

SUPPORTING INFORMATION

Two-photon absorption of dipolar and quadrupolar oligothiophene-cored chromophores derivatives containing terminal dimesitylboryl moieties: A theoretical (DFT) structure-property investigation.

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Dedicated to a long-time friend, collaborator, and leading expert on conjugated materials and their optical properties, Prof. Todd B. Marder, on the occasion of his 66th birthday.

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Computational details

All the structures were fully optimized at the PBE1PBE^{1, 2} -GD3BJ^{3,4} / 6-31G* level of theory, using the Gaussian09⁵ package. During all the calculations, the solvent effects, in our case acetonitrile, were taken into account by means of the Polarizable Continuum Model (PCM)⁶. Frequency calculations have been performed to confirm that the optimized geometry is at a minimum on the potential energy surface (zero imaginary frequencies).

Using previously optimized geometries, 2PA and one-photon absorption (OPA) calculations have been carried out employing the Amsterdam Density Functional (ADF2019) suite of programs⁷.

These properties have been calculated using the SAOP model potential^{8,9} (statistical average of orbital model exchange-correlation potential) using the damped cubic response theory module of Lasse Jensen *and Coll.*¹⁰ implemented in the ADF program package.

The lifetime of the electronic excited states is included in the theory using a damping parameter of 0.0034 au (~ 0.1 eV ~ 800 cm⁻¹) value which was found suitable for 2PA computations^{11,12}.

The 2PA cross-section σ^{2PA} has been obtained from the imaginary part of the third-order hyperpolarizability γ using the following expressions^{13, 14}:

$$(1) \quad \sigma^{TPA} = \frac{N\pi^3 \alpha^2 \hbar^3 \omega^2}{15e^4} \gamma^{TPA}$$

$$(2) \quad \gamma^{TPA} = \sum_{\alpha\beta} (\text{Im}\gamma_{\alpha\alpha\beta\beta} + \text{Im}\gamma_{\alpha\beta\beta\alpha} + \text{Im}\gamma_{\alpha\beta\alpha\beta})$$

Where α is the fine structure constant (not to be confused with the α index of the summation in eq 2), e is the elementary charge, ω is the photon energy, \hbar is the reduced Planck's constant whereas the integer value $N=4$ is used for all simulated 2PA spectra¹⁴. The σ^{2PA} value is usually given in Göppert-Mayer units (1 GM = 10⁻⁵⁰ cm⁴ s photon⁻¹)¹⁵. We first evaluate σ^{2PA} in atomic units and then multiply it by (0.529177 \times 10⁻⁸ cm/a.u.)⁴ \times (2.418884 \times 10⁻¹⁷ s/a.u.) to obtain its value in the conventional units (cm⁴ s photon⁻¹).

References

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Table S1. SAOP/DZP Frontier MO energies. SAOP/DZP and PBE0/6-31G(d) calculated HOMO-LUMO gaps

Cpds	HOMO	LUMO	LUMO+1	Gap SAOP/DZP	Gap PBE0/6-31G(d)
2V	-9.47	-7.68	-7.02	1.79	3.09
2VD	-9.78	-7.21	-5.78	2.57	4.14
3V	-9.31	-7.66	-7.19	1.65	2.90
4V	-9.20	-7.63	-7.28	1.57	2.78
4VD	-9.43	-7.31	-6.24	2.12	3.48
5V	-9.12	-7.60	-7.34	1.52	2.69
2T	-9.63	-7.85	-7.14	1.78	3.16
2TD	-9.85	-7.28	-5.93	2.57	4.08
3T	-9.44	-7.73	-7.27	1.71	2.94
4T	-9.29	-7.69	-7.34	1.60	2.78
4TD	-9.53	-7.37	-6.39	2.16	3.48
5T	-9.20	-7.67	-7.40	1.53	2.67

2TM-H	-9.17	-7.14	-6.98	2.03	3.46
2TM-NH₂	-8.82	-6.80	-6.52	2.02	3.43
2TM-CN	-9.74	-7.98	-7.90	1.76	3.16
2TM(NMe₃⁺)	-14.61	-13.30	-13.22	1.31	3.07
5M-H	-9.19	-7.83	-7.21	1.36	2.58
5M-CN	-9.58	-8.34	-8.03	1.24	2.53
5M(NMe₃⁺)	-14.01	-13.08	-13.00	0.93	2.45

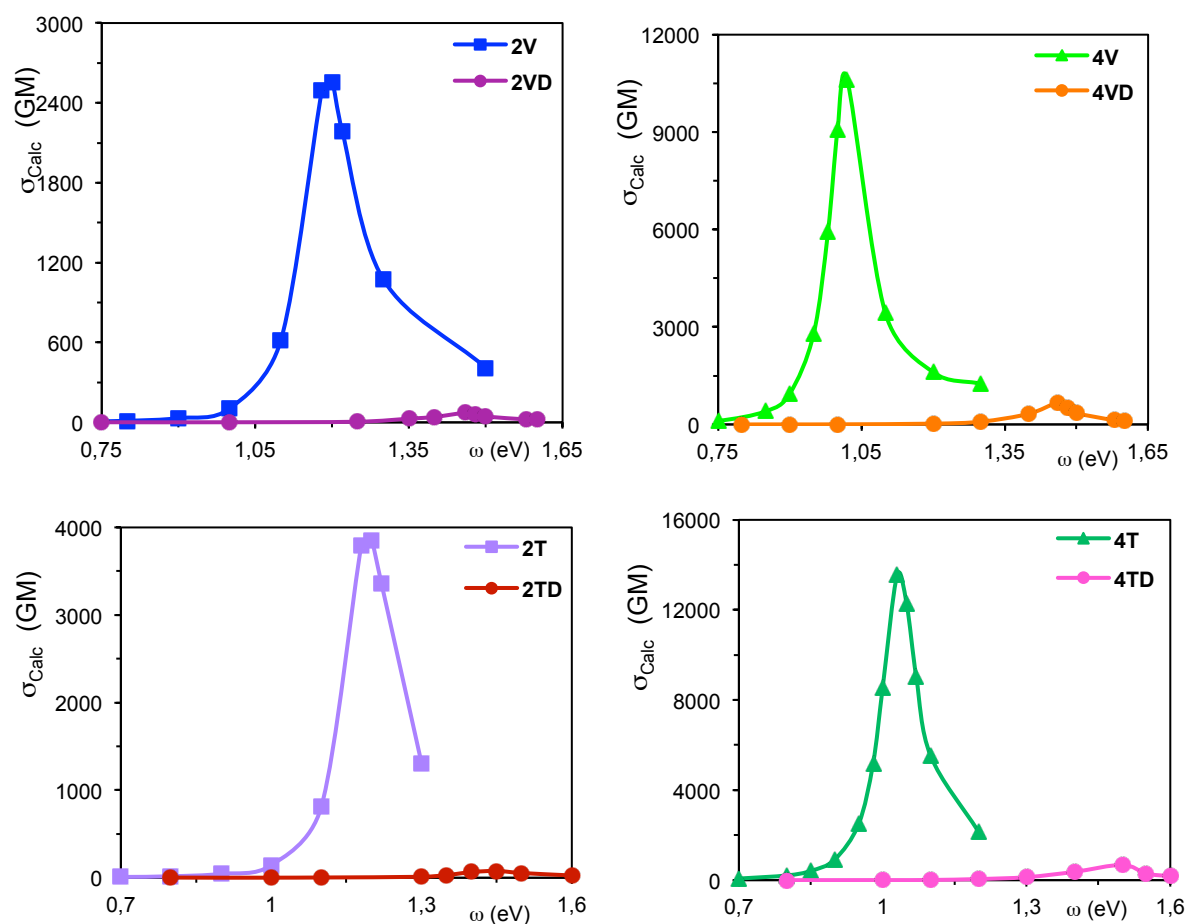


Figure S1: 2PA simulated spectra for 2T, 2TD and 4T, 4TD.

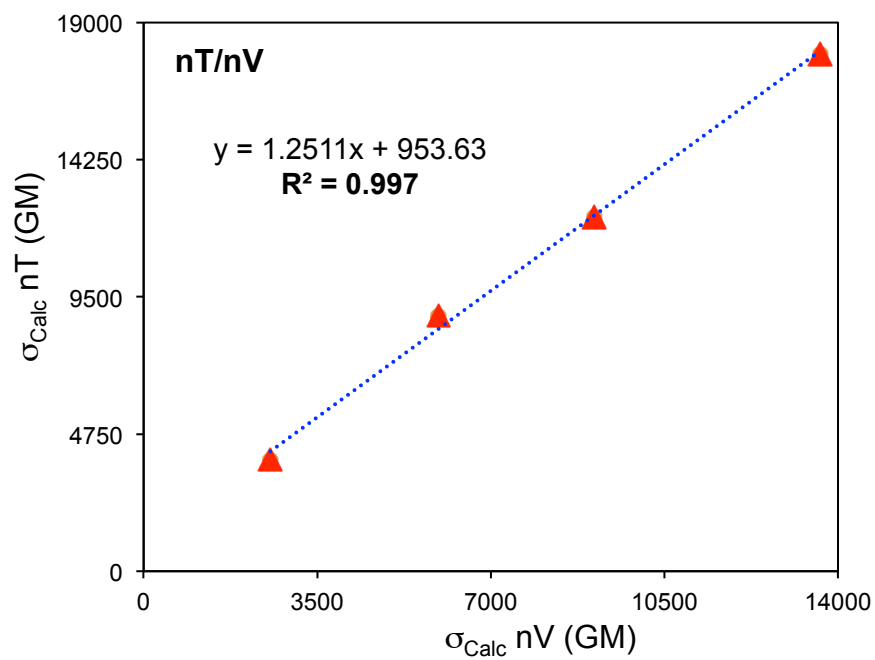


Figure S2: linear regression between the nT and nV 2PA cross-sections

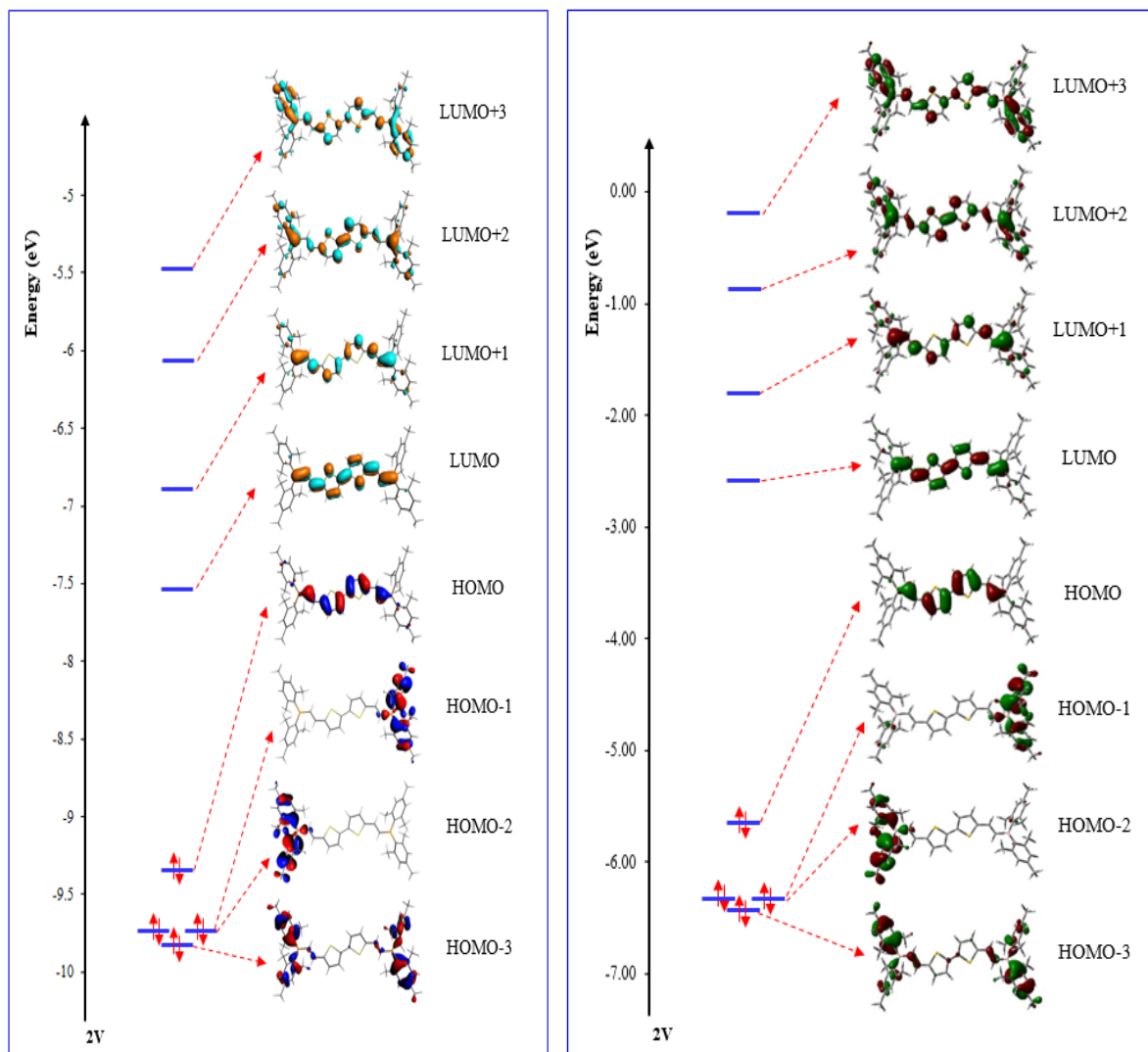


Figure S3: SAOP/DZP (left) and PBE0/6-31G(d) (right) frontier MOs of 2V.

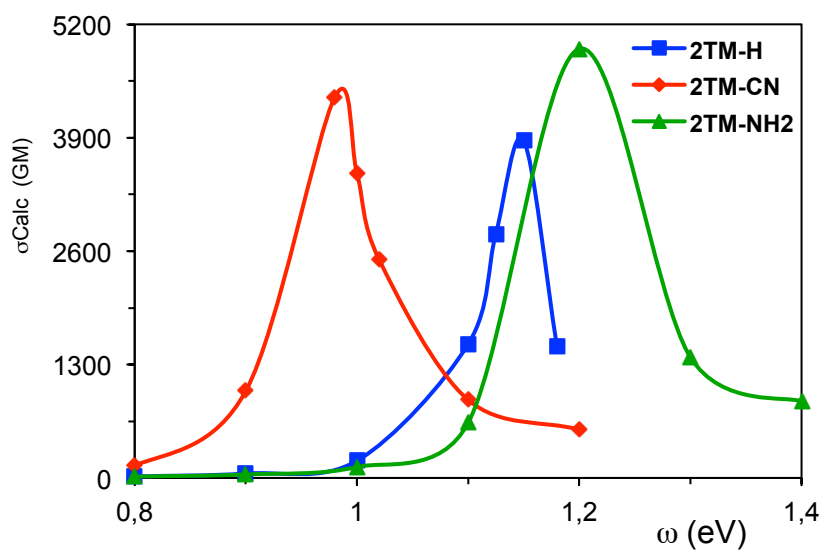
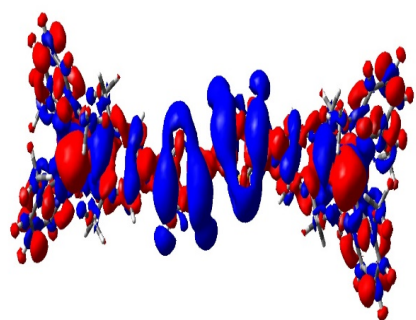
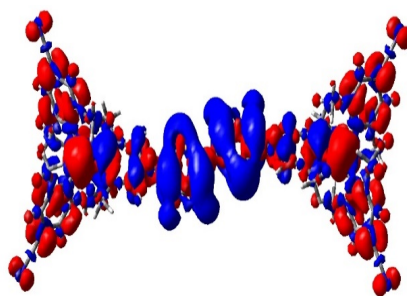


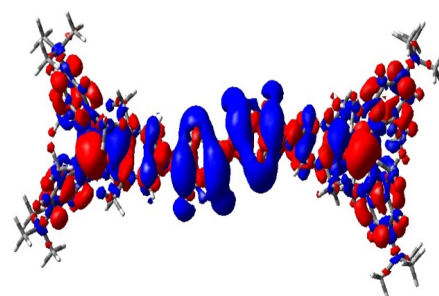
Figure S4: simulated 2PA spectra of 2TM-X (X=H, NH₂, CN)



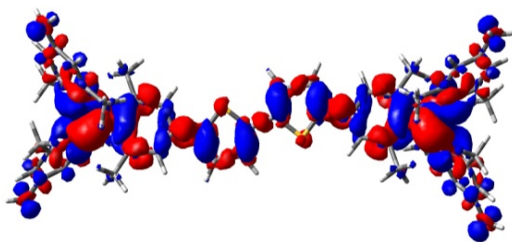
2TM-H
 $q^{\text{CT}} = 0.93 \text{ e}$; $d^{\text{CT}} = 0.24 \text{ \AA}$
 $\Delta\mu_{\text{S2-S0}} = 1.08 \text{ D}$



2TM-CN
 $q^{\text{CT}} = 1.00 \text{ e}$; $d^{\text{CT}} = 0.27 \text{ \AA}$
 $\Delta\mu_{\text{S2-S0}} = 1.33 \text{ D}$



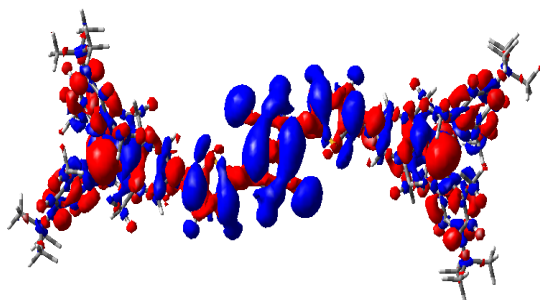
2TM(NMe₃⁺)
 $q^{\text{CT}} = 1.00 \text{ e}$; $d^{\text{CT}} = 0.35 \text{ \AA}$
 $\Delta\mu_{\text{S2-S0}} = 1.70 \text{ D}$



2TM-NH₂

S₄-S₀: $q^{\text{CT}} = 0.58 e$; $d^{\text{CT}} = 0.20 \text{ \AA}$

$\Delta\mu_{\text{S}_4\text{-S}_0} = 0.55 \text{ D}$



5M-NMe₃⁺

$q^{\text{CT}} = 1.112 e$, $d^{\text{CT}} = 0.135 \text{ \AA}$,

$\Delta\mu_{\text{S}_2\text{-S}_0} = 0.72 \text{ D}$

Figure S5: Density differences plots between **S₂-S₀** states (red=increase, blue=decrease of electron density; isovalue 0.03 au) . q^{CT} and d^{CT} are respectively the amount of transferred charge and the distance between the barycenters of the positive and negative charges. $\Delta\mu_{\text{S}_2\text{-S}_0}$ is the difference in Debye between the dipole moments in the S2 and S0 states. PBE0/6-31G(d) calculation.

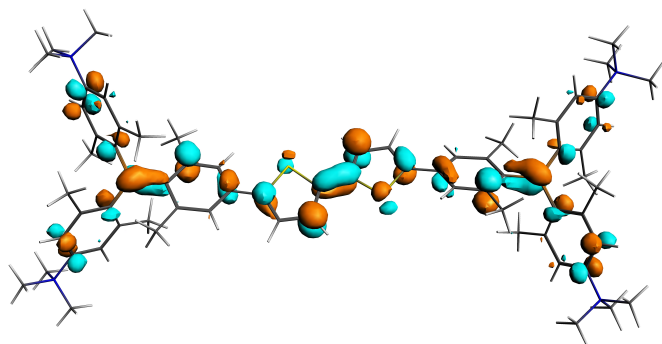


Figure S6: LUMO+10 of the 2TM(NMe₃⁺) compound.

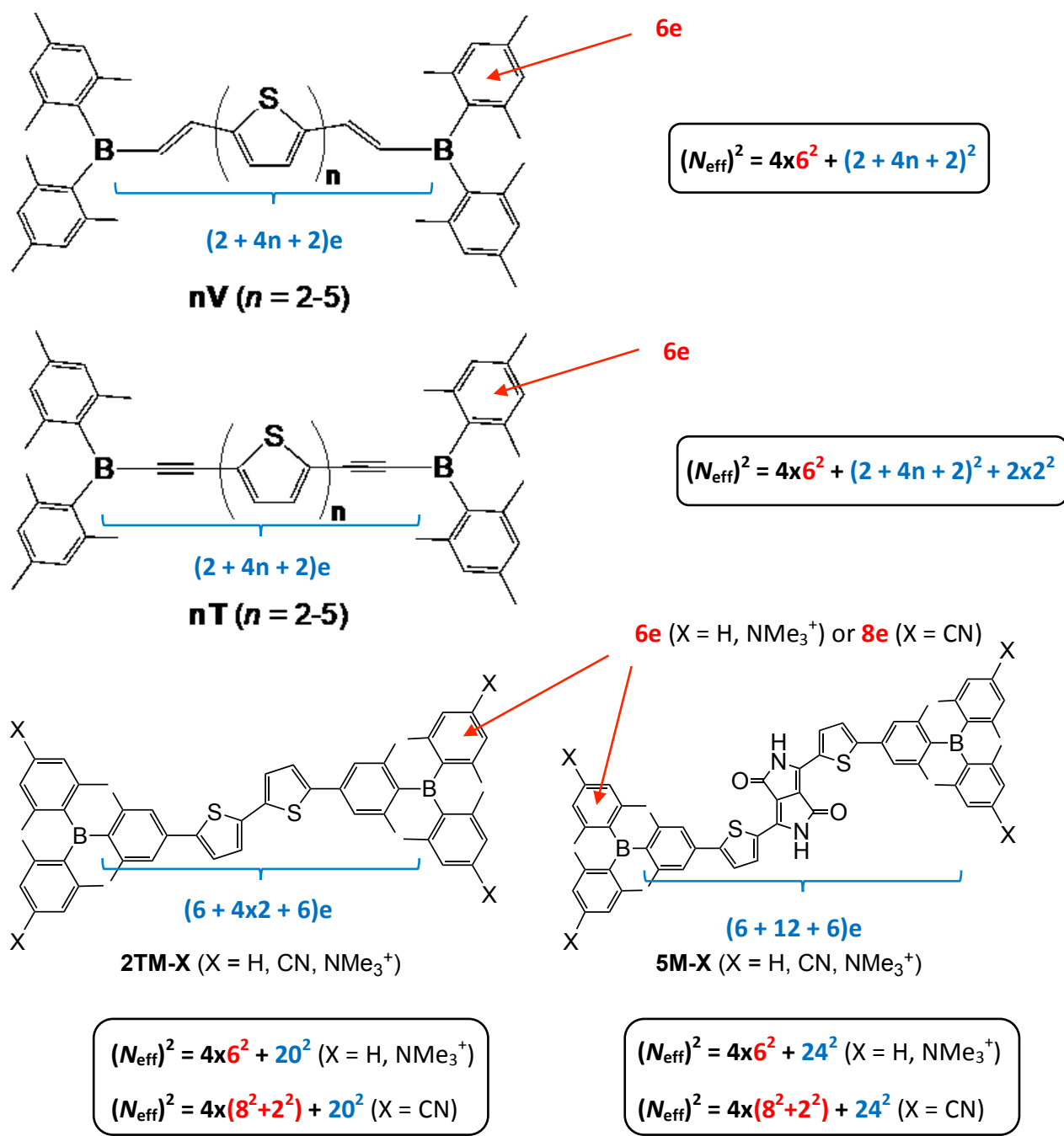
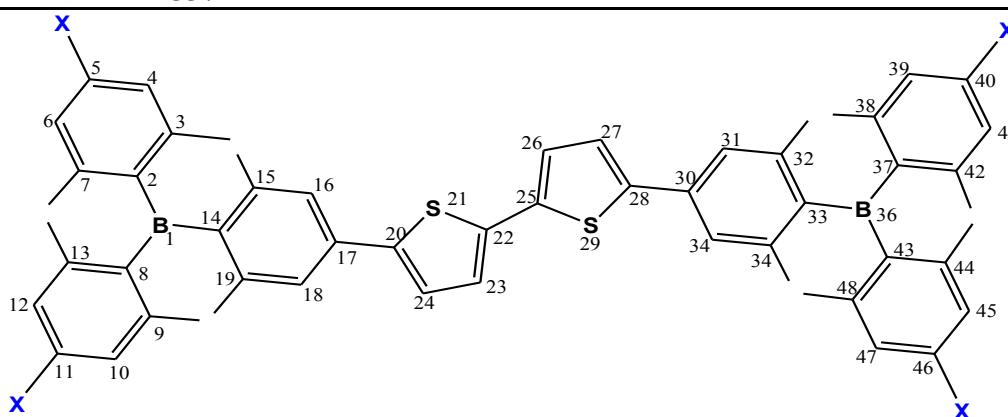


Figure S7: Derivation of the number of effective electrons (N_{eff}) for the various

Table S2. Selected calculated optimized structural parameters for compounds **2M-X**.

		2TM-H	2TM-CN	2TM(NMe₃⁺)
Bond lengths (Å)	B1-C14	1.57	1.57	1.56
	C17-C20	1.46	1.46	1.46
	C22-C25	1.45	1.45	1.44
	C28-C30	1.46	1.46	1.46
	C33-B36	1.57	1.57	1.56
Bond angles (°)	C17-C20-S21	121.26	121.30	121.20
	S21-C22-C25	120.71	120.70	120.68
	C22-C25-S29	128.72	120.75	120.77
	C30-C28-S29	121.27	121.32	121.28
Torsion angles (°)	C2-B1-C14-C15	-49.10	-46.93	-46.00
	C16-C17-C20-S21	24.86	23.91	16.80
	S21-C22-C25-S29	164.57	164.72	165.54
	C27-C28-C30-S31	-23.97	-23.27	-21.00
	C32-C33-B36-C37	49.32	46.94	45.03

**Table S3:** Computed 2PA-cross section values normalized by the number of effective electrons (N_{eff}).

Cmpd	N_{eff}^a	$(\sigma^{2\text{PA}})_{\text{max}}^b$ (GM)	$(\sigma^{2\text{PA}})_{\text{max}}/(N_{\text{eff}})^2{}^c$ (GM)
2V	16.97	2556.00	8.88
2T	17.20	3857.00	13.04
2TM-NH₂	23.32	4919.00	9.05
2TM-H	23.32	2967.00	5.46
2TM-CN	25.92	4365.00	6.50
2TM-NMe₃⁺	23.32	6269.00	11.53
5M-H	26.83	9423.00	13.09
5M-CN	29.12	9096.00	10.73
5M-NMe₃⁺	26.83	7482.00	10.39

^a Number of effective electrons.¹ ^b Computed 2PA cross-section. ^c Normalized 2PA cross-section.²

Table S4: Optimized Cartesian coordinates, PBE0/6-31G(d) calculations (acetonitrile solvent)

2V

C	0.63623972	-0.33892974	-0.01534021
C	0.89457969	-1.65736985	-0.34240024
H	0.11192960	-2.38672987	-0.52236025
C	2.26895978	-1.94977993	-0.41223024
H	2.67143978	-2.92782001	-0.65348026
C	3.08079989	-0.86502987	-0.13844022
S	2.11786987	0.54468027	0.20486981
B	6.86527019	0.10590005	0.08515980
C	7.72693035	1.42263011	0.06487980
C	9.26602053	3.81803024	0.03703979
C	7.36738034	2.51358022	-0.76291027
C	8.88791042	1.55665008	0.86903986
C	9.61631052	2.74479014	0.85703986
C	8.14236048	3.67543027	-0.77204027
H	10.49019060	2.83404012	1.50059991
H	7.85758046	4.49360035	-1.43200032
C	7.52321018	-1.32621008	0.00814979
C	8.70677019	-3.89845033	-0.18662022
C	8.29836024	-1.68405014	-1.11906029
C	7.35255015	-2.27858015	1.03290987
C	7.95390014	-3.53579027	0.92695986
C	8.86437023	-2.95425026	-1.20376030
H	7.83155012	-4.24961032	1.74061993
H	9.45121029	-3.21454031	-2.08361037
C	-0.63815035	0.30932036	0.14424980
C	-0.89710032	1.61381047	0.52283983
S	-2.11891050	-0.55533965	-0.14606022
H	-0.11513023	2.32897049	0.75524985
C	-2.27133041	1.90963055	0.57983984
C	-3.08235052	0.84181050	0.24409981
H	-2.67434040	2.87749064	0.85838986
B	-6.86617085	-0.09674942	-0.10156022
C	-7.73228097	-1.40840949	-0.17971022
C	-7.51994082	1.33152072	0.04859979
C	-7.39595099	-2.54811959	0.59074984
C	-8.87654104	-1.48778945	-1.01386029
C	-8.31447088	1.62434077	1.18134988
C	-7.32582077	2.34372078	-0.91239028
C	-8.17586110	-3.70379965	0.51520983
C	-9.61058117	-2.67066951	-1.08704029
C	-8.87542088	2.89029089	1.33361989
C	-7.92219078	3.59615090	-0.74002027
C	-9.27900119	-3.79420961	-0.32961023
H	-7.91329108	-4.55828972	1.13726988
H	-10.47551122	-2.71453948	-1.74714034

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C	-8.69373084	3.89445095	0.37963982
H	-9.47722093	3.09972093	2.21695996
H	-7.78074075	4.35788096	-1.50574032
C	-6.50725072	2.12115074	-2.16058037
H	-5.47895063	2.48139072	-2.03221036
H	-6.43730074	1.06518065	-2.43500040
H	-6.93861072	2.66517079	-3.00759044
C	-8.55889097	0.58791070	2.24775996
H	-9.12371101	-0.26472934	1.85565993
H	-7.61941090	0.18772063	2.64763000
H	-9.12088097	1.01264075	3.08513003
C	-9.34042105	-0.32742934	-1.85721035
H	-9.69762104	0.50134074	-1.23751030
H	-8.54028097	0.07283066	-2.48803040
H	-10.15878112	-0.63599933	-2.51488040
C	-6.22932090	-2.57275964	1.54831991
H	-5.30333083	-2.88004970	1.04652987
H	-6.03623084	-1.59924957	2.00586994
H	-6.41174095	-3.29402968	2.35147997
C	6.17625025	2.48030026	-1.68949034
H	5.97719022	1.48202019	-2.08730037
H	5.26172020	2.81087032	-1.18152030
H	6.33371027	3.15664030	-2.53586040
C	9.37156043	0.45260998	1.77466993
H	8.58545032	0.09134998	2.44543998
H	9.71867044	-0.41278010	1.20103988
H	10.20211047	0.80322997	2.39494998
C	8.51722033	-0.71377008	-2.25127038
H	7.56848024	-0.33945001	-2.65428041
H	9.08829037	0.16155997	-1.92352036
H	9.06232031	-1.18771014	-3.07328045
C	6.55462013	-1.98386010	2.27952997
H	6.49369013	-0.91409001	2.49696998
H	5.52274000	-2.34466008	2.18671996
H	6.99674010	-2.48310015	3.14824003
C	-9.30158081	5.25560108	0.56906983
H	-8.72527075	5.84802112	1.29105989
H	-9.32709081	5.81620111	-0.37030024
H	-10.32420087	5.18665112	0.95544986
C	-10.07866131	-5.06122967	-0.43436024
H	-11.14141136	-4.85155962	-0.59373025
H	-9.73904127	-5.66981973	-1.28227031
H	-9.97882128	-5.67327971	0.46730983
C	10.09473067	5.07043030	0.00857979
H	11.00249075	4.92734025	-0.59128025
H	9.54066066	5.90709038	-0.42754024
H	10.41763071	5.35815031	1.01473987
C	9.31836018	-5.26609045	-0.30332023
H	8.71430012	-5.91422046	-0.95104028
H	10.32099025	-5.21984050	-0.74168026
H	9.39276017	-5.75539050	0.67264984
C	-4.51701063	0.83562056	0.20367981
H	-4.97499062	1.78086065	0.49765983
C	-5.32510071	-0.19760949	-0.14257022
H	-4.84606073	-1.13855958	-0.42294024
C	4.51597999	-0.85103993	-0.12456022

H	4.97341999	-1.80799002	-0.37894024
C	5.32485009	0.20218012	0.15261980
H	4.84627010	1.15446021	0.39256982

2VD

C	5.52275500	-2.19688200	-0.12133400
C	5.83143700	-0.91057000	0.23316500
S	3.83189600	-2.42070500	-0.33625800
H	6.84410500	-0.56874000	0.41471200
C	4.68196500	-0.08938100	0.33454900
C	3.50528200	-0.75423800	0.05381100
H	4.70287400	0.96165100	0.60360000
B	-0.35464500	-0.12018400	-0.12182400
C	-1.67374000	-0.98012500	-0.13410900
C	-0.38504500	1.45142700	0.02363100
C	-1.78478400	-2.14912300	0.65727700
C	-2.79106900	-0.60742300	-0.92374300
C	-0.94528000	2.03966200	1.18154500
C	0.14377600	2.30053600	-0.96865700
C	-2.96357200	-2.89750600	0.64581300
C	-3.93871700	-1.39894700	-0.93376400
C	-0.95753200	3.42500900	1.32636900
C	0.09470500	3.68771600	-0.80193400
C	-4.04890500	-2.55057400	-0.15443800
H	-3.03524400	-3.77748700	1.28347100
H	-4.77844400	-1.10220100	-1.56033100
C	-0.44370700	4.27164600	0.34106800
H	-1.38547700	3.85893900	2.22910900
H	0.48676500	4.32829900	-1.59091500
C	0.75056700	1.76760600	-2.24357200
H	1.84190900	1.68948400	-2.16280300
H	0.38356000	0.77002900	-2.49915700
H	0.53380000	2.43597900	-3.08364800
C	-1.52257900	1.18862000	2.28314200
H	-2.38792100	0.61484100	1.93439600
H	-0.79213100	0.46206500	2.65917400
H	-1.84101800	1.80566900	3.12888000
C	-2.79026500	0.62947100	-1.78561700
H	-2.75364900	1.54050400	-1.17980200
H	-1.92805800	0.66431000	-2.45933200
H	-3.69415100	0.66763000	-2.40127600
C	-0.68156600	-2.62631300	1.57037100
H	0.02117800	-3.28291100	1.04251600
H	-0.09554000	-1.80562700	1.99142400
H	-1.09858900	-3.20577800	2.40037800
C	-0.46279900	5.76337300	0.52166500
H	0.29979100	6.08363800	1.24280100
H	-0.26426600	6.28245600	-0.42087400
H	-1.42963500	6.10741200	0.90514800
C	-5.29153400	-3.39348000	-0.19055000
H	-6.18795900	-2.77928900	-0.32459800
H	-5.25901200	-4.10402200	-1.02647500
H	-5.40657100	-3.97630900	0.72854400
C	2.18059800	-0.19394200	0.06594700
H	2.14496600	0.85785700	0.35321700
C	1.01555600	-0.82426300	-0.22299500

H	1.06970500	-1.88048500	-0.49678400
H	6.19863400	-3.02951000	-0.26797900

3V

B	8.61777600	0.40595800	0.13589200
C	9.17239800	1.87917300	0.15935500
C	10.15467900	4.55158000	0.20580300
C	8.61347100	2.87855700	-0.67302100
C	10.24795000	2.24981200	1.00726400
C	10.70142800	3.56729700	1.03023900
C	9.11740800	4.18103700	-0.64489800
H	11.51271200	3.83405900	1.70589900
H	8.68461900	4.92789100	-1.30895400
C	9.57659900	-0.84592800	0.06931000
C	11.31305000	-3.08492100	-0.09955000
C	10.44999000	-1.00517500	-1.03175000
C	9.58796300	-1.82806500	1.07963500
C	10.45894900	-2.91764000	0.98667900
C	11.28922600	-2.11455500	-1.10430600
H	10.47088700	-3.65374300	1.78950000
H	11.94888400	-2.22389400	-1.96412200
C	-2.64104700	-1.36670300	-0.18709500
C	-3.18729400	-2.60109500	-0.48764100
S	-3.89056600	-0.18540900	0.07427000
H	-2.58620100	-3.48241400	-0.68529300
C	-4.59426000	-2.59280000	-0.50508100
C	-5.14554700	-1.35873600	-0.21614800
H	-5.20489300	-3.46358700	-0.71910400
B	-8.61916700	0.40741000	0.13351200
C	-9.17302000	1.88098100	0.14430000
C	-9.57764400	-0.84522100	0.07852400
C	-8.61285300	2.87296900	-0.69711000
C	-10.25203500	2.25845800	0.98388300
C	-10.45085200	-1.01529400	-1.02087000
C	-9.58910200	-1.81719800	1.09870500
C	-9.11784200	4.17466400	-0.68347400
C	-10.70675500	3.57628600	0.99255000
C	-11.29018500	-2.12538400	-1.08245100
C	-10.46011900	-2.90749900	1.01662800
C	-10.15439500	4.55411300	0.16517300
H	-8.68848500	4.91353800	-1.35860800
H	-11.52545000	3.84727000	1.65744700
C	-11.31405800	-3.08564400	-0.06814000
H	-11.95000100	-2.24311900	-1.94103100
H	-10.47241200	-3.63540500	1.82688200
C	-8.70243700	-1.71575100	2.31570800
H	-7.77371200	-2.28390100	2.18074400
H	-8.40942200	-0.68597000	2.53770600
H	-9.20819800	-2.12339400	3.19735100
C	-10.48352600	-0.01538900	-2.14791100
H	-10.82694100	0.96582900	-1.80287700
H	-9.48948100	0.13388400	-2.58646200
H	-11.15187600	-0.34832400	-2.94783000
C	-10.93957700	1.27923800	1.90111100
H	-11.48556300	0.51652400	1.33668900
H	-10.23219200	0.74803400	2.54593600

H	-11.65356100	1.79794600	2.54815600
C	-7.49196200	2.58632700	-1.66670900
H	-6.50974000	2.70948700	-1.19373400
H	-7.52769900	1.57019200	-2.06730600
H	-7.53038000	3.28428100	-2.50931100
C	7.49084700	2.60269200	-1.64365200
H	7.52251300	1.58894400	-2.05056100
H	6.50935400	2.72680800	-1.16934300
H	7.53158300	3.30567400	-2.48197000
C	10.92691400	1.26342100	1.92319400
H	10.21427800	0.73265200	2.56267800
H	11.47161100	0.50068800	1.35762100
H	11.64060900	1.77581500	2.57555500
C	10.48250300	0.00543700	-2.14922500
H	9.48819600	0.15984800	-2.58538000
H	10.82717000	0.98300100	-1.79523400
H	11.14978900	-0.32054500	-2.95289100
C	8.70141400	-1.73934800	2.29771200
H	8.40158200	-0.71293100	2.52566700
H	7.77656400	-2.31320600	2.16010900
H	9.21048000	-2.14862200	3.17672200
C	-12.22448400	-4.27779800	-0.15807300
H	-11.84541800	-5.01047600	-0.88172200
H	-12.31556700	-4.78453200	0.80741700
H	-13.22807000	-3.99036100	-0.49023100
C	-10.65361500	5.97018000	0.20085100
H	-11.73225400	6.00967400	0.38460200
H	-10.16808300	6.53664900	1.00586600
H	-10.44386700	6.49216400	-0.73784500
C	10.69094100	5.95456600	0.21962200
H	11.65427200	6.01272100	-0.30261600
H	10.00517600	6.64978900	-0.27378000
H	10.86021500	6.30660200	1.24296900
C	12.22451600	-4.27536300	-0.20092600
H	11.85762700	-4.99142600	-0.94705800
H	13.23359200	-3.98108900	-0.50990200
H	12.29975800	-4.80322700	0.75452700
C	-6.54189800	-1.03622100	-0.15138100
H	-7.20380600	-1.87146700	-0.38376700
C	-7.09434000	0.16663700	0.14787000
H	-6.41248700	0.99189000	0.36597900
C	6.54016900	-1.03526700	-0.15959700
H	7.20181200	-1.86882500	-0.39868200
C	7.09295300	0.16525300	0.14835900
H	6.41134300	0.98893800	0.37308000
C	-1.25372500	-1.00259500	-0.08286200
C	-0.70462000	0.21271600	0.27511200
S	-0.00098300	-2.15968400	-0.43082100
C	0.70326300	0.21306400	0.27332900
H	-1.30372700	1.07811000	0.53784200
C	1.25207500	-1.00196700	-0.08605400
H	1.30257900	1.07885000	0.53429300
C	2.63929900	-1.36538500	-0.19387600
C	3.18523100	-2.59773100	-0.50330600
S	3.88910500	-0.18598300	0.07453900
C	4.59216600	-2.58932500	-0.52217800

H	2.58390200	-3.47757500	-0.70672000
C	5.14376800	-1.35724700	-0.22543700
H	5.20256900	-3.45860400	-0.74289400

4V

B	-10.68129180	0.19813701	0.00099002
C	-11.41180585	1.58791912	0.11667903
C	-12.71554693	4.11131931	0.32050804
C	-10.92145482	2.59713020	0.98013009
C	-12.58281594	1.87025314	-0.63280703
C	-13.19494998	3.11845023	-0.53476902
C	-11.58209287	3.82405529	1.07550010
H	-14.07907705	3.32108125	-1.13735607
H	-11.19762486	4.57767635	1.76134615
C	-11.47297986	-1.16692509	0.03892002
C	-12.89534697	-3.61991228	0.16512503
C	-12.23519994	-1.50523812	1.18089911
C	-11.43667787	-2.07826516	-1.03534706
C	-12.15393392	-3.27570325	-0.96186206
C	-12.91968500	-2.71762221	1.23110211
H	-12.13355891	-3.95625131	-1.81216212
H	-13.49464100	-2.96431823	2.12267318
C	4.51916136	0.70863105	-0.42936802
C	4.89466339	1.98419916	-0.80967005
S	5.91352845	-0.25470902	-0.03800399
H	4.18225434	2.74882321	-1.10098606
C	6.28806249	2.17862417	-0.78969805
C	6.99905255	1.06172908	-0.39302301
H	6.77599852	3.10946624	-1.05877506
B	10.67613184	-0.14116501	0.19134503
C	11.44027691	-1.50873011	0.34786604
C	11.44147989	1.23304610	0.05871502
C	11.07332985	-2.63846420	-0.42326602
C	12.52266797	-1.64963512	1.25342611
C	12.32667098	1.44210611	-1.02420706
C	11.26464489	2.27670918	0.98900609
C	11.76472993	-3.84313629	-0.28014300
C	13.16732704	-2.87798722	1.39117113
C	12.99235701	2.65836721	-1.15906407
C	11.96485090	3.47686427	0.83607208
C	12.80560502	-3.99145130	0.63265607
H	11.48167588	-4.69029736	-0.90328205
H	13.98512507	-2.96728322	2.10463818
C	12.82775701	3.69272729	-0.23472300
H	13.66395708	2.80328022	-2.00424113
H	11.83345990	4.26282333	1.57875014
C	10.35398778	2.14241117	2.18496918
H	9.36370173	2.56877320	1.98192617
H	10.19266577	1.10085609	2.47549521
H	10.76718584	2.67668121	3.04707925
C	12.55802595	0.36847403	-2.05616514
H	13.02933999	-0.51626404	-1.61475611
H	11.61777593	0.03241901	-2.50969917
H	13.20309201	0.73200306	-2.86187720
C	13.01302403	-0.50697003	2.10585918
H	13.46443403	0.28259903	1.49663613

H	12.20499196	-0.04020900	2.67823922
H	13.76569204	-0.85725406	2.81879723
C	9.96836378	-2.60369220	-1.45110209
H	8.99485169	-2.83877221	-1.00310306
H	9.86978176	-1.62838412	-1.93415213
H	10.15009277	-3.35103726	-2.23024716
C	-9.70630875	2.40746218	1.85529016
H	-9.58103773	1.37399010	2.18758219
H	-8.78483563	2.68903020	1.33053112
H	-9.77465173	3.04327423	2.74393323
C	-13.20067097	0.86340506	-1.56949010
H	-12.47588896	0.46280503	-2.28539016
H	-13.61021103	0.00742100	-1.02356306
H	-14.01380605	1.32130810	-2.14101015
C	-12.31326094	-0.57679405	2.36544720
H	-11.31720584	-0.31537203	2.74252223
H	-12.80895497	0.36444902	2.10435518
H	-12.86862495	-1.03733609	3.18820826
C	-10.66138378	-1.79953914	-2.29977316
H	-10.50255578	-0.73105706	-2.46875817
H	-9.66768474	-2.26342818	-2.26800416
H	-11.18338284	-2.20839917	-3.17140922
C	13.54964606	4.99969639	-0.40473201
H	13.06975702	5.61851944	-1.17359007
H	13.55594306	5.57664644	0.52502606
H	14.58730915	4.84544437	-0.71984004
C	13.50763304	-5.30769141	0.80730608
H	14.57082914	-5.16784639	1.02837709
H	13.07612900	-5.87416846	1.64252814
H	13.42019602	-5.92992744	-0.08866899
C	-13.42033800	5.43220539	0.44165605
H	-14.31867909	5.34267839	1.06559410
H	-12.77593495	6.18898447	0.89907009
H	-13.74532803	5.80223544	-0.53657002
C	-13.63405602	-4.92614938	0.24443004
H	-13.07936698	-5.65720245	0.84638408
H	-14.61548810	-4.80278137	0.71480907
H	-13.78187603	-5.36267843	-0.74805304
C	8.42360866	0.95199308	-0.26837100
H	8.96585071	1.85731015	-0.54448302
C	9.13362572	-0.13159801	0.13653903
H	8.57148565	-1.03156707	0.39659705
C	-8.43126363	-0.98916408	0.06592102
H	-8.97172267	-1.91151115	0.28263804
C	-9.14326770	0.15111701	-0.12128899
H	-8.58215265	1.06596008	-0.32557001
C	3.19479126	0.15640301	-0.33463801
C	2.81688023	-1.14345608	-0.06473999
S	1.79307515	1.16275109	-0.56873803
C	1.42091713	-1.33091510	-0.05465299
H	3.52982329	-1.94220515	0.11031003
C	0.71036907	-0.17630301	-0.31590501
H	0.94646909	-2.28920317	0.12842703
C	-0.71406504	0.00908200	-0.38592001
C	-1.42318009	1.13391609	-0.75763304
S	-1.79903712	-1.28415510	0.03820702

C	-2.81972820	0.95596807	-0.71106104
H	-0.94727006	2.05829116	-1.06750806
C	-3.19914823	-0.30700902	-0.30360801
H	-3.53163825	1.72807613	-0.98303106
C	-4.52440933	-0.84226007	-0.14430699
C	-4.90051936	-2.14913117	0.10672503
S	-5.91855542	0.19192801	-0.25246400
C	-6.29458544	-2.31310918	0.20534303
H	-4.18794430	-2.96118423	0.20546203
C	-7.00550952	-1.14102509	0.02873202
H	-6.78305150	-3.26318925	0.39450505

4VD

B	1.80624300	0.13618500	0.09464400
C	2.65783600	1.46080900	0.10169600
C	4.17610300	3.87003000	0.12428400
C	2.30129100	2.55808600	-0.71878900
C	3.80540000	1.59598100	0.92458600
C	4.52366500	2.79031300	0.93691300
C	3.06588400	3.72690700	-0.70290500
H	5.38724900	2.87946900	1.59428700
H	2.78344500	4.55015900	-1.35758500
C	2.47956600	-1.28888700	0.00416700
C	3.69278100	-3.84576900	-0.21679100
C	3.26315100	-1.62496400	-1.12403400
C	2.31505100	-2.25580400	1.01605500
C	2.93065800	-3.50518200	0.89728700
C	3.84415600	-2.88737800	-1.22162800
H	2.81208700	-4.23042000	1.70140200
H	4.43764900	-3.13020800	-2.10204400
C	1.12423500	2.52571400	-1.66325800
H	0.93498100	1.52895600	-2.06940100
H	0.20097500	2.84956200	-1.16685900
H	1.29152100	3.20780600	-2.50315500
C	4.28466500	0.48598000	1.82520700
H	3.49290700	0.11516300	2.48408800
H	4.64173700	-0.37265800	1.24765100
H	5.10672000	0.83463900	2.45780200
C	3.47370700	-0.63927900	-2.24438400
H	2.52122200	-0.27941500	-2.65190200
H	4.02458800	0.24367200	-1.90291600
H	4.03478400	-1.09423900	-3.06638000
C	1.50787700	-1.98637500	2.26244600
H	1.42221400	-0.91963100	2.48560300
H	0.48458300	-2.36983000	2.16473400
H	1.95870500	-2.48102100	3.12938300
C	4.99387500	5.12999600	0.12290500
H	5.91521800	5.00013400	-0.45899200
H	4.44122300	5.96520600	-0.31779200
H	5.29321500	5.41249200	1.13783500
C	4.32103100	-5.20463800	-0.34723700
H	3.73552400	-5.84746300	-1.01688300
H	5.33055000	-5.13994200	-0.76721700
H	4.38423400	-5.71046200	0.62105800
C	-0.53201800	-0.84264300	-0.13113500

H	-0.06329700	-1.79613900	-0.37842400
C	0.26644000	0.21895100	0.14791300
H	-0.22288100	1.16733000	0.38175000
C	-8.13599500	0.79328600	0.11252200
C	-7.37351600	1.83384100	0.56619900
S	-7.17062100	-0.55829100	-0.33615600
C	-5.98640700	1.53907500	0.55802000
H	-7.78973000	2.77795800	0.89892100
C	-5.70251800	0.27220900	0.09599200
H	-5.22078500	2.23230200	0.89097500
C	-4.41859300	-0.36900800	-0.05024300
C	-4.14481400	-1.68747800	-0.35838100
S	-2.94796300	0.53359700	0.16051700
C	-2.76572100	-1.96654600	-0.41938800
H	-4.91935500	-2.42852500	-0.52523900
C	-1.96583800	-0.87168100	-0.15533400
H	-2.35262600	-2.94438100	-0.64362400
H	-9.21223100	0.74038700	0.01382500

5V

B	-12.48387900	0.64163800	-0.04802100
C	-13.01273200	2.12458300	-0.07325100
C	-13.95096000	4.81265800	-0.12157900
C	-12.39891600	3.12775400	0.71459300
C	-14.11918200	2.49995200	-0.87782000
C	-14.55118400	3.82466500	-0.90318700
C	-12.88169700	4.43823600	0.68687400
H	-15.38777600	4.09437400	-1.54603700
H	-12.40610100	5.18843200	1.31704900
C	-13.46134200	-0.58977200	0.09302000
C	-15.22752500	-2.79101000	0.39878000
C	-14.28053200	-0.70893800	1.23990600
C	-13.54263500	-1.59245700	-0.89377700
C	-14.42754300	-2.66275400	-0.73300900
C	-15.13501400	-1.80013400	1.37919300
H	-14.49406300	-3.41495800	-1.51807100
H	-15.75188900	-1.87848300	2.27344600
C	2.64016600	-0.93600900	-0.29354700
C	3.18864600	0.25305800	-0.73083100
S	3.89090800	-2.03890400	0.20462100
H	2.59040800	1.08088400	-1.09651000
C	4.59625200	0.27314400	-0.67726700
C	5.14479900	-0.89952000	-0.19883500
H	5.19597400	1.11911900	-0.99616900
B	12.48473700	0.64423400	-0.04312800
C	13.01199800	2.12788100	-0.04384100
C	13.46251400	-0.58915900	0.07615700
C	12.39588200	3.11743000	0.76033500
C	14.12196800	2.51678100	-0.83628100
C	14.28184400	-0.72889700	1.22042500
C	13.54424300	-1.57329400	-0.92916600
C	12.87870200	4.42764500	0.75754000
C	14.55415000	3.84221700	-0.83678600
C	15.13726700	-1.82190400	1.33928100
C	14.42995300	-2.64564000	-0.78853400
C	13.94735200	4.81752800	-0.04534300

H	12.40553200	5.16500400	1.40447000
H	15.39811200	4.12148500	-1.46572400
C	15.23023500	-2.79430300	0.34066200
H	15.75459600	-1.91627100	2.23166700
H	14.49707100	-3.38300400	-1.58749300
C	12.72000600	-1.50406400	-2.19148400
H	11.80262100	-2.09897000	-2.10150500
H	12.40897900	-0.48466100	-2.43521800
H	13.28292500	-1.90132600	-3.04275900
C	14.23915000	0.28511900	2.33444600
H	14.58051200	1.26865300	1.99402900
H	13.22181600	0.42007500	2.72110500
H	14.87296400	-0.02491200	3.17086200
C	14.86736000	1.54131900	-1.71136300
H	15.40138700	0.79456800	-1.11503200
H	14.19899100	0.99070200	-2.38105100
H	15.60000000	2.06654600	-2.33175900
C	11.23511200	2.81980600	1.67831000
H	10.27479900	2.91739100	1.15687800
H	11.27115800	1.80930700	2.09295800
H	11.21886000	3.52819800	2.51287700
C	-11.23655100	2.84820000	1.63613100
H	-11.26772200	1.84304900	2.06393200
H	-10.27677100	2.94370200	1.11327500
H	-11.22370400	3.56748400	2.46140600
C	-14.85498600	1.51020400	-1.74493200
H	-14.18029900	0.95461000	-2.40419100
H	-15.38848200	0.76827400	-1.14218200
H	-15.58688500	2.02401000	-2.37566800
C	-14.23833700	0.32511200	2.33540600
H	-13.22081500	0.46900400	2.71830400
H	-14.58204200	1.30170100	1.97785400
H	-14.87052800	0.02889800	3.17803900
C	-12.71912500	-1.54659400	-2.15763400
H	-12.39942300	-0.53328600	-2.41472500
H	-11.80704300	-2.14860200	-2.06080400
H	-13.28636800	-1.94997000	-3.00318700
C	16.15557400	-3.96850200	0.49300600
H	15.74277900	-4.70862100	1.19022400
H	16.32091400	-4.47353700	-0.46350500
H	17.12877500	-3.66177600	0.89150700
C	14.42371500	6.24168800	-0.07136700
H	15.50957200	6.29808900	-0.20005500
H	13.97082200	6.79127500	-0.90654200
H	14.15726000	6.76960600	0.84945100
C	-14.46407500	6.22431200	-0.13453200
H	-15.39491700	6.30992100	0.44026600
H	-13.74007500	6.91711900	0.30471900
H	-14.68558100	6.55873900	-1.15376400
C	-16.15258700	-3.96237400	0.57303900
H	-15.74600600	-4.68278100	1.29410000
H	-17.13029100	-3.64675100	0.95328400
H	-16.30759400	-4.49292200	-0.37129300
C	10.42172100	-0.83475500	0.15026400
H	11.08568900	-1.65565000	0.42436900
C	10.96772500	0.37544000	-0.13203100

H	10.28328000	1.18621000	-0.39244500
C	-10.41959100	-0.83296400	0.16673300
H	-11.08267800	-1.65020700	0.45355000
C	-10.96673700	0.37254200	-0.13297200
H	-10.28307700	1.17980300	-0.40610800
C	1.25429300	-1.31205100	-0.21100000
C	0.70582600	-2.55382400	0.03737800
S	0.00051600	-0.12363600	-0.42854200
C	-0.70365000	-2.55394900	0.03854400
H	1.30523200	-3.44431200	0.19489800
C	-1.25269100	-1.31227100	-0.20895700
H	-1.30269100	-3.44454300	0.19681800
C	-2.63873800	-0.93639900	-0.28947400
C	-3.18824900	0.25011100	-0.73234700
S	-3.88818200	-2.03599100	0.21911700
C	-4.59567700	0.27078800	-0.67478500
H	-2.59090200	1.07545500	-1.10501400
C	-5.14307800	-0.89883200	-0.18762100
H	-5.19610600	1.11506700	-0.99684300
C	-6.52856300	-1.23442600	0.00155900
C	-7.07905200	-2.45137400	0.36021200
S	-7.76954700	-0.03521400	-0.21519300
C	-8.48269000	-2.41636200	0.45400300
H	-6.48337700	-3.34014000	0.53992800
C	-9.02786300	-1.17926900	0.16648800
H	-9.09588700	-3.27128300	0.71880100
C	6.53073500	-1.23660300	-0.01561000
C	7.08241200	-2.45775900	0.32649000
S	7.77063100	-0.03379500	-0.21802900
C	8.48617000	-2.42306600	0.41882000
H	6.48753300	-3.34926100	0.49494700
C	9.03019300	-1.18198200	0.14676800
H	9.10027200	-3.28097600	0.67157000

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C	0.66851500	-0.29310000	-0.06528600
C	1.04274700	-1.62422600	-0.14364700
H	0.32706400	-2.43722300	-0.20266600
C	2.43419100	-1.81235400	-0.14734200
H	2.92305600	-2.77766700	-0.20670600
C	3.14500900	-0.62613500	-0.06944200
S	2.05963600	0.73809500	0.01180900
B	7.23733900	-0.04042400	-0.00882600
C	8.19044200	-1.27963000	-0.15141800
C	9.94205600	-3.49542900	-0.43854500
C	8.00397200	-2.45548200	0.61342400
C	9.26700700	-1.23880700	-1.06950700
C	10.10695200	-2.34394500	-1.20713600
C	8.88392200	-3.52751000	0.46901000
H	10.91770900	-2.30289100	-1.93270300
H	8.73742200	-4.41644400	1.08052300
C	7.76381800	1.42972500	0.15965900

C	8.74369700	4.07173200	0.50043000
C	8.75705900	1.71516600	1.12671900
C	7.26920900	2.49341500	-0.63043500
C	7.77657900	3.78142700	-0.46087400
C	9.21617600	3.02220000	1.28781200
H	7.40475700	4.58284900	-1.09727600
H	9.97128200	3.22640800	2.04525700
C	-0.66243800	0.25721600	-0.04656400
C	-1.03508500	1.59101200	-0.03111900
S	-2.05473700	-0.77527100	-0.04129600
H	-0.31826300	2.40514300	-0.03496600
C	-2.42617800	1.78053100	-0.01558300
C	-3.13842700	0.59257300	-0.01980000
H	-2.91395200	2.74812200	-0.00273100
B	-7.23425600	0.02947600	0.00840900
C	-8.16425700	1.29389100	0.05404100
C	-7.78844500	-1.43914500	-0.02855400
C	-7.97955700	2.38536000	-0.82651100
C	-9.22198600	1.35753600	0.99207600
C	-8.81173600	-1.78443400	-0.94367400
C	-7.29303500	-2.44367000	0.83601200
C	-8.84381800	3.47849900	-0.77138500
C	-10.04564300	2.48222200	1.03697100
C	-9.29830400	-3.09101700	-0.98311700
C	-7.82810200	-3.73048600	0.78771000
C	-9.87890600	3.55326400	0.15973000
H	-8.70460000	4.29713000	-1.47565000
H	-10.84696800	2.52014700	1.77320100
C	-8.82507500	-4.08033800	-0.12209500
H	-10.07637500	-3.34258100	-1.70202700
H	-7.45469600	-4.48342900	1.47995000
C	-6.21345000	-2.16898600	1.85132500
H	-5.22929700	-2.09520400	1.37523700
H	-6.37361000	-1.22818600	2.38770000
H	-6.16739700	-2.97447900	2.59047400
C	-9.40583000	-0.78330900	-1.90229800
H	-10.04727700	-0.06348300	-1.38238800
H	-8.63936000	-0.20290500	-2.42586200
H	-10.01372300	-1.29108500	-2.65732600
C	-9.49792200	0.24189400	1.96846800
H	-9.92942500	-0.63117200	1.46688400
H	-8.59000400	-0.10135500	2.47497700
H	-10.20428100	0.57136700	2.73655100
C	-6.88796900	2.40130000	-1.86564300
H	-5.90861300	2.58661300	-1.41090100
H	-6.80897800	1.45005100	-2.40215100
H	-7.07010800	3.18920300	-2.60272100
C	6.88922500	-2.59040100	1.61866900
H	6.78766000	-1.70102500	2.24922400
H	5.92244700	-2.73621200	1.12451500
H	7.06438100	-3.44901000	2.27388000
C	9.54225600	-0.03416100	-1.93398800
H	8.64002600	0.33640300	-2.43122800
H	9.94273600	0.79775000	-1.34467300
H	10.27395600	-0.27948900	-2.70976100
C	9.34586600	0.64643600	2.01287700

H	8.57673900	0.01545100	2.47023600
H	10.00795900	-0.02023500	1.44982000
H	9.93053900	1.09785800	2.82020400
C	6.21975000	2.28438900	-1.69193300
H	6.40673600	1.38967500	-2.29443600
H	5.22506400	2.16208500	-1.24873100
H	6.18042500	3.14369600	-2.36823100
C	-9.35486800	-5.48397100	-0.18917800
H	-8.76161700	-6.09339000	-0.88298800
H	-9.31392000	-5.97393700	0.78871400
H	-10.39030800	-5.50434900	-0.54332400
C	-10.77017600	4.75985200	0.23273600
H	-11.77137500	4.49679000	0.58841800
H	-10.36373900	5.50519500	0.92842700
H	-10.86640600	5.24559600	-0.74332600
C	10.88910600	-4.65414100	-0.56500900
H	11.72473200	-4.55497300	0.13969300
H	10.39114200	-5.60379600	-0.34523600
H	11.31758400	-4.71276100	-1.57038400
C	9.24331100	5.47405400	0.69905600
H	8.64464800	5.99954100	1.45415900
H	10.28171400	5.48359800	1.04521800
H	9.18183100	6.05535900	-0.22621800
C	-4.52182300	0.41185200	-0.00966200
C	-5.73570400	0.23625000	-0.00062400
C	4.52804600	-0.44337300	-0.04936900
C	5.74130500	-0.26428000	-0.03111700

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C	6.203298	-0.304116	-0.015049
C	5.847568	-1.628270	0.034574
H	6.568501	-2.437269	0.060466
C	4.446906	-1.814418	0.049138
H	3.952665	-2.778372	0.088095
C	3.742616	-0.624387	0.008790
S	4.840023	0.733008	-0.047367
B	-0.350819	-0.036027	0.005646
C	-1.297954	-1.285344	0.106284
C	-3.041502	-3.516159	0.312590
C	-1.123518	-2.420502	-0.719706
C	-2.356923	-1.293334	1.044695
C	-3.193276	-2.405633	1.141734
C	-1.999461	-3.500435	-0.613791
H	-3.990790	-2.402725	1.883022
H	-1.862695	-4.357214	-1.271751
C	-0.891341	1.435647	-0.097689
C	-1.902961	4.079634	-0.311109
C	-1.902915	1.751414	-1.035923
C	-0.394148	2.470849	0.728083
C	-0.917020	3.759441	0.621088
C	-2.377613	3.059187	-1.134411
H	-0.542293	4.537471	1.284284
H	-3.147108	3.286983	-1.870361
C	-0.025954	-2.501440	-1.749394
H	0.060546	-1.582134	-2.338035
H	0.949991	-2.664736	-1.279410

H	-0.208531	-3.328574	-2.442051
C	-2.616648	-0.133353	1.972745
H	-1.704970	0.214308	2.469463
H	-3.029792	0.725628	1.432999
H	-3.332310	-0.417865	2.750144
C	-2.495679	0.715500	-1.957757
H	-1.727932	0.112421	-2.453419
H	-3.142487	0.018712	-1.413783
H	-3.097072	1.195083	-2.736084
C	0.674991	2.229355	1.762702
H	0.499882	1.315121	2.338943
H	1.661273	2.122348	1.297534
H	0.725508	3.066308	2.465765
C	-3.985265	-4.681502	0.396963
H	-4.833699	-4.548350	-0.286524
H	-3.490579	-5.617959	0.120384
H	-4.395372	-4.791945	1.405666
C	-2.420012	5.483631	-0.441939
H	-1.837454	6.048161	-1.181294
H	-3.463166	5.496583	-0.773414
H	-2.351942	6.024886	0.506888
C	2.357538	-0.436764	0.007940
C	1.144677	-0.255675	0.007076
H	7.201130	0.115179	-0.033701

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C	2.638631	-0.991170	-0.126609
C	3.177924	-2.266982	-0.158315
H	2.570273	-3.164049	-0.210375
C	4.581606	-2.279829	-0.129362
H	5.187507	-3.178104	-0.152154
C	5.139231	-1.013148	-0.074401
S	3.889263	0.207248	-0.052356
B	9.125822	0.071523	0.025015
C	10.218223	-1.055221	-0.038261
C	12.213815	-3.068596	-0.189247
C	10.160302	-2.197302	0.794699
C	11.290986	-0.945202	-0.954514
C	12.252812	-1.953192	-1.024841
C	11.158239	-3.168106	0.716450
H	13.060015	-1.862194	-1.749842
H	11.108534	-4.030529	1.379359
C	9.476800	1.599812	0.119254
C	10.140801	4.352619	0.323367
C	10.420555	2.049335	1.073572
C	8.870874	2.556652	-0.728437
C	9.223736	3.902021	-0.625103
C	10.723667	3.407544	1.166848
H	8.767883	4.620573	-1.304404
H	11.442522	3.737299	1.915249
C	1.250913	-0.611094	-0.147461
C	0.703766	0.654025	-0.231949
S	-0.000641	-1.815362	-0.058883
H	1.303198	1.555435	-0.302586
C	-0.703739	0.654278	-0.233748
C	-1.251489	-0.610668	-0.150703

H	-1.302746	1.555815	-0.306273
B	-9.126437	0.073244	0.025411
C	-9.478575	1.600165	0.135164
C	-10.217273	-1.054337	-0.049279
C	-8.873302	2.565991	-0.702818
C	-10.422830	2.039299	1.093753
C	-11.292561	-0.935299	-0.961608
C	-10.159482	-2.202303	0.775358
C	-9.227169	3.909935	-0.586021
C	-10.726970	3.396326	1.200657
C	-12.255944	-1.941219	-1.037295
C	-11.159125	-3.171107	0.692070
C	-10.144720	4.350265	0.366868
H	-8.771805	4.635640	-1.258007
H	-11.446174	3.717993	1.952229
C	-12.212712	-3.066581	-0.215250
H	-13.069484	-1.839535	-1.753801
H	-11.113688	-4.034401	1.354097
C	-9.058745	-2.410254	1.783631
H	-8.121052	-2.697001	1.294988
H	-8.846012	-1.504859	2.361416
H	-9.326825	-3.203802	2.487692
C	-11.440154	0.252187	-1.879303
H	-11.737349	1.150319	-1.327097
H	-10.507113	0.494682	-2.398350
H	-12.203320	0.056376	-2.638692
C	-11.123182	1.085236	2.028332
H	-11.865363	0.478307	1.498477
H	-10.428689	0.387806	2.507786
H	-11.641952	1.635921	2.818952
C	-7.866788	2.193295	-1.761031
H	-6.891251	1.962668	-1.318635
H	-8.168844	1.309132	-2.331622
H	-7.727507	3.018091	-2.466468
C	9.057089	-2.400052	1.801256
H	8.843027	-1.491137	2.373008
H	8.120514	-2.689931	1.312333
H	9.323910	-3.189112	2.510806
C	11.433303	0.230848	-1.887715
H	10.498820	0.464394	-2.408289
H	11.728982	1.136584	-1.347254
H	12.195845	0.027679	-2.645796
C	11.121190	1.105193	2.017966
H	10.426936	0.412116	2.504077
H	11.863910	0.493495	1.494437
H	11.639267	1.664133	2.803234
C	7.864549	2.172855	-1.782881
H	8.165938	1.282029	-2.343326
H	6.888581	1.948171	-1.338351
H	7.726310	2.989788	-2.497614
C	-13.253918	-4.143721	-0.321348
H	-12.950947	-4.911319	-1.045046
H	-13.408467	-4.646447	0.638549
H	-14.213775	-3.740406	-0.659055
C	-10.477114	5.808076	0.507754
H	-11.500041	5.952056	0.869730

H	-9.806403	6.294675	1.227540
H	-10.369585	6.336718	-0.444545
C	13.287926	-4.116899	-0.244696
H	14.097457	-3.885444	0.459443
H	12.897993	-5.103913	0.023537
H	13.733578	-4.180598	-1.242271
C	10.472264	5.811978	0.449687
H	9.806963	6.303454	1.171176
H	11.497947	5.960256	0.802072
H	10.356192	6.332726	-0.505928
C	6.487506	-0.659603	-0.038328
C	7.669108	-0.330175	-0.007680
C	-2.639402	-0.990260	-0.133470
C	-3.179251	-2.265545	-0.175355
S	-3.889462	0.208126	-0.050354
C	-4.582947	-2.277939	-0.147361
H	-2.571900	-3.162374	-0.234632
C	-5.140030	-1.011458	-0.082893
H	-5.189263	-3.175717	-0.177632
C	-6.488151	-0.657524	-0.044562
C	-7.669583	-0.327728	-0.011305

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C	4.55213200	-0.56189300	-0.14054900
C	4.98464500	-1.87406800	-0.24876300
H	4.30515000	-2.71427700	-0.34388900
C	6.38249400	-2.00403900	-0.23269700
H	6.91149200	-2.94677600	-0.31053900
C	7.04390100	-0.79325400	-0.11005000
S	5.89863100	0.52304300	-0.00955600
B	11.10379600	-0.03832500	0.03120200
C	12.10730300	-1.23743400	-0.11997300
C	13.94456500	-3.38015200	-0.42666600
C	11.96249400	-2.42955000	0.62803600
C	13.18605200	-1.14277300	-1.03099200
C	14.06902300	-2.21269500	-1.17856500
C	12.88374000	-3.46511600	0.47433000
H	14.88153100	-2.13035500	-1.89869400
H	12.76806800	-4.36737900	1.07284900
C	11.57187500	1.44789600	0.23330200
C	12.44912100	4.11853500	0.63080100
C	12.54500600	1.75303600	1.21471500
C	11.04485200	2.50696700	-0.54214700
C	11.50189600	3.80981500	-0.34444900
C	12.95363200	3.07315200	1.40352600
H	11.10551500	4.60841000	-0.96952900
H	13.69396700	3.29143700	2.17158100
C	3.20151100	-0.06717000	-0.12959000
C	2.76138500	1.24091100	-0.09757200
S	1.85127600	-1.16551600	-0.15874900
H	3.43365600	2.09224400	-0.07934600
C	1.35855400	1.35969800	-0.10071800
C	0.70555400	0.14328500	-0.13484100
H	0.83835700	2.31146300	-0.08377600
B	-11.10409100	0.03540800	0.03859000
C	-12.11298000	1.23879000	0.07178300

C	-11.56401900	-1.46703800	0.04705000
C	-12.00691300	2.32358100	-0.83015200
C	-13.16296900	1.25418500	1.02064800
C	-12.56837200	-1.90220200	-0.84989400
C	-10.99926900	-2.41355600	0.93379900
C	-12.93586800	3.36271000	-0.78296400
C	-14.05429500	2.32657400	1.05583600
C	-12.97091600	-3.23774100	-0.85007200
C	-11.45049000	-3.73314700	0.92427600
C	-13.96334000	3.39040900	0.15907500
H	-12.85506400	4.17576800	-1.50267200
H	-14.84861200	2.32799300	1.80062500
C	-12.42922600	-4.17093000	0.03300000
H	-13.73617200	-3.55790000	-1.55539800
H	-11.02433600	-4.44152100	1.63295500
C	-9.93236800	-2.04247200	1.93181900
H	-8.95812100	-1.92007600	1.44545200
H	-10.14796700	-1.09848400	2.44263300
H	-9.83033500	-2.82193300	2.69299400
C	-13.23019600	-0.96654100	-1.83002700
H	-13.90936800	-0.27174000	-1.32411500
H	-12.50397000	-0.35656600	-2.37711500
H	-13.81258100	-1.53099400	-2.56467000
C	-13.35929800	0.14225900	2.02023000
H	-13.73580000	-0.76677400	1.53877800
H	-12.42762200	-0.13108300	2.52612500
H	-14.08069100	0.44013400	2.78724300
C	-10.93122700	2.38789300	-1.88388300
H	-9.95684800	2.62679400	-1.44397800
H	-10.81034800	1.43742700	-2.41408700
H	-11.16396700	3.15907100	-2.62440000
C	10.84744500	-2.62059000	1.62380100
H	10.70680400	-1.74354400	2.26406400
H	9.89031100	-2.79764000	1.12111500
H	11.05169100	-3.47972500	2.26989800
C	13.41820400	0.08388100	-1.87694300
H	12.50453300	0.42512900	-2.37439700
H	13.78177100	0.92276900	-1.27366400
H	14.16337000	-0.12094400	-2.65168500
C	13.16559000	0.69142800	2.08756400
H	12.41634600	0.02518900	2.52753600
H	13.85587400	0.05903100	1.51890900
H	13.72697700	1.14980800	2.90742600
C	10.01329400	2.27916500	-1.61726800
H	10.24287200	1.40770000	-2.23882600
H	9.02141100	2.10368200	-1.18591500
H	9.94271300	3.15201900	-2.27339900
C	-12.86823100	-5.60700900	0.00807600
H	-12.24394800	-6.19557000	-0.67646800
H	-12.78660500	-6.06735100	0.99776600
H	-13.90363000	-5.70299600	-0.33361500
C	-14.92620300	4.54126700	0.22238700
H	-15.90376900	4.22473500	0.59958300
H	-14.55615900	5.32480800	0.89608100
H	-15.06698200	4.99945400	-0.76158400
C	14.93613900	-4.49991300	-0.56338100

H	15.76397100	-4.37860400	0.14704400
H	14.47391900	-5.47089900	-0.35918900
H	15.37147200	-4.52845800	-1.56713900
C	12.89392400	5.53475000	0.85919900
H	12.26687900	6.02504800	1.61494500
H	13.92688700	5.57665400	1.21896200
H	12.82250800	6.12908100	-0.05706400
C	8.41631600	-0.55395200	-0.06250400
C	9.62076000	-0.32219300	-0.01949600
C	-0.70835500	-0.11965300	-0.15006700
C	-1.36057200	-1.33469300	-0.22441000
S	-1.85498100	1.18591600	-0.06716300
C	-2.76347200	-1.21712200	-0.21898600
H	-0.83965600	-2.28417100	-0.28678900
C	-3.20445800	0.08873000	-0.14099800
H	-3.43501700	-2.06713000	-0.27849700
C	-8.41922200	0.56803000	-0.03365800
C	-9.62285100	0.33011100	-0.00312000
C	-4.55530400	0.58251200	-0.11750100
C	-4.98778500	1.89910800	-0.12905000
S	-5.90180800	-0.50906200	-0.06694100
C	-6.38557300	2.02768900	-0.09957100
H	-4.30811200	2.74382900	-0.16394700
C	-7.04702500	0.81119600	-0.06607000
H	-6.91444600	2.97368800	-0.10457000

4TD

C	4.590998	-0.558604	0.034077
C	4.162156	-1.873520	0.095137
H	4.844884	-2.715009	0.144216
C	2.763290	-2.005900	0.099336
H	2.237231	-2.952303	0.148006
C	2.098439	-0.792968	0.041013
S	3.241902	0.527689	-0.026921
B	-1.963503	-0.038725	0.008233
C	-2.964953	-1.245494	0.104547
C	-4.802711	-3.400160	0.306151
C	-2.833556	-2.389818	-0.716773
C	-4.029858	-1.205426	1.035456
C	-4.913197	-2.281044	1.130297
C	-3.754864	-3.431601	-0.613261
H	-5.714937	-2.241803	1.865983
H	-3.649891	-4.295755	-1.267434
C	-2.437505	1.455658	-0.100810
C	-3.329253	4.141639	-0.325918
C	-3.425966	1.814565	-1.047966
C	-1.901825	2.469214	0.727801
C	-2.366001	3.779550	0.614745
C	-3.841794	3.141926	-1.151810
H	-1.962461	4.541322	1.279952
H	-4.594323	3.402368	-1.894441
C	5.944426	-0.059121	0.016452
C	6.382002	1.246196	0.082455
S	7.297980	-1.147522	-0.102350
H	5.709009	2.093304	0.167091

C	7.793818	1.364992	0.040142
C	8.421253	0.153486	-0.057196
H	8.323449	2.309840	0.083084
C	-1.733318	-2.520925	-1.738374
H	-1.602263	-1.607453	-2.327784
H	-0.768819	-2.726013	-1.261086
H	-1.946968	-3.340717	-2.430879
C	-4.246310	-0.032388	1.958115
H	-3.324332	0.276530	2.461396
H	-4.616829	0.842212	1.412555
H	-4.980144	-0.282931	2.730246
C	-4.055640	0.804380	-1.973805
H	-3.310705	0.166801	-2.461018
H	-4.738044	0.138151	-1.434999
H	-4.627683	1.308656	-2.758646
C	-0.852649	2.182297	1.771223
H	-1.070930	1.275832	2.344954
H	0.132249	2.034152	1.314368
H	-0.772710	3.016007	2.475436
C	-5.795127	-4.524539	0.388160
H	-6.631877	-4.359330	-0.302704
H	-5.337952	-5.482207	0.119752
H	-6.217343	-4.612865	1.394041
C	-3.782305	5.567070	-0.462395
H	-3.158550	6.108882	-1.184960
H	-4.815817	5.626170	-0.818042
H	-3.713441	6.101470	0.490304
C	0.725046	-0.554003	0.030495
C	-0.480239	-0.322447	0.020016
H	9.482454	-0.052441	-0.106073

5T

C	6.529816	-0.853403	-0.139789
C	7.068964	-2.130121	-0.150499
H	6.461052	-3.027139	-0.200125
C	8.471930	-2.144010	-0.102166
H	9.076802	-3.043331	-0.106790
C	9.031178	-0.877746	-0.052298
S	7.781396	0.344456	-0.060947
B	13.016024	0.204322	0.089475
C	14.107552	-0.924638	0.041607
C	16.100613	-2.942390	-0.082880
C	14.041223	-2.061845	0.880406
C	15.187337	-0.821758	-0.867005
C	16.147992	-1.831739	-0.924332
C	15.037932	-3.034936	0.815215
H	16.960887	-1.746181	-1.643638
H	14.981479	-3.893628	1.482443
C	13.369450	1.732474	0.181767
C	14.037933	4.484758	0.382106
C	14.305790	2.183450	1.142687
C	12.773182	2.687845	-0.674467
C	13.128111	4.032817	-0.572672
C	14.611268	3.541314	1.233842
H	12.679701	4.750008	-1.258353
H	15.324371	3.872034	1.987315

C	5.143667	-0.472693	-0.184444
C	4.596690	0.791980	-0.266349
S	3.888570	-1.678641	-0.135782
H	5.196765	1.694686	-0.313260
C	3.188913	0.792499	-0.299068
C	2.638947	-0.473090	-0.241973
H	2.591584	1.694785	-0.375664
B	-13.016820	0.204935	0.089951
C	-13.368932	1.733638	0.177750
C	-14.108392	-0.924050	0.045212
C	-12.772014	2.685881	-0.681544
C	-14.304567	2.188333	1.137536
C	-15.191249	-0.821867	-0.860064
C	-14.043342	-2.056795	0.889920
C	-13.125402	4.031499	-0.583524
C	-14.608545	3.546825	1.224859
C	-16.154996	-1.829079	-0.909508
C	-15.043306	-3.027239	0.832519
C	-14.034405	4.487185	0.370312
H	-12.676511	4.746196	-1.271495
H	-15.321153	3.880474	1.977503
C	-16.104523	-2.939386	-0.067594
H	-16.974562	-1.740469	-1.620898
H	-14.991961	-3.878483	1.509575
C	-12.933864	-2.246070	1.892274
H	-11.999391	-2.537935	1.400534
H	-12.718789	-1.330983	2.453764
H	-13.194060	-3.028958	2.611078
C	-15.346315	0.348807	-1.797919
H	-15.636557	1.257492	-1.259450
H	-14.417998	0.580059	-2.330491
H	-16.117181	0.140388	-2.546100
C	-14.995975	1.249603	2.094035
H	-15.741997	0.633206	1.580792
H	-14.296698	0.560894	2.579110
H	-15.508474	1.813084	2.879728
C	-11.775076	2.296594	-1.742867
H	-10.795220	2.073992	-1.305936
H	-12.081572	1.402820	-2.295816
H	-11.643221	3.109806	-2.463043
C	12.929559	-2.256815	1.879168
H	12.713870	-1.344612	2.445099
H	11.995891	-2.545686	1.384139
H	13.188258	-3.043535	2.594314
C	15.338257	0.348817	-1.805721
H	14.408364	0.579285	-2.335897
H	15.629106	1.257718	-1.267965
H	16.107415	0.141234	-2.555894
C	14.996078	1.241284	2.096628
H	14.296052	0.551538	2.579161
H	15.741916	0.625987	1.581837
H	15.508537	1.801980	2.884342
C	11.775105	2.302935	-1.736312
H	12.079934	1.410294	-2.291977
H	10.795201	2.080500	-1.299399
H	11.643956	3.118377	-2.454093

C	-17.146270	-4.018461	-0.145474
H	-16.852694	-4.795308	-0.863155
H	-17.287512	-4.508562	0.822954
H	-18.110933	-3.620163	-0.475434
C	-14.366186	5.947030	0.490211
H	-15.384830	6.096633	0.861848
H	-13.687276	6.446334	1.193423
H	-14.270459	6.459357	-0.472227
C	17.173232	-3.992922	-0.124332
H	17.977874	-3.759140	0.584633
H	16.779464	-4.977768	0.146295
H	17.626318	-4.062948	-1.118139
C	14.371505	5.943844	0.506210
H	13.699478	6.439889	1.218282
H	15.393608	6.091130	0.869249
H	14.267231	6.460994	-0.452726
C	10.378688	-0.525382	-0.001129
C	11.560196	-0.195764	0.042124
C	1.252451	-0.854775	-0.258680
C	0.703859	-2.118417	-0.345429
S	-0.000681	0.349600	-0.160805
C	-0.704883	-2.118550	-0.344967
H	1.302791	-3.019725	-0.422653
C	-1.253652	-0.855009	-0.257879
H	-1.303696	-3.019971	-0.421785
C	-10.379865	-0.526597	0.002157
C	-11.561227	-0.196283	0.044165
C	-2.640200	-0.473566	-0.240300
C	-3.190415	0.791939	-0.296938
S	-3.889566	-1.679330	-0.133499
C	-4.598158	0.791198	-0.263250
H	-2.593287	1.694336	-0.373778
C	-5.144885	-0.473570	-0.181038
H	-5.198373	1.693846	-0.309451
C	-6.530953	-0.854447	-0.135312
C	-7.069850	-2.131305	-0.142151
S	-7.782792	0.343380	-0.060300
C	-8.472811	-2.145340	-0.093839
H	-6.461758	-3.028364	-0.188791
C	-9.032340	-0.879055	-0.047848
H	-9.077487	-3.044804	-0.095664

2TM-H

C	-0.666694	-0.390942	-0.183235
C	-1.039682	-1.649223	0.209669
H	-0.330106	-2.448832	0.388703
C	-2.444726	-1.807798	0.328048
H	-2.917396	-2.743492	0.600736
C	-3.151578	-0.675402	0.025262
S	-2.066922	0.621965	-0.397257
C	-4.603768	-0.480544	0.032282
C	-7.416308	-0.140183	0.055002
C	-5.214537	0.502920	-0.745370
C	-5.418348	-1.289197	0.826027
C	-6.801143	-1.148542	0.830260

C	-6.591940	0.695262	-0.729535
H	-4.606288	1.130002	-1.390978
H	-4.963140	-2.039042	1.465149
B	-8.979423	0.047231	0.066600
C	-9.597584	1.478099	0.287377
C	-10.701260	4.034889	0.681176
C	-9.165264	2.292049	1.357896
C	-10.595366	1.973337	-0.581264
C	-11.121190	3.248879	-0.381849
C	-9.733275	3.550695	1.548762
H	-11.874370	3.625595	-1.068099
H	-9.405786	4.159148	2.386998
C	-9.920205	-1.197587	-0.142258
C	-11.598980	-3.423644	-0.512407
C	-10.993532	-1.445131	0.742147
C	-9.706693	-2.089974	-1.216245
C	-10.557011	-3.180074	-1.395036
C	-11.806990	-2.561443	0.554144
H	-10.393625	-3.848220	-2.235881
H	-12.617410	-2.751016	1.252285
C	0.666401	0.130531	-0.412681
C	1.037671	1.277301	-1.063757
S	2.068693	-0.722165	0.169814
H	0.326229	1.961056	-1.512373
C	2.442459	1.473913	-1.099223
C	3.150993	0.480492	-0.479195
H	2.911675	2.335349	-1.558541
C	4.603844	0.352768	-0.336447
C	5.175766	-0.392946	0.694000
C	5.458011	0.985873	-1.240278
C	6.554378	-0.525962	0.820509
H	4.534517	-0.875829	1.425950
C	6.840019	0.905840	-1.114567
H	5.036307	1.544550	-2.069749
C	7.416883	0.133853	-0.081599
B	8.980195	0.007892	0.056088
C	9.641146	-1.411374	0.219883
C	9.877336	1.301116	0.028350
C	9.302657	-2.469065	-0.653202
C	10.583480	-1.652560	1.244244
C	11.006462	1.375936	-0.817088
C	9.567929	2.410033	0.846815
C	9.907450	-3.716059	-0.503094
C	11.147186	-2.919434	1.387192
C	11.780481	2.535005	-0.843387
C	10.379975	3.542808	0.820298
C	10.820021	-3.947705	0.515579
H	9.652754	-4.515812	-1.192758
H	11.856283	-3.097108	2.190754
C	11.477530	3.613295	-0.025047
H	12.635209	2.587200	-1.511834
H	10.142304	4.381477	1.468570
C	7.674626	1.644580	-2.135541
H	8.147124	2.528685	-1.698944
H	8.477262	1.026722	-2.547120
H	7.051112	1.974418	-2.970163

C	7.069328	-1.371229	1.962822
H	7.468694	-2.323979	1.604717
H	7.872030	-0.879558	2.518948
H	6.264205	-1.588633	2.668985
C	8.381592	2.419656	1.784072
H	7.440057	2.530264	1.238703
H	8.301671	1.500430	2.370951
H	8.460149	3.252413	2.487572
C	11.413622	0.240086	-1.727972
H	11.851902	-0.588277	-1.164370
H	10.570613	-0.170875	-2.290389
H	12.156476	0.582475	-2.452881
C	11.005193	-0.582953	2.225908
H	11.661624	0.155267	1.756807
H	10.155241	-0.033153	2.639457
H	11.547127	-1.029017	3.063704
C	8.306167	-2.305075	-1.778443
H	7.279961	-2.261961	-1.402578
H	8.470349	-1.391596	-2.356481
H	8.373316	-3.148245	-2.470631
C	-7.149058	1.800572	-1.596997
H	-8.006352	1.474548	-2.192016
H	-7.485195	2.648667	-0.994314
H	-6.385440	2.162527	-2.289847
C	-7.592453	-2.088438	1.710631
H	-8.338682	-1.566906	2.316006
H	-8.129707	-2.832741	1.116614
H	-6.926628	-2.620840	2.394269
C	-8.105005	1.845821	2.339088
H	-8.268642	0.826854	2.700605
H	-7.108033	1.866596	1.889920
H	-8.092662	2.505267	3.210602
C	-11.118653	1.174699	-1.753377
H	-10.317904	0.722925	-2.345356
H	-11.767988	0.358596	-1.424351
H	-11.698956	1.816422	-2.421197
C	-11.296931	-0.546959	1.919800
H	-10.403691	-0.296992	2.499000
H	-11.740735	0.399391	1.598325
H	-12.002032	-1.034863	2.597554
C	-8.585029	-1.906074	-2.213312
H	-8.503595	-0.875880	-2.570474
H	-7.615819	-2.168713	-1.779834
H	-8.744610	-2.544446	-3.086002
H	12.095330	4.506025	-0.045720
H	11.275134	-4.926950	0.629757
H	-11.127367	5.022008	0.833171
H	-12.247139	-4.283042	-0.655303

2TM-CN

C	-0.667332	-0.399492	-0.188584
C	-1.037954	-1.654610	0.217433
H	-0.327455	-2.451986	0.402238

C	-2.441984	-1.812656	0.341474
H	-2.912828	-2.746116	0.624553
C	-3.149943	-0.683070	0.029658
S	-2.067814	0.610539	-0.408945
C	-4.601911	-0.490818	0.037120
C	-7.414198	-0.156193	0.058321
C	-5.213403	0.495994	-0.735924
C	-5.415473	-1.305117	0.826362
C	-6.797976	-1.168743	0.829957
C	-6.590266	0.687156	-0.720958
H	-4.605849	1.126882	-1.377984
H	-4.959613	-2.056361	1.462848
B	-8.970029	0.024130	0.065571
C	-9.609353	1.457359	0.239109
C	-10.754328	3.988265	0.579951
C	-9.206690	2.284978	1.310635
C	-10.595364	1.922201	-0.658018
C	-11.147826	3.186537	-0.488751
C	-9.792210	3.534574	1.479165
H	-11.894131	3.550101	-1.186703
H	-9.494984	4.164701	2.310336
C	-9.919363	-1.226603	-0.101721
C	-11.609840	-3.432871	-0.430533
C	-10.979429	-1.455635	0.802276
C	-9.721479	-2.124579	-1.173966
C	-10.575681	-3.209359	-1.336289
C	-11.805040	-2.561992	0.638709
H	-10.433843	-3.891102	-2.167759
H	-12.610091	-2.746605	1.341606
C	0.664795	0.120471	-0.426491
C	1.032554	1.262323	-1.088724
S	2.068743	-0.727393	0.157064
H	0.319155	1.942212	-1.539936
C	2.436581	1.458296	-1.132483
C	3.147476	0.469460	-0.507264
H	2.903310	2.315891	-1.601292
C	4.600523	0.344932	-0.369625
C	5.177121	-0.404242	0.655784
C	5.449994	0.984592	-1.273485
C	6.555607	-0.535393	0.778383
H	4.539383	-0.891355	1.387579
C	6.831953	0.909299	-1.152831
H	5.024411	1.544739	-2.099564
C	7.413957	0.132904	-0.123868
B	8.969928	0.013552	0.009578
C	9.648275	-1.396211	0.222780
C	9.880758	1.301004	-0.067165
C	9.335837	-2.468219	-0.642354
C	10.579959	-1.599581	1.263807
C	10.995036	1.347519	-0.932831
C	9.593652	2.418104	0.748226
C	9.956046	-3.700553	-0.470951
C	11.167262	-2.847687	1.436226
C	11.786865	2.488894	-0.984781
C	10.414920	3.538866	0.702534
C	10.863276	-3.893519	0.568161

H	9.728618	-4.520044	-1.144022
H	11.871196	-3.008728	2.245444
C	11.503864	3.578698	-0.165021
H	12.633965	2.530909	-1.660737
H	10.205003	4.391024	1.339723
C	7.657380	1.653317	-2.177313
H	8.123213	2.543592	-1.745820
H	8.461143	1.041495	-2.595212
H	7.027195	1.977992	-3.008479
C	7.071213	-1.382442	1.919036
H	7.465077	-2.337901	1.561680
H	7.873695	-0.893378	2.477470
H	6.266079	-1.598482	2.625054
C	8.416927	2.453374	1.695095
H	7.475513	2.575715	1.152731
H	8.326994	1.539345	2.287550
H	8.514231	3.289001	2.391784
C	11.368288	0.195548	-1.835252
H	11.812922	-0.626468	-1.267722
H	10.506521	-0.211128	-2.370769
H	12.096239	0.517204	-2.583305
C	10.967744	-0.504909	2.229204
H	11.627249	0.227557	1.755778
H	10.101252	0.040785	2.611335
H	11.496005	-0.923666	3.088611
C	8.344619	-2.337840	-1.775007
H	7.317400	-2.311861	-1.401363
H	8.493755	-1.427605	-2.361176
H	8.432703	-3.186698	-2.456761
C	-7.144269	1.794430	-1.587788
H	-7.996427	1.470407	-2.191001
H	-7.481063	2.643266	-0.986367
H	-6.376860	2.158073	-2.274971
C	-7.584158	-2.114320	1.708724
H	-8.337694	-1.600688	2.311411
H	-8.107656	-2.869455	1.115790
H	-6.915497	-2.637043	2.396503
C	-8.154031	1.867016	2.310501
H	-8.306228	0.849471	2.679436
H	-7.153694	1.900665	1.870608
H	-8.163722	2.535123	3.174582
C	-11.079801	1.098114	-1.827105
H	-10.257461	0.649945	-2.390719
H	-11.727708	0.281588	-1.497001
H	-11.651412	1.718845	-2.520538
C	-11.256664	-0.543101	1.973212
H	-10.350161	-0.292568	2.530251
H	-11.705310	0.398816	1.646155
H	-11.949004	-1.018228	2.671718
C	-8.607803	-1.957816	-2.181191
H	-8.518640	-0.930392	-2.542672
H	-7.640183	-2.229654	-1.750740
H	-8.781131	-2.598168	-3.048969
C	12.336304	4.745419	-0.214019
C	11.486145	-5.173095	0.744949
C	-11.341648	5.284825	0.755006

C	-12.476114	-4.563250	-0.599285
N	13.008211	5.686839	-0.253060
N	11.988826	-6.205663	0.887636
N	-11.815733	6.331023	0.896275
N	-13.175352	-5.475304	-0.735158

2TM(NMe₃⁺)

C	-0.65222300	-0.41882600	-0.15446200
C	-1.01380000	-1.65066900	0.34885700
H	-0.29311200	-2.42408700	0.59311300
C	-2.40961000	-1.81244600	0.48082700
H	-2.87021500	-2.72818900	0.83376200
C	-3.13453700	-0.71079000	0.08117600
S	-2.06221700	0.55309000	-0.45157100
C	-4.58010700	-0.52858900	0.07080900
C	-7.39955500	-0.19576900	0.06575900
C	-5.18595300	0.49355900	-0.66842000
C	-5.40876700	-1.38171900	0.81039600
C	-6.79234700	-1.24741000	0.79777500
C	-6.56343600	0.68578600	-0.66310600
H	-4.57097400	1.15497700	-1.27463400
H	-4.96493200	-2.16255700	1.42129300
B	-8.95118200	-0.01173500	0.06705800
C	-9.59255300	1.41443500	0.28512200
C	-10.75922900	3.92330800	0.72435200
C	-9.19088500	2.21171600	1.38160400
C	-10.58751200	1.90735900	-0.58210300
C	-11.15508300	3.16657500	-0.36442800
C	-9.78844400	3.45099700	1.59773700
H	-11.90558000	3.51605500	-1.06166600
H	-9.47066900	4.03263100	2.45671700
C	-9.91195000	-1.24499900	-0.15166900
C	-11.66138800	-3.38427300	-0.61097900
C	-10.99674200	-1.48644500	0.71416600
C	-9.71528500	-2.11005000	-1.25239500
C	-10.60133000	-3.16053700	-1.47964600
C	-11.85773100	-2.56416800	0.48650300
H	-10.43658400	-3.79403500	-2.34504600
H	-12.67161700	-2.72329300	1.18213400
N	-11.35864400	5.26392100	0.99727100
N	-12.58330100	-4.52267300	-0.90376100
C	0.66623500	0.09423000	-0.43064000
C	1.02505800	1.19835800	-1.17499300
S	2.07931200	-0.69990300	0.19779500
H	0.30163200	1.84061600	-1.66629400
C	2.42091600	1.39666100	-1.24301600
C	3.14705500	0.45146700	-0.55244600
H	2.88100600	2.22273700	-1.77349700
C	4.59381800	0.34338200	-0.41471400
C	5.18098300	-0.37470200	0.63257100
C	5.44007300	0.96521000	-1.34056300
C	6.56146700	-0.49644300	0.75397800
H	4.54753700	-0.84136200	1.38373100
C	6.82388300	0.89880900	-1.22416500
H	5.00909700	1.49925000	-2.18272700

C	7.41552200	0.15016100	-0.17448100
B	8.96926400	0.03226000	-0.05238900
C	9.64419000	-1.36341100	0.24676100
C	9.89182800	1.30185000	-0.21917700
C	9.30694000	-2.49632000	-0.52839900
C	10.59097000	-1.50744900	1.28032800
C	11.00079000	1.28733600	-1.09387000
C	9.63493000	2.46641700	0.53185500
C	9.90987700	-3.72471600	-0.26769400
C	11.16342900	-2.75500000	1.54530000
C	11.81100800	2.41363500	-1.21275400
C	10.48029200	3.57514200	0.42491100
C	10.82354100	-3.85015400	0.77060800
H	9.63818100	-4.57308000	-0.88755200
H	11.87082500	-2.82904400	2.36094700
C	11.55461300	3.54361300	-0.44712000
H	12.64316100	2.37837300	-1.90824800
H	10.26195200	4.44443000	1.03168900
N	11.41695400	-5.19633100	1.02934600
N	12.46531400	4.71759000	-0.59960800
C	7.64052500	1.60980200	-2.27335800
H	8.11441300	2.51104400	-1.87028500
H	8.44023300	0.98249900	-2.67960100
H	7.00445800	1.91445200	-3.10917500
C	7.08398800	-1.30104700	1.91726300
H	7.45877000	-2.27772900	1.59272000
H	7.90518600	-0.80138300	2.44018800
H	6.28780000	-1.47735400	2.64600800
C	8.46588000	2.57841800	1.47561100
H	7.52668600	2.69268200	0.92397100
H	8.35389200	1.69457700	2.11083000
H	8.57909100	3.44624800	2.13088400
C	11.34505100	0.08597100	-1.93348100
H	11.76932400	-0.71553200	-1.31984500
H	10.46885400	-0.32794400	-2.44243300
H	12.07919400	0.34550400	-2.70079800
C	11.01663200	-0.35598300	2.15302200
H	11.67558300	0.32927800	1.60947300
H	10.16528400	0.23131600	2.51025100
H	11.55954500	-0.71601400	3.03095200
C	8.30451600	-2.43884200	-1.65116100
H	7.28158700	-2.39652900	-1.26231100
H	8.43865700	-1.55859200	-2.28668200
H	8.38633800	-3.32437900	-2.28715600
C	-7.10747200	1.82876400	-1.48205400
H	-7.95460400	1.53205900	-2.10855500
H	-7.45311800	2.64933700	-0.84436900
H	-6.33283800	2.22638700	-2.14374600
C	-7.59247100	-2.22863700	1.61640800
H	-8.34796100	-1.73901800	2.23918000
H	-8.11991200	-2.94595700	0.97859200
H	-6.93546700	-2.79609000	2.28148100
C	-8.13161300	1.77114200	2.35760000
H	-8.28397800	0.74328600	2.70127400
H	-7.13636900	1.80937700	1.90311300
H	-8.12540500	2.41802800	3.23893300

C	-11.07856200	1.12877500	-1.77432600
H	-10.26141300	0.66354300	-2.33308400
H	-11.75778300	0.32571100	-1.46845500
H	-11.62091700	1.78007300	-2.46499300
C	-11.27707700	-0.62159700	1.91491400
H	-10.36750100	-0.37728100	2.47148000
H	-11.73882600	0.32662800	1.61937300
H	-11.96013100	-1.12531600	2.60414100
C	-8.57400300	-1.94212000	-2.22089400
H	-8.45163200	-0.90502800	-2.54739600
H	-7.62508900	-2.24458300	-1.76582000
H	-8.73088100	-2.55500100	-3.11251700
C	12.39785300	5.21506000	-2.01425900
H	11.36398700	5.48126400	-2.23294200
H	13.04598600	6.08716400	-2.10369800
H	12.73336500	4.42987300	-2.68864100
C	13.87169000	4.30808700	-0.27104000
H	14.51613700	5.18148900	-0.37376000
H	13.88831500	3.93657600	0.75327100
H	14.19273300	3.52813000	-0.95807400
C	12.10401800	5.85415000	0.30141100
H	11.10302400	6.20647900	0.05671400
H	12.15941100	5.52355700	1.33773300
H	12.82645500	6.65129300	0.12971900
C	12.39060100	-5.19102700	2.16360200
H	11.87933700	-4.88658200	3.07573000
H	12.77009000	-6.20567700	2.27654200
H	13.21186100	-4.51406500	1.93222000
C	12.14486000	-5.66905100	-0.19564600
H	11.44482900	-5.74998700	-1.02455200
H	12.92330900	-4.94395200	-0.43147000
H	12.58129800	-6.64506800	0.01883500
C	10.32090000	-6.16269000	1.37424400
H	9.80465700	-5.79070800	2.25896700
H	9.62744400	-6.23568300	0.53914000
H	10.77054800	-7.13593600	1.57262000
C	-13.66664400	-4.66844400	0.11593900
H	-14.27718400	-5.52351100	-0.17244800
H	-13.21978700	-4.84819500	1.09290800
H	-14.27742100	-3.76678900	0.12594600
C	-11.80719200	-5.80720900	-0.92761700
H	-12.50109100	-6.62271900	-1.13298100
H	-11.04966300	-5.75997500	-1.70705700
H	-11.33718500	-5.93946400	0.04644300
C	-13.23622800	-4.29946500	-2.23722500
H	-13.77974000	-3.35572600	-2.19808300
H	-12.47214700	-4.25975100	-3.01077100
H	-13.91872300	-5.12770300	-2.42852600
C	-10.28015700	6.30822900	0.97733600
H	-10.73973900	7.27871800	1.16596700
H	-9.54731600	6.08737800	1.75053100
H	-9.80708400	6.29193900	-0.00410400
C	-12.02360600	5.24688400	2.34321400
H	-12.47222300	6.22522200	2.51649700
H	-12.78727200	4.46964400	2.33700900
H	-11.28185300	5.03687000	3.11099900

C	-12.38833100	5.65545000	-0.01346800
H	-11.92741700	5.69947300	-0.99936200
H	-13.20433000	4.93419600	0.00377700
H	-12.76223300	6.64090100	0.26276500

5M-H

C	-1.735229	-0.199551	0.082173
N	-1.420910	-1.436440	0.613002
C	-0.031635	-1.660301	0.712024
O	0.465206	-2.690049	1.154189
C	0.531373	-0.434078	0.187063
C	-0.531418	0.434021	-0.187335
C	1.735174	0.199537	-0.082403
N	1.420847	1.436439	-0.613195
C	0.031565	1.660305	-0.712179
O	-0.465291	2.690097	-1.154211
C	3.065932	-0.267259	0.121458
C	3.429175	-1.500229	0.639095
H	2.688787	-2.237461	0.936416
C	4.821455	-1.670190	0.714570
H	5.294406	-2.578528	1.069697
C	5.541653	-0.580409	0.259448
S	4.470427	0.681938	-0.261678
C	-3.065979	0.267246	-0.121731
C	-3.429276	1.500256	-0.639218
H	-2.688920	2.237562	-0.936433
C	-4.821566	1.670182	-0.714652
H	-5.294552	2.578561	-1.069625
C	-5.541716	0.580322	-0.259654
S	-4.470454	-0.682120	0.261138
C	-6.987977	0.416679	-0.190063
C	-9.805873	0.128546	-0.068696
C	-7.826928	1.215911	-0.975380
C	-7.579381	-0.529861	0.653282
C	-8.959793	-0.697068	0.708867
C	-9.211841	1.099796	-0.909904
H	-7.391874	1.935275	-1.663664
H	-6.952116	-1.144936	1.295153
C	6.987914	-0.416773	0.189902
C	9.805818	-0.128619	0.068654
C	7.579348	0.529810	-0.653375
C	7.826845	-1.216064	0.975185
C	9.211760	-1.099947	0.909763
C	8.959761	0.697029	-0.708901
H	6.952113	1.144922	-1.295240

H	7.391779	-1.935486	1.663401
C	-9.498795	-1.755981	1.636439
H	-9.886474	-2.613647	1.076929
H	-10.320513	-1.387548	2.258942
H	-8.712028	-2.117018	2.305273
C	-10.031400	2.018380	-1.779942
H	-10.814983	1.485879	-2.328454
H	-9.394813	2.520732	-2.514162
H	-10.531422	2.788301	-1.183104
C	9.498800	1.756005	-1.636375
H	9.886598	2.613569	-1.076796
H	8.712031	2.117190	-2.305128
H	10.320447	1.387563	-2.258973
C	10.031297	-2.018599	1.779750
H	9.394629	-2.521328	2.513639
H	10.814581	-1.486052	2.328655
H	10.531700	-2.788205	1.182834
B	-11.372045	-0.029776	-0.000094
B	11.371984	0.029772	0.000178
C	-12.277506	1.239393	0.209970
C	-13.400255	1.466578	-0.621640
C	-11.982598	2.176775	1.228651
C	-12.804022	3.291556	1.407104
C	-14.181514	2.609094	-0.437922
H	-12.579461	3.994457	2.206134
H	-15.029784	2.783736	-1.095873
C	-12.019892	-1.456435	-0.141325
C	-12.993796	-1.897864	0.786047
C	-11.635862	-2.323637	-1.191801
C	-12.227891	-3.582891	-1.305819
C	-13.541598	-3.176282	0.663038
H	-11.939695	-4.232932	-2.128822
H	-14.273994	-3.512764	1.393360
C	12.019801	1.456434	0.141647
C	11.635802	2.323441	1.192296
C	12.993752	1.897999	-0.785607
C	13.541666	3.176338	-0.662300
C	12.227944	3.582620	1.306610
H	14.274095	3.512928	-1.392539
H	11.939771	4.232504	2.129742
C	12.277556	-1.239301	-0.209973
C	13.400321	-1.466457	0.621613
C	11.982795	-2.176563	-1.228810
C	12.804354	-3.291226	-1.407393
C	14.181726	-2.608853	0.437755
H	12.579913	-3.994032	-2.206539
H	15.030013	-2.783468	1.095689
C	-10.610343	-1.932355	-2.225987

H	-10.635739	-2.627045	-3.070989
H	-9.596346	-1.946212	-1.811834
H	-10.776158	-0.925039	-2.622000
C	-13.462770	-1.039845	1.934156
H	-14.115693	-0.231160	1.588522
H	-12.634902	-0.566908	2.472413
H	-14.025454	-1.641025	2.654714
C	-10.808875	2.012848	2.161362
H	-9.861600	2.232534	1.656980
H	-10.726363	0.996297	2.559619
H	-10.899910	2.694173	3.012691
C	-13.787691	0.521238	-1.730945
H	-14.524295	0.989155	-2.391060
H	-14.227916	-0.400493	-1.335608
H	-12.933507	0.222323	-2.347317
C	10.610210	1.932037	2.226362
H	10.776180	0.924781	2.622482
H	9.596270	1.945648	1.812073
H	10.635355	2.626794	3.071315
C	13.462654	1.040194	-1.933904
H	14.115752	0.231556	-1.588478
H	14.025144	1.641547	-2.654473
H	12.634767	0.567214	-2.472088
C	13.787652	-0.521180	1.731008
H	14.524175	-0.989148	2.391178
H	12.933404	-0.222282	2.347291
H	14.227946	0.400565	1.335766
C	10.809089	-2.012661	-2.161544
H	9.861859	-2.232889	-1.657302
H	10.900411	-2.693637	-3.013118
H	10.726226	-0.995991	-2.559410
C	13.170035	4.015135	0.381259
C	13.894413	-3.515379	-0.575394
C	-13.169907	-4.015285	-0.380332
C	-13.894078	3.515717	0.575107
H	-2.089781	-2.129777	0.917300
H	2.089731	2.129931	-0.917108
H	13.613751	5.003036	0.473473
H	14.518510	-4.394011	-0.716325
H	-13.613536	-5.003245	-0.472313
H	-14.518062	4.394446	0.715922

5M-CN

C	-1.73509300	-0.22414800	0.03680700
N	-1.42327300	-1.43998900	0.61498700
C	-0.03442700	-1.66216100	0.72244000
O	0.46106800	-2.67404200	1.20454200
C	0.53065700	-0.45805000	0.14925500

C	-0.53059500	0.39603800	-0.25868600
C	1.73515900	0.16368800	-0.14298700
N	1.42335200	1.37913700	-0.72194200
C	0.03449200	1.60101300	-0.83007000
O	-0.46098900	2.61340100	-1.31109000
C	3.06502400	-0.29630200	0.08375900
C	3.42368200	-1.50659300	0.65559900
H	2.68100400	-2.22995600	0.97993800
C	4.81522100	-1.67311100	0.74787700
H	5.28565000	-2.56515800	1.14510400
C	5.53782100	-0.60351700	0.25104200
S	4.47143700	0.63499300	-0.33190500
C	-3.06494800	0.23956500	-0.18193300
C	-3.42391900	1.45412400	-0.74437100
H	-2.68140700	2.17648000	-1.07128100
C	-4.81545000	1.62698700	-0.82232300
H	-5.28483700	2.52358200	-1.21033800
C	-5.53830900	0.55774200	-0.32462800
S	-4.47121400	-0.68860500	0.24081000
C	-6.98488500	0.40510000	-0.24302200
C	-9.80314500	0.14018700	-0.09546900
C	-7.82375000	1.19570100	-1.03727900
C	-7.57661800	-0.52196800	0.62157500
C	-8.95683400	-0.68010800	0.69028600
C	-9.20840400	1.09314700	-0.95944600
H	-7.38909800	1.89818400	-1.74250900
H	-6.94944700	-1.12926400	1.27040400
C	6.98446800	-0.44296900	0.18644300
C	9.80177300	-0.15329700	0.08346900
C	7.58304800	0.45884900	-0.69976400
C	7.81535500	-1.19880400	1.02161200
C	9.20028100	-1.08395500	0.96697700
C	8.96278000	0.62845700	-0.74820300
H	6.96183500	1.03557700	-1.38136000
H	7.37326500	-1.88089600	1.74217800
C	-9.49119100	-1.71749700	1.64424100
H	-9.88032600	-2.58964900	1.10839400
H	-10.30615000	-1.33556900	2.26705700
H	-8.69963700	-2.06426700	2.31440800
C	-10.02298900	2.00121800	-1.84485900
H	-10.82186200	1.46926700	-2.37081100
H	-9.38624100	2.46993800	-2.60039500
H	-10.49823000	2.80075500	-1.26671300
C	9.50544900	1.63578200	-1.72932600
H	9.87115800	2.53311500	-1.21914400
H	8.72487000	1.94576000	-2.42973300
H	10.33899000	1.24105100	-2.31870400
C	10.00625200	-1.95277900	1.89847600

H	9.35816600	-2.40829400	2.65243000
H	10.78454900	-1.39353500	2.42696600
H	10.50683300	-2.76193500	1.35620100
B	-11.36168400	-0.00130400	-0.00869200
B	11.35952900	0.01193300	0.03213800
C	-12.27131500	1.28105700	0.12710300
C	-13.38337100	1.47207300	-0.72630400
C	-11.98504900	2.24819500	1.12005100
C	-12.80383800	3.36582100	1.25541300
C	-14.17165700	2.61180800	-0.59489600
H	-12.59576500	4.10155100	2.02630700
H	-15.01554700	2.76877000	-1.25981700
C	-12.03779900	-1.42626800	-0.05476200
C	-12.99297500	-1.80409500	0.91791700
C	-11.70034600	-2.33549500	-1.08550900
C	-12.31968300	-3.58094900	-1.14100800
C	-13.57815500	-3.06588500	0.86273500
H	-12.07458200	-4.27452400	-1.93962900
H	-14.29907800	-3.36431500	1.61780000
C	12.00891000	1.45010400	0.04505400
C	11.62739700	2.38941900	1.03259000
C	12.98460400	1.80996100	-0.91394700
C	13.54716800	3.08291200	-0.88811000
C	12.22449600	3.64662400	1.06033000
H	14.28406700	3.36677700	-1.63329000
H	11.94560700	4.36368800	1.82645400
C	12.29664500	-1.25608500	-0.03153200
C	13.38888600	-1.39241800	0.85721800
C	12.05669500	-2.26447000	-0.99529300
C	12.90172700	-3.36825500	-1.06860400
C	14.20377300	-2.51884700	0.78786800
H	12.72945500	-4.13568000	-1.81711700
H	15.03261300	-2.63380200	1.47974400
C	-10.68830100	-2.00892600	-2.15310800
H	-10.75132800	-2.72923400	-2.97336100
H	-9.66871700	-2.04073900	-1.75495500
H	-10.83270000	-1.01052300	-2.57759500
C	-13.40280200	-0.88887200	2.04199600
H	-14.04406600	-0.07829600	1.68028400
H	-12.54372500	-0.42284000	2.53489700
H	-13.95928800	-1.44148700	2.80385800
C	-10.81780800	2.11835000	2.06424900
H	-9.87135000	2.32980900	1.55564000
H	-10.73236200	1.11389700	2.49017900
H	-10.91754200	2.82240200	2.89494800
C	-13.75245800	0.48443400	-1.80214700
H	-14.48126700	0.92085800	-2.49052500
H	-14.19546100	-0.42107600	-1.37447400

H	-12.88755100	0.16957400	-2.39435800
C	10.59073000	2.08412900	2.08277400
H	10.73707500	1.10307500	2.54528800
H	9.58226300	2.08712300	1.65598800
H	10.62077100	2.83295500	2.87901700
C	13.44114500	0.86277700	-1.99261900
H	14.09056800	0.08081500	-1.58526700
H	14.00416900	1.39881400	-2.76150500
H	12.60459900	0.35958400	-2.48756200
C	13.70934200	-0.35950600	1.90585600
H	14.42225100	-0.75860600	2.63249800
H	12.82195800	-0.03590700	2.45863200
H	14.15294700	0.53596400	1.45803300
C	10.91189200	-2.19359400	-1.97259700
H	9.95666700	-2.40229800	-1.47948100
H	11.04491100	-2.92777400	-2.77198500
H	10.81960000	-1.20831300	-2.44000100
C	13.17569000	3.99726800	0.09985000
C	13.96745300	-3.50117900	-0.17599900
C	-13.24989800	-3.95017300	-0.16704400
C	-13.88903300	3.55346500	0.39678800
H	-2.09308400	-2.11957500	0.94700500
H	2.09316700	2.06015100	-1.05100800
C	-14.71338500	4.71266100	0.53364600
C	-13.86785000	-5.23733800	-0.22452400
C	13.77075200	5.29615700	0.12818200
C	14.81922100	-4.64621300	-0.24911500
N	14.25479800	6.35256400	0.15110100
N	15.51204300	-5.57752400	-0.30805700
N	-15.38391900	5.65548600	0.64445600
N	-14.37043600	-6.28426500	-0.27111900

5M(NMe₃⁺)

C	-1.325515	1.040811	0.566702
N	-0.316236	1.880907	1.004200
H	-0.453707	2.776799	1.447898
C	0.975053	1.373611	0.753600
O	2.010484	1.952039	1.051330
C	0.702976	0.104529	0.104774
C	-0.706219	-0.061647	0.004502
C	1.320742	-1.015893	-0.422651
N	0.310644	-1.861695	-0.847084
H	0.448863	-2.743681	-1.317224
C	-0.979415	-1.340359	-0.623935
O	-2.015023	-1.913977	-0.930679
C	2.700302	-1.358678	-0.552401
C	3.238377	-2.544759	-1.024526
H	2.640317	-3.390098	-1.347121

C	4.642362	-2.551907	-1.023061
H	5.234359	-3.403937	-1.335967
C	5.194950	-1.375276	-0.551808
S	3.958702	-0.245431	-0.105351
C	6.606460	-1.037557	-0.417167
C	9.357080	-0.389841	-0.186394
C	7.031671	0.024420	0.388559
C	7.579481	-1.774182	-1.102952
C	8.933738	-1.485479	-0.980011
C	8.374331	0.370680	0.493918
H	6.300168	0.593643	0.957568
H	7.275162	-2.582757	-1.761232
B	10.873103	-0.021796	-0.077334
C	11.342231	1.475862	-0.251814
C	12.166950	4.133637	-0.586489
C	10.900462	2.232645	-1.356508
C	12.213775	2.081995	0.681149
C	12.607453	3.407351	0.512293
C	11.328218	3.553947	-1.522053
H	13.264453	3.847084	1.255331
H	10.975886	4.097791	-2.388819
C	11.946138	-1.146469	0.200218
C	13.828903	-3.158439	0.707549
C	13.101030	-1.270034	-0.604794
C	11.763006	-2.050542	1.266294
C	12.715499	-3.042139	1.521154
C	14.023169	-2.283413	-0.353534
H	12.545843	-3.708415	2.357153
H	14.888013	-2.364303	-1.004322
N	12.625523	5.548972	-0.728395
N	14.848318	-4.226918	0.937823
C	-2.707617	1.358194	0.731951
C	-3.256869	2.475297	1.339927
S	-3.956282	0.291869	0.158521
H	-2.666519	3.277834	1.768046
C	-4.661408	2.469660	1.338409
C	-5.201242	1.353519	0.727256
H	-5.264138	3.271343	1.749471
C	-6.609331	1.023917	0.543662
C	-7.028954	0.141507	-0.457404
C	-7.581846	1.588673	1.376422
C	-8.368559	-0.194811	-0.619954
H	-6.296015	-0.284464	-1.138529
C	-8.933543	1.305346	1.214660
H	-7.275400	2.248767	2.182873
C	-9.352963	0.391502	0.214459
B	-10.863820	0.024717	0.047862
C	-11.304175	-1.482837	-0.117198

C	-11.968791	1.152673	0.055067
C	-10.855507	-2.453788	0.800594
C	-12.159733	-1.883421	-1.167318
C	-13.102474	1.059354	0.893184
C	-11.835418	2.278622	-0.782186
C	-11.267610	-3.784473	0.676969
C	-12.536102	-3.218675	-1.290650
C	-14.049832	2.080494	0.902299
C	-12.814736	3.276855	-0.783801
C	-12.096804	-4.157531	-0.366495
H	-10.914086	-4.497608	1.410563
H	-13.178429	-3.499102	-2.119019
C	-13.905007	3.177273	0.062740
H	-14.896235	1.991404	1.575561
H	-12.684383	4.118883	-1.451440
N	-12.538053	-5.575284	-0.538464
N	-14.947794	4.246611	0.113113
C	-9.898098	1.969037	2.164841
H	-10.484623	2.746434	1.664121
H	-10.610942	1.263047	2.602928
H	-9.356217	2.440786	2.989067
C	-8.712045	-1.159253	-1.726702
H	-8.981523	-2.144459	-1.331812
H	-9.554344	-0.816397	-2.336074
H	-7.857030	-1.292604	-2.395193
C	-10.657497	2.468628	-1.701559
H	-9.774358	2.797693	-1.143203
H	-10.378196	1.548112	-2.221653
H	-10.876676	3.225025	-2.459990
C	-13.328891	-0.110470	1.813850
H	-13.623201	-1.003432	1.252352
H	-12.431220	-0.370541	2.383155
H	-14.121520	0.109534	2.533802
C	-12.680448	-0.910671	-2.191503
H	-13.455885	-0.266035	-1.764478
H	-11.892914	-0.255286	-2.575879
H	-13.114094	-1.437445	-3.045722
C	-9.932221	-2.122174	1.943650
H	-8.903812	-1.988707	1.591428
H	-10.213391	-1.196687	2.453987
H	-9.931841	-2.924195	2.686809
C	8.722212	1.545388	1.372397
H	9.566981	1.340028	2.037546
H	8.989508	2.424249	0.775985
H	7.869445	1.818790	1.999929
C	9.900065	-2.351872	-1.747313
H	10.641261	-1.768285	-2.302724
H	10.453836	-3.020326	-1.079549

H	9.364365	-2.973790	-2.469826
C	9.967807	1.678645	-2.402091
H	10.242236	0.667337	-2.715180
H	8.941249	1.625201	-2.024647
H	9.965482	2.312981	-3.292704
C	12.733903	1.348138	1.888550
H	11.938236	0.823902	2.426815
H	13.478955	0.597418	1.605387
H	13.205886	2.039888	2.591304
C	13.377943	-0.345627	-1.760604
H	12.505452	-0.221401	-2.409647
H	13.661155	0.651871	-1.409242
H	14.194832	-0.729089	-2.377693
C	10.561353	-2.003377	2.173605
H	10.316384	-0.985935	2.491565
H	9.673474	-2.400970	1.670722
H	10.732480	-2.599314	3.074166
C	-14.953975	4.862521	1.482373
H	-13.969482	5.292470	1.666665
H	-15.721676	5.636029	1.509786
H	-15.170611	4.095013	2.222399
C	-16.293873	3.653351	-0.186662
H	-16.546229	2.916627	0.573351
H	-17.031326	4.456873	-0.181938
H	-16.245658	3.180119	-1.167465
C	-14.708111	5.341488	-0.876887
H	-13.754250	5.821482	-0.662559
H	-14.719809	4.927408	-1.884404
H	-15.514928	6.065791	-0.768552
C	-14.037294	-5.644427	-0.507324
H	-14.446250	-5.046749	-1.319398
H	-14.335828	-6.686506	-0.625857
H	-14.377756	-5.256136	0.452002
C	-12.020988	-6.474401	0.537833
H	-10.932058	-6.474105	0.516233
H	-12.392130	-6.130421	1.502659
H	-12.391665	-7.478814	0.336060
C	-12.034967	-6.099654	-1.852395
H	-12.442424	-5.498516	-2.662737
H	-10.946942	-6.038987	-1.850444
H	-12.361051	-7.135078	-1.955961
C	14.928791	-5.108419	-0.275425
H	15.656930	-5.896228	-0.079457
H	13.941973	-5.533935	-0.457133
H	15.244187	-4.516224	-1.132148
C	14.524856	-5.095362	2.111140
H	13.575067	-5.600218	1.939517
H	15.321280	-5.832921	2.202906

H	14.484272	-4.484412	3.012004
C	16.187036	-3.598493	1.195022
H	16.478987	-3.002845	0.332977
H	16.105150	-2.964584	2.077590
H	16.913764	-4.394322	1.361516
C	12.204708	6.336069	0.479001
H	12.672223	5.916373	1.367217
H	12.525075	7.369643	0.343964
H	11.119962	6.277510	0.563390
C	12.050467	6.226418	-1.931047
H	12.369230	5.701315	-2.830298
H	10.963883	6.240948	-1.852816
H	12.431332	7.246873	-1.947649
C	14.121190	5.578871	-0.855198
H	14.436043	6.616012	-0.975189
H	14.568120	5.157001	0.042889
H	14.403732	4.989225	-1.727238