3655920
35	H	0.3140480	-1.1509200	1.8243920
36	H	2.0303000	-1.4732070	1.5779370
37	H	1.4777290	0.1878860	1.8445600

38 Energy: -438.420610844

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42 B3LYP/6-311++G** geometry and energy of conformer: aThr-XXV

44	N	-0.4745510	1.8888600	-0.6668210
45	H	-1.4168640	2.0321000	-1.0150590
46	C	-0.1301400	0.4754950	-0.6909840
47	H	-0.0994220	0.1369900	-1.7320910
48	C	1.2921290	0.3057560	-0.1151160
49	C	-1.1695020	-0.4010630	0.0256040
50	H	1.8751290	1.1052930	-0.5880990
51	O	1.1728320	0.5732660	1.2899320
52	O	-2.0872870	0.0115050	0.6851070
53	H	2.0524420	0.6290890	1.6756320
54	O	-0.9826770	-1.7251040	-0.2105640
55	H	-1.6814210	-2.1990930	0.2661420
56	H	-0.4726320	2.2125680	0.2965460
57	C	1.9707380	-1.0336830	-0.3836690
58	H	2.0305040	-1.2273890	-1.4585670
59	H	2.9942500	-1.0100430	0.0035800
60	H	1.4375730	-1.8579010	0.0888570

Energy: -438.420378965

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B3LYP/6-311++G** geometry and energy of conformer: aThr-XXVI

N	0.0887170	1.9404360	-0.0629900
H	-0.2379260	2.0886900	0.8869430
C	0.0336140	0.5214450	-0.4163080
H	0.2125200	0.4306330	-1.4915170
C	1.1372430	-0.2562770	0.3405290
C	-1.3295100	-0.1267800	-0.1737220
H	1.0236740	-0.0437440	1.4074880
O	0.9161160	-1.6640930	0.2365470
O	-2.0014580	-0.6751930	-1.0101430
H	1.1071550	-1.9473310	-0.6650710
O	-1.7329290	0.0184780	1.1132790
H	-2.5901200	-0.4245240	1.2001590
H	-0.4926990	2.4971170	-0.6798450
C	2.5341780	0.1403610	-0.1199130
H	2.6788990	1.2173480	-0.0225360
H	3.2868710	-0.3791250	0.4766970
H	2.6836240	-0.1281460	-1.1723670

Energy: -438.420301515

B3LYP/6-311++G** geometry and energy of conformer: aThr-XXVII

N	-0.4172310	1.9407700	-0.3528340
H	-1.3701950	2.2039770	-0.5807030
C	-0.1808790	0.5244910	-0.6504790
H	-0.3368820	0.3808760	-1.7214120
C	1.2818920	0.1802810	-0.3464240
C	-1.2141740	-0.3997820	0.0365090
H	1.4519820	0.3756870	1.0808940
O	-2.1888990	-0.8069270	-0.5405590
O	2.3609360	0.1864730	1.3342520
H	-1.0161220	-0.6692430	1.3442660
O	-0.1426900	-0.3276460	1.6174500
H	-0.2576260	2.1417040	0.6291120
H	1.6835560	-1.2282340	-0.7682420
C	1.0838090	-1.9874950	-0.2602630
H	1.5568450	-1.3519850	-1.8469030
H	2.7369220	-1.4126970	-0.5373430
H	1.8914410	0.9247320	-0.8693310

Energy: -438.420126348

B3LYP/6-311++G** geometry and energy of conformer: aThr-XXVIII

N	-0.5144560	1.8248030	-0.7228020
H	-1.4408890	1.9395570	-1.1185240
C	-0.1054560	0.4275490	-0.7351730
H	-0.0198210	0.0957020	-1.7742600
C	1.3022030	0.3183490	-0.1116580
C	-1.0649660	-0.5732320	-0.0738850
H	1.8849730	1.1113040	-0.5963420

3	O	1.1318040	0.6382860	1.2780800
4	O	-1.0225550	-1.7682450	-0.2405790
5	H	1.9964390	0.6806790	1.6977850
6	O	-1.9973410	0.0164320	0.7073200
7	H	-2.5336540	-0.6951690	1.0888480
8	H	-0.5510850	2.1618520	0.2341760
9	C	2.0019510	-1.0219300	-0.3051960
10	H	2.1223060	-1.2434640	-1.3693650
11	H	3.0017860	-0.9830390	0.1391880
12	H	1.4434870	-1.8372360	0.1550320

14 Energy: -438.420018140

20 B3LYP/6-311++G** geometry and energy of conformer: aThr-XXIX

21	N	-0.1258460	1.8768710	0.4103310
22	H	0.0314360	1.8188730	1.4113610
23	C	-0.0035910	0.5654980	-0.2310840
24	H	0.0665930	0.7241820	-1.3105750
25	C	1.1991630	-0.2900310	0.2319350
26	C	-1.3158530	-0.1751890	0.0280230
27	H	1.1205820	-1.6094120	-0.3085740
28	O	-1.4808860	-1.0060490	0.8933250
29	O	0.4097550	-2.0716860	0.1513400
30	H	-2.2973900	0.2098530	-0.8056690
31	O	-3.1038680	-0.2611650	-0.5448450
32	H	0.5214780	2.5489040	0.0186760
33	H	2.5281470	0.2965230	-0.2208460
34	C	2.5798800	0.3181260	-1.3132690
35	H	2.6695400	1.3107310	0.1597720
36	H	3.3488580	-0.3230060	0.1447600
37	H	1.1716070	-0.3389880	1.3296390

39 Energy: -438.419984225

44 B3LYP/6-311++G** geometry and energy of conformer: aThr-XXX

46	N	0.0477930	1.5981070	0.5746330
47	H	0.8722460	2.1447190	0.3490730
48	C	-0.0617450	0.4958820	-0.3780540
49	H	-0.1086820	0.8409760	-1.4271680
50	C	1.1718400	-0.4194810	-0.2993050
51	C	-1.3509030	-0.2878550	-0.1895800
52	H	1.0273360	-1.2291190	-1.0223220
53	O	2.2548640	0.4228160	-0.7334320
54	O	-1.4893290	-1.4708730	-0.3761380
55	H	3.0831680	-0.0481420	-0.6010470
56	O	-2.3840620	0.5175210	0.1551120
57	H	-3.1735050	-0.0406490	0.2218220
58	H	-0.7642060	2.2023480	0.5284480
59	C	1.4352580	-1.0080070	1.0825850
60	H	0.6238320	-1.6785760	1.3737700
	H	2.3572920	-1.5986940	1.0677820
	H	1.5294880	-0.2185520	1.8289980

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4 Energy: -438.419941615
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8 B3LYP/6-311++G** geometry and energy of conformer: aThr-XXXI
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10	N	-0.3052320	1.9290640	-0.5005250
11	H	0.1379480	2.2130500	0.3683950
12	C	-0.0947260	0.4972240	-0.7206240
13	H	-0.2339910	0.2850160	-1.7821520
14	C	1.3133770	-0.0116770	-0.3003430
15	C	-1.2194190	-0.2614730	-0.0213480
16	H	1.6539340	0.4276080	1.0138540
17	O	-2.0771670	-0.9103930	-0.5575160
18	O	1.0160210	0.0513170	1.6339930
19	H	-1.1475590	-0.1346010	1.3363190
20	O	-1.9092500	-0.6022540	1.7124760
21	H	0.1098300	2.4682540	-1.2519740
22	H	1.4903940	-1.5200550	-0.4659720
23	C	0.8187460	-2.0784130	0.1938850
24	H	1.2839880	-1.8306120	-1.4944110
25	H	2.5157040	-1.8011390	-0.2182450
26	H	2.0262000	0.5062990	-0.9498330

27 Energy: -438.419904230
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31 B3LYP/6-311++G** geometry and energy of conformer: aThr-XXXII
32

33	N	-0.1348270	1.8943190	-0.3262450
34	H	-0.3958050	2.1844250	0.6095700
35	C	-0.0198280	0.4499580	-0.4489730
36	H	0.1762220	0.2069170	-1.4994800
37	C	1.1238500	-0.2519510	0.3686660
38	C	-1.3260640	-0.2462220	-0.0989990
39	H	1.2907520	-1.5990110	-0.0492780
40	O	-1.5120590	-1.4352860	-0.2515410
41	O	0.4167930	-2.0117900	-0.1108110
42	H	-2.2485220	0.5532210	0.4654220
43	O	-3.0121870	-0.0033860	0.6841060
44	H	0.7305920	2.3530170	-0.5817000
45	H	2.4702810	0.4329770	0.1815850
46	C	2.7303930	0.4884720	-0.8797340
47	H	2.4790300	1.4371630	0.6096270
48	H	3.2379760	-0.1572890	0.6853330
49	H	0.8499770	-0.2177290	1.4363040

50 Energy: -438.419864927
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54 B3LYP/6-311++G** geometry and energy of conformer: aThr-XXXIII
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56	N	0.0612960	1.9199590	0.0596680
57	H	-0.5237330	2.5057250	-0.5257170
58	C	0.0230810	0.5245530	-0.3868390
59	H	0.1846600	0.5018460	-1.4663370
60	C	1.1445070	-0.2785990	0.2921160
	C	-1.3435420	-0.1215370	-0.1573620

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3	H	1.0164970	-0.1844400	1.3794190
4	O	0.9238850	-1.6384850	-0.0987170
5	O	-2.1223130	-0.4405040	-1.0181120
6	H	1.5735750	-2.1986630	0.3364330
7	O	-1.6338280	-0.2267200	1.1674310
8	H	-2.5189140	-0.6144210	1.2359780
9	H	-0.2699320	2.0056060	1.0156980
10	C	2.5309680	0.2096420	-0.1093870
11	H	2.6493000	1.2665930	0.1343580
12	H	3.3043430	-0.3556000	0.4203630
13	H	2.6830920	0.0749670	-1.1838470

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15 Energy: -438.419811685

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19 B3LYP/6-311++G** geometry and energy of conformer: aThr-XXXIV

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21	N	-0.6448760	1.9569030	-0.2472940
22	H	-0.5704360	2.1156960	0.7545320
23	C	-0.1743860	0.6129430	-0.5547100
24	H	-0.1209950	0.5096420	-1.6468550
25	C	1.2596240	0.4331690	0.0098610
26	C	-1.1687240	-0.4652200	-0.0974780
27	H	1.7203470	1.4180010	-0.0918210
28	O	1.2216850	0.2025040	1.4228810
29	O	-2.3225770	-0.2591350	0.1752450
30	H	1.0162370	-0.7280950	1.5705310
31	O	-0.6356100	-1.7167280	-0.0589770
32	H	-1.3510490	-2.3221640	0.1918660
33	H	-1.6287320	2.0486750	-0.4805640
34	C	2.1288870	-0.5878960	-0.7192000
35	H	2.2131930	-0.3334940	-1.7796160
36	H	3.1324820	-0.5795700	-0.2882040
37	H	1.7227020	-1.5981190	-0.6428360

38 Energy: -438.419695990

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43 B3LYP/6-311++G** geometry and energy of conformer: aThr-XXXV

44				
45	N	0.2133880	1.7984030	-0.3404260
46	H	-0.6538950	2.3132400	-0.2297770
47	C	0.0565040	0.4767580	0.2802730
48	H	-0.0212200	0.5235880	1.3792060
49	C	-1.2142400	-0.1981100	-0.2500480
50	C	1.3125890	-0.3212510	-0.0505270
51	H	-1.1040960	-0.3228410	-1.3331430
52	O	-2.2628370	0.7503790	0.0208560
53	O	1.3903590	-1.3095740	-0.7336400
54	H	-3.0729330	0.4417280	-0.3956850
55	O	2.3978170	0.2487970	0.5305000
56	H	3.1752800	-0.2585800	0.2519930
57	H	0.9595990	2.3170680	0.1091730
58	C	-1.5165090	-1.5392990	0.4107240
59	H	-0.7351570	-2.2682510	0.1928850
60	H	-1.6126560	-1.4207290	1.4936500
	H	-2.4613990	-1.9394590	0.0304180

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3 Energy: -438.419617424
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9 B3LYP/6-311++G** geometry and energy of conformer: aThr-XXXVI
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11	N	0.0060310	1.9204190	-0.3972340
12	H	-0.3972190	2.2598230	0.4691130
13	C	-0.0043250	0.4697090	-0.4622250
14	H	0.1367670	0.1495630	-1.5006730
15	C	1.0886270	-0.2882070	0.3760060
16	C	-1.3772290	0.0039820	-0.0057660
17	H	1.1615230	-1.6620820	0.0040770
18	O	-2.1460760	0.6382080	0.6669170
19	O	0.2711930	-2.0314760	-0.0354510
20	H	-1.6380220	-1.2782110	-0.3905070
21	O	-2.5032850	-1.5190060	-0.0238140
22	H	0.9343880	2.3023950	-0.5178670
23	H	2.4838910	0.2797370	0.1560930
24	C	2.7351940	0.2861890	-0.9085530
25	H	2.5813390	1.2900190	0.5580100
26	H	3.2066110	-0.3572820	0.6693910
27	H	0.8276130	-0.1978110	1.4419290

28 Energy: -438.419573259
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32 B3LYP/6-311++G** geometry and energy of conformer: aThr-XXXVII
33

34	N	0.1817750	1.7319630	0.2297290
35	H	0.9841720	2.2181860	-0.1500650
36	C	-0.0361020	0.4763910	-0.4628620
37	H	-0.0680270	0.5775130	-1.5652790
38	C	1.1139560	-0.5229720	-0.1627380
39	C	-1.4121240	-0.0648180	-0.1094900
40	H	2.3445890	0.0380510	-0.6489190
41	O	-2.2824670	0.5535140	0.4471650
42	O	2.3840390	-0.0777720	-1.6036950
43	H	-1.5867790	-1.3357460	-0.5504920
44	O	-2.4943410	-1.5926570	-0.3275180
45	H	-0.6376870	2.3262340	0.1978920
46	H	1.3023010	-0.8084660	1.3182760
47	C	1.5112110	0.1144630	1.8591870
48	H	0.4025380	-1.2619310	1.7424290
49	H	2.1352430	-1.5007960	1.4536870
50	H	0.8994980	-1.4543410	-0.6958870

51 Energy: -438.419386885
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55 B3LYP/6-311++G** geometry and energy of conformer: aThr-XXXVIII
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57	N	0.1217280	1.7894370	-0.0965360
58	H	1.0897940	2.0825130	-0.1844600
59	C	-0.0137230	0.4224880	-0.5752420
60	H	0.0346880	0.4389510	-1.6702090
	C	1.1079810	-0.5690870	-0.1167500

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3	C	-1.3696230	-0.1852730	-0.2634130
4	H	0.9047870	-1.5375830	-0.5885290
5	O	2.3731940	-0.0642630	-0.5614340
6	O	-1.8262880	-1.1420120	-0.8392560
7	H	2.4433800	-0.1874710	-1.5140110
8	O	-2.0050560	0.4161360	0.7684730
9	H	-2.8430940	-0.0525380	0.9016740
10	H	-0.1513670	1.8747930	0.8758690
11	C	1.2096440	-0.7435270	1.3898780
12	H	0.2820100	-1.1456050	1.8041870
13	H	2.0206390	-1.4350610	1.6241060
14	H	1.4265890	0.2094520	1.8780310

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16 Energy: -438.419206946
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21 B3LYP/6-311++G** geometry and energy of conformer: aThr-XXXIX

22	N	0.6360290	-1.7147460	-0.6782690
23	H	1.4463640	-1.8474740	-1.2763470
24	C	0.1260780	-0.3333750	-0.7607010
25	H	0.0483420	0.0412720	-1.7873440
26	C	-1.2941420	-0.2942860	-0.1382370
27	C	1.0890680	0.6146040	-0.0253170
28	H	-1.8892340	-1.0277730	-0.7077490
29	O	-1.2724610	-0.6689130	1.2366920
30	O	1.1258660	1.7964580	-0.2380460
31	H	-0.8513700	-1.5317270	1.3203570
32	O	1.8895720	0.0227330	0.8783280
33	H	1.6793740	-0.9296760	0.8684910
34	H	-0.0663670	-2.3808020	-0.9872310
35	C	-1.9738470	1.0612120	-0.2317380
36	H	-2.0510870	1.3850840	-1.2722620
37	H	-2.9788360	0.9866720	0.1874840
38	H	-1.4161520	1.8164850	0.3226510

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40 Energy: -438.419197138
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45 B3LYP/6-311++G** geometry and energy of conformer: aThr-XL

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47	N	0.1168490	1.7942960	0.0305650
48	H	-0.1079050	1.8038380	1.0187390
49	C	-0.0144460	0.4664790	-0.5483330
50	H	0.0381530	0.5659550	-1.6365240
51	C	1.1046640	-0.5515510	-0.1812790
52	C	-1.3662090	-0.1692940	-0.2703360
53	H	0.9100480	-1.4657550	-0.7549530
54	O	2.3070470	0.0692350	-0.6551790
55	O	-1.8177810	-1.0967290	-0.8952930
56	H	3.0578080	-0.4868000	-0.4249410
57	O	-2.0079600	0.3747400	0.7895210
58	H	-2.8461970	-0.1013870	0.8906260
59	H	1.0697760	2.1205210	-0.0912600
60	C	1.1972990	-0.8853830	1.3042570
	H	0.2884630	-1.3805060	1.6571220
	H	2.0312690	-1.5700360	1.4875330

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3 H 1.3623510 0.0146320 1.9014630
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Energy: -438.418891187

9 B3LYP/6-311++G** geometry and energy of conformer: aThr-XLI

10
11 N 0.0599990 1.6321440 0.4792430
12 H 0.9234720 2.1254710 0.2785740
13 C -0.0533750 0.4791110 -0.4031710
14 H -0.0900630 0.7569020 -1.4755980
15 C 1.1745770 -0.4496830 -0.2451280
16 C -1.3555570 -0.2821510 -0.1975960
17 H 1.0260490 -1.3100550 -0.9041150
18 O 2.3498320 0.2770920 -0.6461600
19 O -1.5193740 -1.4517870 -0.4420200
20 H 2.3899740 0.2997880 -1.6076230
21 O -2.3600550 0.5185600 0.2276090
22 H -3.1559630 -0.0307380 0.2945600
23 H -0.7192330 2.2694230 0.3682110
24 C 1.4075370 -0.9328440 1.1778130
25 H 0.5521680 -1.5134410 1.5296060
26 H 2.2928790 -1.5708260 1.2032070
27 H 1.5583990 -0.0890520 1.8515290

28 Energy: -438.418624880
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31

32 B3LYP/6-311++G** geometry and energy of conformer: aThr-XLII

33
34 N 0.0268110 1.9494890 -0.2850380
35 H -0.2374930 2.2114810 0.6597180
36 C 0.0267550 0.4973090 -0.4321480
37 H 0.1437040 0.2536750 -1.4934780
38 C 1.1205680 -0.2629990 0.3724790
39 C -1.3393300 0.0003810 0.0239950
40 H 0.8883830 -1.6729650 0.3388900
41 O -1.8727140 0.3438790 1.0484700
42 O 0.9854550 -1.9875030 -0.5674330
43 H -1.8924150 -0.8746120 -0.8413710
44 O -2.7314450 -1.1706370 -0.4549520
45 H 0.9310490 2.3511810 -0.5002150
46 H 2.5329310 0.0747600 -0.0974310
47 C 2.6678520 -0.1911870 -1.1522650
48 H 2.7585780 1.1382450 0.0163480
49 H 3.2597610 -0.4868530 0.4926240
50 H 1.0032910 0.0080470 1.4256370

51 Energy: -438.418486184
52
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55 B3LYP/6-311++G** geometry and energy of conformer: aThr-XLIII

56
57 N 0.0038330 1.9340960 -0.1693510
58 H -0.1052730 2.1421130 0.8183050
59 C 0.0164960 0.4920620 -0.4034210
60 H 0.1032880 0.3117130 -1.4771620
C 1.1320070 -0.2967860 0.3174960

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2				
3	C	-1.3357000	-0.0332250	0.0705410
4	H	0.8920210	-1.6714830	-0.0092250
5	O	-1.7271390	0.0617790	1.2081790
6	O	1.4432230	-2.2300600	0.5473130
7	H	-2.0625820	-0.5888090	-0.9163210
8	O	-2.8983930	-0.8871390	-0.5249990
9	H	0.8461640	2.3795070	-0.5120130
10	H	2.5341250	0.1330920	-0.1030470
11	C	2.6693560	0.0023930	-1.1804340
12	H	2.7294670	1.1766100	0.1577870
13	H	3.2865490	-0.4737720	0.4092930
14	H	0.9988180	-0.1427950	1.3968810

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16 Energy: -438.418452566

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19 B3LYP/6-311++G** geometry and energy of conformer: aThr-XLIV

21	N	-0.0455280	1.9367630	-0.2061400
22	H	-0.1887880	2.1425040	0.7771550
23	C	0.0279720	0.4957670	-0.4449290
24	H	0.2048410	0.3408670	-1.5135940
25	C	1.1194150	-0.2669840	0.3558420
26	C	-1.3398130	-0.1187500	-0.1701290
27	H	0.9247230	-1.6792590	0.2607830
28	O	-1.9807270	-0.7765840	-0.9468330
29	O	1.0125110	-1.9529650	-0.6598550
30	H	-1.7642920	0.1654240	1.0848540
31	O	-2.6297530	-0.2544270	1.2012160
32	H	0.7927250	2.4100440	-0.5211210
33	H	2.5318920	0.1310990	-0.0642680
34	C	2.6996560	-0.0866540	-1.1251800
35	H	2.7172770	1.1962070	0.0980560
36	H	3.2627540	-0.4312410	0.5199490
37	H	0.9730420	-0.0451220	1.4168360

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39 Energy: -438.417538525

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42
43 B3LYP/6-311++G** geometry and energy of conformer: aThr-XLV

46	N	-0.6382970	1.7886960	-0.7431980
47	H	-0.7408820	2.1275400	0.2080560
48	C	-0.1061070	0.4312490	-0.7415080
49	H	-0.0134340	0.0964850	-1.7783520
50	C	1.3005580	0.2887740	-0.0976160
51	C	-1.0849280	-0.5438160	-0.0922730
52	H	1.9208620	1.0546230	-0.5880870
53	O	1.1418100	0.6256430	1.2843090
54	O	-1.1027660	-1.7297610	-0.3195450
55	H	1.9968640	0.5695110	1.7218240
56	O	-1.9215600	0.0416350	0.7856700
57	H	-2.4746650	-0.6596180	1.1615800
58	H	-0.0023670	2.4133430	-1.2283760
59	C	1.9619610	-1.0732440	-0.2838870
60	H	2.0671760	-1.3097660	-1.3464370
	H	2.9656270	-1.0643190	0.1539500
	H	1.3801280	-1.8665770	0.1864610

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4 Energy: -438.417432710
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10 B3LYP/6-311++G** geometry and energy of conformer: aThr-XLVI
11

12	N	0.3558960	1.7481230	0.0362010
13	H	-0.0559220	1.8589370	0.9588270
14	C	-0.0207130	0.4567710	-0.5268660
15	H	-0.0252070	0.5493140	-1.6183380
16	C	1.0893950	-0.5881020	-0.1870610
17	C	-1.4060030	-0.0177110	-0.0714990
18	H	0.9037100	-1.5047740	-0.7576010
19	O	2.3221510	-0.0845930	-0.6723440
20	O	-2.0295290	0.4930570	0.8171010
21	H	2.3587660	0.8394380	-0.3793170
22	O	-1.9064660	-1.1004470	-0.7217200
23	H	-1.3048720	-1.3941080	-1.4177220
24	H	0.0037790	2.5097580	-0.5319310
25	C	1.1636080	-0.9330210	1.2999660
26	H	0.2425560	-1.4046050	1.6544690
27	H	1.9917210	-1.6242730	1.4657910
28	H	1.3472270	-0.0383170	1.9008780

29 Energy: -438.417185763
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34 B3LYP/6-311++G** geometry and energy of conformer: aThr-XLVII
35

36	N	-0.5905490	1.8438300	-0.7329650
37	H	-0.8834180	2.1235550	0.1980120
38	C	-0.1223480	0.4652020	-0.7113660
39	H	-0.0746820	0.0882300	-1.7383740
40	C	1.2938100	0.2717370	-0.1001210
41	C	-1.1690060	-0.3646570	0.0264360
42	H	1.1808860	0.5692470	1.2926410
43	O	-1.9747600	0.0660140	0.8067460
44	O	2.0513210	0.5128730	1.6987630
45	H	-1.0983430	-1.6800000	-0.3012260
46	O	-1.7768140	-2.1359900	0.2200050
47	H	0.1469160	2.4699440	-1.0370480
48	H	1.9292480	-1.0949150	-0.3447810
49	C	1.3617000	-1.8910660	0.1372870
50	H	1.9860430	-1.3103150	-1.4156160
51	H	2.9509190	-1.1062770	0.0483960
52	H	1.9193640	1.0359460	-0.5869620

53 Energy: -438.417177495
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58 B3LYP/6-311++G** geometry and energy of conformer: aThr-XLVIII
59

60	N	-0.0648050	1.9323990	0.2208920
	H	-0.0269270	1.9234190	1.2349290

1				
2				
3	C	0.0275030	0.5807890	-0.3372480
4	H	0.1865160	0.6668680	-1.4138140
5	C	1.1458060	-0.3054290	0.2715670
6	C	-1.3512130	-0.0559220	-0.1865640
7	H	0.9984870	-1.6694720	-0.1353060
8	O	-2.1636270	-0.2075310	-1.0569210
9	O	0.2961250	-2.0745960	0.3840540
10	H	-1.5844570	-0.4332680	1.1053300
11	O	-2.4959840	-0.7607670	1.1480070
12	H	0.6713660	2.5330950	-0.1284930
13	H	2.5295940	0.1412120	-0.1763030
14	C	2.6314650	0.0208920	-1.2584160
15	H	2.7122450	1.1871550	0.0812380
16	H	3.2942640	-0.4689350	0.3075700
17	H	1.0712010	-0.2356560	1.3651460

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19 Energy: -438.417071201

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21
22 B3LYP/6-311++G** geometry and energy of conformer: aThr-XLIX

23				
24				
25	N	-0.0573360	1.9225070	-0.1069100
26	H	-0.1259560	2.0790760	0.8931060
27	C	0.0163750	0.4972920	-0.4275210
28	H	0.1735790	0.3930810	-1.5028890
29	C	1.1212660	-0.2918920	0.3096250
30	C	-1.3570770	-0.1096890	-0.1534670
31	H	0.9221590	-1.6610010	-0.0564140
32	O	-2.1050290	-0.5680630	-0.9733170
33	O	1.5250330	-2.2151420	0.4488010
34	H	-1.6675240	-0.0366070	1.1687650
35	O	-2.5577230	-0.4040030	1.2742000
36	H	0.7406910	2.4308070	-0.4674840
37	H	2.5251150	0.1819250	-0.0562920
38	C	2.6978170	0.0751120	-1.1309000
39	H	2.6827040	1.2255780	0.2283650
40	H	3.2776150	-0.4132740	0.4698370
41	H	0.9566620	-0.1692270	1.3889920

42 Energy: -438.416792961

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44
45 B3LYP/6-311++G** geometry and energy of conformer: aThr-L

46				
47				
48	N	0.1681890	1.7389080	-0.4087770
49	H	-0.4670730	2.2836560	-0.9801700
50	C	-0.0183250	0.3166690	-0.6232220
51	H	0.0232430	0.1278760	-1.7014860
52	C	1.1238950	-0.5400840	0.0105050
53	C	-1.3612990	-0.2869570	-0.1916390
54	H	2.3754000	-0.2792130	-0.6131070
55	O	-1.7794660	-1.3524310	-0.5726170
56	O	2.3071610	-0.4628690	-1.5555890
57	H	-2.0420730	0.4891780	0.6869710
58	O	-2.8582770	0.0158620	0.9101380
59	H	0.0031160	1.9980240	0.5568850
60	H	1.3212950	-0.2806720	1.4973230
	C	1.6503850	0.7473300	1.6645180
	H	0.4017900	-0.4605400	2.0601140

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2
3 H 2.0955880 -0.9464180 1.8822380
4 H 0.8424620 -1.5892830 -0.1429900
5

6 Energy: -438.416002766
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10 B3LYP/6-311++G** geometry and energy of conformer: aThr-LI

11
12 N -0.4560830 1.9232240 -0.4195430
13 H -0.0743350 2.5146910 -1.1486670
14 C -0.1693930 0.5109420 -0.6809320
15 H -0.3422960 0.3238740 -1.7414970
16 C 1.2783350 0.0870220 -0.3536270
17 C -1.2305370 -0.3431150 0.0476840
18 H 1.9435510 0.7268180 -0.9478900
19 O 1.4748170 0.4067580 1.0449650
20 O -2.1378670 -0.8814370 -0.5249900
21 H 2.3408970 0.1030740 1.3346580
22 O -1.0965050 -0.4355490 1.3889240
23 H -0.2345730 -0.0674850 1.6562560
24 H -0.0666300 2.2230240 0.4678870
25 C 1.5766320 -1.3796060 -0.6436350
26 H 1.4160620 -1.5979870 -1.7027930
27 H 2.6199920 -1.6165270 -0.4133000
28 H 0.9361220 -2.0416730 -0.0559820

29 Energy: -438.415697217
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34 B3LYP/6-311++G** geometry and energy of conformer: aThr-LII

35
36 N -0.2979340 1.9441450 -0.3811970
37 H 0.0942490 2.1728720 0.5277890
38 C -0.1508270 0.5101330 -0.6290640
39 H -0.3525630 0.3234100 -1.6918950
40 C 1.3162650 0.1055450 -0.3531960
41 C -1.1205130 -0.3235350 0.2277120
42 H 1.9279550 0.7585170 -0.9814000
43 O 1.6861590 0.4300130 0.9827340
44 O -0.9345540 -0.5919700 1.3879190
45 H 1.0864580 -0.0488240 1.5743480
46 O -2.2725120 -0.7198690 -0.3717610
47 H -2.2686220 -0.4742800 -1.3051620
48 H -1.2642520 2.2512050 -0.4060160
49 C 1.6117010 -1.3540960 -0.6952410
50 H 1.3870720 -1.5669010 -1.7453540
51 H 2.6702320 -1.5586640 -0.5259420
52 H 1.0325060 -2.0400250 -0.0703890

53 Energy: -438.414409825
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59 B3LYP/6-311++G** geometry and energy of conformer: aThr-LIII

60 N 0.5394600 -1.8236570 -0.5196840

1				
2				
3	H	0.4118430	-2.3605190	-1.3680470
4	C	0.1611350	-0.4202560	-0.6876790
5	H	0.1784950	-0.1003080	-1.7412270
6	C	-1.3059190	-0.2835430	-0.1720660
7	C	1.1936210	0.4484110	0.0494620
8	H	-1.8875840	-0.9407390	-0.8379870
9	O	-1.3868380	-0.7562970	1.1572120
10	O	2.1188490	-0.0057680	0.6638590
11	H	-0.8840930	-1.5861340	1.1705140
12	O	1.0537080	1.7886960	-0.0702220
13	H	0.2583350	2.0123770	-0.5684950
14	H	1.5029830	-1.8991330	-0.2092090
15	C	-1.9329870	1.1031540	-0.2153180
16	H	-1.8497330	1.5512310	-1.2123310
17	H	-2.9963540	1.0247820	0.0174550
18	H	-1.4909690	1.7644020	0.5339260

19 Energy: -438.414281429

22
23 B3LYP/6-311++G** geometry and energy of conformer: aThr-LIV

25	N	-0.0934140	1.8185110	0.2926450
26	H	0.6845720	2.3803730	-0.0353470
27	C	-0.0316840	0.4675200	-0.2871040
28	H	0.0127810	0.4783690	-1.3887170
29	C	1.1790620	-0.3289850	0.2294800
30	C	-1.3327980	-0.2359620	0.1019890
31	H	1.2319270	-1.5877900	-0.4488490
32	O	-1.4953010	-0.9951190	1.0165000
33	O	1.5452990	-1.4406870	-1.3484610
34	H	-2.3468760	0.1597710	-0.7149890
35	O	-3.1552870	-0.2728330	-0.3998630
36	H	-0.9433590	2.2895320	-0.0009310
37	H	2.4979840	0.4264400	0.0950950
38	C	2.6826290	0.7297590	-0.9433290
39	H	2.5158020	1.3183490	0.7256610
40	H	3.3190670	-0.2211660	0.4088390
41	H	0.9990120	-0.5802510	1.2755700

42 Energy: -438.414211330

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48 B3LYP/6-311++G** geometry and energy of conformer: aThr-LV

49				
50	N	-0.0923170	1.8388530	-0.2240380
51	H	0.8207470	2.2769010	-0.2565260
52	C	-0.0218520	0.3933800	-0.4971070
53	H	0.1557640	0.1408860	-1.5480230
54	C	1.1102880	-0.2356270	0.3467480
55	C	-1.3810100	-0.2270470	-0.1137440
56	H	0.9043260	-0.0126470	1.4031930
57	O	1.0351990	-1.6385910	0.1179510
58	O	-1.8921470	-1.1424330	-0.6924800
59	H	1.6033460	-2.0901710	0.7493330
60	O	-1.9577400	0.3666120	0.9554630
	H	-1.4366080	1.1719080	1.1410890
	H	-0.6724690	2.3090970	-0.9120520

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3 C 2.4955590 0.2991870 -0.0238290
4 H 2.6161300 1.3599430 0.2147990
5 H 3.2610040 -0.2371380 0.5443170
6 H 2.6935770 0.1451840 -1.0877450
7

8 Energy: -438.413909974
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13 B3LYP/6-311++G** geometry and energy of conformer: aThr-LVI
14

15 N 0.1729360 1.7808940 -0.3190110
16 H -0.1492230 2.0212350 0.6123840
17 C -0.0473200 0.3758020 -0.5961410
18 H -0.0604460 0.2377720 -1.6856410
19 C 1.0541530 -0.5936370 -0.0716840
20 C -1.4054020 -0.0412950 -0.0324290
21 H 0.7876970 -1.6145550 -0.3836120
22 O 2.2361770 -0.1855790 -0.7714420
23 O -1.9178260 0.4719350 0.9223430
24 H 2.9960320 -0.6414570 -0.3955780
25 O -2.0036750 -1.0956010 -0.6453870
26 H -1.5187030 -1.3450850 -1.4419360
27 H 1.1538670 2.0152080 -0.4209140
28 C 1.2539400 -0.5679710 1.4391650
29 H 0.3533960 -0.8935370 1.9648400
30 H 2.0656970 -1.2453640 1.7228090
31 H 1.5114930 0.4361020 1.7831400

32 Energy: -438.412120899
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38 B3LYP/6-311++G** geometry and energy of conformer: aThr-LVII
39

40 N 0.3187900 1.8028530 0.0479700
41 H 0.2347370 2.0148230 -0.9421430
42 C 0.0863860 0.3767240 0.3284250
43 H 0.0081170 0.2881340 1.4198600
44 C -1.1840750 -0.2861280 -0.2709520
45 C 1.3763100 -0.3932440 -0.0498570
46 H -1.4879220 -1.4850970 0.4383800
47 O 1.4049640 -1.5229490 -0.4474460
48 O -1.8601000 -1.2515310 1.2965290
49 H 2.4967130 0.3364110 0.1289710
50 O 2.2022850 1.2482470 0.3237080
51 H -0.3268040 2.4008250 0.5494660
52 H -2.3957220 0.6454340 -0.2982260
53 C -2.6382200 1.0142000 0.7063690
54 H -2.2422650 1.5106050 -0.9474620
55 H -3.2603660 0.0938760 -0.6722290
56 H -0.9563540 -0.6227880 -1.2854760

57 Energy: -438.411872601
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59
60 B3LYP/6-311++G** geometry and energy of conformer: aThr-LVIII

1				
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3				
4	N	0.1622800	1.7398730	0.1035560
5	H	0.8193760	2.2900240	-0.4335420
6	C	-0.0540160	0.4392940	-0.5003720
7	H	-0.0736930	0.4729250	-1.6041720
8	C	1.1037230	-0.5236600	-0.1359360
9	C	-1.4291930	-0.0925400	-0.0858390
10	H	0.9084890	-1.5088040	-0.5911920
11	O	2.2508610	0.0400490	-0.7792000
12	O	-2.2322270	0.5438120	0.5362560
13	H	3.0457870	-0.3302960	-0.3830050
14	O	-1.7368060	-1.3475970	-0.5053510
15	H	-1.0086010	-1.7303140	-1.0106480
16	H	-0.7114600	2.2396760	0.2188030
17	C	1.3065140	-0.6989760	1.3636670
18	H	0.4368250	-1.1783430	1.8219340
19	H	2.1728230	-1.3399780	1.5571890
20	H	1.4577120	0.2711820	1.8369870

21 Energy: -438.411382946

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26 B3LYP/6-311++G** geometry and energy of conformer: aThr-LIX

27				
28	N	0.1973060	1.7887000	-0.2515890
29	H	1.1914510	1.9822820	-0.1999410
30	C	-0.0368080	0.3990620	-0.5867150
31	H	-0.0593550	0.2998290	-1.6846470
32	C	1.0682930	-0.5915500	-0.0867830
33	C	-1.4052840	-0.0297820	-0.0568320
34	H	0.8413830	-1.5927830	-0.4816400
35	O	2.3363210	-0.1588570	-0.5915340
36	O	-1.9621120	0.4999990	0.8629960
37	H	2.3523150	-0.2609410	-1.5494010
38	O	-1.9620990	-1.1124610	-0.6601480
39	H	-1.4422440	-1.3824920	-1.4272010
40	H	-0.2448420	2.0204360	0.6319530
41	C	1.2003810	-0.6689530	1.4251930
42	H	0.2825670	-1.0420120	1.8838310
43	H	2.0197630	-1.3417300	1.6834780
44	H	1.4214510	0.3144000	1.8449920

45 Energy: -438.411204130

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51 B3LYP/6-311++G** geometry and energy of conformer: aThr-LX

52				
53	N	0.4476980	-1.8422390	-0.7662680
54	H	0.4102800	-2.2193410	0.1767970
55	C	0.1474640	-0.4219790	-0.7118200
56	H	0.1492820	-0.0324680	-1.7381650
57	C	-1.2908200	-0.2531880	-0.1713180
58	C	1.1956130	0.3852110	0.0929830
59	H	-1.8953740	-0.9336160	-0.7828860
60	O	-1.2598720	-0.7201940	1.1801800
	O	2.0018680	-0.1101330	0.8252640

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H	-2.1598880	-0.8630190	1.4884840
O	1.2010270	1.7343570	-0.1082910
H	0.5199690	1.9896720	-0.7417690
H	1.3947240	-1.9923400	-1.0985030
C	-1.8785310	1.1552450	-0.2574070
H	-1.8406980	1.5406040	-1.2824830
H	-2.9321750	1.1360300	0.0345710
H	-1.3665430	1.8461750	0.4159890

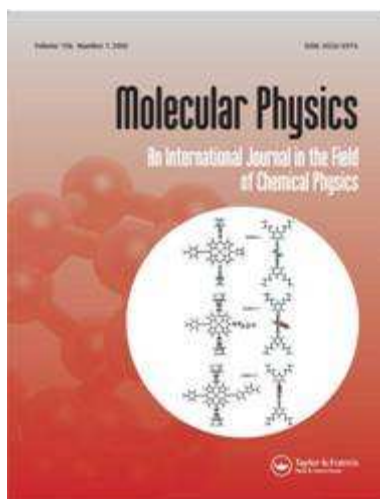
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12 Energy: -438.410386298
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20 B3LYP/6-311++G** geometry and energy of conformer: aThr-LXI

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N	0.5523640	-1.8025000	-0.8192360
H	0.8770620	-2.1110980	0.0925610
C	0.1388480	-0.4117870	-0.7332690
H	0.1348320	0.0165200	-1.7454910
C	-1.2959780	-0.2029840	-0.1695720
C	1.1934550	0.3352170	0.1003260
H	-1.9453450	-0.8242550	-0.8063220
O	-1.2955280	-0.7162050	1.1586600
O	1.8658200	-0.1818210	0.9430890
H	-2.1850160	-0.6604060	1.5213530
O	1.3289090	1.6643680	-0.1620710
H	0.7757050	1.9216400	-0.9089900
H	-0.2219160	-2.3958690	-1.0968940
C	-1.8086660	1.2366410	-0.2205050
H	-1.7638380	1.6379600	-1.2389030
H	-2.8573770	1.2745120	0.0886210
H	-1.2402100	1.8852450	0.4494140

39 Energy: -438.407171053
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Conformers of gaseous threonine

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Conformers of Gaseous Threonine

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Abstract

Following an extensive search on the potential energy surfaces (PES) of the natural amino acid L-threonine (Thr) and its allotropic form L-allo-threonine (aThr), 56 and 61 conformers of Thr and aThr, respectively, have been located with the help of density functional theory (DFT). Accurate structures, relative energies, rotational as well as quartic and sextic centrifugal distortion constants, dipole moments, ^{14}N nuclear quadrupole coupling constants, anharmonic vibrational frequencies and double-harmonic infrared intensities have been determined from *ab initio* electronic structure calculations for the five most stable Thr and aThr conformers. The global minimum, **Thr-I**, has a cyclic triple H-bond motif with strong $\text{OH}\cdots\text{N}$, $\text{C}=\text{O}\cdots\text{HO}$, and a weaker $\text{NH}\cdots\text{OH}$ H-bond, where the latter two involves the side chain OH, and an energetically unfavorable trans $-\text{COOH}$ arrangement. The best relative energies of the conformers, accurate within $\pm 1 \text{ kJ mol}^{-1}$, have been determined through the first-principles composite focal-point analysis (FPA) approach. There are four and three conformers of Thr and aThr, respectively, within a relative energy of 5 kJ mol^{-1} . Similarly to other amino acids investigated, lower levels of electronic structure theory, especially the Hartree–Fock level, are unable to determine the correct relative energies of the conformers. The rotational, the quartic and sextic centrifugal distortion, and the ^{14}N nuclear quadrupole coupling constants as well as the anharmonic vibrational fundamentals and double-harmonic infrared intensities, all determined using DFT, should aid identification and characterization of the conformers of threonine and allo-threonine by rotational and vibrational spectroscopies, respectively.

Keywords: neutral L-threonine • neutral L-allo-threonine • amino acids • *ab initio* calculations • conformational analysis • structure elucidation

This paper is dedicated to Professor Fritz Schaefer on the occasion of his 65th birthday.

I. INTRODUCTION

During the last decades, determination and characterization of the structures of biomolecules, in particular those of proteins and peptides, have been in the focal point of experimental and theoretical research. Since amino acids (AA) are the building blocks of these biopolymers, the structural investigation of AAs, extending from solids to the gas phase, also received considerable attention. Experimental and theoretical structural investigations related to AAs, executed prior to 1999, have been reviewed in ref. 1. During the last decade a considerable number of novel experimental and first-principles computational investigations have been performed on different aspects of the structures of amino acids [2-4], peptides [5,6], and their various complexes [7]. The review of all these studies is out of the scope of the present study and thus only a small number of high-level computational studies originating from our own group are mentioned.

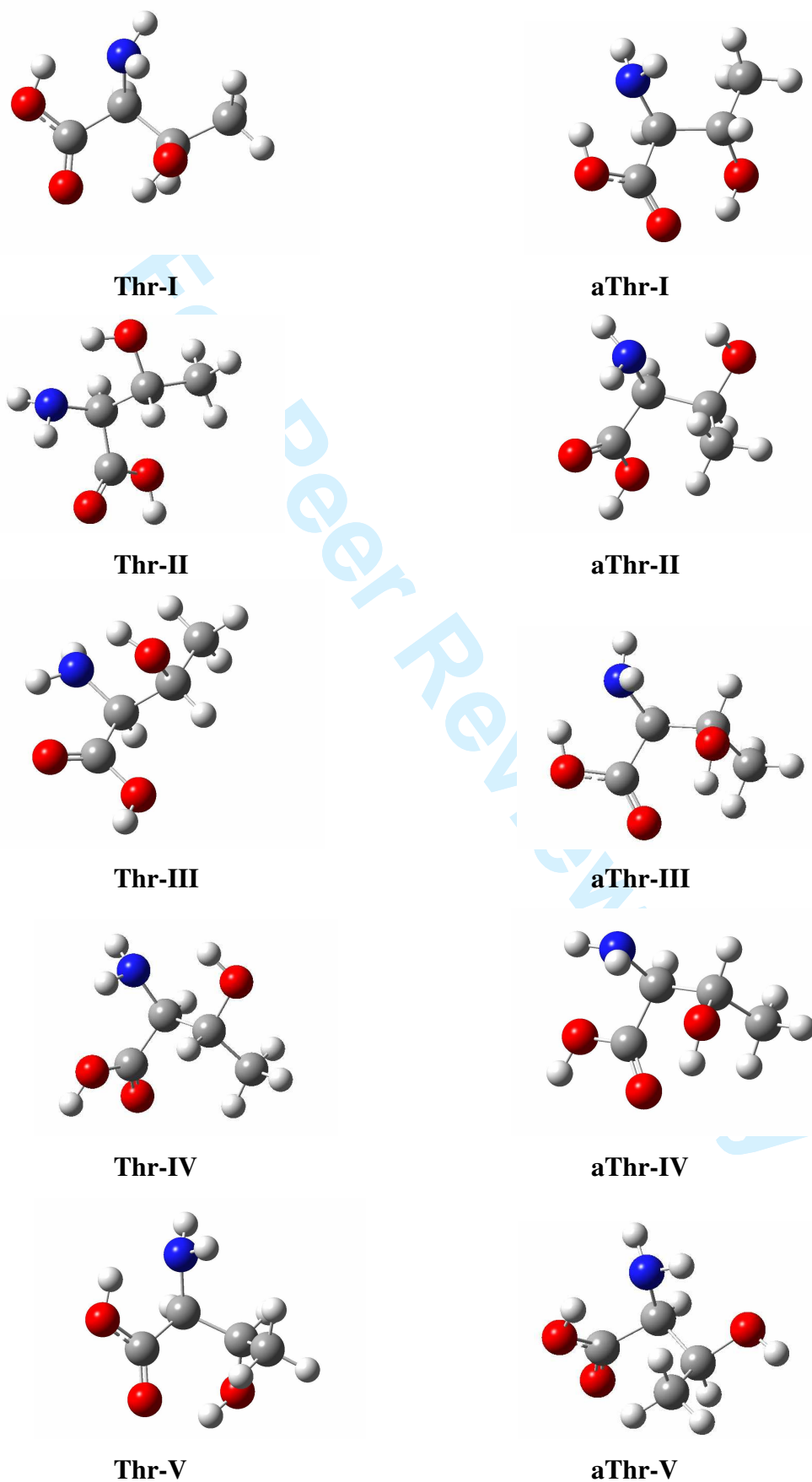
There is only a limited number of natural amino acids and the relatively small size of these molecules allows the application of highly sophisticated experimental and computational techniques during studies related to their equilibrium and dynamical structures usually investigated through their rotational-vibrational spectra. Consequently, we have a detailed understanding of the basics of the structural characteristics of AAs. AAs are chiral, with the sole exception of glycine. In solution and in the solid state, AAs are found in different zwitterionic forms. In the gas phase, however, AAs exist in their neutral form. Furthermore, as AAs are very flexible molecules, all of them exhibit a large number of low-energy conformers and a complex, highly structured potential energy surface (PES). Due partially to the low volatility of AAs and their tendency to decomposition when heated, most of these conformers are not amenable to experimental scrutiny but they can be subjected to detailed quantum chemical investigations. Characterization of the complex PESs of amino acids should precede and supplement related experimental structural studies.

Chiral AAs can play a role in chirally selective organocatalysis, the most important amino acid in this respect appears to be proline (Pro) [8]. As to other applications of AAs in chemistry, one may mention functionalization of fullerenes, carbon nanotubes and semiconductor quantum dots with amino acids [9]. Search for signs of life in the universe is also based principally on structural and spectroscopic characterization of AAs [10]. As of today, it seems that none of the AAs have been found outside of our own planet. Threonine, being an essential amino acid is involved in many studies with biochemical importance, for which the present conformational results could prove useful. As examples, we mention the

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3 studies of metallic complexes of threonine [11-13] and the possible use of Thr and its
4 derivatives in organocatalysis [14].
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7 The number of local minima on the respective PESs and the structural properties of the
8 related conformers, including accurate relative energy estimates, are available for a number of
9 amino acids [1]. The most accurate relative energies, mostly obtained within the focal-point
10 analysis (FPA) approach [15,16], are available for the amino acids glycine (Gly) [4,17-19],
11 alanine (Ala) [18,20], and proline (Pro) [1-3]. The present computational study expands the
12 list of structurally particularly well characterized amino acids by establishing all of the lower-
13 energy and almost all of the higher-energy conformers of L-threonine (see Figure 1), one of
14 the two amino acids, the other one being isoleucine, exhibiting two chirality centers. This
15 feature of threonine was one of the reasons for performing this study. The two diastereomers
16 need to be examined separately during conformational and spectroscopic studies as for all
17 practical purposes they appear as two distinct molecules. Obviously, both L-threonine and L-
18 allo-threonine has an enantiomer pair, D-threonine and D-allo-threonine, respectively. In what
19 follows, L-threonine and L-allo-threonine will be abbreviated as Thr and aThr, respectively. In
20 the biosphere only Thr is abundant. Detailed structural characterization of the lowest-energy
21 conformers of these diastereomers was another important aim of the present study. The
22 present study yielded, as primary information, equilibrium structures, relative energies, and a
23 large number of spectroscopic molecular parameters related to the vibrational and rotational
24 spectra of the most important conformers of the two forms of threonine, Thr and aThr. The
25 computational results obtained should help identification of at least some of the conformers of
26 threonine by means of rotational and vibrational spectroscopies.
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Figure 1. Pictorial representation of the five lowest-energy conformers of L-threonine (Thr) and L-allo-threonine (aThr)



II. COMPUTATIONAL DETAILS

Most of the atom-centered Gaussian basis sets selected for the electronic structure computations of this study contain both polarization and diffuse functions, as they are both needed for the determination of accurate structures and relative energies for H-bonded systems [21]. The subcompact 3-21G basis [22] lacks these functions and thus it has been used only for pre-screening the conformers at the Hartree–Fock [23] level of electronic structure theory. The 6-31G* [24] and 6-311++G** [25] bases, used in this study extensively for geometry optimizations and subsequent force field determinations, contain 260 and 369 contracted Gaussian functions (CGFs), respectively, for threonine. The correlation-consistent, polarized-valence (aug)-cc-p(C)VnZ, $n = 2$ (D), 3 (T), 4 (Q) basis sets of Dunning and coworkers [26,27] have been employed extensively for single-point energy calculations within the FPA approach. (Note that only the augmented (aug) basis set contains diffuse functions, while tight functions, necessary for calculation of core correlation [28] and relativistic effects [29] are only part of core-polarized (C) basis sets.) For Thr, the aug-cc-pVDZ, cc-pVTZ, cc-pCVTZ, aug-cc-pVTZ, and aug-cc-pVQZ basis sets contain 265, 366, 470, 575, and 1054 CGFs, respectively. Only the pure spherical harmonics have been employed in the cc basis sets used in this study.

Electronic wave functions have been determined in this study by the single-configuration, self-consistent-field, restricted Hartree–Fock (RHF) method [23,30,31], by second-order Møller–Plesset perturbation theory, *i.e.*, MP2 [32], by coupled cluster (CC) methods [33] including all single and double excitations (CCSD) [34] and in cases, additionally, a perturbative correction for contributions from connected triple excitations [CCSD(T)] [35], and by a hybrid density functional theory (DFT) approach usually abbreviated as B3LYP [36]. The T_1 diagnostic values of coupled cluster theory [37] are around 0.013 for the different conformers of Thr, suggesting that they can adequately be described by single-reference-based electron correlation methods. The eight lowest 1s-like core orbitals were kept frozen in all post-Hartree–Fock treatments unless otherwise noted.

Rotation barriers corresponding to the methyl group were computed via restricted optimizations [38-40], fixing the methyl torsional coordinate, at the MP2/cc-pVDZ level.

The electronic structure program packages Gaussian03 [41] and MOLPRO [42] have been used extensively during this study. The package MAB-ACESII [43] was employed for the methyl rotational barrier computations.

II.1. Geometry optimizations

Similarly to a scheme first employed for glycine [17], the conformers of Thr and aThr determined in this study are numbered by Roman numerals (see Figure 1) and reflect the energy order of the conformers determined at the B3LYP/6-311++G** level.

Initial structures for the geometry optimizations of the conformers of Thr and aThr were generated by replacing the appropriate H atom of the global minimum of serine with a CH₃ group followed by an optimization at the HF/3-21G level. Then, 5 of the 6 torsional angles characterizing threonine, CCOH (carboxyl), CCC=O, CCNH, CCC-O, and CCOH (side chain), were modified systematically by 60 degrees. This resulted in $6^5 = 7776$ initial structures for one diastereomer. Initial geometry optimizations on the 7776 structures were performed for each diastereomer at the inexpensive RHF/3-21G level. This simple level of electronic structure theory was chosen for the prescreening of the conformers as it was widely assumed [1] that the RHF/3-21G PESs of amino acids and peptides are more structured than their counterparts determined at more sophisticated, and thus computationally more demanding levels of electronic structure theory. Further optimizations were executed at the more reliable B3LYP/6-31G*, B3LYP/6-311++G**, and MP2/aug-cc-pVTZ levels. Initial structures for the latter optimizations were the local minima found on the RHF/3-21G PES of Thr and aThr.

Relative energies of the lowest-energy conformers of Thr and aThr, obtained by geometry optimizations at the HF/3-21G, DFT(B3LYP)/6-31G*, DFT(B3LYP)/6-311++G**, and MP2/aug-cc-pVTZ levels, are given in Table 1. Cartesian coordinates of the optimized structures and energies of all the conformers found in this study are provided as Supplementary Material.

Table 1. Relative energies (kJ mol^{-1}) of the most stable L-threonine and L-allo-threonine conformers obtained from geometry optimizations performed at the MP2/aug-cc-pVTZ, DFT(B3LYP)/6-311++G**, DFT(B3LYP)/6-31G*, and RHF/3-21G levels^[a]

Conformer	MP2/ aug-cc-pVTZ	DFT(B3LYP)/ 6-311++G**	DFT(B3LYP)/ 6-31G*	RHF/ 3-21G
Thr-I	0.00	0.00	0.00	0.00
Thr-II	2.54	1.34	3.18	4.24
Thr-III	4.29	4.33	7.15	-0.96
Thr-IV	4.41	4.80	1.38	3.54
Thr-V	6.77	5.34	9.07	7.69
Thr-VI		7.30		2.68
Thr-VII		7.86		9.95
Thr-VIII		8.06		11.16
Thr-IX		10.82		24.21
Thr-X		11.34		-0.71
Thr-XI		11.47		4.49
Thr-XII		11.91		14.07
aThr-I	0.00	0.00	0.00	0.00
aThr-II	-1.13	0.64	5.48	-0.30
aThr-III	3.18	4.13	4.27	1.39
aThr-IV	5.79	6.43	8.77	1.87
aThr-V	3.50	7.08	13.65	12.53
aThr-VI		7.23		13.02
aThr-VII		7.30		8.32
aThr-VIII		7.42		14.56
aThr-IX		8.11		7.36
aThr-X		8.21		5.62
aThr-XI		10.01		7.81
aThr-XII		10.10		19.49
aThr-XIII		10.13		0.34

^[a] The relative energies of conformer **aThr-I** with respect to conformer **Thr-I** at the MP2, B3LYP/6-311++G**, B3LYP/6-31G*, and RHF levels is 3.67, 2.20, -1.06, and 2.37 kJ mol^{-1} , respectively.

II.2. Focal-point analysis (FPA)

In order to obtain accurate estimates of the relative energies of the conformers of Thr and aThr with corresponding uncertainties, the FPA approach [15,16] was utilized for both diastereomers. The five lowest-energy structures of Thr and aThr (Figure 1), obtained at the B3LYP/6-311++G** level, were included in this investigation.

Extrapolation of the energies to the complete basis set (CBS) limit at the RHF and MP2 levels was performed, as part of the FPA approach, using the formulas $E_n = E_{\text{CBS}} + A(n+1)\exp(-9\sqrt{n})$ [44] and $\varepsilon_n = \varepsilon_{\text{CBS}} + Bn^{-3}$ [45], respectively. In these formulas n is the cardinal number of the augmented, correlation-consistent basis sets aug-cc-pVnZ ($n \in \{3,4\}$), A and B are parameters, E_n is the RHF energy, and ε_n is the MP2 correlation energy increment, and CBS refers to the complete basis set limit. Energy corrections were treated additively, taking advantage of the fact that the contribution of higher-level electron correlation to the requested relative energies does not change significantly with the size of the basis set. CCSD and CCSD(T) correlation energy increments were calculated using the cc-pVTZ basis set.

From the auxiliary corrections needed to be determined within the FPA approach, the core correction was obtained at the MP2/cc-pCVTZ level as the difference between explicit frozen-core (fc) and all-electron (ae) energy computations. The relativistic contributions to the relative energies were estimated within the Douglas-Kroll (DK) formalism [46], as implemented in MOLPRO, at the MP2(ae)/cc-pCVTZ level. After deemed to be unimportant even at the level of precision of this study, the diagonal Born–Oppenheimer corrections (DBOC) [47] were not computed and thus were completely neglected. Zero-point vibrational energies (ZPVE) were obtained as harmonic and anharmonic correction values at the B3LYP/6-311++G** and B3LYP/6-31G* levels, respectively.

The resulting composite single-point relative energies are shown in Tables 2 and 3 for Thr and aThr, respectively.

Table 2. FPA relative energies and energy increments (δ), all in kJ mol^{-1} , for the 5 lowest-energy conformers of L-threonine^[a]

Energy term	Basis	Thr-I	Thr-II	Thr-III	Thr-IV	Thr-V
RHF	aug-cc-pVDZ	0.00	-3.14	-2.01	7.52	0.42
	aug-cc-pVTZ	0.00	-3.01	-2.11	7.80	0.72
	aug-cc-pVQZ	0.00	-2.99	-2.20	7.80	0.77
	CBS	0.00	-2.99	-2.21	7.79	0.78
δ [MP2]	aug-cc-pVDZ	0.00	4.60	6.25	-2.48	5.05
	aug-cc-pVTZ	0.00	5.36	6.47	-3.43	5.90
	aug-cc-pVQZ	0.00	5.36	6.43	-3.47	5.94
	CBS	0.00	5.36	6.39	-3.49	5.98
δ [CCSD]	cc-pVTZ	0.00	-0.74	-1.38	0.66	-0.93
δ [CCSD(T)]	cc-pVTZ	0.00	0.93	1.35	-1.08	1.19
MP2(ae) – MP2(fc)	cc-pCVTZ	0.00	0.08	0.00	0.04	0.08
Relativistic	cc-pCVTZ	0.00	-0.05	0.00	0.03	-0.04
ZPVE(harm)		0.00	-0.41	-1.05	0.68	-0.72
ZPVE(anharm) – ZPVE(harm)		0.00	0.14	0.20	-0.21	0.44
FPA relative energies		0.00	2.32	3.30	4.42	6.77

^[a] All the FPA energy computations were performed employing the fully optimized B3LYP/6-311++G** structures as references. Energy increments (δ) refer to the previous level of theory, MP2 to RHF, CCSD to MP2, and CCSD(T) to CCSD. The abbreviations (fc) and (ae) show that the correlated-level electronic structure computations were done with the frozen core approximation or with all electrons, respectively. The ZPVE(harm)s (harmonic zero-point vibrational energies) correspond to B3LYP/6-311++G** harmonic frequencies. The ZPVE(anharm)s (anharmonic zero-point vibrational energies) were obtained at the B3LYP/6-31G* level based on quartic normal coordinate force fields and second-order vibrational perturbation theory (VPT2).

Table 3. FPA relative energies and energy increments (δ), all in kJ mol^{-1} , for the 5 lowest-energy conformers of L-allo-threonine.^[a]

Energy term	Basis	aThr-I	aThr-II	aThr-III	aThr-IV	aThr-V
RHF	aug-cc-pVDZ	0.00	-8.53	2.19	-3.63	4.70
	aug-cc-pVTZ	0.00	-8.55	2.22	-3.17	4.66
	aug-cc-pVQZ	0.00	-8.42	2.40	-2.98	4.88
	CBS	0.00	-8.41	2.43	-2.95	4.91
δ [MP2]	aug-cc-pVDZ	0.00	6.46	0.47	7.56	-1.77
	aug-cc-pVTZ	0.00	7.94	1.18	9.11	-0.66
	aug-cc-pVQZ	0.00	8.25	1.41	9.39	-0.29
	CBS	0.00	8.48	1.57	9.60	-0.01
δ [CCSD]	cc-pVTZ	0.00	-1.54	-0.68	-2.32	0.26
δ [CCSD(T)]	cc-pVTZ	0.00	2.14	0.53	1.89	0.89
MP2(ae) – MP2(fc)	cc-pCVTZ	0.00	-0.01	0.04	0.08	-0.04
Relativistic	cc-pCVTZ	0.00	-0.05	-0.03	-0.06	-0.02
ZPVE(harm)		0.00	-1.40	-0.53	-0.85	-0.91
ZPVE(anharm) – ZPVE(harm)		0.00	-0.01	0.09	-0.02	0.13
FPA rel. energies		0.00	-0.80	3.42	5.37	5.21

^[a] See footnote [a] to Table 2. The relative energy of conformer **aThr-I** with respect to conformer **Thr-I** is 3.07 kJ mol^{-1} .

II.3. Spectroscopic parameters

For all local minima, quadratic force constants were computed at the B3LYP/6-311++G** level using the B3LYP/6-311++G** optimized structures, thus avoiding the nonzero-force dilemma [48]. For the five lowest-energy conformers of Thr and aThr quartic force fields in normal coordinate space have been determined at the B3LYP/6-31G* level, again at the fully optimized B3LYP/6-31G* structure. The related harmonic and anharmonic vibrational fundamentals of Thr and aThr are reported in Tables 4 and 5, respectively. No scaling of the force fields or of the resulting vibrational wavenumbers has been attempted. The anharmonic vibrational fundamentals were obtained through second-order vibrational perturbation theory (VPT2) [49].

The optimized structures determine the equilibrium rotational constants, while the quadratic and cubic force fields yield the equilibrium quartic and sextic centrifugal distortion constants in the *A*-reduced representation. The anharmonic force fields determined also allow the calculation of vibrationally averaged ground-state rotational constants. For the five lowest-energy Thr and aThr conformers these spectroscopic constants are reported in Tables 6 and 7, respectively.

The ^{14}N nuclear quadruple coupling constants, resulting from the non-spherical distribution of the nuclear charge, have been determined at the B3LYP/6-311++G** level.

Table 4. Harmonic vibrational fundamentals (ω), their VPT2 anharmonic corrections ($\Delta\nu$), and double-harmonic vibrational intensities (I) of the 5 lowest energy conformers of L-threonine^[a]

number	Thr-I			Thr-II			Thr-III			Thr-IV			Thr-V		
	ω	$\Delta\nu$	I	ω	$\Delta\nu$	I	ω	$\Delta\nu$	I	ω	$\Delta\nu$	I	ω	$\Delta\nu$	I
1	3819	-177	46.8	3742	-186	64.9	3762	-188	84.1	3705	-195	131.3	3758	-187	78.7
2	3595	-181	15.3	3708	-199	91.8	3713	-196	60.9	3600	-182	16.1	3718	-198	84.5
3	3495	-108	11.1	3582	-181	12.1	3612	-183	21.9	3518	-129	1.1	3592	-181	11.8
4	3455	-262	277.5	3497	-191	6.2	3516	-142	18.8	3467	-259	264.4	3511	-105	4.8
5	3114	-142	18.4	3115	-142	18.9	3109	-148	23.5	3114	-143	15.6	3113	-143	18.3
6	3098	-141	28.9	3109	-143	24.4	3095	-135	35.2	3086	-113	26.6	3107	-143	24.9
7	3055	-131	9.9	3085	-139	8.3	3078	-130	2.0	3055	-138	5.1	3092	-141	5.7
8	3041	-119	7.7	3040	-133	13.2	3023	-160	23.0	3034	-144	29.1	3038	-134	11.9
9	3033	-132	13.5	2959	-106	38.3	3000	-137	19.8	3021	-165	21.4	2964	-109	39.5
10	1824	-31	324.4	1800	-31	296.8	1808	-33	304.2	1808	-31	287.4	1811	-29	321.0
11	1651	-50	32.9	1662	-31	39.5	1642	-58	77.4	1658	-48	38.1	1659	-57	36.8
12	1503	-42	4.4	1502	-36	3.2	1501	-73	4.8	1502	-51	9.7	1502	-39	4.0
13	1484	-9	6.7	1484	-20	6.0	1489	-39	6.0	1491	-48	5.5	1483	-19	3.6
14	1430	-34	6.3	1441	-46	54.3	1431	-30	55.5	1445	-39	16.5	1439	-47	44.4
15	1418	-40	427.2	1425	-32	4.4	1416	-44	23.4	1419	-45	232.8	1409	-32	29.7
16	1409	-34	9.6	1404	-34	23.6	1401	-17	5.6	1409	-33	215.9	1400	-36	0.9
17	1387	-36	4.9	1375	-5	20.3	1370	-34	11.6	1394	-39	21.4	1377	-5	3.6
18	1359	-35	8.0	1339	-19	31.8	1337	-4	24.0	1371	-33	41.7	1333	-14	53.6
19	1280	-32	57.0	1311	-11	81.1	1302	-30	3.1	1311	-30	18.0	1309	-26	59.6
20	1276	-37	0.4	1265	-39	7.5	1258	-31	21.0	1270	-23	2.5	1289	-29	14.8
21	1209	-40	21.5	1226	-33	20.0	1221	-35	49.2	1220	-46	23.6	1229	-18	17.5
22	1197	-37	9.7	1158	-34	75.1	1162	-33	112.9	1192	-36	9.6	1163	-37	213.1
23	1151	-29	24.6	1136	-31	167.6	1136	-32	154.5	1140	-32	8.9	1138	-31	43.8
24	1084	-24	14.4	1113	-40	54.7	1104	-28	27.3	1106	-31	50.5	1110	-37	7.7
25	1052	-18	55.9	1074	-29	12.9	1076	-30	52.8	1090	-31	79.6	1072	-31	14.8
26	1017	-24	11.5	1052	-21	35.6	1026	-22	25.2	1045	-21	5.2	1050	-19	31.7
27	984	-35	88.3	958	-41	46.6	937	-28	0.7	968	-32	23.1	932	-41	16.9
28	909	-24	54.3	925	-22	35.3	892	-45	77.0	903	-41	84.1	921	-23	88.3
29	878	-47	103.5	872	-29	38.8	869	-24	23.9	872	-40	83.5	868	-20	36.4
30	854	-26	51.0	854	-14	98.7	830	-27	75.8	837	-52	61.4	831	-21	92.2
31	822	-18	13.7	742	-19	37.1	728	-14	28.6	799	-18	26.7	752	-16	24.0
32	751	-15	6.7	666	-16	17.3	659	-3	34.0	754	-10	3.1	643	-20	58.8
33	650	-11	8.9	610	-41	108.9	630	-31	58.1	609	-29	18.0	595	-46	56.3
34	559	-12	9.3	601	-18	125.4	575	-41	163.9	575	-19	117.5	586	-19	160.0
35	532	-23	3.9	543	-11	1.0	545	-12	22.0	549	-11	3.8	548	-11	6.9
36	453	-50	7.9	469	-1	8.8	476	-10	28.5	491	-5	7.3	467	0	10.6
37	403	-11	88.0	385	-6	21.8	450	-3	4.6	456	-6	3.1	396	-8	6.7
38	368	-17	34.8	366	-3	6.3	349	-4	3.3	377	-5	7.8	365	-3	9.4
39	356	-7	24.7	307	-7	4.1	301	-3	0.5	337	-11	18.2	309	-8	8.3
40	310	-2	3.7	290	-21	7.4	270	-8	6.0	298	-29	13.0	291	-2	2.3
41	251	-2	12.6	267	-3	3.2	240	-12	0.9	251	-16	3.5	260	-1	1.5
42	225	-19	1.2	230	5	0.5	215	-23	11.8	245	-12	3.6	221	-4	0.6
43	179	-1	5.4	171	-1	1.0	181	-1	0.5	203	-11	8.0	162	-1	0.7
44	86	-3	3.1	84	0	5.3	81	2	1.2	111	-9	3.0	86	-2	3.5
45	51	-4	5.7	47	-2	0.9	69	7	2.2	67	-9	1.2	41	-3	1.6

^[a] Harmonic frequencies and intensities were calculated at the B3LYP/6-311++G** level, while anharmonic corrections correspond to the B3LYP/6-31G* level of theory. Frequencies and intensities are given in cm^{-1} and in $\text{km} \cdot \text{mol}^{-1}$, respectively.

Table 5. Harmonic vibrational fundamentals (ω), their VPT2 anharmonic corrections ($\Delta\nu$), and double-harmonic vibrational intensities (I) of the 5 lowest energy conformers of L-allo-threonine^[a]

number	aThr-I			aThr-II			aThr-III			aThr-IV			aThr-V		
	ω	$\Delta\nu$	I	ω	$\Delta\nu$	I	ω	$\Delta\nu$	I	ω	$\Delta\nu$	I	ω	$\Delta\nu$	I
1	3690	-197	191.6	3751	-186	70.1	3789	-182	38.5	3752	-190	56.6	3837	-175	35.5
2	3596	-180	12.5	3718	-196	67.3	3586	-182	14.0	3740	-186	85.5	3574	-182	19.3
3	3506	-125	1.6	3589	-182	13.4	3493	-103	9.8	3595	-182	12.3	3507	-100	1.4
4	3464	-263	268.4	3512	-188	6.8	3455	-265	279.7	3505	-131	4.9	3453	-251	273.3
5	3114	-142	16.0	3111	-142	20.3	3128	-141	7.0	3110	-142	20.6	3112	-143	15.5
6	3101	-141	27.5	3096	-137	36.5	3095	-137	25.1	3094	-128	32.1	3092	-137	22.6
7	3041	-140	7.3	3076	-138	9.1	3043	-106	19.6	3066	-133	7.3	3049	-132	20.6
8	3034	-117	15.4	3068	-130	1.6	3035	-116	24.0	3059	-136	13.2	3037	-128	5.6
9	2937	-85	50.2	3029	-101	13.8	3032	-128	14.0	3028	-151	13.8	3031	-121	15.2
10	1808	-21	307.4	1804	-33	299.0	1821	-28	305.2	1780	-34	279.2	1834	-30	338.2
11	1660	-45	32.5	1672	-8	40.7	1653	-45	35.2	1643	-80	39.6	1668	-33	45.6
12	1501	-37	5.5	1503	-100	5.0	1507	-69	3.5	1505	-68	5.9	1501	-42	10.3
13	1488	-6	4.0	1489	17	5.1	1490	11	13.0	1493	-40	10.4	1497	-43	3.5
14	1446	-54	11.0	1429	-30	45.2	1429	-46	174.6	1444	-39	31.2	1426	-58	128.5
15	1416	-52	435.3	1425	-35	26.8	1415	-41	158.8	1412	-14	14.9	1417	-20	232.0
16	1405	-30	61.4	1412	-19	13.8	1408	-30	107.8	1395	-54	19.3	1405	-46	30.6
17	1385	-38	12.3	1377	-40	7.6	1400	-36	42.5	1394	-41	31.4	1384	-33	5.3
18	1369	-5	0.3	1330	-28	36.2	1352	-34	14.5	1343	-32	12.7	1364	-39	14.6
19	1315	-1	76.0	1295	-27	16.1	1316	-34	7.6	1317	-34	9.3	1317	-41	1.5
20	1269	-32	4.4	1263	-33	9.6	1267	-39	4.5	1285	-35	2.9	1260	-34	11.6
21	1216	-42	36.9	1215	-36	31.0	1204	-41	27.4	1212	-34	10.7	1228	-36	14.4
22	1189	-28	4.8	1173	-35	14.3	1194	-32	19.2	1147	-37	243.0	1192	-34	25.8
23	1152	-31	15.1	1130	-34	250.5	1141	-30	33.6	1143	-30	129.4	1125	-30	34.9
24	1111	-31	26.0	1111	-28	98.6	1091	-27	34.9	1090	-26	11.2	1109	-28	79.0
25	1084	-32	57.0	1072	-29	18.5	1074	-25	8.9	1080	-34	19.9	1063	-27	4.7
26	1056	-30	10.9	1027	-28	17.7	1035	-21	42.3	1045	-22	32.6	1021	-29	37.4
27	975	-28	26.3	958	-39	30.9	973	-36	106.9	943	-23	7.8	964	-34	109.8
28	919	-34	78.2	921	-20	48.2	915	-26	46.6	901	-42	32.5	930	-26	42.1
29	884	-29	63.6	850	-41	131.1	880	-45	110.3	829	-52	136.2	883	-56	72.8
30	847	-62	18.9	828	-18	4.7	860	-23	38.2	816	-23	25.2	867	-25	25.9
31	840	-14	102.8	723	-21	19.4	813	-17	8.7	771	-17	34.4	829	-15	8.9
32	736	-12	5.8	650	-13	15.8	754	-14	8.2	709	-9	9.6	731	-10	17.0
33	631	-20	126.3	644	-8	78.3	607	-9	0.6	629	-30	99.3	648	-13	16.6
34	591	-9	3.9	570	-64	20.4	552	-34	11.0	569	-49	207.7	623	-10	8.5
35	571	-8	5.7	549	-21	152.0	524	-27	11.6	531	-9	19.6	495	-7	0.6
36	485	-1	15.6	457	-5	25.9	476	-15	20.1	498	-5	6.9	424	-5	11.7
37	406	-10	1.6	414	-2	4.0	437	-9	102.2	391	-2	0.9	362	-10	12.1
38	357	-10	10.2	362	-5	7.2	366	-18	31.0	358	-6	26.1	325	-32	5.6
39	347	-32	25.7	302	-10	5.1	349	-6	9.7	324	-3	14.7	306	-7	38.7
40	331	-7	3.7	255	-19	1.7	331	-3	8.0	269	-4	3.7	280	3	73.4
41	302	-13	10.6	249	-2	3.2	241	-1	3.0	241	-7	0.2	272	1	25.4
42	235	-18	6.2	228	-18	8.6	229	-1	5.1	230	-6	3.6	248	-11	0.3
43	208	-7	6.7	166	0	1.9	199	0	5.5	187	-5	3.6	174	-1	10.5
44	94	-2	0.9	82	-1	6.0	86	-2	4.1	120	-6	3.5	86	-7	3.9
45	71	-8	2.0	62	1	0.9	47	-4	5.1	45	-5	0.6	80	-4	2.2

^[a] See footnote [a] to table 4.

III. CONFORMATIONAL ANALYSIS

III.1. Preliminary tests

The method described in section II.1 for studying the conformational space of Thr and aThr systematically was tested on the neutral amino acids glycine (Gly) and L-alanine (Ala), where the number of conformers are well established as a result of previous high-level first-principles studies [17-20].

At the RHF/3-21G level, only 6 of the 8 and 11 of the 13 conformers were found for Gly and Ala, respectively. The RHF/3-21G optimizations failed to yield the high-energy conformers **Gly-VIIp** and **Gly-VIIIIn** for Gly. The most stable conformers {**Gly-Ip,Gly-IIIn**} [4] were obtained {28,49} times out of a total of 216 initial structures. Using the same conformational search but this time at the RHF/6-31G** level, all Gly conformers were found. These observations show the possible dangers of using RHF/3-21G optimizations for prescreening the possible conformers of amino acids (and most likely peptides). It is comforting, nevertheless, that RHF/3-21G optimizations always missed only the highest-energy conformers.

The discrepancies obtained for the amino acids Gly and Ala based on the initial prescreening of the conformers at the RHF/3-21G level led us to an extended study of the role of initial geometry optimizations. Taking the Thr conformers determined at the B3LYP/6-311++G** level, preliminary optimizations at the RHF/3-21G, RHF/3-21G**, and RHF/3-21+G** levels were done, continued by B3LYP/6-311++G** level optimizations. It was found that the final B3LYP/6-311++G** structures were often different from the initial B3LYP/6-311++G** structures when using the different basis sets for the preoptimizations at the RHF level. Thus, the conformers found on the PES corresponding to the final optimization level depend somewhat on the level of the initial optimizations. Since the conformers found by only one of the methods were of high relative energy (above 15 kJ mol⁻¹ in all cases), it is safely concluded that this effect is due to the fine structure of the high-energy regions of the different PESs. While this observation is certainly somewhat disturbing, it seems to be not relevant for the low-energy conformers, of highest relevance for practical applications.

III.2. Initial optimizations

Using the inexpensive RHF/3-21G method, 68 and 66 conformers were found for L-threonine and L-allo-threonine, respectively. When B3LYP/6-311++G** geometry optimizations were performed, using the RHF/3-21G conformers as initial structures, some of the higher-energy RHF/3-21G conformers disappeared, thus finally 56 and 61 conformers were found this way for Thr and aThr, respectively. Of the 7776 initial structures for each diastereomer, {202, 455, 328, 78, 146} and {220, 422, 534, 336, 131} ended up as {**Thr-I, Thr-II, Thr-III, Thr-IV, Thr-V**} and {**aThr-I, aThr-II, aThr-III, aThr-IV, aThr-V**}, respectively. This clearly shows that these lowest-energy conformers have substantial catchment regions. The smallest region corresponds to **Thr-XV** with only 12 initial structures ending up at that conformer.

III.3. Comparison with the study of Zhang and Lin [50]

The recent investigation of Zhang and Lin [50] is similar to our work in many respects. An important distinction is that in that paper only the L-threonine diastereomer was considered. For L-Thr, Zhang and Lin found 71 conformers at the B3LYP/6-311++G** level, while, as stated above, we found only 56 conformers. This result is the more curious as their grid for the initial optimization was somewhat less systematic, it was based partially on chemical intuition, and they included much less (only 1296) initial points than the grid corresponding to the present study contains (7776). The difference is due to the different theoretical levels used for the initial optimizations, and in this case show that the RHF/3-21G PES is less structured (68 conformers found) than the PES obtained at the B3LYP/6-311++G** level (71 conformers found). Overall, Zhang and Lin obtained 16 conformers which were not found and missed one conformer which was found in the present study. Since the dependence of the results of the conformational search on the method of initial optimization seems to be only relevant for higher-energy conformers, it is important to stress that all conformers of L-Thr up to a relative energy of 19 kJ mol^{-1} agree in the two studies.

IV. STRUCTURES

The MP2 and DFT(B3LYP) levels of electronic structure theory yield equilibrium structures which may suffer from different problems. It is the intramolecular basis set superposition error (BSSE) that can be quite significant at the MP2 level, especially when smaller basis sets are used, hindering the determination of truly accurate equilibrium structures. By design, this is much less of a problem at the DFT levels. The usual functionals of DFT theory, like B3LYP, suffer, however, from the inability to describe dispersion effects. Therefore, it is comforting to note that the RHF, DFT(B3LYP), and MP2 levels produce the same minima for the five lowest-energy conformers of Thr and aThr. This means that the structures predicted for the lowest-energy conformers are as dependable as can be expected at these levels of electronic structure theory.

It is of fundamental interest to investigate which intramolecular factors (electronic effects including exchange, electrostatic, and hyperconjugative interactions, steric repulsion, H-bonding capabilities, and dispersive interactions) lead to stabilization of the many possible conformers of Thr and aThr. Most of these effects are operative in stabilizing the configurations resulting from rotations around the appropriate single bonds of these molecules.

Threonine is a representative of the three hydroxyamino acids whereby the OH group in the side chain is capable of strong intramolecular H-bonds. The subsequent increase in the number of low-energy conformations has been proved in this study. The presence of NH, carboxylic OH, and side-chain OH H-bond donors and N, C=O, carboxylic OH, and side-chain OH H-bond acceptors allow for the existence of the following types of H-bonds: (a) bifurcated H-bonds between NH₂ and C=O, similar to that found in the most stable conformers of glycine [4,17] and alanine [18,20]; (b) simple H-bonds, like N-H to side-chain OH, carboxylic O-H, and C=O; (c) carboxylic O-H to C=O, side-chain O-H, and NH₂; and (d) side-chain O-H to carbonyl oxygen, nitrogen, and carboxylic OH.

The structure of the global minimum, **Thr-I**, is stabilized by strong OH \cdots N, OH \cdots O=C and weaker NH \cdots O H-bonds, whereby the COOH, NH₂, and the side-chain OH functional groups are interconnected via the three intramolecular H-bonds, while the -COOH group is in an energetically unfavorable trans conformation. In the case of **Thr-II**, although the -COOH group is now in the favorable cis conformation, this substantial energy gain, on the order of 20 kJ mol⁻¹, is not able to compensate for the energy difference between the H-bonds in **Thr-I** and **Thr-II**. **Thr-II** exhibits weaker NH \cdots O=C and OH \cdots N H-bonds. The H-bond arrangements in the most stable conformers of Thr are completely different from those for

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2
3 glycine and α -alanine, where the global minima have a cis $-\text{COOH}$ arrangement with a
4 bifurcated (and thus less strong) $\text{NH}\cdots\text{O}=\text{C}$ H-bonds, while the second lowest energy
5 conformers have a trans $-\text{COOH}$ arrangement and strong $\text{OH}\cdots\text{N}$ H-bonds. This shows, and
6 this conclusion is similar to that obtained in a MW study on the conformers of cysteine [51],
7 that the presence of a polar side chain has a major effect on the conformational preferences of
8 amino acids.
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14 In the case of L-allo-threonine, the global minimum, **aThr-I**, is stabilized, very similarly
15 to **Thr-I**, by strong $\text{OH}\cdots\text{O}=\text{C}$ and $\text{OH}\cdots\text{N}$ H-bonds, while the $-\text{COOH}$ group is again in the
16 less favorable trans conformation. As to **aThr-II**, the $-\text{COOH}$ group is in a cis conformation,
17 while $\text{OH}\cdots\text{N}$ and $\text{NH}\cdots\text{O}=\text{C}$ H-bonds can be found.
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21 A number of different secondary structural effects characterize the other conformers.
22 Among them one can find the $\text{OH}\cdots\text{NH}\cdots\text{O}=\text{C}$ structural motif in **Thr-III** whereby the same
23 NH group is included in a H-bond chain. In **Thr-IV**, the stability is due to the $\text{OH}\cdots\text{O}=\text{C}$ and
24 $\text{OH}\cdots\text{N}$ bonds. While **aThr-III** has the same H-bonds as **Thr-I**, the change in chirality causes
25 the methyl group to be in a highly unfavorable position. Furthermore, **aThr-IV** is stabilized
26 by a sequential $\text{NH}\cdots\text{OH}\cdots\text{O}=\text{C}$ H-bond arrangement involving $\text{NH}\cdots\text{OH}$ and $\text{OH}\cdots\text{O}=\text{C}$ H-
27 bond, including the same side-chain OH group.
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33 In all five low-energy Thr and aThr conformers, the methyl group is found in a
34 staggered position with respect to the β -carbon atom. One can compute straightforwardly the
35 pure (vibrationless) internal rotation barrier of the CH_3 group in Thr and aThr. This was done
36 in the present study at the MP2(fc)/cc-pVDZ level. The rotation barriers determined for the
37 methyl group in Thr and aThr are between 1100 and 1300 cm^{-1} . Furthermore, note that for
38 the three lowest-energy conformers of alanine [20], the methyl rotation barrier is also about
39 1200 cm^{-1} , computed, as part of this study, at the same level of theory. The characteristic
40 increase of the rotation barrier in these natural amino acids with respect to ethane, where the
41 barrier is 1140 cm^{-1} at this level [16], originates most probably from increased
42 hyperconjugation, due to the presence of CC and CX ($\text{X} = \text{O}, \text{N}$) bonds. Note also that the
43 internal rotation barrier of the methyl group can be substantially smaller than the barriers
44 reported; for example, it is only about 400 cm^{-1} in acetaldehyde [40] and much smaller in
45 toluene. Observation of transitions between the energy levels under the slightly different
46 barriers, aimed compounded by different reduced masses due to the structural differences of
47 the conformers, should help identification of the low-energy conformers of Thr and Ala, as
48 well.
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Note, finally, that the only threonine conformer considered by Lakard [52] in a study of the vibrational fundamentals of hydroxyamino acids at the harmonic level, though the figure included in that paper is not particularly instructive, is definitely not the global minimum and it is not even among the five most stable conformers.

V. RELATIVE ENERGIES

As observed repeatedly for amino acids, the introductory Hartree–Fock level of electronic structure theory, independently of the basis set used, is unable to yield the correct relative energies of the conformers of Thr and aThr (see Tables 2 and 3). At the extrapolated RHF/CBS level, **Thr-II** and **Thr-III** both have lower energies than **Thr-I**, while **Thr-IV** has a very high relative energy. These RHF/CBS results clearly show the inadequacy of this level of theory in predicting relative conformational energies for this class of compounds due to its inadequacy in describing fine electrostatic and H-bonding effects. The MP2 level of theory stabilizes **Thr-IV** substantially, while it destabilizes all the other conformers considered. For Thr, the explicit MP2/aug-cc-pVQZ and the extrapolated MP2/CBS relative energies deviate at most by 0.04 kJ mol^{-1} , an excellent agreement indeed, contributing greatly to the overall accuracy of the FPA relative conformational energies. For aThr, the extrapolation contributions are larger by almost an order of magnitude but they are still surprisingly small on an absolute scale; consequently, the error due to MP2 extrapolation remains a small factor of the overall estimated precision of the FPA relative energies. Compared to $\delta[\text{MP2}]$, the $\delta[\text{CCSD}]$ and $\delta[\text{CCSD(T)}]$ energy increments are relatively small though can affect relative energies by at most 2 kJ mol^{-1} . Overall, it seems safe to attribute about 0.7 kJ mol^{-1} accuracy to the CCSD(T)/CBS limit FPA relative energies. Based on the CCSD – HF and CCSD(T) – CCSD increments, the relative energy corrections due to electron correlation effects beyond CCSD(T) are estimated to be considerably less than 0.5 kJ mol^{-1} , thus these missing corrections should not affect significantly the CCSD(T)/CBS limit FPA relative energies and their uncertainty estimates.

The DFT(B3LYP) level performs reasonably well, the FPA relative energies, including the ZPVE corrections, are quite similar to the B3LYP/6-311++G** relative energies. This shows again the utility of the DFT approach for conformational energy studies.

Interestingly, but again in line with our study on the conformers of Pro [2], the relative energies are barely affected by consideration of the core-core and core-valence correlation

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3 and the relativistic effects. Even the largest change is smaller than 0.1 kJ mol^{-1} . This is
4 comforting and makes accurate relative energy predictions for the conformers of the building
5 blocks of biopolymers considerably less expensive.
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9 ZPVE corrections are substantial and can affect relative energies on the order of 2
10 kJ mol^{-1} . It is also of general interest to compare harmonic and anharmonic ZPVE corrections
11 to the relative energies. The anharmonic contributions to relative energies of the Thr
12 conformers are on the order of 0.5 kJ mol^{-1} . This is significant but not substantial given the
13 other sources of error in the present computations contributing to the final FPA relative
14 energy estimates.
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18 The above statements nearly stand for aThr, as well. The RHF level of theory gives
19 relative energies with considerable error, underestimating the relative energies of **aThr-II** and
20 **aThr-IV**. The MP2 increment compensates most of this error by destabilizing these
21 conformers. Compared to MP2, $\delta[\text{CCSD}]$ and $\delta[\text{CCSD(T)}]$ energy corrections are fairly
22 small yet can affect relative energies by over 2 kJ mol^{-1} . Core correlation and relativistic
23 effects are on the order of 0.01 kJ mol^{-1} , while ZPVE corrections can reach nearly 1.5
24 kJ mol^{-1} .
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28 In the case of aThr, the B3LYP/6-311++G** level gives a different relative energy order
29 than the FPA approach. In the cases of **aThr-I** and **aThr-II**, this is due to the ZPVE
30 corrections, which shows the importance of including ZPVE for conformational studies. It is
31 interesting to find that the FPA relative energies give the same relative energy order as the
32 MP2/aug-cc-pVTZ level for the optimized structures.
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36 Since the FPA energy difference between **aThr-I** and **aThr-II** is only 0.8 kJ mol^{-1} and
37 the assumed uncertainty of the present FPA relative energies is $\pm 1 \text{ kJ mol}^{-1}$, even the present
38 extensive computations are insufficient to determine the lowest-energy conformer of aThr.
39 Similarly, the small FPA energy difference between **aThr-IV** and **aThr-V** does not allow an
40 unambiguous determination of their energy order.
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44 In order to estimate the uncertainty on the FPA energies resulting from the choice of
45 reference structures, MP2/aug-cc-pVTZ//B3LYP/6-311++G** relative energies were
46 compared to MP2/aug-cc-pVTZ//MP2/aug-cc-pVTZ energies. The average effect is 0.1 and
47 0.3 kJ mol^{-1} for Thr and aThr, respectively, suggesting that the DFT reference structures
48 chosen are appropriate for the purposes of the present study.
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VI. VIBRATIONAL FUNDAMENTALS

Many vibrational fundamentals are found to be characteristic for some of the conformers of Thr and aThr (*cf.* Tables 4 and 5). One of the most useful fundamentals characterizing the conformers is the intense stretching vibrational motion of the carboxyl group, ω_{10} , at about 1800 cm^{-1} . The spread in ω_{10} is substantial, from 1780 cm^{-1} (**aThr-IV**) to 1834 cm^{-1} (**aThr-V**). The anharmonic corrections alter this picture only slightly as all the VPT2 corrections are between 28 and 34 cm^{-1} . When the C=O group is not involved in H-bonding, *e.g.*, for **Thr-V**, the fundamental is at a high wavenumber, while a strong H-bond between C=O and the side-chain OH results in a substantially lower wavenumber, as for **aThr-IV**. The exact wavenumber of this fundamental should also depend on the *cis vs trans* arrangement of the carboxylic group, though this effect cannot be seen clearly from the data of Tables 4 and 5.

Other simple nuclear motions, such as OH stretching (ω_1, ω_2) and NH stretching (ω_3, ω_4), should also be discussed. The OH stretching motion characterizes conformers by intensity ratios (I_1/I_2) varying from 0.7 to 15.3, and by frequency differences ($\omega_1 - \omega_2$) varying between 12 and 263 cm^{-1} , with anharmonic corrections altering only slightly these differences. Correlation between the H-bond structure and the OH band origins cannot be so easily used for identification purposes as ω_{10} . Nearly the same stands for the NH stretching motion. The NH stretches also characterize conformers by their relative intensities (I_3/I_4) and frequency differences ($\omega_3 - \omega_4$). Interestingly, in most cases the $\omega_3 - \omega_4$ frequency differences are considerably modified by the anharmonic corrections.

Various other fundamentals, including $\omega_{14}, \omega_{15}, \omega_{18}, \omega_{21}, \omega_{22}, \omega_{24}$, and ω_{26} , can also be found where the intensities or the wavenumbers are characteristic of the different conformers. Nevertheless, in these cases the use of this information to identify conformers based on the availability of the infrared spectrum, for example in a matrix isolation study, is not straightforward due to the presence of nearby fundamentals of similar energies.

VII. ROTATIONAL SPECTRA

There are three possible routes to identify conformers via rotational spectroscopy if results from related electronic structure computations are available. The most obvious route is based on the comparison of measured effective rotational constants with equilibrium or vibrationally averaged computed rotational constants. The second route uses the information contained in computed dipole moments and selection rules and thus allows interpretation of measured relative intensities of rotational lines. In the case of amino acids a third route is also open, namely one can use computed ^{14}N nuclear quadruple coupling constants for the identification of a conformer.

At the B3LYP/6-311++G** level, the rotational constants corresponding to the optimized equilibrium structures are accurate enough to be useful to deduce the presence of most of the conformers when evaluating experimental data of microwave and millimeterwave spectroscopic studies. Furthermore, some of the conformers (*e.g.*, **Thr-I** and **Thr-IV**, as well as **aThr-I**) have substantial dipole moments thus helping the observation of the related rotational transitions. Nevertheless, given the limited accuracy of the rotational constants obtained at the B3LYP and MP2 levels, in certain cases it might be quite difficult to distinguish the conformers of Thr and aThr based on this information alone. This holds, for example, for **Thr-II** and **Thr-V**. Unfortunately, in this case the ^{14}N nuclear quadruple coupling constants are also rather similar, hindering further the unequivocal identification of these conformers. In contrast, while the rotational constants of **Thr-I** and **Thr-III** are rather similar, in this case the ^{14}N nuclear quadruple coupling constants allow for an easy distinction between the measured spectroscopic data of the two conformers.

The relatively accurate rotational and quartic centrifugal distortion (QCD) constants determined should facilitate the observation of the low-energy conformers of L-Thr and L-aThr, especially **Thr-I** and **aThr-I**. The sextic centrifugal distortion constants are so small (they are given in mHz units in Tables 6 and 7) that it is unlikely that they could be determined experimentally with any reasonable certainty. Their smallness also means that the experimental spectrum could straightforwardly be fitted with just the effective rotational and quartic centrifugal distortion constants.

Table 6. Equilibrium rotational constants (A_e , B_e , C_e), their vibrational corrections (ΔA , ΔB , ΔC) leading to ground-state rotational constants A_0 , B_0 , and C_0 , A -reduced quartic (ΔJ , ΔK , Δ_{JK} , δ_J , δ_K) and sextic (Φ_J , Φ_K , Φ_{JK} , Φ_{KJ} , ϕ_j , ϕ_k , ϕ_{jk}) centrifugal distortion constants, ^{14}N nuclear quadrupole coupling tensor elements (χ_{aa} , χ_{bb} , χ_{cc}), and total dipole moments (μ_{total}) of the five lowest-energy conformers of L-threonine^[a]

	Thr-I	Thr-II	Thr-III	Thr-IV	Thr-V
A_e	3 201.77	2 865.57	3 128.28	2 679.22	2 882.14
ΔA	-32.91	-24.61	-38.07	-27.82	-25.09
B_e	1 498.69	1 587.52	1 476.30	1 749.67	1 549.45
ΔB	-25.80	-13.55	-14.75	-17.45	-17.18
C_e	1 256.81	1 194.30	1 294.91	1 354.93	1 222.85
ΔC	-8.64	-10.49	-9.29	-10.67	-6.24
ΔJ	0.258	0.270	0.172	0.211	0.300
ΔK	-0.017	-0.142	-0.118	0.192	-0.526
Δ_{JK}	0.404	0.269	0.723	0.006	0.697
δ_J	0.065	0.052	0.020	0.035	0.069
δ_K	0.155	0.620	-1.217	-0.028	-0.727
Φ_J	-0.15	-0.10	0.08	-0.02	-0.15
Φ_K	20.45	13.57	-1.49	-0.20	61.88
Φ_{JK}	6.61	4.77	-4.70	0.10	26.28
Φ_{KJ}	-27.18	-18.09	5.05	-0.47	-87.56
ϕ_j	-0.08	-0.04	0.02	0.00	-0.04
ϕ_k	70.70	27.48	-59.03	1.89	138.08
ϕ_{jk}	-0.36	-1.23	2.03	-0.06	-1.54
χ_{aa}	-4.08	-4.83	-0.94	-4.51	-4.80
χ_{bb}	2.12	2.92	3.24	2.66	2.84
χ_{cc}	1.96	1.90	-2.30	1.85	1.95
μ_{total}	4.37	2.36	3.02	5.14	3.00

Table 6. cont.

[a] The equilibrium rotational and quartic centrifugal distortion constants, given in MHz and kHz, respectively, correspond to the parent isotopologue, and were determined at the B3LYP/6-311++G** level. Vibrational corrections and sextic centrifugal distortion constants, given in MHz and mHz, respectively, were determined from anharmonic force fields obtained at the B3LYP/6-31G* level. The nuclear quadrupole coupling tensor elements given correspond to the ^{14}N nucleus (in MHz). Dipole moments are given in debye.

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Table 7. Equilibrium (A_e , B_e , C_e) rotational constants, their vibrational corrections (ΔA , ΔB , ΔC) leading to ground-state rotational constants A_0 , B_0 , and C_0 , A -reduced quartic (Δ_J , Δ_K , Δ_{JK} , δ_J , δ_K) and sextic (Φ_J , Φ_K , Φ_{JK} , Φ_{KJ} , ϕ_j , ϕ_k , ϕ_{jk}) centrifugal distortion constants, ^{14}N nuclear quadrupole coupling constants (χ_{aa} , χ_{bb} , χ_{cc}), and total dipole moments (μ_{total}) of the five lowest-energy conformers of L-allo-threonine^[a]

	aThr-I	aThr-II	aThr-III	aThr-IV	aThr-V
A_e	3 076.01	3 019.18	2 773.73	2 738.22	3 059.09
ΔA	-25.24	-29.23	-29.65	-24.31	-28.66
B_e	1 639.65	1 464.42	1 702.83	1 627.34	1 483.53
ΔB	-15.83	-9.65	-15.32	-17.21	-14.60
C_e	1 117.74	1 316.22	1 341.31	1 417.04	1 336.00
ΔC	-9.71	-16.16	-13.67	-15.98	-14.96
Δ_J	0.102	0.278	0.250	0.277	0.244
Δ_K	0.248	0.084	0.157	0.909	0.055
Δ_{JK}	0.027	0.170	0.438	0.226	0.190
δ_J	0.032	0.048	0.060	0.016	0.030
δ_K	0.170	2.004	-1.337	-0.661	1.386
Φ_J	0.00	-0.13	0.03	-0.11	0.01
Φ_K	-0.37	28.67	1.20	7.30	18.87
Φ_{JK}	-0.06	11.43	-0.45	4.46	6.76
Φ_{KJ}	0.10	-40.04	-1.50	-16.01	-25.65
ϕ_j	0.00	0.01	0.04	0.03	0.04
ϕ_k	0.00	117.36	-1.27	20.51	89.59
ϕ_{jk}	0.00	-5.55	1.60	-6.23	-1.09
χ_{aa}	-4.64	-5.02	-4.65	-0.34	-0.21
χ_{bb}	2.67	3.02	2.75	0.67	2.86
χ_{cc}	1.97	2.00	1.90	-0.33	-2.65
μ_{total}	5.31	1.85	4.41	2.75	4.57

^[a] See footnote [a] to Table 6.

VIII. SUMMARY

Following an extensive search utilizing $6^5 = 7776$ initial structures for each diastereomer, 68 and 66 conformers (local minima on their related PESs) were found for L-threonine and L-allo-threonine, respectively, at the RHF/3-21G level of electronic structure theory. After geometry optimizations at the B3LYP/6-311++G** level, 56 and 61 conformers remained for L-threonine and L-allo-threonine, respectively, within an energy range of 51 and 52 kJ mol⁻¹, respectively. The PESs of the Thr and aThr molecules clearly depend on the level of theory used for their determination. Lacking high-level definitive computational studies, only conformers obtained at several medium theoretical levels should be considered as ones whose likely existence is confirmed by theory. Fortunately, the results obtained show that the conformers found in the lower-energy regions of the PESs have the same bonding arrangements at the HF, DFT(B3LYP), and MP2 levels of theory, thus these conformers should in fact exist.

Following the FPA approach, relative energy predictions with an accuracy of ± 1 kJ mol⁻¹ were determined for the five lowest-energy conformers of both diastereomers of Thr. The computations clearly predict the global minimum for Thr, called **Thr-I**. However, for aThr the relative energies of two conformers, **aThr-I** and **aThr-II** are the same within the uncertainty of the FPA approach. In contrast to the global minimum of Gly and Ala, **Thr-I** contains an energetically unfavorable trans carboxylic group, and it is stabilized by strong OH \cdots N, OH \cdots O=C and weaker NH \cdots O H-bonds, whereby the COOH, NH₂, and the side-chain OH functional groups are interconnected via three intramolecular H-bonds. **aThr-I** is stabilized, very similarly to **Thr-I**, by strong OH \cdots O=C and OH \cdots N H-bonds, while the COOH group, to allow for these bonds, is again in the less favorable trans conformation. **Thr-II** and **aThr-II** also have similar structures, with energetically favorable cis carboxylic groups, but weaker H-bonds, NH \cdots O=C and OH \cdots N for both **Thr-II** and **aThr-II**. The structural differences between the most stable conformers of Gly and Ala and those of Thr and aThr are clearly due to the presence of the polar side chain. The side chain's significant effect on conformer stability was already observed for cysteine [51]. In the notation of Alonso et al., the presence of OH and SH polar side chains favor type-**III** conformers over type-**I** conformers known as global minima for Gly and Ala. As expected, the methyl group is in a staggered conformation for all the low-energy conformers of Thr and aThr, with rotational barriers varying between 1100 and 1300 cm⁻¹.

Spectroscopic parameters (harmonic and anharmonic frequencies, double-harmonic vibrational intensities, rotational constants with corresponding vibrational corrections, A-

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3 reduced quartic and sextic centrifugal distortion constants, dipole moments and nuclear
4 quadrupole coupling constants) were calculated for the conformers of Thr and aThr. Several
5 of these parameters show the possibility for the experimental distinction of the conformers.
6 Most important are the characteristic stretching C=O (ω_{10}), NH (ω_3, ω_4) and OH (ω_1, ω_2)
7 vibrational fundamentals if the vibrational spectra of the conformers were available.
8 Assignment of the conformers based on pure rotational spectra can be based on rotational
9 constant (equilibrium, $A_e, B_e,$ and $C_e,$ as well as vibrationally averaged $A_0, B_0,$ and C_0
10 constants are provided), A-reduced quartic centrifugal distortion constants ($\Delta_J, \Delta_K, \Delta_{JK}, \delta_J,$ and
11 δ_K) and nuclear quadrupole coupling constants ($\chi_{aa}, \chi_{bb},$ and χ_{cc}) corresponding to the ^{14}N
12 nucleus. It seems feasible that conformers of Thr (and similarly those of Ala) could be
13 identified if transitions between the energy levels corresponding to internal rotation
14 characterized by slightly different methyl rotation barriers became available.
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REFERENCES

- [1] A. G. Császár, A. Perczel, *Progr. Biophys. Mol. Biol.* **71**, 243 (1999).
- [2] E. Czinki, A. G. Császár, *Chem. Eur. J.* **9**, 1008 (2003).
- [3] W. D. Allen, E. Czinki, A. G. Császár, *Chem. Eur. J.* **10**, 4512 (2004).
- [4] V. Kasalová, W. D. Allen, H. F. Schaefer III, E. Czinki, A. G. Császár, *J. Comp. Chem.* **28**, 1373 (2007).
- [5] P. Hudáky, I. Jákli, A. G. Császár, A. Perczel, *J. Comp. Chem.* **22**, 732 (2001).
- [6] I. Jákli, A. Perczel, Ö. Farkas, A. G. Császár, C. Sosa, I. G. Csizmadia, *J. Comp. Chem.* **21**, 626 (2000).
- [7] F. Pollreisz, Á. Gömöröy, G. Schlosser, K. Vékey, I. Solt, A. G. Császár, *Chem. Eur. J.* **11**, 5908 (2005).
- [8] (a) G. Guillea, D. T. Ramon, *Tetrahedron-Asymmetry* **17**, 1675 (2006). (b) B. List, *Synlett* **11**, 1675 (2001).
- [9] (a) X. Michalat, F. F. Pinaud, L. A. Bentolila, J. M. Tsay, S. Doose, G. Sundaresan, S. S. Wu, S. S. Gambhir, S. Weiss, *Science* **307**, 538 (2005). (b) A. Mavrandonakis, S. C. Farantos, G. E. Froudakis, *J. Phys. Chem. B* **110**, 6048 (2006).
- [10] F. Combes, Q. R. Nguyeu, G. Wlodarczak, *Astron. Astrophys.* **308**, 618 (1996).
- [11] S. Daydé, D. Champmartin, P. Rubini, G. Berthon, *Inorg. Chim. Acta* **339**, 513 (2002).
- [12] Y. Inomata, T. Takeuchi, T. Moriwaki, *Spectrochim. Acta* **40A**, 179 (1984).
- [13] S. Boudesocque, Z. Damaj, L. Dupont, J.-B. Behr, E. Guillon, *J. Inorg. Biochem.* **102**, 1514 (2008).
- [14] (a) S. S. V. Ramasastry, H. Zhang, F. Tanaka, C. F. Barbes III, *J. Am. Chem. Soc.* **129**, 288 (2007). (b) N. Utsumi, M. Imai, F. Tanaka, S. S. V. Ramasastry, C. F. Barbes III, *Org. Lett.* **17**, 3445 (2007).
- [15] W. D. Allen, A. L. L. East, A. G. Császár, *Structures and Conformations of Non-Rigid Molecules*, eds. J. Laane, M. Dakkori, B. van der Veken, H. Oberhammer, Kluwer: Dordrecht, 1993, p.343.
- [16] A. G. Császár, W. D. Allen, H. F. Schaefer III, *J. Chem. Phys.* **108**, 9751 (1998).
- [17] A. G. Császár, *J. Am. Chem. Soc.* **114**, 9568 (1992).
- [18] C. H. Hu, M. Z. Shen, H. F. Schaefer, *J. Am. Chem. Soc.* **115**, 2923 (1993).
- [19] A. G. Császár, *J. Mol. Struct.* **346**, 141 (1995).
- [20] A. G. Császár, *J. Phys. Chem.* **100**, 3541 (1996).
- [21] M. J. Frisch, J. A. Pople, J. E. Del Bene, *J. Phys. Chem.* **89**, 3664 (1985).

- 1
2
3
4
5 [22] J. S. Binkley, J. A. Pople, W. J. Hehre, J. Am. Chem. Soc. **102**, 939 (1980).
6
7 [23] C. C. J. Roothaan, Rev. Mod. Phys. **23**, 69 (1951); Ibid. **32**, 179 (1960).
8
9 [24] R. Ditchfield, W. J. Hehre, J. A. Pople, J. Chem. Phys. **54**, 724 (1971).
10
11 [25] (a) R. Krishnan, J. S. Binkley, R. Seeger, J. A. Pople, J. Chem. Phys. **72**, 650 (1980). (b)
12 T. Clark, J. Chandrasekhar, G. W. Spitznagel, P. v. R. Schleyer, J. Comp. Chem. **4**, 294
13 (1983). (c) M. J. Frisch, J. A. Pople, J. S. Binkley, J. Chem. Phys. **80**, 3265 (1984).
14
15 [26] T. H. Dunning Jr., J. Chem. Phys. **90**, 1007 (1989).
16
17 [27] R. A. Kendall, T. H., Dunning, Jr., R. J. Harrison, J. Chem. Phys. **96**, 6796 (1992).
18
19 [28] A. G. Császár, W. D. Allen, J. Chem. Phys. **104**, 2746 (1996).
20
21 [29] G. Tarczay, A. G. Császár, W. Klopper, H. M. Quiney, Mol. Phys. **99**, 1769 (2001).
22
23 [30] P. Pulay, Mol. Phys. **17**, 197 (1969).
24
25 [31] W. J. Hehre, L. Radom, P. v. R. Schleyer, J. A. Pople, *Ab Initio Molecular Orbital*
26 *Theory*, Wiley-Interscience, New York, **1986**.
27
28 [32] (a) C. Møller, M. S. Plesset, Phys. Rev. **46**, 618 (1934). (b) R. Krishnan, M. J. Frisch, J.
29 A. Pople, J. Chem. Phys. **72**, 4244 (1980).
30
31 [33] (a) J. Čížek, J. Chem. Phys. **45**, 4256 (1966). (b) J. Čížek, J. Paldus, Physica Scripta **21**,
32 251 (1980).
33
34 [34] R. J. Bartlett, C. E. Dykstra, J. Paldus, in *Advanced Theories and Computational*
35 *Approaches to the Electronic Structure of Molecules*, ed. C. E. Dykstra, Reidel,
36 Dordrecht, **1984**, p. 127.
37
38 [35] K. Raghavachari, G. W. Trucks, J. A. Pople, M. Head-Gordon, Chem. Phys. Lett. **157**,
39 479 (1989).
40
41 [36] (a) P. A. M. Dirac, Proc. Cambridge Philos. Soc. **26**, 376 (1930). (b) A. D. Becke, Phys.
42 Rev. B **38**, 3098 (1988). (c) A. D. Becke, J. Chem. Phys. **98**, 5648 (1993). (d) C. Lee, W.
43 Yang, R. G. Parr, Phys. Rev. B **37**, 785 (1988). (e) S. H. Vosko, L. Wilk, M. Nusair, Can.
44 J. Phys. **58**, 1200 (1980).
45
46 [37] T. J. Lee, P. R. Taylor, Int. J. Quantum Chem. Symp. **23**, 199 (1989).
47
48 [38] V. Szalay, A. G. Császár, M. L. Senent, J. Chem. Phys. **117**, 6489 (2002).
49
50 [39] W. D. Allen, A. Bódi, V. Szalay, A. G. Császár, J. Chem. Phys. **124**, 224310 (2006).
51
52 [40] A. G. Császár, V. Szalay, M. L. Senent, J. Chem. Phys. **120**, 1203 (2004).
53
54 [41] Gaussian 03, Revision C.02, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria,
55 M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C.
56 Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G.
57
58
59
60

1
2
3
4
5 Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R.
6 Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene,
7 X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R.
8 Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W.
9 Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G.
10 Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D.
11 Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford,
12 J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komáromi, R. L.
13 Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M.
14 Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, J. A.
15 Pople, Gaussian, Inc., Wallingford CT, 2004.

16
17
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20
21
22
23
24 [42] MOLPRO is a package of *ab initio* programs written by H.-J. Werner, P. J. Knowles, R.
25 Lindh, F. R. Manby, M. Schütz, P. Celani, T. Korona, G. Rauhut, R. D. Amos, A.
26 Bernhardsson, A. Berning, D. L. Cooper, M. J. O. Deegan, A. J. Dobbyn, F. Eckert, C.
27 Hampel, G. Hetzer, A. W. Lloyd, S. J. McNicholas, W. Meyer, M. E. Mura, A. Nicklaß,
28 P. Palmieri, R. Pitzer, U. Schumann, H. Stoll, A. J. Stone, R. Tarroni, T. Thorsteinsson.

29
30
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32
33 [43] The Mainz-Austin-Budapest version of ACESII was written by J. F. Stanton, J. Gauss, J.
34 D. Watts, P. G. Szalay, and R. J. Bartlett with contributions from A. A. Auer, D. E.
35 Bernholdt, O. Christiansen, M. E. Harding, M. Heckert, O. Heun, C. Huber, D. Jonsson, J.
36 Jusélius, W. J. Lauderdale, T. Metzroth, C. Michauk, D. P. O'Neill, D. R. Price, K. Ruud,
37 F. Schiffmann, M. E. Varner, J. Vázquez. The program contains the integral packages
38 *MOLECULE* (J. Almlöf and P. R. Taylor), *PROPS* (P. R. Taylor), and *ABACUS* (T.
39 Helgaker, H. J. Aa. Jensen, P. Jørgensen, and J. Olsen). For the current version, see
40 <http://www.aces2.de>.

41
42
43
44
45
46
47 [44] (a) W. Klopper, W. Kutzelnigg, J. Mol. Struct. (THEOCHEM) **135**, 339 (1986); (b) A.
48 Karton, J. M. L. Martin, Theor. Chem. Acc. **115**, 330 (2006); (c) G. Tasi, A. G. Császár,
49 Chem. Phys. Lett. **438**, 139 (2007).

50
51
52 [45] W. M. Klopper, K. L. Bak, P. Jørgensen, J. Olsen, T. Helgaker, J. Phys. B **32**, 103 (1999).

53 [46] M. Douglas, N. M. Kroll, Ann. Phys. **82**, 89 (1974).

54 [47] N. C. Handy, Y. Yamaguchi, H. F. Schaefer, J. Chem. Phys. **84**, 4481 (1986).

55 [48] W. D. Allen, A. G. Császár, J. Chem. Phys. **98**, 2983 (1993).

56 [49] (a) D. A. Clabo Jr., W. D. Allen, R. B. Remington, Y. Yamaguchi, H. F. Schaefer, Chem.
57 Phys. **123**, 187 (1988). (c) W. D. Allen, Y. Yamaguchi, A. G. Császár, D. A. Clabo Jr., R.
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1
2
3
4
5 B. Remington, H. F. Schaefer, Chem. Phys. **145**, 427 (1990). (d) H. H. Nielsen, Rev.
6 Mod. Phys. **23**, 90 (1951). (e) D. Papousek, M. R. Aliev, *Molecular Vibrational-*
7 *Rotational Spectra*, Elsevier: Amsterdam, 1982. (e) J. K. G. Watson, In *Vibrational*
8 *Spectra and Structure*, Vol. 6; J. R. Durig, Ed., Elsevier: Amsterdam, 1997; p. 1.

9
10
11 [50] M. Zhang, Z. Lin, J. Mol. Struct. (THEOCHEM) **760**, 159 (2006).

12
13 [51] M. E. Sanz, S. Blanco, J. C. López, J. L. Alonso, Angew. Chem. Int. Ed. **47**, 6216 (2008).

14
15 [52] B. Lakard, J. Mol. Struct. (THEOCHEM) **681**, 183 (2004).
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Supplementary material to

Conformers of Gaseous Threonine

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Coordinates and energies are given in angstroms and Hartrees, respectively.

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3 B3LYP/6-311++G** geometry and energy of conformer: Thr-I
4

5	N	-0.0533470	1.7038990	0.2314590
6	H	0.3590150	1.5838260	1.1539310
7	C	-0.0442190	0.4246410	-0.4896880
8	H	-0.0363780	0.6334110	-1.5655940
9	C	1.1430510	-0.5037890	-0.1593510
10	C	-1.3815210	-0.3070190	-0.2275860
11	H	0.9807530	-1.4445550	-0.6929990
12	O	1.1738110	-0.7476170	1.2544990
13	O	-1.5379430	-1.4843320	-0.4334870
14	H	0.5281650	-1.4335760	1.4592670
15	O	-2.3522510	0.4880920	0.2309000
16	H	-1.9233980	1.3640610	0.3658960
17	H	0.4619530	2.4261160	-0.2564510
18	C	2.4888610	0.0865890	-0.5502360
19	H	2.6921460	1.0080080	0.0020550
20	H	3.2850080	-0.6229850	-0.3194590
21	H	2.5202000	0.3067220	-1.6209910

22 Energy: -438.426915844
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24 MP2/aug-cc-pVTZ geometry and energy of conformer: Thr-I
25

26	N	-0.0228480	1.6903810	0.2688530
27	H	0.3571380	1.5014330	1.1926450
28	C	-0.0325080	0.4464470	-0.4999460
29	H	-0.0298410	0.6933330	-1.5652570
30	C	1.1266340	-0.5049620	-0.2019770
31	C	-1.3566840	-0.2788850	-0.2338380
32	H	0.9942280	-1.3951460	-0.8198310
33	O	1.0926700	-0.8586950	1.1824380
34	O	-1.5115450	-1.4644300	-0.4282970
35	H	0.3890420	-1.5121760	1.2899200
36	O	-2.3254110	0.5169110	0.2285460
37	H	-1.8749420	1.3828820	0.3633260
38	H	0.5611700	2.3913320	-0.1672090
39	C	2.4747650	0.1241160	-0.4701750
40	H	2.6378010	0.9763930	0.1888130
41	H	3.2640720	-0.6010270	-0.2850380
42	H	2.5423180	0.4597270	-1.5052230

43 Energy: -437.569506052
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B3LYP/6-311++G** geometry and energy of conformer: Thr-II

N	0.1698080	1.9023870	-0.2684410
H	-0.2646530	2.2031330	0.6005130
C	0.0095320	0.4556970	-0.4335040
H	0.1436610	0.2014940	-1.4869980
C	1.1509880	-0.2394760	0.3675790
C	-1.3579540	-0.0283770	0.0303600
H	0.9800490	-0.0154010	1.4325370
O	2.3843380	0.3221540	-0.0481070
O	-1.9633040	0.4334080	0.9670390
H	2.2258460	1.2762680	-0.1233500
O	-1.8319130	-1.0523370	-0.7148490
H	-2.6858660	-1.3164590	-0.3376500
H	-0.2736900	2.4134800	-1.0233540
C	1.2294720	-1.7442590	0.1711070
H	2.0924090	-2.1322730	0.7155260
H	0.3336330	-2.2460040	0.5428480
H	1.3547640	-1.9882530	-0.8868970

Energy: -438.426405842

MP2/aug-cc-pVTZ geometry and energy of conformer: Thr-II

N	0.2150230	1.8995500	-0.2575850
H	-0.1945680	2.1704510	0.6322350
C	0.0255610	0.4647260	-0.4423400
H	0.1655710	0.2119030	-1.4929450
C	1.1255050	-0.2468140	0.3655030
C	-1.3322570	-0.0060160	0.0244210
H	0.9583930	0.0023120	1.4228040
O	2.3791580	0.2520800	-0.0617590
O	-1.9065580	0.4302560	0.9989700
H	2.2461020	1.2094890	-0.1537030
O	-1.8337900	-0.9937040	-0.7499910
H	-2.6799650	-1.2499270	-0.3476670
H	-0.2729080	2.4221520	-0.9748690
C	1.1348810	-1.7470710	0.1852070
H	1.9852550	-2.1657050	0.7198930
H	0.2231230	-2.1980880	0.5736040
H	1.2312190	-1.9974390	-0.8707660

Energy: -437.568537183

B3LYP/6-311++G** geometry and energy of conformer: Thr-III

N	0.2094330	1.7152330	-0.1760860
H	-0.6680670	2.1553750	0.0824120
C	-0.0118720	0.3237980	-0.5681810
H	0.0155870	0.1764700	-1.6565370
C	1.0858580	-0.5745470	0.0705780
C	-1.4037190	-0.1054630	-0.1245350
H	0.7987080	-1.6203050	-0.0509580
O	1.1203250	-0.3330130	1.4690640
O	-2.2215460	0.6197410	0.3847900
H	1.1141340	0.6321260	1.5671760
O	-1.6434660	-1.4057260	-0.3949310
H	-2.5376390	-1.6066530	-0.0800330
H	0.6467190	2.2569870	-0.9096480
C	2.4509340	-0.3415200	-0.5768270
H	3.1999520	-0.9598210	-0.0783840
H	2.4364200	-0.6061270	-1.6392160
H	2.7584420	0.7036820	-0.4798050

Energy: -438.425267222

MP2/aug-cc-pVTZ geometry and energy of conformer: Thr-III

N	0.2492490	1.7005400	-0.0943430
H	-0.6354210	2.1587430	0.0954840
C	0.0053990	0.3490860	-0.5806540
H	0.0293140	0.2596820	-1.6725250
C	1.0622810	-0.5943080	0.0167490
C	-1.3768040	-0.0776380	-0.1403450
H	0.7963960	-1.6228230	-0.2230430
O	1.0116590	-0.4870430	1.4301680
O	-2.1809450	0.6371420	0.4151040
H	0.9905650	0.4688270	1.6009130
O	-1.6271430	-1.3628440	-0.4648840
H	-2.5218930	-1.5520120	-0.1410080
H	0.7611310	2.2526500	-0.7679740
C	2.4464370	-0.2736420	-0.5189330
H	3.1775120	-0.9316470	-0.0533970
H	2.4894600	-0.4120260	-1.6005470
H	2.7157510	0.7557890	-0.2815170

Energy: -437.567871617

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B3LYP/6-311++G** geometry and energy of conformer: Thr-IV

N	-0.8186040	1.7821470	-0.3309400
H	-0.4205930	2.2264530	0.4902180
C	-0.1907550	0.4827140	-0.6154870
H	-0.2403160	0.3129490	-1.6958070
C	1.3049830	0.3558530	-0.2214000
C	-1.0409900	-0.6447280	0.0052240
H	1.8278280	1.1798690	-0.7182750
O	1.8587050	-0.8277410	-0.7734890
O	-0.6466930	-1.7830180	0.1086290
H	1.2999960	-1.5654680	-0.4817550
O	-2.2578630	-0.2671330	0.3987980
H	-2.2986430	0.7001230	0.2224650
H	-0.7310480	2.4259210	-1.1077820
C	1.5543040	0.4490370	1.2868790
H	2.6267670	0.3784660	1.4762780
H	1.2076150	1.3994270	1.7078940
H	1.0601870	-0.3668810	1.8205460

Energy: -438.425087806

MP2/aug-cc-pVTZ geometry and energy of conformer: Thr-IV

N	-0.8469700	1.7575370	-0.3515190
H	-0.4202520	2.2160600	0.4449560
C	-0.1880080	0.4816160	-0.6407020
H	-0.2058270	0.3118280	-1.7189970
C	1.2812450	0.3921050	-0.1960970
C	-0.9985460	-0.6609140	-0.0233860
H	1.8031190	1.2381650	-0.6495230
O	1.8855410	-0.7690010	-0.7349080
O	-0.5854010	-1.8013960	0.0445680
H	1.3019170	-1.5067420	-0.4896980
O	-2.1993670	-0.3017450	0.4305310
H	-2.2366340	0.6681460	0.2544960
H	-0.7843440	2.3915280	-1.1365740
C	1.4380670	0.4501610	1.3170880
H	2.4963730	0.4107630	1.5663950
H	1.0286300	1.3685400	1.7429320
H	0.9430750	-0.4017230	1.7837030

Energy: -437.568109398

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3 B3LYP/6-311++G** geometry and energy of conformer: Thr-V
4

5	N	0.0878610	1.8845440	-0.2474540
6	H	-0.3917680	2.3981650	-0.9779090
7	C	0.0107380	0.4342910	-0.4629700
8	H	0.1992680	0.2340690	-1.5192340
9	C	1.1514520	-0.2329730	0.3539300
10	C	-1.3471450	-0.1754040	-0.1421140
11	H	0.9439590	-0.0532130	1.4202630
12	O	2.3757110	0.3865930	-0.0067480
13	O	-1.9674510	-0.9263050	-0.8509510
14	H	2.1852190	1.3350420	-0.0707650
15	O	-1.8030990	0.2224500	1.0760170
16	H	-2.6616110	-0.2041570	1.2184690
17	H	-0.3257800	2.1450650	0.6425700
18	C	1.2860290	-1.7265050	0.1067550
19	H	0.3901020	-2.2680380	0.4198280
20	H	1.4616040	-1.9248700	-0.9535260
21	H	2.1362480	-2.1122220	0.6723260

22 Energy: -438.424882619
23

24 MP2/aug-cc-pVTZ geometry and energy of conformer: Thr-V
25

26	N	0.1323170	1.8850100	-0.2398030
27	H	-0.3851820	2.4055810	-0.9373440
28	C	0.0255380	0.4460660	-0.4714850
29	H	0.2234190	0.2429400	-1.5234790
30	C	1.1249650	-0.2390800	0.3539410
31	C	-1.3254930	-0.1491490	-0.1490500
32	H	0.9202350	-0.0342170	1.4133990
33	O	2.3721180	0.3200200	-0.0177380
34	O	-1.9554290	-0.9057310	-0.8526960
35	H	2.2067270	1.2729040	-0.0975950
36	O	-1.7604520	0.2515710	1.0750780
37	H	-2.6155270	-0.1864530	1.2124170
38	H	-0.2621800	2.1194620	0.6649800
39	C	1.1905960	-1.7306230	0.1205030
40	H	0.2719570	-2.2211660	0.4408860
41	H	1.3476350	-1.9355180	-0.9379430
42	H	2.0231640	-2.1487700	0.6826920

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44 Energy: -437.566928008
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B3LYP/6-311++G** geometry and energy of conformer: Thr-VI

N	-0.1205910	-1.3994510	0.9934550
H	0.6843540	-1.9870540	1.1766820
C	0.0453620	-0.6034940	-0.2238470
H	0.1076370	-1.2881030	-1.0755180
C	-1.1634380	0.3346920	-0.4254480
C	1.3463630	0.2005650	-0.1861960
H	-0.9657120	0.9360790	-1.3234400
O	-1.3228340	1.1989520	0.7008040
O	1.4524000	1.3773840	0.0802880
H	-0.5447420	1.7724370	0.7281070
O	2.4247430	-0.5770420	-0.4372330
H	3.2153660	-0.0241560	-0.3365820
H	-0.2848060	-0.7932050	1.7912620
C	-2.4662010	-0.4274630	-0.6119270
H	-2.4117260	-1.0770210	-1.4898120
H	-2.6786830	-1.0439070	0.2621090
H	-3.2845380	0.2809320	-0.7533560

Energy: -438.424133922

B3LYP/6-311++G** geometry and energy of conformer: Thr-VII

N	-0.2126490	-1.8206810	0.2695310
H	0.6963680	-2.2371360	0.0915470
C	-0.0588590	-0.3743060	0.4934350
H	0.1337270	-0.1187090	1.5409580
C	1.1198260	0.1563020	-0.3520380
C	-1.3643260	0.3376500	0.0770720
H	0.8613840	0.0300670	-1.4131850
O	2.2224130	-0.7126690	-0.0397190
O	-1.6463270	1.4582080	0.4133890
H	2.9926440	-0.4272070	-0.5413650
O	-2.1464320	-0.4043400	-0.7179290
H	-1.6964710	-1.2791270	-0.7789300
H	-0.6015280	-2.2763270	1.0887040
C	1.4670790	1.6123580	-0.0711460
H	0.6175860	2.2674990	-0.2664390
H	1.7673000	1.7364090	0.9722120
H	2.2979840	1.9276830	-0.7100800

Energy: -438.423921028

B3LYP/6-311++G** geometry and energy of conformer: Thr-VIII

N	-0.2084540	-1.8209760	0.2747170
H	-0.5884260	-2.2874110	1.0915720
C	-0.0611780	-0.3761680	0.4970470
H	0.1300150	-0.1147640	1.5449710
C	1.1216980	0.1503630	-0.3647410
C	-1.3683130	0.3333540	0.0879310
H	0.8590060	0.0084350	-1.4175870

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3	O	2.2620890	-0.6977210	-0.1707490
4	O	-1.6539280	1.4500480	0.4350620
5	H	2.7424990	-0.3963070	0.6088270
6	O	-2.1450690	-0.4006600	-0.7198480
7	H	-1.6980480	-1.2759530	-0.7845350
8	H	0.6994060	-2.2316040	0.0752000
9	C	1.4647860	1.6096880	-0.1035720
10	H	0.6032420	2.2577260	-0.2648960
11	H	1.7896870	1.7492970	0.9339650
12	H	2.2751070	1.9206650	-0.7662380

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14 Energy: -438.423845140

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19 B3LYP/6-311++G** geometry and energy of conformer: Thr-IX

21	N	-0.0413720	-1.2438400	1.2151860
22	H	-0.4512880	-0.5827480	1.8688640
23	C	0.0489910	-0.6334050	-0.1137760
24	H	0.1221530	-1.4314140	-0.8563140
25	C	-1.1244190	0.3107930	-0.4859690
26	C	1.3669610	0.1376410	-0.1436700
27	H	-0.8688630	0.8061800	-1.4346770
28	O	-1.3193560	1.2905110	0.5314350
29	O	1.5026810	1.2866770	0.2175540
30	H	-0.4926710	1.7887950	0.6097410
31	O	2.3929550	-0.5994420	-0.6046390
32	H	3.1961640	-0.0599000	-0.5337760
33	H	-0.6188080	-2.0753080	1.1987160
34	C	-2.4390040	-0.4345690	-0.6583710
35	H	-3.2299950	0.2721390	-0.9154470
36	H	-2.3656490	-1.1788380	-1.4561210
37	H	-2.7268480	-0.9367590	0.2686250

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39 Energy: -438.422793907

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44 B3LYP/6-311++G** geometry and energy of conformer: Thr-X

47	N	-0.7159900	1.8667120	-0.3779960
48	H	-1.6256120	1.8132780	0.0724060
49	C	-0.2274210	0.5196140	-0.6370400
50	H	-0.2443500	0.2711770	-1.7078130
51	C	1.2519180	0.4003020	-0.1951320
52	C	-1.1431430	-0.5226050	0.0383960
53	H	1.7960570	1.1940310	-0.7177100
54	O	1.7132030	-0.8796130	-0.6972480
55	O	-2.2010150	-0.2314190	0.5339270
56	H	2.5869850	-1.0707420	-0.3407960
57	O	-0.7044020	-1.7898210	0.0132530
58	H	0.2085550	-1.8088900	-0.3413880
59	H	-0.8149610	2.4009910	-1.2315750
60	C	1.4653320	0.5363510	1.3051990
	H	2.5324730	0.5170550	1.5479870
	H	1.0589610	1.4912200	1.6428960

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H	0.9714170	-0.2702470	1.8539750
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Energy: -438.422596879

B3LYP/6-311++G** geometry and energy of conformer: Thr-XI

N	0.2721470	1.7740430	-0.1393730
H	-0.4706620	2.3967660	-0.4377880
C	-0.0160480	0.4107210	-0.5430580
H	-0.0100170	0.3536420	-1.6383150
C	1.0771350	-0.5531780	-0.0418440
C	-1.4075120	-0.0760430	-0.1107240
H	0.8021700	-1.5640000	-0.3625790
O	1.0197440	-0.4778630	1.3906870
O	-2.2209430	0.5799150	0.4862410
H	1.7380740	-0.9988080	1.7621040
O	-1.6549650	-1.3431230	-0.5296150
H	-2.5487490	-1.5733900	-0.2340880
H	0.3044390	1.8222300	0.8747980
C	2.4625120	-0.2056670	-0.5753600
H	3.2066290	-0.9019880	-0.1746780
H	2.4863000	-0.2915600	-1.6655790
H	2.7395710	0.8123810	-0.3008560

Energy: -438.422545547

B3LYP/6-311++G** geometry and energy of conformer: Thr-XII

N	-0.3918680	-1.8080200	0.0591660
H	0.2072020	-2.4092460	0.6133980
C	-0.0940770	-0.3946940	0.3435790
H	0.0322280	-0.3089030	1.4295700
C	1.1925940	0.1328910	-0.3226840
C	-1.3475190	0.4463280	0.0038290
H	1.0098690	0.2263680	-1.4036040
O	2.1675350	-0.9003230	-0.0999060
O	-1.3404290	1.6372420	-0.1713370
H	3.0300670	-0.5665560	-0.3662960
O	-2.4704220	-0.2815410	-0.0416310
H	-2.1822440	-1.2144770	0.0855630
H	-0.1835860	-2.0259460	-0.9124850
C	1.6762110	1.4681240	0.2313580
H	0.9374760	2.2493880	0.0579500
H	1.8636890	1.3864030	1.3060920
H	2.6116440	1.7601980	-0.2578590

Energy: -438.422381394

B3LYP/6-311++G** geometry and energy of conformer: Thr-XIII

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4	N	0.1393900	1.6827480	-0.1833630
5	H	-0.7556280	2.1431390	-0.0768630
6	C	-0.0061670	0.2798290	-0.5857260
7	H	0.0586770	0.1388500	-1.6733230
8	C	1.1242110	-0.5572270	0.0774390
9	C	-1.3538260	-0.3194580	-0.2039090
10	H	0.8804760	-1.6138220	-0.0470670
11	O	1.1221560	-0.3064010	1.4749940
12	O	-1.6529560	-1.4685890	-0.4001350
13	H	1.0374890	0.6556750	1.5669090
14	O	-2.2069690	0.5721520	0.3554310
15	H	-3.0252280	0.0955100	0.5619860
16	H	0.6947530	2.2056200	-0.8488730
17	C	2.4892440	-0.2671130	-0.5466740
18	H	3.2540710	-0.8530160	-0.0335630
19	H	2.5046460	-0.5340110	-1.6083410
20	H	2.7563950	0.7893370	-0.4464240

Energy: -438.422193322

B3LYP/6-311++G** geometry and energy of conformer: Thr-XIV

28	N	-0.4677310	1.9484360	-0.5428900
29	H	-0.7951780	2.1586770	0.3949690
30	C	-0.1411500	0.5362040	-0.6702830
31	H	-0.1310180	0.2699140	-1.7313490
32	C	1.3092720	0.2621520	-0.1624140
33	C	-1.1642830	-0.3732770	0.0134630
34	H	1.9153790	1.0352330	-0.6370180
35	O	1.8202810	-0.9690960	-0.6604630
36	O	-2.0967840	-0.0082680	0.6809700
37	H	1.2333110	-1.6835630	-0.3847850
38	O	-0.8992500	-1.6951330	-0.1933110
39	H	-1.5737260	-2.2049340	0.2825270
40	H	-1.2235650	2.1996050	-1.1702620
41	C	1.4548000	0.3706860	1.3545110
42	H	0.8641450	-0.3922640	1.8726270
43	H	2.5015340	0.2302420	1.6303540
44	H	1.1374230	1.3534360	1.7139430

Energy: -438.421670064

B3LYP/6-311++G** geometry and energy of conformer: Thr-XV

52	N	-0.5212800	1.9195560	-0.3539110
53	H	-1.4085510	2.1468730	-0.7876350
54	C	-0.1467790	0.5362390	-0.6136420
55	H	-0.1970690	0.3730820	-1.6967470
56	C	1.3370160	0.2839400	-0.2277290
57	C	-1.0622550	-0.5410210	-0.0179100
58	H	1.9017020	1.0668540	-0.7374530
59	O	1.8064530	-0.9417070	-0.7728690
60	O	-0.7584980	-1.7042820	0.1308880
	H	1.2328330	-1.6470070	-0.4412700

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O	-2.2863880	-0.0781620	0.3159760
H	-2.7965040	-0.8339630	0.6471060
H	-0.6232490	2.0984370	0.6392250
C	1.6039220	0.3789600	1.2759790
H	1.0468580	-0.3812500	1.8317710
H	2.6675240	0.2186430	1.4617960
H	1.3414620	1.3659440	1.6684320

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11 Energy: -438.421541581
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16 B3LYP/6-311++G** geometry and energy of conformer: Thr-XVI

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N	-0.5784370	1.9273800	-0.3001630
H	-1.5639310	1.9610530	-0.0624250
C	-0.1618670	0.5658300	-0.6153250
H	-0.1575770	0.3509260	-1.6947020
C	1.3032400	0.3231520	-0.1345260
C	-1.1604060	-0.4132230	-0.0195820
H	1.8698550	1.1737450	-0.5220660
O	1.8822860	-0.8134290	-0.7654910
O	-2.2139900	-0.1214550	0.4850880
H	1.3800660	-1.5932590	-0.5006030
O	-0.7477020	-1.7048750	-0.1311570
H	-1.4365850	-2.2635080	0.2607090
H	-0.4038050	2.5579800	-1.0721420
C	1.4435010	0.2902270	1.3847650
H	0.9465270	-0.5871630	1.8114230
H	2.4995740	0.2429680	1.6573180
H	1.0033700	1.1877580	1.8241070

35 Energy: -438.421498297
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40 B3LYP/6-311++G** geometry and energy of conformer: Thr-XVII

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N	0.1925480	1.7437770	-0.1447390
H	-0.5504030	2.3440600	-0.4826600
C	-0.0084330	0.3694890	-0.5689890
H	0.0439780	0.3267250	-1.6628590
C	1.1174410	-0.5363630	-0.0338600
C	-1.3566760	-0.2851970	-0.2228820
H	0.8860490	-1.5606770	-0.3458350
O	1.0254870	-0.4406310	1.3969590
O	-1.6657180	-1.4048070	-0.5485520
H	1.7152420	-0.9816570	1.7928540
O	-2.1919900	0.5317220	0.4580840
H	-3.0037250	0.0282580	0.6235180
H	0.1913940	1.7957730	0.8687470
C	2.4967900	-0.1348560	-0.5426870
H	3.2632900	-0.7851120	-0.1088520
H	2.5510850	-0.2432930	-1.6298490
H	2.7183000	0.9007690	-0.2833100

59 Energy: -438.421395397
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B3LYP/6-311++G** geometry and energy of conformer: Thr-XVIII

N	-0.2129830	-1.0623770	1.3729630
H	0.5188070	-1.6573580	1.7433640
C	0.0265030	-0.6918630	-0.0182400
H	0.0102800	-1.5990650	-0.6270800
C	-1.0985340	0.2484450	-0.5228210
C	1.4190500	-0.1000950	-0.2463730
H	-0.8162340	0.5952760	-1.5273860
O	-1.2696890	1.3717290	0.3430670
O	2.3385430	-0.6609470	-0.7850040
H	-0.4479210	1.8772640	0.3501910
O	1.5504410	1.1615820	0.2656620
H	2.4644810	1.4448560	0.1089310
H	-0.3111580	-0.2398700	1.9584330
C	-2.4403560	-0.4649240	-0.6019200
H	-2.7207720	-0.8558160	0.3767910
H	-3.2060500	0.2376930	-0.9358340
H	-2.3948850	-1.2946280	-1.3118270

Energy: -438.421382922

B3LYP/6-311++G** geometry and energy of conformer: Thr-XIX

N	-0.5696310	1.8862950	-0.1508650
H	-1.5710780	2.0111070	-0.2426360
C	-0.1522570	0.5515110	-0.5758770
H	-0.2093940	0.4004490	-1.6680100
C	1.3336840	0.2989270	-0.1978800
C	-1.0591820	-0.5347480	-0.0200670
H	1.8968610	1.1266370	-0.6414560
O	1.8244570	-0.8656270	-0.8487910
O	-0.7348240	-1.6908140	0.1298040
H	1.2963020	-1.6117610	-0.5327560
O	-2.3110320	-0.1028440	0.2416540
H	-2.8232490	-0.8662890	0.5502290
H	-0.1119810	2.5931520	-0.7162030
C	1.5928720	0.2824840	1.3075740
H	1.1042200	-0.5727850	1.7822870
H	2.6663120	0.2023140	1.4900590
H	1.2199140	1.1983370	1.7707060

Energy: -438.421129086

B3LYP/6-311++G** geometry and energy of conformer: Thr-XX

N	-0.7308580	1.8669150	-0.3601330
H	-1.6534570	1.8017010	0.0615410
C	-0.2256480	0.5281620	-0.6279700
H	-0.2417900	0.2921640	-1.7038690
C	1.2540160	0.4061920	-0.1696320
C	-1.1396460	-0.5302060	0.0254530
H	1.8113110	1.2031620	-0.6714560

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3 O 1.7894760 -0.8786780 -0.5895420
4 O -2.2222220 -0.2589620 0.4762090
5 H 2.0945190 -0.8200270 -1.5009370
6 O -0.6704930 -1.7866820 0.0312010
7 H 0.2600400 -1.7900010 -0.2772600
8 H -0.8053110 2.4195510 -1.2044330
9 C 1.4446210 0.5224260 1.3319580
10 H 2.5077960 0.5170690 1.5785010
11 H 1.0000950 1.4547610 1.6825500
12 H 0.9686570 -0.3116490 1.8544930

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14 Energy: -438.421075307
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18 B3LYP/6-311++G** geometry and energy of conformer: Thr-XXI
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20 N -0.1193650 -1.2422280 1.1368790
21 H -0.7776110 -2.0136960 1.1012910
22 C 0.0657780 -0.6525800 -0.2053300
23 H 0.0930950 -1.4052590 -1.0012280
24 C -1.0959750 0.3286130 -0.4698970
25 C 1.4563490 0.0192130 -0.2394780
26 H -0.8754030 0.9044240 -1.3728620
27 O -1.1315500 1.2969050 0.5950170
28 O 2.4368950 -0.5963240 -0.5696990
29 H -1.1403550 0.7782500 1.4164830
30 O 1.5240350 1.3032300 0.1397980
31 H 0.6327720 1.6133520 0.4136110
32 H 0.7547210 -1.6216240 1.4865990
33 C -2.4455210 -0.3617540 -0.6339720
34 H -3.2215390 0.3827010 -0.8204340
35 H -2.4251390 -1.0579320 -1.4775960
36 H -2.7238110 -0.9160590 0.2671200

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38 Energy: -438.420967528
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43 B3LYP/6-311++G** geometry and energy of conformer: Thr-XXII
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45 N 0.1782550 1.7228290 0.2842200
46 H -0.6668530 2.2807450 0.3206010
47 C -0.0392250 0.4883760 -0.4518520
48 H -0.0672370 0.6306060 -1.5468320
49 C 1.1089650 -0.5127620 -0.2017160
50 C -1.4107930 -0.0678890 -0.1098930
51 H 0.8946880 -1.4207490 -0.7753650
52 O 2.2625080 0.1367780 -0.7610310
53 O -2.2905550 0.5491840 0.4347260
54 H 3.0496880 -0.3488870 -0.4963900
55 O -1.5753610 -1.3417690 -0.5425510
56 H -2.4864820 -1.5973140 -0.3326620
57 H 0.9279740 2.2566180 -0.1373290
58 C 1.3134620 -0.8632360 1.2677040
59 H 0.4443980 -1.3956850 1.6643090
60 H 2.1782030 -1.5253940 1.3813450
H 1.4706580 0.0397710 1.8581780

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3 Energy: -438.420596988
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8 B3LYP/6-311++G** geometry and energy of conformer: Thr-XXIII
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10 N	0.0120870	1.9356770	-0.3341160
11 H	-0.3803690	2.2146210	0.5608410
12 C	0.0014210	0.4814200	-0.4447510
13 H	0.1248570	0.2008000	-1.4964290
14 C	1.1377810	-0.2121200	0.3696660
15 C	-1.3554650	-0.0168880	0.0213570
16 H	1.0035400	0.0601490	1.4204530
17 O	2.3872280	0.3820180	0.0007360
18 O	-1.9293540	0.3867380	1.0022350
19 H	2.6817810	-0.0087930	-0.8301520
20 O	-1.8542620	-0.9951490	-0.7680010
21 H	-2.7049560	-1.2656010	-0.3882800
22 H	0.9723890	2.2634540	-0.3721110
23 C	1.1824480	-1.7285930	0.2222510
24 H	0.2711830	-2.1973010	0.6001650
25 H	1.2910510	-2.0191660	-0.8287740
26 H	2.0299150	-2.1296730	0.7821950

27 Energy: -438.420534409
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32 B3LYP/6-311++G** geometry and energy of conformer: Thr-XXIV
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34 N	0.0119250	1.9373550	-0.3075720
35 H	-0.2756370	2.2039380	0.6298530
36 C	0.0074290	0.4839820	-0.4356370
37 H	0.1266720	0.2233540	-1.4904560
38 C	1.1383400	-0.2289210	0.3504060
39 C	-1.3473670	-0.0157720	0.0411010
40 H	1.0170610	0.0255590	1.4123780
41 O	2.3440630	0.3653650	-0.1502420
42 O	-1.8764470	0.3305740	1.0681020
43 H	3.0886180	0.0467400	0.3691960
44 O	-1.9031380	-0.9129260	-0.8025300
45 H	-2.7533580	-1.1802360	-0.4193160
46 H	0.9543590	2.2806180	-0.4612160
47 C	1.1577340	-1.7445970	0.1751410
48 H	0.2548410	-2.2063460	0.5830840
49 H	1.2380620	-2.0100760	-0.8819350
50 H	2.0132750	-2.1772930	0.7027090

51 Energy: -438.420532603
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56 B3LYP/6-311++G** geometry and energy of conformer: Thr-XXV
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58 N	-0.0982090	-0.9222640	1.5056010
59 H	-0.4033540	-0.0727720	1.9712700
C	0.0241960	-0.6964720	0.0660630
H	-0.0069430	-1.6612420	-0.4428670

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3	C	-1.0699750	0.2239260	-0.5571600
4	C	1.4178810	-0.1519790	-0.2274710
5	H	-0.7621570	0.4686480	-1.5845570
6	O	-1.2291980	1.4238350	0.1999730
7	O	2.2628330	-0.6897130	-0.8921060
8	H	-0.3823340	1.8864730	0.2251450
9	O	1.6133590	1.0745110	0.3401930
10	H	2.5212570	1.3481780	0.1375670
11	H	-0.7767400	-1.6484490	1.7007460
12	C	-2.4306990	-0.4553140	-0.5986290
13	H	-2.7618690	-0.7198500	0.4087850
14	H	-3.1688490	0.2253430	-1.0263690
15	H	-2.3959110	-1.3605100	-1.2102240

Energy: -438.420255853

B3LYP/6-311++G** geometry and energy of conformer: Thr-XXVI

23	N	0.0633420	1.8760450	-0.8002950
24	H	-0.6911350	2.2811890	-1.3437440
25	C	-0.0618980	0.4246150	-0.7404920
26	H	-0.2839710	0.0592170	-1.7473250
27	C	1.2982590	-0.2071300	-0.3158400
28	C	-1.1897900	-0.0476620	0.1774590
29	H	2.0078960	0.0821460	-1.1011540
30	O	1.2036510	-1.6294900	-0.2295240
31	O	-1.5031670	0.4832820	1.2141990
32	H	0.8956790	-1.9844830	-1.0702380
33	O	-1.8235030	-1.1400740	-0.3082810
34	H	-2.4854800	-1.4087570	0.3478570
35	H	0.0023140	2.2714150	0.1334010
36	C	1.8210300	0.2769900	1.0274330
37	H	2.7765770	-0.2096730	1.2322450
38	H	1.9845790	1.3559740	1.0136360
39	H	1.1286850	0.0300450	1.8348720

Energy: -438.419934224

B3LYP/6-311++G** geometry and energy of conformer: Thr-XXVII

48	N	-0.1477480	-1.2451090	1.2118140
49	H	0.5851420	-1.9075620	1.4414960
50	C	0.0718540	-0.6750820	-0.1209180
51	H	0.0987670	-1.4998220	-0.8359600
52	C	-1.0995360	0.2391890	-0.5135570
53	C	1.4566250	0.0029070	-0.2447220
54	H	-0.8773570	0.6694560	-1.4987920
55	O	-1.1125680	1.3122150	0.4627730
56	O	2.4141490	-0.5827170	-0.6802200
57	H	-1.8417980	1.9129960	0.2790870
58	O	1.5649110	1.2627530	0.2257370
59	H	0.6808940	1.5922380	0.4806670
60	H	-0.1570900	-0.5225230	1.9244680
	C	-2.4393920	-0.4807500	-0.5560590
	H	-2.6576680	-0.9415590	0.4072180

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2
3 H -3.2413630 0.2181820 -0.8141730
4 H -2.4245310 -1.2612310 -1.3214940
5

6 Energy: -438.419811701
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9

10
11 B3LYP/6-311++G** geometry and energy of conformer: Thr-XXVIII
12

13 N -0.6588050 1.8625360 -0.5595770
14 H -0.8737180 2.1075010 0.4000050
15 C -0.1266380 0.5143400 -0.6877920
16 H -0.0600670 0.2732550 -1.7542180
17 C 1.3184760 0.2840640 -0.1258770
18 C -1.0548320 -0.5348160 -0.1000970
19 H 1.9287600 1.0845780 -0.5567530
20 O 1.8753450 -0.9201020 -0.6324910
21 O -0.8413310 -1.7259050 -0.1781570
22 H 1.2382390 -1.6322210 -0.4753670
23 O -2.1114040 -0.0377660 0.5676020
24 H -2.6090450 -0.7930570 0.9182420
25 H -0.0077870 2.5449210 -0.9316010
26 C 1.4101950 0.3578180 1.3984430
27 H 0.8479970 -0.4538100 1.8703310
28 H 2.4534480 0.2621220 1.7046720
29 H 1.0297100 1.3107010 1.7780340

30 Energy: -438.419618259
31
32
33

34
35 B3LYP/6-311++G** geometry and energy of conformer: Thr-XXIX
36

37 N -0.0871570 1.9085340 -0.3383170
38 H 0.8440900 2.3005820 -0.4424250
39 C -0.0019850 0.4566440 -0.4779060
40 H 0.1923090 0.2206870 -1.5288930
41 C 1.1339210 -0.1940040 0.3705940
42 C -1.3450910 -0.1778920 -0.1611230
43 H 0.9463610 0.0433070 1.4218420
44 O 2.3638060 0.4730740 0.0648070
45 O -1.8944520 -1.0257130 -0.8164930
46 H 2.7266250 0.0944400 -0.7443420
47 O -1.8615880 0.2943260 1.0021790
48 H -2.7138580 -0.1457640 1.1410130
49 H -0.4192310 2.1558790 0.5889780
50 C 1.2605670 -1.7019010 0.1872100
51 H 0.3531380 -2.2245160 0.4975750
52 H 1.4391160 -1.9549470 -0.8639970
53 H 2.0949480 -2.0799850 0.7818750

54 Energy: -438.419484049
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58
59 B3LYP/6-311++G** geometry and energy of conformer: Thr-XXX
60

N -0.0859000 1.9079330 -0.3251160

1				
2				
3	H	-0.3394860	2.1550230	0.6266150
4	C	0.0020860	0.4569830	-0.4730680
5	H	0.1949150	0.2311420	-1.5244370
6	C	1.1319070	-0.2085120	0.3550460
7	C	-1.3445060	-0.1710060	-0.1495830
8	H	0.9485110	0.0075140	1.4169540
9	O	2.3226510	0.4689490	-0.0699170
10	O	-1.9255980	-0.9801220	-0.8250050
11	H	3.0684270	0.1400290	0.4412950
12	O	-1.8296330	0.2700200	1.0397620
13	H	-2.6914500	-0.1521820	1.1750310
14	H	0.8253190	2.3116030	-0.5171120
15	C	1.2462170	-1.7147260	0.1400390
16	H	0.3470720	-2.2376420	0.4754280
17	H	1.4024770	-1.9410030	-0.9175840
18	H	2.0919340	-2.1172240	0.7062960

Energy: -438.419445973

B3LYP/6-311++G** geometry and energy of conformer: Thr-XXXI

26	N	0.0226880	1.8829110	-0.7477320
27	H	-0.0475930	2.2518860	0.1961090
28	C	-0.0780880	0.4250940	-0.7315620
29	H	-0.3173430	0.0781800	-1.7377690
30	C	1.2917580	-0.1916710	-0.3632020
31	C	-1.1765330	-0.0745510	0.2105690
32	H	1.9746650	0.1220520	-1.1627080
33	O	1.1024600	-1.6101060	-0.4094690
34	O	-1.3502240	0.3354120	1.3341080
35	H	1.9148880	-2.0402240	-0.1257220
36	O	-1.9709380	-1.0041770	-0.3579820
37	H	-2.6198160	-1.2768510	0.3094590
38	H	-0.7344130	2.2887150	-1.2864540
39	C	1.8584040	0.2592780	0.9793800
40	H	1.1961620	-0.0108780	1.8036750
41	H	2.8334410	-0.2111340	1.1445750
42	H	2.0175620	1.3399410	0.9885940

Energy: -438.419177858

B3LYP/6-311++G** geometry and energy of conformer: Thr-XXXII

51	N	0.2123150	1.7949590	-0.3540140
52	H	-0.6767870	2.2832420	-0.3203950
53	C	0.0569650	0.4803330	0.2767830
54	H	-0.0193580	0.5335320	1.3775230
55	C	-1.2174430	-0.1968910	-0.2613670
56	C	1.3191750	-0.3137730	-0.0449410
57	H	-1.1067690	-0.3137230	-1.3410020
58	O	-2.3212590	0.7096960	-0.0993030
59	O	1.4054250	-1.2877890	-0.7470460
60	H	-2.6666440	0.6159610	0.7955320
	O	2.3952080	0.2415500	0.5669980
	H	3.1774180	-0.2592300	0.2892040

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2
3 H 0.9145200 2.3493500 0.1220400
4 C -1.5167480 -1.5426150 0.3866820
5 H -0.7189440 -2.2590610 0.1894470
6 H -1.6275550 -1.4392730 1.4731840
7 H -2.4487760 -1.9454950 -0.0155640

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9 Energy: -438.418743997

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12
13 B3LYP/6-311++G** geometry and energy of conformer: Thr-XXXIII

14
15 N 0.1397450 1.8101650 -0.2514790
16 H -0.0758470 1.9704100 0.7270110
17 C -0.0141670 0.4038760 -0.5759280
18 H 0.0054740 0.2835100 -1.6651870
19 C 1.0553640 -0.5714780 -0.0099780
20 C -1.3937160 -0.0493330 -0.1107970
21 H 0.7677450 -1.5828450 -0.3236360
22 O 0.9793940 -0.4663570 1.4144760
23 O -2.1132080 0.5439400 0.6462270
24 H 1.6144900 -1.0712790 1.8097940
25 O -1.7279690 -1.2479100 -0.6563910
26 H -2.5939090 -1.4910480 -0.2961730
27 H 1.0828410 2.1319050 -0.4321430
28 C 2.4603480 -0.2720870 -0.5254650
29 H 2.7932880 0.7235320 -0.2209950
30 H 3.1748030 -0.9969400 -0.1233010
31 H 2.5001960 -0.3416580 -1.6164960

32 Energy: -438.418617731

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35
36 B3LYP/6-311++G** geometry and energy of conformer: Thr-XXXIV

37
38 N -0.0864220 1.8827520 -0.3881530
39 H -0.2161500 2.1985570 0.5669810
40 C -0.0010770 0.4273660 -0.4907660
41 H 0.1749660 0.1758490 -1.5384330
42 C 1.1311440 -0.2344060 0.3526040
43 C -1.3535260 -0.1684670 -0.1313090
44 H 0.9098310 -0.0636140 1.4151150
45 O 2.3847960 0.3704120 0.0237010
46 O -1.9740550 -0.9640620 -0.7870780
47 H 2.4158190 1.2504100 0.4118210
48 O -1.7894910 0.2860150 1.0726780
49 H -2.6553420 -0.1165290 1.2386080
50 H 0.7242920 2.3317870 -0.7964030
51 C 1.2769300 -1.7244850 0.0857050
52 H 1.5242280 -1.8972410 -0.9649690
53 H 2.0815620 -2.1339670 0.6989200
54 H 0.3549300 -2.2634800 0.3136280

55 Energy: -438.418555341

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58
59 B3LYP/6-311++G** geometry and energy of conformer: Thr-XXXV

60 N 0.0917630 1.6853540 -0.2798000

1				
2				
3	H	-0.4573790	2.2698680	-0.9028850
4	C	-0.0286220	0.2636940	-0.6443290
5	H	0.0338930	0.0834860	-1.7237960
6	C	1.0799940	-0.5797020	0.0323560
7	C	-1.4007230	-0.2774530	-0.2038580
8	H	0.8497840	-1.6226300	-0.1935980
9	O	1.0101390	-0.4903110	1.4529150
10	O	-1.8562380	-1.2992030	-0.6415960
11	H	1.1248270	0.4298200	1.7167150
12	O	-2.0433920	0.4716800	0.7065130
13	H	-1.4565220	1.2216190	0.9216580
14	H	1.0504170	2.0097190	-0.3530370
15	C	2.4818140	-0.2565940	-0.4865930
16	H	3.2025490	-0.9315590	-0.0218990
17	H	2.5402450	-0.3805410	-1.5715970
18	H	2.7909960	0.7657420	-0.2410720

Energy: -438.418544325

B3LYP/6-311++G** geometry and energy of conformer: Thr-XXXVI

25	N	0.0708310	1.7809980	-0.1976800
26	H	0.0381060	1.8727830	0.8122810
27	C	-0.0054870	0.3829930	-0.5890670
28	H	0.0662670	0.3254570	-1.6797750
29	C	1.0896840	-0.5581780	-0.0195660
30	C	-1.3608240	-0.2378110	-0.2528200
31	H	0.8456220	-1.5733960	-0.3543720
32	O	0.9684250	-0.4745010	1.4062670
33	O	-1.7204550	-1.3074780	-0.6828650
34	H	1.5656060	-1.1104280	1.8115760
35	O	-2.1098740	0.5017770	0.5853340
36	H	-2.9204380	-0.0015630	0.7557710
37	H	0.9318380	2.2026780	-0.5260350
38	C	2.4941150	-0.1908780	-0.4875280
39	H	3.2286470	-0.8853190	-0.0687510
40	H	2.5702870	-0.2492170	-1.5774300
41	H	2.7685560	0.8168790	-0.1655030

Energy: -438.418434988

B3LYP/6-311++G** geometry and energy of conformer: Thr-XXXVII

49	N	0.1090110	1.9085680	-0.2778820
50	H	-0.3578410	2.1975030	0.5789480
51	C	-0.0143240	0.4593990	-0.4314020
52	H	0.1500950	0.2129880	-1.4866650
53	C	1.1425100	-0.1986680	0.3784840
54	C	-1.3823120	-0.0619370	0.0293890
55	H	0.9671800	0.0404480	1.4388440
56	O	2.3633750	0.3772310	-0.0516370
57	O	-2.0275380	0.4690960	0.8914280
58	H	2.1914600	1.3290880	-0.1272750
59	O	-1.8428990	-1.1886880	-0.5711610
60	H	-1.2186910	-1.4986880	-1.2390940
	H	-0.3412570	2.4005820	-1.0417190
	C	1.2544310	-1.7061750	0.2142150

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2
3 H 0.3869450 -2.2252250 0.6278000
4 H 1.3719730 -1.9740750 -0.8411230
5 H 2.1417280 -2.0594170 0.7423000
6

7 Energy: -438.418268937
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11 B3LYP/6-311++G** geometry and energy of conformer: Thr-XXXVIII

12
13 N -0.0445150 1.8411230 -0.8161040
14 H -0.0854710 2.2370770 0.1167920
15 C -0.0751130 0.3824500 -0.7732460
16 H -0.2465950 0.0247420 -1.7923700
17 C 1.3084440 -0.1752870 -0.3296780
18 C -1.2177640 -0.2315310 0.0386100
19 H 2.0057670 0.1160630 -1.1257520
20 O 1.2658630 -1.5965570 -0.2013670
21 O -1.9137270 -1.1417590 -0.3353580
22 H 0.9285230 -1.9878970 -1.0146650
23 O -1.3906670 0.3723350 1.2411960
24 H -2.1212720 -0.0818210 1.6879910
25 H -0.8311320 2.2083060 -1.3400340
26 C 1.8274690 0.3648290 0.9943180
27 H 1.1554670 0.1140490 1.8169030
28 H 2.8026100 -0.0815240 1.1987580
29 H 1.9537470 1.4482280 0.9493130

30 Energy: -438.418218677
31
32

33
34 B3LYP/6-311++G** geometry and energy of conformer: Thr-XXXIX

35
36 N -0.0830810 1.8518360 0.3146390
37 H -0.7244710 2.4595480 -0.1843000
38 C -0.0226530 0.5332950 -0.3298020
39 H 0.1033300 0.5918830 -1.4199590
40 C 1.1584090 -0.2637270 0.2390910
41 C -1.3827400 -0.1201750 -0.1003520
42 H 1.0219930 -0.3505930 1.3222030
43 O 2.3102310 0.5542040 -0.0344630
44 O -2.3156460 -0.0052540 -0.8557080
45 H 3.0688680 0.1872910 0.4293310
46 O -1.4680440 -0.8050750 1.0623800
47 H -2.3826060 -1.1161140 1.1440460
48 H 0.8412870 2.2700580 0.2776170
49 C 1.3094350 -1.6443720 -0.3930080
50 H 0.4419370 -2.2737740 -0.1816120
51 H 1.4348690 -1.5600170 -1.4755450
52 H 2.1893350 -2.1522550 0.0125080

53 Energy: -438.418020902
54
55

56 B3LYP/6-311++G** geometry and energy of conformer: Thr-XL

57
58 N -0.1612090 1.8585250 -0.8496080
59 H -0.2908270 2.2675740 0.0700790
60 C -0.0719470 0.4070660 -0.7559960
H -0.2420690 -0.0169090 -1.7519930

1				
2				
3	C	1.3092720	-0.1388770	-0.2645430
4	C	-1.1976090	-0.0803980	0.1421810
5	H	2.0437980	0.2427830	-0.9914770
6	O	1.3369470	-1.5651060	-0.2603410
7	O	-1.5739050	0.4855770	1.1379730
8	H	1.0143320	-1.8980920	-1.1048840
9	O	-1.7295370	-1.2433400	-0.2904530
10	H	-2.3948350	-1.5177750	0.3596680
11	H	0.6710300	2.2549010	-1.2724080
12	C	1.7203040	0.3100540	1.1293340
13	H	1.0170000	-0.0498200	1.8826770
14	H	2.7078920	-0.0951210	1.3579690
15	H	1.7739890	1.3986790	1.1943340

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17 Energy: -438.417869111

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20
21 B3LYP/6-311++G** geometry and energy of conformer: Thr-XLI

22	N	-0.0324190	1.8809760	0.2178140
23	H	0.9174830	2.2371620	0.2617440
24	C	-0.0102640	0.5346410	-0.3572560
25	H	0.1228490	0.5293260	-1.4499360
26	C	1.1478610	-0.2671260	0.2737380
27	C	-1.3777240	-0.1002820	-0.1168230
28	H	1.0090450	-0.2649770	1.3560960
29	O	2.3755060	0.4448480	0.0638300
30	O	-2.2342510	-0.2074120	-0.9598840
31	H	2.6717170	0.2893440	-0.8405110
32	O	-1.5506410	-0.5192870	1.1561710
33	H	-2.4564920	-0.8566440	1.2268390
34	H	-0.5859150	2.5130440	-0.3499110
35	C	1.2422390	-1.6966610	-0.2461360
36	H	1.3817710	-1.7127060	-1.3331180
37	H	2.0902380	-2.2044780	0.2175360
38	H	0.3386540	-2.2655300	-0.0155120

39
40 Energy: -438.417733846

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43
44 B3LYP/6-311++G** geometry and energy of conformer: Thr-XLII

45				
46	N	-0.1222980	1.8873060	-0.6396680
47	H	-0.9207210	2.2735960	-1.1306130
48	C	-0.1057810	0.4266650	-0.7363740
49	H	-0.3007800	0.1536900	-1.7742100
50	C	1.2991960	-0.1167110	-0.3963820
51	C	-1.2320710	-0.2469870	0.0532940
52	H	1.9536850	0.2695470	-1.1885170
53	O	1.1888910	-1.5395840	-0.5044280
54	O	-2.1162890	-0.9078920	-0.4258930
55	H	2.0349580	-1.9367710	-0.2766300
56	O	-1.1830250	0.0428670	1.3828920
57	H	-1.9451560	-0.3911980	1.7953530
58	H	-0.1740100	2.1940600	0.3259880
59	C	1.8713840	0.3069440	0.9536610
60	H	1.2604830	-0.0579250	1.7798680
	H	2.8845130	-0.0937390	1.0639980
	H	1.9501240	1.3950000	1.0166830

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4 Energy: -438.416965250
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8 B3LYP/6-311++G** geometry and energy of conformer: Thr-XLIII
9

10 N	-0.1884010	1.8592180	-0.8039330
11 H	-0.1763880	2.2626160	0.1269550
12 C	-0.0866920	0.4043140	-0.7457610
13 H	-0.2827200	-0.0034590	-1.7391440
14 C	1.3024700	-0.1417190	-0.3132850
15 C	-1.1871910	-0.0894740	0.1855540
16 H	2.0128020	0.2516140	-1.0572480
17 O	1.2184370	-1.5635710	-0.4432620
18 O	-1.3958530	0.3624570	1.2860100
19 H	2.0395800	-1.9559420	-0.1303880
20 O	-1.9183050	-1.0843050	-0.3492670
21 H	-2.5748520	-1.3471760	0.3144420
22 H	0.5650520	2.2627820	-1.3494770
23 C	1.7707250	0.2713900	1.0785380
24 H	1.0997700	-0.1051910	1.8520370
25 H	2.7758950	-0.1222930	1.2622740
26 H	1.8295590	1.3588160	1.1699600

27 Energy: -438.416792867
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31 B3LYP/6-311++G** geometry and energy of conformer: Thr-XLIV
32

33 N	-0.2539740	1.8118220	-0.8630330
34 H	-0.2459270	2.2387700	0.0565390
35 C	-0.0767670	0.3649860	-0.7832200
36 H	-0.1973930	-0.0377650	-1.7938440
37 C	1.3197120	-0.1199840	-0.2759520
38 C	-1.2101560	-0.2684040	0.0115920
39 H	2.0404690	0.2451540	-1.0250510
40 O	1.3789220	-1.5431340	-0.2061510
41 O	-1.7867480	-1.2773090	-0.3034450
42 H	0.9824640	-1.9282970	-0.9956810
43 O	-1.4976270	0.4183110	1.1431320
44 H	-2.2231820	-0.0470650	1.5866210
45 H	0.4770620	2.2372970	-1.4232810
46 C	1.7377930	0.3991930	1.0918970
47 H	1.0432690	0.0726830	1.8678610
48 H	2.7288430	0.0087860	1.3312460
49 H	1.7923410	1.4899920	1.1026350

50 Energy: -438.416053844
51
52

53 B3LYP/6-311++G** geometry and energy of conformer: Thr-XLV
54

55 N	0.1630950	1.7075640	-0.0322460
56 H	0.6465600	2.2990720	-0.6956160
57 C	-0.0323770	0.3508990	-0.5364590
58 H	-0.0172260	0.2965400	-1.6365640
59 C	1.1050810	-0.5521540	0.0129250
60 C	-1.4378860	-0.1215240	-0.1233730
H	0.9027210	-1.6052370	-0.2222720

1				
2				
3	O	1.1227050	-0.4729230	1.4261710
4	O	-2.2778080	0.6232810	0.3020840
5	H	1.0406050	0.4712750	1.6354030
6	O	-1.7249500	-1.4252630	-0.3255160
7	H	-0.9362300	-1.9165780	-0.5858770
8	H	-0.7359660	2.1251710	0.1899360
9	C	2.4618020	-0.1940790	-0.5961350
10	H	3.2345380	-0.8329170	-0.1648700
11	H	2.4612040	-0.3342800	-1.6819950
12	H	2.7228330	0.8443880	-0.3760850

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14 Energy: -438.415737637

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18 B3LYP/6-311++G** geometry and energy of conformer: Thr-XLVI

19				
20	N	-0.0508300	-1.1284500	1.3522490
21	H	-0.6861400	-1.9103200	1.4493350
22	C	0.0711170	-0.6923310	-0.0389100
23	H	0.0900770	-1.5796180	-0.6728010
24	C	-1.0662360	0.2298520	-0.5392520
25	C	1.4626880	-0.0503900	-0.2307850
26	H	-0.7933010	0.6024960	-1.5352830
27	O	-1.0968310	1.3452070	0.3845800
28	O	2.3657060	-0.6138380	-0.7865340
29	H	-1.7358810	2.0007760	0.0876010
30	O	1.6209510	1.1885430	0.2828700
31	H	0.7556060	1.5358060	0.5672710
32	H	-0.3629500	-0.3778700	1.9583500
33	C	-2.4219130	-0.4597790	-0.6051170
34	H	-3.1953000	0.2378440	-0.9401650
35	H	-2.3951920	-1.2888550	-1.3176150
36	H	-2.7136560	-0.8445110	0.3746140

37 Energy: -438.415355600

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41 B3LYP/6-311++G** geometry and energy of conformer: Thr-XLVII

42				
43	N	-0.1393770	-1.2392960	1.1878900
44	H	-0.3759920	-0.5238630	1.8692910
45	C	0.0673120	-0.6225140	-0.1232850
46	H	0.1245600	-1.4196460	-0.8763400
47	C	-1.1396880	0.2800330	-0.4790320
48	C	1.3687840	0.1981300	-0.1669470
49	H	-0.9078410	0.7730600	-1.4337810
50	O	-1.3412220	1.2622190	0.5326770
51	O	1.4511120	1.3587170	0.1476190
52	H	-0.5372540	1.8011280	0.5688900
53	O	2.4918700	-0.4744940	-0.5292080
54	H	2.2734510	-1.3720590	-0.8091390
55	H	0.6729020	-1.7485960	1.5174310
56	C	-2.4327160	-0.5075230	-0.6253210
57	H	-3.2466560	0.1773170	-0.8700350
58	H	-2.3487600	-1.2473270	-1.4261320
59	H	-2.6749960	-1.0252380	0.3033930

60 Energy: -438.414630711

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5 B3LYP/6-311++G** geometry and energy of conformer: Thr-XLVIII
6

7 N	-0.3093120	1.8173620	-0.7919380
8 H	-0.2057330	2.2298510	0.1281830
9 C	-0.0999250	0.3707870	-0.7688310
10 H	-0.2361820	-0.0079360	-1.7828960
11 C	1.3125220	-0.0918840	-0.3201590
12 C	-1.2294770	-0.2713500	0.0324150
13 H	2.0031750	0.3357620	-1.0639610
14 O	1.3047620	-1.5160080	-0.4408370
15 O	-1.9866440	-1.1099910	-0.3741840
16 H	2.1526800	-1.8621870	-0.1453820
17 O	-1.3149460	0.2418950	1.2901770
18 H	-2.0754660	-0.1803350	1.7176260
19 H	0.3338500	2.2725790	-1.4301000
20 C	1.7646010	0.3529890	1.0682660
21 H	1.1241500	-0.0610000	1.8476480
22 H	2.7923170	0.0187060	1.2443580
23 H	1.7646980	1.4425990	1.1567000

24 Energy: -438.414283769
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28
29 B3LYP/6-311++G** geometry and energy of conformer: Thr-XLIX
30

31 N	0.0188040	1.8879400	0.0602360
32 H	-0.5314530	2.4781900	-0.5539310
33 C	-0.0264390	0.4795030	-0.3705270
34 H	0.1084390	0.4689370	-1.4534090
35 C	1.1736440	-0.2618220	0.2594430
36 C	-1.3957570	-0.1640140	-0.1133930
37 H	1.0365350	-0.2901230	1.3597310
38 O	2.3587350	0.4569650	-0.0276790
39 O	-2.2322540	-0.3006710	-0.9614520
40 H	2.1259980	1.3965790	0.0348010
41 O	-1.6698960	-0.5232730	1.1736700
42 H	-0.8831860	-0.4457880	1.7293170
43 H	-0.3321940	2.0166600	1.0051110
44 C	1.3369480	-1.6842380	-0.2537480
45 H	1.4735680	-1.6795700	-1.3377740
46 H	2.2195680	-2.1392410	0.1990630
47 H	0.4680530	-2.3019720	-0.0115240

48 Energy: -438.413726133
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52 B3LYP/6-311++G** geometry and energy of conformer: Thr-L
53

54 N	-0.0193390	1.9348650	-0.3129230
55 H	-0.3476760	2.2004530	0.6114240
56 C	-0.0090690	0.4826610	-0.4315110
57 H	0.1272900	0.2295700	-1.4911420
58 C	1.1328590	-0.2189090	0.3460590
59 C	-1.3600240	-0.0349790	0.0716030
60 H	1.0153220	0.0412290	1.4059820
O	2.3318790	0.3744670	-0.1702150

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3	O	-1.8122780	0.2717380	1.1399960
4	H	3.0780050	0.0978320	0.3706940
5	O	-2.0288580	-0.8953150	-0.7341780
6	H	-1.5665320	-0.9928420	-1.5754600
7	H	0.9246910	2.2878880	-0.4322790
8	C	1.1505470	-1.7360270	0.1795160
9	H	0.2485640	-2.1954970	0.5927880
10	H	1.2375320	-2.0083120	-0.8766420
11	H	2.0063500	-2.1679780	0.7062730

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13 Energy: -438.412787935

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16
17 B3LYP/6-311++G** geometry and energy of conformer: Thr-LI

18	N	-0.5499040	1.8495380	0.1823190
19	H	-0.0445280	2.6264980	-0.2302400
20	C	-0.1538490	0.5868590	-0.4496230
21	H	-0.2720030	0.6103460	-1.5498140
22	C	1.3446910	0.3140810	-0.1723850
23	C	-1.1011110	-0.5257980	-0.0040250
24	H	1.8557720	1.2563750	-0.4261020
25	O	1.8486280	-0.7301690	-1.0040560
26	O	-0.8150630	-1.6338890	0.3571310
27	H	1.7896270	-0.4590360	-1.9259660
28	O	-2.3956750	-0.1113140	-0.1141420
29	H	-2.9562530	-0.8505220	0.1658840
30	H	-1.5415740	2.0209590	0.0618960
31	C	1.6794420	-0.0382060	1.2687200
32	H	1.2878900	-1.0241720	1.5170040
33	H	2.7633910	-0.0489780	1.3990150
34	H	1.2488460	0.7031260	1.9445180

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36 Energy: -438.412520745

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40 B3LYP/6-311++G** geometry and energy of conformer: Thr-LII

41				
42	N	0.2369850	1.7669510	-0.1157790
43	H	0.2444820	1.8058290	0.8996530
44	C	-0.0356190	0.4048080	-0.5330590
45	H	-0.0339100	0.3710630	-1.6310630
46	C	1.0887910	-0.5364620	-0.0545660
47	C	-1.4372410	-0.0943320	-0.0974050
48	H	0.8829370	-1.5551740	-0.4236540
49	O	1.0122230	-0.5341990	1.3717490
50	O	-2.2380670	0.5957790	0.4653890
51	H	1.7946760	-0.9600330	1.7355520
52	O	-1.7673000	-1.3651360	-0.4534940
53	H	-1.0163640	-1.8135060	-0.8609330
54	H	-0.5136290	2.3788050	-0.4179000
55	C	2.4664660	-0.1225380	-0.5617240
56	H	3.2306520	-0.8089680	-0.1825880
57	H	2.5021720	-0.1599360	-1.6541430
58	H	2.7008570	0.8928550	-0.2430900

59 Energy: -438.412327313

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4 B3LYP/6-311++G** geometry and energy of conformer: Thr-LIII

5
6 N -0.0157450 1.9284530 -0.3551070
7 H 0.9425150 2.2644440 -0.3771390
8 C -0.0158390 0.4747840 -0.4465130
9 H 0.1186900 0.1948500 -1.5023330
10 C 1.1299630 -0.2047700 0.3631430
11 C -1.3684510 -0.0339030 0.0573790
12 H 0.9882930 0.0659390 1.4127010
13 O 2.3744590 0.3975370 -0.0057140
14 O -1.8472690 0.3249370 1.0974490
15 H 2.6899450 -0.0091940 -0.8209040
16 O -2.0025540 -0.9595760 -0.7047700
17 H -1.5308170 -1.0890570 -1.5363530
18 H -0.4294060 2.2119870 0.5289950
19 C 1.1782850 -1.7214480 0.2168190
20 H 0.2673790 -2.1918950 0.5950210
21 H 1.2992960 -2.0137530 -0.8338880
22 H 2.0234900 -2.1236540 0.7789650

23 Energy: -438.411988888

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26
27 B3LYP/6-311++G** geometry and energy of conformer: Thr-LIV

28
29 N 0.0406680 1.9300640 -0.1267260
30 H 0.8995460 2.3176010 -0.4983940
31 C -0.0186320 0.5051050 -0.3983340
32 H 0.1265710 0.2537380 -1.4657010
33 C 1.1322660 -0.1816700 0.3724040
34 C -1.3863840 -0.0457010 0.0328150
35 H 1.0330280 0.1279170 1.4188160
36 O 2.3222680 0.3924520 -0.1922470
37 O -2.0734610 0.4245080 0.8916290
38 H 3.0523630 0.2677310 0.4216880
39 O -1.8035300 -1.1529370 -0.6434010
40 H -1.1673720 -1.3880820 -1.3302720
41 H -0.7545930 2.4290070 -0.5067970
42 C 1.1693010 -1.7035160 0.2692830
43 H 0.2937940 -2.1644340 0.7324840
44 H 1.2368310 -2.0247000 -0.7749220
45 H 2.0536300 -2.0867110 0.7853140

46 Energy: -438.408744171

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50 B3LYP/6-311++G** geometry and energy of conformer: Thr-LV

51
52 N 0.1042250 1.7712250 -0.4127240
53 H -0.2829180 2.0351080 0.4878570
54 C -0.0332940 0.3410080 -0.6030150
55 H -0.0080720 0.1205260 -1.6806800
56 C 1.0600600 -0.5563650 0.0447560
57 C -1.4157890 -0.0784180 -0.0789080
58 H 0.7997590 -1.6055380 -0.1687220
59 O 0.9984480 -0.3258250 1.4481010
60 O -2.0775670 0.5768820 0.6709500
H 1.6653060 -0.8613930 1.8890180

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O	-1.8655080	-1.2888320	-0.5103240
H	-1.2568720	-1.6726490	-1.1530050
H	1.0706490	2.0700050	-0.4541640
C	2.4547590	-0.2890290	-0.5180950
H	3.1844500	-0.9626690	-0.0587450
H	2.4836260	-0.4576530	-1.5985310
H	2.7771010	0.7347090	-0.3122020

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11 Energy: -438.407983479
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15 B3LYP/6-311++G** geometry and energy of conformer: Thr-LVI

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N	0.0930600	1.9231390	-0.0296460
H	1.0479800	2.2371380	-0.1661680
C	-0.0137050	0.5165040	-0.3755210
H	0.0834070	0.3232590	-1.4628520
C	1.1342270	-0.2502140	0.3279310
C	-1.3654200	-0.0382280	0.1110090
H	1.0294650	-0.0553320	1.3968950
O	2.3859230	0.3411080	-0.0395730
O	-1.7407760	0.0029640	1.2455530
H	2.6739060	-0.0359060	-0.8786200
O	-2.1348580	-0.6361750	-0.8438090
H	-1.7035400	-0.5759120	-1.7048350
H	-0.5335310	2.5085680	-0.5689720
C	1.1251160	-1.7493860	0.0570910
H	1.2180240	-1.9604610	-1.0153740
H	1.9642800	-2.2220950	0.5710840
H	0.2049640	-2.2164690	0.4159390

34 Energy: -438.407467696
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3 B3LYP/6-311++G** geometry and energy of conformer: aThr-I
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5	N	0.2923440	1.8515520	0.0058230
6	H	0.0289510	2.0580980	-0.9537200
7	C	0.0568290	0.4377930	0.3400420
8	H	-0.0800310	0.3642720	1.4251160
9	C	-1.1837500	-0.2176340	-0.3222290
10	C	1.3458670	-0.3568710	0.0329220
11	H	-1.0098190	-0.2383200	-1.4117690
12	O	-1.3712230	-1.5348850	0.1653400
13	O	1.3762730	-1.5610510	-0.0738490
14	H	-0.5259760	-2.0018520	0.0657870
15	O	2.4389950	0.3972740	-0.0854610
16	H	2.1233100	1.3260630	-0.0065920
17	H	-0.2275260	2.4764410	0.6096490
18	C	-2.4695860	0.5477090	-0.0373330
19	H	-2.6399370	0.6192240	1.0409560
20	H	-2.4542010	1.5531140	-0.4640690
21	H	-3.3096980	0.0054080	-0.4747620

22 Energy: -438.426076096
23

24 MP2/aug-cc-pVTZ geometry and energy of conformer: aThr-I
25

26	N	0.2779100	1.8412290	0.0116870
27	H	0.0219000	2.0222540	-0.9537360
28	C	0.0504700	0.4334780	0.3478070
29	H	-0.0983050	0.3549570	1.4284760
30	C	-1.1651990	-0.2188160	-0.3265250
31	C	1.3314440	-0.3491660	0.0377150
32	H	-0.9799290	-0.2326860	-1.4114700
33	O	-1.3534250	-1.5333810	0.1594760
34	O	1.3699800	-1.5584090	-0.0706310
35	H	-0.4906890	-1.9749690	0.0787340
36	O	2.4182540	0.4132350	-0.0918330
37	H	2.0755600	1.3332470	-0.0058470
38	H	-0.2853630	2.4505600	0.5896710
39	C	-2.4433220	0.5407600	-0.0398110
40	H	-2.5984810	0.6093950	1.0375240
41	H	-2.4271300	1.5425680	-0.4658640
42	H	-3.2817580	-0.0030290	-0.4705160

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44 Energy: -435.933243196
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B3LYP/6-311++G** geometry and energy of conformer: aThr-II

N	0.3845910	1.7459650	0.1091240
H	-0.0076120	1.8208290	1.0430750
C	-0.0023820	0.4823340	-0.5098950
H	-0.0121850	0.6105720	-1.5953050
C	1.0913670	-0.5924520	-0.2199330
C	-1.3845200	0.0038690	-0.0869770
H	0.8795460	-1.4680330	-0.8372570
O	2.3333930	-0.0789570	-0.6746890
O	-2.0387470	0.4683270	0.8134310
H	2.3787120	0.8301190	-0.3403510
O	-1.8044800	-1.0422640	-0.8358020
H	-2.6737640	-1.3113630	-0.5009800
H	0.0344840	2.5356120	-0.4203560
C	1.1635060	-1.0059530	1.2505090
H	1.9840080	-1.7134110	1.3829300
H	1.3567510	-0.1432830	1.8944120
H	0.2387730	-1.4864350	1.5842230

Energy: -438.425833825

MP2/aug-cc-pVTZ geometry and energy of conformer: aThr-II

N	0.4252700	1.7279270	0.0802170
H	0.0052150	1.8007140	1.0015020
C	0.0140320	0.4777880	-0.5389850
H	0.0133340	0.5931430	-1.6230830
C	1.0628600	-0.6080150	-0.2122960
C	-1.3582370	0.0215490	-0.1021900
H	0.8484860	-1.4893660	-0.8162380
O	2.3283540	-0.1285860	-0.6299060
O	-2.0001310	0.5004240	0.8064990
H	2.3531660	0.7904650	-0.3172260
O	-1.7805750	-1.0365590	-0.8313230
H	-2.6448750	-1.2891150	-0.4685780
H	0.0771310	2.5161590	-0.4503700
C	1.0708360	-0.9743800	1.2627500
H	1.8646780	-1.6953590	1.4465340
H	1.2658770	-0.0925510	1.8739110
H	0.1219680	-1.4134730	1.5741970

Energy: -437.568540604

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3 B3LYP/6-311++G** geometry and energy of conformer: aThr-III
4

5	N	-0.9006290	1.7481870	-0.2100110
6	H	-0.6137430	2.0552030	0.7168340
7	C	-0.1875900	0.5111930	-0.5698130
8	H	-0.1835870	0.4335630	-1.6630430
9	C	1.2722380	0.4666440	-0.0591800
10	C	-1.0282340	-0.6883160	-0.0699370
11	H	1.7022080	1.4472520	-0.2879700
12	O	1.2802490	0.4061520	1.3696180
13	O	-0.5803840	-1.7937070	0.1077570
14	H	1.0651210	-0.4986610	1.6300760
15	O	-2.3148780	-0.3914370	0.1338070
16	H	-2.3802580	0.5818950	0.0004750
17	H	-0.7090630	2.4992030	-0.8627630
18	C	2.1481710	-0.6083830	-0.6969090
19	H	3.1679950	-0.5168610	-0.3163470
20	H	1.7698160	-1.6072410	-0.4775380
21	H	2.1785030	-0.4865580	-1.7840710

22 Energy: -438.424501996
23

24 MP2/aug-cc-pVTZ geometry and energy of conformer: aThr-III
25

26	N	-0.9211890	1.7352070	-0.1692450
27	H	-0.6547970	1.9815240	0.7804080
28	C	-0.1861370	0.5300810	-0.5660090
29	H	-0.1727840	0.4844290	-1.6583880
30	C	1.2509350	0.4858440	-0.0337820
31	C	-0.9952070	-0.6850570	-0.0925070
32	H	1.6698990	1.4823170	-0.1922880
33	O	1.2223290	0.3330430	1.3840800
34	O	-0.5186200	-1.7837330	0.0919080
35	H	0.9784000	-0.5877200	1.5545360
36	O	-2.2918140	-0.4223490	0.0948870
37	H	-2.3581610	0.5531170	-0.0294690
38	H	-0.6841900	2.5181670	-0.7647840
39	C	2.1425890	-0.5374470	-0.7122100
40	H	3.1506690	-0.4583060	-0.3087350
41	H	1.7656160	-1.5444030	-0.5502960
42	H	2.1854330	-0.3517910	-1.7862180

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44 Energy: -437.566898070
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B3LYP/6-311++G** geometry and energy of conformer: aThr-IV

N	-0.3892980	1.9484780	-0.1407350
H	-1.3630650	2.2121010	-0.2407070
C	-0.1382820	0.5713100	-0.5719860
H	-0.3208970	0.5120350	-1.6485280
C	1.3359430	0.2164080	-0.2936370
C	-1.0971610	-0.3984880	0.1209660
H	1.9254210	1.0006590	-0.7751470
O	1.6341190	0.3370720	1.0967300
O	-0.8841980	-1.0018660	1.1498550
H	1.0848210	-0.3093910	1.5626510
O	-2.2873330	-0.4716000	-0.5179610
H	-2.8675950	-1.0442020	0.0082530
H	-0.1034020	2.0691190	0.8262380
C	1.7475030	-1.1443130	-0.8542200
H	1.1907290	-1.9588570	-0.3827620
H	1.5802620	-1.1908490	-1.9347820
H	2.8100860	-1.3083240	-0.6658000

Energy: -438.423629378

MP2/aug-cc-pVTZ geometry and energy of conformer: aThr-IV

N	-0.3790920	1.9401160	-0.1350980
H	-1.3619210	2.1786020	-0.1948500
C	-0.1361750	0.5698900	-0.5795430
H	-0.3283600	0.5140030	-1.6518560
C	1.3248370	0.2154370	-0.3096790
C	-1.0760710	-0.3933950	0.1202200
H	1.9206620	0.9816240	-0.8071580
O	1.6271250	0.3510920	1.0752350
O	-0.8475650	-1.0032430	1.1478020
H	1.0600390	-0.2873130	1.5333150
O	-2.2743230	-0.4559280	-0.5027490
H	-2.8354310	-1.0309440	0.0432130
H	-0.0834380	2.0268120	0.8320320
C	1.6964820	-1.1580140	-0.8407310
H	1.1271970	-1.9375410	-0.3339980
H	1.5036750	-1.2242780	-1.9123370
H	2.7548810	-1.3406460	-0.6665720

Energy: -437.565902301

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3 B3LYP/6-311++G** geometry and energy of conformer: aThr-V
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5	N	0.1053490	1.7111100	0.1581730
6	H	1.0854160	1.8783950	0.3668560
7	C	-0.0393510	0.4423970	-0.5739110
8	H	-0.0127820	0.5804690	-1.6593570
9	C	1.0977130	-0.5395250	-0.2258400
10	C	-1.3942710	-0.2099300	-0.2411520
11	H	0.9531240	-1.4190970	-0.8614810
12	O	2.3017990	0.1453140	-0.6037880
13	O	-1.8242730	-1.1610560	-0.8398760
14	H	3.0564300	-0.4151700	-0.3967810
15	O	-2.0341380	0.3603780	0.7885420
16	H	-1.4518760	1.1001040	1.0774480
17	H	-0.2076160	2.4909730	-0.4107310
18	C	1.1397260	-0.9718500	1.2393900
19	H	0.2342920	-1.5187110	1.5132360
20	H	1.9877770	-1.6432220	1.4051720
21	H	1.2477870	-0.1151550	1.9084820

22 Energy: -438.423380829
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24 MP2/aug-cc-pVTZ geometry and energy of conformer: aThr-V
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26	N	0.1575090	1.6961910	0.1338620
27	H	1.1507150	1.8483260	0.2787810
28	C	-0.0267150	0.4433150	-0.6005700
29	H	0.0049130	0.5677780	-1.6845700
30	C	1.0655250	-0.5594850	-0.2244650
31	C	-1.3735630	-0.1825210	-0.2475020
32	H	0.9077530	-1.4438650	-0.8462870
33	O	2.2921070	0.0872120	-0.5783160
34	O	-1.8372570	-1.1236860	-0.8481290
35	H	3.0186070	-0.4872490	-0.3119620
36	O	-1.9674870	0.3778160	0.8156470
37	H	-1.3507070	1.1005680	1.0784340
38	H	-0.1774380	2.4784930	-0.4160750
39	C	1.0498910	-0.9506280	1.2428630
40	H	0.1217560	-1.4618460	1.4974000
41	H	1.8734260	-1.6350450	1.4502990
42	H	1.1586800	-0.0753150	1.8813740

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44 Energy: -437.566777895
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B3LYP/6-311++G** geometry and energy of conformer: aThr-VI

N	-0.0955450	1.7052140	0.3193320
H	0.4774690	2.4074860	-0.1340140
C	-0.0726050	0.4494920	-0.4424550
H	-0.0935300	0.7230100	-1.5029350
C	1.1660500	-0.4430630	-0.2519370
C	-1.3814260	-0.3300020	-0.2062950
H	1.0391450	-1.3050670	-0.9143420
O	2.2670620	0.3635170	-0.6976100
O	-1.5236910	-1.4897210	-0.4952410
H	3.0725230	-0.1617450	-0.6601850
O	-2.3635310	0.4165420	0.3158280
H	-1.9670610	1.3036330	0.4661020
H	0.2796840	1.5796930	1.2549450
C	1.3732850	-0.9397380	1.1771510
H	0.5289080	-1.5519480	1.5021080
H	2.2705950	-1.5630170	1.2320000
H	1.5105320	-0.1113850	1.8784040

Energy: -438.423320511

B3LYP/6-311++G** geometry and energy of conformer: aThr-VII

N	0.3060560	1.7244680	0.1537380
H	-0.1197550	2.5140820	-0.3165110
C	0.0042770	0.4681200	-0.5281790
H	0.0490430	0.6474130	-1.6051200
C	1.1338870	-0.5646780	-0.2303070
C	-1.3627410	-0.1561850	-0.2693680
H	0.9785260	-1.4255290	-0.8836850
O	2.3685730	0.0158680	-0.6187760
O	-1.8233390	-1.0663460	-0.9112650
H	2.3554670	0.9213590	-0.2726940
O	-2.0152340	0.3964180	0.7843780
H	-2.8531700	-0.0812000	0.8831160
H	-0.0324240	1.7235720	1.1093950
C	1.1692200	-1.0283630	1.2269030
H	0.2530000	-1.5574210	1.5061570
H	2.0108700	-1.7094250	1.3645110
H	1.3081970	-0.1850180	1.9096770

Energy: -438.423294504

B3LYP/6-311++G** geometry and energy of conformer: aThr-VIII

N	0.1061950	1.7130560	0.1089890
H	-0.1991930	2.4812620	-0.4789130
C	-0.0383150	0.4234250	-0.5794570
H	-0.0144500	0.5241650	-1.6712780
C	1.1022820	-0.5531840	-0.1850540
C	-1.3976000	-0.2148360	-0.2416990
H	0.9465960	-1.4692210	-0.7630410
O	2.3680850	0.0337640	-0.5154930
O	-1.8281630	-1.1729800	-0.8291910

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H	2.4833750	0.0216670	-1.4715890
O	-2.0386790	0.3711110	0.7783210
H	-1.4611440	1.1180690	1.0548850
H	1.0816620	1.8813750	0.3382470
C	1.1502810	-0.8954490	1.2981160
H	0.2271110	-1.3841240	1.6161150
H	1.9825600	-1.5764890	1.4822410
H	1.3002780	-0.0029870	1.9098790

12 Energy: -438.423250569

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19 B3LYP/6-311++G** geometry and energy of conformer: aThr-IX

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N	-0.4700340	1.8581390	-0.5036360
H	-1.4462760	1.9687400	-0.2517430
C	-0.1257190	0.4457680	-0.6907120
H	-0.1321780	0.1326500	-1.7441580
C	1.3210010	0.2523440	-0.1432150
C	-1.1790270	-0.3999110	0.0137780
H	1.9279470	0.9503350	-0.7419440
O	1.3624510	0.6402260	1.2200270
O	-2.1056740	0.0418210	0.6466070
H	0.9028030	1.4924160	1.2653450
O	-0.9978990	-1.7232300	-0.1820470
H	-1.7060930	-2.1812740	0.2962030
H	-0.2695600	2.4092260	-1.3285370
C	1.9286460	-1.1343720	-0.2701480
H	1.4156750	-1.8533090	0.3676070
H	1.8801800	-1.4887520	-1.3033210
l	2.9773190	-1.0905170	0.0310880

38 Energy: -438.422988926

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42 B3LYP/6-311++G** geometry and energy of conformer: aThr-X

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N	-0.0706400	1.8513750	0.4304850
H	-0.8015610	2.4343720	0.0385110
C	-0.0101110	0.5454640	-0.2349080
H	0.0760400	0.7191310	-1.3115900
C	1.2292760	-0.2438020	0.2365980
C	-1.2956410	-0.2494770	-0.0007820
H	1.1981220	-0.2971060	1.3346710
O	1.2224710	-1.5620190	-0.3071070
O	-1.4205870	-1.2122340	0.7220080
H	0.5050680	-2.0484850	0.1173620
O	-2.3426980	0.2900380	-0.6666500
H	-3.1317400	-0.2263660	-0.4407460
H	-0.2479070	1.7503990	1.4255420
C	2.5238650	0.4218880	-0.2028810
H	2.5651170	1.4547350	0.1438520
H	3.3764300	-0.1287220	0.1989890
H	2.5970890	0.4116940	-1.2941580

Energy: -438.422948728

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B3LYP/6-311++G** geometry and energy of conformer: aThr-XI

N	0.1469390	1.8441480	-0.2188930
H	1.0444240	2.2507980	0.0186950
C	0.0351320	0.4793590	0.3014670
H	-0.0666100	0.4326210	1.4009690
C	-1.1978290	-0.2503050	-0.2873520
C	1.3115900	-0.2963660	0.0005650
H	-1.0387560	-0.3553120	-1.3687040
O	-1.3557960	-1.5292520	0.3169630
O	1.3707050	-1.4626870	-0.3127690
H	-0.5713950	-2.0479690	0.0936400
O	2.4222800	0.4552640	0.1637220
H	3.1873610	-0.1094880	-0.0254090
H	-0.5749010	2.4347970	0.1768420
C	-2.4894680	0.5163650	-0.0415430
H	-2.4908480	1.4749640	-0.5638340
H	-3.3296370	-0.0738430	-0.4114660
H	-2.6422690	0.6834710	1.0293620

Energy: -438.422264697

B3LYP/6-311++G** geometry and energy of conformer: aThr-XII

N	-0.0891570	1.7228900	0.2217640
H	0.3490020	1.6604070	1.1358180
C	-0.0683190	0.4272240	-0.4702970
H	-0.0849100	0.6348470	-1.5464650
C	1.1644080	-0.4688090	-0.1974050
C	-1.3859740	-0.3326680	-0.2056250
H	1.0185890	-1.3940950	-0.7617110
O	2.3541240	0.2023690	-0.6368980
O	-1.5480790	-1.4878790	-0.5032730
H	2.4512550	0.0833850	-1.5868230
O	-2.3423230	0.4190980	0.3532350
H	-1.9349630	1.3055260	0.4803420
H	0.4217430	2.4252430	-0.2994180
C	1.3607160	-0.8135510	1.2725730
H	0.4789450	-1.3142930	1.6782660
H	2.2164130	-1.4819000	1.3784580
H	1.5732560	0.0787700	1.8691920

Energy: -438.422230945

B3LYP/6-311++G** geometry and energy of conformer: aThr-XIII

N	0.1158580	1.9111030	0.0026970
H	1.0805230	2.1701190	-0.1850590
C	0.0641450	0.4990990	0.3560990
H	-0.0762030	0.3375390	1.4366790
C	-1.1334750	-0.1856550	-0.3450930
C	1.4228810	-0.1587480	0.0152710
H	-0.9381290	-0.2058440	-1.4241570
O	-1.1676360	-1.5454070	0.1603980

3	O	2.4008870	0.4959440	-0.2412560
4	H	-1.8436190	-2.0486490	-0.3050580
5	O	1.4683700	-1.4957880	0.0562940
6	H	0.5635150	-1.8470890	0.1931630
7	H	-0.2344520	2.4998300	0.7473510
8	C	-2.4552460	0.5147660	-0.0707120
9	H	-2.4264030	1.5341060	-0.4572570
10	H	-3.2774300	-0.0122920	-0.5647450
11	H	-2.6615990	0.5397900	1.0033220

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13 Energy: -438.422218686

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18 B3LYP/6-311++G** geometry and energy of conformer: aThr-XIV

19	N	0.7751260	-1.7248190	-0.4758970
20	H	0.3038300	-2.2180650	0.2770570
21	C	0.1719150	-0.3943200	-0.6706380
22	H	0.1789760	-0.1529840	-1.7376480
23	C	-1.2909930	-0.3575850	-0.1876570
24	C	1.0742560	0.6783180	-0.0042650
25	H	-1.2372330	-0.7751200	1.1853570
26	O	0.8024680	1.8510420	0.0140900
27	O	-2.1070570	-0.6731630	1.5834840
28	H	2.2102410	0.1884310	0.4995500
29	O	2.1805470	-0.7773710	0.3073910
30	H	0.7408280	-2.2929180	-1.3129930
31	H	-2.0291190	0.9633640	-0.3637190
32	C	-1.5644350	1.7582940	0.2168870
33	H	-2.0313080	1.2653700	-1.4147540
34	H	-3.0729760	0.8433870	-0.0537440
35	H	-1.8144520	-1.1323040	-0.7687000

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37 Energy: -438.422129382

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41 B3LYP/6-311++G** geometry and energy of conformer: aThr-XV

42	N	-0.3833390	1.9501280	-0.2376000
43	H	0.0990310	2.1654390	0.6307180
44	C	-0.1203530	0.5557770	-0.6070070
45	H	-0.3389180	0.4368510	-1.6703970
46	C	1.3293600	0.0862610	-0.3259530
47	C	-1.1302340	-0.2856700	0.1698980
48	H	1.9831030	0.7405290	-0.9123140
49	O	1.6866600	0.3380700	1.0309350
50	O	-0.9880250	-0.6435880	1.3188490
51	H	1.0558260	-0.1410600	1.5883970
52	O	-2.2269680	-0.5845690	-0.5492320
53	H	-2.8373550	-1.0631780	0.0338280
54	H	-0.0366960	2.5801960	-0.9520110
55	C	1.5882770	-1.3652690	-0.7310060
56	H	1.3713220	-1.5223760	-1.7923260
57	H	2.6363210	-1.6146280	-0.5545420
58	H	0.9750950	-2.0585680	-0.1481520

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60 Energy: -438.422021799

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B3LYP/6-311++G** geometry and energy of conformer: aThr-XVI

N	-0.4278870	1.9034380	-0.0420630
H	-0.0323130	2.6176180	-0.6469940
C	-0.1849850	0.5620140	-0.6134030
H	-0.3578330	0.5204760	-1.6948000
C	1.2850930	0.2017140	-0.3222380
C	-1.2172610	-0.4082460	0.0015880
H	1.9082510	0.9677570	-0.8042200
O	1.5089420	0.2606320	1.0997010
O	-2.2611460	-0.6424840	-0.5497270
H	1.2070720	1.1403910	1.3766870
O	-0.9146800	-0.9439810	1.1935370
H	-0.0204370	-0.6463270	1.4688160
H	-1.4222640	2.0964830	0.0275360
C	1.7123820	-1.1684240	-0.8211510
H	1.5809770	-1.2343430	-1.9041250
H	2.7658190	-1.3357760	-0.5906460
H	1.1296390	-1.9660320	-0.3546830

Energy: -438.421535885

B3LYP/6-311++G** geometry and energy of conformer: aThr-XVII

N	-0.2297340	1.9470650	-0.4745560
H	-1.1646910	2.2910160	-0.6614080
C	-0.1088510	0.5104460	-0.7039720
H	-0.2467870	0.3173010	-1.7706480
C	1.3174410	0.0555880	-0.3161510
C	-1.2106510	-0.2979920	-0.0140570
H	1.6468340	0.4338870	1.0201920
O	-2.1376670	-0.8320280	-0.5668760
O	1.0524110	-0.0328280	1.6211000
H	-1.0722580	-0.3295370	1.3460660
O	-1.8286000	-0.8212050	1.7019970
H	0.0360520	2.1838420	0.4755720
H	1.5644250	-1.4303980	-0.5677110
C	0.9216780	-2.0586030	0.0574810
H	1.3760510	-1.6899050	-1.6134420
H	2.6023200	-1.6734370	-0.3333070
H	1.9902490	0.6499230	-0.9391650

Energy: -438.421431774

B3LYP/6-311++G** geometry and energy of conformer: aThr-XVIII

N	0.1367420	1.9111710	-0.0195110
H	1.1092390	2.1729220	-0.1564180
C	0.0685810	0.5042900	0.3503230
H	-0.0690430	0.3585950	1.4360650
C	-1.1321920	-0.1829680	-0.3512630
C	1.4246690	-0.1664190	0.0236070

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3	H	-0.9404890	-0.2019300	-1.4268040
4	O	-1.2010840	-1.5780670	0.0407520
5	O	2.4198160	0.4811200	-0.1788630
6	H	-1.7302420	-1.6579050	0.8426370
7	O	1.4462850	-1.5042150	0.0141820
8	H	0.5319020	-1.8473900	0.1104770
9	H	-0.2606610	2.5112030	0.6918150
10	C	-2.4541690	0.5153590	-0.0788160
11	H	-2.4182110	1.5435650	-0.4396280
12	H	-3.2678850	-0.0044110	-0.5895460
13	H	-2.6732730	0.5348780	0.9963060

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15 Energy: -438.421364331

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18 B3LYP/6-311++G** geometry and energy of conformer: aThr-XIX

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20				
21	N	0.1671450	1.9561490	-0.1718390
22	H	-0.3723320	2.4885980	-0.8459240
23	C	0.0342680	0.5218640	-0.4094280
24	H	0.1674140	0.3279530	-1.4779020
25	C	1.1390660	-0.2372620	0.3747630
26	C	-1.3327830	-0.0205040	0.0104540
27	H	1.0692050	0.0804310	1.4194270
28	O	0.8723870	-1.6394320	0.4137580
29	O	-1.9223610	0.3189850	1.0059460
30	H	1.0153240	-2.0108990	-0.4642360
31	O	-1.8300440	-0.9182520	-0.8702630
32	H	-2.6680760	-1.2460920	-0.5079580
33	H	-0.1966740	2.1851100	0.7495690
34	C	2.5301180	0.0657240	-0.1669890
35	H	2.7120540	1.1411190	-0.1758400
36	H	3.2861900	-0.4228710	0.4511410
37	H	2.6330140	-0.3057310	-1.1937160

38 Energy: -438.421204845

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42 B3LYP/6-311++G** geometry and energy of conformer: aThr-XX

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44				
45	N	-0.4951630	1.8015490	-0.5771520
46	H	-1.5005070	1.9208360	-0.5652420
47	C	-0.0938610	0.3975930	-0.7380120
48	H	-0.0341500	0.0748980	-1.7856670
49	C	1.3288430	0.2623880	-0.1160000
50	C	-1.0782190	-0.5614060	-0.0851940
51	H	1.9502370	0.9697670	-0.6898680
52	O	1.2897060	0.6617970	1.2443070
53	O	-1.0718660	-1.7535550	-0.2596650
54	H	0.7689090	1.4788490	1.2666600
55	O	-1.9855560	0.0526560	0.7102510
56	H	-2.5499500	-0.6417760	1.0831530
57	H	-0.1096510	2.3741530	-1.3195130
58	C	1.9603920	-1.1157170	-0.2012190
59	H	2.0137860	-1.4552020	-1.2388610
60	H	2.9742960	-1.0679840	0.2013200
	H	1.3919620	-1.8487140	0.3714800

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3 Energy: -438.421165644
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8 B3LYP/6-311++G** geometry and energy of conformer: aThr-XXI
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10	N	0.1550590	1.9403860	-0.1050090
11	H	-0.1862400	2.1358790	0.8323630
12	C	0.0300920	0.5121720	-0.3937590
13	H	0.1395260	0.3546680	-1.4686200
14	C	1.1462050	-0.2640180	0.3308230
15	C	-1.3260100	-0.0425950	0.0496940
16	H	1.0597460	-0.0335880	1.4019900
17	O	0.8543870	-1.6499770	0.1152550
18	O	-1.7922750	0.1196250	1.1517150
19	H	1.4723300	-2.1816090	0.6258860
20	O	-1.9773990	-0.6946550	-0.9352320
21	H	-2.8111690	-1.0219750	-0.5629610
22	H	-0.3995170	2.4908820	-0.7513510
23	C	2.5351150	0.1079310	-0.1713640
24	H	2.7059130	1.1797390	-0.0606470
25	H	3.3028570	-0.4255870	0.3979590
26	H	2.6410210	-0.1620040	-1.2258180

27 Energy: -438.421106779
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31 B3LYP/6-311++G** geometry and energy of conformer: aThr-XXII
32

33	N	-0.1124730	1.9266840	0.2569850
34	H	0.2871330	2.2110180	-0.6328570
35	C	-0.0008280	0.4857490	0.4222260
36	H	-0.1516610	0.2316800	1.4761780
37	C	-1.1208590	-0.2676600	-0.3698590
38	C	1.3827810	-0.0286220	0.0087170
39	H	-0.8929340	-0.1798850	-1.4443190
40	O	-1.1885150	-1.6423510	-0.0013230
41	O	2.2193330	0.6104530	-0.5747550
42	H	-0.3046750	-2.0272800	-0.0214280
43	O	1.5837780	-1.3349320	0.3472720
44	H	2.4655530	-1.5860110	0.0292480
45	H	0.4189510	2.4093410	0.9731870
46	C	-2.4987920	0.3171920	-0.1027020
47	H	-2.5527210	1.3587760	-0.4145730
48	H	-3.2416440	-0.2685830	-0.6482270
49	H	-2.7312760	0.2588410	0.9640520

50 Energy: -438.420944975
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54 B3LYP/6-311++G** geometry and energy of conformer: aThr-XXIII
55

56	N	0.2097500	1.8057310	-0.1676450
57	H	-0.1877190	1.9895030	0.7473180
58	C	-0.0217050	0.4297000	-0.5665910
59	H	-0.0423750	0.3713030	-1.6627930
60	C	1.0714630	-0.5912140	-0.1048360
	C	-1.3885330	-0.0185340	-0.0863530

3	H	0.8179830	-1.5692990	-0.5311040
4	O	2.3414320	-0.1580460	-0.6080570
5	O	-2.0218220	0.4941680	0.8010970
6	H	2.3556710	-0.2694490	-1.5647710
7	O	-1.8192840	-1.1148880	-0.7564950
8	H	-2.6757500	-1.3657910	-0.3780900
9	H	1.2041230	2.0049380	-0.1519620
10	C	1.2175380	-0.7105330	1.4035170
11	H	0.2901000	-1.0572990	1.8651450
12	H	2.0103750	-1.4227020	1.6383170
13	H	1.4841610	0.2522940	1.8446700

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15 Energy: -438.420921096

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18 B3LYP/6-311++G** geometry and energy of conformer: aThr-XXIV

21	N	0.1990200	1.8121770	-0.1094000
22	H	-0.0969370	1.9402520	0.8520420
23	C	-0.0254920	0.4496320	-0.5552190
24	H	-0.0384780	0.4320180	-1.6496890
25	C	1.0619570	-0.5854300	-0.1404790
26	C	-1.3873510	-0.0188260	-0.0773540
27	H	0.7965950	-1.5458740	-0.5997710
28	O	2.2631170	-0.0846300	-0.7432940
29	O	-1.9996800	0.4452380	0.8507490
30	H	3.0049420	-0.6274440	-0.4584330
31	O	-1.8409650	-1.0700160	-0.8016230
32	H	-2.6942080	-1.3324490	-0.4236850
33	H	1.1788750	2.0541600	-0.2034550
34	C	1.2265880	-0.7611090	1.3655920
35	H	0.3140480	-1.1509200	1.8243920
36	H	2.0303000	-1.4732070	1.5779370
37	H	1.4777290	0.1878860	1.8445600

38 Energy: -438.420610844

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42 B3LYP/6-311++G** geometry and energy of conformer: aThr-XXV

44	N	-0.4745510	1.8888600	-0.6668210
45	H	-1.4168640	2.0321000	-1.0150590
46	C	-0.1301400	0.4754950	-0.6909840
47	H	-0.0994220	0.1369900	-1.7320910
48	C	1.2921290	0.3057560	-0.1151160
49	C	-1.1695020	-0.4010630	0.0256040
50	H	1.8751290	1.1052930	-0.5880990
51	O	1.1728320	0.5732660	1.2899320
52	O	-2.0872870	0.0115050	0.6851070
53	H	2.0524420	0.6290890	1.6756320
54	O	-0.9826770	-1.7251040	-0.2105640
55	H	-1.6814210	-2.1990930	0.2661420
56	H	-0.4726320	2.2125680	0.2965460
57	C	1.9707380	-1.0336830	-0.3836690
58	H	2.0305040	-1.2273890	-1.4585670
59	H	2.9942500	-1.0100430	0.0035800
60	H	1.4375730	-1.8579010	0.0888570

Energy: -438.420378965

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B3LYP/6-311++G** geometry and energy of conformer: aThr-XXVI

N	0.0887170	1.9404360	-0.0629900
H	-0.2379260	2.0886900	0.8869430
C	0.0336140	0.5214450	-0.4163080
H	0.2125200	0.4306330	-1.4915170
C	1.1372430	-0.2562770	0.3405290
C	-1.3295100	-0.1267800	-0.1737220
H	1.0236740	-0.0437440	1.4074880
O	0.9161160	-1.6640930	0.2365470
O	-2.0014580	-0.6751930	-1.0101430
H	1.1071550	-1.9473310	-0.6650710
O	-1.7329290	0.0184780	1.1132790
H	-2.5901200	-0.4245240	1.2001590
H	-0.4926990	2.4971170	-0.6798450
C	2.5341780	0.1403610	-0.1199130
H	2.6788990	1.2173480	-0.0225360
H	3.2868710	-0.3791250	0.4766970
H	2.6836240	-0.1281460	-1.1723670

Energy: -438.420301515

B3LYP/6-311++G** geometry and energy of conformer: aThr-XXVII

N	-0.4172310	1.9407700	-0.3528340
H	-1.3701950	2.2039770	-0.5807030
C	-0.1808790	0.5244910	-0.6504790
H	-0.3368820	0.3808760	-1.7214120
C	1.2818920	0.1802810	-0.3464240
C	-1.2141740	-0.3997820	0.0365090
H	1.4519820	0.3756870	1.0808940
O	-2.1888990	-0.8069270	-0.5405590
O	2.3609360	0.1864730	1.3342520
H	-1.0161220	-0.6692430	1.3442660
O	-0.1426900	-0.3276460	1.6174500
H	-0.2576260	2.1417040	0.6291120
H	1.6835560	-1.2282340	-0.7682420
C	1.0838090	-1.9874950	-0.2602630
H	1.5568450	-1.3519850	-1.8469030
H	2.7369220	-1.4126970	-0.5373430
H	1.8914410	0.9247320	-0.8693310

Energy: -438.420126348

B3LYP/6-311++G** geometry and energy of conformer: aThr-XXVIII

N	-0.5144560	1.8248030	-0.7228020
H	-1.4408890	1.9395570	-1.1185240
C	-0.1054560	0.4275490	-0.7351730
H	-0.0198210	0.0957020	-1.7742600
C	1.3022030	0.3183490	-0.1116580
C	-1.0649660	-0.5732320	-0.0738850
H	1.8849730	1.1113040	-0.5963420

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3	O	1.1318040	0.6382860	1.2780800
4	O	-1.0225550	-1.7682450	-0.2405790
5	H	1.9964390	0.6806790	1.6977850
6	O	-1.9973410	0.0164320	0.7073200
7	H	-2.5336540	-0.6951690	1.0888480
8	H	-0.5510850	2.1618520	0.2341760
9	C	2.0019510	-1.0219300	-0.3051960
10	H	2.1223060	-1.2434640	-1.3693650
11	H	3.0017860	-0.9830390	0.1391880
12	H	1.4434870	-1.8372360	0.1550320

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14 Energy: -438.420018140

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20 B3LYP/6-311++G** geometry and energy of conformer: aThr-XXIX

21				
22	N	-0.1258460	1.8768710	0.4103310
23	H	0.0314360	1.8188730	1.4113610
24	C	-0.0035910	0.5654980	-0.2310840
25	H	0.0665930	0.7241820	-1.3105750
26	C	1.1991630	-0.2900310	0.2319350
27	C	-1.3158530	-0.1751890	0.0280230
28	H	1.1205820	-1.6094120	-0.3085740
29	O	-1.4808860	-1.0060490	0.8933250
30	O	0.4097550	-2.0716860	0.1513400
31	H	-2.2973900	0.2098530	-0.8056690
32	O	-3.1038680	-0.2611650	-0.5448450
33	H	0.5214780	2.5489040	0.0186760
34	H	2.5281470	0.2965230	-0.2208460
35	C	2.5798800	0.3181260	-1.3132690
36	H	2.6695400	1.3107310	0.1597720
37	H	3.3488580	-0.3230060	0.1447600
38	H	1.1716070	-0.3389880	1.3296390

39 Energy: -438.419984225

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44 B3LYP/6-311++G** geometry and energy of conformer: aThr-XXX

45				
46	N	0.0477930	1.5981070	0.5746330
47	H	0.8722460	2.1447190	0.3490730
48	C	-0.0617450	0.4958820	-0.3780540
49	H	-0.1086820	0.8409760	-1.4271680
50	C	1.1718400	-0.4194810	-0.2993050
51	C	-1.3509030	-0.2878550	-0.1895800
52	H	1.0273360	-1.2291190	-1.0223220
53	O	2.2548640	0.4228160	-0.7334320
54	O	-1.4893290	-1.4708730	-0.3761380
55	H	3.0831680	-0.0481420	-0.6010470
56	O	-2.3840620	0.5175210	0.1551120
57	H	-3.1735050	-0.0406490	0.2218220
58	H	-0.7642060	2.2023480	0.5284480
59	C	1.4352580	-1.0080070	1.0825850
60	H	0.6238320	-1.6785760	1.3737700
	H	2.3572920	-1.5986940	1.0677820
	H	1.5294880	-0.2185520	1.8289980

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4 Energy: -438.419941615
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8 B3LYP/6-311++G** geometry and energy of conformer: aThr-XXXI
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10	N	-0.3052320	1.9290640	-0.5005250
11	H	0.1379480	2.2130500	0.3683950
12	C	-0.0947260	0.4972240	-0.7206240
13	H	-0.2339910	0.2850160	-1.7821520
14	C	1.3133770	-0.0116770	-0.3003430
15	C	-1.2194190	-0.2614730	-0.0213480
16	H	1.6539340	0.4276080	1.0138540
17	O	-2.0771670	-0.9103930	-0.5575160
18	O	1.0160210	0.0513170	1.6339930
19	H	-1.1475590	-0.1346010	1.3363190
20	O	-1.9092500	-0.6022540	1.7124760
21	H	0.1098300	2.4682540	-1.2519740
22	H	1.4903940	-1.5200550	-0.4659720
23	C	0.8187460	-2.0784130	0.1938850
24	H	1.2839880	-1.8306120	-1.4944110
25	H	2.5157040	-1.8011390	-0.2182450
26	H	2.0262000	0.5062990	-0.9498330

27 Energy: -438.419904230
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31 B3LYP/6-311++G** geometry and energy of conformer: aThr-XXXII
32

33	N	-0.1348270	1.8943190	-0.3262450
34	H	-0.3958050	2.1844250	0.6095700
35	C	-0.0198280	0.4499580	-0.4489730
36	H	0.1762220	0.2069170	-1.4994800
37	C	1.1238500	-0.2519510	0.3686660
38	C	-1.3260640	-0.2462220	-0.0989990
39	H	1.2907520	-1.5990110	-0.0492780
40	O	-1.5120590	-1.4352860	-0.2515410
41	O	0.4167930	-2.0117900	-0.1108110
42	H	-2.2485220	0.5532210	0.4654220
43	O	-3.0121870	-0.0033860	0.6841060
44	H	0.7305920	2.3530170	-0.5817000
45	H	2.4702810	0.4329770	0.1815850
46	C	2.7303930	0.4884720	-0.8797340
47	H	2.4790300	1.4371630	0.6096270
48	H	3.2379760	-0.1572890	0.6853330
49	H	0.8499770	-0.2177290	1.4363040

50 Energy: -438.419864927
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54 B3LYP/6-311++G** geometry and energy of conformer: aThr-XXXIII
55

56	N	0.0612960	1.9199590	0.0596680
57	H	-0.5237330	2.5057250	-0.5257170
58	C	0.0230810	0.5245530	-0.3868390
59	H	0.1846600	0.5018460	-1.4663370
60	C	1.1445070	-0.2785990	0.2921160
	C	-1.3435420	-0.1215370	-0.1573620

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3	H	1.0164970	-0.1844400	1.3794190
4	O	0.9238850	-1.6384850	-0.0987170
5	O	-2.1223130	-0.4405040	-1.0181120
6	H	1.5735750	-2.1986630	0.3364330
7	O	-1.6338280	-0.2267200	1.1674310
8	H	-2.5189140	-0.6144210	1.2359780
9	H	-0.2699320	2.0056060	1.0156980
10	C	2.5309680	0.2096420	-0.1093870
11	H	2.6493000	1.2665930	0.1343580
12	H	3.3043430	-0.3556000	0.4203630
13	H	2.6830920	0.0749670	-1.1838470

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15 Energy: -438.419811685

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18 B3LYP/6-311++G** geometry and energy of conformer: aThr-XXXIV

19				
20				
21	N	-0.6448760	1.9569030	-0.2472940
22	H	-0.5704360	2.1156960	0.7545320
23	C	-0.1743860	0.6129430	-0.5547100
24	H	-0.1209950	0.5096420	-1.6468550
25	C	1.2596240	0.4331690	0.0098610
26	C	-1.1687240	-0.4652200	-0.0974780
27	H	1.7203470	1.4180010	-0.0918210
28	O	1.2216850	0.2025040	1.4228810
29	O	-2.3225770	-0.2591350	0.1752450
30	H	1.0162370	-0.7280950	1.5705310
31	O	-0.6356100	-1.7167280	-0.0589770
32	H	-1.3510490	-2.3221640	0.1918660
33	H	-1.6287320	2.0486750	-0.4805640
34	C	2.1288870	-0.5878960	-0.7192000
35	H	2.2131930	-0.3334940	-1.7796160
36	H	3.1324820	-0.5795700	-0.2882040
37	H	1.7227020	-1.5981190	-0.6428360

38 Energy: -438.419695990

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42 B3LYP/6-311++G** geometry and energy of conformer: aThr-XXXV

43				
44				
45	N	0.2133880	1.7984030	-0.3404260
46	H	-0.6538950	2.3132400	-0.2297770
47	C	0.0565040	0.4767580	0.2802730
48	H	-0.0212200	0.5235880	1.3792060
49	C	-1.2142400	-0.1981100	-0.2500480
50	C	1.3125890	-0.3212510	-0.0505270
51	H	-1.1040960	-0.3228410	-1.3331430
52	O	-2.2628370	0.7503790	0.0208560
53	O	1.3903590	-1.3095740	-0.7336400
54	H	-3.0729330	0.4417280	-0.3956850
55	O	2.3978170	0.2487970	0.5305000
56	H	3.1752800	-0.2585800	0.2519930
57	H	0.9595990	2.3170680	0.1091730
58	C	-1.5165090	-1.5392990	0.4107240
59	H	-0.7351570	-2.2682510	0.1928850
60	H	-1.6126560	-1.4207290	1.4936500
	H	-2.4613990	-1.9394590	0.0304180

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3 Energy: -438.419617424
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9 B3LYP/6-311++G** geometry and energy of conformer: aThr-XXXVI
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11	N	0.0060310	1.9204190	-0.3972340
12	H	-0.3972190	2.2598230	0.4691130
13	C	-0.0043250	0.4697090	-0.4622250
14	H	0.1367670	0.1495630	-1.5006730
15	C	1.0886270	-0.2882070	0.3760060
16	C	-1.3772290	0.0039820	-0.0057660
17	H	1.1615230	-1.6620820	0.0040770
18	O	-2.1460760	0.6382080	0.6669170
19	O	0.2711930	-2.0314760	-0.0354510
20	H	-1.6380220	-1.2782110	-0.3905070
21	O	-2.5032850	-1.5190060	-0.0238140
22	H	0.9343880	2.3023950	-0.5178670
23	H	2.4838910	0.2797370	0.1560930
24	C	2.7351940	0.2861890	-0.9085530
25	H	2.5813390	1.2900190	0.5580100
26	H	3.2066110	-0.3572820	0.6693910
27	H	0.8276130	-0.1978110	1.4419290

28 Energy: -438.419573259
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32 B3LYP/6-311++G** geometry and energy of conformer: aThr-XXXVII
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34	N	0.1817750	1.7319630	0.2297290
35	H	0.9841720	2.2181860	-0.1500650
36	C	-0.0361020	0.4763910	-0.4628620
37	H	-0.0680270	0.5775130	-1.5652790
38	C	1.1139560	-0.5229720	-0.1627380
39	C	-1.4121240	-0.0648180	-0.1094900
40	H	2.3445890	0.0380510	-0.6489190
41	O	-2.2824670	0.5535140	0.4471650
42	O	2.3840390	-0.0777720	-1.6036950
43	H	-1.5867790	-1.3357460	-0.5504920
44	O	-2.4943410	-1.5926570	-0.3275180
45	H	-0.6376870	2.3262340	0.1978920
46	H	1.3023010	-0.8084660	1.3182760
47	C	1.5112110	0.1144630	1.8591870
48	H	0.4025380	-1.2619310	1.7424290
49	H	2.1352430	-1.5007960	1.4536870
50	H	0.8994980	-1.4543410	-0.6958870

51 Energy: -438.419386885
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55 B3LYP/6-311++G** geometry and energy of conformer: aThr-XXXVIII
56

57	N	0.1217280	1.7894370	-0.0965360
58	H	1.0897940	2.0825130	-0.1844600
59	C	-0.0137230	0.4224880	-0.5752420
60	H	0.0346880	0.4389510	-1.6702090
	C	1.1079810	-0.5690870	-0.1167500

3	C	-1.3696230	-0.1852730	-0.2634130
4	H	0.9047870	-1.5375830	-0.5885290
5	O	2.3731940	-0.0642630	-0.5614340
6	O	-1.8262880	-1.1420120	-0.8392560
7	H	2.4433800	-0.1874710	-1.5140110
8	O	-2.0050560	0.4161360	0.7684730
9	H	-2.8430940	-0.0525380	0.9016740
10	H	-0.1513670	1.8747930	0.8758690
11	C	1.2096440	-0.7435270	1.3898780
12	H	0.2820100	-1.1456050	1.8041870
13	H	2.0206390	-1.4350610	1.6241060
14	H	1.4265890	0.2094520	1.8780310

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16 Energy: -438.419206946

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21 B3LYP/6-311++G** geometry and energy of conformer: aThr-XXXIX

22	N	0.6360290	-1.7147460	-0.6782690
23	H	1.4463640	-1.8474740	-1.2763470
24	C	0.1260780	-0.3333750	-0.7607010
25	H	0.0483420	0.0412720	-1.7873440
26	C	-1.2941420	-0.2942860	-0.1382370
27	C	1.0890680	0.6146040	-0.0253170
28	H	-1.8892340	-1.0277730	-0.7077490
29	O	-1.2724610	-0.6689130	1.2366920
30	O	1.1258660	1.7964580	-0.2380460
31	H	-0.8513700	-1.5317270	1.3203570
32	O	1.8895720	0.0227330	0.8783280
33	H	1.6793740	-0.9296760	0.8684910
34	H	-0.0663670	-2.3808020	-0.9872310
35	C	-1.9738470	1.0612120	-0.2317380
36	H	-2.0510870	1.3850840	-1.2722620
37	H	-2.9788360	0.9866720	0.1874840
38	H	-1.4161520	1.8164850	0.3226510

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40 Energy: -438.419197138

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45 B3LYP/6-311++G** geometry and energy of conformer: aThr-XL

46	N	0.1168490	1.7942960	0.0305650
47	H	-0.1079050	1.8038380	1.0187390
48	C	-0.0144460	0.4664790	-0.5483330
49	H	0.0381530	0.5659550	-1.6365240
50	C	1.1046640	-0.5515510	-0.1812790
51	C	-1.3662090	-0.1692940	-0.2703360
52	H	0.9100480	-1.4657550	-0.7549530
53	O	2.3070470	0.0692350	-0.6551790
54	O	-1.8177810	-1.0967290	-0.8952930
55	H	3.0578080	-0.4868000	-0.4249410
56	O	-2.0079600	0.3747400	0.7895210
57	H	-2.8461970	-0.1013870	0.8906260
58	H	1.0697760	2.1205210	-0.0912600
59	C	1.1972990	-0.8853830	1.3042570
60	H	0.2884630	-1.3805060	1.6571220
	H	2.0312690	-1.5700360	1.4875330

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H	1.3623510	0.0146320	1.9014630
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Energy: -438.418891187

B3LYP/6-311++G** geometry and energy of conformer: aThr-XLI

N	0.0599990	1.6321440	0.4792430
H	0.9234720	2.1254710	0.2785740
C	-0.0533750	0.4791110	-0.4031710
H	-0.0900630	0.7569020	-1.4755980
C	1.1745770	-0.4496830	-0.2451280
C	-1.3555570	-0.2821510	-0.1975960
H	1.0260490	-1.3100550	-0.9041150
O	2.3498320	0.2770920	-0.6461600
O	-1.5193740	-1.4517870	-0.4420200
H	2.3899740	0.2997880	-1.6076230
O	-2.3600550	0.5185600	0.2276090
H	-3.1559630	-0.0307380	0.2945600
H	-0.7192330	2.2694230	0.3682110
C	1.4075370	-0.9328440	1.1778130
H	0.5521680	-1.5134410	1.5296060
H	2.2928790	-1.5708260	1.2032070
H	1.5583990	-0.0890520	1.8515290

Energy: -438.418624880

B3LYP/6-311++G** geometry and energy of conformer: aThr-XLII

N	0.0268110	1.9494890	-0.2850380
H	-0.2374930	2.2114810	0.6597180
C	0.0267550	0.4973090	-0.4321480
H	0.1437040	0.2536750	-1.4934780
C	1.1205680	-0.2629990	0.3724790
C	-1.3393300	0.0003810	0.0239950
H	0.8883830	-1.6729650	0.3388900
O	-1.8727140	0.3438790	1.0484700
O	0.9854550	-1.9875030	-0.5674330
H	-1.8924150	-0.8746120	-0.8413710
O	-2.7314450	-1.1706370	-0.4549520
H	0.9310490	2.3511810	-0.5002150
H	2.5329310	0.0747600	-0.0974310
C	2.6678520	-0.1911870	-1.1522650
H	2.7585780	1.1382450	0.0163480
H	3.2597610	-0.4868530	0.4926240
H	1.0032910	0.0080470	1.4256370

Energy: -438.418486184

B3LYP/6-311++G** geometry and energy of conformer: aThr-XLIII

N	0.0038330	1.9340960	-0.1693510
H	-0.1052730	2.1421130	0.8183050
C	0.0164960	0.4920620	-0.4034210
H	0.1032880	0.3117130	-1.4771620
C	1.1320070	-0.2967860	0.3174960

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3	C	-1.3357000	-0.0332250	0.0705410
4	H	0.8920210	-1.6714830	-0.0092250
5	O	-1.7271390	0.0617790	1.2081790
6	O	1.4432230	-2.2300600	0.5473130
7	H	-2.0625820	-0.5888090	-0.9163210
8	O	-2.8983930	-0.8871390	-0.5249990
9	H	0.8461640	2.3795070	-0.5120130
10	H	2.5341250	0.1330920	-0.1030470
11	C	2.6693560	0.0023930	-1.1804340
12	H	2.7294670	1.1766100	0.1577870
13	H	3.2865490	-0.4737720	0.4092930
14	H	0.9988180	-0.1427950	1.3968810

Energy: -438.418452566

B3LYP/6-311++G** geometry and energy of conformer: aThr-XLIV

21				
22	N	-0.0455280	1.9367630	-0.2061400
23	H	-0.1887880	2.1425040	0.7771550
24	C	0.0279720	0.4957670	-0.4449290
25	H	0.2048410	0.3408670	-1.5135940
26	C	1.1194150	-0.2669840	0.3558420
27	C	-1.3398130	-0.1187500	-0.1701290
28	H	0.9247230	-1.6792590	0.2607830
29	O	-1.9807270	-0.7765840	-0.9468330
30	O	1.0125110	-1.9529650	-0.6598550
31	H	-1.7642920	0.1654240	1.0848540
32	O	-2.6297530	-0.2544270	1.2012160
33	H	0.7927250	2.4100440	-0.5211210
34	H	2.5318920	0.1310990	-0.0642680
35	C	2.6996560	-0.0866540	-1.1251800
36	H	2.7172770	1.1962070	0.0980560
37	H	3.2627540	-0.4312410	0.5199490
38	H	0.9730420	-0.0451220	1.4168360

Energy: -438.417538525

B3LYP/6-311++G** geometry and energy of conformer: aThr-XLV

46	N	-0.6382970	1.7886960	-0.7431980
47	H	-0.7408820	2.1275400	0.2080560
48	C	-0.1061070	0.4312490	-0.7415080
49	H	-0.0134340	0.0964850	-1.7783520
50	C	1.3005580	0.2887740	-0.0976160
51	C	-1.0849280	-0.5438160	-0.0922730
52	H	1.9208620	1.0546230	-0.5880870
53	O	1.1418100	0.6256430	1.2843090
54	O	-1.1027660	-1.7297610	-0.3195450
55	H	1.9968640	0.5695110	1.7218240
56	O	-1.9215600	0.0416350	0.7856700
57	H	-2.4746650	-0.6596180	1.1615800
58	H	-0.0023670	2.4133430	-1.2283760
59	C	1.9619610	-1.0732440	-0.2838870
60	H	2.0671760	-1.3097660	-1.3464370
	H	2.9656270	-1.0643190	0.1539500
	H	1.3801280	-1.8665770	0.1864610

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4 Energy: -438.417432710
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10 B3LYP/6-311++G** geometry and energy of conformer: aThr-XLVI
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12	N	0.3558960	1.7481230	0.0362010
13	H	-0.0559220	1.8589370	0.9588270
14	C	-0.0207130	0.4567710	-0.5268660
15	H	-0.0252070	0.5493140	-1.6183380
16	C	1.0893950	-0.5881020	-0.1870610
17	C	-1.4060030	-0.0177110	-0.0714990
18	H	0.9037100	-1.5047740	-0.7576010
19	O	2.3221510	-0.0845930	-0.6723440
20	O	-2.0295290	0.4930570	0.8171010
21	H	2.3587660	0.8394380	-0.3793170
22	O	-1.9064660	-1.1004470	-0.7217200
23	H	-1.3048720	-1.3941080	-1.4177220
24	H	0.0037790	2.5097580	-0.5319310
25	C	1.1636080	-0.9330210	1.2999660
26	H	0.2425560	-1.4046050	1.6544690
27	H	1.9917210	-1.6242730	1.4657910
28	H	1.3472270	-0.0383170	1.9008780

29 Energy: -438.417185763
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34 B3LYP/6-311++G** geometry and energy of conformer: aThr-XLVII
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36	N	-0.5905490	1.8438300	-0.7329650
37	H	-0.8834180	2.1235550	0.1980120
38	C	-0.1223480	0.4652020	-0.7113660
39	H	-0.0746820	0.0882300	-1.7383740
40	C	1.2938100	0.2717370	-0.1001210
41	C	-1.1690060	-0.3646570	0.0264360
42	H	1.1808860	0.5692470	1.2926410
43	O	-1.9747600	0.0660140	0.8067460
44	O	2.0513210	0.5128730	1.6987630
45	H	-1.0983430	-1.6800000	-0.3012260
46	O	-1.7768140	-2.1359900	0.2200050
47	H	0.1469160	2.4699440	-1.0370480
48	H	1.9292480	-1.0949150	-0.3447810
49	C	1.3617000	-1.8910660	0.1372870
50	H	1.9860430	-1.3103150	-1.4156160
51	H	2.9509190	-1.1062770	0.0483960
52	H	1.9193640	1.0359460	-0.5869620

53 Energy: -438.417177495
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58 B3LYP/6-311++G** geometry and energy of conformer: aThr-XLVIII
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60	N	-0.0648050	1.9323990	0.2208920
	H	-0.0269270	1.9234190	1.2349290

3	C	0.0275030	0.5807890	-0.3372480
4	H	0.1865160	0.6668680	-1.4138140
5	C	1.1458060	-0.3054290	0.2715670
6	C	-1.3512130	-0.0559220	-0.1865640
7	H	0.9984870	-1.6694720	-0.1353060
8	O	-2.1636270	-0.2075310	-1.0569210
9	O	0.2961250	-2.0745960	0.3840540
10	H	-1.5844570	-0.4332680	1.1053300
11	O	-2.4959840	-0.7607670	1.1480070
12	H	0.6713660	2.5330950	-0.1284930
13	H	2.5295940	0.1412120	-0.1763030
14	C	2.6314650	0.0208920	-1.2584160
15	H	2.7122450	1.1871550	0.0812380
16	H	3.2942640	-0.4689350	0.3075700
17	H	1.0712010	-0.2356560	1.3651460

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19 Energy: -438.417071201

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22 B3LYP/6-311++G** geometry and energy of conformer: aThr-XLIX

24	N	-0.0573360	1.9225070	-0.1069100
25	H	-0.1259560	2.0790760	0.8931060
26	C	0.0163750	0.4972920	-0.4275210
27	H	0.1735790	0.3930810	-1.5028890
28	C	1.1212660	-0.2918920	0.3096250
29	C	-1.3570770	-0.1096890	-0.1534670
30	H	0.9221590	-1.6610010	-0.0564140
31	O	-2.1050290	-0.5680630	-0.9733170
32	O	1.5250330	-2.2151420	0.4488010
33	H	-1.6675240	-0.0366070	1.1687650
34	O	-2.5577230	-0.4040030	1.2742000
35	H	0.7406910	2.4308070	-0.4674840
36	H	2.5251150	0.1819250	-0.0562920
37	C	2.6978170	0.0751120	-1.1309000
38	H	2.6827040	1.2255780	0.2283650
39	H	3.2776150	-0.4132740	0.4698370
40	H	0.9566620	-0.1692270	1.3889920

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42 Energy: -438.416792961

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45 B3LYP/6-311++G** geometry and energy of conformer: aThr-L

48	N	0.1681890	1.7389080	-0.4087770
49	H	-0.4670730	2.2836560	-0.9801700
50	C	-0.0183250	0.3166690	-0.6232220
51	H	0.0232430	0.1278760	-1.7014860
52	C	1.1238950	-0.5400840	0.0105050
53	C	-1.3612990	-0.2869570	-0.1916390
54	H	2.3754000	-0.2792130	-0.6131070
55	O	-1.7794660	-1.3524310	-0.5726170
56	O	2.3071610	-0.4628690	-1.5555890
57	H	-2.0420730	0.4891780	0.6869710
58	O	-2.8582770	0.0158620	0.9101380
59	H	0.0031160	1.9980240	0.5568850
60	H	1.3212950	-0.2806720	1.4973230
	C	1.6503850	0.7473300	1.6645180
	H	0.4017900	-0.4605400	2.0601140

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H	2.0955880	-0.9464180	1.8822380
H	0.8424620	-1.5892830	-0.1429900

Energy: -438.416002766

B3LYP/6-311++G** geometry and energy of conformer: aThr-LI

N	-0.4560830	1.9232240	-0.4195430
H	-0.0743350	2.5146910	-1.1486670
C	-0.1693930	0.5109420	-0.6809320
H	-0.3422960	0.3238740	-1.7414970
C	1.2783350	0.0870220	-0.3536270
C	-1.2305370	-0.3431150	0.0476840
H	1.9435510	0.7268180	-0.9478900
O	1.4748170	0.4067580	1.0449650
O	-2.1378670	-0.8814370	-0.5249900
H	2.3408970	0.1030740	1.3346580
O	-1.0965050	-0.4355490	1.3889240
H	-0.2345730	-0.0674850	1.6562560
H	-0.0666300	2.2230240	0.4678870
C	1.5766320	-1.3796060	-0.6436350
H	1.4160620	-1.5979870	-1.7027930
H	2.6199920	-1.6165270	-0.4133000
H	0.9361220	-2.0416730	-0.0559820

Energy: -438.415697217

B3LYP/6-311++G** geometry and energy of conformer: aThr-LII

N	-0.2979340	1.9441450	-0.3811970
H	0.0942490	2.1728720	0.5277890
C	-0.1508270	0.5101330	-0.6290640
H	-0.3525630	0.3234100	-1.6918950
C	1.3162650	0.1055450	-0.3531960
C	-1.1205130	-0.3235350	0.2277120
H	1.9279550	0.7585170	-0.9814000
O	1.6861590	0.4300130	0.9827340
O	-0.9345540	-0.5919700	1.3879190
H	1.0864580	-0.0488240	1.5743480
O	-2.2725120	-0.7198690	-0.3717610
H	-2.2686220	-0.4742800	-1.3051620
H	-1.2642520	2.2512050	-0.4060160
C	1.6117010	-1.3540960	-0.6952410
H	1.3870720	-1.5669010	-1.7453540
H	2.6702320	-1.5586640	-0.5259420
H	1.0325060	-2.0400250	-0.0703890

Energy: -438.414409825

B3LYP/6-311++G** geometry and energy of conformer: aThr-LIII

N	0.5394600	-1.8236570	-0.5196840
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1				
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3	H	0.4118430	-2.3605190	-1.3680470
4	C	0.1611350	-0.4202560	-0.6876790
5	H	0.1784950	-0.1003080	-1.7412270
6	C	-1.3059190	-0.2835430	-0.1720660
7	C	1.1936210	0.4484110	0.0494620
8	H	-1.8875840	-0.9407390	-0.8379870
9	O	-1.3868380	-0.7562970	1.1572120
10	O	2.1188490	-0.0057680	0.6638590
11	H	-0.8840930	-1.5861340	1.1705140
12	O	1.0537080	1.7886960	-0.0702220
13	H	0.2583350	2.0123770	-0.5684950
14	H	1.5029830	-1.8991330	-0.2092090
15	C	-1.9329870	1.1031540	-0.2153180
16	H	-1.8497330	1.5512310	-1.2123310
17	H	-2.9963540	1.0247820	0.0174550
18	H	-1.4909690	1.7644020	0.5339260

19 Energy: -438.414281429

22 B3LYP/6-311++G** geometry and energy of conformer: aThr-LIV

23				
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25	N	-0.0934140	1.8185110	0.2926450
26	H	0.6845720	2.3803730	-0.0353470
27	C	-0.0316840	0.4675200	-0.2871040
28	H	0.0127810	0.4783690	-1.3887170
29	C	1.1790620	-0.3289850	0.2294800
30	C	-1.3327980	-0.2359620	0.1019890
31	H	1.2319270	-1.5877900	-0.4488490
32	O	-1.4953010	-0.9951190	1.0165000
33	O	1.5452990	-1.4406870	-1.3484610
34	H	-2.3468760	0.1597710	-0.7149890
35	O	-3.1552870	-0.2728330	-0.3998630
36	H	-0.9433590	2.2895320	-0.0009310
37	H	2.4979840	0.4264400	0.0950950
38	C	2.6826290	0.7297590	-0.9433290
39	H	2.5158020	1.3183490	0.7256610
40	H	3.3190670	-0.2211660	0.4088390
41	H	0.9990120	-0.5802510	1.2755700

42 Energy: -438.414211330

45 B3LYP/6-311++G** geometry and energy of conformer: aThr-LV

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50	N	-0.0923170	1.8388530	-0.2240380
51	H	0.8207470	2.2769010	-0.2565260
52	C	-0.0218520	0.3933800	-0.4971070
53	H	0.1557640	0.1408860	-1.5480230
54	C	1.1102880	-0.2356270	0.3467480
55	C	-1.3810100	-0.2270470	-0.1137440
56	H	0.9043260	-0.0126470	1.4031930
57	O	1.0351990	-1.6385910	0.1179510
58	O	-1.8921470	-1.1424330	-0.6924800
59	H	1.6033460	-2.0901710	0.7493330
60	O	-1.9577400	0.3666120	0.9554630
	H	-1.4366080	1.1719080	1.1410890
	H	-0.6724690	2.3090970	-0.9120520

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3 C 2.4955590 0.2991870 -0.0238290
4 H 2.6161300 1.3599430 0.2147990
5 H 3.2610040 -0.2371380 0.5443170
6 H 2.6935770 0.1451840 -1.0877450
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8 Energy: -438.413909974
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13 B3LYP/6-311++G** geometry and energy of conformer: aThr-LVI
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15 N 0.1729360 1.7808940 -0.3190110
16 H -0.1492230 2.0212350 0.6123840
17 C -0.0473200 0.3758020 -0.5961410
18 H -0.0604460 0.2377720 -1.6856410
19 C 1.0541530 -0.5936370 -0.0716840
20 C -1.4054020 -0.0412950 -0.0324290
21 H 0.7876970 -1.6145550 -0.3836120
22 O 2.2361770 -0.1855790 -0.7714420
23 O -1.9178260 0.4719350 0.9223430
24 H 2.9960320 -0.6414570 -0.3955780
25 O -2.0036750 -1.0956010 -0.6453870
26 H -1.5187030 -1.3450850 -1.4419360
27 H 1.1538670 2.0152080 -0.4209140
28 C 1.2539400 -0.5679710 1.4391650
29 H 0.3533960 -0.8935370 1.9648400
30 H 2.0656970 -1.2453640 1.7228090
31 H 1.5114930 0.4361020 1.7831400

32 Energy: -438.412120899
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38 B3LYP/6-311++G** geometry and energy of conformer: aThr-LVII
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40 N 0.3187900 1.8028530 0.0479700
41 H 0.2347370 2.0148230 -0.9421430
42 C 0.0863860 0.3767240 0.3284250
43 H 0.0081170 0.2881340 1.4198600
44 C -1.1840750 -0.2861280 -0.2709520
45 C 1.3763100 -0.3932440 -0.0498570
46 H -1.4879220 -1.4850970 0.4383800
47 O 1.4049640 -1.5229490 -0.4474460
48 O -1.8601000 -1.2515310 1.2965290
49 H 2.4967130 0.3364110 0.1289710
50 O 2.2022850 1.2482470 0.3237080
51 H -0.3268040 2.4008250 0.5494660
52 H -2.3957220 0.6454340 -0.2982260
53 C -2.6382200 1.0142000 0.7063690
54 H -2.2422650 1.5106050 -0.9474620
55 H -3.2603660 0.0938760 -0.6722290
56 H -0.9563540 -0.6227880 -1.2854760

57 Energy: -438.411872601
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B3LYP/6-311++G** geometry and energy of conformer: aThr-LVIII

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4	N	0.1622800	1.7398730	0.1035560
5	H	0.8193760	2.2900240	-0.4335420
6	C	-0.0540160	0.4392940	-0.5003720
7	H	-0.0736930	0.4729250	-1.6041720
8	C	1.1037230	-0.5236600	-0.1359360
9	C	-1.4291930	-0.0925400	-0.0858390
10	H	0.9084890	-1.5088040	-0.5911920
11	O	2.2508610	0.0400490	-0.7792000
12	O	-2.2322270	0.5438120	0.5362560
13	H	3.0457870	-0.3302960	-0.3830050
14	O	-1.7368060	-1.3475970	-0.5053510
15	H	-1.0086010	-1.7303140	-1.0106480
16	H	-0.7114600	2.2396760	0.2188030
17	C	1.3065140	-0.6989760	1.3636670
18	H	0.4368250	-1.1783430	1.8219340
19	H	2.1728230	-1.3399780	1.5571890
20	H	1.4577120	0.2711820	1.8369870

21 Energy: -438.411382946

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26 B3LYP/6-311++G** geometry and energy of conformer: aThr-LIX

27				
28	N	0.1973060	1.7887000	-0.2515890
29	H	1.1914510	1.9822820	-0.1999410
30	C	-0.0368080	0.3990620	-0.5867150
31	H	-0.0593550	0.2998290	-1.6846470
32	C	1.0682930	-0.5915500	-0.0867830
33	C	-1.4052840	-0.0297820	-0.0568320
34	H	0.8413830	-1.5927830	-0.4816400
35	O	2.3363210	-0.1588570	-0.5915340
36	O	-1.9621120	0.4999990	0.8629960
37	H	2.3523150	-0.2609410	-1.5494010
38	O	-1.9620990	-1.1124610	-0.6601480
39	H	-1.4422440	-1.3824920	-1.4272010
40	H	-0.2448420	2.0204360	0.6319530
41	C	1.2003810	-0.6689530	1.4251930
42	H	0.2825670	-1.0420120	1.8838310
43	H	2.0197630	-1.3417300	1.6834780
44	H	1.4214510	0.3144000	1.8449920

45 Energy: -438.411204130

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51 B3LYP/6-311++G** geometry and energy of conformer: aThr-LX

52				
53	N	0.4476980	-1.8422390	-0.7662680
54	H	0.4102800	-2.2193410	0.1767970
55	C	0.1474640	-0.4219790	-0.7118200
56	H	0.1492820	-0.0324680	-1.7381650
57	C	-1.2908200	-0.2531880	-0.1713180
58	C	1.1956130	0.3852110	0.0929830
59	H	-1.8953740	-0.9336160	-0.7828860
60	O	-1.2598720	-0.7201940	1.1801800
	O	2.0018680	-0.1101330	0.8252640

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H	-2.1598880	-0.8630190	1.4884840
O	1.2010270	1.7343570	-0.1082910
H	0.5199690	1.9896720	-0.7417690
H	1.3947240	-1.9923400	-1.0985030
C	-1.8785310	1.1552450	-0.2574070
H	-1.8406980	1.5406040	-1.2824830
H	-2.9321750	1.1360300	0.0345710
H	-1.3665430	1.8461750	0.4159890

12 Energy: -438.410386298
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20 B3LYP/6-311++G** geometry and energy of conformer: aThr-LXI

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N	0.5523640	-1.8025000	-0.8192360
H	0.8770620	-2.1110980	0.0925610
C	0.1388480	-0.4117870	-0.7332690
H	0.1348320	0.0165200	-1.7454910
C	-1.2959780	-0.2029840	-0.1695720
C	1.1934550	0.3352170	0.1003260
H	-1.9453450	-0.8242550	-0.8063220
O	-1.2955280	-0.7162050	1.1586600
O	1.8658200	-0.1818210	0.9430890
H	-2.1850160	-0.6604060	1.5213530
O	1.3289090	1.6643680	-0.1620710
H	0.7757050	1.9216400	-0.9089900
H	-0.2219160	-2.3958690	-1.0968940
C	-1.8086660	1.2366410	-0.2205050
H	-1.7638380	1.6379600	-1.2389030
H	-2.8573770	1.2745120	0.0886210
H	-1.2402100	1.8852450	0.4494140

39 Energy: -438.407171053
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