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Revisiting carbenium chemistry
on Amorphous Silica Alumina:
unraveling their milder acidity as compared to zeolites

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Abstract

Amorphous silica-aluminas (ASA) are prominent solids for their acidic properties. They are of first interest in catalysis, in particular for cracking reactions. Their relative acidity as compared to zeolites is a long-lasting general issue, driven by the limited knowledge of the surface structure of ASA, due to their amorphous nature. In the present contribution, thanks to a first principles approach based on our original ASA surface model, and on the study of a model mordenite zeolite (MOR), we propose a rational explanation for this feature. We compare by density functional theory calculations the ability of ASA and MOR to generate carbenium species from isobutene, *versus* π -complexes and alkoxide species. On ASA, carbenium species can be formed on Pseudo-Bridging Silanols (PBS) only, and are much less stable than in MOR. Then, we investigate the cracking pathway of a model alkene, 2,4,4-trimethyl-2-pentene (DIB), by quantifying the stability of relevant intermediates of carbocationic and alkoxide natures. The carbocationic pathway is favored in MOR, whereas on ASA this pathway is strongly activated. By contrast, the PBS on ASA initiate preferentially a tertiary alkoxide route, or possibly a combined carbocationic/alkoxy route. Finally, the *i*-butene desorption step is also limiting in MOR due to the confinement effect induced by the zeolite pores. As a result, the higher cracking reactivity of zeolites as compared to ASA is mainly attributed to the favored nature of the carbenium route, stabilized by higher electrostatic confinement effect.

Keywords

Heterogeneous catalysis, amorphous silica alumina, zeolite, cracking, carbocation, carbenium, alkoxide, DFT, isobutene, 2,4,4-trimethyl-2-pentene, confinement effect.

1. Introduction

The concept of Brønsted acidity[1] has been studied for a long time in the context of aqueous solutions, but its application to solid surfaces still remains an issue. One significant example is the case of amorphous silica-alumina (ASA) materials, which are widely used in fine chemistry,[2-4] biomass conversion[5, 6] and in industrial refining processes.[7] Indeed, the intimate chemical mixing of silica with alumina in ASA materials is empirically known to promote an enhanced surface Brønsted acidity with respect to the reference alumina or silica solids themselves. At the same time, this acidity is milder than the one observed in microporous alumino-silicates such as zeolites.[8, 9] This milder acidity is targeted in industrial processes such as hydrocracking (HCK) in order to reach optimal cracking selectivity into middle distillate products.[10, 11] However, the origin of this milder acidity as compared to zeolites is still questioned, due to the difficulty to reach a resolution at the molecular scale of ASA surfaces – amorphous systems – and of the intermediates involved during reactions even by using cutting edge operando techniques. Understanding the acidity of ASA is moreover of prominent interest because they are also suspected to be present as debris in (non-leached) de-aluminated zeolites.[12, 13] Interestingly, ASA and ultrastable-Y zeolite have been found to exhibit similar hydrocracking patterns in the conversion of the pristane model molecule.[14]

Bifunctional catalysts such as used in HCK processes require an optimal control of the balance between the hydrogenation function and the acidic function.[7, 15-18] For that purpose, various types of catalytic supports exhibiting a tuneable acidity scale (mesoporous alumina, ASA or zeolites) are industrially used in combination with a hydrogenating active phase (either a transition metal sulfide or a reduced metal).[7, 17] Indeed, it is crucial to optimize the acidic function of the HCK support: the milder acidity of ASA as compared to

zeolites is profitably used to convert petroleum feeds containing also refractory compounds (such as nitrogen organic ones) in a selective way.

Many experimental studies[19-29] have analyzed the nature of possible Brønsted acid sites (BAS) on ASA: zeolite-like Si-(OH)-Al groups,[19-22] silanols in the vicinity of aluminum atoms[23-25] and water molecules adsorbed on aluminum atoms[26, 27]. However, at a molecular scale, it remains crucial to understand the precise chemical behavior of the ASA Brønsted acid sites, how they catalyze cracking reactions and the reasons of their milder acidity of ASA as compared to zeolites. In particular, it is proposed that ASA surface would exhibit very few BAS with an acidic character very similar to BAS found in zeolite.[21, 30] However, this interpretation remains questionable because it is also well known that the strength depends on both the local BAS atomic structure and the confinement effect depending on the pores' size surrounding the BAS.[31, 32]

Using density functional theory (DFT) calculations, some of us recently established a relevant ASA surface model which renders the diversity of surface Brønsted acid sites and highlights the existence of pseudo-bridging silanols (PBS).[33] In particular, PBS-Al sites consist of silanols whose oxygen atom is close to an aluminum atom, and able to be bonded to it upon deprotonation (**Figure 1**). The surface model also shows the presence of silicic PBS site (PBS-Si, see **Figure 1**), other silanols, for which Si-O-Al bridges coexist (called hereafter Silanol-Al), and water molecules adsorbed on aluminum atoms (III_1 in **figure 1**).

-- HERE FIGURE 1 --

So far, DFT approaches investigated the surface Brønsted acidity by calculating the adsorption of probe molecules,[34] in particular 2,6-lutidine[35] and CO.[36] The lutidine protonation was shown to be favored when the conjugated base of the BAS is stabilized. In

particular, the PBS-Si site depicted in **Figure 1** and the PBS-Al site called $\text{Si(V}_1\text{)-OH}\cdots\text{Al}_{\text{IV}}$ (III_3) are both able to transfer their proton to lutidine, thanks to the formation of a new Si-O and Al-O bond after deprotonation, respectively. Other PBS-Al sites were not able to do so due to angular constraints,[33] while Silanol-Al sites are not deprotonated because the conjugated silanolate cannot be stabilized. The water molecule adsorbed on the III_1 aluminum atom can generate lutidinium, as an Al-OH group is formed. Cascade proton transfer can also occur from this adsorbed water molecule to the neighboring silanol group.[35] The vibrational stretching of CO was found sensitive to the electrostatic field at the surface of aluminosilicic materials.[36] In the course of a reaction involving a hydrocarbon, both aspects (proton transfer and local electrostatic field) are expected to play a role. In particular the relation between the structure of the sites, the protonation ability towards lutidine, the electrostatic field, and the reactivity in cracking reactions, remains to be understood.

For zeolite catalysts, it is quite widely admitted that olefin cracking proceeds via carbenium ions (formed on protonic sites of the material),[37] well known in organic chemistry.[38-40] After formation, and possible isomerization, these species are considered to undergo β -scission (**Figure 2**).[16, 18, 41-44]

-- HERE FIGURE 2 --

However, isolating carbocations within or on the surface of aluminosilicates remains a challenging task due to their supposed short lifetime.[45, 46] Highly resonant species mainly could be observed in zeolites,[45, 47, 48] even if indirect evidence was provided by ^{13}C NMR for the transient formation of short-live carbenium ions in the case of long-chain or branched

olefins.[49-51] Alternative proposals to carbenium β -scission can thus be recorded. Sie[52] proposes a pathway invoking hydride shifts and highly non classical cyclopropane-like intermediates, by analogy with what is known about isomerization reactions.[53] Up to date, no confirmation of this kind of pathway could ever be given.[16] Moreover, alkoxides (**Figure 3**) were characterized in zeolites thanks to ^{13}C NMR[51, 54, 55] and FTIR[56, 57] and were calculated as stable species by earlier quantum chemical calculations,[58-64] which led some authors to refute the existence of carbenium ions as cracking intermediates in zeolites, even for tertiary carbenium. The intermediate or transition state nature of carbenium in zeolites as calculated by quantum chemistry however appears to be strongly dependant on the alkene considered,[65] but also on the level of theory (DFT, with or without dispersion corrections, *versus* post-Hartree-Fock methods for example),[66, 67] on the kind of model – small clusters versus periodic cells – and on the local geometry of the active site.[65, 68-75] Indeed, taking into account the electrostatics induced by the porosity leads to a stabilization of charged species whereas the stability of the neutral species remains almost unchanged. Temperature effects are also shown to affect the alkoxide existence probability over that of carbenium, according to DFT calculations.[76-78]

-- HERE FIGURE 3 --

In the case of ASA, the formation of carbenium ions thanks to surface proton transfers was also invoked for a long time[15, 79, 80] even if alkoxides are mainly observed by FTIR.[56] Generally, the catalytic activity of ASA in acid-catalyzed reactions is lower than zeolites.[18, 81] This could be either due to intrinsically weaker sites,[82] or to a lower amount of the same kind of sites (bridging Si-(OH)-Al groups) than in zeolites.[21, 30] There

is however a lack of detailed data both on the stability of carbenium species on these solids, and on their implication in the conversion of hydrocarbons, in particular cracking of alkenes.

In the present work, we propose to determine the energetics of carbocation / alkoxide formation followed by C-C β -scission for BAS located on ASA surface and in a reference zeolite (mordenite, MOR), thanks to periodic DFT+D calculations. As indicated above, we suspect that confinement effects may play a key role, so it is mandatory to include dispersion corrections. We chose a model molecule, 2,4,4-trimethyl-2-pentene (DIB, 8 carbon atoms), as its branched character is expected to render the formation of carbocations and the β -scission favorable, with stable intermediates (**Figure 2**). Indeed, the β -scission of carbocations produced from linear alkenes generates a primary carbenium ion, which is energetically highly unfavorable.[16] Thus, the n-alkylcarbenium ions undergo skeletal isomerization first, leading to branched isomers. In the present study, we do not address any preliminary isomerization reaction, but focus on the C-C bond cleavage from a multi-branched species. This is the archetype of the so-called "type A" β -scission,[83] which both starts and ends up with tertiary carbenium ions.

So as to investigate such mechanism, the physicochemical interaction of isobutene (formed upon DIB cracking) with the acid sites of the surface has to be understood first. Stable intermediates and energy profiles will be investigated, but at this stage activation energies are not evaluated: however we will show that the quantitative analysis of the thermodynamic profiles is very much insightful for discriminating the two acid solids. The relative stabilities of the π -complex, the tert-butyl cation and isobutoxy species (**Figure 3**) were studied on various sites of the ASA surface model, in comparison with mordenite. The existence of a possible link between the lutidine (results from ref. [35]) *versus* alkene protonation abilities will be looked at, also in comparison with CO adsorption features (results from ref. [36]). Then, the implication of the stability of the various intermediates in the shape

of the reaction profile for the cracking of DIB will be detailed on the most important site of ASA, PBS-Al (**Figure 1**), in comparison with the acid site of mordenite. PBS-Al site was indeed shown to protonate lutidine,[35] and induces a strong electrostatic field.[36] Temperature effects are taken into account thanks to a statistical thermodynamic approach to understand the nature of the preferred pathways. We will finally show how the confinement effects,[31, 32, 69, 84] existing in zeolites but absent from ASA, are determining the nature of the preferred pathway on each solid and the lower acidity of ASA as compared to the reference MOR zeolite.

2. Methodology

The ASA supercell was the same as in references [33, 35] for $\theta_{\text{OH}} = 5.4 \text{ nm}^{-2}$ (**Figure 1**), with dimensions of $11.13 \times 16.77 \times 43 \text{ \AA}^3$. The OH content chosen represents typical reaction conditions used in catalysis and characterization experiments (see ref. [33] for a full thermodynamic diagram). Model mordenite (with a main channel circumscribed by twelve-membered rings - 12 MR) was considered to depict the behavior of a typical proton exchanged zeolite. The primitive cell, doubled in the c direction was considered (dimensions: $13.78 \times 13.78 \times 15.15 \text{ \AA}^3$). One T_4 site was substituted by an Al atom, with a proton in the O_{10} position (see for example reference [85] for structural details).

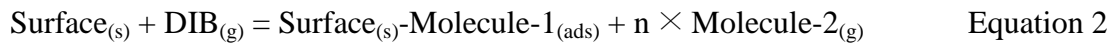
Periodic DFT calculations were carried out with the PBE exchange-correlation functional[86] as implemented in VASP 5.2.[87, 88] The projected augmented wave (PAW) method[89] was used to describe the core-electrons interactions and the plane wave basis set was limited to a kinetic cut-off energy of 500 eV. Van der Waals corrections as proposed within the Grimme formalism[90] was applied. These corrections are mandatory to evaluate reasonably accurate energies of hydrocarbons adsorbed on aluminosilicates, even if systematic deviation from experimental values is still observed.[66, 91, 92] $2 \times 1 \times 1$ and $2 \times 2 \times 2$

K-points meshes were used for the ASA and MOR supercells respectively. A dipolar correction was applied to account for the arbitrary interaction between asymmetric - thus polar - slabs in the case of ASA. We achieved geometry optimizations with a convergence criterion on forces on relaxed atoms ($< 2 \cdot 10^{-2} \text{ eV} \cdot \text{\AA}^{-1}$). We also explored the energy potential landscape by performing velocity scaled molecular dynamics (time step: 3 fs, artificial mass for hydrogen: 5 u.a., 500 K, energy cutoff: 400 eV), followed by quenching performed with an energy cutoff of 500 eV, to solve the configurations of the DIB molecule adsorbed on BAS.

The stability of each adsorbed species was first quantified by an energetic approach, calculating the reaction energy $\Delta_r U$, and decomposing it into Kohn-Sham (DFT-PBE, $\Delta_r U_{\text{DFT}}$ term) and dispersion (Grimme, $\Delta_r U_{\text{disp}}$ term) contributions, according to equation 1.

$$\Delta_r U = U_{\text{adsorbed-species}} - U_{\text{alkene}} - U_{\text{site}} = \Delta_r U_{\text{DFT}} + \Delta_r U_{\text{disp}} \quad \text{Equation 1}$$

Thermal corrections were then introduced as explained below, to obtain the reaction Gibbs energy $\Delta_r G$. Then, we considered DIB cracking (equation 2).



$\text{Surface}_{(s)}$ depicts the surface (external surface of ASA or internal surface of MOR) on which the $\text{DIB}_{(g)}$ adsorbs to generate the $\text{Surface}_{(s)}\text{-Molecule-1}_{(ads)}$ system, together with the possible release of n $\text{Molecule-2}_{(g)}$ (when DIB is transformed into isobutene, $n=1$ then $n=2$). Thermal and entropic corrections were then included for evaluating the reaction Gibbs free energy (equation 3 and 4), considering a temperature of 500 K, which is typical of hydrocracking reaction conditions,[16] and standard pressure.

$$\Delta_r G(T) = G_{\text{Surface}_{(s)}\text{-Molecule-1}_{(ads)}} + n \times G_{\text{Molecule-2}_{(g)}} - G_{\text{Surface}_{(s)}} - G_{\text{DIB}_{(g)}} \quad \text{Equation 3}$$

$$\text{with : } G(T) = U_{\text{elec}} + F_{\text{trans}(T)} + F_{\text{rot}(T)} + F_{\text{vib}(T)} + PV_m + \text{ZPE} \quad \text{Equation 4}$$

where $F_{\text{trans}(T)}$, $F_{\text{rot}(T)}$ and $F_{\text{vib}(T)}$ are translational, rotational and vibrational contributions to free energy, V_m the molar volume, U_{elec} the electronic (DFT+D) contribution to energy, ZPE

the zero-point vibrational energy.

To evaluate $F_{\text{trans}(T)}$, $F_{\text{rot}(T)}$ and $F_{\text{vib}(T)}$, we calculated the partition function of each gaseous and adsorbed species, considering each gaseous species as ideal gas (see **Supporting Information S1.1.**) and adsorbed species as partially immobile gaseous species. For each adsorbed molecules (see **Supporting Information S1.2.** for details), we assumed that some translational contributions to enthalpy and entropy are lost upon adsorption: one over three degree of freedom is lost for carbenium and π -complexes (2D gas model), whereas alkoxy species are supposed to be immobile from a translational point of view. Indeed, the latter are linked to the surface by an additional C-O bond. In the same spirit, we also considered that one rotational degree of freedom over three is lost upon adsorption for π -complexes and carbenium species, two degrees of freedom being lost for alkoxides. Indeed, partial rotational freedom has been experimentally evidenced on related systems.[93] In a first approach, we kept unchanged the vibrational contribution to enthalpy H and entropy S as compared to gas phase species. Although some of the approximations performed here differ from previously published calculations dealing with isobutene reactivity in zeolites,[77, 78] it can be noted that difference in Gibbs free energy corrections between the tertiary alkoxides and carbenium species are of the same order of magnitude: $(\Delta_r G - \Delta_r U)_{\text{carbenium}} - (\Delta_r G - \Delta_r U)_{\text{alkoxide}}$ equals to $70 \text{ kJ}\cdot\text{mol}^{-1}$ at 500 K in our case, whereas it was evaluated around $70 \text{ kJ}\cdot\text{mol}^{-1}$ in mordenite by Nguyen et al.,[78] and about $80 \text{ kJ}\cdot\text{mol}^{-1}$ from extrapolated values after Tuma and Sauer.[77] This validates the $\Delta_r G$ values which will be presented in the following, even if refinements could be brought to check the assumptions made for their calculation.

As mentioned in Introduction, activation reaction energies were not evaluated at this stage but we will show that the chemical behaviors of the two acid materials can already be differentiated according to the trends revealed by the energy profiles. Note also that the present study lacks from self-interactions corrections due to the level of theory used (DFT),

which is expected to affect the overall energetics.[67] Main trends regarding the ASA *versus* MOR comparison might however not be strongly affected.

Electrostatic field was calculated in the surrounding of the C=C bond of the isobutene molecule when adsorbed as a π -complex mode. For that purpose, we calculated the local electrostatic potential on the system, after removing the isobutene molecule, but keeping all other geometric features constrained. The gradient of the electrostatic potential (ionic *plus* Hartree *plus* exchange-correlation) was estimated between two points A and B distant by 1 Å, aligned perpendicular to the π -bonding of the molecule, the middle of the [AB] segment being also the middle of the [C=C] one. Note that the electrostatic field determined in the present work differs from previous values reported in ref. [36] due to the inclusion of the exchange-correlation potential (available in the present version of VASP) and to the different geometry of the acid site after CO versus isobutene adsorption.

3. Results and discussion

3.1. Isobutene interaction with surface acid sites

We firstly investigate the stability of key intermediates obtained upon interaction of isobutene with the acid sites of ASA and MOR. The stability and structures of the π -complex, carbenium and alkoxides are compared in **Table 1**.

Table 1. Formation energies $\Delta_r U$ of the π -complex (physisorption), the carbenium ion and the alkoxide from isobutene on various sites of the ASA surface and in MOR ; decomposition (see eq. 1) of $\Delta_r U$ into the DFT energy ($\Delta_r U_{\text{DFT}}$) and dispersion correction terms ($\Delta_r U_{\text{disp}}$) ; distance between the π -complex (terminal C atom of the C=C bond) and the acid site ($\text{H}\cdots\pi$), and $\text{O}_{\text{site}}\text{-C}_{\text{alkoxide}}$ bond length ;

Acid site ¹	Protonation ability of lutidine ²	Location and terminology (see figure 1)	$\Delta_r U$ (kJ/mol)			Decomposition of $\Delta_r U$: $\Delta_r U_{\text{DFT}}$ ($\Delta_r U_{\text{disp}}$) (kJ/mol)			H $\cdots\pi$ distance, O _{site} -C _{alkoxide} bond length (Å)		Electrostatic field (V.nm ⁻¹) ³
			π -complex	Carbenium	Alkoxide	π -complex	Carbenium	Alkoxide	π -complex	Alkoxide	
PBS-Si	protonation	Si(U ₁)-OH \cdots Si(V ₂)	-13	+61	-16	+19 (-32)	+112 (-51)	+40 (-56)	2.179	1.502	21.48
PBS-Al	protonation	Si(V ₁)-OH \cdots Al _{IV} (III ₃)	-18	+30	-59	+37 (-55)	+100 (-70)	+5 (-64)	2.042	1.484	27.64
PBS-Al	No protonation	Si(Z ₂)-OH \cdots Al _V (III ₂)	-50	—	-75	-12 (-38)	—	-19 (-56)	2.053	1.482	30.18
		Si(Y ₂)-OH \cdots Al _V (III ₄)	-26	—	-33	+8 (-34)	—	+21 (-54)	2.364	1.447	16.44
Silanol-Al	No protonation	Si(W ₂)-OH	-9	—	-54	+7 (-16)	—	-12 (-42)	2.052	1.480	24.59
Al-OH	protonation	Al(III ₁)-HOH ₍₂₎	-11	—	-6	+16 (-27)	—	+49 (-55)	2.785	1.521	5.32
Mordenite	protonation		-95	-88	-95	-44 (-51)	-1 (-87)	-22 (-73)	1.821	1.624	34.10

¹ For the nature of acid sites, the reader is referred to Figure 1 (and introduction) : PBS = pseudo-bridging silanols, PBS-Si = silicic PBS, PBS-Al= aluminic PBS, Silanol-Al = silanol with Si-O-Al bridges.

² From ref. [35]

³ At the surrounding of the isobutene molecule adsorbed according to a π -complex mode, see text.

3.1.1. Structure and stability of the π -complex

The physisorption of isobutene takes place through the interaction of the C=C double bond with the acidic proton of the surface. After geometry optimisation, the molecule slightly orients the terminal C atom of the C=C bond near the surface proton (see structures in **Figure 4**).

-- HERE FIGURE 4 --

The distance between this carbon atom and the proton (**table 1**) is as high as 2.0-2.8 Å whereas it is only 1.8 Å in mordenite. On ASA, the adsorption is most favorable ($-50 \text{ kJ}\cdot\text{mol}^{-1}$) on $\text{Si}(Z_2)\text{-OH}\cdots\text{Al}_V(\text{III}_2)$, which belongs to the PBS-Al family, but does not protonate lutidine.[35] The adsorption is however much more favorable in mordenite ($-95 \text{ kJ}\cdot\text{mol}^{-1}$). This effect is assigned to:

- van der Waals interactions between isobutene and the surrounding framework of MOR. For the π -complexes in weak interaction as mainly found on ASA, van der Waals forces represent the major part of the attractive part of the interaction but they are weaker by about 13 to 35 $\text{kJ}\cdot\text{mol}^{-1}$ than in MOR with one exception: the PBS-Al site (V_1) for which van der Waals interactions are as high as in MOR.
- Electrostatic interactions, which are weaker on the planar surface of ASA than in MOR (see electrostatic field values in Table 1). Even for this neutral complex, it is interesting to notice that the electrostatic contributions exert a strongly stabilizing effect in MOR ($-44 \text{ kJ}\cdot\text{mol}^{-1}$) whereas they are destabilizing on ASA ($+7$ to $+37 \text{ kJ}\cdot\text{mol}^{-1}$) with the exception of the PBS-Al site (Z_2).

Note that the two π -complexes with higher $|\Delta_r U|$ and $|\Delta_r U_{\text{DFT}}|$ values (MOR and PBS-Al site (Z_2)) exhibit high frequency shifts of CO [36] (see **Supporting Information S2**) and the

highest electrostatic field value (see Table 1), which suggests that the electrostatic part of the interaction becomes critical in their case. Moreover, the value of the electrostatic field was found to be directly correlated to the distance between the molecule and the framework (Figure 5). By formally displacing the position of the molecule within the MOR main channel, perpendicularly to it, we calculate a depletion of the electrostatic field (line in Figure 5), in a very similar fashion as the values obtained on the various sites of ASA. This demonstrates that the enhanced electrostatic field in the zeolite in the surrounding of the molecule, at the origin of more stable adsorption complexes, is a direct consequence of the proximity of the molecule with the framework.

-- HERE FIGURE 5 --

As expected, no correlation could be found between the adsorption energy of isobutene into π -complex and the lutidine protonation ability of the acid site involved (see **Supporting Information S2**). As previously discussed in Ref. [36], in which no direct correlation between CO adsorption and lutidine protonation was reported, the stability of the π -complexes cannot be deduced from the analysis of BAS strength probed by lutidine or CO molecule because it results from multi-contribution effects.

Note that regarding mordenite, our energy results compare well with previous ab initio reports in the literature,[78, 94] in particular DFT+D.[59, 66, 67, 95-97]

3.1.2. Carbenium formation

The $C_4H_9^+$ species is well-known to be planar. For the systems investigated here the $C_{\text{molecule}} \cdots O_{\text{surf}}$ distance is higher than 1.7 Å. In mordenite, we obtained a carbenium as local energy minimum (-88 kJ.mol⁻¹), depicted in **Figure 6-a**. Note that the carbocation is

positioned, after geometry optimization, above the aluminum atom, each of the methyl groups being oriented towards framework oxygen atoms, similarly to previous results reported for H-ZSM-5.[74] The energetics are comparable to most recent reports on various zeolite frameworks using similar levels of theory[78, 94] (although Δ_rU being more negative than most advanced hybrid MP2/DFT results[66, 67]).

On ASA however, it appeared to be very difficult to obtain carbenium as local energy minimum, as the geometry optimizations very often led to the restitution of the proton to the surface, to regenerate isobutene and the acid site, or to the formation of a C–O_{surf} bond to provide the alkoxide (see next section). Only two local energy minima were obtained on the PBS-Al Si(V₁)–OH···Al_{IV} (III₃) and on the PBS-Si (**Figure 6-b-to d**), although they correspond to endothermic formation reactions. The existence of this carbenium ion as a transition state on this site or on other ASA sites cannot be excluded at present time, but it is beyond the scope of the present work.

The protonation of isobutene to form a carbenium species is quite comparable with the formation of lutidinium from lutidine: it involves a concomitant stabilization of the silanolate species in the case of ASA. For a given site (bridging OH group of mordenite or PBS-Al of ASA), the formation of lutidinium is favored over that of the tert-butyl carbenium ion (**Table 2**). This is an illustration of the different basic characters of the two molecules, linked to different stabilization of the protonated species on the surface. When comparing the Si(V₁)–OH···Al_{IV} (III₃) site of ASA (PBS-Al which protonates lutidine) with the bridging OH group in mordenite, it appears that both ionic species are more strongly stabilized in the zeolite than on the ASA surface. As the dispersion interaction corrections are rather comparable for both solids, this trend must be assigned to electrostatic effects, also measured by the electrostatic field on the different solids. Table 2 reports electrostatic field values calculated for π -

complexes. Note that the protocol we applied to calculate this field -see section 2- cannot be transposed to systems in which atom transfers have occurred, and that the value of the electrostatic field is expected to be significantly different after proton transfer (negatively charged framework). The electrostatic field evolves from 27.6 V.nm^{-1} on the PBS-Al site up to 34.1 V.nm^{-1} on the MOR site, which induces a stabilizing effect on charged species such as tert-butyl carbenium ions. As mentioned in section 3.1.1., the electrostatic interaction is conditioned by the proximity of the molecule with the framework, allowed in MOR by the three hydrogen bonds illustrated in Figure 6a) and b) for the most stable tert-butyl carbenium ion. A similar trend was inferred for aromatics isomerization reactions on the basis of a charge analysis, which reveals that charged species are stabilized by the surrounding negatively charged oxygen atoms of the zeolitic framework.[69] So the higher acidity of zeolites with regard to ASA can thus be attributed mainly to electrostatic confinement effect rather than van der Waals confinement. This different stabilization of ions pairs is expected to have significant impact on catalysis,[98, 99] as it will be shown further.

Table 2. Formation energy of tert-butyl carbenium ion and of lutidinium on the bridging OH group of mordenite and on the $\text{Si(V}_1\text{)-OH}\cdots\text{Al}_{\text{IV}}(\text{III}_3)$ PBS-Al site of the ASA surface. All energies are expressed in kJ/mol.

Site	$\Delta_r\text{U}$		Decomposition of $\Delta_r\text{U}$: $\Delta_r\text{U}_{\text{DFT}} (\Delta_r\text{U}_{\text{disp}})$		Electrostatic field* (V.nm^{-1})
	tert-butyl carbenium	Lutidinium*	tert-butyl carbenium	Lutidinium*	
PBS-Al	+30	-101	+100 (-70)	-41 (-60)	27.6
Mordenite	-88	-241	-1 (-87)	-172 (-69)	34.1

* These calculations were performed with the same functional (PBE) as for the formation of tert-butyl carbenium ion, and include dispersion corrections (DFT-D2).

* as calculated for π -complexes, see Table 1.

-- HERE FIGURE 6 --

3.1.3. Tert-butoxide formation

Contrary to the carbenium ion, the alkoxide species is not planar anymore and exhibits an umbrella like conformation with the formation of a covalent C-O_{surf} bond (**Table 1**). The newly formed C-O_{surf} bond length is almost constant from one site to another ($1.48 \pm 0.04 \text{ \AA}$). We consider here that the alkoxide intermediates is anchored either on the O_{surf} atom of the BAS itself or on the neighboring O_{surf} atom as reported in the literature devoted to zeolitic materials.[58, 59, 65, 68, 70, 77, 95, 97, 100-103] The various possible kinds of intermediates and their energetics are exemplified in **Figure 7** without making any assumptions on the mechanisms leading to them. These mechanisms will be briefly discussed in the next section.

In the case of the ASA site Si(V₁)-OH···Al_{IV} (III₃) (PBS-Al which protonates lutidine) the energy difference between the two plausible products (**Figure 7-c and d**) is higher than for mordenite (32 kJ.mol^{-1} versus 7 kJ.mol^{-1} respectively), in line with the different local structures. Once the proton of PBS-Al is transferred to isobutene, the silanolate has to be stabilized, by analogy to the proton transfer to lutidine,[35] and this stabilization occurs as follows:

- the tert-butyl cation is the stabilizing group by forming the new C-O_{surf} bond capping the PBS (**Figure 7-c**)
- or the PBS-Al closes its bridge (in the same way as after proton transfer to lutidine), by forming a new O-Al bond, while the alkoxide forms a new C-O bond on the neighboring site (**Figure 7-d**).

-- HERE FIGURE 7 --

The intermediate formed on the BAS appears to be more stable, likely in relation with

the less sterically hindered nature of the terminal Si-O-R group (**Figure 7-c**) as compared to the multicoordinated nature of the O atom of the alkoxide formed on the neighboring O site (**Figure 7-d**). This is illustrated by the higher position of carbon atoms along the perpendicular to the surface for the configuration reported in **Figure 7-c** as compared to the one shown in **Figure 7-d** (central carbon atom : difference in height of 0.47 Å, other carbon atoms : mean difference in height of 0.44 Å). Note that the stabilization of the silanolate obtained after proton transfer by the protonated species itself (the possible carbenium ion) instead of the implication of surface atoms (as for lutidine) is an illustration of the amphoteric character of the alkene molecule.

The alkoxide intermediates formed on the BAS itself were then systematically investigated for the whole set of ASA sites under study. The formation energy of the *tert*-butoxide species lies between -6 and -75 kJ.mol⁻¹ (**Table 1**), whereas it is more negative in mordenite (-95 kJ.mol⁻¹), which is due to both dispersion and electronic contributions. Note that this energy interval is compatible with previous reports,[59, 66, 67, 70, 95-97] including DFT+D,[78, 94] in various zeolitic frameworks and site positions.

No correlation could be revealed between $\Delta_r U$ value and the adsorption energy of lutidine or the shift of its ν_{8a} mode, even if a proton transfer occurs in each case. This is due to the strong differences in the adsorbed structures, with a strong charge separation in the case of the lutidinium–deprotonated surface interaction. Moreover, due to the amphoteric nature of isobutene, the formation energy of the alkoxide according to a 4-center mechanism is not dependent on the ability of the silanolate to stabilize on other surface atoms, which was critical in the case of lutidine.

Surprisingly, a good correlation is obtained between the formation energy of the *tert*-butoxy species and the CO frequency shift (**Figure 8**). In our previous work, we showed that the CO frequency shift is directly related to the local electrostatic field.[36] Such a correlation

is quite unexpected because contrary to the case of CO, the surface proton was transferred to the isobutene molecule. This indicates that not only the proton, but also a large piece of the surface, play a role in the local electrostatic field, as already shown in reference [36]. **Table 1** also shows that dispersion forces also play a significant role in the interaction, but the fluctuation from one site to another (from -42 to -64 kJ.mol⁻¹) is lower than for the π -complex due to the rather constrained C-O_{surf} distance ($1.48 \pm 0.04 \text{ \AA}$). However, as for the π -complex, variation of the electronic contribution is rather large and impacts strongly the overall adsorption energy.

-- HERE FIGURE 8 --

3.1.4. Protonation energy profiles at 0 K

The adsorption energies of isobutene according to the three modes previously exposed are gathered in **Figure 9-a and b**. Note that this representation does not imply any consequence on the mechanisms involved in the formation of the carbocation and alkoxide species (see further).

Without dispersion corrections (**Figure 9-a**), the π -complex is the most stable species within mordenite, whereas the alkoxide is the most stable on some sites of ASA. Including dispersion corrections (**Figure 9-b**), all profiles are lower in energy. In mordenite, the energy profile becomes also nearly isoenergetic for the protonation reaction and much more favorable than all profiles calculated on the ASA sites. On ASA, the formation of the carbenium ion seems to be preferentially formed on the single PBS-Al able to protonate lutidine. In any case, **Figure 9-b** unambiguously shows that carbenium ions and alkoxides formation is much easier in zeolites than on ASA. It could also be that carbenium ions are energetically stronger competitors to alkoxide species in zeolites.

Comparing the various sites of the ASA surface (taking into account dispersion forces), it appears that the two sites stabilizing carbenium ion are one PBS-Al (V₁) and the PBS-Si

(U₁), which are also able to protonate lutidine. Thus the proton transfer ability as formerly revealed by the lutidine probe molecule is qualitatively linked with the carbenium formation. By contrast, the more stable alkoxide species are not directly linked to it, as already discussed: some sites exhibiting high frequency shifts when CO is used as a probe molecule, lead to the formation of stable alkoxides but neither to carbenium ions nor lutidinium ions. This is the case of one PBS-Al which is not able to protonate lutidine, Si(Z₂)-OH···Al_V(III₂).

-- HERE FIGURE 9 --

If the lifetime of the tert-butyl carbenium species is already questioned in the case of zeolites,[51, 67] it can be anticipated that the lifetime of such species on ASA will be even shorter. Whereas carbenium chemistry is often supposed to be at the core of hydrocarbon conversion for aluminosilicates, our present results suggest that it would hardly be the case on ASA.

Regarding the possible mechanisms connecting the tertiary alkoxide to the two other intermediates (π -complex and carbocation), three pathways are usually invoked for the formation of tertiary alkoxides:

- one “indirect” mechanism as investigated in Ref. [67]: the carbocation is a precursor of the tertiary alkoxide either anchored on the O site of the BAS itself or on the neighbouring O site (see also previous section)
- two “direct” mechanisms (without formation of carbocation):
 - o the so-called "4-center mechanism": the acid site protonates isobutene and stabilizes subsequently the alkoxide on the conjugated base (deprotonated O atom).
 - o the so-called "6-center mechanism": the alkoxide species is formed on a

neighbouring O atom.

Regarding zeolites, the 6-center mechanism is mostly presented in the literature.[58, 59, 65, 70, 77, 95, 97, 100-103] Bhan et al.[101] compared the two mechanisms in the case of propene and hexene adsorbed on 10T-clusters of ZSM-5 and concluded that the stability of both the transition states and the products are in favor of a 6-center mechanism, although the reaction and activation energies differ from less than 20 kJ.mol⁻¹. In addition, they report that the activation energy is about 80 kJ.mol⁻¹ and involves a carbocation like transition state. This value is close to the one reported by Tuma et al. in Ref. [67], involved in the formation of the tert-butyl carbenium species in H-ferrierite. In MOR, Rozanska et al. [70] reported also moderate activation energies (similar to the one leading to the carbocation intermediates, ~30 kJ.mol⁻¹) leading to butoxy species via a carbocation like transition state. So even if these results are much dependant on the location of the acid site, the nature of the alumina-silicate materials and the level of theory itself, the formation of alkoxy species is possible from a kinetic point of view and might occur according to the two mechanisms listed above. We will thus consider alkoxy and carbocation pathways in the forthcoming sections.

3.1.5. Protonation energy profiles: thermal effects

Figure 9-c depicts the $\Delta_r G$ values for all species derived from isobutene adsorption on ASA and MOR, according to the methods exposed in section 2. For mordenite, the alkoxides become much less favorable (their formation becomes an endergonic reaction) than the carbenium, due to their lower number of degree of freedom (translational and rotational). On ASA, despite the application of similar thermal corrections, the carbenium remains a highly improbable species as compared to the alkoxide, although the formation of both compounds is endergonic. This trend will have a direct impact on the cracking reaction pathway investigated in the forthcoming section.

3.2. DIB cracking pathway

To further investigate this aspect, we calculate the DFT energy and Gibbs energy profiles of the cracking reaction of a relevant olefin molecule: DIB (2,4,4-trimethyl-2-pentene). Our main aim is to compare cracking pathways between MOR and ASA. As carbenium ions are very often invoked in the cracking pathways of alkenes on zeolites, one may choose to investigate first on ASA a site which is able to stabilize both carbenium and alkoxide intermediates. For this reason, we focus on the PBS-Al site ($\text{Si(V}_1\text{)-OH}\cdots\text{Al}_{\text{IV}}(\text{III}_3)$), which allows the investigation of carbenium *versus* alkoxides routes, and according to the previous section, with intermediates being more stable on it than on the PBS-Si sites (see **Figure 9**). We compare it with the bridging Si-(OH)-Al group in mordenite. Note that in the future, other ASA sites will deserve attention, even if they do not stabilize carbenium ions as intermediates, in particular those leading to most stable alkoxides (PBS-Al $\text{Si(Z}_2\text{)-OH}\cdots\text{Al}_{\text{V}}(\text{III}_2)$).

3.2.1. Reaction pathways under study

The various intermediates and reaction pathways considered are depicted in **Figure 10**, on the PBS-Al site $\text{Si(V}_1\text{)-OH}\cdots\text{Al}_{\text{IV}}(\text{III}_3)$ of ASA. Strictly analogous pathways are investigated on MOR. They involve either secondary or tertiary carbocations/alkoxides according to six formal steps (likely not elementary steps):

- physisorption of DIB on the BAS of the ASA surface or mordenite
- proton transfer from PBS-Al (ASA) or Si-(OH)-Al (MOR) to DIB, leading either to a carbenium or to an alkoxide. We consider here tertiary carbenium (C_{III}) only and either secondary (A_{II} , B_{II}) or tertiary alkoxides (A_{III} , B_{III}). The alkoxide can be stabilized either on the deprotonated oxygen atom (A), or on a neighboring one (B)

according to the previous analysis made for isobutene.

- the cracking step occurs via β -scission leading to a physisorbed isobutene molecule and either a *tert*-butyl cation (5) or isobutoxy species (1, 2, 3, 4). In the following, for sake of clarity, we report pathways involving only either carbenium intermediate or alkoxides. Note that according to the discussion on 3.1.4, we cannot exclude that carbenium intermediate may be precursor of alkoxide species, however for sake or clarity the energy profiles presented in Figure 11 will not illustrate explicitly the combination of the two routes. However, we will discuss this point in 3.2.2.
- the first isobutene molecule formed is then desorbed (loss of the physisorption energy) leading either to adsorbed *tert*-butyl cation (3') or isobutoxy species (1', 2')
- the carbenium or alkoxide remaining at the surface then transfers one proton to regenerate the surface BAS (A or B) and produces a second physisorbed isobutene molecule.
- finally, the secondly formed isobutene molecule desorbs.

-- HERE FIGURE 10 --

3.2.2. *Gibbs free energy profiles*

In what follows, we directly report the $\Delta_r G$ profiles of the adsorbed intermediates (including thermal and entropy contributions) as explained in the Methods section. Note that in the conditions considered (500 K, all partial pressures of gaseous compounds equal to 1 bar), the overall $\Delta_r G$ value for the cracking reaction of DIB into isobutene is almost zero (-3 kJ.mol⁻¹). Energy profiles at 0 K, as well as $\Delta_r U$ and $\Delta_r G$ values of all intermediates for ASA and MOR are reported in **Supporting Information S3**. Considering firstly the alkoxide routes only, it appears on ASA that the A_{III} pathway is favored over the A_{II} one, as well as the

B_{III} route over the B_{II} one. Thus on a given site, tertiary alkoxides are more stabilized. In the following, for the sake of clarity, we plot in **Figure 11** mainly the A_{III} and B_{II} routes, as being representative for the reactivity of tertiary and secondary alkoxide routes. Regarding mordenite, the A_{III} and A_{II} routes will be shown. Considering the whole set of energy data reported in **Supporting Information S3** does not affect the conclusions drawn in the following. From a general point of view, it appears that all pathways are favored (Δ_rU and Δ_rG) in mordenite as compared to ASA. This is related to the electrostatic confinement effect already mentioned in section 3.1.2. Moreover in MOR, the carbenium route is favored over all other routes, at each stage of the reaction. This is due to higher entropy of adsorbed carbenium species as compared to alkoxides, as shown by the comparison of Δ_rG and Δ_rU profiles (Supporting Information S3). This finding is in agreement with the classical description of carbenium chemistry considered to take place in zeolites.[16, 41-43, 80, 104] The drawing is not the same for ASA, and to understand this, we detail each reaction step in the following.

a) DIB adsorption and protonation

In a similar way as for isobutene, the adsorption of the DIB molecule as a π -complex is much stronger in mordenite ($\Delta_rG = -88 \text{ kJ.mol}^{-1}$) than on ASA ($\Delta_rG = +12 \text{ kJ.mol}^{-1}$). Moreover, on ASA, protonated DIB is much more stabilized in a tertiary alkoxide form ($\Delta_rG = 36 \text{ kJ.mol}^{-1}$) rather than in a secondary alkoxide one ($\Delta_rG = 86 \text{ kJ.mol}^{-1}$) or than in a carbenium one ($\Delta_rG = 63 \text{ kJ.mol}^{-1}$). In MOR, the trend is the opposite, with the carbenium ion being the most favorable species at this stage ($\Delta_rG = -87 \text{ kJ.mol}^{-1}$, almost iso-G with the π -complex) with regard to alkoxides.

Considering kinetic data available on zeolites (see section 3.1.4), the activation energy for the formation of the alkoxy intermediate would be similar with the one leading to the

carbenium. Assuming that this trend is still valid for ASA, and that barriers will all be higher in ASA than in MOR (if a Brønsted-Evans-Polanyi relationship exists), kinetics may not change our conclusions for the comparison of MOR and ASA, neither for the probability of alkoxides versus carbenium formation.

b) Cracking step

Considering first $\Delta_r U$ values, the cracking reaction is most of the time endothermic on ASA and in MOR ($>70 \text{ kJ}\cdot\text{mol}^{-1}$). Note that this is also the case for the gas phase cracking reaction (DIB = 2 isobutene, computed $\Delta_r U$: $+87 \text{ kJ}\cdot\text{mol}^{-1}$). This trend is explained from the energy loss of one C-C bond due to β -scission, which is not compensated by the energy gain induced by the conversion of a C-C bond into a C=C one. Calculated reaction energies for β -scission steps of various alkenes reported in the literature for zeolites differ quite strongly from one study to another: from $\sim 10 \text{ kJ}\cdot\text{mol}^{-1}$ to more than $100 \text{ kJ}\cdot\text{mol}^{-1}$ (in the same interval as our results)[64, 75, 105-110] with a very strong impact of the size of the model and the type of zeolite, thus of steric and confinement effects. Coming back to $\Delta_r G$ profiles, it appears that including thermal and entropic effects counterbalances the internal energy variations (as observed for gas phase, for which $\Delta_r G \approx 0$ at 500 K).

Analysing the $\Delta_r G$ profiles on ASA shows that the most favorable one involves the tertiary alkoxy: $A_{\text{III}} \rightarrow 2$ ($+12 \text{ kJ}\cdot\text{mol}^{-1}$). The scenario involving $B_{\text{II}} \rightarrow 3$ ($-53 \text{ kJ}\cdot\text{mol}^{-1}$) should be ruled out since this secondary alkoxy is far less stable than A_{III} . However, $A_{\text{III}} \rightarrow 2$ would occur on the same site for the formation of the first and second alkoxide species (before and after cracking) which might be mechanistically difficult to envisage (to be confirmed by more detailed mechanistic studies). So, we report in figure 11 also the $A_{\text{III}} \rightarrow 1$ reaction ($+50 \text{ kJ}\cdot\text{mol}^{-1}$) in which two neighboring sites are involved during cracking (as it is for $B_{\text{II}} \rightarrow 3$). In MOR, the most favorable pathway would be $A_{\text{II}} \rightarrow 2$ ($+7 \text{ kJ}\cdot\text{mol}^{-1}$) or $A_{\text{III}} \rightarrow 1$ ($+3 \text{ kJ}\cdot\text{mol}^{-1}$). For the

same reason, we also plot $B_{III \rightarrow 3}$ (-13 kJ.mol^{-1}). The pathway involving the carbocationic intermediate $C_{III \rightarrow 5}$, is slightly more endergonic ($+28 \text{ kJ.mol}^{-1}$).

At this stage, one could also suggest the existence of an alternative cracking pathway combining carbocation and alkoxy routes during the cracking step. For MOR, this would not bring any gain in Gibbs energy, as carbenium species are by far more stable than alkoxides: a purely carbenium pathway remains the most probable. By contrast, on ASA we can propose that the optimal cracking step could occur along the route $C_{III \rightarrow 1}$ or $C_{III \rightarrow 3}$, 1 and 3 being significantly more stable than the carbocation 5. Although we previously underlined that the probability of existence of C_{III} is certainly lower than A_{III} , C_{III} may offer a favorable alternative if too high barriers have to be overcome for the cracking of alkoxy A_{III} . In that case, the energy demanding step would be the formation of C_{III} , whereas it is the cracking step for the A_{III} pathway. In such a scenario, A_{III} would be a dormant species and the relative concentration of C_{III} versus A_{III} species on the ASA surface would be the determining parameter for cracking.

-- HERE FIGURE 11 --

In the literature, energy barriers for β -scission steps in zeolites were evaluated mainly from alkoxides, with values as high as $150\text{-}200 \text{ kJ.mol}^{-1}$. [108-112] Earlier studies performed on small clusters (neglecting confinement effect) even concluded to barriers above 200 kJ.mol^{-1} . [62-64, 105-107] Starting from a carbenium species, [75, 112] barriers between 65 and 115 kJ.mol^{-1} were reported in H-ZSM5. Kinetic modelling (compared to octane hydrocracking experiments on Pt/H-USY) leads to energy barriers for β -scission close to 125 kJ.mol^{-1} , however with strong dependence on the hypothesis retained for the kinetic model used for fitting the experimental data. [104] On ASA, the identification of transition states and activation energies is still required to determine which of the cracking step and carbocation

formation is the kinetic limiting step on ASA. Even in absence of such kinetic values, considering the higher energy levels of the carbocationic intermediates (C_{III} and 5) on ASA (both Δ_rU and Δ_rG profiles), this route seems to be thermodynamically difficult to envisage. Thus we suggest in the future to also explore kinetic parameters of the mixed route leading from carbocationic intermediate to cracked alkoxide intermediates particularly on ASA, as this route seems to be thermodynamically relevant.

c) Deprotonation/Desorption steps

On ASA and MOR, the deprotonation steps are all exergonic (opposite trends as the protonation step discussed before). In MOR, the isobutene desorption step is endergonic ($\Delta_rG = +68 \text{ kJ.mol}^{-1}$), which can be a limitation to the reaction rate due to the confinement effect induced by the zeolite pores, whereas it is generally admitted that the β -scission step is rate controlling.[16-18] It is beyond the scope of the present study to identify the rate limiting step, however it is clear from this Δ_rG profile, that product desorption limitation in MOR may also be at the origin of hydrocarbon overcracking. As a complementary analysis, let us consider the situation in which a protonated DIB intermediate is formed in the zeolitic micropore, from the cracking of longer chain hydrocarbons. In that case, after deprotonation, the desorption of DIB is also strongly limiting ($\Delta_rG = +87 \text{ kJ.mol}^{-1}$) which implies that DIB would preferentially remain in the pore and be cracked according to the pathway described above. The situation is different on ASA in which the desorption steps of DIB and isobutene molecules are slightly exergonic: it appears thermodynamically more favorable to reversely deprotonate and desorb it, than to further crack it into lighter hydrocarbons. This is first theoretical explanation of the origin of the milder acidic character of ASA wished for specific applications in which overcracking must be avoided. In particular, cracking being activated, the corresponding energy barrier is expected to reinforce this trend, which is contrasting with

the scenario in MOR. To a certain extent this interpretation is also coherent with previous kinetic modelling of phenantrene hydrocracking which has highlighted that an optimal pore size is required for controlling the selectivity towards targeted products of intermediate molecular weight in hydrocracking.[10, 32] In particular, the relative positions of the Δ_rG profiles as plotted in **Figure 11** may directly be correlated on the size of micropores and mesopores of the considered aluminosilicates, hopefully leading to the discovery of an optimal pocket size.[113, 114] This concept may open new routes for future investigations.

4. Conclusions

Thanks to DFT+D2 calculations led on original Amorphous Silica Alumina surface models, we propose a rational interpretation of the lower acidity of ASA surface with respect to zeolite, as probed by alkene cracking reactivity.

Regarding the interaction of isobutene with aluminosilicates, three key intermediates (π -complex, carbocation and alkoxide) are less stable on the ASA surface than in MOR. This is mainly due to the combined effect of the electrostatic and van der Waals contributions, being stronger in zeolites by confinement effect. Moreover, the tert-butyl carbenium ion is significantly higher in energy on the ASA surface than in MOR. Since the calculated van der Waals contributions are close in both cases, the origin of the carbocation stabilization in MOR is attributed to an electrostatic confinement effect as quantified by the large electrostatic field in the zeolite[36]. As a consequence, the formation of the tert-butyl carbenium ion is nearly isoenergetic in MOR, whereas it is endergonic on the PBS-Al site of ASA. By contrast, alkoxy species are more stabilized on the PBS-Al site than carbocationic ones: this is a first indication discriminating the chemical reactivity of BAS located in MOR versus BAS on ASA surface.

By investigating the cracking pathway of DIB, we highlighted that the carbocationic pathways are less favored on ASA with respect to the alkoxy route. A reverse trend was found in MOR, in which the formation of carbocationic intermediates is stabilized again by electrostatic confinement effects. In the case of ASA, the reaction profile goes through slightly positive Δ_rG values. The preferred nature of the tertiary alkoxy route was also revealed, whereas the carbenium route appears very unlikely. From the stability of the intermediates, the protonation and β -scission steps are likely the limiting ones for the “pure” carbocationic or alkoxy routes. For the cracking step, on ASA we also highlighted an alternative pathway combining minority carbocationic species and cracked alkoxy intermediates. Further kinetic analyses are mandatory to confirm this proposal.

Moreover, we furnished a quantified picture based on the Gibbs free enthalpy of each intermediate, which reveal a thermodynamic reason for the formation of overcracked products in zeolites with small micropores while these are less stabilized on ASA. This thermodynamic analysis provides the first theoretical explanation of the origin of the empirically observed milder acidic character of ASA targeted for specific applications in which selective cracking is sought.

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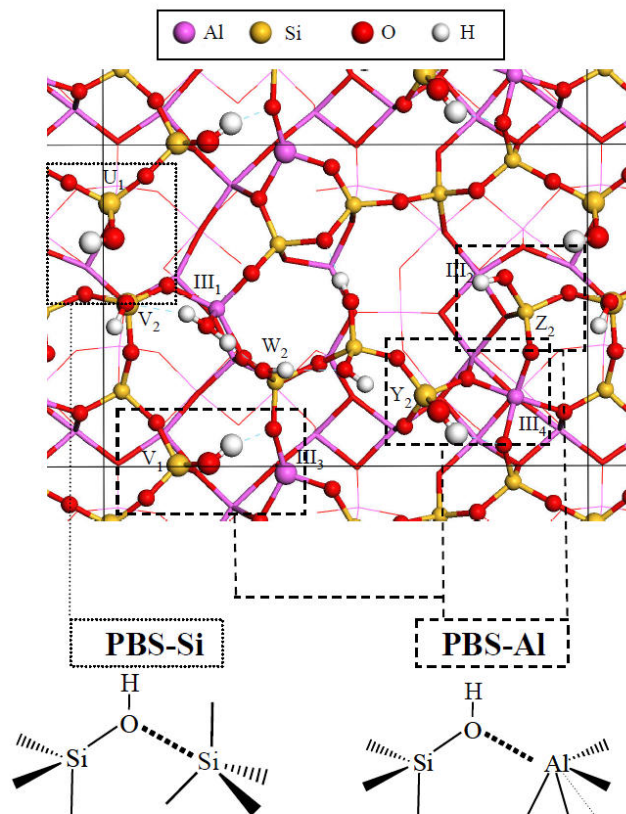


Figure 1. ASA surface model for $\theta_{\text{OH}} = 5.4 \text{ nm}^{-2}$, as established in ref. [37, 38]. Some Pseudo-Bridging Silanols (PBS) are shown, in particular silicic PBS (PBS-Si, Si(U₁)-OH...Si(V₂)) and aluminic PBS (PBS-Al, Si(V₁)-OH...Al_{IV}(III₃)) are able to protonate lutidine, others are not.

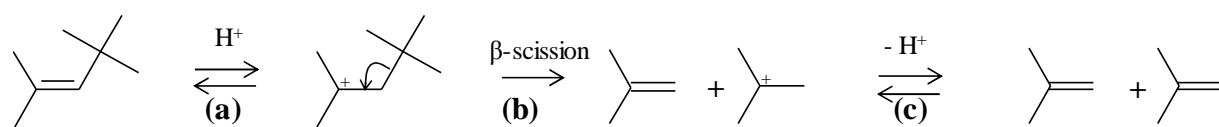


Figure 2. Expected reaction steps leading to the cracking of 2,4,4-trimethyl-2-pentene (DIB): (a) protonation step, (b) β -scission step, (c) product formation and regeneration of the protonic site.

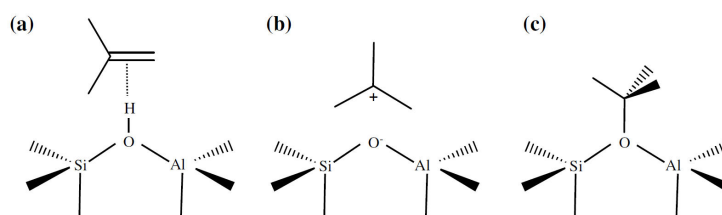


Figure 3. Species likely formed upon interaction of isobutene with the protonic site of a zeolite (omitting further reactions, like dimerization [63,64]): (a) π -complex, (b) carbenium ion – *tert*-butyl – , (c) alkoxide – isobutoxide – also called σ -complex. The tertiary species is exemplified here.

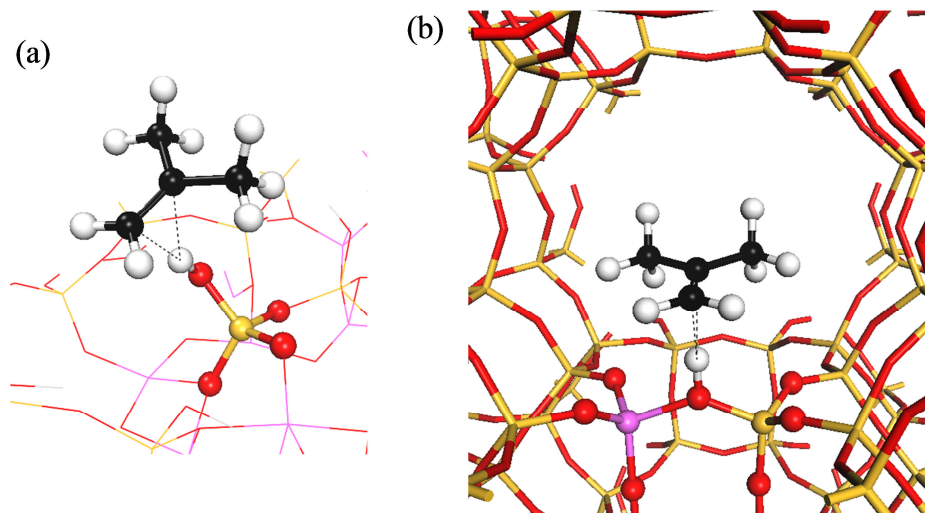


Figure 4. π -complex adsorption mode of isobutene on ASA (Si(Z₂)-OH site) (a) and MOR (b). Same color code as figure 1, carbon atoms are in black.

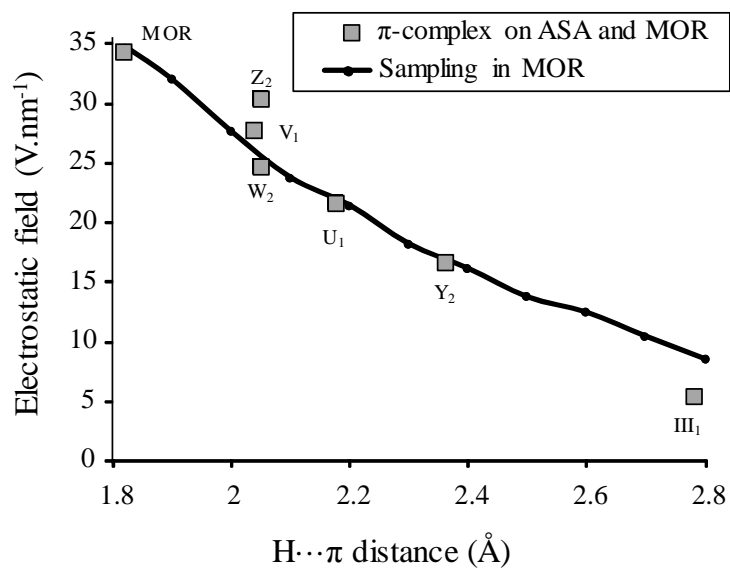


Figure 5. Electrostatic field evaluated in the surrounding of the isobutene molecule adsorbed in a π -complex mode, as a function of the distance between the acid site (H) and the nearer C atom of the C=C bond (terminal atom) (grey squares). The electrostatic field was also evaluated in the cavity of MOR, by formally increasing the H...C distance, perpendicularly to the channel direction, and is depicted by the solid line (increment: 0.1 Å).

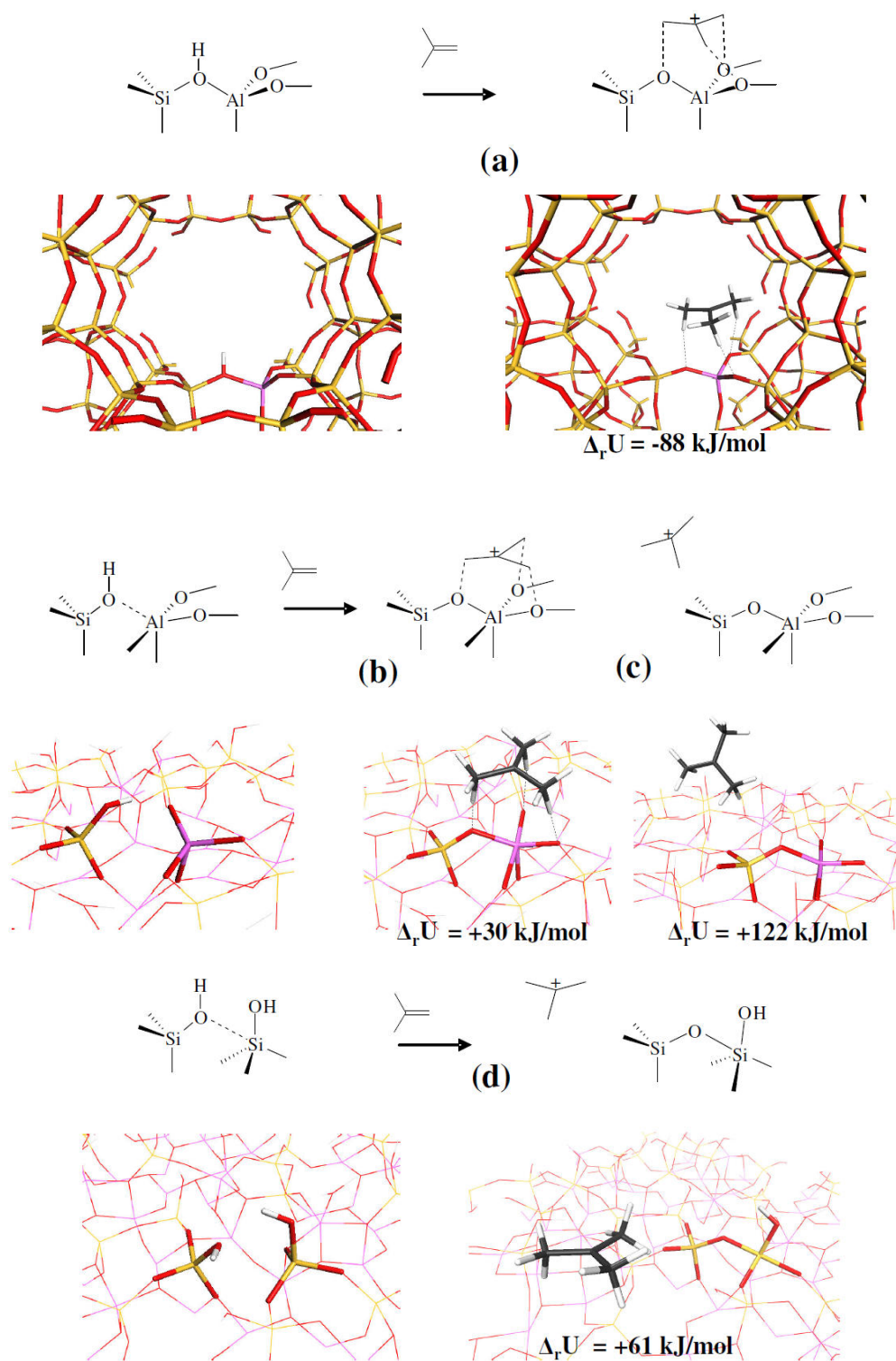


Figure 6. Geometries and energetics of the formation of tertibutoxonium from isobutene on mordenite (a), PBS-Al site of ASA (this site is able to protonate lutidine) (b and c), and PBS-Si site of ASA (d).

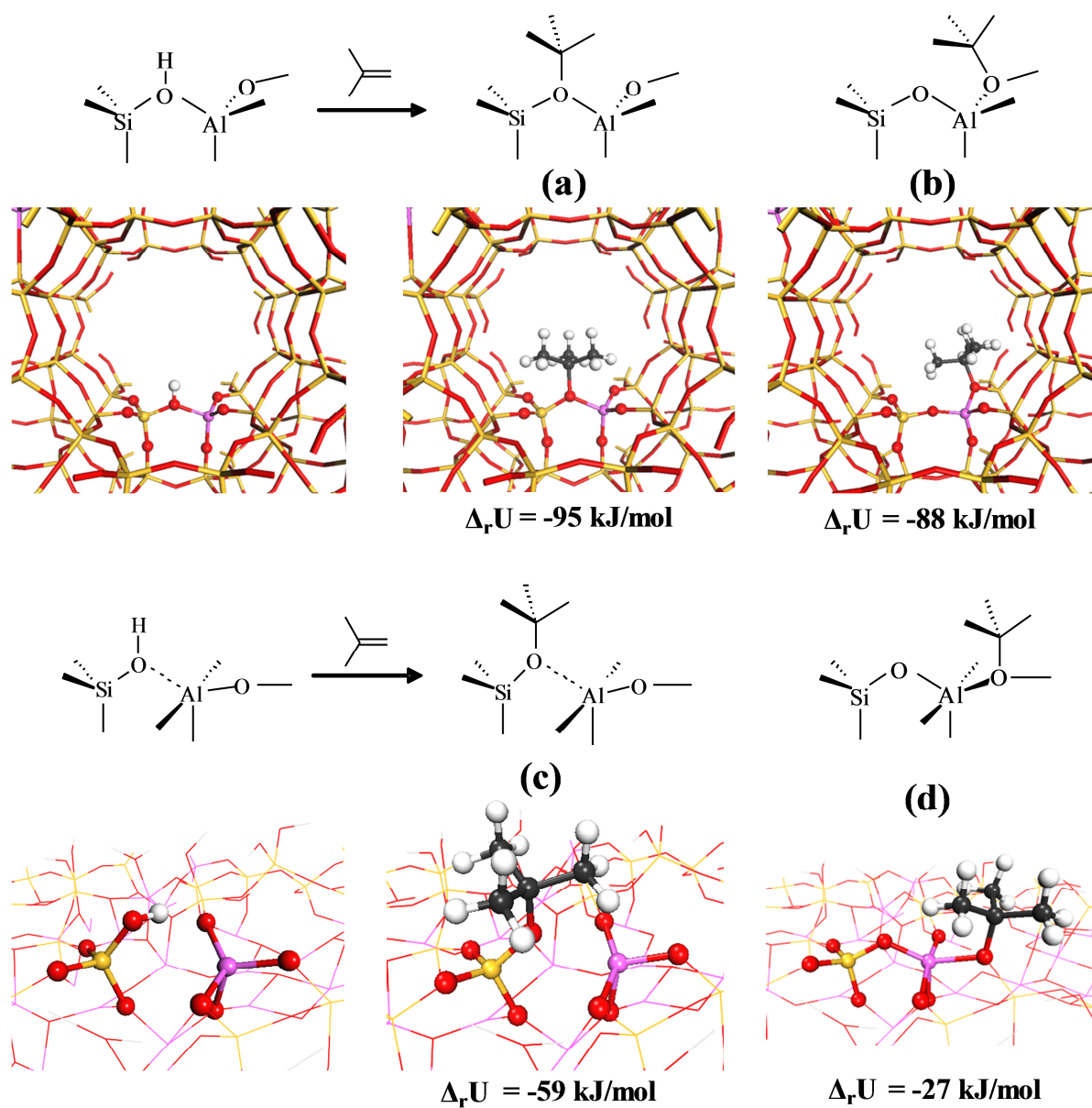


Figure 7. Geometries and adsorption energies of isobutene to form an alkoxide on mordenite (a and b) and ASA (PBS-Al which protonates lutidine, c and d), according to a 4-center (a and c) or 6-center (b and d) mechanism. Same color code as figure 1, carbon atoms are in black.

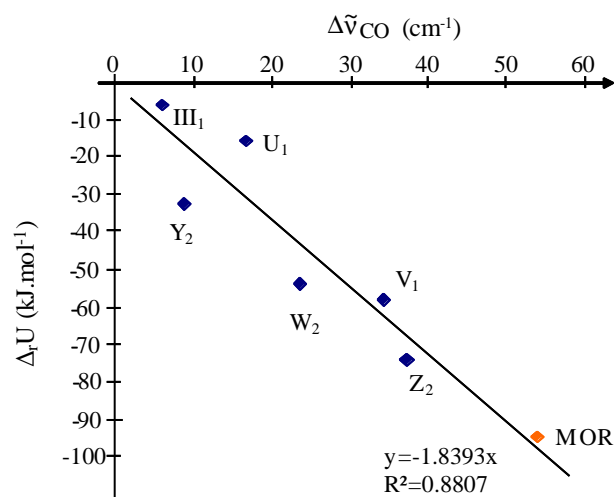


Figure 8. Formation energy of *tert*-butoxy on ASA (blue) and mordenite (orange) from isobutene, as a function of the frequency shift of CO when adsorbed on the same surface site. Values of CO frequency shifts are extracted from [36].

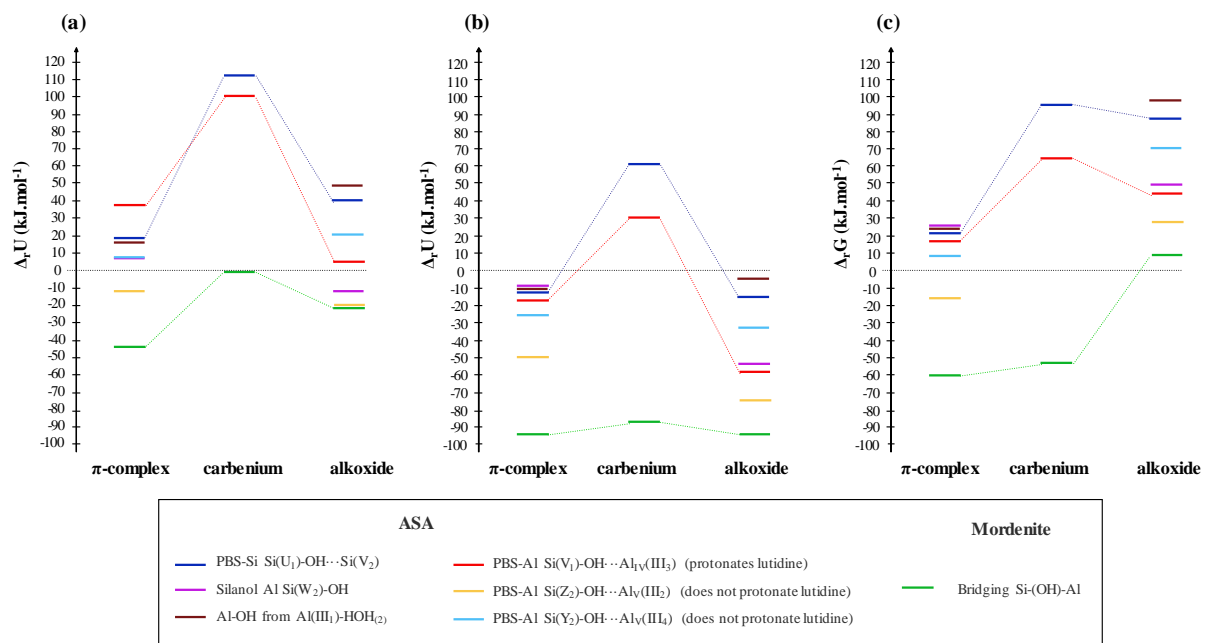


Figure 9. Energy diagram representing the formation energy of adsorbed isobutene according to the three modes investigated, without dispersion corrections (a) or taking into account dispersion corrections (b). Gibbs energy diagram (c) at 500 K.

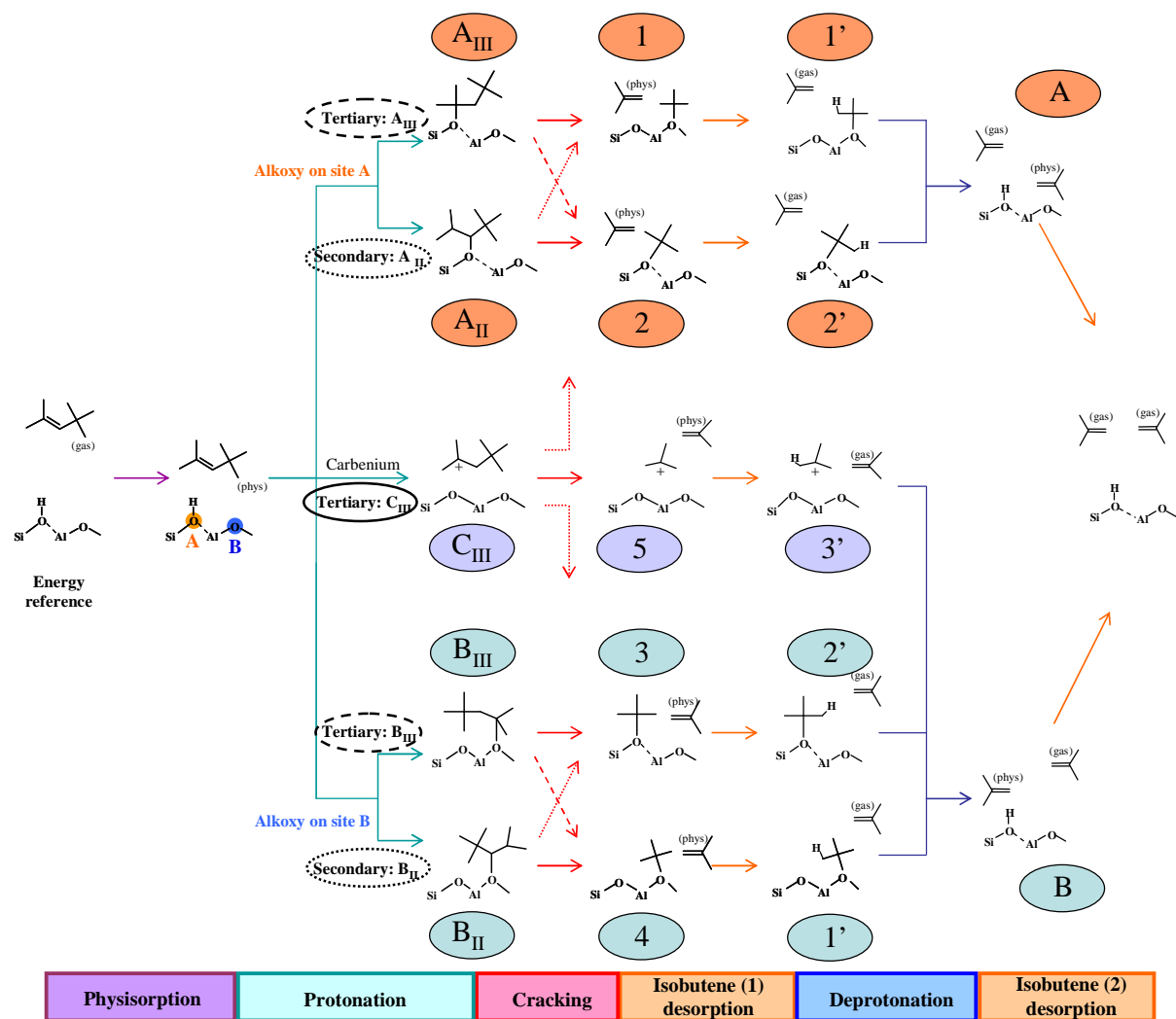


Figure 10. Reaction pathway investigated for DIB cracking reaction, from tertiary and secondary alkoxydes or from a tertiary carbenium ion (C_{III}). Reactions are illustrated in the case of the strongest PBS-Al site of ASA.

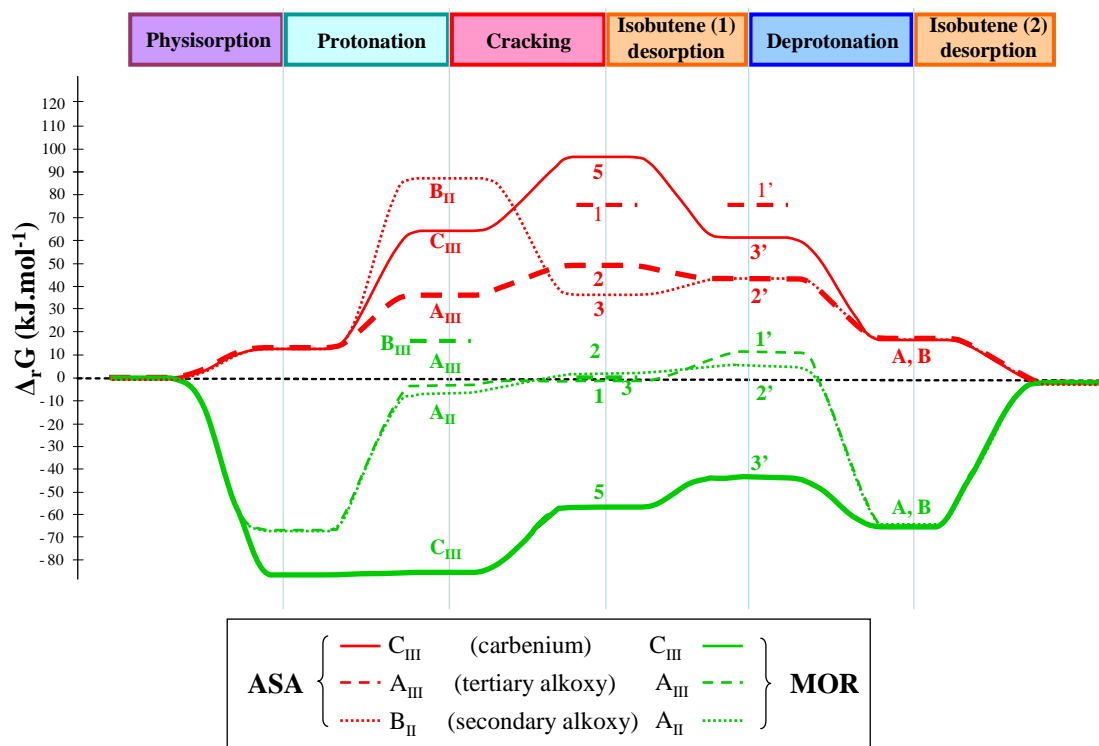


Figure 11. Gibbs free energy profiles for the selected cracking pathways of diisobutene on the ASA surface (PBS-Al site) and in mordenite, at 500 K and all partial pressures equal to 1 bar. Labels refer to intermediates depicted in Figure 10. Lines relate to the selected pathways, as explained in the main text.

Table 1. Formation energies $\Delta_f U$ of the π -complex (physisorption), the carbenium ion and the alkoxide from isobutene on various sites of the ASA surface and in MOR ; decomposition (see eq. 1) of $\Delta_f U$ into the DFT energy ($\Delta_f U_{\text{DFT}}$) and dispersion correction terms ($\Delta_f U_{\text{disp}}$) ; distance between the π -complex (terminal C atom of the C=C bond) and the acid site ($\text{H}\cdots\pi$), and $\text{O}_{\text{site}}\text{-C}_{\text{alkoxide}}$ bond length ;

Acid site ¹	Protonation ability of lutidine ²	Location and terminology (see figure 1)	$\Delta_f U$ (kJ/mol)		Decomposition of $\Delta_f U$: $\Delta_f U_{\text{DFT}}$ ($\Delta_f U_{\text{disp}}$) (kJ/mol)		$\text{H}\cdots\pi$ distance, $\text{O}_{\text{site}}\text{-C}_{\text{alkoxide}}$ bond length (Å)		Electrostatic field (V.nm ⁻¹) ³	
			π -complex	Carbenium	Alkoxide	π -complex	Carbenium	Alkoxide		π -complex
PBS-Si	protonation	Si(U ₁)-OH...Si(V ₂)	-13	+61	-16	+112 (-51)	+40 (-56)	2.179	1.502	21.48
PBS-Al	protonation	Si(V ₁)-OH...Al _{IV} (III ₃)	-18	+30	-59	+100 (-70)	+5 (-64)	2.042	1.484	27.64
PBS-Al	No protonation	Si(Z ₂)-OH...Al _V (III ₂)	-50	—	-75	—	-19 (-56)	2.053	1.482	30.18
		Si(Y ₂)-OH...Al _V (III ₄)	-26	—	-33	—	+21 (-54)	2.364	1.447	16.44
Silanol-Al	No protonation	Si(W ₂)-OH	-9	—	-54	—	-12 (-42)	2.052	1.480	24.59
Al-OH	protonation	Al(III ₁)-HOH ₍₂₎	-11	—	-6	—	+49 (-55)	2.785	1.521	5.32
Mordenite	protonation		-95	-88	-95	-1 (-87)	-22 (-73)	1.821	1.624	34.10

¹ For the nature of acid sites, the reader is referred to Figure 1 (and introduction) : PBS = pseudo-bridging silanols, PBS-Si = silicic PBS, PBS-Al= aluminic PBS, Silanol-Al = silanol with Si-O-Al bridges.

² From ref. [35]

³ At the surrounding of the isobutene molecule adsorbed according to a π -complex mode, see text.

Table 2. Formation energy of tert-butyl carbenium ion and of lutidinium on the bridging OH group of mordenite and on the Si(V₁)–OH···Al_{IV} (III₃) PBS-Al site of the ASA surface. All energies are expressed in kJ/mol.

Site	$\Delta_r U$		Decomposition of $\Delta_r U$: $\Delta_r U_{\text{DFT}} (\Delta_r U_{\text{disp}})$		Electrostatic field* (V.nm ⁻¹)
	tert-butyl carbenium	Lutidinium*	tert-butyl carbenium	Lutidinium*	
PBS-Al	+30	-101	+100 (-70)	-41 (-60)	27.6
Mordenite	-88	-241	-1 (-87)	-172 (-69)	34.1

* These calculations were performed with the same functional (PBE) as for the formation of tert-butyl carbenium ion, and include dispersion corrections (DFT–D2).

* as calculated for π -complexes, see Table 1.

SUPPORTING INFORMATION

Revisiting carbenium chemistry

on Amorphous Silica Alumina:

unraveling their milder acidity as compared to zeolites

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S1. Gibbs free energy calculations

S1.1. Calculation of the various corrections (H, S, translational, rotational and vibrational) for ideal gases

To take into account temperature (T) and pressure (P) effects from the energies U calculated with VASP, the Gibbs free energy G has to be estimated thanks to equations S1., S2. and S3, with H the enthalpy, S the entropy, V_m the molar volume, U_{elec} the electronic (DFT+D) contribution to energy, U_{trans} , U_{rot} , U_{vib} the translational, rotational and vibrational contributions to enthalpy respectively, ZPE the zero-point vibrational energy, S_{trans} , S_{rot} , $S_{vib(T)}$ the translational, rotational and vibrational contributions to entropy respectively.

$$G_{(T)} = H_{(T)} - T \times S_{(T)} \quad \text{Equation S1}$$

$$H_{(T)} = U_{(T)} + PV_m = U_{elec} + U_{trans(T)} + U_{rot(T)} + U_{vib(T)} + ZPE + PV_m \quad \text{Equation S2}$$

$$S_{(T)} = S_{trans(T)} + S_{rot(T)} + S_{vib(T)} \quad \text{Equation S3}$$

This can also be written as :

$$G_{(T)} = U_{elec} + F_{trans(T)} + F_{rot(T)} + F_{vib(T)} + PV_m + ZPE \quad \text{Equation S4}$$

where $F_{trans(T)}$, $F_{rot(T)}$ and $F_{vib(T)}$ are translational, rotational and vibrational contributions to free energy.

Each term was evaluated thanks to statistical thermodynamics, within the ideal gas model for gaseous species, according to equations S4-S8. In particular, the S_{trans} term is given by the Sackur-Tetrode equation (equation S7).¹⁻³

$$U_{trans(T)} = U_{rot(T)} = \frac{3}{2} \mathcal{N} kT \quad \text{Equation S5}$$

$$ZPE + U_{vib(T)} = \mathcal{N} \left(\frac{1}{2} \sum_i h\nu_i + \sum_i \frac{h\nu_i \times \exp\left(\frac{-h\nu_i}{kT}\right)}{1 - \exp\left(\frac{-h\nu_i}{kT}\right)} \right) \quad \text{Equation S6}$$

$$S_{trans(T)} = \mathcal{N} k \left(\frac{5}{2} \ln T - \ln P + \frac{3}{2} \ln \mathcal{M} - 1,165 \right) \quad \text{Equation S7}$$

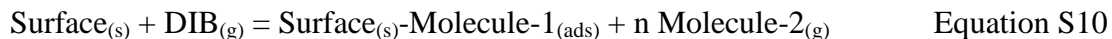
$$S_{rot(T)} = \mathcal{N} k \ln \left(\frac{\sqrt{\pi}}{\sigma} \left(\frac{8\pi^2 kT}{h^2} \right)^{3/2} \sqrt{A_e \times B_e \times C_e} \right) \quad \text{Equation S8}$$

$$S_{vib(T)} = \mathcal{N} k \sum_i \frac{\frac{h\nu_i}{kT} \times \exp\left(\frac{-h\nu_i}{kT}\right)}{1 - \exp\left(\frac{-h\nu_i}{kT}\right)} - \mathcal{N} k \sum_i \ln \left(1 - \exp\left(\frac{-h\nu_i}{kT}\right) \right) \quad \text{Equation S9}$$

with \mathcal{N} : Avogadro constant; k: Boltzmann constant; h : Planck constant; c : speed of light; ν_i : vibration eigenvalues; \mathcal{M} : molar mass; σ : symmetry number; A_e , B_e , C_e : moments of inertia according to the three eigenaxis of the molecule.

S1.2. Calculation of Gibbs free energy of reaction for DIB cracking into isobutene

The reaction profiles, taking into account temperature and pressure effects, are estimated for the following reaction :



$\text{Surface}_{(s)}$ depicts the surface (external surface of ASA or internal surface of MOR) on which the $\text{DIB}_{(g)}$ adsorbs to generate the $\text{Surface}_{(s)}\text{-Molecule-1}_{(ads)}$ system, with $n \text{Molecule-2}_{(g)}$ in case of DIB ($n=1$) or isobutene ($n=1$ or 2) possible release.

$\text{DIB}_{(g)}$ and $\text{Molecule-2}_{(g)}$ are considered as ideal gases, their Gibbs free energies are calculated according to section S1.1. The pressure of each compound is taken equal to 1 bar. The entropy and PV terms relative to $\text{Surface}_{(s)}$ are supposed to be compensated along the reaction depicted by Equation S10.

Regarding the adsorbed molecule $\text{Molecule-1}_{(ads)}$, the translational contributions (Equations S5 and S7) present for the gas phase are supposed to be lost for alkoxide species, whereas two degrees of freedom over 3 are expected to be kept in the adsorbed phase for carbenium and π -complexes. ZPE variations (Equation S6) are neglected between gas phase and adsorbed state.

The reaction Gibbs free energy $\Delta_r G$ corresponding to equation S10 is given in equations S11 and S12, G_i representing the molar Gibbs free energy for each compound i , $\Delta_r U_{elec}$ being the electronic contribution to the reaction energy, ΔF the corresponding thermal correction in free energy, Δ_{ZPE} the variation in ZPE.

$$\Delta_r G_{(T)} = G_{\text{Surface}_{(s)}\text{-Molecule-1}_{(ads)}} + nG_{\text{Molecule-2}_{(g)}} - G_{\text{Surface}_{(s)}} - G_{\text{DIB}_{(g)}} \quad \text{Equation S11}$$

$$\Delta_r G_{(T)} \approx \Delta_r U_{elec} + \Delta F + ((n-1)RT) + \Delta_{ZPE} \quad \text{Equation S12}$$

S2. Isobutene adsorption according to the π -complex mode: variation of adsorption energies with spectroscopic features

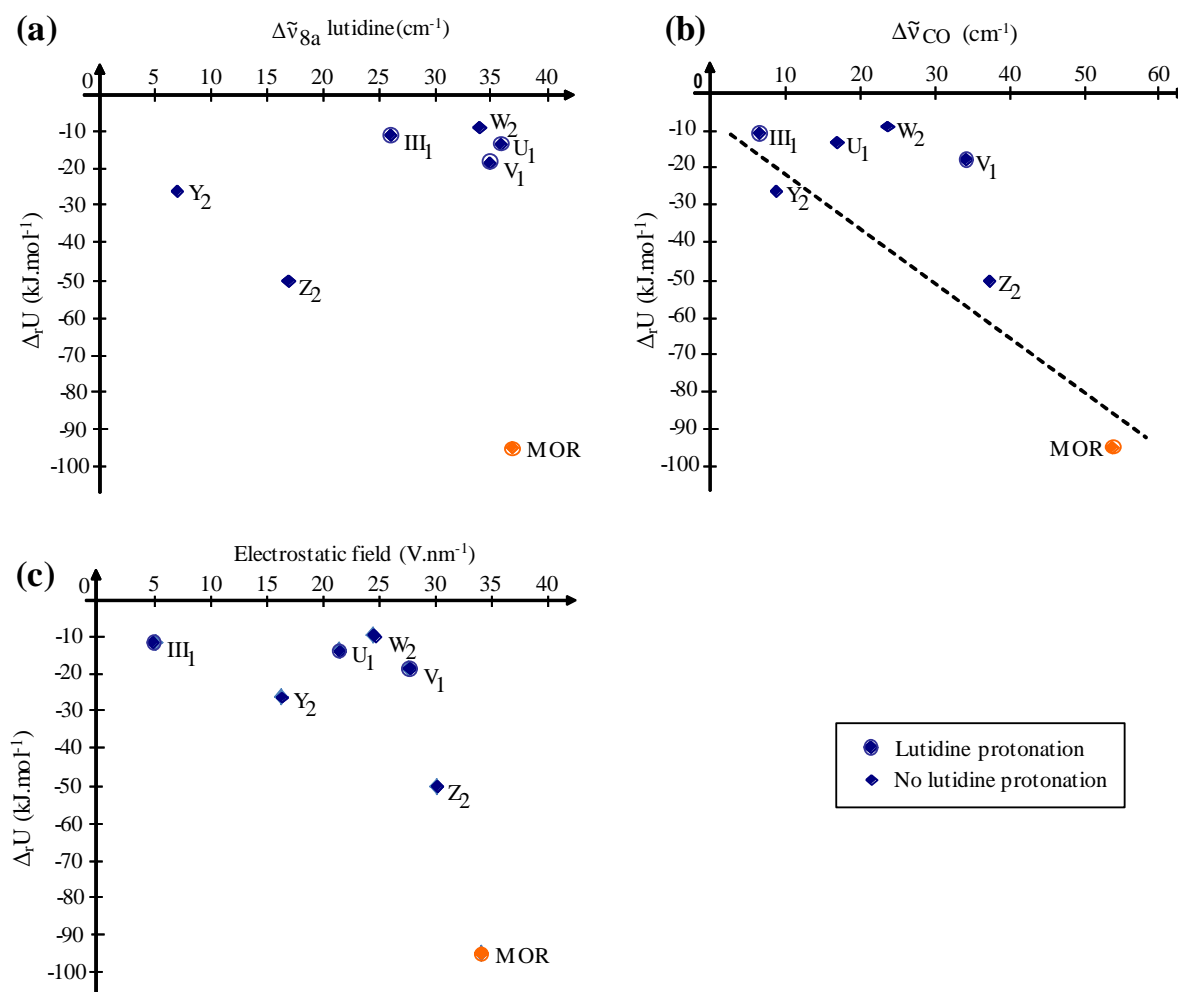


Figure S2.1. Formation energy of the π -complex on ASA (blue) and mordenite (orange) from isobutene, as a function of one vibration frequency of lutidine (a), the frequency shift of CO (b) when adsorbed on the same surface site, (c) the electrostatic field in the π -complex adsorption configuration. Values of lutidine frequencies and CO frequency shifts are extracted from ref. 4 and 5 respectively.

S3. Numerical data for DIB cracking profiles, and energy plot

Table S3.1. Δ_rU and Δ_rG (T=500 K, 1 bar of each gas species) values for the various intermediates calculated on ASA (PBS-Al) and in MOR, for DIB cracking into isobutene (see figure 9 in the manuscript for the terminology). The reference state is the isolated surface site and DIB molecule in gas phase.

Species	Δ_rU (kJ.mol ⁻¹)		Δ_rG (kJ.mol ⁻¹)	
	MOR	ASA	MOR	ASA
DIB _(phys)	-131	-31	-88	12
A _{III}	-122	-82	-4	36
A _{II}	-124	-78	-6	40
C _{III}	-130	20	-87	63
B _{III}	-104	-55	14	63
B _{II}	-77	-32	41	86
1	-54	23	-1	76
2	-52	-5	1	48
3	-52	-20	1	33
4	-54	24	-1	77
5	-44	111	-59	96
1'	-2	60	10	75
2'	-9	27	3	43
3'	11	117	-45	61
A	-8	68	-65	16
B	-8	68	-65	16
Final state	87	87	-3	-3

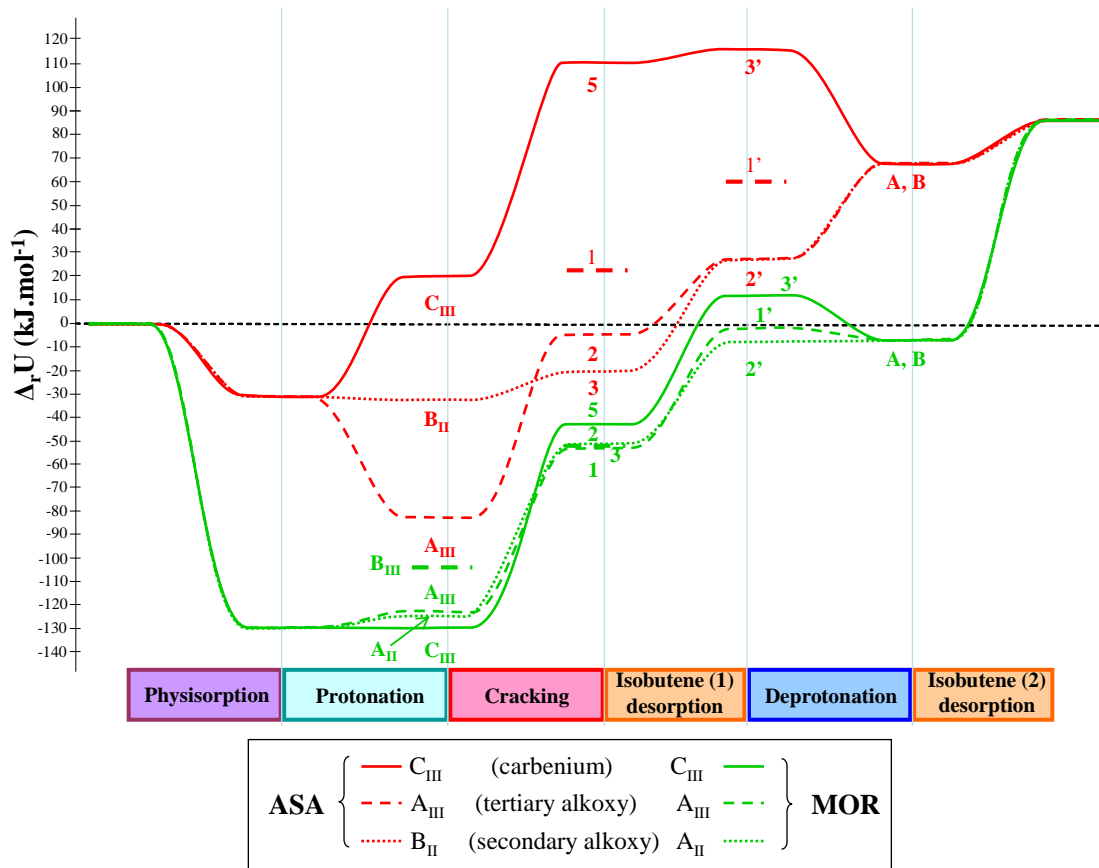


Figure S3.1. Energy profiles for the selected cracking pathways of diisobutene on the ASA surface (PBS-Al site) and in mordenite. Labels refer to intermediates depicted in Figure 9. Lines relate to the selected pathways, as explained in the main text.

S4. .cif files for most important structures involved in DIB reaction on ASA and in MOR

Table S4.1 indicates the number of the file reported below, corresponding to the structures on MOR and ASA.

Table S4.1. Number of the files for the systems which coordinate are reported below.

Species	File number	
	MOR	ASA
DIB _(phys)	1	11
A _{III}	2	12
C _{III}	3	13
1	4	14
2	5	15
5	6	16
1'	7	17
2'	8	18
3'	9	19
A	10	20

The common first lines for files n°1 to 10 are the following in the .cif files:

```
data_File
_audit_creation_date      2014-10-29
_audit_creation_method    'Leydier et al.'
_symmetry_space_group_name_H-M  'P1'
_symmetry_Int_Tables_number  1
_symmetry_cell_setting    triclinic
loop_
_symmetry_equiv_pos_as_xyz
x,y,z
_cell_length_a            13.7839
_cell_length_b            13.7839
_cell_length_c            15.1482
_cell_angle_alpha         90.0000
_cell_angle_beta          90.0000
_cell_angle_gamma        83.1126
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_U_iso_or_equiv
_atom_site_adp_type
_atom_site_occupancy
```

The common first lines for files n°11 to 20 are the following in the .cif files:

```
data_File
_audit_creation_date      2014-10-29
_audit_creation_method    'Leydier et al.'
_symmetry_space_group_name_H-M  'P1'
_symmetry_Int_Tables_number  1
_symmetry_cell_setting    triclinic
loop_
_symmetry_equiv_pos_as_xyz
x,y,z
_cell_length_a            43.0000
_cell_length_b            16.7682
_cell_length_c            11.1308
_cell_angle_alpha         89.9903
```

```

_cell_angle_beta      90.0000
_cell_angle_gamma     90.0000
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_U_iso_or_equiv
_atom_site_adp_type
_atom_site_occupancy

```

Then come the coordinates :

File n°1

```

Si2 Si 0.37635 0.76224 0.02399 0.00000 Uiso 1.00
Si3 Si 0.60998 0.00605 0.02213 0.00000 Uiso 1.00
Si4 Si 0.61276 0.23289 0.27342 0.00000 Uiso 1.00
Si5 Si 0.37603 0.98743 0.27484 0.00000 Uiso 1.00
Si6 Si 0.76183 0.37630 0.23162 0.00000 Uiso 1.00
Si7 Si 0.00743 0.60133 0.22567 0.00000 Uiso 1.00
Si8 Si 0.23320 0.61310 0.47975 0.00000 Uiso 1.00
Si9 Si 0.98763 0.38190 0.47806 0.00000 Uiso 1.00
Si10 Si 0.61599 0.23035 0.48027 0.00000 Uiso 1.00
Si11 Si 0.37397 0.99002 0.48146 0.00000 Uiso 1.00
Si12 Si 0.37363 0.76351 0.23056 0.00000 Uiso 1.00
Si13 Si 0.60226 0.00744 0.22857 0.00000 Uiso 1.00
Si14 Si 0.23068 0.61073 0.27227 0.00000 Uiso 1.00
Si15 Si 0.98867 0.37519 0.27338 0.00000 Uiso 1.00
Si16 Si 0.76363 0.37945 0.02694 0.00000 Uiso 1.00
Si17 Si 0.00587 0.60456 0.01884 0.00000 Uiso 1.00
Si18 Si 0.46337 0.28870 0.12564 0.00000 Uiso 1.00
Si19 Si 0.31154 0.13426 0.12669 0.00000 Uiso 1.00
Si20 Si 0.53622 0.70496 0.37567 0.00000 Uiso 1.00
Si21 Si 0.68767 0.86587 0.37482 0.00000 Uiso 1.00
Si22 Si 0.28800 0.46222 0.12705 0.00000 Uiso 1.00
Si23 Si 0.13541 0.30797 0.12751 0.00000 Uiso 1.00
Si24 Si 0.69847 0.53397 0.37986 0.00000 Uiso 1.00
Si25 Si 0.37608 0.76587 0.52261 0.00000 Uiso 1.00
Si26 Si 0.60173 0.00601 0.52554 0.00000 Uiso 1.00
Si27 Si 0.62203 0.22622 0.77484 0.00000 Uiso 1.00
Si28 Si 0.37891 0.99077 0.77306 0.00000 Uiso 1.00
Si29 Si 0.76380 0.37305 0.72890 0.00000 Uiso 1.00
Si30 Si 0.00658 0.60475 0.73461 0.00000 Uiso 1.00
Si31 Si 0.22787 0.62046 0.97997 0.00000 Uiso 1.00
Si32 Si 0.98997 0.37863 0.97926 0.00000 Uiso 1.00
Si33 Si 0.62282 0.22881 0.98133 0.00000 Uiso 1.00
Si34 Si 0.38365 0.98899 0.97769 0.00000 Uiso 1.00
Si35 Si 0.37449 0.76504 0.72878 0.00000 Uiso 1.00
Si36 Si 0.60737 0.00346 0.73141 0.00000 Uiso 1.00
Si37 Si 0.22999 0.61899 0.77447 0.00000 Uiso 1.00
Si38 Si 0.98887 0.37996 0.77686 0.00000 Uiso 1.00
Si39 Si 0.76054 0.37520 0.52324 0.00000 Uiso 1.00
Si40 Si 0.01029 0.60608 0.52675 0.00000 Uiso 1.00
Si41 Si 0.46504 0.28842 0.62868 0.00000 Uiso 1.00
Si42 Si 0.30836 0.13835 0.62655 0.00000 Uiso 1.00
Si43 Si 0.53108 0.70222 0.87713 0.00000 Uiso 1.00
Si44 Si 0.68734 0.85795 0.87837 0.00000 Uiso 1.00
Si45 Si 0.29148 0.46445 0.62603 0.00000 Uiso 1.00
Si46 Si 0.13457 0.31433 0.62610 0.00000 Uiso 1.00
Si47 Si 0.70264 0.53078 0.87549 0.00000 Uiso 1.00
Si48 Si 0.85897 0.68625 0.87467 0.00000 Uiso 1.00
Al49 Al 0.86746 0.68462 0.37948 0.00000 Uiso 1.00
O50 O 0.52569 0.29401 0.21653 0.00000 Uiso 1.00
O51 O 0.31053 0.06899 0.21610 0.00000 Uiso 1.00
O52 O 0.34754 0.88294 0.51000 0.00000 Uiso 1.00
O53 O 0.47331 0.72886 0.46536 0.00000 Uiso 1.00
O54 O 0.67113 0.92884 0.46462 0.00000 Uiso 1.00
O55 O 0.62541 0.11870 0.24321 0.00000 Uiso 1.00
O56 O 0.28182 0.53375 0.04164 0.00000 Uiso 1.00
O57 O 0.06881 0.31067 0.03889 0.00000 Uiso 1.00
O58 O 0.87886 0.35436 0.24673 0.00000 Uiso 1.00
O59 O 0.71188 0.46544 0.29181 0.00000 Uiso 1.00
O60 O 0.93517 0.67508 0.28361 0.00000 Uiso 1.00
O61 O 0.11219 0.64077 0.00197 0.00000 Uiso 1.00
O62 O 0.46711 0.71990 0.28922 0.00000 Uiso 1.00
O63 O 0.67864 0.93539 0.28843 0.00000 Uiso 1.00
O64 O 0.64304 0.11409 0.00844 0.00000 Uiso 1.00
O65 O 0.53422 0.28450 0.03981 0.00000 Uiso 1.00
O66 O 0.31495 0.06460 0.03996 0.00000 Uiso 1.00
O67 O 0.34865 0.88030 0.24749 0.00000 Uiso 1.00
O68 O 0.70264 0.46299 0.46632 0.00000 Uiso 1.00
O69 O 0.93866 0.68475 0.47312 0.00000 Uiso 1.00
O70 O 0.12034 0.62542 0.23423 0.00000 Uiso 1.00
O71 O 0.29568 0.52351 0.21807 0.00000 Uiso 1.00
O72 O 0.06727 0.30445 0.21483 0.00000 Uiso 1.00
O73 O 0.87722 0.36380 0.50522 0.00000 Uiso 1.00
O74 O 0.49209 -0.00679 0.25929 0.00000 Uiso 1.00
O75 O 0.49796 0.00466 0.98923 0.00000 Uiso 1.00
O76 O 0.00862 0.49244 0.98463 0.00000 Uiso 1.00
O77 O 0.00273 0.48841 0.25625 0.00000 Uiso 1.00

```

O78	O	0.38537	0.38511	0.11773	0.00000	Uiso	1.00
O79	O	0.21314	0.21035	0.12433	0.00000	Uiso	1.00
O80	O	0.58840	0.59369	0.37740	0.00000	Uiso	1.00
O81	O	0.80482	0.81387	0.37784	0.00000	Uiso	1.00
O82	O	0.40918	0.19003	0.12780	0.00000	Uiso	1.00
O83	O	0.61873	0.78052	0.36889	0.00000	Uiso	1.00
O84	O	0.19096	0.40572	0.13054	0.00000	Uiso	1.00
O85	O	0.77863	0.60817	0.38461	0.00000	Uiso	1.00
O86	O	0.34994	0.00931	0.37778	0.00000	Uiso	1.00
O87	O	0.58349	0.24166	0.37728	0.00000	Uiso	1.00
O88	O	0.61936	0.97614	0.12603	0.00000	Uiso	1.00
O89	O	0.40202	0.74263	0.12761	0.00000	Uiso	1.00
O90	O	0.00853	0.34747	0.37658	0.00000	Uiso	1.00
O91	O	0.23271	0.58145	0.37637	0.00000	Uiso	1.00
O92	O	0.97640	0.61222	0.12194	0.00000	Uiso	1.00
O93	O	0.73804	0.40589	0.12927	0.00000	Uiso	1.00
O94	O	0.71596	0.27544	0.25577	0.00000	Uiso	1.00
O95	O	0.27335	0.72223	-0.00066	0.00000	Uiso	1.00
O96	O	0.27786	0.71253	0.25812	0.00000	Uiso	1.00
O97	O	0.72251	0.27752	-0.00012	0.00000	Uiso	1.00
O98	O	0.53404	0.28296	0.71597	0.00000	Uiso	1.00
O99	O	0.31035	0.07022	0.71429	0.00000	Uiso	1.00
O100	O	0.36638	0.87844	0.00373	0.00000	Uiso	1.00
O101	O	0.46336	0.70443	0.96504	0.00000	Uiso	1.00
O102	O	0.68223	0.92761	0.96555	0.00000	Uiso	1.00
O103	O	0.63916	0.11100	0.74987	0.00000	Uiso	1.00
O104	O	0.29834	0.52739	0.53576	0.00000	Uiso	1.00
O105	O	0.06421	0.31332	0.54024	0.00000	Uiso	1.00
O106	O	0.88105	0.36180	0.74260	0.00000	Uiso	1.00
O107	O	0.70877	0.45931	0.79016	0.00000	Uiso	1.00
O108	O	0.92754	0.68127	0.78695	0.00000	Uiso	1.00
O109	O	0.12343	0.63039	0.51940	0.00000	Uiso	1.00
O110	O	0.46500	0.71461	0.78817	0.00000	Uiso	1.00
O111	O	0.67683	0.92353	0.78872	0.00000	Uiso	1.00
O112	O	0.62938	0.11525	0.50756	0.00000	Uiso	1.00
O113	O	0.53084	0.29070	0.53969	0.00000	Uiso	1.00
O114	O	0.30600	0.07199	0.53786	0.00000	Uiso	1.00
O115	O	0.35719	0.88214	0.74458	0.00000	Uiso	1.00
O116	O	0.71123	0.46807	0.96648	0.00000	Uiso	1.00
O117	O	0.92494	0.67573	0.96374	0.00000	Uiso	1.00
O118	O	0.11470	0.63663	0.75071	0.00000	Uiso	1.00
O119	O	0.28703	0.53349	0.71324	0.00000	Uiso	1.00
O120	O	0.07027	0.31690	0.71603	0.00000	Uiso	1.00
O121	O	0.88089	0.36534	0.01323	0.00000	Uiso	1.00
O122	O	0.49362	0.00183	0.75785	0.00000	Uiso	1.00
O123	O	0.48878	-0.00167	0.50011	0.00000	Uiso	1.00
O124	O	0.00388	0.49581	0.48855	0.00000	Uiso	1.00
O125	O	0.00205	0.49532	0.77329	0.00000	Uiso	1.00
O126	O	0.38865	0.38656	0.63332	0.00000	Uiso	1.00
O127	O	0.21080	0.21555	0.62739	0.00000	Uiso	1.00
O128	O	0.59768	0.59742	0.87347	0.00000	Uiso	1.00
O129	O	0.79227	0.79148	0.87664	0.00000	Uiso	1.00
O130	O	0.40733	0.19211	0.62532	0.00000	Uiso	1.00
O131	O	0.59808	0.79114	0.88271	0.00000	Uiso	1.00
O132	O	0.19288	0.41022	0.62232	0.00000	Uiso	1.00
O133	O	0.79113	0.59792	0.87073	0.00000	Uiso	1.00
O134	O	0.35114	0.01102	0.87601	0.00000	Uiso	1.00
O135	O	0.59148	0.24021	0.87807	0.00000	Uiso	1.00
O136	O	0.62336	0.97558	0.62759	0.00000	Uiso	1.00
O137	O	0.40079	0.74128	0.62570	0.00000	Uiso	1.00
O138	O	0.00380	0.34156	0.87776	0.00000	Uiso	1.00
O139	O	0.24586	0.58732	0.87747	0.00000	Uiso	1.00
O140	O	0.97996	0.60817	0.63082	0.00000	Uiso	1.00
O141	O	0.73784	0.39955	0.62670	0.00000	Uiso	1.00
O142	O	0.72440	0.26995	0.75530	0.00000	Uiso	1.00
O143	O	0.28278	0.71417	0.48928	0.00000	Uiso	1.00
O144	O	0.27423	0.72149	0.75615	0.00000	Uiso	1.00
O145	O	0.72025	0.27180	0.49689	0.00000	Uiso	1.00
H146	H	0.85327	0.86547	0.38240	0.00000	Uiso	1.00
H147	H	0.85747	0.96686	0.19324	0.00000	Uiso	1.00
H148	H	0.96343	0.10052	0.23380	0.00000	Uiso	1.00
H149	H	0.86295	0.02357	0.34200	0.00000	Uiso	1.00
H150	H	0.81455	0.05802	0.47907	0.00000	Uiso	1.00
H151	H	0.91449	0.05603	0.55378	0.00000	Uiso	1.00
H152	H	0.89795	0.84203	0.21932	0.00000	Uiso	1.00
H153	H	0.96267	0.90483	0.14038	0.00000	Uiso	1.00
H154	H	0.06599	0.03088	0.18319	0.00000	Uiso	1.00
H155	H	0.07366	0.07048	0.29492	0.00000	Uiso	1.00
H156	H	0.13233	0.89406	0.33203	0.00000	Uiso	1.00
H157	H	0.11307	0.85544	0.22245	0.00000	Uiso	1.00
H158	H	0.05636	0.79987	0.31077	0.00000	Uiso	1.00
H159	H	0.99938	0.85608	0.54620	0.00000	Uiso	1.00
H160	H	0.07824	0.94300	0.51662	0.00000	Uiso	1.00
H161	H	0.06750	0.84097	0.44675	0.00000	Uiso	1.00
H162	H	0.84170	0.95893	0.55519	0.00000	Uiso	1.00
C163	C	0.02507	0.04342	0.24542	0.00000	Uiso	1.00
C164	C	0.87359	0.01030	0.51115	0.00000	Uiso	1.00
C165	C	0.98897	0.94681	0.27587	0.00000	Uiso	1.00
C166	C	0.92222	0.91298	0.20311	0.00000	Uiso	1.00
C167	C	0.07772	0.86954	0.28702	0.00000	Uiso	1.00
C168	C	0.92805	0.97239	0.35799	0.00000	Uiso	1.00
C169	C	0.94323	0.95679	0.44580	0.00000	Uiso	1.00
C170	C	0.02693	0.89488	0.48974	0.00000	Uiso	1.00

File n°2

Si2	Si	0.36932	0.76300	0.02632	0.00000	Uiso	1.00
Si3	Si	0.60222	0.00080	0.02551	0.00000	Uiso	1.00
Si4	Si	0.61474	0.23027	0.27519	0.00000	Uiso	1.00
Si5	Si	0.37466	0.98716	0.27724	0.00000	Uiso	1.00

Si6	Si	0.75690	0.37866	0.23196	0.00000	Uiso	1.00
Si7	Si	0.00858	0.60622	0.23057	0.00000	Uiso	1.00
Si8	Si	0.22783	0.61377	0.48225	0.00000	Uiso	1.00
Si9	Si	0.98908	0.37392	0.48201	0.00000	Uiso	1.00
Si10	Si	0.61465	0.22547	0.48223	0.00000	Uiso	1.00
Si11	Si	0.36684	0.99097	0.48339	0.00000	Uiso	1.00
Si12	Si	0.37814	0.76019	0.23182	0.00000	Uiso	1.00
Si13	Si	0.59952	0.00798	0.23195	0.00000	Uiso	1.00
Si14	Si	0.23161	0.61310	0.27538	0.00000	Uiso	1.00
Si15	Si	0.98495	0.38163	0.27690	0.00000	Uiso	1.00
Si16	Si	0.76389	0.36923	0.02685	0.00000	Uiso	1.00
Si17	Si	0.00139	0.60138	0.02255	0.00000	Uiso	1.00
Si18	Si	0.46230	0.28680	0.12849	0.00000	Uiso	1.00
Si19	Si	0.30744	0.13481	0.13016	0.00000	Uiso	1.00
Si20	Si	0.53784	0.70334	0.37696	0.00000	Uiso	1.00
Si21	Si	0.68826	0.86440	0.37876	0.00000	Uiso	1.00
Si22	Si	0.28876	0.46260	0.13082	0.00000	Uiso	1.00
Si23	Si	0.13353	0.31086	0.13060	0.00000	Uiso	1.00
Si24	Si	0.69863	0.53489	0.37711	0.00000	Uiso	1.00
Si25	Si	0.37368	0.76625	0.52344	0.00000	Uiso	1.00
Si26	Si	0.59425	0.00428	0.52863	0.00000	Uiso	1.00
Si27	Si	0.61753	0.22628	0.77556	0.00000	Uiso	1.00
Si28	Si	0.37945	0.98516	0.77781	0.00000	Uiso	1.00
Si29	Si	0.75701	0.37791	0.72935	0.00000	Uiso	1.00
Si30	Si	0.00627	0.60346	0.73944	0.00000	Uiso	1.00
Si31	Si	0.22597	0.61677	0.98183	0.00000	Uiso	1.00
Si32	Si	0.98701	0.37368	0.98182	0.00000	Uiso	1.00
Si33	Si	0.61807	0.22313	0.98239	0.00000	Uiso	1.00
Si34	Si	0.37463	0.98793	0.98185	0.00000	Uiso	1.00
Si35	Si	0.37922	0.75738	0.72909	0.00000	Uiso	1.00
Si36	Si	0.60422	0.00461	0.73497	0.00000	Uiso	1.00
Si37	Si	0.23029	0.61605	0.77631	0.00000	Uiso	1.00
Si38	Si	0.98366	0.38029	0.77940	0.00000	Uiso	1.00
Si39	Si	0.76232	0.37208	0.52338	0.00000	Uiso	1.00
Si40	Si	0.00599	0.59964	0.53078	0.00000	Uiso	1.00
Si41	Si	0.46062	0.28486	0.62982	0.00000	Uiso	1.00
Si42	Si	0.30453	0.13348	0.63070	0.00000	Uiso	1.00
Si43	Si	0.52936	0.69908	0.87826	0.00000	Uiso	1.00
Si44	Si	0.68443	0.85649	0.87908	0.00000	Uiso	1.00
Si45	Si	0.28694	0.46094	0.62789	0.00000	Uiso	1.00
Si46	Si	0.13158	0.30892	0.62948	0.00000	Uiso	1.00
Si47	Si	0.70119	0.52936	0.87780	0.00000	Uiso	1.00
Si48	Si	0.85701	0.68608	0.87803	0.00000	Uiso	1.00
Al49	Al	0.86386	0.69007	0.37981	0.00000	Uiso	1.00
O50	O	0.52796	0.29084	0.21756	0.00000	Uiso	1.00
O51	O	0.30637	0.06446	0.21635	0.00000	Uiso	1.00
O52	O	0.34366	0.88379	0.51555	0.00000	Uiso	1.00
O53	O	0.46828	0.73423	0.46144	0.00000	Uiso	1.00
O54	O	0.65909	0.92186	0.46997	0.00000	Uiso	1.00
O55	O	0.63142	0.11701	0.24185	0.00000	Uiso	1.00
O56	O	0.28279	0.53195	0.04387	0.00000	Uiso	1.00
O57	O	0.07286	0.31134	0.03865	0.00000	Uiso	1.00
O58	O	0.87369	0.36673	0.25000	0.00000	Uiso	1.00
O59	O	0.70006	0.46835	0.28749	0.00000	Uiso	1.00
O60	O	0.93939	0.68366	0.28791	0.00000	Uiso	1.00
O61	O	0.10967	0.63096	0.00169	0.00000	Uiso	1.00
O62	O	0.47377	0.71392	0.28674	0.00000	Uiso	1.00
O63	O	0.67321	0.93494	0.29293	0.00000	Uiso	1.00
O64	O	0.63539	0.10861	0.01062	0.00000	Uiso	1.00
O65	O	0.53054	0.28118	0.04079	0.00000	Uiso	1.00
O66	O	0.30868	0.07025	0.04018	0.00000	Uiso	1.00
O67	O	0.35875	0.87748	0.24748	0.00000	Uiso	1.00
O68	O	0.71635	0.46132	0.46159	0.00000	Uiso	1.00
O69	O	0.92604	0.67024	0.47829	0.00000	Uiso	1.00
O70	O	0.12190	0.63072	0.23565	0.00000	Uiso	1.00
O71	O	0.29632	0.52606	0.22059	0.00000	Uiso	1.00
O72	O	0.05988	0.31150	0.21438	0.00000	Uiso	1.00
O73	O	0.88027	0.35247	0.51204	0.00000	Uiso	1.00
O74	O	0.48883	0.00439	0.26690	0.00000	Uiso	1.00
O75	O	0.49002	-0.00088	0.99335	0.00000	Uiso	1.00
O76	O	-0.00517	0.48983	0.99036	0.00000	Uiso	1.00
O77	O	0.00393	0.49471	0.26603	0.00000	Uiso	1.00
O78	O	0.38576	0.38467	0.12287	0.00000	Uiso	1.00
O79	O	0.20950	0.21173	0.13313	0.00000	Uiso	1.00
O80	O	0.58766	0.59172	0.38776	0.00000	Uiso	1.00
O81	O	0.80853	0.82315	0.38306	0.00000	Uiso	1.00
O82	O	0.40571	0.18964	0.13309	0.00000	Uiso	1.00
O83	O	0.62354	0.77527	0.36950	0.00000	Uiso	1.00
O84	O	0.19101	0.40715	0.13530	0.00000	Uiso	1.00
O85	O	0.77630	0.61158	0.37125	0.00000	Uiso	1.00
O86	O	0.34175	0.00559	0.37927	0.00000	Uiso	1.00
O87	O	0.58310	0.23464	0.37872	0.00000	Uiso	1.00
O88	O	0.61157	0.97225	0.12995	0.00000	Uiso	1.00
O89	O	0.39979	0.73687	0.12805	0.00000	Uiso	1.00
O90	O	0.00536	0.34639	0.37830	0.00000	Uiso	1.00
O91	O	0.23099	0.58176	0.37882	0.00000	Uiso	1.00
O92	O	0.97648	0.61234	0.12667	0.00000	Uiso	1.00
O93	O	0.73432	0.39953	0.12778	0.00000	Uiso	1.00
O94	O	0.71714	0.27587	0.26095	0.00000	Uiso	1.00
O95	O	0.26735	0.72049	0.00218	0.00000	Uiso	1.00
O96	O	0.28111	0.71413	0.26471	0.00000	Uiso	1.00
O97	O	0.71974	0.26876	0.99994	0.00000	Uiso	1.00
O98	O	0.52811	0.28257	0.71803	0.00000	Uiso	1.00
O99	O	0.31063	0.05894	0.71417	0.00000	Uiso	1.00
O100	O	0.35251	0.88076	0.01433	0.00000	Uiso	1.00
O101	O	0.45618	0.71388	0.96243	0.00000	Uiso	1.00
O102	O	0.67409	0.92160	0.96929	0.00000	Uiso	1.00
O103	O	0.63894	0.11238	0.74585	0.00000	Uiso	1.00
O104	O	0.28977	0.52692	0.53920	0.00000	Uiso	1.00
O105	O	0.06878	0.30239	0.53914	0.00000	Uiso	1.00
O106	O	0.87347	0.36820	0.74777	0.00000	Uiso	1.00

O107	O	0.70006	0.46711	0.78667	0.00000	Uiso	1.00
O108	O	0.92745	0.68077	0.79143	0.00000	Uiso	1.00
O109	O	0.11590	0.63241	0.51723	0.00000	Uiso	1.00
O110	O	0.46811	0.69967	0.78637	0.00000	Uiso	1.00
O111	O	0.67668	0.92658	0.79201	0.00000	Uiso	1.00
O112	O	0.63094	0.11033	0.51051	0.00000	Uiso	1.00
O113	O	0.52781	0.28369	0.54129	0.00000	Uiso	1.00
O114	O	0.29758	0.07343	0.53862	0.00000	Uiso	1.00
O115	O	0.36869	0.87351	0.75003	0.00000	Uiso	1.00
O116	O	0.71877	0.45728	0.96235	0.00000	Uiso	1.00
O117	O	0.92156	0.67508	0.96823	0.00000	Uiso	1.00
O118	O	0.11454	0.63586	0.75460	0.00000	Uiso	1.00
O119	O	0.28469	0.52799	0.71626	0.00000	Uiso	1.00
O120	O	0.06002	0.31617	0.71488	0.00000	Uiso	1.00
O121	O	0.88185	0.34927	0.01834	0.00000	Uiso	1.00
O122	O	0.49277	0.00597	0.77009	0.00000	Uiso	1.00
O123	O	0.48058	0.00533	0.50103	0.00000	Uiso	1.00
O124	O	0.00685	0.48633	0.49863	0.00000	Uiso	1.00
O125	O	0.00226	0.49441	0.77918	0.00000	Uiso	1.00
O126	O	0.38495	0.38367	0.63047	0.00000	Uiso	1.00
O127	O	0.20734	0.21048	0.63993	0.00000	Uiso	1.00
O128	O	0.59591	0.59466	0.88889	0.00000	Uiso	1.00
O129	O	0.79051	0.79166	0.87926	0.00000	Uiso	1.00
O130	O	0.40287	0.18843	0.62938	0.00000	Uiso	1.00
O131	O	0.59665	0.78790	0.87584	0.00000	Uiso	1.00
O132	O	0.18949	0.40505	0.62619	0.00000	Uiso	1.00
O133	O	0.78816	0.59848	0.87279	0.00000	Uiso	1.00
O134	O	0.34356	0.00457	0.87908	0.00000	Uiso	1.00
O135	O	0.58675	0.23419	0.87912	0.00000	Uiso	1.00
O136	O	0.61111	0.97332	0.63135	0.00000	Uiso	1.00
O137	O	0.40360	0.73814	0.62502	0.00000	Uiso	1.00
O138	O	0.00052	0.33939	0.87953	0.00000	Uiso	1.00
O139	O	0.24736	0.58541	0.87943	0.00000	Uiso	1.00
O140	O	0.97999	0.60544	0.63576	0.00000	Uiso	1.00
O141	O	0.73503	0.40018	0.62560	0.00000	Uiso	1.00
O142	O	0.71732	0.27562	0.75822	0.00000	Uiso	1.00
O143	O	0.27934	0.71375	0.49345	0.00000	Uiso	1.00
O144	O	0.27674	0.71695	0.75517	0.00000	Uiso	1.00
O145	O	0.71693	0.27115	0.49769	0.00000	Uiso	1.00
H146	H	0.92204	0.12467	0.29672	0.00000	Uiso	1.00
H147	H	0.89374	0.05117	0.43246	0.00000	Uiso	1.00
H148	H	0.82077	0.98035	0.49642	0.00000	Uiso	1.00
H149	H	0.77662	0.03387	0.39347	0.00000	Uiso	1.00
H150	H	0.91969	0.85129	0.25233	0.00000	Uiso	1.00
H151	H	0.90326	0.04642	0.14301	0.00000	Uiso	1.00
H152	H	0.97117	0.93125	0.11752	0.00000	Uiso	1.00
H153	H	0.03195	0.03820	0.12522	0.00000	Uiso	1.00
H154	H	0.04615	0.12225	0.26413	0.00000	Uiso	1.00
H155	H	0.01877	0.07274	0.36737	0.00000	Uiso	1.00
H156	H	0.14776	0.95851	0.22674	0.00000	Uiso	1.00
H157	H	0.09334	0.84774	0.23285	0.00000	Uiso	1.00
H158	H	0.11747	0.91226	0.33061	0.00000	Uiso	1.00
H159	H	0.83869	0.96167	0.25567	0.00000	Uiso	1.00
H160	H	0.01774	0.80138	0.39904	0.00000	Uiso	1.00
H161	H	0.95549	0.84180	0.49891	0.00000	Uiso	1.00
H162	H	0.02596	0.92072	0.44035	0.00000	Uiso	1.00
C163	C	0.84053	0.99812	0.42880	0.00000	Uiso	1.00
C164	C	0.99230	0.98142	0.25262	0.00000	Uiso	1.00
C165	C	0.97326	0.00037	0.15349	0.00000	Uiso	1.00
C166	C	0.99415	0.08062	0.29831	0.00000	Uiso	1.00
C167	C	0.09308	0.92098	0.26177	0.00000	Uiso	1.00
C168	C	0.90671	0.92387	0.28310	0.00000	Uiso	1.00
C169	C	0.89058	0.90986	0.38105	0.00000	Uiso	1.00
C170	C	0.97710	0.86369	0.43294	0.00000	Uiso	1.00

File n°3

Si2	Si	0.37548	0.76534	0.02423	0.00000	Uiso	1.00
Si3	Si	0.60800	0.00145	0.02323	0.00000	Uiso	1.00
Si4	Si	0.61635	0.23147	0.27219	0.00000	Uiso	1.00
Si5	Si	0.37983	0.98552	0.27478	0.00000	Uiso	1.00
Si6	Si	0.76114	0.37662	0.22990	0.00000	Uiso	1.00
Si7	Si	0.01357	0.60542	0.22778	0.00000	Uiso	1.00
Si8	Si	0.23427	0.60967	0.48055	0.00000	Uiso	1.00
Si9	Si	0.99035	0.37861	0.47958	0.00000	Uiso	1.00
Si10	Si	0.61630	0.22984	0.47939	0.00000	Uiso	1.00
Si11	Si	0.37751	0.98724	0.47951	0.00000	Uiso	1.00
Si12	Si	0.38184	0.75958	0.23047	0.00000	Uiso	1.00
Si13	Si	0.60552	0.00615	0.22981	0.00000	Uiso	1.00
Si14	Si	0.23821	0.60808	0.27239	0.00000	Uiso	1.00
Si15	Si	0.98843	0.38117	0.27492	0.00000	Uiso	1.00
Si16	Si	0.76662	0.37179	0.02410	0.00000	Uiso	1.00
Si17	Si	0.00665	0.60349	0.02052	0.00000	Uiso	1.00
Si18	Si	0.46717	0.28731	0.12494	0.00000	Uiso	1.00
Si19	Si	0.31260	0.13507	0.12757	0.00000	Uiso	1.00
Si20	Si	0.54023	0.70672	0.37655	0.00000	Uiso	1.00
Si21	Si	0.69456	0.86498	0.37653	0.00000	Uiso	1.00
Si22	Si	0.29297	0.46144	0.12610	0.00000	Uiso	1.00
Si23	Si	0.13729	0.30999	0.12893	0.00000	Uiso	1.00
Si24	Si	0.70840	0.53248	0.37611	0.00000	Uiso	1.00
Si25	Si	0.37591	0.76305	0.52174	0.00000	Uiso	1.00
Si26	Si	0.60451	0.00435	0.52411	0.00000	Uiso	1.00
Si27	Si	0.62648	0.22546	0.77344	0.00000	Uiso	1.00
Si28	Si	0.38533	0.98943	0.77424	0.00000	Uiso	1.00
Si29	Si	0.76504	0.37634	0.72813	0.00000	Uiso	1.00
Si30	Si	0.00987	0.60490	0.73555	0.00000	Uiso	1.00
Si31	Si	0.22973	0.62026	0.97992	0.00000	Uiso	1.00
Si32	Si	0.99238	0.37619	0.97918	0.00000	Uiso	1.00
Si33	Si	0.62468	0.22248	0.97971	0.00000	Uiso	1.00
Si34	Si	0.38039	0.99062	0.97866	0.00000	Uiso	1.00

Si35	Si	0.37960	0.76219	0.72795	0.00000	Uiso	1.00
Si36	Si	0.61126	0.00477	0.73102	0.00000	Uiso	1.00
Si37	Si	0.23224	0.62201	0.77446	0.00000	Uiso	1.00
Si38	Si	0.99202	0.37990	0.77630	0.00000	Uiso	1.00
Si39	Si	0.76512	0.37141	0.52206	0.00000	Uiso	1.00
Si40	Si	0.00978	0.60385	0.52763	0.00000	Uiso	1.00
Si41	Si	0.46887	0.28937	0.62806	0.00000	Uiso	1.00
Si42	Si	0.31394	0.13674	0.62644	0.00000	Uiso	1.00
Si43	Si	0.53265	0.70076	0.87563	0.00000	Uiso	1.00
Si44	Si	0.68863	0.85693	0.87604	0.00000	Uiso	1.00
Si45	Si	0.29446	0.46384	0.62837	0.00000	Uiso	1.00
Si46	Si	0.13886	0.31181	0.62697	0.00000	Uiso	1.00
Si47	Si	0.70368	0.52960	0.87564	0.00000	Uiso	1.00
Si48	Si	0.86011	0.68555	0.87668	0.00000	Uiso	1.00
Al49	Al	0.86916	0.68984	0.37611	0.00000	Uiso	1.00
O50	O	0.53082	0.29485	0.21471	0.00000	Uiso	1.00
O51	O	0.31294	0.06285	0.21264	0.00000	Uiso	1.00
O52	O	0.34881	0.88036	0.50767	0.00000	Uiso	1.00
O53	O	0.46805	0.72015	0.46180	0.00000	Uiso	1.00
O54	O	0.68146	0.93352	0.46539	0.00000	Uiso	1.00
O55	O	0.62842	0.11852	0.23923	0.00000	Uiso	1.00
O56	O	0.28531	0.53433	0.04156	0.00000	Uiso	1.00
O57	O	0.07377	0.31036	0.03839	0.00000	Uiso	1.00
O58	O	0.87822	0.36268	0.24779	0.00000	Uiso	1.00
O59	O	0.70474	0.46504	0.28717	0.00000	Uiso	1.00
O60	O	0.94965	0.68555	0.28630	0.00000	Uiso	1.00
O61	O	0.11369	0.63714	0.00097	0.00000	Uiso	1.00
O62	O	0.47615	0.71230	0.28586	0.00000	Uiso	1.00
O63	O	0.68233	0.93662	0.28962	0.00000	Uiso	1.00
O64	O	0.64375	0.10807	0.00745	0.00000	Uiso	1.00
O65	O	0.53670	0.27929	0.03818	0.00000	Uiso	1.00
O66	O	0.31304	0.07205	0.03669	0.00000	Uiso	1.00
O67	O	0.35647	0.87605	0.24986	0.00000	Uiso	1.00
O68	O	0.71449	0.46018	0.46214	0.00000	Uiso	1.00
O69	O	0.94020	0.68407	0.47323	0.00000	Uiso	1.00
O70	O	0.12863	0.62532	0.23229	0.00000	Uiso	1.00
O71	O	0.30291	0.52092	0.21814	0.00000	Uiso	1.00
O72	O	0.06563	0.31112	0.21414	0.00000	Uiso	1.00
O73	O	0.88298	0.35315	0.50921	0.00000	Uiso	1.00
O74	O	0.49473	0.99598	0.26208	0.00000	Uiso	1.00
O75	O	0.49532	0.00268	0.99141	0.00000	Uiso	1.00
O76	O	0.00524	0.49135	0.98751	0.00000	Uiso	1.00
O77	O	0.00551	0.49429	0.26185	0.00000	Uiso	1.00
O78	O	0.38992	0.38426	0.11453	0.00000	Uiso	1.00
O79	O	0.21394	0.21124	0.13113	0.00000	Uiso	1.00
O80	O	0.60327	0.60066	0.38253	0.00000	Uiso	1.00
O81	O	0.80144	0.80571	0.37506	0.00000	Uiso	1.00
O82	O	0.41043	0.19031	0.13127	0.00000	Uiso	1.00
O83	O	0.60709	0.79540	0.37551	0.00000	Uiso	1.00
O84	O	0.19507	0.40630	0.13071	0.00000	Uiso	1.00
O85	O	0.79843	0.59453	0.37278	0.00000	Uiso	1.00
O86	O	0.34826	0.00831	0.37671	0.00000	Uiso	1.00
O87	O	0.58537	0.23847	0.37581	0.00000	Uiso	1.00
O88	O	0.61833	0.97243	0.12712	0.00000	Uiso	1.00
O89	O	0.40513	0.74084	0.12637	0.00000	Uiso	1.00
O90	O	0.00934	0.34819	0.37683	0.00000	Uiso	1.00
O91	O	0.23702	0.57947	0.37663	0.00000	Uiso	1.00
O92	O	0.98045	0.61333	0.12429	0.00000	Uiso	1.00
O93	O	0.73952	0.40001	0.12592	0.00000	Uiso	1.00
O94	O	0.72048	0.27357	0.25653	0.00000	Uiso	1.00
O95	O	0.27356	0.72275	-0.00003	0.00000	Uiso	1.00
O96	O	0.28531	0.71024	0.26019	0.00000	Uiso	1.00
O97	O	0.72568	0.26957	0.99736	0.00000	Uiso	1.00
O98	O	0.53944	0.28318	0.71426	0.00000	Uiso	1.00
O99	O	0.31712	0.06686	0.71318	0.00000	Uiso	1.00
O100	O	0.35899	0.88277	0.01017	0.00000	Uiso	1.00
O101	O	0.46303	0.71420	0.96221	0.00000	Uiso	1.00
O102	O	0.67816	0.92148	0.96628	0.00000	Uiso	1.00
O103	O	0.64719	0.11182	0.74325	0.00000	Uiso	1.00
O104	O	0.29948	0.52413	0.53620	0.00000	Uiso	1.00
O105	O	0.07268	0.31220	0.53809	0.00000	Uiso	1.00
O106	O	0.88205	0.36769	0.74402	0.00000	Uiso	1.00
O107	O	0.70814	0.46556	0.78539	0.00000	Uiso	1.00
O108	O	0.92974	0.67827	0.78963	0.00000	Uiso	1.00
O109	O	0.12358	0.62566	0.51785	0.00000	Uiso	1.00
O110	O	0.46759	0.70448	0.78586	0.00000	Uiso	1.00
O111	O	0.68241	0.92623	0.78868	0.00000	Uiso	1.00
O112	O	0.62637	0.11659	0.51125	0.00000	Uiso	1.00
O113	O	0.53168	0.29384	0.53741	0.00000	Uiso	1.00
O114	O	0.31254	0.07012	0.53776	0.00000	Uiso	1.00
O115	O	0.37103	0.87911	0.74449	0.00000	Uiso	1.00
O116	O	0.71574	0.45927	0.96176	0.00000	Uiso	1.00
O117	O	0.92559	0.67562	0.96625	0.00000	Uiso	1.00
O118	O	0.11688	0.64021	0.75076	0.00000	Uiso	1.00
O119	O	0.28935	0.53677	0.71291	0.00000	Uiso	1.00
O120	O	0.06978	0.31356	0.71407	0.00000	Uiso	1.00
O121	O	0.88435	0.35676	0.01202	0.00000	Uiso	1.00
O122	O	0.49934	0.00714	0.76574	0.00000	Uiso	1.00
O123	O	0.49333	0.99220	0.49381	0.00000	Uiso	1.00
O124	O	0.00049	0.49343	0.49288	0.00000	Uiso	1.00
O125	O	0.01075	0.49395	0.77236	0.00000	Uiso	1.00
O126	O	0.39241	0.38734	0.63628	0.00000	Uiso	1.00
O127	O	0.21515	0.21277	0.62882	0.00000	Uiso	1.00
O128	O	0.59814	0.59532	0.88133	0.00000	Uiso	1.00
O129	O	0.79438	0.79136	0.87684	0.00000	Uiso	1.00
O130	O	0.41134	0.19275	0.62512	0.00000	Uiso	1.00
O131	O	0.60068	0.78870	0.87223	0.00000	Uiso	1.00
O132	O	0.19693	0.40794	0.62773	0.00000	Uiso	1.00
O133	O	0.79132	0.59799	0.87397	0.00000	Uiso	1.00
O134	O	0.35032	0.00739	0.87583	0.00000	Uiso	1.00
O135	O	0.59316	0.23352	0.87640	0.00000	Uiso	1.00

O136	O	0.61873	0.97352	0.62754	0.00000	Uiso	1.00
O137	O	0.40305	0.73917	0.62442	0.00000	Uiso	1.00
O138	O	0.00823	0.34148	0.87718	0.00000	Uiso	1.00
O139	O	0.24868	0.58903	0.87709	0.00000	Uiso	1.00
O140	O	0.98137	0.61027	0.63212	0.00000	Uiso	1.00
O141	O	0.73997	0.39762	0.62494	0.00000	Uiso	1.00
O142	O	0.72746	0.27373	0.75895	0.00000	Uiso	1.00
O143	O	0.27906	0.71323	0.49333	0.00000	Uiso	1.00
O144	O	0.27629	0.72483	0.75616	0.00000	Uiso	1.00
O145	O	0.72131	0.27010	0.49535	0.00000	Uiso	1.00
H146	H	0.15807	0.81047	0.41595	0.00000	Uiso	1.00
H147	H	0.05455	0.89052	0.52419	0.00000	Uiso	1.00
H148	H	0.92986	0.94505	0.49739	0.00000	Uiso	1.00
H149	H	0.97029	0.81623	0.48320	0.00000	Uiso	1.00
H150	H	0.91380	0.01349	0.35839	0.00000	Uiso	1.00
H151	H	0.90104	0.89793	0.31890	0.00000	Uiso	1.00
H152	H	0.15598	0.87688	0.31265	0.00000	Uiso	1.00
H153	H	0.08834	0.77813	0.32201	0.00000	Uiso	1.00
H154	H	0.86363	0.09990	0.23010	0.00000	Uiso	1.00
H155	H	0.83639	0.98803	0.18207	0.00000	Uiso	1.00
H156	H	0.91024	0.06452	0.12373	0.00000	Uiso	1.00
H157	H	0.09486	0.85947	0.18862	0.00000	Uiso	1.00
H158	H	0.02657	0.92139	0.10259	0.00000	Uiso	1.00
H159	H	0.97079	0.83988	0.17236	0.00000	Uiso	1.00
H160	H	0.03694	0.11822	0.27746	0.00000	Uiso	1.00
H161	H	0.08132	0.07928	0.17170	0.00000	Uiso	1.00
H162	H	0.13266	0.01996	0.26727	0.00000	Uiso	1.00
C163	C	0.95655	0.95185	0.32406	0.00000	Uiso	1.00
C164	C	0.02303	0.89898	0.38696	0.00000	Uiso	1.00
C165	C	0.99243	0.89274	0.47826	0.00000	Uiso	1.00
C166	C	0.11319	0.83955	0.36022	0.00000	Uiso	1.00
C167	C	0.98641	0.98258	0.23071	0.00000	Uiso	1.00
C168	C	0.89329	0.03703	0.18942	0.00000	Uiso	1.00
C169	C	0.02201	0.89524	0.17090	0.00000	Uiso	1.00
C170	C	0.06383	0.05360	0.23787	0.00000	Uiso	1.00

File n°4

Si2	Si	0.37035	0.76445	0.02680	0.00000	Uiso	1.00
Si3	Si	0.59976	0.99351	0.02419	0.00000	Uiso	1.00
Si4	Si	0.61038	0.22169	0.27670	0.00000	Uiso	1.00
Si5	Si	0.37576	0.97702	0.27525	0.00000	Uiso	1.00
Si6	Si	0.75209	0.36992	0.23605	0.00000	Uiso	1.00
Si7	Si	0.01298	0.60193	0.23256	0.00000	Uiso	1.00
Si8	Si	0.23129	0.60338	0.48670	0.00000	Uiso	1.00
Si9	Si	0.98443	0.36701	0.48821	0.00000	Uiso	1.00
Si10	Si	0.60486	0.22951	0.48329	0.00000	Uiso	1.00
Si11	Si	0.37629	0.98231	0.48127	0.00000	Uiso	1.00
Si12	Si	0.37940	0.75102	0.23224	0.00000	Uiso	1.00
Si13	Si	0.60248	-0.00313	0.23007	0.00000	Uiso	1.00
Si14	Si	0.24164	0.59481	0.27804	0.00000	Uiso	1.00
Si15	Si	0.97699	0.38602	0.28358	0.00000	Uiso	1.00
Si16	Si	0.75958	0.36067	0.02965	0.00000	Uiso	1.00
Si17	Si	0.00352	0.59635	0.02508	0.00000	Uiso	1.00
Si18	Si	0.45948	0.27537	0.12759	0.00000	Uiso	1.00
Si19	Si	0.29655	0.12870	0.13429	0.00000	Uiso	1.00
Si20	Si	0.53083	0.70170	0.38174	0.00000	Uiso	1.00
Si21	Si	0.67772	0.85909	0.38352	0.00000	Uiso	1.00
Si22	Si	0.29295	0.45219	0.12843	0.00000	Uiso	1.00
Si23	Si	0.12856	0.30655	0.13317	0.00000	Uiso	1.00
Si24	Si	0.70857	0.53055	0.37279	0.00000	Uiso	1.00
Si25	Si	0.36935	0.75641	0.52472	0.00000	Uiso	1.00
Si26	Si	0.60156	0.00495	0.53025	0.00000	Uiso	1.00
Si27	Si	0.62276	0.22115	0.77496	0.00000	Uiso	1.00
Si28	Si	0.38479	0.97855	0.78066	0.00000	Uiso	1.00
Si29	Si	0.75956	0.37493	0.72950	0.00000	Uiso	1.00
Si30	Si	0.00212	0.60262	0.74082	0.00000	Uiso	1.00
Si31	Si	0.22727	0.61534	0.98562	0.00000	Uiso	1.00
Si32	Si	0.98513	0.36920	0.98259	0.00000	Uiso	1.00
Si33	Si	0.61951	0.21141	0.98037	0.00000	Uiso	1.00
Si34	Si	0.36997	0.99061	0.98590	0.00000	Uiso	1.00
Si35	Si	0.37485	0.75152	0.73198	0.00000	Uiso	1.00
Si36	Si	0.61095	-0.00203	0.73624	0.00000	Uiso	1.00
Si37	Si	0.22257	0.61523	0.78026	0.00000	Uiso	1.00
Si38	Si	0.98691	0.37554	0.77801	0.00000	Uiso	1.00
Si39	Si	0.76045	0.37251	0.52405	0.00000	Uiso	1.00
Si40	Si	0.00437	0.59381	0.53277	0.00000	Uiso	1.00
Si41	Si	0.45811	0.28163	0.63226	0.00000	Uiso	1.00
Si42	Si	0.30657	0.12345	0.63038	0.00000	Uiso	1.00
Si43	Si	0.52503	0.69004	0.87513	0.00000	Uiso	1.00
Si44	Si	0.67953	0.84467	0.87625	0.00000	Uiso	1.00
Si45	Si	0.28469	0.45361	0.63352	0.00000	Uiso	1.00
Si46	Si	0.13230	0.29666	0.62972	0.00000	Uiso	1.00
Si47	Si	0.69502	0.51980	0.88331	0.00000	Uiso	1.00
Si48	Si	0.85132	0.67593	0.88533	0.00000	Uiso	1.00
Al49	Al	0.86031	0.68424	0.37936	0.00000	Uiso	1.00
O50	O	0.52559	0.28137	0.21585	0.00000	Uiso	1.00
O51	O	0.30176	0.04989	0.21464	0.00000	Uiso	1.00
O52	O	0.35154	0.87245	0.50291	0.00000	Uiso	1.00
O53	O	0.45468	0.69971	0.46368	0.00000	Uiso	1.00
O54	O	0.67408	0.93621	0.46593	0.00000	Uiso	1.00
O55	O	0.62661	0.10747	0.24834	0.00000	Uiso	1.00
O56	O	0.28368	0.53134	0.04858	0.00000	Uiso	1.00
O57	O	0.06605	0.30321	0.04225	0.00000	Uiso	1.00
O58	O	0.86797	0.36192	0.25965	0.00000	Uiso	1.00
O59	O	0.68923	0.45638	0.29166	0.00000	Uiso	1.00
O60	O	0.95301	0.70056	0.28550	0.00000	Uiso	1.00
O61	O	0.11072	0.62908	0.00628	0.00000	Uiso	1.00
O62	O	0.47239	0.70020	0.28792	0.00000	Uiso	1.00
O63	O	0.67226	0.92115	0.29079	0.00000	Uiso	1.00

O64	O	0.64090	0.09377	-0.00685	0.00000	Uiso	1.00
O65	O	0.52762	0.25585	0.04076	0.00000	Uiso	1.00
O66	O	0.29666	0.07158	0.03973	0.00000	Uiso	1.00
O67	O	0.35283	0.86545	0.25857	0.00000	Uiso	1.00
O68	O	0.72493	0.46693	0.46390	0.00000	Uiso	1.00
O69	O	0.93419	0.66454	0.47071	0.00000	Uiso	1.00
O70	O	0.12887	0.60488	0.24376	0.00000	Uiso	1.00
O71	O	0.30237	0.50531	0.22399	0.00000	Uiso	1.00
O72	O	0.05480	0.32659	0.21656	0.00000	Uiso	1.00
O73	O	0.87668	0.33782	0.51174	0.00000	Uiso	1.00
O74	O	0.48806	0.98850	0.25042	0.00000	Uiso	1.00
O75	O	0.48208	0.00506	0.01005	0.00000	Uiso	1.00
O76	O	-0.00184	0.48424	0.99552	0.00000	Uiso	1.00
O77	O	0.98303	0.50382	0.27716	0.00000	Uiso	1.00
O78	O	0.39147	0.37826	0.11301	0.00000	Uiso	1.00
O79	O	0.19601	0.20242	0.14466	0.00000	Uiso	1.00
O80	O	0.60937	0.60565	0.38689	0.00000	Uiso	1.00
O81	O	0.77635	0.78627	0.38762	0.00000	Uiso	1.00
O82	O	0.39164	0.18772	0.13985	0.00000	Uiso	1.00
O83	O	0.57971	0.80296	0.38862	0.00000	Uiso	1.00
O84	O	0.19592	0.39570	0.12794	0.00000	Uiso	1.00
O85	O	0.80179	0.58510	0.35002	0.00000	Uiso	1.00
O86	O	0.35441	0.00630	0.37777	0.00000	Uiso	1.00
O87	O	0.57557	0.23188	0.37920	0.00000	Uiso	1.00
O88	O	0.62540	0.97011	0.12717	0.00000	Uiso	1.00
O89	O	0.40535	0.73947	0.12778	0.00000	Uiso	1.00
O90	O	0.00597	0.35112	0.38319	0.00000	Uiso	1.00
O91	O	0.24690	0.57306	0.38297	0.00000	Uiso	1.00
O92	O	0.97981	0.60851	0.13025	0.00000	Uiso	1.00
O93	O	0.73641	0.39279	0.13127	0.00000	Uiso	1.00
O94	O	0.71363	0.26575	0.26104	0.00000	Uiso	1.00
O95	O	0.26887	0.71876	0.00628	0.00000	Uiso	1.00
O96	O	0.28270	0.69771	0.25503	0.00000	Uiso	1.00
O97	O	0.71871	0.25676	0.00935	0.00000	Uiso	1.00
O98	O	0.53386	0.27241	0.71457	0.00000	Uiso	1.00
O99	O	0.31599	0.04878	0.71403	0.00000	Uiso	1.00
O100	O	0.34774	0.88185	0.01455	0.00000	Uiso	1.00
O101	O	0.45702	0.71813	0.96126	0.00000	Uiso	1.00
O102	O	0.65235	0.90303	0.96731	0.00000	Uiso	1.00
O103	O	0.64460	0.10531	0.75318	0.00000	Uiso	1.00
O104	O	0.29505	0.51929	0.54536	0.00000	Uiso	1.00
O105	O	0.06574	0.29333	0.54125	0.00000	Uiso	1.00
O106	O	0.87618	0.36448	0.74758	0.00000	Uiso	1.00
O107	O	0.70237	0.46167	0.78968	0.00000	Uiso	1.00
O108	O	0.91559	0.66739	0.79525	0.00000	Uiso	1.00
O109	O	0.11778	0.61056	0.51401	0.00000	Uiso	1.00
O110	O	0.45809	0.68307	0.78748	0.00000	Uiso	1.00
O111	O	0.68283	0.91879	0.79291	0.00000	Uiso	1.00
O112	O	0.62302	0.11777	0.51971	0.00000	Uiso	1.00
O113	O	0.51519	0.28912	0.53872	0.00000	Uiso	1.00
O114	O	0.30506	0.06089	0.53924	0.00000	Uiso	1.00
O115	O	0.37110	0.86495	0.76224	0.00000	Uiso	1.00
O116	O	0.70422	0.44379	0.96546	0.00000	Uiso	1.00
O117	O	0.92201	0.66867	0.97216	0.00000	Uiso	1.00
O118	O	0.10554	0.64057	0.76698	0.00000	Uiso	1.00
O119	O	0.26746	0.52335	0.71991	0.00000	Uiso	1.00
O120	O	0.06353	0.30630	0.71733	0.00000	Uiso	1.00
O121	O	0.87674	0.34815	0.01289	0.00000	Uiso	1.00
O122	O	0.49865	-0.00385	0.76925	0.00000	Uiso	1.00
O123	O	0.48887	-0.00606	0.50495	0.00000	Uiso	1.00
O124	O	0.99230	0.47883	0.51671	0.00000	Uiso	1.00
O125	O	0.00736	0.48856	0.76998	0.00000	Uiso	1.00
O126	O	0.38466	0.38091	0.64686	0.00000	Uiso	1.00
O127	O	0.20524	0.19568	0.63786	0.00000	Uiso	1.00
O128	O	0.58916	0.58494	0.89104	0.00000	Uiso	1.00
O129	O	0.78577	0.78142	0.88677	0.00000	Uiso	1.00
O130	O	0.39983	0.18567	0.63042	0.00000	Uiso	1.00
O131	O	0.59619	0.77344	0.85712	0.00000	Uiso	1.00
O132	O	0.19275	0.39090	0.62283	0.00000	Uiso	1.00
O133	O	0.78326	0.58767	0.88956	0.00000	Uiso	1.00
O134	O	0.35019	0.00685	0.88101	0.00000	Uiso	1.00
O135	O	0.59200	0.23771	0.87813	0.00000	Uiso	1.00
O136	O	0.62134	0.97054	0.63217	0.00000	Uiso	1.00
O137	O	0.40057	0.74031	0.62770	0.00000	Uiso	1.00
O138	O	0.00314	0.33948	0.87982	0.00000	Uiso	1.00
O139	O	0.24709	0.58539	0.88285	0.00000	Uiso	1.00
O140	O	0.98019	0.61729	0.63668	0.00000	Uiso	1.00
O141	O	0.73691	0.40215	0.62675	0.00000	Uiso	1.00
O142	O	0.72180	0.27066	0.75458	0.00000	Uiso	1.00
O143	O	0.26812	0.70984	0.50458	0.00000	Uiso	1.00
O144	O	0.26958	0.71403	0.75295	0.00000	Uiso	1.00
O145	O	0.70447	0.27938	0.49703	0.00000	Uiso	1.00
H146	H	0.11314	0.75667	0.17930	0.00000	Uiso	1.00
H147	H	0.08741	0.88456	0.35119	0.00000	Uiso	1.00
H148	H	0.02548	0.80215	0.41484	0.00000	Uiso	1.00
H149	H	0.12868	0.75793	0.34841	0.00000	Uiso	1.00
H150	H	0.88020	0.89542	0.34388	0.00000	Uiso	1.00
H151	H	0.84945	0.86598	0.23339	0.00000	Uiso	1.00
H152	H	0.93422	0.95080	0.25319	0.00000	Uiso	1.00
H153	H	0.06629	0.88158	0.17823	0.00000	Uiso	1.00
H154	H	-0.00400	0.79592	0.13079	0.00000	Uiso	1.00
H155	H	0.88390	0.90663	0.08416	0.00000	Uiso	1.00
H156	H	0.81433	0.02952	0.06620	0.00000	Uiso	1.00
H157	H	0.96673	0.87118	0.86682	0.00000	Uiso	1.00
H158	H	0.05939	0.92812	0.91947	0.00000	Uiso	1.00
H159	H	0.00175	0.83723	-0.02305	0.00000	Uiso	1.00
H160	H	0.85980	0.04305	0.84251	0.00000	Uiso	1.00
H161	H	0.95823	0.09740	0.88833	0.00000	Uiso	1.00
H162	H	0.83920	0.12181	0.93618	0.00000	Uiso	1.00
C163	C	0.90864	0.88293	0.27696	0.00000	Uiso	1.00
C164	C	-0.00457	0.80409	0.27430	0.00000	Uiso	1.00

C165	C	0.06329	0.81130	0.35214	0.00000	Uiso	1.00
C166	C	0.04600	0.80723	0.18510	0.00000	Uiso	1.00
C167	C	0.91384	0.97810	-0.03518	0.00000	Uiso	1.00
C168	C	0.86871	0.97124	0.04258	0.00000	Uiso	1.00
C169	C	0.98929	0.89902	0.93097	0.00000	Uiso	1.00
C170	C	0.89114	0.06523	0.90537	0.00000	Uiso	1.00

File n°5

Si2	Si	0.37058	0.75561	0.02941	0.00000	Uiso	1.00
Si3	Si	0.60129	-0.00578	0.02805	0.00000	Uiso	1.00
Si4	Si	0.61952	0.22494	0.27603	0.00000	Uiso	1.00
Si5	Si	0.37673	0.98556	0.27968	0.00000	Uiso	1.00
Si6	Si	0.75839	0.37696	0.23121	0.00000	Uiso	1.00
Si7	Si	0.01273	0.60127	0.23073	0.00000	Uiso	1.00
Si8	Si	0.22972	0.60578	0.48032	0.00000	Uiso	1.00
Si9	Si	0.98993	0.36849	0.48302	0.00000	Uiso	1.00
Si10	Si	0.61371	0.22282	0.48328	0.00000	Uiso	1.00
Si11	Si	0.36946	0.98462	0.48601	0.00000	Uiso	1.00
Si12	Si	0.38483	0.75727	0.23416	0.00000	Uiso	1.00
Si13	Si	0.60181	0.00453	0.23468	0.00000	Uiso	1.00
Si14	Si	0.23481	0.61045	0.27370	0.00000	Uiso	1.00
Si15	Si	0.98749	0.37785	0.27728	0.00000	Uiso	1.00
Si16	Si	0.76154	0.36266	0.02591	0.00000	Uiso	1.00
Si17	Si	0.00319	0.59498	0.02275	0.00000	Uiso	1.00
Si18	Si	0.46182	0.27766	0.12905	0.00000	Uiso	1.00
Si19	Si	0.30598	0.12752	0.13165	0.00000	Uiso	1.00
Si20	Si	0.53985	0.69647	0.38168	0.00000	Uiso	1.00
Si21	Si	0.68882	0.85903	0.38311	0.00000	Uiso	1.00
Si22	Si	0.28791	0.45364	0.12978	0.00000	Uiso	1.00
Si23	Si	0.13186	0.30363	0.13107	0.00000	Uiso	1.00
Si24	Si	0.69990	0.52845	0.37755	0.00000	Uiso	1.00
Si25	Si	0.37198	0.76058	0.52433	0.00000	Uiso	1.00
Si26	Si	0.59710	-0.00081	0.53188	0.00000	Uiso	1.00
Si27	Si	0.62314	0.22324	0.77526	0.00000	Uiso	1.00
Si28	Si	0.38515	0.98319	0.78079	0.00000	Uiso	1.00
Si29	Si	0.75881	0.37703	0.72902	0.00000	Uiso	1.00
Si30	Si	0.00848	0.60217	0.74113	0.00000	Uiso	1.00
Si31	Si	0.22921	0.60581	0.98191	0.00000	Uiso	1.00
Si32	Si	0.98564	0.36781	0.98141	0.00000	Uiso	1.00
Si33	Si	0.61479	0.21838	0.98193	0.00000	Uiso	1.00
Si34	Si	0.37314	0.97929	0.98510	0.00000	Uiso	1.00
Si35	Si	0.38027	0.75614	0.73014	0.00000	Uiso	1.00
Si36	Si	0.60973	0.00173	0.73855	0.00000	Uiso	1.00
Si37	Si	0.23069	0.61844	0.77662	0.00000	Uiso	1.00
Si38	Si	0.98625	0.37894	0.77965	0.00000	Uiso	1.00
Si39	Si	0.76536	0.36467	0.52388	0.00000	Uiso	1.00
Si40	Si	0.00630	0.59534	0.53144	0.00000	Uiso	1.00
Si41	Si	0.46269	0.28398	0.63069	0.00000	Uiso	1.00
Si42	Si	0.30724	0.13039	0.63341	0.00000	Uiso	1.00
Si43	Si	0.52829	0.69600	0.87876	0.00000	Uiso	1.00
Si44	Si	0.68325	0.85105	0.88170	0.00000	Uiso	1.00
Si45	Si	0.28856	0.45828	0.62898	0.00000	Uiso	1.00
Si46	Si	0.13345	0.30414	0.63059	0.00000	Uiso	1.00
Si47	Si	0.70066	0.52346	0.87788	0.00000	Uiso	1.00
Si48	Si	0.85693	0.67764	0.88032	0.00000	Uiso	1.00
Al49	Al	0.86537	0.68285	0.38072	0.00000	Uiso	1.00
O50	O	0.53196	0.27916	0.21534	0.00000	Uiso	1.00
O51	O	0.30415	0.05924	0.21916	0.00000	Uiso	1.00
O52	O	0.34120	0.87765	0.51329	0.00000	Uiso	1.00
O53	O	0.46674	0.72579	0.46363	0.00000	Uiso	1.00
O54	O	0.66766	0.92048	0.47348	0.00000	Uiso	1.00
O55	O	0.64115	0.10978	0.24885	0.00000	Uiso	1.00
O56	O	0.28453	0.51476	0.03789	0.00000	Uiso	1.00
O57	O	0.06973	0.30480	0.03982	0.00000	Uiso	1.00
O58	O	0.87471	0.36881	0.25088	0.00000	Uiso	1.00
O59	O	0.69886	0.46616	0.28567	0.00000	Uiso	1.00
O60	O	0.93922	0.67428	0.28822	0.00000	Uiso	1.00
O61	O	0.11265	0.61875	-0.00100	0.00000	Uiso	1.00
O62	O	0.48039	0.71022	0.28901	0.00000	Uiso	1.00
O63	O	0.66814	0.92498	0.29544	0.00000	Uiso	1.00
O64	O	0.62844	0.10286	0.00649	0.00000	Uiso	1.00
O65	O	0.52528	0.27563	0.03851	0.00000	Uiso	1.00
O66	O	0.30662	0.06121	0.04284	0.00000	Uiso	1.00
O67	O	0.36500	0.87397	0.25265	0.00000	Uiso	1.00
O68	O	0.72104	0.45150	0.45893	0.00000	Uiso	1.00
O69	O	0.92727	0.66803	0.47965	0.00000	Uiso	1.00
O70	O	0.12362	0.63220	0.23785	0.00000	Uiso	1.00
O71	O	0.29501	0.52420	0.21493	0.00000	Uiso	1.00
O72	O	0.05893	0.30339	0.21541	0.00000	Uiso	1.00
O73	O	0.88308	0.34125	0.51327	0.00000	Uiso	1.00
O74	O	0.48893	0.00804	0.26545	0.00000	Uiso	1.00
O75	O	0.48862	0.98513	0.00223	0.00000	Uiso	1.00
O76	O	0.99165	0.48366	0.99298	0.00000	Uiso	1.00
O77	O	0.01350	0.48855	0.26495	0.00000	Uiso	1.00
O78	O	0.38455	0.37498	0.12902	0.00000	Uiso	1.00
O79	O	0.20907	0.20558	0.13235	0.00000	Uiso	1.00
O80	O	0.58909	0.58458	0.39172	0.00000	Uiso	1.00
O81	O	0.80994	0.81753	0.38093	0.00000	Uiso	1.00
O82	O	0.40563	0.18037	0.13332	0.00000	Uiso	1.00
O83	O	0.62611	0.76830	0.38163	0.00000	Uiso	1.00
O84	O	0.18911	0.40022	0.13665	0.00000	Uiso	1.00
O85	O	0.77705	0.60570	0.37328	0.00000	Uiso	1.00
O86	O	0.34644	0.00500	0.38217	0.00000	Uiso	1.00
O87	O	0.58590	0.23346	0.37902	0.00000	Uiso	1.00
O88	O	0.61722	0.97046	0.13272	0.00000	Uiso	1.00
O89	O	0.40841	0.73668	0.13029	0.00000	Uiso	1.00
O90	O	0.00639	0.34341	0.37901	0.00000	Uiso	1.00
O91	O	0.23666	0.57595	0.37646	0.00000	Uiso	1.00
O92	O	0.98094	0.60796	0.12706	0.00000	Uiso	1.00

O93	O	0.73705	0.39717	0.12681	0.00000	Uiso	1.00
O94	O	0.71997	0.27355	0.26033	0.00000	Uiso	1.00
O95	O	0.27057	0.70636	0.01330	0.00000	Uiso	1.00
O96	O	0.28754	0.70980	0.26440	0.00000	Uiso	1.00
O97	O	0.71666	0.26082	0.00572	0.00000	Uiso	1.00
O98	O	0.53469	0.27774	0.71578	0.00000	Uiso	1.00
O99	O	0.31581	0.05788	0.71831	0.00000	Uiso	1.00
O100	O	0.34576	0.87208	0.01216	0.00000	Uiso	1.00
O101	O	0.45523	0.70734	0.96306	0.00000	Uiso	1.00
O102	O	0.67421	0.91508	0.97250	0.00000	Uiso	1.00
O103	O	0.64673	0.10856	0.74874	0.00000	Uiso	1.00
O104	O	0.29118	0.51793	0.53637	0.00000	Uiso	1.00
O105	O	0.07332	0.29959	0.53849	0.00000	Uiso	1.00
O106	O	0.87442	0.37252	0.74964	0.00000	Uiso	1.00
O107	O	0.69746	0.46508	0.78472	0.00000	Uiso	1.00
O108	O	0.92514	0.67515	0.79234	0.00000	Uiso	1.00
O109	O	0.11720	0.62261	0.51340	0.00000	Uiso	1.00
O110	O	0.46725	0.69445	0.78691	0.00000	Uiso	1.00
O111	O	0.68092	0.92248	0.79557	0.00000	Uiso	1.00
O112	O	0.62569	0.10793	0.51210	0.00000	Uiso	1.00
O113	O	0.52602	0.28374	0.53972	0.00000	Uiso	1.00
O114	O	0.30285	0.06739	0.54280	0.00000	Uiso	1.00
O115	O	0.37620	0.87200	0.75026	0.00000	Uiso	1.00
O116	O	0.71209	0.44742	0.96004	0.00000	Uiso	1.00
O117	O	0.92369	0.66916	0.96884	0.00000	Uiso	1.00
O118	O	0.11404	0.63968	0.75947	0.00000	Uiso	1.00
O119	O	0.28232	0.53277	0.71243	0.00000	Uiso	1.00
O120	O	0.05881	0.31213	0.71372	0.00000	Uiso	1.00
O121	O	0.87892	0.34187	0.01243	0.00000	Uiso	1.00
O122	O	0.49811	0.00594	0.77439	0.00000	Uiso	1.00
O123	O	0.48465	-0.00898	0.50506	0.00000	Uiso	1.00
O124	O	0.00087	0.48212	0.50185	0.00000	Uiso	1.00
O125	O	0.01020	0.49155	0.77930	0.00000	Uiso	1.00
O126	O	0.38864	0.38394	0.63672	0.00000	Uiso	1.00
O127	O	0.20762	0.20443	0.64135	0.00000	Uiso	1.00
O128	O	0.59869	0.59402	0.88928	0.00000	Uiso	1.00
O129	O	0.78572	0.78031	0.88219	0.00000	Uiso	1.00
O130	O	0.40312	0.18883	0.63031	0.00000	Uiso	1.00
O131	O	0.59087	0.78849	0.87594	0.00000	Uiso	1.00
O132	O	0.19339	0.39905	0.63037	0.00000	Uiso	1.00
O133	O	0.79287	0.58609	0.87691	0.00000	Uiso	1.00
O134	O	0.34781	0.00010	0.88172	0.00000	Uiso	1.00
O135	O	0.58916	0.23392	0.87791	0.00000	Uiso	1.00
O136	O	0.61560	0.97026	0.63488	0.00000	Uiso	1.00
O137	O	0.40253	0.73523	0.62614	0.00000	Uiso	1.00
O138	O	0.00383	0.33593	0.87891	0.00000	Uiso	1.00
O139	O	0.25297	0.58425	0.87813	0.00000	Uiso	1.00
O140	O	0.98450	0.60448	0.63701	0.00000	Uiso	1.00
O141	O	0.73826	0.39787	0.62495	0.00000	Uiso	1.00
O142	O	0.72272	0.27310	0.75831	0.00000	Uiso	1.00
O143	O	0.27833	0.70681	0.49540	0.00000	Uiso	1.00
O144	O	0.27583	0.72049	0.75720	0.00000	Uiso	1.00
O145	O	0.71745	0.26431	0.50200	0.00000	Uiso	1.00
H146	H	0.92151	0.83244	0.23768	0.00000	Uiso	1.00
H147	H	0.02998	0.91416	0.40483	0.00000	Uiso	1.00
H148	H	0.96888	0.84360	0.48106	0.00000	Uiso	1.00
H149	H	0.01631	0.79103	0.37934	0.00000	Uiso	1.00
H150	H	0.90111	0.04351	0.39654	0.00000	Uiso	1.00
H151	H	0.83404	0.98691	0.47812	0.00000	Uiso	1.00
H152	H	0.77808	0.02763	0.37532	0.00000	Uiso	1.00
H153	H	0.95453	0.95226	0.25324	0.00000	Uiso	1.00
H154	H	0.82990	0.93654	0.23421	0.00000	Uiso	1.00
H155	H	0.10577	0.81701	0.07724	0.00000	Uiso	1.00
H156	H	0.97738	0.86779	0.10407	0.00000	Uiso	1.00
H157	H	0.08143	0.83441	0.85033	0.00000	Uiso	1.00
H158	H	0.11821	0.94942	0.87697	0.00000	Uiso	1.00
H159	H	0.17245	0.84248	0.93316	0.00000	Uiso	1.00
H160	H	0.90416	0.91765	0.88308	0.00000	Uiso	1.00
H161	H	0.94115	0.02574	0.92792	0.00000	Uiso	1.00
H162	H	0.87282	0.95071	0.99431	0.00000	Uiso	1.00
C163	C	0.84538	-0.00615	0.40689	0.00000	Uiso	1.00
C164	C	0.88602	0.89712	0.36511	0.00000	Uiso	1.00
C165	C	0.98056	0.85752	0.41084	0.00000	Uiso	1.00
C166	C	0.89763	0.90445	0.26601	0.00000	Uiso	1.00
C167	C	0.02474	0.89342	-0.02592	0.00000	Uiso	1.00
C168	C	0.03689	0.85785	0.05621	0.00000	Uiso	1.00
C169	C	0.10406	0.87887	0.90557	0.00000	Uiso	1.00
C170	C	0.93033	0.94969	0.94400	0.00000	Uiso	1.00

File n°6

Si2	Si	0.37940	0.75931	0.02356	0.00000	Uiso	1.00
Si3	Si	0.60962	-0.00533	0.02306	0.00000	Uiso	1.00
Si4	Si	0.61990	0.22601	0.27345	0.00000	Uiso	1.00
Si5	Si	0.38319	0.98265	0.27462	0.00000	Uiso	1.00
Si6	Si	0.76165	0.37476	0.22880	0.00000	Uiso	1.00
Si7	Si	0.01465	0.60036	0.22672	0.00000	Uiso	1.00
Si8	Si	0.23611	0.60587	0.47819	0.00000	Uiso	1.00
Si9	Si	0.99208	0.37273	0.47770	0.00000	Uiso	1.00
Si10	Si	0.61930	0.22321	0.48109	0.00000	Uiso	1.00
Si11	Si	0.37913	0.98318	0.47986	0.00000	Uiso	1.00
Si12	Si	0.38374	0.75602	0.22997	0.00000	Uiso	1.00
Si13	Si	0.60949	0.00256	0.22945	0.00000	Uiso	1.00
Si14	Si	0.23872	0.60664	0.26979	0.00000	Uiso	1.00
Si15	Si	0.98991	0.37689	0.27370	0.00000	Uiso	1.00
Si16	Si	0.76750	0.36571	0.02321	0.00000	Uiso	1.00
Si17	Si	0.01027	0.59840	0.01953	0.00000	Uiso	1.00
Si18	Si	0.46889	0.28027	0.12659	0.00000	Uiso	1.00
Si19	Si	0.31241	0.12953	0.12794	0.00000	Uiso	1.00
Si20	Si	0.54043	0.70205	0.37696	0.00000	Uiso	1.00

Si21	Si	0.69470	0.85992	0.37728	0.00000	Uiso	1.00
Si22	Si	0.29529	0.45553	0.12550	0.00000	Uiso	1.00
Si23	Si	0.13819	0.30529	0.12756	0.00000	Uiso	1.00
Si24	Si	0.70836	0.52769	0.37587	0.00000	Uiso	1.00
Si25	Si	0.37636	0.75968	0.52165	0.00000	Uiso	1.00
Si26	Si	0.60610	-0.00163	0.52638	0.00000	Uiso	1.00
Si27	Si	0.62660	0.22312	0.77328	0.00000	Uiso	1.00
Si28	Si	0.38743	0.98507	0.77544	0.00000	Uiso	1.00
Si29	Si	0.76718	0.37277	0.72650	0.00000	Uiso	1.00
Si30	Si	0.01063	0.59841	0.73389	0.00000	Uiso	1.00
Si31	Si	0.23376	0.61170	0.97857	0.00000	Uiso	1.00
Si32	Si	0.99314	0.37211	0.97760	0.00000	Uiso	1.00
Si33	Si	0.62635	0.21625	0.97957	0.00000	Uiso	1.00
Si34	Si	0.38084	0.98481	0.97970	0.00000	Uiso	1.00
Si35	Si	0.37928	0.75833	0.72831	0.00000	Uiso	1.00
Si36	Si	0.61362	0.00085	0.73225	0.00000	Uiso	1.00
Si37	Si	0.23227	0.61698	0.77290	0.00000	Uiso	1.00
Si38	Si	0.99363	0.37366	0.77476	0.00000	Uiso	1.00
Si39	Si	0.76638	0.36603	0.52109	0.00000	Uiso	1.00
Si40	Si	0.01229	0.59751	0.52570	0.00000	Uiso	1.00
Si41	Si	0.47003	0.28565	0.62769	0.00000	Uiso	1.00
Si42	Si	0.31602	0.13208	0.62655	0.00000	Uiso	1.00
Si43	Si	0.53525	0.69578	0.87348	0.00000	Uiso	1.00
Si44	Si	0.69180	0.85127	0.87497	0.00000	Uiso	1.00
Si45	Si	0.29497	0.45953	0.62546	0.00000	Uiso	1.00
Si46	Si	0.14029	0.30629	0.62540	0.00000	Uiso	1.00
Si47	Si	0.70555	0.52481	0.87565	0.00000	Uiso	1.00
Si48	Si	0.86286	0.68035	0.87710	0.00000	Uiso	1.00
Al49	Al	0.86972	0.68429	0.37582	0.00000	Uiso	1.00
O50	O	0.53188	0.28676	0.21685	0.00000	Uiso	1.00
O51	O	0.31276	0.05849	0.21382	0.00000	Uiso	1.00
O52	O	0.34865	0.87669	0.50687	0.00000	Uiso	1.00
O53	O	0.46922	0.71654	0.46281	0.00000	Uiso	1.00
O54	O	0.68200	0.92748	0.46667	0.00000	Uiso	1.00
O55	O	0.63598	0.11370	0.23870	0.00000	Uiso	1.00
O56	O	0.28963	0.52382	0.03778	0.00000	Uiso	1.00
O57	O	0.07562	0.30727	0.03641	0.00000	Uiso	1.00
O58	O	0.87869	0.36252	0.24641	0.00000	Uiso	1.00
O59	O	0.70487	0.46449	0.28438	0.00000	Uiso	1.00
O60	O	0.94834	0.67916	0.28485	0.00000	Uiso	1.00
O61	O	0.11864	0.62986	0.00285	0.00000	Uiso	1.00
O62	O	0.47559	0.70549	0.28685	0.00000	Uiso	1.00
O63	O	0.68370	0.93204	0.29086	0.00000	Uiso	1.00
O64	O	0.64503	0.10067	0.00334	0.00000	Uiso	1.00
O65	O	0.53929	0.27160	0.04021	0.00000	Uiso	1.00
O66	O	0.31285	0.06537	0.03780	0.00000	Uiso	1.00
O67	O	0.36260	0.87246	0.24973	0.00000	Uiso	1.00
O68	O	0.71340	0.45172	0.45918	0.00000	Uiso	1.00
O69	O	0.94257	0.67879	0.47210	0.00000	Uiso	1.00
O70	O	0.12860	0.62363	0.23126	0.00000	Uiso	1.00
O71	O	0.30347	0.52011	0.21481	0.00000	Uiso	1.00
O72	O	0.06524	0.30625	0.21182	0.00000	Uiso	1.00
O73	O	0.88412	0.34966	0.50784	0.00000	Uiso	1.00
O74	O	0.49718	0.99651	0.26002	0.00000	Uiso	1.00
O75	O	0.49576	-0.00445	0.99479	0.00000	Uiso	1.00
O76	O	0.00638	0.48737	0.98372	0.00000	Uiso	1.00
O77	O	0.01036	0.48932	0.26299	0.00000	Uiso	1.00
O78	O	0.39251	0.37810	0.11754	0.00000	Uiso	1.00
O79	O	0.21391	0.20592	0.12998	0.00000	Uiso	1.00
O80	O	0.60372	0.59629	0.38397	0.00000	Uiso	1.00
O81	O	0.80150	0.80007	0.37636	0.00000	Uiso	1.00
O82	O	0.41062	0.18428	0.13110	0.00000	Uiso	1.00
O83	O	0.60673	0.79116	0.37440	0.00000	Uiso	1.00
O84	O	0.19719	0.40081	0.13136	0.00000	Uiso	1.00
O85	O	0.79892	0.58913	0.37588	0.00000	Uiso	1.00
O86	O	0.35294	0.00503	0.37683	0.00000	Uiso	1.00
O87	O	0.58934	0.23031	0.37721	0.00000	Uiso	1.00
O88	O	0.62352	0.96780	0.12711	0.00000	Uiso	1.00
O89	O	0.40863	0.73676	0.12614	0.00000	Uiso	1.00
O90	O	0.01039	0.34149	0.37517	0.00000	Uiso	1.00
O91	O	0.23927	0.57721	0.37402	0.00000	Uiso	1.00
O92	O	0.98187	0.60434	0.12307	0.00000	Uiso	1.00
O93	O	0.73948	0.39539	0.12450	0.00000	Uiso	1.00
O94	O	0.72172	0.27231	0.25809	0.00000	Uiso	1.00
O95	O	0.28001	0.71274	-0.00134	0.00000	Uiso	1.00
O96	O	0.28476	0.70946	0.25756	0.00000	Uiso	1.00
O97	O	0.72798	0.26216	0.99811	0.00000	Uiso	1.00
O98	O	0.53909	0.28118	0.71488	0.00000	Uiso	1.00
O99	O	0.32015	0.06239	0.71348	0.00000	Uiso	1.00
O100	O	0.35808	0.87649	0.00858	0.00000	Uiso	1.00
O101	O	0.46953	0.71203	0.96240	0.00000	Uiso	1.00
O102	O	0.67741	0.91212	0.96696	0.00000	Uiso	1.00
O103	O	0.64654	0.10951	0.74246	0.00000	Uiso	1.00
O104	O	0.30113	0.51972	0.53333	0.00000	Uiso	1.00
O105	O	0.07336	0.30583	0.53701	0.00000	Uiso	1.00
O106	O	0.88454	0.36070	0.74062	0.00000	Uiso	1.00
O107	O	0.71418	0.46411	0.78351	0.00000	Uiso	1.00
O108	O	0.92826	0.67009	0.78729	0.00000	Uiso	1.00
O109	O	0.12548	0.62078	0.51582	0.00000	Uiso	1.00
O110	O	0.46655	0.69915	0.78608	0.00000	Uiso	1.00
O111	O	0.68693	0.92508	0.79072	0.00000	Uiso	1.00
O112	O	0.62837	0.11048	0.51404	0.00000	Uiso	1.00
O113	O	0.53441	0.28857	0.53780	0.00000	Uiso	1.00
O114	O	0.31381	0.06593	0.53776	0.00000	Uiso	1.00
O115	O	0.37130	0.87487	0.74643	0.00000	Uiso	1.00
O116	O	0.71485	0.45093	0.95934	0.00000	Uiso	1.00
O117	O	0.93218	0.67280	0.96414	0.00000	Uiso	1.00
O118	O	0.11653	0.63580	0.75038	0.00000	Uiso	1.00
O119	O	0.28860	0.53283	0.70978	0.00000	Uiso	1.00
O120	O	0.07248	0.30775	0.71328	0.00000	Uiso	1.00
O121	O	0.88532	0.35299	0.01153	0.00000	Uiso	1.00

O122	O	0.50201	0.00080	0.76721	0.00000	Uiso	1.00
O123	O	0.49467	0.98665	0.49716	0.00000	Uiso	1.00
O124	O	0.00372	0.48751	0.49002	0.00000	Uiso	1.00
O125	O	0.01273	0.48751	0.77069	0.00000	Uiso	1.00
O126	O	0.39315	0.38345	0.63400	0.00000	Uiso	1.00
O127	O	0.21696	0.20769	0.62843	0.00000	Uiso	1.00
O128	O	0.59928	0.58949	0.87923	0.00000	Uiso	1.00
O129	O	0.79830	0.78703	0.87633	0.00000	Uiso	1.00
O130	O	0.41306	0.18861	0.62511	0.00000	Uiso	1.00
O131	O	0.60528	0.78182	0.86519	0.00000	Uiso	1.00
O132	O	0.19778	0.40296	0.62429	0.00000	Uiso	1.00
O133	O	0.79234	0.59420	0.88051	0.00000	Uiso	1.00
O134	O	0.35237	0.00422	0.87678	0.00000	Uiso	1.00
O135	O	0.59419	0.23082	0.87657	0.00000	Uiso	1.00
O136	O	0.62192	0.96710	0.62948	0.00000	Uiso	1.00
O137	O	0.40260	0.73649	0.62458	0.00000	Uiso	1.00
O138	O	0.00778	0.33566	0.87588	0.00000	Uiso	1.00
O139	O	0.24944	0.58230	0.87497	0.00000	Uiso	1.00
O140	O	0.98360	0.60333	0.63013	0.00000	Uiso	1.00
O141	O	0.74113	0.39457	0.62353	0.00000	Uiso	1.00
O142	O	0.72733	0.27163	0.75835	0.00000	Uiso	1.00
O143	O	0.27975	0.70985	0.49232	0.00000	Uiso	1.00
O144	O	0.27584	0.72035	0.75559	0.00000	Uiso	1.00
O145	O	0.72454	0.26282	0.49733	0.00000	Uiso	1.00
H146	H	0.16331	0.81087	0.40183	0.00000	Uiso	1.00
H147	H	0.07241	0.86142	0.53257	0.00000	Uiso	1.00
H148	H	0.94935	0.93000	0.52577	0.00000	Uiso	1.00
H149	H	0.97447	0.80410	0.49077	0.00000	Uiso	1.00
H150	H	0.91037	0.01650	0.38619	0.00000	Uiso	1.00
H151	H	0.88965	0.90235	0.34288	0.00000	Uiso	1.00
H152	H	0.97074	0.97132	0.28322	0.00000	Uiso	1.00
H153	H	0.13110	0.88043	0.30116	0.00000	Uiso	1.00
H154	H	0.07264	0.77790	0.32589	0.00000	Uiso	1.00
H155	H	0.07893	0.80598	0.16417	0.00000	Uiso	1.00
H156	H	0.94380	0.83233	0.17723	0.00000	Uiso	1.00
H157	H	0.08979	0.87794	0.94664	0.00000	Uiso	1.00
H158	H	0.10445	0.98679	0.00429	0.00000	Uiso	1.00
H159	H	0.16191	0.87196	0.04439	0.00000	Uiso	1.00
H160	H	0.89756	0.91699	0.96369	0.00000	Uiso	1.00
H161	H	0.91372	0.02544	0.02138	0.00000	Uiso	1.00
H162	H	0.84864	0.93511	0.07204	0.00000	Uiso	1.00
C163	C	0.94712	0.95357	0.34978	0.00000	Uiso	1.00
C164	C	0.02136	0.89532	0.40171	0.00000	Uiso	1.00
C165	C	0.00487	0.87789	0.49411	0.00000	Uiso	1.00
C166	C	0.10455	0.84034	0.35713	0.00000	Uiso	1.00
C167	C	0.00568	0.89707	0.06621	0.00000	Uiso	1.00
C168	C	0.00960	0.84360	0.14040	0.00000	Uiso	1.00
C169	C	0.09569	0.90892	0.01332	0.00000	Uiso	1.00
C170	C	0.91103	0.94630	0.02970	0.00000	Uiso	1.00

File n°7

Si2	Si	0.37526	0.76740	0.02615	0.00000	Uiso	1.00
Si3	Si	0.60590	-0.00255	0.02375	0.00000	Uiso	1.00
Si4	Si	0.61248	0.22733	0.27424	0.00000	Uiso	1.00
Si5	Si	0.37588	0.98111	0.27519	0.00000	Uiso	1.00
Si6	Si	0.75567	0.37319	0.23123	0.00000	Uiso	1.00
Si7	Si	0.01434	0.60325	0.22821	0.00000	Uiso	1.00
Si8	Si	0.23527	0.60785	0.48351	0.00000	Uiso	1.00
Si9	Si	0.98987	0.37276	0.48268	0.00000	Uiso	1.00
Si10	Si	0.61420	0.22912	0.48150	0.00000	Uiso	1.00
Si11	Si	0.37792	0.98598	0.48019	0.00000	Uiso	1.00
Si12	Si	0.37875	0.75473	0.23153	0.00000	Uiso	1.00
Si13	Si	0.60204	0.00245	0.22956	0.00000	Uiso	1.00
Si14	Si	0.24241	0.59864	0.27528	0.00000	Uiso	1.00
Si15	Si	0.98027	0.38742	0.27886	0.00000	Uiso	1.00
Si16	Si	0.76528	0.36723	0.02554	0.00000	Uiso	1.00
Si17	Si	0.00781	0.60026	0.02082	0.00000	Uiso	1.00
Si18	Si	0.46434	0.28208	0.12742	0.00000	Uiso	1.00
Si19	Si	0.30355	0.13370	0.13244	0.00000	Uiso	1.00
Si20	Si	0.53455	0.70435	0.37851	0.00000	Uiso	1.00
Si21	Si	0.68129	0.86278	0.38023	0.00000	Uiso	1.00
Si22	Si	0.29647	0.45831	0.12515	0.00000	Uiso	1.00
Si23	Si	0.13398	0.31166	0.12913	0.00000	Uiso	1.00
Si24	Si	0.71174	0.53230	0.37072	0.00000	Uiso	1.00
Si25	Si	0.37570	0.75873	0.52333	0.00000	Uiso	1.00
Si26	Si	0.60351	0.00631	0.52771	0.00000	Uiso	1.00
Si27	Si	0.62387	0.22498	0.77508	0.00000	Uiso	1.00
Si28	Si	0.38532	0.98507	0.77871	0.00000	Uiso	1.00
Si29	Si	0.76208	0.37739	0.72707	0.00000	Uiso	1.00
Si30	Si	0.00642	0.60434	0.73517	0.00000	Uiso	1.00
Si31	Si	0.23061	0.62104	0.98254	0.00000	Uiso	1.00
Si32	Si	0.99080	0.37376	0.97870	0.00000	Uiso	1.00
Si33	Si	0.62556	0.21585	0.98112	0.00000	Uiso	1.00
Si34	Si	0.37634	0.99337	0.98327	0.00000	Uiso	1.00
Si35	Si	0.37810	0.75769	0.73022	0.00000	Uiso	1.00
Si36	Si	0.61064	0.00322	0.73433	0.00000	Uiso	1.00
Si37	Si	0.22871	0.61869	0.77665	0.00000	Uiso	1.00
Si38	Si	0.98917	0.37807	0.77466	0.00000	Uiso	1.00
Si39	Si	0.76510	0.37408	0.52154	0.00000	Uiso	1.00
Si40	Si	0.00903	0.59965	0.52750	0.00000	Uiso	1.00
Si41	Si	0.46471	0.28443	0.63009	0.00000	Uiso	1.00
Si42	Si	0.31160	0.12997	0.62855	0.00000	Uiso	1.00
Si43	Si	0.53085	0.69695	0.87534	0.00000	Uiso	1.00
Si44	Si	0.68673	0.85176	0.87497	0.00000	Uiso	1.00
Si45	Si	0.29064	0.45935	0.63116	0.00000	Uiso	1.00
Si46	Si	0.13703	0.30542	0.62718	0.00000	Uiso	1.00
Si47	Si	0.70116	0.52627	0.87837	0.00000	Uiso	1.00
Si48	Si	0.85806	0.68209	0.87980	0.00000	Uiso	1.00
Al49	Al	0.86400	0.68803	0.37618	0.00000	Uiso	1.00

O50	O	0.52625	0.29142	0.21790	0.00000	Uiso	1.00
O51	O	0.30523	0.05595	0.21341	0.00000	Uiso	1.00
O52	O	0.35804	0.87549	0.50475	0.00000	Uiso	1.00
O53	O	0.46444	0.70435	0.46485	0.00000	Uiso	1.00
O54	O	0.67625	0.93273	0.46770	0.00000	Uiso	1.00
O55	O	0.62409	0.11482	0.24046	0.00000	Uiso	1.00
O56	O	0.28817	0.53749	0.04539	0.00000	Uiso	1.00
O57	O	0.07238	0.30792	0.03775	0.00000	Uiso	1.00
O58	O	0.87199	0.36285	0.25306	0.00000	Uiso	1.00
O59	O	0.69473	0.45980	0.28788	0.00000	Uiso	1.00
O60	O	0.95383	0.70276	0.27935	0.00000	Uiso	1.00
O61	O	0.11466	0.63566	0.00588	0.00000	Uiso	1.00
O62	O	0.46967	0.70219	0.28854	0.00000	Uiso	1.00
O63	O	0.67570	0.93235	0.29196	0.00000	Uiso	1.00
O64	O	0.64826	0.09962	0.00117	0.00000	Uiso	1.00
O65	O	0.53630	0.26417	0.04288	0.00000	Uiso	1.00
O66	O	0.30602	0.07531	0.03859	0.00000	Uiso	1.00
O67	O	0.35365	0.86990	0.25534	0.00000	Uiso	1.00
O68	O	0.72477	0.46710	0.46121	0.00000	Uiso	1.00
O69	O	0.94018	0.67286	0.46633	0.00000	Uiso	1.00
O70	O	0.13015	0.60657	0.23981	0.00000	Uiso	1.00
O71	O	0.30591	0.51119	0.22085	0.00000	Uiso	1.00
O72	O	0.05945	0.32955	0.21211	0.00000	Uiso	1.00
O73	O	0.88252	0.34629	0.51098	0.00000	Uiso	1.00
O74	O	0.48928	-0.00747	0.25496	0.00000	Uiso	1.00
O75	O	0.49036	0.00742	0.99920	0.00000	Uiso	1.00
O76	O	0.00572	0.48886	0.98761	0.00000	Uiso	1.00
O77	O	-0.01527	0.50563	0.27410	0.00000	Uiso	1.00
O78	O	0.39391	0.38288	0.10993	0.00000	Uiso	1.00
O79	O	0.20359	0.20874	0.14014	0.00000	Uiso	1.00
O80	O	0.61229	0.60764	0.38199	0.00000	Uiso	1.00
O81	O	0.78049	0.79062	0.38136	0.00000	Uiso	1.00
O82	O	0.39955	0.19155	0.13857	0.00000	Uiso	1.00
O83	O	0.58425	0.80521	0.37912	0.00000	Uiso	1.00
O84	O	0.19873	0.40285	0.12469	0.00000	Uiso	1.00
O85	O	0.80580	0.58714	0.35200	0.00000	Uiso	1.00
O86	O	0.34977	0.00802	0.37736	0.00000	Uiso	1.00
O87	O	0.58217	0.23319	0.37799	0.00000	Uiso	1.00
O88	O	0.62191	0.96952	0.12732	0.00000	Uiso	1.00
O89	O	0.40605	0.74017	0.12759	0.00000	Uiso	1.00
O90	O	0.00820	0.35035	0.37808	0.00000	Uiso	1.00
O91	O	0.24660	0.57533	0.37997	0.00000	Uiso	1.00
O92	O	0.98147	0.60771	0.12577	0.00000	Uiso	1.00
O93	O	0.73826	0.39754	0.12693	0.00000	Uiso	1.00
O94	O	0.71633	0.26943	0.25649	0.00000	Uiso	1.00
O95	O	0.27353	0.72426	0.00106	0.00000	Uiso	1.00
O96	O	0.28070	0.70334	0.25389	0.00000	Uiso	1.00
O97	O	0.72553	0.26367	0.00211	0.00000	Uiso	1.00
O98	O	0.53441	0.27928	0.71679	0.00000	Uiso	1.00
O99	O	0.31727	0.05938	0.71491	0.00000	Uiso	1.00
O100	O	0.35617	0.88527	0.01585	0.00000	Uiso	1.00
O101	O	0.46344	0.72012	0.96265	0.00000	Uiso	1.00
O102	O	0.66767	0.91152	0.96697	0.00000	Uiso	1.00
O103	O	0.64549	0.11061	0.74758	0.00000	Uiso	1.00
O104	O	0.29929	0.52402	0.54207	0.00000	Uiso	1.00
O105	O	0.07255	0.30236	0.53736	0.00000	Uiso	1.00
O106	O	0.87903	0.36544	0.74348	0.00000	Uiso	1.00
O107	O	0.70716	0.46702	0.78544	0.00000	Uiso	1.00
O108	O	0.92454	0.67368	0.79109	0.00000	Uiso	1.00
O109	O	0.12269	0.61911	0.51453	0.00000	Uiso	1.00
O110	O	0.46320	0.69448	0.78777	0.00000	Uiso	1.00
O111	O	0.68407	0.92499	0.79055	0.00000	Uiso	1.00
O112	O	0.63152	0.11691	0.51632	0.00000	Uiso	1.00
O113	O	0.52753	0.29015	0.53953	0.00000	Uiso	1.00
O114	O	0.30793	0.06378	0.53982	0.00000	Uiso	1.00
O115	O	0.37210	0.87307	0.75348	0.00000	Uiso	1.00
O116	O	0.71240	0.45175	0.96146	0.00000	Uiso	1.00
O117	O	0.92677	0.67357	0.96807	0.00000	Uiso	1.00
O118	O	0.11283	0.63866	0.75564	0.00000	Uiso	1.00
O119	O	0.28238	0.52922	0.71788	0.00000	Uiso	1.00
O120	O	0.06664	0.31026	0.71359	0.00000	Uiso	1.00
O121	O	0.88301	0.35538	0.01281	0.00000	Uiso	1.00
O122	O	0.49945	0.00297	0.77061	0.00000	Uiso	1.00
O123	O	0.49122	0.00124	0.49712	0.00000	Uiso	1.00
O124	O	-0.00018	0.48592	0.50362	0.00000	Uiso	1.00
O125	O	0.00759	0.49181	0.76779	0.00000	Uiso	1.00
O126	O	0.38803	0.38215	0.63909	0.00000	Uiso	1.00
O127	O	0.21330	0.20670	0.63341	0.00000	Uiso	1.00
O128	O	0.59521	0.59121	0.88660	0.00000	Uiso	1.00
O129	O	0.79348	0.78839	0.88066	0.00000	Uiso	1.00
O130	O	0.40856	0.18695	0.62631	0.00000	Uiso	1.00
O131	O	0.60152	0.78150	0.86210	0.00000	Uiso	1.00
O132	O	0.19399	0.40244	0.62514	0.00000	Uiso	1.00
O133	O	0.78874	0.59499	0.88187	0.00000	Uiso	1.00
O134	O	0.34934	0.00745	0.87955	0.00000	Uiso	1.00
O135	O	0.59337	0.23524	0.87874	0.00000	Uiso	1.00
O136	O	0.61660	0.97335	0.63064	0.00000	Uiso	1.00
O137	O	0.40319	0.73929	0.62660	0.00000	Uiso	1.00
O138	O	0.00533	0.34129	0.87625	0.00000	Uiso	1.00
O139	O	0.24713	0.58880	0.88001	0.00000	Uiso	1.00
O140	O	0.98030	0.61632	0.63151	0.00000	Uiso	1.00
O141	O	0.73821	0.40158	0.62402	0.00000	Uiso	1.00
O142	O	0.72276	0.27529	0.75648	0.00000	Uiso	1.00
O143	O	0.27542	0.71332	0.49777	0.00000	Uiso	1.00
O144	O	0.27369	0.72001	0.75444	0.00000	Uiso	1.00
O145	O	0.71528	0.27729	0.49317	0.00000	Uiso	1.00
H146	H	0.11043	0.75366	0.16821	0.00000	Uiso	1.00
H147	H	0.08808	0.88929	0.33840	0.00000	Uiso	1.00
H148	H	0.02458	0.81106	0.40531	0.00000	Uiso	1.00
H149	H	0.12781	0.76240	0.34098	0.00000	Uiso	1.00
H150	H	0.87923	0.89978	0.33136	0.00000	Uiso	1.00

H151	H	0.84994	0.86659	0.22144	0.00000	Uiso	1.00
H152	H	0.93472	0.95205	0.24001	0.00000	Uiso	1.00
H153	H	0.07054	0.87978	0.16946	0.00000	Uiso	1.00
H154	H	-0.00597	0.79956	0.12125	0.00000	Uiso	1.00
C155	C	0.90852	0.88499	0.26509	0.00000	Uiso	1.00
C156	C	-0.00460	0.80620	0.26486	0.00000	Uiso	1.00
C157	C	0.06297	0.81659	0.34235	0.00000	Uiso	1.00
C158	C	0.04565	0.80720	0.17527	0.00000	Uiso	1.00

File n°8

Si2	Si	0.37320	0.76592	0.02462	0.00000	Uiso	1.00
Si3	Si	0.60534	0.00367	0.02389	0.00000	Uiso	1.00
Si4	Si	0.61757	0.23342	0.27309	0.00000	Uiso	1.00
Si5	Si	0.37656	0.99083	0.27479	0.00000	Uiso	1.00
Si6	Si	0.75941	0.38199	0.23051	0.00000	Uiso	1.00
Si7	Si	0.01407	0.60637	0.22805	0.00000	Uiso	1.00
Si8	Si	0.23179	0.61721	0.48117	0.00000	Uiso	1.00
Si9	Si	0.99291	0.37735	0.48064	0.00000	Uiso	1.00
Si10	Si	0.61895	0.22962	0.48005	0.00000	Uiso	1.00
Si11	Si	0.37419	0.99408	0.48130	0.00000	Uiso	1.00
Si12	Si	0.38276	0.76458	0.23008	0.00000	Uiso	1.00
Si13	Si	0.60211	0.01088	0.22969	0.00000	Uiso	1.00
Si14	Si	0.23653	0.61504	0.27427	0.00000	Uiso	1.00
Si15	Si	0.98839	0.38297	0.27546	0.00000	Uiso	1.00
Si16	Si	0.76562	0.37322	0.02566	0.00000	Uiso	1.00
Si17	Si	0.00536	0.60412	0.01965	0.00000	Uiso	1.00
Si18	Si	0.46402	0.28836	0.12704	0.00000	Uiso	1.00
Si19	Si	0.30939	0.13712	0.12844	0.00000	Uiso	1.00
Si20	Si	0.54107	0.70735	0.37652	0.00000	Uiso	1.00
Si21	Si	0.69233	0.86776	0.37825	0.00000	Uiso	1.00
Si22	Si	0.28940	0.46366	0.12935	0.00000	Uiso	1.00
Si23	Si	0.13444	0.31251	0.12893	0.00000	Uiso	1.00
Si24	Si	0.69987	0.53739	0.37569	0.00000	Uiso	1.00
Si25	Si	0.37621	0.77051	0.52230	0.00000	Uiso	1.00
Si26	Si	0.60196	0.00741	0.52679	0.00000	Uiso	1.00
Si27	Si	0.62335	0.23012	0.77449	0.00000	Uiso	1.00
Si28	Si	0.38429	0.98827	0.77645	0.00000	Uiso	1.00
Si29	Si	0.76124	0.38101	0.72773	0.00000	Uiso	1.00
Si30	Si	0.00995	0.60751	0.73798	0.00000	Uiso	1.00
Si31	Si	0.22953	0.61906	0.98015	0.00000	Uiso	1.00
Si32	Si	0.98931	0.37719	0.97910	0.00000	Uiso	1.00
Si33	Si	0.62067	0.22664	0.98147	0.00000	Uiso	1.00
Si34	Si	0.37735	0.99107	0.98023	0.00000	Uiso	1.00
Si35	Si	0.38211	0.76066	0.72775	0.00000	Uiso	1.00
Si36	Si	0.60926	0.00806	0.73391	0.00000	Uiso	1.00
Si37	Si	0.23345	0.61988	0.77486	0.00000	Uiso	1.00
Si38	Si	0.98809	0.38413	0.77717	0.00000	Uiso	1.00
Si39	Si	0.76577	0.37596	0.52205	0.00000	Uiso	1.00
Si40	Si	0.00939	0.60351	0.52903	0.00000	Uiso	1.00
Si41	Si	0.46624	0.28949	0.62879	0.00000	Uiso	1.00
Si42	Si	0.31006	0.13720	0.62944	0.00000	Uiso	1.00
Si43	Si	0.53175	0.70221	0.87604	0.00000	Uiso	1.00
Si44	Si	0.68671	0.85905	0.87714	0.00000	Uiso	1.00
Si45	Si	0.29163	0.46386	0.62660	0.00000	Uiso	1.00
Si46	Si	0.13598	0.31084	0.62770	0.00000	Uiso	1.00
Si47	Si	0.70346	0.53163	0.87598	0.00000	Uiso	1.00
Si48	Si	0.85933	0.68763	0.87710	0.00000	Uiso	1.00
Al49	Al	0.86732	0.68969	0.37704	0.00000	Uiso	1.00
O50	O	0.53000	0.29324	0.21580	0.00000	Uiso	1.00
O51	O	0.30677	0.06822	0.21538	0.00000	Uiso	1.00
O52	O	0.34776	0.88811	0.51386	0.00000	Uiso	1.00
O53	O	0.47001	0.73665	0.46002	0.00000	Uiso	1.00
O54	O	0.67187	0.92673	0.46995	0.00000	Uiso	1.00
O55	O	0.63415	0.11951	0.24150	0.00000	Uiso	1.00
O56	O	0.28352	0.53255	0.04208	0.00000	Uiso	1.00
O57	O	0.07367	0.31407	0.03696	0.00000	Uiso	1.00
O58	O	0.87584	0.37128	0.25034	0.00000	Uiso	1.00
O59	O	0.70062	0.46994	0.28683	0.00000	Uiso	1.00
O60	O	0.94143	0.68119	0.28466	0.00000	Uiso	1.00
O61	O	0.11276	0.63489	0.99748	0.00000	Uiso	1.00
O62	O	0.47998	0.72224	0.28490	0.00000	Uiso	1.00
O63	O	0.67279	0.93648	0.29199	0.00000	Uiso	1.00
O64	O	0.63747	0.11153	0.00741	0.00000	Uiso	1.00
O65	O	0.53196	0.28359	0.03916	0.00000	Uiso	1.00
O66	O	0.31046	0.07201	0.03889	0.00000	Uiso	1.00
O67	O	0.35843	0.88140	0.24613	0.00000	Uiso	1.00
O68	O	0.71816	0.46524	0.46102	0.00000	Uiso	1.00
O69	O	0.92941	0.67388	0.47590	0.00000	Uiso	1.00
O70	O	0.12611	0.63408	0.23581	0.00000	Uiso	1.00
O71	O	0.29890	0.52700	0.21891	0.00000	Uiso	1.00
O72	O	0.06088	0.31051	0.21267	0.00000	Uiso	1.00
O73	O	0.88364	0.35729	0.51062	0.00000	Uiso	1.00
O74	O	0.49036	0.00718	0.26079	0.00000	Uiso	1.00
O75	O	0.49254	0.00139	0.99426	0.00000	Uiso	1.00
O76	O	0.99886	0.49299	0.98651	0.00000	Uiso	1.00
O77	O	0.01139	0.49449	0.26276	0.00000	Uiso	1.00
O78	O	0.38582	0.38496	0.12124	0.00000	Uiso	1.00
O79	O	0.21230	0.21498	0.12976	0.00000	Uiso	1.00
O80	O	0.58916	0.59497	0.38550	0.00000	Uiso	1.00
O81	O	0.81315	0.82484	0.37608	0.00000	Uiso	1.00
O82	O	0.40872	0.19041	0.13160	0.00000	Uiso	1.00
O83	O	0.62831	0.77803	0.37462	0.00000	Uiso	1.00
O84	O	0.19074	0.40973	0.13496	0.00000	Uiso	1.00
O85	O	0.77797	0.61365	0.36934	0.00000	Uiso	1.00
O86	O	0.34777	0.00963	0.37760	0.00000	Uiso	1.00
O87	O	0.58678	0.23932	0.37677	0.00000	Uiso	1.00
O88	O	0.61816	0.97532	0.12809	0.00000	Uiso	1.00
O89	O	0.40567	0.74228	0.12635	0.00000	Uiso	1.00
O90	O	0.00908	0.34903	0.37714	0.00000	Uiso	1.00

O91	O	0.23673	0.58454	0.37789	0.00000	Uiso	1.00
O92	O	0.98282	0.61313	0.12418	0.00000	Uiso	1.00
O93	O	0.73824	0.40531	0.12658	0.00000	Uiso	1.00
O94	O	0.71992	0.27838	0.25699	0.00000	Uiso	1.00
O95	O	0.27159	0.72172	0.00294	0.00000	Uiso	1.00
O96	O	0.28793	0.71476	0.26274	0.00000	Uiso	1.00
O97	O	0.72211	0.27154	0.00190	0.00000	Uiso	1.00
O98	O	0.53526	0.28719	0.71595	0.00000	Uiso	1.00
O99	O	0.31586	0.06132	0.71186	0.00000	Uiso	1.00
O100	O	0.35463	0.88316	0.00999	0.00000	Uiso	1.00
O101	O	0.45946	0.71597	0.96071	0.00000	Uiso	1.00
O102	O	0.67633	0.92424	0.96718	0.00000	Uiso	1.00
O103	O	0.64347	0.11579	0.74608	0.00000	Uiso	1.00
O104	O	0.29374	0.53064	0.53832	0.00000	Uiso	1.00
O105	O	0.07230	0.30555	0.53774	0.00000	Uiso	1.00
O106	O	0.87775	0.37376	0.74483	0.00000	Uiso	1.00
O107	O	0.70279	0.46942	0.78489	0.00000	Uiso	1.00
O108	O	0.92965	0.68260	0.79047	0.00000	Uiso	1.00
O109	O	0.11939	0.63558	0.51489	0.00000	Uiso	1.00
O110	O	0.47022	0.70115	0.78452	0.00000	Uiso	1.00
O111	O	0.68154	0.92931	0.79025	0.00000	Uiso	1.00
O112	O	0.63555	0.11446	0.50804	0.00000	Uiso	1.00
O113	O	0.53186	0.28713	0.53929	0.00000	Uiso	1.00
O114	O	0.30750	0.07821	0.53647	0.00000	Uiso	1.00
O115	O	0.37287	0.87632	0.75040	0.00000	Uiso	1.00
O116	O	0.71770	0.45935	0.96061	0.00000	Uiso	1.00
O117	O	0.92394	0.67805	0.96731	0.00000	Uiso	1.00
O118	O	0.11749	0.64095	0.75427	0.00000	Uiso	1.00
O119	O	0.28661	0.53122	0.71485	0.00000	Uiso	1.00
O120	O	0.06460	0.31918	0.71323	0.00000	Uiso	1.00
O121	O	0.88331	0.35455	0.01471	0.00000	Uiso	1.00
O122	O	0.49772	0.00845	0.76843	0.00000	Uiso	1.00
O123	O	0.48954	0.00359	0.49671	0.00000	Uiso	1.00
O124	O	0.01044	0.48993	0.49723	0.00000	Uiso	1.00
O125	O	0.00818	0.49769	0.77672	0.00000	Uiso	1.00
O126	O	0.39134	0.38897	0.62975	0.00000	Uiso	1.00
O127	O	0.21083	0.21158	0.63749	0.00000	Uiso	1.00
O128	O	0.59924	0.59850	0.88618	0.00000	Uiso	1.00
O129	O	0.79163	0.79237	0.87808	0.00000	Uiso	1.00
O130	O	0.40711	0.19407	0.63061	0.00000	Uiso	1.00
O131	O	0.59742	0.79233	0.87269	0.00000	Uiso	1.00
O132	O	0.19579	0.40565	0.62378	0.00000	Uiso	1.00
O133	O	0.79224	0.59862	0.87246	0.00000	Uiso	1.00
O134	O	0.34825	0.00992	0.87733	0.00000	Uiso	1.00
O135	O	0.59161	0.23994	0.87777	0.00000	Uiso	1.00
O136	O	0.61669	0.97808	0.62999	0.00000	Uiso	1.00
O137	O	0.40678	0.74268	0.62368	0.00000	Uiso	1.00
O138	O	0.00363	0.34233	0.87706	0.00000	Uiso	1.00
O139	O	0.25241	0.58907	0.87770	0.00000	Uiso	1.00
O140	O	0.98387	0.61020	0.63412	0.00000	Uiso	1.00
O141	O	0.73784	0.40297	0.62424	0.00000	Uiso	1.00
O142	O	0.72417	0.27770	0.75720	0.00000	Uiso	1.00
O143	O	0.28164	0.71811	0.49294	0.00000	Uiso	1.00
O144	O	0.27923	0.72084	0.75289	0.00000	Uiso	1.00
O145	O	0.72128	0.27488	0.49551	0.00000	Uiso	1.00
H146	H	0.92555	0.84092	0.23225	0.00000	Uiso	1.00
H147	H	0.03482	0.91847	0.40017	0.00000	Uiso	1.00
H148	H	0.97321	0.84818	0.47617	0.00000	Uiso	1.00
H149	H	0.01951	0.79589	0.37398	0.00000	Uiso	1.00
H150	H	0.90710	0.04902	0.39472	0.00000	Uiso	1.00
H151	H	0.83927	0.99154	0.47510	0.00000	Uiso	1.00
H152	H	0.78368	0.03494	0.37301	0.00000	Uiso	1.00
H153	H	0.95821	0.96079	0.24992	0.00000	Uiso	1.00
H154	H	0.83372	0.94492	0.23053	0.00000	Uiso	1.00
C155	C	0.85075	0.99983	0.40403	0.00000	Uiso	1.00
C156	C	0.89027	0.90353	0.36083	0.00000	Uiso	1.00
C157	C	0.98469	0.86245	0.40599	0.00000	Uiso	1.00
C158	C	0.90160	0.91237	0.26174	0.00000	Uiso	1.00

File n°9

Si2	Si	0.37386	0.76556	0.02404	0.00000	Uiso	1.00
Si3	Si	0.60721	0.00176	0.02280	0.00000	Uiso	1.00
Si4	Si	0.61492	0.23206	0.27242	0.00000	Uiso	1.00
Si5	Si	0.37956	0.98518	0.27457	0.00000	Uiso	1.00
Si6	Si	0.75919	0.37838	0.22987	0.00000	Uiso	1.00
Si7	Si	0.01304	0.60514	0.22668	0.00000	Uiso	1.00
Si8	Si	0.23281	0.61169	0.47956	0.00000	Uiso	1.00
Si9	Si	0.98957	0.37920	0.47938	0.00000	Uiso	1.00
Si10	Si	0.61651	0.22928	0.48026	0.00000	Uiso	1.00
Si11	Si	0.37746	0.98885	0.47964	0.00000	Uiso	1.00
Si12	Si	0.38174	0.75893	0.22996	0.00000	Uiso	1.00
Si13	Si	0.60503	0.00706	0.22906	0.00000	Uiso	1.00
Si14	Si	0.23722	0.60808	0.27158	0.00000	Uiso	1.00
Si15	Si	0.98700	0.38160	0.27458	0.00000	Uiso	1.00
Si16	Si	0.76548	0.37277	0.02438	0.00000	Uiso	1.00
Si17	Si	0.00542	0.60354	0.01962	0.00000	Uiso	1.00
Si18	Si	0.46515	0.28670	0.12602	0.00000	Uiso	1.00
Si19	Si	0.31049	0.13434	0.12780	0.00000	Uiso	1.00
Si20	Si	0.53959	0.70770	0.37567	0.00000	Uiso	1.00
Si21	Si	0.69386	0.86589	0.37582	0.00000	Uiso	1.00
Si22	Si	0.29128	0.46075	0.12610	0.00000	Uiso	1.00
Si23	Si	0.13548	0.30924	0.12870	0.00000	Uiso	1.00
Si24	Si	0.70759	0.53350	0.37603	0.00000	Uiso	1.00
Si25	Si	0.37430	0.76477	0.52035	0.00000	Uiso	1.00
Si26	Si	0.60486	0.00420	0.52495	0.00000	Uiso	1.00
Si27	Si	0.62535	0.22642	0.77346	0.00000	Uiso	1.00
Si28	Si	0.38467	0.98887	0.77412	0.00000	Uiso	1.00
Si29	Si	0.76317	0.37732	0.72792	0.00000	Uiso	1.00
Si30	Si	0.00858	0.60607	0.73486	0.00000	Uiso	1.00

Si31	Si	0.22816	0.62026	0.98003	0.00000	Uiso	1.00
Si32	Si	0.99105	0.37638	0.97901	0.00000	Uiso	1.00
Si33	Si	0.62330	0.22306	0.98006	0.00000	Uiso	1.00
Si34	Si	0.37938	0.99066	0.97876	0.00000	Uiso	1.00
Si35	Si	0.37902	0.76190	0.72671	0.00000	Uiso	1.00
Si36	Si	0.61066	0.00492	0.73138	0.00000	Uiso	1.00
Si37	Si	0.23117	0.62213	0.77436	0.00000	Uiso	1.00
Si38	Si	0.99014	0.38141	0.77611	0.00000	Uiso	1.00
Si39	Si	0.76447	0.37255	0.52223	0.00000	Uiso	1.00
Si40	Si	0.00868	0.60476	0.52681	0.00000	Uiso	1.00
Si41	Si	0.46784	0.29042	0.62828	0.00000	Uiso	1.00
Si42	Si	0.31267	0.13723	0.62720	0.00000	Uiso	1.00
Si43	Si	0.53110	0.70098	0.87474	0.00000	Uiso	1.00
Si44	Si	0.68753	0.85687	0.87607	0.00000	Uiso	1.00
Si45	Si	0.29353	0.46496	0.62761	0.00000	Uiso	1.00
Si46	Si	0.13779	0.31216	0.62686	0.00000	Uiso	1.00
Si47	Si	0.70212	0.53010	0.87529	0.00000	Uiso	1.00
Si48	Si	0.85877	0.68579	0.87580	0.00000	Uiso	1.00
Al49	Al	0.86826	0.69062	0.37443	0.00000	Uiso	1.00
O50	O	0.52798	0.29516	0.21618	0.00000	Uiso	1.00
O51	O	0.31091	0.06093	0.21215	0.00000	Uiso	1.00
O52	O	0.34789	0.88231	0.50798	0.00000	Uiso	1.00
O53	O	0.46661	0.72272	0.46029	0.00000	Uiso	1.00
O54	O	0.68075	0.93300	0.46555	0.00000	Uiso	1.00
O55	O	0.62746	0.11965	0.23785	0.00000	Uiso	1.00
O56	O	0.28277	0.53372	0.04155	0.00000	Uiso	1.00
O57	O	0.07291	0.31039	0.03758	0.00000	Uiso	1.00
O58	O	0.87612	0.36481	0.24830	0.00000	Uiso	1.00
O59	O	0.70233	0.46676	0.28693	0.00000	Uiso	1.00
O60	O	0.94966	0.68572	0.28535	0.00000	Uiso	1.00
O61	O	0.11197	0.63805	0.00013	0.00000	Uiso	1.00
O62	O	0.47619	0.71068	0.28471	0.00000	Uiso	1.00
O63	O	0.68197	0.93871	0.28981	0.00000	Uiso	1.00
O64	O	0.64294	0.10815	0.00599	0.00000	Uiso	1.00
O65	O	0.53511	0.27793	0.03948	0.00000	Uiso	1.00
O66	O	0.31197	0.07259	0.03615	0.00000	Uiso	1.00
O67	O	0.35722	0.87510	0.25088	0.00000	Uiso	1.00
O68	O	0.71446	0.46101	0.46179	0.00000	Uiso	1.00
O69	O	0.93938	0.68548	0.47206	0.00000	Uiso	1.00
O70	O	0.12799	0.62552	0.23062	0.00000	Uiso	1.00
O71	O	0.30183	0.52037	0.21800	0.00000	Uiso	1.00
O72	O	0.06291	0.31071	0.21336	0.00000	Uiso	1.00
O73	O	0.88239	0.35423	0.51000	0.00000	Uiso	1.00
O74	O	0.49404	-0.00325	0.26069	0.00000	Uiso	1.00
O75	O	0.49424	0.00277	0.99176	0.00000	Uiso	1.00
O76	O	0.00461	0.49136	0.98682	0.00000	Uiso	1.00
O77	O	0.00550	0.49434	0.26152	0.00000	Uiso	1.00
O78	O	0.38830	0.38382	0.11419	0.00000	Uiso	1.00
O79	O	0.21150	0.21007	0.13153	0.00000	Uiso	1.00
O80	O	0.60287	0.60203	0.38396	0.00000	Uiso	1.00
O81	O	0.80076	0.80656	0.37420	0.00000	Uiso	1.00
O82	O	0.40795	0.19011	0.13285	0.00000	Uiso	1.00
O83	O	0.60620	0.79657	0.37337	0.00000	Uiso	1.00
O84	O	0.19367	0.40530	0.13139	0.00000	Uiso	1.00
O85	O	0.79802	0.59507	0.37183	0.00000	Uiso	1.00
O86	O	0.34920	0.00930	0.37659	0.00000	Uiso	1.00
O87	O	0.58564	0.23697	0.37652	0.00000	Uiso	1.00
O88	O	0.61851	0.97283	0.12657	0.00000	Uiso	1.00
O89	O	0.40498	0.74088	0.12580	0.00000	Uiso	1.00
O90	O	0.00794	0.34876	0.37659	0.00000	Uiso	1.00
O91	O	0.23518	0.58010	0.37597	0.00000	Uiso	1.00
O92	O	0.97919	0.61278	0.12346	0.00000	Uiso	1.00
O93	O	0.73806	0.40201	0.12588	0.00000	Uiso	1.00
O94	O	0.71822	0.27550	0.25623	0.00000	Uiso	1.00
O95	O	0.27195	0.72256	0.00093	0.00000	Uiso	1.00
O96	O	0.28502	0.70979	0.25936	0.00000	Uiso	1.00
O97	O	0.72386	0.27073	-0.00169	0.00000	Uiso	1.00
O98	O	0.53829	0.28464	0.71454	0.00000	Uiso	1.00
O99	O	0.31619	0.06624	0.71315	0.00000	Uiso	1.00
O100	O	0.35728	0.88311	0.01069	0.00000	Uiso	1.00
O101	O	0.46032	0.71503	0.96051	0.00000	Uiso	1.00
O102	O	0.67688	0.92111	0.96628	0.00000	Uiso	1.00
O103	O	0.64527	0.11259	0.74361	0.00000	Uiso	1.00
O104	O	0.29798	0.52715	0.53636	0.00000	Uiso	1.00
O105	O	0.07201	0.31277	0.53768	0.00000	Uiso	1.00
O106	O	0.88013	0.36951	0.74378	0.00000	Uiso	1.00
O107	O	0.70528	0.46571	0.78534	0.00000	Uiso	1.00
O108	O	0.92847	0.67964	0.78876	0.00000	Uiso	1.00
O109	O	0.12208	0.62767	0.51696	0.00000	Uiso	1.00
O110	O	0.46751	0.70409	0.78406	0.00000	Uiso	1.00
O111	O	0.68190	0.92687	0.78922	0.00000	Uiso	1.00
O112	O	0.62789	0.11618	0.51256	0.00000	Uiso	1.00
O113	O	0.53104	0.29273	0.53766	0.00000	Uiso	1.00
O114	O	0.31232	0.07197	0.53752	0.00000	Uiso	1.00
O115	O	0.37064	0.87872	0.74367	0.00000	Uiso	1.00
O116	O	0.71546	0.46010	0.96149	0.00000	Uiso	1.00
O117	O	0.92398	0.67511	0.96542	0.00000	Uiso	1.00
O118	O	0.11587	0.64085	0.75014	0.00000	Uiso	1.00
O119	O	0.28790	0.53639	0.71317	0.00000	Uiso	1.00
O120	O	0.06814	0.31559	0.71363	0.00000	Uiso	1.00
O121	O	0.88326	0.35720	0.01265	0.00000	Uiso	1.00
O122	O	0.49855	0.00685	0.76538	0.00000	Uiso	1.00
O123	O	0.49322	-0.00649	0.49496	0.00000	Uiso	1.00
O124	O	-0.00043	0.49440	0.49204	0.00000	Uiso	1.00
O125	O	0.00898	0.49542	0.77218	0.00000	Uiso	1.00
O126	O	0.39234	0.38934	0.63454	0.00000	Uiso	1.00
O127	O	0.21306	0.21237	0.62985	0.00000	Uiso	1.00
O128	O	0.59661	0.59568	0.88195	0.00000	Uiso	1.00
O129	O	0.79324	0.79153	0.87675	0.00000	Uiso	1.00
O130	O	0.40920	0.19453	0.62695	0.00000	Uiso	1.00
O131	O	0.59931	0.78890	0.87161	0.00000	Uiso	1.00

O132	O	0.19693	0.40765	0.62635	0.00000	Uiso	1.00
O133	O	0.78976	0.59846	0.87198	0.00000	Uiso	1.00
O134	O	0.34978	0.00655	0.87572	0.00000	Uiso	1.00
O135	O	0.59231	0.23539	0.87659	0.00000	Uiso	1.00
O136	O	0.61946	0.97294	0.62815	0.00000	Uiso	1.00
O137	O	0.40087	0.73899	0.62286	0.00000	Uiso	1.00
O138	O	0.00605	0.34224	0.87675	0.00000	Uiso	1.00
O139	O	0.24744	0.58954	0.87710	0.00000	Uiso	1.00
O140	O	0.98022	0.61133	0.63128	0.00000	Uiso	1.00
O141	O	0.73831	0.39939	0.62479	0.00000	Uiso	1.00
O142	O	0.72654	0.27404	0.75805	0.00000	Uiso	1.00
O143	O	0.27710	0.71595	0.49042	0.00000	Uiso	1.00
O144	O	0.27588	0.72455	0.75574	0.00000	Uiso	1.00
O145	O	0.72083	0.27103	0.49585	0.00000	Uiso	1.00
H146	H	0.16728	0.81389	0.38645	0.00000	Uiso	1.00
H147	H	0.07476	0.86798	0.51557	0.00000	Uiso	1.00
H148	H	0.95072	0.93441	0.50654	0.00000	Uiso	1.00
H149	H	-0.02169	0.80787	0.47533	0.00000	Uiso	1.00
H150	H	0.92142	0.02467	0.36499	0.00000	Uiso	1.00
H151	H	0.89012	0.91182	0.32761	0.00000	Uiso	1.00
H152	H	0.97622	0.97167	0.26364	0.00000	Uiso	1.00
H153	H	0.13896	0.88575	0.28685	0.00000	Uiso	1.00
H154	H	0.07837	0.78318	0.30776	0.00000	Uiso	1.00
C155	C	0.95210	0.95748	0.33081	0.00000	Uiso	1.00
C156	C	0.02546	0.89892	0.38415	0.00000	Uiso	1.00
C157	C	0.00758	0.88264	0.47626	0.00000	Uiso	1.00
C158	C	0.10987	0.84471	0.34101	0.00000	Uiso	1.00

File n°10

Si2	Si	0.37713	0.76567	0.02183	0.00000	Uiso	1.00
Si3	Si	0.60853	0.00662	0.02057	0.00000	Uiso	1.00
Si4	Si	0.61971	0.23182	0.27137	0.00000	Uiso	1.00
Si5	Si	0.37651	0.99281	0.27158	0.00000	Uiso	1.00
Si6	Si	0.76326	0.37763	0.22794	0.00000	Uiso	1.00
Si7	Si	0.01192	0.60690	0.22447	0.00000	Uiso	1.00
Si8	Si	0.23047	0.61638	0.47839	0.00000	Uiso	1.00
Si9	Si	0.98902	0.38177	0.47683	0.00000	Uiso	1.00
Si10	Si	0.61757	0.23182	0.47876	0.00000	Uiso	1.00
Si11	Si	0.37761	0.99039	0.47771	0.00000	Uiso	1.00
Si12	Si	0.37784	0.76793	0.22795	0.00000	Uiso	1.00
Si13	Si	0.60338	0.00905	0.22653	0.00000	Uiso	1.00
Si14	Si	0.23388	0.61712	0.27062	0.00000	Uiso	1.00
Si15	Si	0.99092	0.38219	0.27233	0.00000	Uiso	1.00
Si16	Si	0.76482	0.37687	0.02242	0.00000	Uiso	1.00
Si17	Si	0.00782	0.60673	0.01721	0.00000	Uiso	1.00
Si18	Si	0.46776	0.29077	0.12376	0.00000	Uiso	1.00
Si19	Si	0.31230	0.13992	0.12498	0.00000	Uiso	1.00
Si20	Si	0.53631	0.70569	0.37562	0.00000	Uiso	1.00
Si21	Si	0.68785	0.86700	0.37553	0.00000	Uiso	1.00
Si22	Si	0.29322	0.46651	0.12621	0.00000	Uiso	1.00
Si23	Si	0.13763	0.31546	0.12546	0.00000	Uiso	1.00
Si24	Si	0.69978	0.53447	0.37361	0.00000	Uiso	1.00
Si25	Si	0.37433	0.76624	0.52124	0.00000	Uiso	1.00
Si26	Si	0.60440	0.00738	0.52318	0.00000	Uiso	1.00
Si27	Si	0.62290	0.23017	0.77072	0.00000	Uiso	1.00
Si28	Si	0.38159	0.99234	0.77291	0.00000	Uiso	1.00
Si29	Si	0.76528	0.37859	0.72580	0.00000	Uiso	1.00
Si30	Si	0.00727	0.60584	0.73332	0.00000	Uiso	1.00
Si31	Si	0.23155	0.62048	0.97772	0.00000	Uiso	1.00
Si32	Si	0.99045	0.38169	0.97567	0.00000	Uiso	1.00
Si33	Si	0.62317	0.22898	0.97743	0.00000	Uiso	1.00
Si34	Si	0.38131	0.99212	0.97738	0.00000	Uiso	1.00
Si35	Si	0.37591	0.76583	0.72752	0.00000	Uiso	1.00
Si36	Si	0.60880	0.00734	0.72910	0.00000	Uiso	1.00
Si37	Si	0.23029	0.62152	0.77232	0.00000	Uiso	1.00
Si38	Si	0.99082	0.38043	0.77379	0.00000	Uiso	1.00
Si39	Si	0.76241	0.37706	0.52065	0.00000	Uiso	1.00
Si40	Si	0.00779	0.60670	0.52579	0.00000	Uiso	1.00
Si41	Si	0.46634	0.29209	0.62583	0.00000	Uiso	1.00
Si42	Si	0.31221	0.13935	0.62493	0.00000	Uiso	1.00
Si43	Si	0.53317	0.70508	0.87400	0.00000	Uiso	1.00
Si44	Si	0.68931	0.86126	0.87470	0.00000	Uiso	1.00
Si45	Si	0.29123	0.46680	0.62369	0.00000	Uiso	1.00
Si46	Si	0.13680	0.31404	0.62402	0.00000	Uiso	1.00
Si47	Si	0.70466	0.53374	0.87500	0.00000	Uiso	1.00
Si48	Si	0.86100	0.68970	0.87558	0.00000	Uiso	1.00
Al49	Al	0.86864	0.68551	0.37485	0.00000	Uiso	1.00
O50	O	0.53375	0.29245	0.21285	0.00000	Uiso	1.00
O51	O	0.30962	0.07479	0.21437	0.00000	Uiso	1.00
O52	O	0.35138	0.88353	0.50684	0.00000	Uiso	1.00
O53	O	0.46777	0.72190	0.46255	0.00000	Uiso	1.00
O54	O	0.67989	0.93390	0.46370	0.00000	Uiso	1.00
O55	O	0.63440	0.11752	0.24146	0.00000	Uiso	1.00
O56	O	0.28930	0.53510	0.03870	0.00000	Uiso	1.00
O57	O	0.07175	0.31840	0.03645	0.00000	Uiso	1.00
O58	O	0.88049	0.36553	0.24351	0.00000	Uiso	1.00
O59	O	0.70702	0.46574	0.28564	0.00000	Uiso	1.00
O60	O	0.94061	0.68306	0.28127	0.00000	Uiso	1.00
O61	O	0.11636	0.63829	0.00213	0.00000	Uiso	1.00
O62	O	0.47294	0.72681	0.28602	0.00000	Uiso	1.00
O63	O	0.67465	0.93258	0.28686	0.00000	Uiso	1.00
O64	O	0.64098	0.11480	0.00658	0.00000	Uiso	1.00
O65	O	0.53604	0.28768	0.03605	0.00000	Uiso	1.00
O66	O	0.31398	0.07039	0.03819	0.00000	Uiso	1.00
O67	O	0.35324	0.88534	0.24094	0.00000	Uiso	1.00
O68	O	0.70795	0.46419	0.46076	0.00000	Uiso	1.00
O69	O	0.93461	0.68361	0.47174	0.00000	Uiso	1.00
O70	O	0.12443	0.63330	0.23013	0.00000	Uiso	1.00
O71	O	0.29959	0.53057	0.21597	0.00000	Uiso	1.00

O72	O	0.06851	0.31236	0.21212	0.00000	Uiso	1.00
O73	O	0.87951	0.36152	0.50474	0.00000	Uiso	1.00
O74	O	0.49165	0.00344	0.25707	0.00000	Uiso	1.00
O75	O	0.49616	0.00517	0.98926	0.00000	Uiso	1.00
O76	O	0.00422	0.49687	0.97915	0.00000	Uiso	1.00
O77	O	0.00863	0.49546	0.26051	0.00000	Uiso	1.00
O78	O	0.39020	0.38815	0.12049	0.00000	Uiso	1.00
O79	O	0.21527	0.21779	0.12271	0.00000	Uiso	1.00
O80	O	0.59014	0.59516	0.37449	0.00000	Uiso	1.00
O81	O	0.80388	0.81303	0.37065	0.00000	Uiso	1.00
O82	O	0.41161	0.19327	0.12572	0.00000	Uiso	1.00
O83	O	0.61717	0.78316	0.37977	0.00000	Uiso	1.00
O84	O	0.19457	0.41232	0.12946	0.00000	Uiso	1.00
O85	O	0.78141	0.60717	0.37348	0.00000	Uiso	1.00
O86	O	0.34924	0.01052	0.37491	0.00000	Uiso	1.00
O87	O	0.58797	0.24030	0.37481	0.00000	Uiso	1.00
O88	O	0.61962	0.97643	0.12433	0.00000	Uiso	1.00
O89	O	0.40316	0.74297	0.12510	0.00000	Uiso	1.00
O90	O	0.00893	0.34934	0.37464	0.00000	Uiso	1.00
O91	O	0.23236	0.58663	0.37438	0.00000	Uiso	1.00
O92	O	0.97944	0.61137	0.12077	0.00000	Uiso	1.00
O93	O	0.73800	0.40154	0.12484	0.00000	Uiso	1.00
O94	O	0.72341	0.27456	0.25569	0.00000	Uiso	1.00
O95	O	0.27607	0.72310	0.99512	0.00000	Uiso	1.00
O96	O	0.28243	0.71866	0.26002	0.00000	Uiso	1.00
O97	O	0.72515	0.27465	0.99364	0.00000	Uiso	1.00
O98	O	0.53547	0.28928	0.71287	0.00000	Uiso	1.00
O99	O	0.31389	0.07084	0.71242	0.00000	Uiso	1.00
O100	O	0.36194	0.88268	0.00534	0.00000	Uiso	1.00
O101	O	0.46686	0.71319	0.96288	0.00000	Uiso	1.00
O102	O	0.68035	0.92801	0.96377	0.00000	Uiso	1.00
O103	O	0.64066	0.11618	0.74077	0.00000	Uiso	1.00
O104	O	0.29589	0.52981	0.53321	0.00000	Uiso	1.00
O105	O	0.06731	0.31297	0.53741	0.00000	Uiso	1.00
O106	O	0.88275	0.36431	0.73874	0.00000	Uiso	1.00
O107	O	0.71367	0.46765	0.78604	0.00000	Uiso	1.00
O108	O	0.92773	0.68047	0.78682	0.00000	Uiso	1.00
O109	O	0.12033	0.63197	0.51691	0.00000	Uiso	1.00
O110	O	0.46553	0.71208	0.78597	0.00000	Uiso	1.00
O111	O	0.68131	0.93054	0.78714	0.00000	Uiso	1.00
O112	O	0.63039	0.11779	0.50921	0.00000	Uiso	1.00
O113	O	0.53106	0.29351	0.53594	0.00000	Uiso	1.00
O114	O	0.31263	0.07258	0.53629	0.00000	Uiso	1.00
O115	O	0.36265	0.88287	0.74435	0.00000	Uiso	1.00
O116	O	0.71132	0.46527	0.96246	0.00000	Uiso	1.00
O117	O	0.92930	0.68255	0.96353	0.00000	Uiso	1.00
O118	O	0.11488	0.63953	0.74885	0.00000	Uiso	1.00
O119	O	0.28721	0.53663	0.71034	0.00000	Uiso	1.00
O120	O	0.07163	0.31570	0.71346	0.00000	Uiso	1.00
O121	O	0.88228	0.36467	0.00987	0.00000	Uiso	1.00
O122	O	0.49650	0.00584	0.76111	0.00000	Uiso	1.00
O123	O	0.49383	0.99690	0.49112	0.00000	Uiso	1.00
O124	O	0.00320	0.49569	0.48919	0.00000	Uiso	1.00
O125	O	0.00596	0.49530	0.77033	0.00000	Uiso	1.00
O126	O	0.38912	0.38967	0.62963	0.00000	Uiso	1.00
O127	O	0.21386	0.21569	0.62478	0.00000	Uiso	1.00
O128	O	0.59931	0.59985	0.87430	0.00000	Uiso	1.00
O129	O	0.79459	0.79523	0.87475	0.00000	Uiso	1.00
O130	O	0.41017	0.19464	0.62471	0.00000	Uiso	1.00
O131	O	0.60060	0.79374	0.87296	0.00000	Uiso	1.00
O132	O	0.19369	0.41091	0.62170	0.00000	Uiso	1.00
O133	O	0.79251	0.60181	0.87731	0.00000	Uiso	1.00
O134	O	0.35016	0.01250	0.87510	0.00000	Uiso	1.00
O135	O	0.59131	0.23868	0.87414	0.00000	Uiso	1.00
O136	O	0.61953	0.97528	0.62571	0.00000	Uiso	1.00
O137	O	0.40080	0.74284	0.62416	0.00000	Uiso	1.00
O138	O	0.00514	0.34248	0.87492	0.00000	Uiso	1.00
O139	O	0.24678	0.58786	0.87483	0.00000	Uiso	1.00
O140	O	0.97859	0.61041	0.63002	0.00000	Uiso	1.00
O141	O	0.73856	0.40433	0.62349	0.00000	Uiso	1.00
O142	O	0.72431	0.27684	0.75438	0.00000	Uiso	1.00
O143	O	0.27734	0.71856	0.49134	0.00000	Uiso	1.00
O144	O	0.27450	0.72438	0.75508	0.00000	Uiso	1.00
O145	O	0.72118	0.27388	0.49607	0.00000	Uiso	1.00
H146	H	0.85214	0.86197	0.35368	0.00000	Uiso	1.00
H147	H	0.08811	0.94954	0.45722	0.00000	Uiso	1.00
H148	H	0.00512	0.86931	0.49322	0.00000	Uiso	1.00
H149	H	0.07179	0.84353	0.39325	0.00000	Uiso	1.00
H150	H	0.94951	0.09833	0.45353	0.00000	Uiso	1.00
H151	H	0.86761	0.02037	0.49519	0.00000	Uiso	1.00
H152	H	0.84015	0.08498	0.39396	0.00000	Uiso	1.00
H153	H	0.97304	0.88104	0.26454	0.00000	Uiso	1.00
H154	H	0.87411	0.98667	0.26445	0.00000	Uiso	1.00
C155	C	0.89900	0.04598	0.43376	0.00000	Uiso	1.00
C156	C	0.95384	0.96212	0.38451	0.00000	Uiso	1.00
C157	C	0.03423	0.90227	0.43406	0.00000	Uiso	1.00
C158	C	0.93129	0.94099	0.30031	0.00000	Uiso	1.00

File n°11

H2	H	0.46876	0.44985	0.76074	0.00000	Uiso	1.00
H3	H	0.45149	0.29296	0.88021	0.00000	Uiso	1.00
H4	H	0.46784	0.62771	0.70636	0.00000	Uiso	1.00
H5	H	0.43215	0.51104	0.41816	0.00000	Uiso	1.00
H6	H	0.43802	0.21671	0.43750	0.00000	Uiso	1.00
H7	H	0.45680	0.94704	0.40636	0.00000	Uiso	1.00
H8	H	0.44601	0.77295	0.01946	0.00000	Uiso	1.00
H9	H	0.43378	0.04830	0.30083	0.00000	Uiso	1.00
H10	H	0.45428	0.84237	0.54805	0.00000	Uiso	1.00

H11	H	0.45323	0.75218	0.61816	0.00000	Uiso	1.00
H12	H	0.46681	0.62248	0.94418	0.00000	Uiso	1.00
H13	H	0.45510	0.63074	0.09838	0.00000	Uiso	1.00
H14	H	0.48169	0.55575	0.05496	0.00000	Uiso	1.00
H15	H	0.52607	0.64852	0.89677	0.00000	Uiso	1.00
H16	H	0.53692	0.58671	0.02031	0.00000	Uiso	1.00
H17	H	0.55063	0.68718	0.01213	0.00000	Uiso	1.00
H18	H	0.52763	0.71149	0.22641	0.00000	Uiso	1.00
H19	H	0.51713	0.60883	0.21988	0.00000	Uiso	1.00
H20	H	0.48842	0.68057	0.25555	0.00000	Uiso	1.00
H21	H	0.49211	0.75557	0.91771	0.00000	Uiso	1.00
H22	H	0.46504	0.87997	0.21625	0.00000	Uiso	1.00
H23	H	0.50553	0.89754	0.21501	0.00000	Uiso	1.00
H24	H	0.49107	0.80186	0.25774	0.00000	Uiso	1.00
H25	H	0.46231	0.93411	0.00988	0.00000	Uiso	1.00
H26	H	0.48135	0.88299	0.88882	0.00000	Uiso	1.00
H27	H	0.50286	0.94276	0.99200	0.00000	Uiso	1.00
A128	Al	0.35127	0.05697	0.89405	0.00000	Uiso	1.00
A129	Al	0.35016	0.03672	0.38039	0.00000	Uiso	1.00
A130	Al	0.34427	0.56633	0.89986	0.00000	Uiso	1.00
A131	Al	0.34388	0.53285	0.38242	0.00000	Uiso	1.00
A132	Al	0.34430	0.87459	0.89718	0.00000	Uiso	1.00
A133	Al	0.34999	0.85096	0.41039	0.00000	Uiso	1.00
A134	Al	0.35322	0.40171	0.88391	0.00000	Uiso	1.00
A135	Al	0.32880	0.38674	0.51910	0.00000	Uiso	1.00
A136	Al	0.30475	0.80226	0.26181	0.00000	Uiso	1.00
A137	Al	0.30074	0.80731	0.76480	0.00000	Uiso	1.00
A138	Al	0.30453	0.30669	0.26025	0.00000	Uiso	1.00
A139	Al	0.30162	0.31416	0.77249	0.00000	Uiso	1.00
A140	Al	0.30633	0.13411	0.26127	0.00000	Uiso	1.00
A141	Al	0.30316	0.13612	0.75846	0.00000	Uiso	1.00
A142	Al	0.29754	0.63493	0.26782	0.00000	Uiso	1.00
A143	Al	0.29902	0.64130	0.76050	0.00000	Uiso	1.00
A144	Al	0.21191	0.97110	0.25381	0.00000	Uiso	1.00
A145	Al	0.21176	0.97245	0.75450	0.00000	Uiso	1.00
A146	Al	0.20935	0.47056	0.25063	0.00000	Uiso	1.00
A147	Al	0.21015	0.47068	0.75172	0.00000	Uiso	1.00
A148	Al	0.32931	0.97024	0.12991	0.00000	Uiso	1.00
A149	Al	0.32690	0.96657	0.62732	0.00000	Uiso	1.00
A150	Al	0.32458	0.47527	0.12735	0.00000	Uiso	1.00
A151	Al	0.33979	0.53546	0.65873	0.00000	Uiso	1.00
A152	Al	0.28081	0.22013	0.02363	0.00000	Uiso	1.00
A153	Al	0.28186	0.22140	0.51692	0.00000	Uiso	1.00
A154	Al	0.28101	0.71859	0.00729	0.00000	Uiso	1.00
A155	Al	0.28101	0.72099	0.50702	0.00000	Uiso	1.00
A156	Al	0.34591	0.23237	0.91679	0.00000	Uiso	1.00
A157	Al	0.35637	0.24065	0.65621	0.00000	Uiso	1.00
A158	Al	0.35266	0.73115	0.12544	0.00000	Uiso	1.00
A159	Al	0.35167	0.73154	0.66594	0.00000	Uiso	1.00
A160	Al	0.21198	0.97156	0.00634	0.00000	Uiso	1.00
A161	Al	0.21143	0.97204	0.50418	0.00000	Uiso	1.00
A162	Al	0.21023	0.46983	0.00295	0.00000	Uiso	1.00
A163	Al	0.20960	0.47001	0.50306	0.00000	Uiso	1.00
A164	Al	0.28284	0.96110	0.37883	0.00000	Uiso	1.00
A165	Al	0.28189	0.97621	0.87927	0.00000	Uiso	1.00
A166	Al	0.27839	0.46744	0.37677	0.00000	Uiso	1.00
A167	Al	0.28082	0.47475	0.87728	0.00000	Uiso	1.00
A168	Al	0.23655	0.21902	0.25537	0.00000	Uiso	1.00
A169	Al	0.23539	0.22002	0.75396	0.00000	Uiso	1.00
A170	Al	0.23490	0.72406	0.25056	0.00000	Uiso	1.00
A171	Al	0.23417	0.72320	0.74999	0.00000	Uiso	1.00
A172	Al	0.26186	0.05810	0.13329	0.00000	Uiso	1.00
A173	Al	0.26127	0.05827	0.62615	0.00000	Uiso	1.00
A174	Al	0.25841	0.55813	0.12481	0.00000	Uiso	1.00
A175	Al	0.25901	0.55861	0.62456	0.00000	Uiso	1.00
A176	Al	0.26183	0.88315	0.12666	0.00000	Uiso	1.00
A177	Al	0.25962	0.88322	0.62709	0.00000	Uiso	1.00
A178	Al	0.25952	0.38232	0.13199	0.00000	Uiso	1.00
A179	Al	0.25925	0.38332	0.63006	0.00000	Uiso	1.00
A180	Al	0.21396	0.80723	0.00144	0.00000	Uiso	1.00
A181	Al	0.21308	0.80675	0.50080	0.00000	Uiso	1.00
A182	Al	0.21299	0.30593	0.00341	0.00000	Uiso	1.00
A183	Al	0.21299	0.30600	0.50084	0.00000	Uiso	1.00
A184	Al	0.21369	0.13512	0.00596	0.00000	Uiso	1.00
A185	Al	0.21368	0.13572	0.50169	0.00000	Uiso	1.00
A186	Al	0.21270	0.63517	0.99915	0.00000	Uiso	1.00
A187	Al	0.21272	0.63523	0.49872	0.00000	Uiso	1.00
A188	Al	0.40261	0.15166	0.78370	0.00000	Uiso	1.00
A189	Al	0.35104	0.22617	0.39951	0.00000	Uiso	1.00
A190	Al	0.39731	0.62849	0.01946	0.00000	Uiso	1.00
A191	Al	0.40237	0.76534	0.50808	0.00000	Uiso	1.00
O92	O	0.30862	0.87737	0.38125	0.00000	Uiso	1.00
O93	O	0.30392	0.88794	0.88223	0.00000	Uiso	1.00
O94	O	0.30654	0.38908	0.38504	0.00000	Uiso	1.00
O95	O	0.30650	0.39350	0.88053	0.00000	Uiso	1.00
O96	O	0.30842	0.04362	0.36946	0.00000	Uiso	1.00
O97	O	0.30942	0.05812	0.87192	0.00000	Uiso	1.00
O98	O	0.30385	0.55061	0.37163	0.00000	Uiso	1.00
O99	O	0.30298	0.56353	0.87893	0.00000	Uiso	1.00
O100	O	0.30737	0.22367	0.38766	0.00000	Uiso	1.00
O101	O	0.30455	0.21997	0.88853	0.00000	Uiso	1.00
O102	O	0.30179	0.71602	0.37048	0.00000	Uiso	1.00
O103	O	0.30064	0.72221	0.87094	0.00000	Uiso	1.00
O104	O	0.35154	0.13442	0.31388	0.00000	Uiso	1.00
O105	O	0.35608	0.15404	0.78218	0.00000	Uiso	1.00
O106	O	0.35953	0.62700	0.36776	0.00000	Uiso	1.00
O107	O	0.34596	0.63203	0.73639	0.00000	Uiso	1.00
O108	O	0.34948	0.79796	0.26277	0.00000	Uiso	1.00
O109	O	0.34562	0.80661	0.77475	0.00000	Uiso	1.00
O110	O	0.35603	0.31052	0.02384	0.00000	Uiso	1.00
O111	O	0.41707	0.39839	0.64539	0.00000	Uiso	1.00

O112	O	0.35372	0.96574	0.75580	0.00000	Uiso	1.00
O113	O	0.35538	0.48785	0.23987	0.00000	Uiso	1.00
O114	O	0.35415	0.48758	0.78379	0.00000	Uiso	1.00
O115	O	0.30491	0.88681	0.14315	0.00000	Uiso	1.00
O116	O	0.30157	0.88685	0.64343	0.00000	Uiso	1.00
O117	O	0.30234	0.38934	0.15024	0.00000	Uiso	1.00
O118	O	0.30227	0.38174	0.63782	0.00000	Uiso	1.00
O119	O	0.30546	0.05553	0.13920	0.00000	Uiso	1.00
O120	O	0.30485	0.05595	0.63897	0.00000	Uiso	1.00
O121	O	0.30108	0.55970	0.14383	0.00000	Uiso	1.00
O122	O	0.30062	0.55970	0.63915	0.00000	Uiso	1.00
O123	O	0.30655	0.22066	0.15021	0.00000	Uiso	1.00
O124	O	0.31017	0.21890	0.64661	0.00000	Uiso	1.00
O125	O	0.30982	0.71777	0.13652	0.00000	Uiso	1.00
O126	O	0.30662	0.72451	0.63823	0.00000	Uiso	1.00
O127	O	0.35921	0.14313	0.00323	0.00000	Uiso	1.00
O128	O	0.35671	0.64583	0.00027	0.00000	Uiso	1.00
O129	O	0.36447	0.81150	0.01687	0.00000	Uiso	1.00
O130	O	0.35991	0.77779	0.52186	0.00000	Uiso	1.00
O131	O	0.34501	0.30492	0.78759	0.00000	Uiso	1.00
O132	O	0.35332	0.30376	0.52021	0.00000	Uiso	1.00
O133	O	0.35086	0.96791	0.99185	0.00000	Uiso	1.00
O134	O	0.34971	0.95664	0.49366	0.00000	Uiso	1.00
O135	O	0.34838	0.47876	0.00201	0.00000	Uiso	1.00
O136	O	0.34939	0.48202	0.52098	0.00000	Uiso	1.00
O137	O	0.20714	0.89410	0.88748	0.00000	Uiso	1.00
O138	O	0.20694	0.89349	0.38613	0.00000	Uiso	1.00
O139	O	0.20580	0.39218	0.88554	0.00000	Uiso	1.00
O140	O	0.20555	0.39232	0.38447	0.00000	Uiso	1.00
O141	O	0.20727	0.05009	0.88889	0.00000	Uiso	1.00
O142	O	0.20705	0.04986	0.38642	0.00000	Uiso	1.00
O143	O	0.20574	0.54782	0.88445	0.00000	Uiso	1.00
O144	O	0.20531	0.54773	0.38375	0.00000	Uiso	1.00
O145	O	0.21095	0.22046	0.88651	0.00000	Uiso	1.00
O146	O	0.21090	0.22066	0.38494	0.00000	Uiso	1.00
O147	O	0.21040	0.72146	0.88361	0.00000	Uiso	1.00
O148	O	0.21029	0.72184	0.38227	0.00000	Uiso	1.00
O149	O	0.26215	0.13521	0.25359	0.00000	Uiso	1.00
O150	O	0.26141	0.13781	0.74601	0.00000	Uiso	1.00
O151	O	0.25707	0.63595	0.24359	0.00000	Uiso	1.00
O152	O	0.25710	0.63729	0.74183	0.00000	Uiso	1.00
O153	O	0.26170	0.80403	0.24292	0.00000	Uiso	1.00
O154	O	0.25846	0.80743	0.74601	0.00000	Uiso	1.00
O155	O	0.26074	0.30527	0.25416	0.00000	Uiso	1.00
O156	O	0.25984	0.30508	0.75079	0.00000	Uiso	1.00
O157	O	0.25642	0.96842	0.25014	0.00000	Uiso	1.00
O158	O	0.25571	0.97390	0.75027	0.00000	Uiso	1.00
O159	O	0.25338	0.47022	0.24795	0.00000	Uiso	1.00
O160	O	0.25437	0.47040	0.74746	0.00000	Uiso	1.00
O161	O	0.21592	0.89300	0.12150	0.00000	Uiso	1.00
O162	O	0.21497	0.89461	0.62121	0.00000	Uiso	1.00
O163	O	0.21420	0.39217	0.12082	0.00000	Uiso	1.00
O164	O	0.21407	0.39200	0.62043	0.00000	Uiso	1.00
O165	O	0.21590	0.04853	0.12485	0.00000	Uiso	1.00
O166	O	0.21583	0.04998	0.62089	0.00000	Uiso	1.00
O167	O	0.21366	0.54798	0.11865	0.00000	Uiso	1.00
O168	O	0.21380	0.54805	0.61841	0.00000	Uiso	1.00
O169	O	0.20848	0.21991	0.12777	0.00000	Uiso	1.00
O170	O	0.20818	0.22101	0.62578	0.00000	Uiso	1.00
O171	O	0.20815	0.72182	0.12286	0.00000	Uiso	1.00
O172	O	0.20752	0.72170	0.62177	0.00000	Uiso	1.00
O173	O	0.25600	0.13646	0.01719	0.00000	Uiso	1.00
O174	O	0.25648	0.13831	0.51274	0.00000	Uiso	1.00
O175	O	0.25471	0.63737	0.01157	0.00000	Uiso	1.00
O176	O	0.25487	0.63733	0.50809	0.00000	Uiso	1.00
O177	O	0.25632	0.80362	0.01316	0.00000	Uiso	1.00
O178	O	0.25525	0.80440	0.51081	0.00000	Uiso	1.00
O179	O	0.25541	0.30358	0.01769	0.00000	Uiso	1.00
O180	O	0.25553	0.30338	0.51503	0.00000	Uiso	1.00
O181	O	0.25884	0.97248	0.01255	0.00000	Uiso	1.00
O182	O	0.25840	0.97017	0.50951	0.00000	Uiso	1.00
O183	O	0.25710	0.47055	0.01117	0.00000	Uiso	1.00
O184	O	0.25616	0.46930	0.51001	0.00000	Uiso	1.00
O185	O	0.35220	0.29827	0.27093	0.00000	Uiso	1.00
O186	O	0.39615	0.71319	0.65902	0.00000	Uiso	1.00
O187	O	0.41533	0.18288	0.92845	0.00000	Uiso	1.00
O188	O	0.39887	0.88720	0.86768	0.00000	Uiso	1.00
O189	O	0.39758	0.38902	0.17666	0.00000	Uiso	1.00
O190	O	0.39440	0.37950	0.87131	0.00000	Uiso	1.00
O191	O	0.39821	0.25448	0.71337	0.00000	Uiso	1.00
O192	O	0.41036	0.55941	0.65147	0.00000	Uiso	1.00
O193	O	0.46490	0.49488	0.70722	0.00000	Uiso	1.00
O194	O	0.40838	0.54454	0.29831	0.00000	Uiso	1.00
O195	O	0.40542	0.53194	0.07049	0.00000	Uiso	1.00
O196	O	0.39814	0.22974	0.14753	0.00000	Uiso	1.00
O197	O	0.39556	0.04527	0.84347	0.00000	Uiso	1.00
O198	O	0.40602	0.07249	0.10519	0.00000	Uiso	1.00
O199	O	0.41427	0.69615	0.39808	0.00000	Uiso	1.00
O200	O	0.45041	0.32191	0.80448	0.00000	Uiso	1.00
O201	O	0.45313	0.67218	0.70669	0.00000	Uiso	1.00
O202	O	0.40983	0.63102	0.86941	0.00000	Uiso	1.00
O203	O	0.44577	0.48979	0.48168	0.00000	Uiso	1.00
O204	O	0.37041	0.16780	0.53181	0.00000	Uiso	1.00
O205	O	0.42078	0.11417	0.65222	0.00000	Uiso	1.00
O206	O	0.40930	0.94029	0.64891	0.00000	Uiso	1.00
O207	O	0.39804	0.87015	0.43272	0.00000	Uiso	1.00
O208	O	0.42688	0.16799	0.41824	0.00000	Uiso	1.00
O209	O	0.39735	0.03752	0.46012	0.00000	Uiso	1.00
O210	O	0.45077	0.94591	0.49098	0.00000	Uiso	1.00
O211	O	0.40940	0.91022	0.10291	0.00000	Uiso	1.00
O212	O	0.42322	0.76796	0.00520	0.00000	Uiso	1.00

O213	O	0.42959	0.99346	0.27573	0.00000	Uiso	1.00
O214	O	0.39039	0.67837	0.17301	0.00000	Uiso	1.00
O215	O	0.36448	0.98267	0.23685	0.00000	Uiso	1.00
O216	O	0.44356	0.79092	0.56005	0.00000	Uiso	1.00
Si217	Si	0.39217	0.96056	0.77267	0.00000	Uiso	1.00
Si218	Si	0.41382	0.34052	0.76471	0.00000	Uiso	1.00
Si219	Si	0.43388	0.48407	0.61984	0.00000	Uiso	1.00
Si220	Si	0.39302	0.48642	0.18758	0.00000	Uiso	1.00
Si221	Si	0.39615	0.15801	0.04837	0.00000	Uiso	1.00
Si222	Si	0.39421	0.63974	0.31212	0.00000	Uiso	1.00
Si223	Si	0.37542	0.30908	0.15306	0.00000	Uiso	1.00
Si224	Si	0.41604	0.64200	0.72877	0.00000	Uiso	1.00
Si225	Si	0.41210	0.94838	0.50192	0.00000	Uiso	1.00
Si226	Si	0.40531	0.12655	0.52317	0.00000	Uiso	1.00
Si227	Si	0.40071	0.99024	0.17789	0.00000	Uiso	1.00
Si228	Si	0.40039	0.84501	0.00175	0.00000	Uiso	1.00
C229	C	0.50175	0.67541	0.06542	0.00000	Uiso	1.00
C230	C	0.47474	0.61785	0.03777	0.00000	Uiso	1.00
C231	C	0.53065	0.64793	0.99407	0.00000	Uiso	1.00
C232	C	0.50913	0.66976	0.19994	0.00000	Uiso	1.00
C233	C	0.49342	0.75711	0.01632	0.00000	Uiso	1.00
C234	C	0.48854	0.82990	0.06543	0.00000	Uiso	1.00
C235	C	0.48766	0.85192	0.19650	0.00000	Uiso	1.00
C236	C	0.48328	0.90063	0.98363	0.00000	Uiso	1.00

File n°12 :

H2	H	0.46805	0.44900	0.75979	0.00000	Uiso	1.00
H3	H	0.45182	0.29453	0.87894	0.00000	Uiso	1.00
H4	H	0.46745	0.62242	0.69868	0.00000	Uiso	1.00
H5	H	0.43072	0.51242	0.41925	0.00000	Uiso	1.00
H6	H	0.43815	0.21653	0.43800	0.00000	Uiso	1.00
H7	H	0.45666	0.94868	0.40565	0.00000	Uiso	1.00
H8	H	0.43380	0.04936	0.30189	0.00000	Uiso	1.00
H9	H	0.45459	0.84210	0.54554	0.00000	Uiso	1.00
H10	H	0.45383	0.75055	0.61136	0.00000	Uiso	1.00
H11	H	0.44932	0.68806	0.16097	0.00000	Uiso	1.00
H12	H	0.48870	0.54395	0.08260	0.00000	Uiso	1.00
H13	H	0.47490	0.56568	0.23002	0.00000	Uiso	1.00
H14	H	0.51546	0.55176	0.20498	0.00000	Uiso	1.00
H15	H	0.52027	0.65271	0.96636	0.00000	Uiso	1.00
H16	H	0.54615	0.64739	0.09122	0.00000	Uiso	1.00
H17	H	0.53142	0.74124	0.04436	0.00000	Uiso	1.00
H18	H	0.52471	0.67432	0.30678	0.00000	Uiso	1.00
H19	H	0.48506	0.70338	0.32364	0.00000	Uiso	1.00
H20	H	0.51237	0.76877	0.25392	0.00000	Uiso	1.00
H21	H	0.46036	0.65153	0.01644	0.00000	Uiso	1.00
H22	H	0.45938	0.83907	0.20724	0.00000	Uiso	1.00
H23	H	0.46433	0.90343	0.08076	0.00000	Uiso	1.00
H24	H	0.49585	0.84390	0.12999	0.00000	Uiso	1.00
H25	H	0.50169	0.79384	0.91969	0.00000	Uiso	1.00
H26	H	0.46802	0.84695	0.87290	0.00000	Uiso	1.00
H27	H	0.47023	0.74165	0.85026	0.00000	Uiso	1.00
Al28	Al	0.35118	0.05703	0.89432	0.00000	Uiso	1.00
Al29	Al	0.34989	0.03737	0.38127	0.00000	Uiso	1.00
Al30	Al	0.34382	0.56544	0.90029	0.00000	Uiso	1.00
Al31	Al	0.34394	0.53311	0.38199	0.00000	Uiso	1.00
Al32	Al	0.34488	0.87439	0.89694	0.00000	Uiso	1.00
Al33	Al	0.34999	0.85134	0.40989	0.00000	Uiso	1.00
Al34	Al	0.35313	0.40125	0.88438	0.00000	Uiso	1.00
Al35	Al	0.32885	0.38705	0.51942	0.00000	Uiso	1.00
Al36	Al	0.30483	0.80232	0.26139	0.00000	Uiso	1.00
Al37	Al	0.30084	0.80741	0.76492	0.00000	Uiso	1.00
Al38	Al	0.30446	0.30687	0.26077	0.00000	Uiso	1.00
Al39	Al	0.30159	0.31414	0.77253	0.00000	Uiso	1.00
Al40	Al	0.30629	0.13426	0.26135	0.00000	Uiso	1.00
Al41	Al	0.30316	0.13607	0.75859	0.00000	Uiso	1.00
Al42	Al	0.29764	0.63510	0.26726	0.00000	Uiso	1.00
Al43	Al	0.29903	0.64138	0.76010	0.00000	Uiso	1.00
Al44	Al	0.21191	0.97107	0.25381	0.00000	Uiso	1.00
Al45	Al	0.21176	0.97236	0.75450	0.00000	Uiso	1.00
Al46	Al	0.20935	0.47053	0.25063	0.00000	Uiso	1.00
Al47	Al	0.21015	0.47060	0.75172	0.00000	Uiso	1.00
Al48	Al	0.32927	0.97034	0.12995	0.00000	Uiso	1.00
Al49	Al	0.32691	0.96659	0.62752	0.00000	Uiso	1.00
Al50	Al	0.32452	0.47518	0.12773	0.00000	Uiso	1.00
Al51	Al	0.33998	0.53568	0.65872	0.00000	Uiso	1.00
Al52	Al	0.28078	0.22011	0.02383	0.00000	Uiso	1.00
Al53	Al	0.28184	0.22134	0.51698	0.00000	Uiso	1.00
Al54	Al	0.28100	0.71861	0.00697	0.00000	Uiso	1.00
Al55	Al	0.28103	0.72100	0.50676	0.00000	Uiso	1.00
Al56	Al	0.34579	0.23238	0.91688	0.00000	Uiso	1.00
Al57	Al	0.35622	0.24057	0.65625	0.00000	Uiso	1.00
Al58	Al	0.35294	0.73191	0.12421	0.00000	Uiso	1.00
Al59	Al	0.35172	0.73161	0.66542	0.00000	Uiso	1.00
Al60	Al	0.21198	0.97156	0.00634	0.00000	Uiso	1.00
Al61	Al	0.21143	0.97199	0.50418	0.00000	Uiso	1.00
Al62	Al	0.21023	0.46983	0.00295	0.00000	Uiso	1.00
Al63	Al	0.20960	0.46996	0.50306	0.00000	Uiso	1.00
Al64	Al	0.28282	0.96130	0.37880	0.00000	Uiso	1.00
Al65	Al	0.28200	0.97575	0.87935	0.00000	Uiso	1.00
Al66	Al	0.27841	0.46774	0.37687	0.00000	Uiso	1.00
Al67	Al	0.28072	0.47447	0.87717	0.00000	Uiso	1.00
Al68	Al	0.23655	0.21899	0.25537	0.00000	Uiso	1.00
Al69	Al	0.23539	0.21993	0.75396	0.00000	Uiso	1.00
Al70	Al	0.23490	0.72403	0.25056	0.00000	Uiso	1.00
Al71	Al	0.23417	0.72311	0.74999	0.00000	Uiso	1.00
Al72	Al	0.26186	0.05808	0.13329	0.00000	Uiso	1.00

AI73	AI	0.26127	0.05820	0.62615	0.00000	Uiso	1.00
AI74	AI	0.25841	0.55811	0.12481	0.00000	Uiso	1.00
AI75	AI	0.25901	0.55854	0.62456	0.00000	Uiso	1.00
AI76	AI	0.26183	0.88314	0.12666	0.00000	Uiso	1.00
AI77	AI	0.25962	0.88314	0.62709	0.00000	Uiso	1.00
AI78	AI	0.25952	0.38231	0.13199	0.00000	Uiso	1.00
AI79	AI	0.25925	0.38325	0.63006	0.00000	Uiso	1.00
AI80	AI	0.21396	0.80723	0.00144	0.00000	Uiso	1.00
AI81	AI	0.21308	0.80669	0.50080	0.00000	Uiso	1.00
AI82	AI	0.21299	0.30593	0.00341	0.00000	Uiso	1.00
AI83	AI	0.21299	0.30594	0.50084	0.00000	Uiso	1.00
AI84	AI	0.21369	0.13512	0.00596	0.00000	Uiso	1.00
AI85	AI	0.21368	0.13566	0.50169	0.00000	Uiso	1.00
AI86	AI	0.21270	0.63505	0.99915	0.00000	Uiso	1.00
AI87	AI	0.21272	0.63517	0.49872	0.00000	Uiso	1.00
AI88	AI	0.40253	0.15197	0.78416	0.00000	Uiso	1.00
AI89	AI	0.35102	0.22655	0.39955	0.00000	Uiso	1.00
AI90	AI	0.39734	0.62760	0.01827	0.00000	Uiso	1.00
AI91	AI	0.40233	0.76575	0.50699	0.00000	Uiso	1.00
O92	O	0.30863	0.87757	0.38072	0.00000	Uiso	1.00
O93	O	0.30430	0.88773	0.88239	0.00000	Uiso	1.00
O94	O	0.30655	0.38942	0.38531	0.00000	Uiso	1.00
O95	O	0.30640	0.39331	0.88095	0.00000	Uiso	1.00
O96	O	0.30820	0.04426	0.37013	0.00000	Uiso	1.00
O97	O	0.30935	0.05807	0.87211	0.00000	Uiso	1.00
O98	O	0.30391	0.55084	0.37136	0.00000	Uiso	1.00
O99	O	0.30272	0.56347	0.87878	0.00000	Uiso	1.00
O100	O	0.30734	0.22401	0.38779	0.00000	Uiso	1.00
O101	O	0.30448	0.22001	0.88856	0.00000	Uiso	1.00
O102	O	0.30187	0.71614	0.37014	0.00000	Uiso	1.00
O103	O	0.30076	0.72214	0.87079	0.00000	Uiso	1.00
O104	O	0.35143	0.13491	0.31410	0.00000	Uiso	1.00
O105	O	0.35589	0.15406	0.78238	0.00000	Uiso	1.00
O106	O	0.35951	0.62731	0.36522	0.00000	Uiso	1.00
O107	O	0.34609	0.63209	0.73608	0.00000	Uiso	1.00
O108	O	0.34960	0.79839	0.26189	0.00000	Uiso	1.00
O109	O	0.34577	0.80666	0.77414	0.00000	Uiso	1.00
O110	O	0.35584	0.31084	0.02376	0.00000	Uiso	1.00
O111	O	0.41614	0.39782	0.64461	0.00000	Uiso	1.00
O112	O	0.35385	0.96631	0.75560	0.00000	Uiso	1.00
O113	O	0.35548	0.48806	0.23940	0.00000	Uiso	1.00
O114	O	0.35382	0.48723	0.78431	0.00000	Uiso	1.00
O115	O	0.30494	0.88671	0.14277	0.00000	Uiso	1.00
O116	O	0.30157	0.88684	0.64353	0.00000	Uiso	1.00
O117	O	0.30231	0.38938	0.15052	0.00000	Uiso	1.00
O118	O	0.30227	0.38186	0.63800	0.00000	Uiso	1.00
O119	O	0.30542	0.05556	0.13945	0.00000	Uiso	1.00
O120	O	0.30485	0.05596	0.63908	0.00000	Uiso	1.00
O121	O	0.30111	0.55981	0.14353	0.00000	Uiso	1.00
O122	O	0.30071	0.55968	0.63905	0.00000	Uiso	1.00
O123	O	0.30656	0.22082	0.15038	0.00000	Uiso	1.00
O124	O	0.31013	0.21897	0.64666	0.00000	Uiso	1.00
O125	O	0.31004	0.71788	0.13568	0.00000	Uiso	1.00
O126	O	0.30664	0.72450	0.63800	0.00000	Uiso	1.00
O127	O	0.35910	0.14353	0.00354	0.00000	Uiso	1.00
O128	O	0.35686	0.64480	-0.00155	0.00000	Uiso	1.00
O129	O	0.36594	0.81016	0.01492	0.00000	Uiso	1.00
O130	O	0.35986	0.77773	0.52099	0.00000	Uiso	1.00
O131	O	0.34496	0.30499	0.78773	0.00000	Uiso	1.00
O132	O	0.35332	0.30402	0.52042	0.00000	Uiso	1.00
O133	O	0.35075	0.96789	0.99187	0.00000	Uiso	1.00
O134	O	0.34957	0.95680	0.49369	0.00000	Uiso	1.00
O135	O	0.34838	0.47839	0.00253	0.00000	Uiso	1.00
O136	O	0.34954	0.48239	0.52070	0.00000	Uiso	1.00
O137	O	0.20714	0.89400	0.88748	0.00000	Uiso	1.00
O138	O	0.20694	0.89345	0.38613	0.00000	Uiso	1.00
O139	O	0.20580	0.39208	0.88554	0.00000	Uiso	1.00
O140	O	0.20555	0.39227	0.38447	0.00000	Uiso	1.00
O141	O	0.20727	0.04999	0.88889	0.00000	Uiso	1.00
O142	O	0.20705	0.04981	0.38642	0.00000	Uiso	1.00
O143	O	0.20574	0.54772	0.88445	0.00000	Uiso	1.00
O144	O	0.20531	0.54768	0.38375	0.00000	Uiso	1.00
O145	O	0.21095	0.22036	0.88651	0.00000	Uiso	1.00
O146	O	0.21090	0.22062	0.38494	0.00000	Uiso	1.00
O147	O	0.21040	0.72136	0.88361	0.00000	Uiso	1.00
O148	O	0.21029	0.72180	0.38227	0.00000	Uiso	1.00
O149	O	0.26215	0.13518	0.25359	0.00000	Uiso	1.00
O150	O	0.26141	0.13773	0.74601	0.00000	Uiso	1.00
O151	O	0.25707	0.63592	0.24359	0.00000	Uiso	1.00
O152	O	0.25710	0.63721	0.74183	0.00000	Uiso	1.00
O153	O	0.26170	0.80400	0.24292	0.00000	Uiso	1.00
O154	O	0.25846	0.80735	0.74601	0.00000	Uiso	1.00
O155	O	0.26074	0.30524	0.25416	0.00000	Uiso	1.00
O156	O	0.25984	0.30500	0.75079	0.00000	Uiso	1.00
O157	O	0.25642	0.96839	0.25014	0.00000	Uiso	1.00
O158	O	0.25570	0.97382	0.75027	0.00000	Uiso	1.00
O159	O	0.25338	0.47019	0.24795	0.00000	Uiso	1.00
O160	O	0.25437	0.47031	0.74746	0.00000	Uiso	1.00
O161	O	0.21592	0.89298	0.12150	0.00000	Uiso	1.00
O162	O	0.21497	0.89454	0.62121	0.00000	Uiso	1.00
O163	O	0.21420	0.39216	0.12082	0.00000	Uiso	1.00
O164	O	0.21407	0.39193	0.62043	0.00000	Uiso	1.00
O165	O	0.21590	0.04852	0.12485	0.00000	Uiso	1.00
O166	O	0.21583	0.04991	0.62089	0.00000	Uiso	1.00
O167	O	0.21366	0.54797	0.11865	0.00000	Uiso	1.00
O168	O	0.21380	0.54798	0.61841	0.00000	Uiso	1.00
O169	O	0.20848	0.21989	0.12777	0.00000	Uiso	1.00
O170	O	0.20818	0.22094	0.62578	0.00000	Uiso	1.00
O171	O	0.20815	0.72181	0.12286	0.00000	Uiso	1.00
O172	O	0.20752	0.72163	0.62177	0.00000	Uiso	1.00
O173	O	0.25600	0.13645	0.01719	0.00000	Uiso	1.00

O174	O	0.25648	0.13825	0.51274	0.00000	Uiso	1.00
O175	O	0.25471	0.63737	0.01157	0.00000	Uiso	1.00
O176	O	0.25487	0.63727	0.50809	0.00000	Uiso	1.00
O177	O	0.25632	0.80362	0.01316	0.00000	Uiso	1.00
O178	O	0.25525	0.80434	0.51081	0.00000	Uiso	1.00
O179	O	0.25541	0.30358	0.01769	0.00000	Uiso	1.00
O180	O	0.25553	0.30333	0.51503	0.00000	Uiso	1.00
O181	O	0.25884	0.97248	0.01255	0.00000	Uiso	1.00
O182	O	0.25840	0.97011	0.50951	0.00000	Uiso	1.00
O183	O	0.25710	0.47055	0.01117	0.00000	Uiso	1.00
O184	O	0.25616	0.46925	0.51001	0.00000	Uiso	1.00
O185	O	0.35212	0.29894	0.27115	0.00000	Uiso	1.00
O186	O	0.39627	0.71350	0.65805	0.00000	Uiso	1.00
O187	O	0.41511	0.18402	0.92863	0.00000	Uiso	1.00
O188	O	0.39904	0.88817	0.86715	0.00000	Uiso	1.00
O189	O	0.39760	0.38938	0.17623	0.00000	Uiso	1.00
O190	O	0.39436	0.37955	0.87173	0.00000	Uiso	1.00
O191	O	0.39801	0.25434	0.71357	0.00000	Uiso	1.00
O192	O	0.40870	0.55811	0.65763	0.00000	Uiso	1.00
O193	O	0.46383	0.49450	0.70755	0.00000	Uiso	1.00
O194	O	0.40848	0.54523	0.29641	0.00000	Uiso	1.00
O195	O	0.40577	0.53152	0.06883	0.00000	Uiso	1.00
O196	O	0.39808	0.23091	0.14785	0.00000	Uiso	1.00
O197	O	0.39557	0.04603	0.84409	0.00000	Uiso	1.00
O198	O	0.40592	0.07490	0.10790	0.00000	Uiso	1.00
O199	O	0.41419	0.69679	0.39610	0.00000	Uiso	1.00
O200	O	0.45028	0.32264	0.80263	0.00000	Uiso	1.00
O201	O	0.45311	0.66768	0.69521	0.00000	Uiso	1.00
O202	O	0.41180	0.63743	0.87143	0.00000	Uiso	1.00
O203	O	0.44437	0.49255	0.48361	0.00000	Uiso	1.00
O204	O	0.37027	0.16792	0.53208	0.00000	Uiso	1.00
O205	O	0.42074	0.11456	0.65262	0.00000	Uiso	1.00
O206	O	0.40946	0.94100	0.64881	0.00000	Uiso	1.00
O207	O	0.39799	0.87062	0.43279	0.00000	Uiso	1.00
O208	O	0.42675	0.16824	0.41856	0.00000	Uiso	1.00
O209	O	0.39717	0.03790	0.46093	0.00000	Uiso	1.00
O210	O	0.45081	0.94636	0.49040	0.00000	Uiso	1.00
O211	O	0.40786	0.91443	0.10255	0.00000	Uiso	1.00
O212	O	0.42715	0.77738	0.01243	0.00000	Uiso	1.00
O213	O	0.42929	0.99462	0.27714	0.00000	Uiso	1.00
O214	O	0.39051	0.67875	0.17060	0.00000	Uiso	1.00
O215	O	0.36399	0.98405	0.23827	0.00000	Uiso	1.00
O216	O	0.44368	0.79092	0.55745	0.00000	Uiso	1.00
Si217	Si	0.39233	0.96161	0.77246	0.00000	Uiso	1.00
Si218	Si	0.41351	0.34037	0.76463	0.00000	Uiso	1.00
Si219	Si	0.43255	0.48421	0.62145	0.00000	Uiso	1.00
Si220	Si	0.39308	0.48663	0.18630	0.00000	Uiso	1.00
Si221	Si	0.39600	0.15932	0.04873	0.00000	Uiso	1.00
Si222	Si	0.39421	0.64021	0.31010	0.00000	Uiso	1.00
Si223	Si	0.37528	0.30978	0.15310	0.00000	Uiso	1.00
Si224	Si	0.41611	0.64252	0.72839	0.00000	Uiso	1.00
Si225	Si	0.41216	0.94890	0.50182	0.00000	Uiso	1.00
Si226	Si	0.40522	0.12684	0.52364	0.00000	Uiso	1.00
Si227	Si	0.40020	0.99281	0.17999	0.00000	Uiso	1.00
Si228	Si	0.40155	0.84735	0.00242	0.00000	Uiso	1.00
C229	C	0.49802	0.66632	0.14198	0.00000	Uiso	1.00
C230	C	0.49398	0.57640	0.16611	0.00000	Uiso	1.00
C231	C	0.52544	0.67787	0.05551	0.00000	Uiso	1.00
C232	C	0.50533	0.70616	0.26337	0.00000	Uiso	1.00
C233	C	0.46655	0.69415	0.08829	0.00000	Uiso	1.00
C234	C	0.46136	0.77776	0.03428	0.00000	Uiso	1.00
C235	C	0.47050	0.84520	0.11894	0.00000	Uiso	1.00
C236	C	0.47631	0.79034	0.91151	0.00000	Uiso	1.00

File n°13

Al2	Al	0.35118	0.05661	0.89454	0.00000	Uiso	1.00
Al3	Al	0.35054	0.03692	0.37826	0.00000	Uiso	1.00
Al4	Al	0.34540	0.56746	0.89959	0.00000	Uiso	1.00
Al5	Al	0.34400	0.53245	0.38488	0.00000	Uiso	1.00
Al6	Al	0.34411	0.87462	0.89694	0.00000	Uiso	1.00
Al7	Al	0.34964	0.85220	0.41146	0.00000	Uiso	1.00
Al8	Al	0.35361	0.40152	0.88455	0.00000	Uiso	1.00
Al9	Al	0.32882	0.38549	0.51913	0.00000	Uiso	1.00
Al10	Al	0.30447	0.80309	0.26366	0.00000	Uiso	1.00
Al11	Al	0.30077	0.80705	0.76467	0.00000	Uiso	1.00
Al12	Al	0.30463	0.30702	0.25967	0.00000	Uiso	1.00
Al13	Al	0.30171	0.31431	0.77300	0.00000	Uiso	1.00
Al14	Al	0.30645	0.13419	0.26050	0.00000	Uiso	1.00
Al15	Al	0.30313	0.13586	0.75840	0.00000	Uiso	1.00
Al16	Al	0.29740	0.63518	0.26728	0.00000	Uiso	1.00
Al17	Al	0.29913	0.64080	0.76102	0.00000	Uiso	1.00
Al18	Al	0.21191	0.97110	0.25381	0.00000	Uiso	1.00
Al19	Al	0.21176	0.97245	0.75450	0.00000	Uiso	1.00
Al20	Al	0.20935	0.47056	0.25063	0.00000	Uiso	1.00
Al21	Al	0.21015	0.47068	0.75172	0.00000	Uiso	1.00
Al22	Al	0.32934	0.96977	0.12968	0.00000	Uiso	1.00
Al23	Al	0.32697	0.96646	0.62759	0.00000	Uiso	1.00
Al24	Al	0.32453	0.47611	0.12630	0.00000	Uiso	1.00
Al25	Al	0.33986	0.53460	0.65882	0.00000	Uiso	1.00
Al26	Al	0.28083	0.22011	0.02343	0.00000	Uiso	1.00
Al27	Al	0.28199	0.22129	0.51628	0.00000	Uiso	1.00
Al28	Al	0.28096	0.71863	0.00713	0.00000	Uiso	1.00
Al29	Al	0.28102	0.72093	0.50720	0.00000	Uiso	1.00
Al30	Al	0.34600	0.23208	0.91654	0.00000	Uiso	1.00
Al31	Al	0.35615	0.23923	0.65562	0.00000	Uiso	1.00
Al32	Al	0.35161	0.73334	0.12742	0.00000	Uiso	1.00
Al33	Al	0.35156	0.73100	0.66497	0.00000	Uiso	1.00
Al34	Al	0.21198	0.97156	0.00634	0.00000	Uiso	1.00

AI35	AI	0.21143	0.97204	0.50418	0.00000	Uiso	1.00
AI36	AI	0.21023	0.46983	0.00295	0.00000	Uiso	1.00
AI37	AI	0.20960	0.47001	0.50306	0.00000	Uiso	1.00
AI38	AI	0.28282	0.96215	0.37888	0.00000	Uiso	1.00
AI39	AI	0.28188	0.97617	0.87928	0.00000	Uiso	1.00
AI40	AI	0.27849	0.46755	0.37671	0.00000	Uiso	1.00
AI41	AI	0.28100	0.47512	0.87725	0.00000	Uiso	1.00
AI42	AI	0.23655	0.21902	0.25537	0.00000	Uiso	1.00
AI43	AI	0.23539	0.22002	0.75396	0.00000	Uiso	1.00
AI44	AI	0.23490	0.72406	0.25056	0.00000	Uiso	1.00
AI45	AI	0.23417	0.72320	0.74999	0.00000	Uiso	1.00
AI46	AI	0.26186	0.05810	0.13329	0.00000	Uiso	1.00
AI47	AI	0.26127	0.05827	0.62615	0.00000	Uiso	1.00
AI48	AI	0.25841	0.55813	0.12481	0.00000	Uiso	1.00
AI49	AI	0.25901	0.55861	0.62456	0.00000	Uiso	1.00
AI50	AI	0.26183	0.88315	0.12666	0.00000	Uiso	1.00
AI51	AI	0.25962	0.88322	0.62709	0.00000	Uiso	1.00
AI52	AI	0.25952	0.38232	0.13199	0.00000	Uiso	1.00
AI53	AI	0.25925	0.38332	0.63006	0.00000	Uiso	1.00
AI54	AI	0.21396	0.80723	0.00144	0.00000	Uiso	1.00
AI55	AI	0.21308	0.80675	0.50080	0.00000	Uiso	1.00
AI56	AI	0.21299	0.30593	0.00341	0.00000	Uiso	1.00
AI57	AI	0.21299	0.30600	0.50084	0.00000	Uiso	1.00
AI58	AI	0.21369	0.13512	0.00596	0.00000	Uiso	1.00
AI59	AI	0.21368	0.13572	0.50169	0.00000	Uiso	1.00
AI60	AI	0.21270	0.63517	0.99915	0.00000	Uiso	1.00
AI61	AI	0.21272	0.63523	0.49872	0.00000	Uiso	1.00
AI62	AI	0.40247	0.14893	0.78432	0.00000	Uiso	1.00
AI63	AI	0.35146	0.22621	0.39783	0.00000	Uiso	1.00
AI64	AI	0.39867	0.64549	0.01221	0.00000	Uiso	1.00
AI65	AI	0.40216	0.76638	0.50612	0.00000	Uiso	1.00
O66	O	0.30820	0.87817	0.38335	0.00000	Uiso	1.00
O67	O	0.30372	0.88782	0.88192	0.00000	Uiso	1.00
O68	O	0.30662	0.38890	0.38465	0.00000	Uiso	1.00
O69	O	0.30686	0.39398	0.88103	0.00000	Uiso	1.00
O70	O	0.30868	0.04425	0.36912	0.00000	Uiso	1.00
O71	O	0.30930	0.05825	0.87203	0.00000	Uiso	1.00
O72	O	0.30403	0.55067	0.37087	0.00000	Uiso	1.00
O73	O	0.30374	0.56312	0.87970	0.00000	Uiso	1.00
O74	O	0.30767	0.22401	0.38678	0.00000	Uiso	1.00
O75	O	0.30461	0.22016	0.88832	0.00000	Uiso	1.00
O76	O	0.30187	0.71578	0.37075	0.00000	Uiso	1.00
O77	O	0.30046	0.72188	0.87072	0.00000	Uiso	1.00
O78	O	0.35187	0.13470	0.31167	0.00000	Uiso	1.00
O79	O	0.35605	0.15271	0.78245	0.00000	Uiso	1.00
O80	O	0.36089	0.62507	0.38877	0.00000	Uiso	1.00
O81	O	0.34631	0.63135	0.73471	0.00000	Uiso	1.00
O82	O	0.34870	0.79974	0.26501	0.00000	Uiso	1.00
O83	O	0.34545	0.80562	0.77462	0.00000	Uiso	1.00
O84	O	0.35606	0.31136	0.02176	0.00000	Uiso	1.00
O85	O	0.41561	0.39468	0.64054	0.00000	Uiso	1.00
O86	O	0.35358	0.96393	0.75707	0.00000	Uiso	1.00
O87	O	0.35519	0.49313	0.23777	0.00000	Uiso	1.00
O88	O	0.35462	0.48736	0.78434	0.00000	Uiso	1.00
O89	O	0.30464	0.88703	0.14405	0.00000	Uiso	1.00
O90	O	0.30160	0.88669	0.64312	0.00000	Uiso	1.00
O91	O	0.30248	0.38982	0.14986	0.00000	Uiso	1.00
O92	O	0.30227	0.38118	0.63791	0.00000	Uiso	1.00
O93	O	0.30548	0.05549	0.13906	0.00000	Uiso	1.00
O94	O	0.30484	0.05574	0.63912	0.00000	Uiso	1.00
O95	O	0.30093	0.56005	0.14281	0.00000	Uiso	1.00
O96	O	0.30062	0.55890	0.63995	0.00000	Uiso	1.00
O97	O	0.30669	0.22108	0.14987	0.00000	Uiso	1.00
O98	O	0.31023	0.21842	0.64623	0.00000	Uiso	1.00
O99	O	0.30937	0.71722	0.13753	0.00000	Uiso	1.00
O100	O	0.30656	0.72386	0.63819	0.00000	Uiso	1.00
O101	O	0.35936	0.14351	0.00350	0.00000	Uiso	1.00
O102	O	0.35762	0.65026	0.99194	0.00000	Uiso	1.00
O103	O	0.36177	0.81390	0.01978	0.00000	Uiso	1.00
O104	O	0.35979	0.77919	0.52257	0.00000	Uiso	1.00
O105	O	0.34516	0.30444	0.78689	0.00000	Uiso	1.00
O106	O	0.35352	0.30285	0.51967	0.00000	Uiso	1.00
O107	O	0.35068	0.96862	0.99178	0.00000	Uiso	1.00
O108	O	0.35001	0.95782	0.49383	0.00000	Uiso	1.00
O109	O	0.34979	0.47962	0.00402	0.00000	Uiso	1.00
O110	O	0.34930	0.47987	0.52203	0.00000	Uiso	1.00
O111	O	0.20714	0.89410	0.88748	0.00000	Uiso	1.00
O112	O	0.20694	0.89349	0.38613	0.00000	Uiso	1.00
O113	O	0.20580	0.39218	0.88554	0.00000	Uiso	1.00
O114	O	0.20555	0.39232	0.38447	0.00000	Uiso	1.00
O115	O	0.20727	0.05009	0.88889	0.00000	Uiso	1.00
O116	O	0.20705	0.04986	0.38642	0.00000	Uiso	1.00
O117	O	0.20574	0.54782	0.88445	0.00000	Uiso	1.00
O118	O	0.20531	0.54773	0.38375	0.00000	Uiso	1.00
O119	O	0.21095	0.22046	0.88651	0.00000	Uiso	1.00
O120	O	0.21090	0.22066	0.38494	0.00000	Uiso	1.00
O121	O	0.21040	0.72146	0.88361	0.00000	Uiso	1.00
O122	O	0.21029	0.72184	0.38227	0.00000	Uiso	1.00
O123	O	0.26215	0.13521	0.25359	0.00000	Uiso	1.00
O124	O	0.26141	0.13781	0.74601	0.00000	Uiso	1.00
O125	O	0.25707	0.63595	0.24359	0.00000	Uiso	1.00
O126	O	0.25710	0.63729	0.74183	0.00000	Uiso	1.00
O127	O	0.26170	0.80403	0.24292	0.00000	Uiso	1.00
O128	O	0.25846	0.80743	0.74601	0.00000	Uiso	1.00
O129	O	0.26074	0.30527	0.25416	0.00000	Uiso	1.00
O130	O	0.25984	0.30508	0.75079	0.00000	Uiso	1.00
O131	O	0.25642	0.96842	0.25014	0.00000	Uiso	1.00
O132	O	0.25571	0.97390	0.75027	0.00000	Uiso	1.00
O133	O	0.25338	0.47022	0.24795	0.00000	Uiso	1.00
O134	O	0.25437	0.47040	0.74746	0.00000	Uiso	1.00
O135	O	0.21592	0.89300	0.12150	0.00000	Uiso	1.00

O136	O	0.21497	0.89461	0.62121	0.00000	Uiso	1.00
O137	O	0.21420	0.39217	0.12082	0.00000	Uiso	1.00
O138	O	0.21407	0.39200	0.62043	0.00000	Uiso	1.00
O139	O	0.21590	0.04853	0.12485	0.00000	Uiso	1.00
O140	O	0.21583	0.04998	0.62089	0.00000	Uiso	1.00
O141	O	0.21366	0.54798	0.11865	0.00000	Uiso	1.00
O142	O	0.21380	0.54805	0.61841	0.00000	Uiso	1.00
O143	O	0.20848	0.21991	0.12777	0.00000	Uiso	1.00
O144	O	0.20818	0.22101	0.62578	0.00000	Uiso	1.00
O145	O	0.20815	0.72182	0.12286	0.00000	Uiso	1.00
O146	O	0.20752	0.72170	0.62177	0.00000	Uiso	1.00
O147	O	0.25600	0.13646	0.01719	0.00000	Uiso	1.00
O148	O	0.25648	0.13831	0.51274	0.00000	Uiso	1.00
O149	O	0.25471	0.63737	0.01157	0.00000	Uiso	1.00
O150	O	0.25487	0.63733	0.50809	0.00000	Uiso	1.00
O151	O	0.25632	0.80362	0.01316	0.00000	Uiso	1.00
O152	O	0.25525	0.80440	0.51081	0.00000	Uiso	1.00
O153	O	0.25541	0.30358	0.01769	0.00000	Uiso	1.00
O154	O	0.25553	0.30338	0.51503	0.00000	Uiso	1.00
O155	O	0.25884	0.97248	0.01255	0.00000	Uiso	1.00
O156	O	0.25840	0.97017	0.50951	0.00000	Uiso	1.00
O157	O	0.25710	0.47055	0.01117	0.00000	Uiso	1.00
O158	O	0.25616	0.46930	0.51001	0.00000	Uiso	1.00
O159	O	0.35318	0.29961	0.26949	0.00000	Uiso	1.00
O160	O	0.39627	0.71160	0.65503	0.00000	Uiso	1.00
O161	O	0.41567	0.18064	0.92833	0.00000	Uiso	1.00
O162	O	0.39840	0.88200	0.86854	0.00000	Uiso	1.00
O163	O	0.39699	0.39498	0.16672	0.00000	Uiso	1.00
O164	O	0.39491	0.37891	0.87008	0.00000	Uiso	1.00
O165	O	0.39811	0.25215	0.71380	0.00000	Uiso	1.00
O166	O	0.41002	0.55651	0.64165	0.00000	Uiso	1.00
O167	O	0.46436	0.48822	0.69383	0.00000	Uiso	1.00
O168	O	0.40821	0.54618	0.29450	0.00000	Uiso	1.00
O169	O	0.40643	0.54442	0.06724	0.00000	Uiso	1.00
O170	O	0.39876	0.23165	0.14426	0.00000	Uiso	1.00
O171	O	0.39554	0.04281	0.84465	0.00000	Uiso	1.00
O172	O	0.40561	0.07058	0.10616	0.00000	Uiso	1.00
O173	O	0.41511	0.69761	0.39662	0.00000	Uiso	1.00
O174	O	0.45056	0.32222	0.79882	0.00000	Uiso	1.00
O175	O	0.45363	0.66701	0.68972	0.00000	Uiso	1.00
O176	O	0.41246	0.62653	0.86044	0.00000	Uiso	1.00
O177	O	0.44332	0.48279	0.47014	0.00000	Uiso	1.00
O178	O	0.37005	0.16636	0.53177	0.00000	Uiso	1.00
O179	O	0.42063	0.11264	0.65213	0.00000	Uiso	1.00
O180	O	0.40888	0.93985	0.64988	0.00000	Uiso	1.00
O181	O	0.39775	0.87075	0.43236	0.00000	Uiso	1.00
O182	O	0.42659	0.17172	0.42106	0.00000	Uiso	1.00
O183	O	0.39789	0.03810	0.45713	0.00000	Uiso	1.00
O184	O	0.45027	0.94626	0.49009	0.00000	Uiso	1.00
O185	O	0.40926	0.90416	0.09851	0.00000	Uiso	1.00
O186	O	0.41775	0.75132	0.00970	0.00000	Uiso	1.00
O187	O	0.42992	0.98810	0.27056	0.00000	Uiso	1.00
O188	O	0.38605	0.67739	0.18190	0.00000	Uiso	1.00
O189	O	0.36460	0.98070	0.23557	0.00000	Uiso	1.00
O190	O	0.44319	0.79328	0.55943	0.00000	Uiso	1.00
Si191	Si	0.39204	0.95722	0.77573	0.00000	Uiso	1.00
Si192	Si	0.41340	0.33859	0.76236	0.00000	Uiso	1.00
Si193	Si	0.43237	0.47934	0.61008	0.00000	Uiso	1.00
Si194	Si	0.39217	0.49334	0.17784	0.00000	Uiso	1.00
Si195	Si	0.39637	0.15689	0.04905	0.00000	Uiso	1.00
Si196	Si	0.39331	0.64040	0.31744	0.00000	Uiso	1.00
Si197	Si	0.37601	0.31144	0.15008	0.00000	Uiso	1.00
Si198	Si	0.41641	0.63907	0.71852	0.00000	Uiso	1.00
Si199	Si	0.41154	0.94867	0.50310	0.00000	Uiso	1.00
Si200	Si	0.40525	0.12655	0.52321	0.00000	Uiso	1.00
Si201	Si	0.40077	0.98490	0.17301	0.00000	Uiso	1.00
Si202	Si	0.39941	0.83477	0.00202	0.00000	Uiso	1.00
H203	H	0.46820	0.44066	0.74254	0.00000	Uiso	1.00
H204	H	0.45220	0.29182	0.87317	0.00000	Uiso	1.00
H205	H	0.46757	0.62153	0.68011	0.00000	Uiso	1.00
H206	H	0.42942	0.50664	0.40874	0.00000	Uiso	1.00
H207	H	0.43680	0.22100	0.44440	0.00000	Uiso	1.00
H208	H	0.45520	0.94711	0.40419	0.00000	Uiso	1.00
H209	H	0.43379	0.04324	0.29449	0.00000	Uiso	1.00
H210	H	0.45387	0.84479	0.54635	0.00000	Uiso	1.00
H211	H	0.45359	0.75256	0.61161	0.00000	Uiso	1.00
H212	H	0.49539	0.75710	0.04736	0.00000	Uiso	1.00
H213	H	0.45514	0.62525	0.91533	0.00000	Uiso	1.00
H214	H	0.48492	0.55409	0.91981	0.00000	Uiso	1.00
H215	H	0.47034	0.59817	0.24588	0.00000	Uiso	1.00
H216	H	0.48499	0.72810	0.20155	0.00000	Uiso	1.00
H217	H	0.45631	0.73810	0.08344	0.00000	Uiso	1.00
H218	H	0.45359	0.54372	0.12450	0.00000	Uiso	1.00
H219	H	0.49326	0.65884	0.88523	0.00000	Uiso	1.00
H220	H	0.52434	0.50655	0.99286	0.00000	Uiso	1.00
H221	H	0.47725	0.42048	0.05020	0.00000	Uiso	1.00
H222	H	0.46635	0.41175	0.20397	0.00000	Uiso	1.00
H223	H	0.50324	0.37531	0.15525	0.00000	Uiso	1.00
H224	H	0.54727	0.47165	0.11388	0.00000	Uiso	1.00
H225	H	0.53980	0.57562	0.09926	0.00000	Uiso	1.00
H226	H	0.52926	0.45964	0.31636	0.00000	Uiso	1.00
H227	H	0.49239	0.49791	0.36365	0.00000	Uiso	1.00
H228	H	0.52301	0.56469	0.32159	0.00000	Uiso	1.00
C229	C	0.48046	0.61664	0.94195	0.00000	Uiso	1.00
C230	C	0.48094	0.63548	0.06904	0.00000	Uiso	1.00
C231	C	0.48116	0.71859	0.10532	0.00000	Uiso	1.00
C232	C	0.47530	0.57278	0.15713	0.00000	Uiso	1.00
C233	C	0.50104	0.50414	0.16990	0.00000	Uiso	1.00
C234	C	0.48599	0.42318	0.14309	0.00000	Uiso	1.00
C235	C	0.52953	0.51582	0.08844	0.00000	Uiso	1.00
C236	C	0.51193	0.50699	0.30137	0.00000	Uiso	1.00

File n°14.

AI2	AI	0.35095	0.05625	0.89194	0.00000	Uiso	1.00
AI3	AI	0.35065	0.03573	0.37578	0.00000	Uiso	1.00
AI4	AI	0.34899	0.57666	0.89097	0.00000	Uiso	1.00
AI5	AI	0.34315	0.53139	0.38215	0.00000	Uiso	1.00
AI6	AI	0.34457	0.87518	0.89523	0.00000	Uiso	1.00
AI7	AI	0.34933	0.85223	0.40954	0.00000	Uiso	1.00
AI8	AI	0.35527	0.39912	0.88560	0.00000	Uiso	1.00
AI9	AI	0.32875	0.38514	0.51812	0.00000	Uiso	1.00
AI10	AI	0.30426	0.80287	0.26330	0.00000	Uiso	1.00
AI11	AI	0.30063	0.80726	0.76557	0.00000	Uiso	1.00
AI12	AI	0.30462	0.30637	0.25882	0.00000	Uiso	1.00
AI13	AI	0.30182	0.31595	0.77543	0.00000	Uiso	1.00
AI14	AI	0.30643	0.13377	0.26004	0.00000	Uiso	1.00
AI15	AI	0.30314	0.13597	0.75641	0.00000	Uiso	1.00
AI16	AI	0.29776	0.63497	0.26944	0.00000	Uiso	1.00
AI17	AI	0.29900	0.64023	0.76314	0.00000	Uiso	1.00
AI18	AI	0.21191	0.97110	0.25381	0.00000	Uiso	1.00
AI19	AI	0.21176	0.97245	0.75450	0.00000	Uiso	1.00
AI20	AI	0.20935	0.47056	0.25063	0.00000	Uiso	1.00
AI21	AI	0.21015	0.47068	0.75172	0.00000	Uiso	1.00
AI22	AI	0.32927	0.96962	0.12789	0.00000	Uiso	1.00
AI23	AI	0.32671	0.96628	0.62493	0.00000	Uiso	1.00
AI24	AI	0.32385	0.47562	0.12615	0.00000	Uiso	1.00
AI25	AI	0.33940	0.53145	0.66229	0.00000	Uiso	1.00
AI26	AI	0.28080	0.22001	0.02295	0.00000	Uiso	1.00
AI27	AI	0.28199	0.22108	0.51564	0.00000	Uiso	1.00
AI28	AI	0.28097	0.71872	0.00838	0.00000	Uiso	1.00
AI29	AI	0.28083	0.72114	0.50740	0.00000	Uiso	1.00
AI30	AI	0.34598	0.23073	0.91316	0.00000	Uiso	1.00
AI31	AI	0.35608	0.23881	0.65352	0.00000	Uiso	1.00
AI32	AI	0.35146	0.73459	0.12630	0.00000	Uiso	1.00
AI33	AI	0.35055	0.73165	0.66252	0.00000	Uiso	1.00
AI34	AI	0.21198	0.97156	0.00634	0.00000	Uiso	1.00
AI35	AI	0.21143	0.97204	0.50418	0.00000	Uiso	1.00
AI36	AI	0.21023	0.46983	0.00295	0.00000	Uiso	1.00
AI37	AI	0.20960	0.47001	0.50306	0.00000	Uiso	1.00
AI38	AI	0.28274	0.96214	0.37849	0.00000	Uiso	1.00
AI39	AI	0.28189	0.97627	0.87919	0.00000	Uiso	1.00
AI40	AI	0.27816	0.46656	0.37683	0.00000	Uiso	1.00
AI41	AI	0.28161	0.47735	0.87798	0.00000	Uiso	1.00
AI42	AI	0.23655	0.21902	0.25537	0.00000	Uiso	1.00
AI43	AI	0.23539	0.22002	0.75396	0.00000	Uiso	1.00
AI44	AI	0.23490	0.72406	0.25056	0.00000	Uiso	1.00
AI45	AI	0.23417	0.72320	0.74999	0.00000	Uiso	1.00
AI46	AI	0.26186	0.05810	0.13329	0.00000	Uiso	1.00
AI47	AI	0.26127	0.05827	0.62615	0.00000	Uiso	1.00
AI48	AI	0.25841	0.55813	0.12481	0.00000	Uiso	1.00
AI49	AI	0.25901	0.55861	0.62456	0.00000	Uiso	1.00
AI50	AI	0.26183	0.88315	0.12666	0.00000	Uiso	1.00
AI51	AI	0.25962	0.88322	0.62709	0.00000	Uiso	1.00
AI52	AI	0.25952	0.38232	0.13199	0.00000	Uiso	1.00
AI53	AI	0.25925	0.38332	0.63006	0.00000	Uiso	1.00
AI54	AI	0.21396	0.80723	0.00144	0.00000	Uiso	1.00
AI55	AI	0.21308	0.80675	0.50080	0.00000	Uiso	1.00
AI56	AI	0.21299	0.30593	0.00341	0.00000	Uiso	1.00
AI57	AI	0.21299	0.30600	0.50084	0.00000	Uiso	1.00
AI58	AI	0.21369	0.13512	0.00596	0.00000	Uiso	1.00
AI59	AI	0.21368	0.13572	0.50169	0.00000	Uiso	1.00
AI60	AI	0.21270	0.63517	0.99915	0.00000	Uiso	1.00
AI61	AI	0.21272	0.63523	0.49872	0.00000	Uiso	1.00
AI62	AI	0.40271	0.14853	0.78208	0.00000	Uiso	1.00
AI63	AI	0.35141	0.22520	0.39640	0.00000	Uiso	1.00
AI64	AI	0.39903	0.65408	0.00629	0.00000	Uiso	1.00
AI65	AI	0.40093	0.76264	0.50291	0.00000	Uiso	1.00
O66	O	0.30797	0.87818	0.38238	0.00000	Uiso	1.00
O67	O	0.30398	0.88828	0.88142	0.00000	Uiso	1.00
O68	O	0.30624	0.38782	0.38459	0.00000	Uiso	1.00
O69	O	0.30841	0.39700	0.88527	0.00000	Uiso	1.00
O70	O	0.30873	0.04393	0.36833	0.00000	Uiso	1.00
O71	O	0.30910	0.05884	0.87085	0.00000	Uiso	1.00
O72	O	0.30301	0.55005	0.37334	0.00000	Uiso	1.00
O73	O	0.30603	0.56290	0.88443	0.00000	Uiso	1.00
O74	O	0.30762	0.22322	0.38595	0.00000	Uiso	1.00
O75	O	0.30446	0.22153	0.88719	0.00000	Uiso	1.00
O76	O	0.30129	0.71663	0.37126	0.00000	Uiso	1.00
O77	O	0.30038	0.72174	0.87142	0.00000	Uiso	1.00
O78	O	0.35189	0.13379	0.31009	0.00000	Uiso	1.00
O79	O	0.35564	0.15308	0.78062	0.00000	Uiso	1.00
O80	O	0.35639	0.62761	0.36037	0.00000	Uiso	1.00
O81	O	0.34541	0.63081	0.73466	0.00000	Uiso	1.00
O82	O	0.34853	0.79976	0.26387	0.00000	Uiso	1.00
O83	O	0.34510	0.80536	0.77353	0.00000	Uiso	1.00
O84	O	0.35560	0.31133	0.01737	0.00000	Uiso	1.00
O85	O	0.41396	0.39390	0.63695	0.00000	Uiso	1.00
O86	O	0.35335	0.96551	0.75324	0.00000	Uiso	1.00
O87	O	0.35246	0.48260	0.24275	0.00000	Uiso	1.00
O88	O	0.35517	0.48753	0.79128	0.00000	Uiso	1.00
O89	O	0.30457	0.88708	0.14340	0.00000	Uiso	1.00
O90	O	0.30154	0.88634	0.64264	0.00000	Uiso	1.00
O91	O	0.30229	0.38865	0.14651	0.00000	Uiso	1.00
O92	O	0.30254	0.38203	0.63937	0.00000	Uiso	1.00
O93	O	0.30542	0.05537	0.13840	0.00000	Uiso	1.00
O94	O	0.30471	0.05571	0.63766	0.00000	Uiso	1.00
O95	O	0.30088	0.55983	0.14270	0.00000	Uiso	1.00
O96	O	0.30037	0.55714	0.64413	0.00000	Uiso	1.00
O97	O	0.30662	0.22062	0.14898	0.00000	Uiso	1.00
O98	O	0.31033	0.21840	0.64464	0.00000	Uiso	1.00

O99	O	0.30915	0.71772	0.13809	0.00000	Uiso	1.00
O100	O	0.30624	0.72299	0.63858	0.00000	Uiso	1.00
O101	O	0.35912	0.14276	0.00139	0.00000	Uiso	1.00
O102	O	0.35716	0.65145	0.00121	0.00000	Uiso	1.00
O103	O	0.36185	0.81489	0.01887	0.00000	Uiso	1.00
O104	O	0.35865	0.77816	0.51940	0.00000	Uiso	1.00
O105	O	0.34534	0.30522	0.78541	0.00000	Uiso	1.00
O106	O	0.35343	0.30249	0.51786	0.00000	Uiso	1.00
O107	O	0.35053	0.96923	0.98991	0.00000	Uiso	1.00
O108	O	0.34985	0.95704	0.49153	0.00000	Uiso	1.00
O109	O	0.35737	0.48433	0.02535	0.00000	Uiso	1.00
O110	O	0.34887	0.48099	0.52227	0.00000	Uiso	1.00
O111	O	0.20714	0.89410	0.88748	0.00000	Uiso	1.00
O112	O	0.20694	0.89349	0.38613	0.00000	Uiso	1.00
O113	O	0.20580	0.39218	0.88554	0.00000	Uiso	1.00
O114	O	0.20555	0.39232	0.38447	0.00000	Uiso	1.00
O115	O	0.20727	0.05009	0.88889	0.00000	Uiso	1.00
O116	O	0.20705	0.04986	0.38642	0.00000	Uiso	1.00
O117	O	0.20574	0.54782	0.88445	0.00000	Uiso	1.00
O118	O	0.20531	0.54773	0.38375	0.00000	Uiso	1.00
O119	O	0.21095	0.22046	0.88651	0.00000	Uiso	1.00
O120	O	0.21090	0.22066	0.38494	0.00000	Uiso	1.00
O121	O	0.21040	0.72146	0.88361	0.00000	Uiso	1.00
O122	O	0.21029	0.72184	0.38227	0.00000	Uiso	1.00
O123	O	0.26215	0.13521	0.25359	0.00000	Uiso	1.00
O124	O	0.26141	0.13781	0.74601	0.00000	Uiso	1.00
O125	O	0.25707	0.63595	0.24359	0.00000	Uiso	1.00
O126	O	0.25710	0.63729	0.74183	0.00000	Uiso	1.00
O127	O	0.26170	0.80403	0.24292	0.00000	Uiso	1.00
O128	O	0.25846	0.80743	0.74601	0.00000	Uiso	1.00
O129	O	0.26074	0.30527	0.25416	0.00000	Uiso	1.00
O130	O	0.25984	0.30508	0.75079	0.00000	Uiso	1.00
O131	O	0.25642	0.96842	0.25014	0.00000	Uiso	1.00
O132	O	0.25571	0.97390	0.75027	0.00000	Uiso	1.00
O133	O	0.25338	0.47022	0.24795	0.00000	Uiso	1.00
O134	O	0.25437	0.47040	0.74746	0.00000	Uiso	1.00
O135	O	0.21592	0.89300	0.12150	0.00000	Uiso	1.00
O136	O	0.21497	0.89461	0.62121	0.00000	Uiso	1.00
O137	O	0.21420	0.39217	0.12082	0.00000	Uiso	1.00
O138	O	0.21407	0.39200	0.62043	0.00000	Uiso	1.00
O139	O	0.21590	0.04853	0.12485	0.00000	Uiso	1.00
O140	O	0.21583	0.04998	0.62089	0.00000	Uiso	1.00
O141	O	0.21366	0.54798	0.11865	0.00000	Uiso	1.00
O142	O	0.21380	0.54805	0.61841	0.00000	Uiso	1.00
O143	O	0.20848	0.21991	0.12777	0.00000	Uiso	1.00
O144	O	0.20818	0.22101	0.62578	0.00000	Uiso	1.00
O145	O	0.20815	0.72182	0.12286	0.00000	Uiso	1.00
O146	O	0.20752	0.72170	0.62177	0.00000	Uiso	1.00
O147	O	0.25600	0.13646	0.01719	0.00000	Uiso	1.00
O148	O	0.25648	0.13831	0.51274	0.00000	Uiso	1.00
O149	O	0.25471	0.63737	0.01157	0.00000	Uiso	1.00
O150	O	0.25487	0.63733	0.50809	0.00000	Uiso	1.00
O151	O	0.25632	0.80362	0.01316	0.00000	Uiso	1.00
O152	O	0.25525	0.80440	0.51081	0.00000	Uiso	1.00
O153	O	0.25541	0.30358	0.01769	0.00000	Uiso	1.00
O154	O	0.25553	0.30338	0.51503	0.00000	Uiso	1.00
O155	O	0.25884	0.97248	0.01255	0.00000	Uiso	1.00
O156	O	0.25840	0.97017	0.50951	0.00000	Uiso	1.00
O157	O	0.25710	0.47055	0.01117	0.00000	Uiso	1.00
O158	O	0.25616	0.46930	0.51001	0.00000	Uiso	1.00
O159	O	0.35254	0.29799	0.26721	0.00000	Uiso	1.00
O160	O	0.39427	0.70991	0.65187	0.00000	Uiso	1.00
O161	O	0.41542	0.18027	0.92659	0.00000	Uiso	1.00
O162	O	0.39660	0.88333	0.86483	0.00000	Uiso	1.00
O163	O	0.39560	0.39273	0.15853	0.00000	Uiso	1.00
O164	O	0.39633	0.37785	0.86947	0.00000	Uiso	1.00
O165	O	0.39794	0.25142	0.71249	0.00000	Uiso	1.00
O166	O	0.40671	0.55469	0.63246	0.00000	Uiso	1.00
O167	O	0.46254	0.49226	0.66659	0.00000	Uiso	1.00
O168	O	0.40258	0.54454	0.27621	0.00000	Uiso	1.00
O169	O	0.41240	0.54482	0.06055	0.00000	Uiso	1.00
O170	O	0.39790	0.23001	0.14236	0.00000	Uiso	1.00
O171	O	0.39541	0.04318	0.84121	0.00000	Uiso	1.00
O172	O	0.40566	0.06921	0.10315	0.00000	Uiso	1.00
O173	O	0.41213	0.68954	0.39785	0.00000	Uiso	1.00
O174	O	0.45123	0.32184	0.78803	0.00000	Uiso	1.00
O175	O	0.44977	0.66124	0.70631	0.00000	Uiso	1.00
O176	O	0.40113	0.61744	0.85289	0.00000	Uiso	1.00
O177	O	0.43607	0.47676	0.45173	0.00000	Uiso	1.00
O178	O	0.37031	0.16572	0.52944	0.00000	Uiso	1.00
O179	O	0.42076	0.11228	0.64981	0.00000	Uiso	1.00
O180	O	0.40912	0.93876	0.64705	0.00000	Uiso	1.00
O181	O	0.39766	0.86797	0.43122	0.00000	Uiso	1.00
O182	O	0.42666	0.16887	0.41720	0.00000	Uiso	1.00
O183	O	0.39824	0.03570	0.45588	0.00000	Uiso	1.00
O184	O	0.45078	0.94156	0.48805	0.00000	Uiso	1.00
O185	O	0.40957	0.90319	0.09422	0.00000	Uiso	1.00
O186	O	0.42964	0.98601	0.26870	0.00000	Uiso	1.00
O187	O	0.38862	0.68428	0.17297	0.00000	Uiso	1.00
O188	O	0.36467	0.97974	0.23300	0.00000	Uiso	1.00
O189	O	0.44229	0.78579	0.55841	0.00000	Uiso	1.00
O190	O	0.41755	0.75151	0.98913	0.00000	Uiso	1.00
Si191	Si	0.39178	0.95809	0.77095	0.00000	Uiso	1.00
Si192	Si	0.41385	0.33772	0.75821	0.00000	Uiso	1.00
Si193	Si	0.42905	0.47849	0.59449	0.00000	Uiso	1.00
Si194	Si	0.38650	0.48929	0.15566	0.00000	Uiso	1.00
Si195	Si	0.39616	0.15552	0.04687	0.00000	Uiso	1.00
Si196	Si	0.39130	0.63957	0.30501	0.00000	Uiso	1.00
Si197	Si	0.37513	0.30939	0.14745	0.00000	Uiso	1.00
Si198	Si	0.41228	0.63449	0.71688	0.00000	Uiso	1.00
Si199	Si	0.41221	0.94581	0.50000	0.00000	Uiso	1.00

Si200	Si	0.40539	0.12473	0.52048	0.00000	Uiso	1.00
Si201	Si	0.40087	0.98337	0.16979	0.00000	Uiso	1.00
Si202	Si	0.39959	0.83472	0.99623	0.00000	Uiso	1.00
H203	H	0.46922	0.44674	0.71462	0.00000	Uiso	1.00
H204	H	0.45437	0.29192	0.86198	0.00000	Uiso	1.00
H205	H	0.46358	0.61492	0.69903	0.00000	Uiso	1.00
H206	H	0.42245	0.50191	0.39079	0.00000	Uiso	1.00
H207	H	0.43741	0.21770	0.43902	0.00000	Uiso	1.00
H208	H	0.45650	0.94141	0.40301	0.00000	Uiso	1.00
H209	H	0.43375	0.04086	0.29348	0.00000	Uiso	1.00
H210	H	0.45368	0.83626	0.54658	0.00000	Uiso	1.00
H211	H	0.45140	0.74724	0.61711	0.00000	Uiso	1.00
H212	H	0.49980	0.75060	0.04062	0.00000	Uiso	1.00
H213	H	0.45821	0.61319	0.91840	0.00000	Uiso	1.00
H214	H	0.44925	0.51143	0.88519	0.00000	Uiso	1.00
H215	H	0.48590	0.53784	0.95074	0.00000	Uiso	1.00
H216	H	0.45168	0.66417	0.13291	0.00000	Uiso	1.00
H217	H	0.48554	0.60567	0.14912	0.00000	Uiso	1.00
H218	H	0.45452	0.59308	0.25290	0.00000	Uiso	1.00
H219	H	0.44929	0.44586	0.21290	0.00000	Uiso	1.00
H220	H	0.48272	0.45441	0.12056	0.00000	Uiso	1.00
H221	H	0.44818	0.40999	0.06102	0.00000	Uiso	1.00
H222	H	0.47668	0.93550	0.14737	0.00000	Uiso	1.00
H223	H	0.51398	0.95536	0.08677	0.00000	Uiso	1.00
H224	H	0.50732	0.86442	0.16679	0.00000	Uiso	1.00
H225	H	0.45435	0.95762	0.93260	0.00000	Uiso	1.00
H226	H	0.46531	0.88934	0.81616	0.00000	Uiso	1.00
H227	H	0.49120	0.96624	0.86431	0.00000	Uiso	1.00
H228	H	0.48197	0.76073	0.88852	0.00000	Uiso	1.00
C229	C	0.44792	0.53898	0.07496	0.00000	Uiso	1.00
C230	C	0.46086	0.55126	0.94894	0.00000	Uiso	1.00
C231	C	0.46006	0.60440	0.15842	0.00000	Uiso	1.00
C232	C	0.45716	0.45678	0.12057	0.00000	Uiso	1.00
C233	C	0.49006	0.78918	0.97102	0.00000	Uiso	1.00
C234	C	0.48727	0.86788	0.98852	0.00000	Uiso	1.00
C235	C	0.49697	0.90742	0.10384	0.00000	Uiso	1.00
C236	C	0.47373	0.92252	0.89486	0.00000	Uiso	1.00

File n°15:

Al2	Al	0.35125	0.05679	0.89452	0.00000	Uiso	1.00
Al3	Al	0.35008	0.03694	0.38063	0.00000	Uiso	1.00
Al4	Al	0.34413	0.56591	0.89966	0.00000	Uiso	1.00
Al5	Al	0.34386	0.53271	0.38260	0.00000	Uiso	1.00
Al6	Al	0.34447	0.87433	0.89712	0.00000	Uiso	1.00
Al7	Al	0.35000	0.85122	0.41037	0.00000	Uiso	1.00
Al8	Al	0.35336	0.40130	0.88417	0.00000	Uiso	1.00
Al9	Al	0.32883	0.38648	0.51923	0.00000	Uiso	1.00
Al10	Al	0.30476	0.80229	0.26183	0.00000	Uiso	1.00
Al11	Al	0.30076	0.80726	0.76482	0.00000	Uiso	1.00
Al12	Al	0.30453	0.30668	0.26029	0.00000	Uiso	1.00
Al13	Al	0.30163	0.31414	0.77259	0.00000	Uiso	1.00
Al14	Al	0.30632	0.13413	0.26128	0.00000	Uiso	1.00
Al15	Al	0.30317	0.13599	0.75866	0.00000	Uiso	1.00
Al16	Al	0.29754	0.63492	0.26782	0.00000	Uiso	1.00
Al17	Al	0.29901	0.64121	0.76050	0.00000	Uiso	1.00
Al18	Al	0.21191	0.97110	0.25381	0.00000	Uiso	1.00
Al19	Al	0.21176	0.97245	0.75450	0.00000	Uiso	1.00
Al20	Al	0.20935	0.47056	0.25063	0.00000	Uiso	1.00
Al21	Al	0.21015	0.47068	0.75172	0.00000	Uiso	1.00
Al22	Al	0.32933	0.97014	0.13018	0.00000	Uiso	1.00
Al23	Al	0.32695	0.96649	0.62769	0.00000	Uiso	1.00
Al24	Al	0.32458	0.47531	0.12735	0.00000	Uiso	1.00
Al25	Al	0.33978	0.53519	0.65873	0.00000	Uiso	1.00
Al26	Al	0.28079	0.22011	0.02367	0.00000	Uiso	1.00
Al27	Al	0.28186	0.22138	0.51694	0.00000	Uiso	1.00
Al28	Al	0.28100	0.71860	0.00725	0.00000	Uiso	1.00
Al29	Al	0.28101	0.72098	0.50697	0.00000	Uiso	1.00
Al30	Al	0.34586	0.23225	0.91703	0.00000	Uiso	1.00
Al31	Al	0.35625	0.24023	0.65632	0.00000	Uiso	1.00
Al32	Al	0.35264	0.73144	0.12540	0.00000	Uiso	1.00
Al33	Al	0.35163	0.73136	0.66579	0.00000	Uiso	1.00
Al34	Al	0.21198	0.97156	0.00634	0.00000	Uiso	1.00
Al35	Al	0.21143	0.97204	0.50418	0.00000	Uiso	1.00
Al36	Al	0.21023	0.46983	0.00295	0.00000	Uiso	1.00
Al37	Al	0.20960	0.47001	0.50306	0.00000	Uiso	1.00
Al38	Al	0.28284	0.96122	0.37886	0.00000	Uiso	1.00
Al39	Al	0.28193	0.97594	0.87932	0.00000	Uiso	1.00
Al40	Al	0.27839	0.46739	0.37680	0.00000	Uiso	1.00
Al41	Al	0.28078	0.47449	0.87721	0.00000	Uiso	1.00
Al42	Al	0.23655	0.21902	0.25537	0.00000	Uiso	1.00
Al43	Al	0.23539	0.22002	0.75396	0.00000	Uiso	1.00
Al44	Al	0.23490	0.72406	0.25056	0.00000	Uiso	1.00
Al45	Al	0.23417	0.72320	0.74999	0.00000	Uiso	1.00
Al46	Al	0.26186	0.05810	0.13329	0.00000	Uiso	1.00
Al47	Al	0.26127	0.05827	0.62615	0.00000	Uiso	1.00
Al48	Al	0.25841	0.55813	0.12481	0.00000	Uiso	1.00
Al49	Al	0.25901	0.55861	0.62456	0.00000	Uiso	1.00
Al50	Al	0.26183	0.88315	0.12666	0.00000	Uiso	1.00
Al51	Al	0.25962	0.88322	0.62709	0.00000	Uiso	1.00
Al52	Al	0.25952	0.38232	0.13199	0.00000	Uiso	1.00
Al53	Al	0.25925	0.38332	0.63006	0.00000	Uiso	1.00
Al54	Al	0.21396	0.80723	0.00144	0.00000	Uiso	1.00
Al55	Al	0.21308	0.80675	0.50080	0.00000	Uiso	1.00
Al56	Al	0.21299	0.30593	0.00341	0.00000	Uiso	1.00
Al57	Al	0.21299	0.30600	0.50084	0.00000	Uiso	1.00
Al58	Al	0.21369	0.13512	0.00596	0.00000	Uiso	1.00
Al59	Al	0.21368	0.13572	0.50169	0.00000	Uiso	1.00
Al60	Al	0.21270	0.63517	0.99915	0.00000	Uiso	1.00
Al61	Al	0.21272	0.63523	0.49872	0.00000	Uiso	1.00

Al62	Al	0.40250	0.15132	0.78416	0.00000	Uiso	1.00
Al63	Al	0.35104	0.22612	0.39951	0.00000	Uiso	1.00
Al64	Al	0.39693	0.62818	0.01967	0.00000	Uiso	1.00
Al65	Al	0.40229	0.76557	0.50797	0.00000	Uiso	1.00
O66	O	0.30865	0.87752	0.38122	0.00000	Uiso	1.00
O67	O	0.30403	0.88771	0.88234	0.00000	Uiso	1.00
O68	O	0.30656	0.38909	0.38513	0.00000	Uiso	1.00
O69	O	0.30650	0.39336	0.88070	0.00000	Uiso	1.00
O70	O	0.30835	0.04387	0.36984	0.00000	Uiso	1.00
O71	O	0.30941	0.05794	0.87208	0.00000	Uiso	1.00
O72	O	0.30386	0.55062	0.37161	0.00000	Uiso	1.00
O73	O	0.30289	0.56330	0.87872	0.00000	Uiso	1.00
O74	O	0.30735	0.22375	0.38769	0.00000	Uiso	1.00
O75	O	0.30452	0.21989	0.88858	0.00000	Uiso	1.00
O76	O	0.30182	0.71602	0.37045	0.00000	Uiso	1.00
O77	O	0.30063	0.72210	0.87089	0.00000	Uiso	1.00
O78	O	0.35150	0.13452	0.31376	0.00000	Uiso	1.00
O79	O	0.35598	0.15364	0.78233	0.00000	Uiso	1.00
O80	O	0.35967	0.62672	0.36902	0.00000	Uiso	1.00
O81	O	0.34595	0.63179	0.73638	0.00000	Uiso	1.00
O82	O	0.34950	0.79814	0.26258	0.00000	Uiso	1.00
O83	O	0.34565	0.80629	0.77472	0.00000	Uiso	1.00
O84	O	0.35598	0.31059	0.02383	0.00000	Uiso	1.00
O85	O	0.41676	0.39773	0.64515	0.00000	Uiso	1.00
O86	O	0.35384	0.96507	0.75641	0.00000	Uiso	1.00
O87	O	0.35541	0.48817	0.23975	0.00000	Uiso	1.00
O88	O	0.35414	0.48723	0.78387	0.00000	Uiso	1.00
O89	O	0.30491	0.88672	0.14312	0.00000	Uiso	1.00
O90	O	0.30158	0.88681	0.64349	0.00000	Uiso	1.00
O91	O	0.30235	0.38941	0.15037	0.00000	Uiso	1.00
O92	O	0.30228	0.38165	0.63789	0.00000	Uiso	1.00
O93	O	0.30546	0.05544	0.13939	0.00000	Uiso	1.00
O94	O	0.30487	0.05585	0.63921	0.00000	Uiso	1.00
O95	O	0.30108	0.55974	0.14377	0.00000	Uiso	1.00
O96	O	0.30062	0.55961	0.63907	0.00000	Uiso	1.00
O97	O	0.30654	0.22067	0.15022	0.00000	Uiso	1.00
O98	O	0.31016	0.21881	0.64668	0.00000	Uiso	1.00
O99	O	0.30983	0.71787	0.13647	0.00000	Uiso	1.00
O100	O	0.30661	0.72441	0.63817	0.00000	Uiso	1.00
O101	O	0.35916	0.14325	0.00338	0.00000	Uiso	1.00
O102	O	0.35643	0.64526	0.00029	0.00000	Uiso	1.00
O103	O	0.36505	0.81045	0.01572	0.00000	Uiso	1.00
O104	O	0.35985	0.77793	0.52178	0.00000	Uiso	1.00
O105	O	0.34500	0.30472	0.78774	0.00000	Uiso	1.00
O106	O	0.35334	0.30352	0.52033	0.00000	Uiso	1.00
O107	O	0.35080	0.96761	0.99206	0.00000	Uiso	1.00
O108	O	0.34976	0.95694	0.49401	0.00000	Uiso	1.00
O109	O	0.34845	0.47851	0.00210	0.00000	Uiso	1.00
O110	O	0.34940	0.48178	0.52104	0.00000	Uiso	1.00
O111	O	0.20714	0.89410	0.88748	0.00000	Uiso	1.00
O112	O	0.20694	0.89349	0.38613	0.00000	Uiso	1.00
O113	O	0.20580	0.39218	0.88554	0.00000	Uiso	1.00
O114	O	0.20555	0.39232	0.38447	0.00000	Uiso	1.00
O115	O	0.20727	0.05009	0.88889	0.00000	Uiso	1.00
O116	O	0.20705	0.04986	0.38642	0.00000	Uiso	1.00
O117	O	0.20574	0.54782	0.88445	0.00000	Uiso	1.00
O118	O	0.20531	0.54773	0.38375	0.00000	Uiso	1.00
O119	O	0.21095	0.22046	0.88651	0.00000	Uiso	1.00
O120	O	0.21090	0.22066	0.38494	0.00000	Uiso	1.00
O121	O	0.21040	0.72146	0.88361	0.00000	Uiso	1.00
O122	O	0.21029	0.72184	0.38227	0.00000	Uiso	1.00
O123	O	0.26215	0.13521	0.25359	0.00000	Uiso	1.00
O124	O	0.26141	0.13781	0.74601	0.00000	Uiso	1.00
O125	O	0.25707	0.63595	0.24359	0.00000	Uiso	1.00
O126	O	0.25710	0.63729	0.74183	0.00000	Uiso	1.00
O127	O	0.26170	0.80403	0.24292	0.00000	Uiso	1.00
O128	O	0.25846	0.80743	0.74601	0.00000	Uiso	1.00
O129	O	0.26074	0.30527	0.25416	0.00000	Uiso	1.00
O130	O	0.25984	0.30508	0.75079	0.00000	Uiso	1.00
O131	O	0.25642	0.96842	0.25014	0.00000	Uiso	1.00
O132	O	0.25571	0.97390	0.75027	0.00000	Uiso	1.00
O133	O	0.25338	0.47022	0.24795	0.00000	Uiso	1.00
O134	O	0.25437	0.47040	0.74746	0.00000	Uiso	1.00
O135	O	0.21592	0.89300	0.12150	0.00000	Uiso	1.00
O136	O	0.21497	0.89461	0.62121	0.00000	Uiso	1.00
O137	O	0.21420	0.39217	0.12082	0.00000	Uiso	1.00
O138	O	0.21407	0.39200	0.62043	0.00000	Uiso	1.00
O139	O	0.21590	0.04853	0.12485	0.00000	Uiso	1.00
O140	O	0.21583	0.04998	0.62089	0.00000	Uiso	1.00
O141	O	0.21366	0.54798	0.11865	0.00000	Uiso	1.00
O142	O	0.21380	0.54805	0.61841	0.00000	Uiso	1.00
O143	O	0.20848	0.21991	0.12777	0.00000	Uiso	1.00
O144	O	0.20818	0.22101	0.62578	0.00000	Uiso	1.00
O145	O	0.20815	0.72182	0.12286	0.00000	Uiso	1.00
O146	O	0.20752	0.72170	0.62177	0.00000	Uiso	1.00
O147	O	0.25600	0.13646	0.01719	0.00000	Uiso	1.00
O148	O	0.25648	0.13831	0.51274	0.00000	Uiso	1.00
O149	O	0.25471	0.63737	0.01157	0.00000	Uiso	1.00
O150	O	0.25487	0.63733	0.50809	0.00000	Uiso	1.00
O151	O	0.25632	0.80362	0.01316	0.00000	Uiso	1.00
O152	O	0.25525	0.80440	0.51081	0.00000	Uiso	1.00
O153	O	0.25541	0.30358	0.01769	0.00000	Uiso	1.00
O154	O	0.25553	0.30338	0.51503	0.00000	Uiso	1.00
O155	O	0.25884	0.97248	0.01255	0.00000	Uiso	1.00
O156	O	0.25840	0.97017	0.50951	0.00000	Uiso	1.00
O157	O	0.25710	0.47055	0.01117	0.00000	Uiso	1.00
O158	O	0.25616	0.46930	0.51001	0.00000	Uiso	1.00
O159	O	0.35219	0.29831	0.27093	0.00000	Uiso	1.00
O160	O	0.39609	0.71281	0.65828	0.00000	Uiso	1.00
O161	O	0.41526	0.18274	0.92864	0.00000	Uiso	1.00
O162	O	0.39940	0.88623	0.86705	0.00000	Uiso	1.00

O163	O	0.39756	0.38913	0.17670	0.00000	Uiso	1.00
O164	O	0.39455	0.37896	0.87136	0.00000	Uiso	1.00
O165	O	0.39807	0.25388	0.71337	0.00000	Uiso	1.00
O166	O	0.41026	0.55878	0.65322	0.00000	Uiso	1.00
O167	O	0.46470	0.49371	0.70771	0.00000	Uiso	1.00
O168	O	0.40848	0.54461	0.29817	0.00000	Uiso	1.00
O169	O	0.40558	0.53200	0.07046	0.00000	Uiso	1.00
O170	O	0.39824	0.23026	0.14731	0.00000	Uiso	1.00
O171	O	0.39554	0.04499	0.84435	0.00000	Uiso	1.00
O172	O	0.40547	0.07358	0.10876	0.00000	Uiso	1.00
O173	O	0.41428	0.69685	0.39705	0.00000	Uiso	1.00
O174	O	0.45047	0.32078	0.80215	0.00000	Uiso	1.00
O175	O	0.45306	0.67186	0.70628	0.00000	Uiso	1.00
O176	O	0.40978	0.63291	0.87000	0.00000	Uiso	1.00
O177	O	0.44552	0.48960	0.48230	0.00000	Uiso	1.00
O178	O	0.37030	0.16732	0.53209	0.00000	Uiso	1.00
O179	O	0.42077	0.11391	0.65281	0.00000	Uiso	1.00
O180	O	0.40932	0.94080	0.64896	0.00000	Uiso	1.00
O181	O	0.39800	0.87031	0.43286	0.00000	Uiso	1.00
O182	O	0.42692	0.16953	0.42003	0.00000	Uiso	1.00
O183	O	0.39759	0.03782	0.45967	0.00000	Uiso	1.00
O184	O	0.45080	0.94566	0.49087	0.00000	Uiso	1.00
O185	O	0.40874	0.91193	0.10076	0.00000	Uiso	1.00
O186	O	0.42974	0.99206	0.27545	0.00000	Uiso	1.00
O187	O	0.39009	0.67795	0.17319	0.00000	Uiso	1.00
O188	O	0.36434	0.98240	0.23792	0.00000	Uiso	1.00
O189	O	0.44340	0.79120	0.56047	0.00000	Uiso	1.00
O190	O	0.42455	0.76916	0.01233	0.00000	Uiso	1.00
Si191	Si	0.39234	0.96032	0.77335	0.00000	Uiso	1.00
Si192	Si	0.41377	0.33973	0.76444	0.00000	Uiso	1.00
Si193	Si	0.43368	0.48335	0.62045	0.00000	Uiso	1.00
Si194	Si	0.39305	0.48645	0.18746	0.00000	Uiso	1.00
Si195	Si	0.39612	0.15811	0.04881	0.00000	Uiso	1.00
Si196	Si	0.39418	0.63955	0.31235	0.00000	Uiso	1.00
Si197	Si	0.37541	0.30916	0.15305	0.00000	Uiso	1.00
Si198	Si	0.41596	0.64199	0.72885	0.00000	Uiso	1.00
Si199	Si	0.41212	0.94859	0.50194	0.00000	Uiso	1.00
Si200	Si	0.40534	0.12665	0.52360	0.00000	Uiso	1.00
Si201	Si	0.40055	0.99050	0.17862	0.00000	Uiso	1.00
Si202	Si	0.40098	0.84462	0.00192	0.00000	Uiso	1.00
H203	H	0.46879	0.44819	0.76003	0.00000	Uiso	1.00
H204	H	0.45200	0.28966	0.87580	0.00000	Uiso	1.00
H205	H	0.46785	0.62759	0.70682	0.00000	Uiso	1.00
H206	H	0.43195	0.51075	0.41864	0.00000	Uiso	1.00
H207	H	0.43783	0.21822	0.44145	0.00000	Uiso	1.00
H208	H	0.45659	0.94672	0.40598	0.00000	Uiso	1.00
H209	H	0.43466	0.04688	0.29848	0.00000	Uiso	1.00
H210	H	0.45421	0.84250	0.54799	0.00000	Uiso	1.00
H211	H	0.45319	0.75225	0.61779	0.00000	Uiso	1.00
H212	H	0.47000	0.87063	0.94402	0.00000	Uiso	1.00
H213	H	0.45282	0.64596	0.12359	0.00000	Uiso	1.00
H214	H	0.46134	0.64791	0.96494	0.00000	Uiso	1.00
H215	H	0.49066	0.66950	0.07357	0.00000	Uiso	1.00
H216	H	0.44648	0.77504	0.23750	0.00000	Uiso	1.00
H217	H	0.45884	0.86684	0.17079	0.00000	Uiso	1.00
H218	H	0.48647	0.79013	0.20112	0.00000	Uiso	1.00
H219	H	0.47272	0.77817	0.86328	0.00000	Uiso	1.00
H220	H	0.50148	0.80479	0.97240	0.00000	Uiso	1.00
H221	H	0.48120	0.21835	0.98654	0.00000	Uiso	1.00
H222	H	0.48392	0.15177	0.86135	0.00000	Uiso	1.00
H223	H	0.51765	0.17737	0.94724	0.00000	Uiso	1.00
H224	H	0.46720	0.01763	0.90628	0.00000	Uiso	1.00
H225	H	0.46951	0.97852	0.06331	0.00000	Uiso	1.00
H226	H	0.48147	0.15973	0.20301	0.00000	Uiso	1.00
H227	H	0.51983	0.12715	0.17400	0.00000	Uiso	1.00
H228	H	0.49117	0.05659	0.22114	0.00000	Uiso	1.00
C229	C	0.46246	0.80212	0.17201	0.00000	Uiso	1.00
C230	C	0.45788	0.76514	0.04779	0.00000	Uiso	1.00
C231	C	0.46589	0.67657	0.05186	0.00000	Uiso	1.00
C232	C	0.47657	0.80743	0.95037	0.00000	Uiso	1.00
C233	C	0.47397	0.02678	0.99984	0.00000	Uiso	1.00
C234	C	0.48659	0.09558	0.03649	0.00000	Uiso	1.00
C235	C	0.49257	0.16392	0.95235	0.00000	Uiso	1.00
C236	C	0.49517	0.10986	0.16570	0.00000	Uiso	1.00

File n°16:

Al2	Al	0.35085	0.05566	0.89374	0.00000	Uiso	1.00
Al3	Al	0.35015	0.03670	0.37607	0.00000	Uiso	1.00
Al4	Al	0.34663	0.56923	0.89875	0.00000	Uiso	1.00
Al5	Al	0.34413	0.53279	0.38443	0.00000	Uiso	1.00
Al6	Al	0.34424	0.87356	0.89786	0.00000	Uiso	1.00
Al7	Al	0.35033	0.85180	0.40972	0.00000	Uiso	1.00
Al8	Al	0.35363	0.40239	0.88336	0.00000	Uiso	1.00
Al9	Al	0.32908	0.38487	0.51877	0.00000	Uiso	1.00
Al10	Al	0.30479	0.80291	0.26326	0.00000	Uiso	1.00
Al11	Al	0.30085	0.80713	0.76413	0.00000	Uiso	1.00
Al12	Al	0.30436	0.30716	0.26036	0.00000	Uiso	1.00
Al13	Al	0.30155	0.31470	0.77372	0.00000	Uiso	1.00
Al14	Al	0.30624	0.13411	0.26032	0.00000	Uiso	1.00
Al15	Al	0.30289	0.13541	0.75923	0.00000	Uiso	1.00
Al16	Al	0.29752	0.63541	0.26697	0.00000	Uiso	1.00
Al17	Al	0.29922	0.64076	0.76146	0.00000	Uiso	1.00
Al18	Al	0.21191	0.97110	0.25381	0.00000	Uiso	1.00
Al19	Al	0.21176	0.97245	0.75450	0.00000	Uiso	1.00
Al20	Al	0.20935	0.47056	0.25063	0.00000	Uiso	1.00
Al21	Al	0.21015	0.47068	0.75172	0.00000	Uiso	1.00
Al22	Al	0.32925	0.96948	0.12902	0.00000	Uiso	1.00
Al23	Al	0.32707	0.96719	0.62619	0.00000	Uiso	1.00
Al24	Al	0.32455	0.47619	0.12492	0.00000	Uiso	1.00

AI25	AI	0.33977	0.53444	0.65858	0.00000	Uiso	1.00
AI26	AI	0.28072	0.22012	0.02404	0.00000	Uiso	1.00
AI27	AI	0.28183	0.22123	0.51690	0.00000	Uiso	1.00
AI28	AI	0.28106	0.71861	0.00738	0.00000	Uiso	1.00
AI29	AI	0.28104	0.72090	0.50710	0.00000	Uiso	1.00
AI30	AI	0.34570	0.23210	0.91779	0.00000	Uiso	1.00
AI31	AI	0.35512	0.23790	0.65700	0.00000	Uiso	1.00
AI32	AI	0.35216	0.73070	0.12552	0.00000	Uiso	1.00
AI33	AI	0.35160	0.73091	0.66493	0.00000	Uiso	1.00
AI34	AI	0.21198	0.97156	0.00634	0.00000	Uiso	1.00
AI35	AI	0.21143	0.97204	0.50418	0.00000	Uiso	1.00
AI36	AI	0.21023	0.46983	0.00295	0.00000	Uiso	1.00
AI37	AI	0.20960	0.47001	0.50306	0.00000	Uiso	1.00
AI38	AI	0.28282	0.96168	0.37881	0.00000	Uiso	1.00
AI39	AI	0.28183	0.97554	0.87925	0.00000	Uiso	1.00
AI40	AI	0.27856	0.46767	0.37676	0.00000	Uiso	1.00
AI41	AI	0.28120	0.47615	0.87746	0.00000	Uiso	1.00
AI42	AI	0.23655	0.21902	0.25537	0.00000	Uiso	1.00
AI43	AI	0.23539	0.22002	0.75396	0.00000	Uiso	1.00
AI44	AI	0.23490	0.72406	0.25056	0.00000	Uiso	1.00
AI45	AI	0.23417	0.72320	0.74999	0.00000	Uiso	1.00
AI46	AI	0.26186	0.05810	0.13329	0.00000	Uiso	1.00
AI47	AI	0.26127	0.05827	0.62615	0.00000	Uiso	1.00
AI48	AI	0.25841	0.55813	0.12481	0.00000	Uiso	1.00
AI49	AI	0.25901	0.55861	0.62456	0.00000	Uiso	1.00
AI50	AI	0.26183	0.88315	0.12666	0.00000	Uiso	1.00
AI51	AI	0.25962	0.88322	0.62709	0.00000	Uiso	1.00
AI52	AI	0.25952	0.38232	0.13199	0.00000	Uiso	1.00
AI53	AI	0.25925	0.38332	0.63006	0.00000	Uiso	1.00
AI54	AI	0.21396	0.80723	0.00144	0.00000	Uiso	1.00
AI55	AI	0.21308	0.80675	0.50080	0.00000	Uiso	1.00
AI56	AI	0.21299	0.30593	0.00341	0.00000	Uiso	1.00
AI57	AI	0.21299	0.30600	0.50084	0.00000	Uiso	1.00
AI58	AI	0.21369	0.13512	0.00596	0.00000	Uiso	1.00
AI59	AI	0.21368	0.13572	0.50169	0.00000	Uiso	1.00
AI60	AI	0.21270	0.63517	0.99915	0.00000	Uiso	1.00
AI61	AI	0.21272	0.63523	0.49872	0.00000	Uiso	1.00
AI62	AI	0.40183	0.14785	0.78620	0.00000	Uiso	1.00
AI63	AI	0.35103	0.22481	0.39932	0.00000	Uiso	1.00
AI64	AI	0.40012	0.64450	0.01226	0.00000	Uiso	1.00
AI65	AI	0.40224	0.76563	0.50903	0.00000	Uiso	1.00
O66	O	0.30876	0.87883	0.38304	0.00000	Uiso	1.00
O67	O	0.30387	0.88780	0.88167	0.00000	Uiso	1.00
O68	O	0.30658	0.38821	0.38493	0.00000	Uiso	1.00
O69	O	0.30686	0.39436	0.88085	0.00000	Uiso	1.00
O70	O	0.30847	0.04453	0.36865	0.00000	Uiso	1.00
O71	O	0.30902	0.05820	0.87274	0.00000	Uiso	1.00
O72	O	0.30409	0.55058	0.37072	0.00000	Uiso	1.00
O73	O	0.30437	0.56326	0.88003	0.00000	Uiso	1.00
O74	O	0.30756	0.22339	0.38729	0.00000	Uiso	1.00
O75	O	0.30447	0.22013	0.88921	0.00000	Uiso	1.00
O76	O	0.30183	0.71595	0.37080	0.00000	Uiso	1.00
O77	O	0.30046	0.72213	0.87070	0.00000	Uiso	1.00
O78	O	0.35222	0.13459	0.31101	0.00000	Uiso	1.00
O79	O	0.35581	0.15243	0.78554	0.00000	Uiso	1.00
O80	O	0.36067	0.62570	0.38610	0.00000	Uiso	1.00
O81	O	0.34578	0.63129	0.73550	0.00000	Uiso	1.00
O82	O	0.34889	0.79925	0.26436	0.00000	Uiso	1.00
O83	O	0.34532	0.80612	0.77371	0.00000	Uiso	1.00
O84	O	0.35611	0.31061	0.02348	0.00000	Uiso	1.00
O85	O	0.41520	0.39368	0.63975	0.00000	Uiso	1.00
O86	O	0.35353	0.96658	0.75534	0.00000	Uiso	1.00
O87	O	0.35503	0.49108	0.23786	0.00000	Uiso	1.00
O88	O	0.35503	0.48701	0.78282	0.00000	Uiso	1.00
O89	O	0.30456	0.88710	0.14403	0.00000	Uiso	1.00
O90	O	0.30166	0.88735	0.64250	0.00000	Uiso	1.00
O91	O	0.30254	0.38960	0.14986	0.00000	Uiso	1.00
O92	O	0.30242	0.38046	0.63747	0.00000	Uiso	1.00
O93	O	0.30554	0.05562	0.13896	0.00000	Uiso	1.00
O94	O	0.30472	0.05609	0.63920	0.00000	Uiso	1.00
O95	O	0.30089	0.55976	0.14286	0.00000	Uiso	1.00
O96	O	0.30054	0.55849	0.63986	0.00000	Uiso	1.00
O97	O	0.30672	0.22115	0.15034	0.00000	Uiso	1.00
O98	O	0.31003	0.21837	0.64744	0.00000	Uiso	1.00
O99	O	0.30941	0.71702	0.13793	0.00000	Uiso	1.00
O100	O	0.30654	0.72393	0.63797	0.00000	Uiso	1.00
O101	O	0.35953	0.14353	0.00505	0.00000	Uiso	1.00
O102	O	0.35791	0.65001	0.99735	0.00000	Uiso	1.00
O103	O	0.36150	0.81379	0.02012	0.00000	Uiso	1.00
O104	O	0.35989	0.78023	0.52320	0.00000	Uiso	1.00
O105	O	0.34503	0.30411	0.78797	0.00000	Uiso	1.00
O106	O	0.35380	0.30134	0.52011	0.00000	Uiso	1.00
O107	O	0.35056	0.96867	0.99146	0.00000	Uiso	1.00
O108	O	0.35084	0.96027	0.49321	0.00000	Uiso	1.00
O109	O	0.34985	0.47908	0.00287	0.00000	Uiso	1.00
O110	O	0.34924	0.47955	0.52138	0.00000	Uiso	1.00
O111	O	0.20714	0.89410	0.88748	0.00000	Uiso	1.00
O112	O	0.20694	0.89349	0.38613	0.00000	Uiso	1.00
O113	O	0.20580	0.39218	0.88554	0.00000	Uiso	1.00
O114	O	0.20555	0.39232	0.38447	0.00000	Uiso	1.00
O115	O	0.20727	0.05009	0.88889	0.00000	Uiso	1.00
O116	O	0.20705	0.04986	0.38642	0.00000	Uiso	1.00
O117	O	0.20574	0.54782	0.88445	0.00000	Uiso	1.00
O118	O	0.20531	0.54773	0.38375	0.00000	Uiso	1.00
O119	O	0.21095	0.22046	0.88651	0.00000	Uiso	1.00
O120	O	0.21090	0.22066	0.38494	0.00000	Uiso	1.00
O121	O	0.21040	0.72146	0.88361	0.00000	Uiso	1.00
O122	O	0.21029	0.72184	0.38227	0.00000	Uiso	1.00
O123	O	0.26215	0.13521	0.25359	0.00000	Uiso	1.00
O124	O	0.26141	0.13781	0.74601	0.00000	Uiso	1.00
O125	O	0.25707	0.63595	0.24359	0.00000	Uiso	1.00

O126	O	0.25710	0.63729	0.74183	0.00000	Uiso	1.00
O127	O	0.26170	0.80403	0.24292	0.00000	Uiso	1.00
O128	O	0.25846	0.80743	0.74601	0.00000	Uiso	1.00
O129	O	0.26074	0.30527	0.25416	0.00000	Uiso	1.00
O130	O	0.25984	0.30508	0.75079	0.00000	Uiso	1.00
O131	O	0.25642	0.96842	0.25014	0.00000	Uiso	1.00
O132	O	0.25571	0.97390	0.75027	0.00000	Uiso	1.00
O133	O	0.25338	0.47022	0.24795	0.00000	Uiso	1.00
O134	O	0.25437	0.47040	0.74746	0.00000	Uiso	1.00
O135	O	0.21592	0.89300	0.12150	0.00000	Uiso	1.00
O136	O	0.21497	0.89461	0.62121	0.00000	Uiso	1.00
O137	O	0.21420	0.39217	0.12082	0.00000	Uiso	1.00
O138	O	0.21407	0.39200	0.62043	0.00000	Uiso	1.00
O139	O	0.21590	0.04853	0.12485	0.00000	Uiso	1.00
O140	O	0.21583	0.04998	0.62089	0.00000	Uiso	1.00
O141	O	0.21366	0.54798	0.11865	0.00000	Uiso	1.00
O142	O	0.21380	0.54805	0.61841	0.00000	Uiso	1.00
O143	O	0.20848	0.21991	0.12777	0.00000	Uiso	1.00
O144	O	0.20818	0.22101	0.62578	0.00000	Uiso	1.00
O145	O	0.20815	0.72182	0.12286	0.00000	Uiso	1.00
O146	O	0.20752	0.72170	0.62177	0.00000	Uiso	1.00
O147	O	0.25600	0.13646	0.01719	0.00000	Uiso	1.00
O148	O	0.25648	0.13831	0.51274	0.00000	Uiso	1.00
O149	O	0.25471	0.63737	0.01157	0.00000	Uiso	1.00
O150	O	0.25487	0.63733	0.50809	0.00000	Uiso	1.00
O151	O	0.25632	0.80362	0.01316	0.00000	Uiso	1.00
O152	O	0.25525	0.80440	0.51081	0.00000	Uiso	1.00
O153	O	0.25541	0.30358	0.01769	0.00000	Uiso	1.00
O154	O	0.25553	0.30338	0.51503	0.00000	Uiso	1.00
O155	O	0.25884	0.97248	0.01255	0.00000	Uiso	1.00
O156	O	0.25840	0.97017	0.50951	0.00000	Uiso	1.00
O157	O	0.25710	0.47055	0.01117	0.00000	Uiso	1.00
O158	O	0.25616	0.46930	0.51001	0.00000	Uiso	1.00
O159	O	0.35326	0.29855	0.27096	0.00000	Uiso	1.00
O160	O	0.39552	0.70930	0.65500	0.00000	Uiso	1.00
O161	O	0.41620	0.17988	0.93011	0.00000	Uiso	1.00
O162	O	0.39732	0.88175	0.86591	0.00000	Uiso	1.00
O163	O	0.39738	0.39372	0.16999	0.00000	Uiso	1.00
O164	O	0.39502	0.37657	0.87039	0.00000	Uiso	1.00
O165	O	0.39746	0.25055	0.71258	0.00000	Uiso	1.00
O166	O	0.41014	0.55572	0.63526	0.00000	Uiso	1.00
O167	O	0.46435	0.48744	0.68949	0.00000	Uiso	1.00
O168	O	0.40770	0.54510	0.29754	0.00000	Uiso	1.00
O169	O	0.40594	0.54244	0.06803	0.00000	Uiso	1.00
O170	O	0.39960	0.23218	0.14445	0.00000	Uiso	1.00
O171	O	0.39550	0.04268	0.84696	0.00000	Uiso	1.00
O172	O	0.40619	0.07088	0.10939	0.00000	Uiso	1.00
O173	O	0.41515	0.69702	0.40025	0.00000	Uiso	1.00
O174	O	0.45016	0.31688	0.79216	0.00000	Uiso	1.00
O175	O	0.45219	0.66721	0.69849	0.00000	Uiso	1.00
O176	O	0.40802	0.61851	0.85776	0.00000	Uiso	1.00
O177	O	0.44258	0.47562	0.46602	0.00000	Uiso	1.00
O178	O	0.36726	0.16056	0.53700	0.00000	Uiso	1.00
O179	O	0.41993	0.11191	0.65422	0.00000	Uiso	1.00
O180	O	0.40922	0.94303	0.64928	0.00000	Uiso	1.00
O181	O	0.39809	0.87127	0.43355	0.00000	Uiso	1.00
O182	O	0.42222	0.19056	0.43852	0.00000	Uiso	1.00
O183	O	0.40053	0.04059	0.45352	0.00000	Uiso	1.00
O184	O	0.45117	0.94445	0.48927	0.00000	Uiso	1.00
O185	O	0.40912	0.90354	0.09322	0.00000	Uiso	1.00
O186	O	0.41716	0.74931	0.00123	0.00000	Uiso	1.00
O187	O	0.43016	0.98251	0.26745	0.00000	Uiso	1.00
O188	O	0.38713	0.67811	0.18291	0.00000	Uiso	1.00
O189	O	0.36469	0.98041	0.23420	0.00000	Uiso	1.00
O190	O	0.44231	0.79300	0.56949	0.00000	Uiso	1.00
Si191	Si	0.39185	0.95782	0.77483	0.00000	Uiso	1.00
Si192	Si	0.41293	0.33724	0.76038	0.00000	Uiso	1.00
Si193	Si	0.43230	0.47815	0.60698	0.00000	Uiso	1.00
Si194	Si	0.39202	0.49432	0.17948	0.00000	Uiso	1.00
Si195	Si	0.39623	0.15595	0.05045	0.00000	Uiso	1.00
Si196	Si	0.39375	0.64090	0.31789	0.00000	Uiso	1.00
Si197	Si	0.37557	0.31048	0.15151	0.00000	Uiso	1.00
Si198	Si	0.41526	0.63605	0.72022	0.00000	Uiso	1.00
Si199	Si	0.41247	0.94917	0.50249	0.00000	Uiso	1.00
Si200	Si	0.40339	0.12701	0.52774	0.00000	Uiso	1.00
Si201	Si	0.40084	0.98269	0.17044	0.00000	Uiso	1.00
Si202	Si	0.39932	0.83235	0.99857	0.00000	Uiso	1.00
H203	H	0.46841	0.44233	0.74236	0.00000	Uiso	1.00
H204	H	0.45140	0.27368	0.85022	0.00000	Uiso	1.00
H205	H	0.46760	0.62484	0.70569	0.00000	Uiso	1.00
H206	H	0.42975	0.50502	0.40631	0.00000	Uiso	1.00
H207	H	0.42604	0.24046	0.48141	0.00000	Uiso	1.00
H208	H	0.45611	0.93955	0.40374	0.00000	Uiso	1.00
H209	H	0.43319	0.03599	0.29925	0.00000	Uiso	1.00
H210	H	0.45428	0.84164	0.55129	0.00000	Uiso	1.00
H211	H	0.45253	0.75109	0.62087	0.00000	Uiso	1.00
H212	H	0.51251	0.75782	0.11084	0.00000	Uiso	1.00
H213	H	0.46924	0.68422	0.91883	0.00000	Uiso	1.00
H214	H	0.47445	0.58088	0.95002	0.00000	Uiso	1.00
H215	H	0.46820	0.61881	0.27849	0.00000	Uiso	1.00
H216	H	0.48669	0.75119	0.23712	0.00000	Uiso	1.00
H217	H	0.47279	0.78507	0.09459	0.00000	Uiso	1.00
H218	H	0.46311	0.54604	0.15316	0.00000	Uiso	1.00
H219	H	0.50732	0.64646	0.94116	0.00000	Uiso	1.00
H220	H	0.45566	0.24040	0.03003	0.00000	Uiso	1.00
H221	H	0.49643	0.24273	0.03674	0.00000	Uiso	1.00
H222	H	0.47498	0.33323	0.00025	0.00000	Uiso	1.00
H223	H	0.47232	0.42041	0.17241	0.00000	Uiso	1.00
H224	H	0.48937	0.24422	0.34771	0.00000	Uiso	1.00
H225	H	0.46435	0.38187	0.32420	0.00000	Uiso	1.00
H226	H	0.43744	0.37200	0.20051	0.00000	Uiso	1.00

H227	H	0.45246	0.21261	0.30393	0.00000	Uiso	1.00
H228	H	0.48553	0.17289	0.22529	0.00000	Uiso	1.00
C229	C	0.48294	0.64110	0.97139	0.00000	Uiso	1.00
C230	C	0.48036	0.65923	0.10323	0.00000	Uiso	1.00
C231	C	0.48864	0.74285	0.13950	0.00000	Uiso	1.00
C232	C	0.47052	0.60496	0.18311	0.00000	Uiso	1.00
C233	C	0.47570	0.27924	0.05554	0.00000	Uiso	1.00
C234	C	0.47255	0.29383	0.18463	0.00000	Uiso	1.00
C235	C	0.46333	0.37079	0.22710	0.00000	Uiso	1.00
C236	C	0.47603	0.22672	0.26749	0.00000	Uiso	1.00

File n°17 :

A12	Al	0.35094	0.05667	0.89357	0.00000	Uiso	1.00
A13	Al	0.35052	0.03596	0.37806	0.00000	Uiso	1.00
A14	Al	0.34715	0.57026	0.89732	0.00000	Uiso	1.00
A15	Al	0.34343	0.53329	0.38568	0.00000	Uiso	1.00
A16	Al	0.34424	0.87514	0.89701	0.00000	Uiso	1.00
A17	Al	0.34961	0.85159	0.41216	0.00000	Uiso	1.00
A18	Al	0.35443	0.40138	0.88620	0.00000	Uiso	1.00
A19	Al	0.32873	0.38567	0.51934	0.00000	Uiso	1.00
A110	Al	0.30443	0.80285	0.26387	0.00000	Uiso	1.00
A111	Al	0.30073	0.80721	0.76526	0.00000	Uiso	1.00
A112	Al	0.30455	0.30672	0.25997	0.00000	Uiso	1.00
A113	Al	0.30176	0.31538	0.77462	0.00000	Uiso	1.00
A114	Al	0.30640	0.13384	0.26077	0.00000	Uiso	1.00
A115	Al	0.30314	0.13618	0.75725	0.00000	Uiso	1.00
A116	Al	0.29739	0.63528	0.26788	0.00000	Uiso	1.00
A117	Al	0.29909	0.64055	0.76267	0.00000	Uiso	1.00
A118	Al	0.21191	0.97110	0.25381	0.00000	Uiso	1.00
A119	Al	0.21176	0.97245	0.75450	0.00000	Uiso	1.00
A120	Al	0.20935	0.47056	0.25063	0.00000	Uiso	1.00
A121	Al	0.21015	0.47068	0.75172	0.00000	Uiso	1.00
A122	Al	0.32929	0.96979	0.12958	0.00000	Uiso	1.00
A123	Al	0.32682	0.96649	0.62676	0.00000	Uiso	1.00
A124	Al	0.32435	0.47636	0.12377	0.00000	Uiso	1.00
A125	Al	0.33956	0.53347	0.66102	0.00000	Uiso	1.00
A126	Al	0.28084	0.22002	0.02345	0.00000	Uiso	1.00
A127	Al	0.28194	0.22121	0.51658	0.00000	Uiso	1.00
A128	Al	0.28094	0.71874	0.00797	0.00000	Uiso	1.00
A129	Al	0.28099	0.72101	0.50780	0.00000	Uiso	1.00
A130	Al	0.34594	0.23159	0.91453	0.00000	Uiso	1.00
A131	Al	0.35637	0.23992	0.65562	0.00000	Uiso	1.00
A132	Al	0.35161	0.73319	0.12776	0.00000	Uiso	1.00
A133	Al	0.35132	0.73085	0.66581	0.00000	Uiso	1.00
A134	Al	0.21198	0.97156	0.00634	0.00000	Uiso	1.00
A135	Al	0.21143	0.97204	0.50418	0.00000	Uiso	1.00
A136	Al	0.21023	0.46983	0.00295	0.00000	Uiso	1.00
A137	Al	0.20960	0.47001	0.50306	0.00000	Uiso	1.00
A138	Al	0.28280	0.96166	0.37884	0.00000	Uiso	1.00
A139	Al	0.28186	0.97642	0.87924	0.00000	Uiso	1.00
A140	Al	0.27834	0.46722	0.37667	0.00000	Uiso	1.00
A141	Al	0.28118	0.47618	0.87756	0.00000	Uiso	1.00
A142	Al	0.23655	0.21902	0.25537	0.00000	Uiso	1.00
A143	Al	0.23539	0.22002	0.75396	0.00000	Uiso	1.00
A144	Al	0.23490	0.72406	0.25056	0.00000	Uiso	1.00
A145	Al	0.23417	0.72320	0.74999	0.00000	Uiso	1.00
A146	Al	0.26186	0.05810	0.13329	0.00000	Uiso	1.00
A147	Al	0.26127	0.05827	0.62615	0.00000	Uiso	1.00
A148	Al	0.25841	0.55813	0.12481	0.00000	Uiso	1.00
A149	Al	0.25901	0.55861	0.62456	0.00000	Uiso	1.00
A150	Al	0.26183	0.88315	0.12666	0.00000	Uiso	1.00
A151	Al	0.25962	0.88322	0.62709	0.00000	Uiso	1.00
A152	Al	0.25952	0.38232	0.13199	0.00000	Uiso	1.00
A153	Al	0.25925	0.38332	0.63006	0.00000	Uiso	1.00
A154	Al	0.21396	0.80723	0.00144	0.00000	Uiso	1.00
A155	Al	0.21308	0.80675	0.50080	0.00000	Uiso	1.00
A156	Al	0.21299	0.30593	0.00341	0.00000	Uiso	1.00
A157	Al	0.21299	0.30600	0.50084	0.00000	Uiso	1.00
A158	Al	0.21369	0.13512	0.00596	0.00000	Uiso	1.00
A159	Al	0.21368	0.13572	0.50169	0.00000	Uiso	1.00
A160	Al	0.21270	0.63517	0.99915	0.00000	Uiso	1.00
A161	Al	0.21272	0.63523	0.49872	0.00000	Uiso	1.00
A162	Al	0.40268	0.14918	0.78406	0.00000	Uiso	1.00
A163	Al	0.35125	0.22549	0.39876	0.00000	Uiso	1.00
A164	Al	0.39927	0.65336	0.00941	0.00000	Uiso	1.00
A165	Al	0.40198	0.76505	0.50824	0.00000	Uiso	1.00
O66	O	0.30818	0.87767	0.38332	0.00000	Uiso	1.00
O67	O	0.30377	0.88815	0.88185	0.00000	Uiso	1.00
O68	O	0.30655	0.38889	0.38490	0.00000	Uiso	1.00
O69	O	0.30750	0.39566	0.88338	0.00000	Uiso	1.00
O70	O	0.30864	0.04372	0.36887	0.00000	Uiso	1.00
O71	O	0.30912	0.05885	0.87141	0.00000	Uiso	1.00
O72	O	0.30352	0.55073	0.37170	0.00000	Uiso	1.00
O73	O	0.30479	0.56278	0.88216	0.00000	Uiso	1.00
O74	O	0.30753	0.22372	0.38715	0.00000	Uiso	1.00
O75	O	0.30449	0.22103	0.88792	0.00000	Uiso	1.00
O76	O	0.30160	0.71589	0.37125	0.00000	Uiso	1.00
O77	O	0.30042	0.72186	0.87150	0.00000	Uiso	1.00
O78	O	0.35175	0.13417	0.31235	0.00000	Uiso	1.00
O79	O	0.35582	0.15350	0.78183	0.00000	Uiso	1.00
O80	O	0.35931	0.62712	0.38108	0.00000	Uiso	1.00
O81	O	0.34581	0.63085	0.73721	0.00000	Uiso	1.00
O82	O	0.34878	0.79849	0.26578	0.00000	Uiso	1.00
O83	O	0.34530	0.80558	0.77518	0.00000	Uiso	1.00
O84	O	0.35547	0.31119	0.02047	0.00000	Uiso	1.00
O85	O	0.41853	0.39431	0.64787	0.00000	Uiso	1.00
O86	O	0.35332	0.96529	0.75572	0.00000	Uiso	1.00
O87	O	0.35408	0.49184	0.23893	0.00000	Uiso	1.00
O88	O	0.35506	0.48693	0.78609	0.00000	Uiso	1.00

O89	O	0.30466	0.88696	0.14442	0.00000	Uiso	1.00
O90	O	0.30156	0.88654	0.64310	0.00000	Uiso	1.00
O91	O	0.30256	0.38979	0.14902	0.00000	Uiso	1.00
O92	O	0.30232	0.38181	0.63893	0.00000	Uiso	1.00
O93	O	0.30543	0.05553	0.13896	0.00000	Uiso	1.00
O94	O	0.30477	0.05591	0.63834	0.00000	Uiso	1.00
O95	O	0.30089	0.55996	0.14270	0.00000	Uiso	1.00
O96	O	0.30050	0.55837	0.64169	0.00000	Uiso	1.00
O97	O	0.30660	0.22087	0.14994	0.00000	Uiso	1.00
O98	O	0.31032	0.21876	0.64574	0.00000	Uiso	1.00
O99	O	0.30927	0.71722	0.13831	0.00000	Uiso	1.00
O100	O	0.30654	0.72338	0.63888	0.00000	Uiso	1.00
O101	O	0.35915	0.14337	0.00255	0.00000	Uiso	1.00
O102	O	0.35768	0.64963	0.99984	0.00000	Uiso	1.00
O103	O	0.36150	0.81463	0.02101	0.00000	Uiso	1.00
O104	O	0.35956	0.77864	0.52336	0.00000	Uiso	1.00
O105	O	0.34526	0.30543	0.78685	0.00000	Uiso	1.00
O106	O	0.35351	0.30325	0.51949	0.00000	Uiso	1.00
O107	O	0.35039	0.96922	0.99134	0.00000	Uiso	1.00
O108	O	0.34977	0.95700	0.49326	0.00000	Uiso	1.00
O109	O	0.35312	0.48199	0.00992	0.00000	Uiso	1.00
O110	O	0.34909	0.48071	0.52260	0.00000	Uiso	1.00
O111	O	0.20714	0.89410	0.88748	0.00000	Uiso	1.00
O112	O	0.20694	0.89349	0.38613	0.00000	Uiso	1.00
O113	O	0.20580	0.39218	0.88554	0.00000	Uiso	1.00
O114	O	0.20555	0.39232	0.38447	0.00000	Uiso	1.00
O115	O	0.20727	0.05009	0.88889	0.00000	Uiso	1.00
O116	O	0.20705	0.04986	0.38642	0.00000	Uiso	1.00
O117	O	0.20574	0.54782	0.88445	0.00000	Uiso	1.00
O118	O	0.20531	0.54773	0.38375	0.00000	Uiso	1.00
O119	O	0.21095	0.22046	0.88651	0.00000	Uiso	1.00
O120	O	0.21090	0.22066	0.38494	0.00000	Uiso	1.00
O121	O	0.21040	0.72146	0.88361	0.00000	Uiso	1.00
O122	O	0.21029	0.72184	0.38227	0.00000	Uiso	1.00
O123	O	0.26215	0.13521	0.25359	0.00000	Uiso	1.00
O124	O	0.26141	0.13781	0.74601	0.00000	Uiso	1.00
O125	O	0.25707	0.63595	0.24359	0.00000	Uiso	1.00
O126	O	0.25710	0.63729	0.74183	0.00000	Uiso	1.00
O127	O	0.26170	0.80403	0.24292	0.00000	Uiso	1.00
O128	O	0.25846	0.80743	0.74601	0.00000	Uiso	1.00
O129	O	0.26074	0.30527	0.25416	0.00000	Uiso	1.00
O130	O	0.25984	0.30508	0.75079	0.00000	Uiso	1.00
O131	O	0.25642	0.96842	0.25014	0.00000	Uiso	1.00
O132	O	0.25571	0.97390	0.75027	0.00000	Uiso	1.00
O133	O	0.25338	0.47022	0.24795	0.00000	Uiso	1.00
O134	O	0.25437	0.47040	0.74746	0.00000	Uiso	1.00
O135	O	0.21592	0.89300	0.12150	0.00000	Uiso	1.00
O136	O	0.21497	0.89461	0.62121	0.00000	Uiso	1.00
O137	O	0.21420	0.39217	0.12082	0.00000	Uiso	1.00
O138	O	0.21407	0.39200	0.62043	0.00000	Uiso	1.00
O139	O	0.21590	0.04853	0.12485	0.00000	Uiso	1.00
O140	O	0.21583	0.04998	0.62089	0.00000	Uiso	1.00
O141	O	0.21366	0.54798	0.11865	0.00000	Uiso	1.00
O142	O	0.21380	0.54805	0.61841	0.00000	Uiso	1.00
O143	O	0.20848	0.21991	0.12777	0.00000	Uiso	1.00
O144	O	0.20818	0.22101	0.62578	0.00000	Uiso	1.00
O145	O	0.20815	0.72182	0.12286	0.00000	Uiso	1.00
O146	O	0.20752	0.72170	0.62177	0.00000	Uiso	1.00
O147	O	0.25600	0.13646	0.01719	0.00000	Uiso	1.00
O148	O	0.25648	0.13831	0.51274	0.00000	Uiso	1.00
O149	O	0.25471	0.63737	0.01157	0.00000	Uiso	1.00
O150	O	0.25487	0.63733	0.50809	0.00000	Uiso	1.00
O151	O	0.25632	0.80362	0.01316	0.00000	Uiso	1.00
O152	O	0.25525	0.80440	0.51081	0.00000	Uiso	1.00
O153	O	0.25541	0.30358	0.01769	0.00000	Uiso	1.00
O154	O	0.25553	0.30338	0.51503	0.00000	Uiso	1.00
O155	O	0.25884	0.97248	0.01255	0.00000	Uiso	1.00
O156	O	0.25840	0.97017	0.50951	0.00000	Uiso	1.00
O157	O	0.25710	0.47055	0.01117	0.00000	Uiso	1.00
O158	O	0.25616	0.46930	0.51001	0.00000	Uiso	1.00
O159	O	0.35237	0.29851	0.26962	0.00000	Uiso	1.00
O160	O	0.39537	0.70908	0.65529	0.00000	Uiso	1.00
O161	O	0.41561	0.18041	0.92884	0.00000	Uiso	1.00
O162	O	0.39714	0.88359	0.86808	0.00000	Uiso	1.00
O163	O	0.39540	0.39302	0.16680	0.00000	Uiso	1.00
O164	O	0.39567	0.37873	0.87321	0.00000	Uiso	1.00
O165	O	0.39814	0.25264	0.71549	0.00000	Uiso	1.00
O166	O	0.41048	0.55477	0.64030	0.00000	Uiso	1.00
O167	O	0.46712	0.49435	0.67637	0.00000	Uiso	1.00
O168	O	0.40587	0.54519	0.29335	0.00000	Uiso	1.00
O169	O	0.41197	0.53966	0.07076	0.00000	Uiso	1.00
O170	O	0.39797	0.23085	0.14409	0.00000	Uiso	1.00
O171	O	0.39528	0.04369	0.84359	0.00000	Uiso	1.00
O172	O	0.40544	0.07025	0.10627	0.00000	Uiso	1.00
O173	O	0.41431	0.69537	0.39916	0.00000	Uiso	1.00
O174	O	0.45085	0.31573	0.80775	0.00000	Uiso	1.00
O175	O	0.45204	0.66654	0.70682	0.00000	Uiso	1.00
O176	O	0.40592	0.61991	0.85944	0.00000	Uiso	1.00
O177	O	0.44087	0.47747	0.46349	0.00000	Uiso	1.00
O178	O	0.37047	0.16710	0.53135	0.00000	Uiso	1.00
O179	O	0.42077	0.11311	0.65184	0.00000	Uiso	1.00
O180	O	0.40892	0.93999	0.64962	0.00000	Uiso	1.00
O181	O	0.39790	0.86941	0.43373	0.00000	Uiso	1.00
O182	O	0.42693	0.16931	0.41937	0.00000	Uiso	1.00
O183	O	0.39777	0.03697	0.45824	0.00000	Uiso	1.00
O184	O	0.45068	0.94485	0.49135	0.00000	Uiso	1.00
O185	O	0.40914	0.90444	0.09798	0.00000	Uiso	1.00
O186	O	0.42958	0.98764	0.27205	0.00000	Uiso	1.00
O187	O	0.38762	0.67797	0.17896	0.00000	Uiso	1.00
O188	O	0.36451	0.98029	0.23548	0.00000	Uiso	1.00
O189	O	0.44262	0.79053	0.56597	0.00000	Uiso	1.00

O190	O	0.41735	0.75281	0.00000	0.00000	Uiso	1.00
Si191	Si	0.39175	0.95831	0.77417	0.00000	Uiso	1.00
Si192	Si	0.41464	0.33710	0.76712	0.00000	Uiso	1.00
Si193	Si	0.43345	0.47905	0.60642	0.00000	Uiso	1.00
Si194	Si	0.39049	0.49007	0.17869	0.00000	Uiso	1.00
Si195	Si	0.39609	0.15610	0.04866	0.00000	Uiso	1.00
Si196	Si	0.39270	0.64091	0.31578	0.00000	Uiso	1.00
Si197	Si	0.37477	0.30932	0.14964	0.00000	Uiso	1.00
Si198	Si	0.41489	0.63627	0.72180	0.00000	Uiso	1.00
Si199	Si	0.41206	0.94757	0.50263	0.00000	Uiso	1.00
Si200	Si	0.40543	0.12575	0.52255	0.00000	Uiso	1.00
Si201	Si	0.40079	0.98464	0.17349	0.00000	Uiso	1.00
Si202	Si	0.39918	0.83587	0.00071	0.00000	Uiso	1.00
H203	H	0.47250	0.45378	0.73532	0.00000	Uiso	1.00
H204	H	0.45138	0.28049	0.87738	0.00000	Uiso	1.00
H205	H	0.46655	0.62191	0.69806	0.00000	Uiso	1.00
H206	H	0.42703	0.50551	0.40671	0.00000	Uiso	1.00
H207	H	0.43841	0.21678	0.44247	0.00000	Uiso	1.00
H208	H	0.45643	0.94479	0.40636	0.00000	Uiso	1.00
H209	H	0.43382	0.04265	0.29571	0.00000	Uiso	1.00
H210	H	0.45404	0.84068	0.55175	0.00000	Uiso	1.00
H211	H	0.45228	0.75116	0.62270	0.00000	Uiso	1.00
H212	H	0.48265	0.49616	0.94861	0.00000	Uiso	1.00
H213	H	0.48340	0.45598	0.14967	0.00000	Uiso	1.00
H214	H	0.45103	0.45952	0.24624	0.00000	Uiso	1.00
H215	H	0.44949	0.40091	0.11096	0.00000	Uiso	1.00
H216	H	0.48710	0.60053	0.12622	0.00000	Uiso	1.00
H217	H	0.45488	0.61340	0.22445	0.00000	Uiso	1.00
H218	H	0.45539	0.65885	0.07827	0.00000	Uiso	1.00
H219	H	0.45650	0.57040	0.89491	0.00000	Uiso	1.00
H220	H	0.44374	0.46910	0.90755	0.00000	Uiso	1.00
C221	C	0.46159	0.60511	0.13022	0.00000	Uiso	1.00
C222	C	0.44807	0.52890	0.07711	0.00000	Uiso	1.00
C223	C	0.45783	0.45651	0.15138	0.00000	Uiso	1.00
C224	C	0.45823	0.51580	0.94803	0.00000	Uiso	1.00

File n°18 :

Al2	Al	0.35124	0.05687	0.89424	0.00000	Uiso	1.00
Al3	Al	0.35004	0.03692	0.38075	0.00000	Uiso	1.00
Al4	Al	0.34401	0.56579	0.90006	0.00000	Uiso	1.00
Al5	Al	0.34387	0.53294	0.38217	0.00000	Uiso	1.00
Al6	Al	0.34458	0.87426	0.89724	0.00000	Uiso	1.00
Al7	Al	0.34997	0.85104	0.41093	0.00000	Uiso	1.00
Al8	Al	0.35328	0.40136	0.88386	0.00000	Uiso	1.00
Al9	Al	0.32880	0.38683	0.51911	0.00000	Uiso	1.00
Al10	Al	0.30477	0.80229	0.26183	0.00000	Uiso	1.00
Al11	Al	0.30076	0.80734	0.76494	0.00000	Uiso	1.00
Al12	Al	0.30451	0.30667	0.26031	0.00000	Uiso	1.00
Al13	Al	0.30162	0.31414	0.77250	0.00000	Uiso	1.00
Al14	Al	0.30632	0.13415	0.26132	0.00000	Uiso	1.00
Al15	Al	0.30315	0.13612	0.75850	0.00000	Uiso	1.00
Al16	Al	0.29759	0.63498	0.26762	0.00000	Uiso	1.00
Al17	Al	0.29898	0.64125	0.76058	0.00000	Uiso	1.00
Al18	Al	0.21191	0.97110	0.25381	0.00000	Uiso	1.00
Al19	Al	0.21176	0.97245	0.75450	0.00000	Uiso	1.00
Al20	Al	0.20935	0.47056	0.25063	0.00000	Uiso	1.00
Al21	Al	0.21015	0.47068	0.75172	0.00000	Uiso	1.00
Al22	Al	0.32928	0.97028	0.12998	0.00000	Uiso	1.00
Al23	Al	0.32688	0.96663	0.62749	0.00000	Uiso	1.00
Al24	Al	0.32460	0.47511	0.12741	0.00000	Uiso	1.00
Al25	Al	0.33977	0.53536	0.65881	0.00000	Uiso	1.00
Al26	Al	0.28081	0.22011	0.02367	0.00000	Uiso	1.00
Al27	Al	0.28185	0.22140	0.51692	0.00000	Uiso	1.00
Al28	Al	0.28101	0.71861	0.00731	0.00000	Uiso	1.00
Al29	Al	0.28101	0.72099	0.50703	0.00000	Uiso	1.00
Al30	Al	0.34592	0.23208	0.91659	0.00000	Uiso	1.00
Al31	Al	0.35632	0.24061	0.65615	0.00000	Uiso	1.00
Al32	Al	0.35281	0.73152	0.12580	0.00000	Uiso	1.00
Al33	Al	0.35164	0.73124	0.66629	0.00000	Uiso	1.00
Al34	Al	0.21198	0.97156	0.00634	0.00000	Uiso	1.00
Al35	Al	0.21143	0.97204	0.50418	0.00000	Uiso	1.00
Al36	Al	0.21023	0.46983	0.00295	0.00000	Uiso	1.00
Al37	Al	0.20960	0.47001	0.50306	0.00000	Uiso	1.00
Al38	Al	0.28283	0.96115	0.37888	0.00000	Uiso	1.00
Al39	Al	0.28195	0.97601	0.87928	0.00000	Uiso	1.00
Al40	Al	0.27839	0.46754	0.37680	0.00000	Uiso	1.00
Al41	Al	0.28074	0.47443	0.87723	0.00000	Uiso	1.00
Al42	Al	0.23655	0.21902	0.25537	0.00000	Uiso	1.00
Al43	Al	0.23539	0.22002	0.75396	0.00000	Uiso	1.00
Al44	Al	0.23490	0.72406	0.25056	0.00000	Uiso	1.00
Al45	Al	0.23417	0.72320	0.74999	0.00000	Uiso	1.00
Al46	Al	0.26186	0.05810	0.13329	0.00000	Uiso	1.00
Al47	Al	0.26127	0.05827	0.62615	0.00000	Uiso	1.00
Al48	Al	0.25841	0.55813	0.12481	0.00000	Uiso	1.00
Al49	Al	0.25901	0.55861	0.62456	0.00000	Uiso	1.00
Al50	Al	0.26183	0.88315	0.12666	0.00000	Uiso	1.00
Al51	Al	0.25962	0.88322	0.62709	0.00000	Uiso	1.00
Al52	Al	0.25952	0.38232	0.13199	0.00000	Uiso	1.00
Al53	Al	0.25925	0.38332	0.63006	0.00000	Uiso	1.00
Al54	Al	0.21396	0.80723	0.00144	0.00000	Uiso	1.00
Al55	Al	0.21308	0.80675	0.50080	0.00000	Uiso	1.00
Al56	Al	0.21299	0.30593	0.00341	0.00000	Uiso	1.00
Al57	Al	0.21299	0.30600	0.50084	0.00000	Uiso	1.00
Al58	Al	0.21369	0.13512	0.00596	0.00000	Uiso	1.00
Al59	Al	0.21368	0.13572	0.50169	0.00000	Uiso	1.00
Al60	Al	0.21270	0.63517	0.99915	0.00000	Uiso	1.00
Al61	Al	0.21272	0.63523	0.49872	0.00000	Uiso	1.00
Al62	Al	0.40258	0.15166	0.78382	0.00000	Uiso	1.00
Al63	Al	0.35104	0.22626	0.39950	0.00000	Uiso	1.00

Al64	Al	0.39710	0.62750	0.01995	0.00000	Uiso	1.00
Al65	Al	0.40224	0.76533	0.50846	0.00000	Uiso	1.00
O66	O	0.30863	0.87741	0.38125	0.00000	Uiso	1.00
O67	O	0.30410	0.88782	0.88239	0.00000	Uiso	1.00
O68	O	0.30654	0.38922	0.38502	0.00000	Uiso	1.00
O69	O	0.30648	0.39337	0.88074	0.00000	Uiso	1.00
O70	O	0.30832	0.04383	0.36978	0.00000	Uiso	1.00
O71	O	0.30939	0.05811	0.87201	0.00000	Uiso	1.00
O72	O	0.30385	0.55069	0.37164	0.00000	Uiso	1.00
O73	O	0.30282	0.56331	0.87893	0.00000	Uiso	1.00
O74	O	0.30735	0.22382	0.38769	0.00000	Uiso	1.00
O75	O	0.30454	0.21994	0.88853	0.00000	Uiso	1.00
O76	O	0.30178	0.71607	0.37042	0.00000	Uiso	1.00
O77	O	0.30065	0.72213	0.87100	0.00000	Uiso	1.00
O78	O	0.35147	0.13455	0.31396	0.00000	Uiso	1.00
O79	O	0.35602	0.15402	0.78227	0.00000	Uiso	1.00
O80	O	0.35928	0.62732	0.36536	0.00000	Uiso	1.00
O81	O	0.34594	0.63181	0.73684	0.00000	Uiso	1.00
O82	O	0.34955	0.79809	0.26285	0.00000	Uiso	1.00
O83	O	0.34563	0.80645	0.77471	0.00000	Uiso	1.00
O84	O	0.35617	0.30999	0.02365	0.00000	Uiso	1.00
O85	O	0.41713	0.39792	0.64477	0.00000	Uiso	1.00
O86	O	0.35372	0.96605	0.75561	0.00000	Uiso	1.00
O87	O	0.35542	0.48761	0.23982	0.00000	Uiso	1.00
O88	O	0.35402	0.48734	0.78396	0.00000	Uiso	1.00
O89	O	0.30493	0.88674	0.14317	0.00000	Uiso	1.00
O90	O	0.30157	0.88684	0.64352	0.00000	Uiso	1.00
O91	O	0.30234	0.38926	0.15020	0.00000	Uiso	1.00
O92	O	0.30228	0.38182	0.63788	0.00000	Uiso	1.00
O93	O	0.30544	0.05553	0.13935	0.00000	Uiso	1.00
O94	O	0.30483	0.05600	0.63902	0.00000	Uiso	1.00
O95	O	0.30111	0.55960	0.14377	0.00000	Uiso	1.00
O96	O	0.30062	0.55969	0.63918	0.00000	Uiso	1.00
O97	O	0.30655	0.22066	0.15024	0.00000	Uiso	1.00
O98	O	0.31016	0.21895	0.64663	0.00000	Uiso	1.00
O99	O	0.30993	0.71788	0.13640	0.00000	Uiso	1.00
O100	O	0.30661	0.72438	0.63832	0.00000	Uiso	1.00
O101	O	0.35925	0.14308	0.00331	0.00000	Uiso	1.00
O102	O	0.35659	0.64479	0.00084	0.00000	Uiso	1.00
O103	O	0.36522	0.81055	0.01627	0.00000	Uiso	1.00
O104	O	0.35982	0.77755	0.52211	0.00000	Uiso	1.00
O105	O	0.34499	0.30488	0.78761	0.00000	Uiso	1.00
O106	O	0.35331	0.30386	0.52022	0.00000	Uiso	1.00
O107	O	0.35077	0.96774	0.99193	0.00000	Uiso	1.00
O108	O	0.34964	0.95670	0.49381	0.00000	Uiso	1.00
O109	O	0.34851	0.47837	0.00222	0.00000	Uiso	1.00
O110	O	0.34942	0.48226	0.52085	0.00000	Uiso	1.00
O111	O	0.20714	0.89410	0.88748	0.00000	Uiso	1.00
O112	O	0.20694	0.89349	0.38613	0.00000	Uiso	1.00
O113	O	0.20580	0.39218	0.88554	0.00000	Uiso	1.00
O114	O	0.20555	0.39232	0.38447	0.00000	Uiso	1.00
O115	O	0.20727	0.05009	0.88889	0.00000	Uiso	1.00
O116	O	0.20705	0.04986	0.38642	0.00000	Uiso	1.00
O117	O	0.20574	0.54782	0.88445	0.00000	Uiso	1.00
O118	O	0.20531	0.54773	0.38375	0.00000	Uiso	1.00
O119	O	0.21095	0.22046	0.88651	0.00000	Uiso	1.00
O120	O	0.21090	0.22066	0.38494	0.00000	Uiso	1.00
O121	O	0.21040	0.72146	0.88361	0.00000	Uiso	1.00
O122	O	0.21029	0.72184	0.38227	0.00000	Uiso	1.00
O123	O	0.26215	0.13521	0.25359	0.00000	Uiso	1.00
O124	O	0.26141	0.13781	0.74601	0.00000	Uiso	1.00
O125	O	0.25707	0.63595	0.24359	0.00000	Uiso	1.00
O126	O	0.25710	0.63729	0.74183	0.00000	Uiso	1.00
O127	O	0.26170	0.80403	0.24292	0.00000	Uiso	1.00
O128	O	0.25846	0.80743	0.74601	0.00000	Uiso	1.00
O129	O	0.26074	0.30527	0.25416	0.00000	Uiso	1.00
O130	O	0.25984	0.30508	0.75079	0.00000	Uiso	1.00
O131	O	0.25642	0.96842	0.25014	0.00000	Uiso	1.00
O132	O	0.25571	0.97390	0.75027	0.00000	Uiso	1.00
O133	O	0.25338	0.47022	0.24795	0.00000	Uiso	1.00
O134	O	0.25437	0.47040	0.74746	0.00000	Uiso	1.00
O135	O	0.21592	0.89300	0.12150	0.00000	Uiso	1.00
O136	O	0.21497	0.89461	0.62121	0.00000	Uiso	1.00
O137	O	0.21420	0.39217	0.12082	0.00000	Uiso	1.00
O138	O	0.21407	0.39200	0.62043	0.00000	Uiso	1.00
O139	O	0.21590	0.04853	0.12485	0.00000	Uiso	1.00
O140	O	0.21583	0.04998	0.62089	0.00000	Uiso	1.00
O141	O	0.21366	0.54798	0.11865	0.00000	Uiso	1.00
O142	O	0.21380	0.54805	0.61841	0.00000	Uiso	1.00
O143	O	0.20848	0.21991	0.12777	0.00000	Uiso	1.00
O144	O	0.20818	0.22101	0.62578	0.00000	Uiso	1.00
O145	O	0.20815	0.72182	0.12286	0.00000	Uiso	1.00
O146	O	0.20752	0.72170	0.62177	0.00000	Uiso	1.00
O147	O	0.25600	0.13646	0.01719	0.00000	Uiso	1.00
O148	O	0.25648	0.13831	0.51274	0.00000	Uiso	1.00
O149	O	0.25471	0.63737	0.01157	0.00000	Uiso	1.00
O150	O	0.25487	0.63733	0.50809	0.00000	Uiso	1.00
O151	O	0.25632	0.80362	0.01316	0.00000	Uiso	1.00
O152	O	0.25525	0.80440	0.51081	0.00000	Uiso	1.00
O153	O	0.25541	0.30358	0.01769	0.00000	Uiso	1.00
O154	O	0.25553	0.30338	0.51503	0.00000	Uiso	1.00
O155	O	0.25884	0.97248	0.01255	0.00000	Uiso	1.00
O156	O	0.25840	0.97017	0.50951	0.00000	Uiso	1.00
O157	O	0.25710	0.47055	0.01117	0.00000	Uiso	1.00
O158	O	0.25616	0.46930	0.51001	0.00000	Uiso	1.00
O159	O	0.35218	0.29833	0.27088	0.00000	Uiso	1.00
O160	O	0.39610	0.71268	0.65905	0.00000	Uiso	1.00
O161	O	0.41534	0.18307	0.92836	0.00000	Uiso	1.00
O162	O	0.39867	0.88706	0.86682	0.00000	Uiso	1.00
O163	O	0.39762	0.38889	0.17675	0.00000	Uiso	1.00
O164	O	0.39447	0.37952	0.87075	0.00000	Uiso	1.00

O165	O	0.39815	0.25433	0.71322	0.00000	Uiso	1.00
O166	O	0.41031	0.55854	0.65496	0.00000	Uiso	1.00
O167	O	0.46507	0.49401	0.70750	0.00000	Uiso	1.00
O168	O	0.40824	0.54453	0.29888	0.00000	Uiso	1.00
O169	O	0.40592	0.53171	0.07133	0.00000	Uiso	1.00
O170	O	0.39826	0.23007	0.14771	0.00000	Uiso	1.00
O171	O	0.39555	0.04534	0.84387	0.00000	Uiso	1.00
O172	O	0.40608	0.07380	0.10715	0.00000	Uiso	1.00
O173	O	0.41405	0.69624	0.39798	0.00000	Uiso	1.00
O174	O	0.45043	0.32147	0.80401	0.00000	Uiso	1.00
O175	O	0.45314	0.67174	0.70498	0.00000	Uiso	1.00
O176	O	0.41030	0.63377	0.87123	0.00000	Uiso	1.00
O177	O	0.44572	0.49102	0.48270	0.00000	Uiso	1.00
O178	O	0.37034	0.16778	0.53186	0.00000	Uiso	1.00
O179	O	0.42072	0.11405	0.65243	0.00000	Uiso	1.00
O180	O	0.40931	0.94055	0.64873	0.00000	Uiso	1.00
O181	O	0.39789	0.87011	0.43301	0.00000	Uiso	1.00
O182	O	0.42687	0.16824	0.41874	0.00000	Uiso	1.00
O183	O	0.39730	0.03761	0.46023	0.00000	Uiso	1.00
O184	O	0.45073	0.94562	0.49072	0.00000	Uiso	1.00
O185	O	0.40885	0.91302	0.10104	0.00000	Uiso	1.00
O186	O	0.42952	0.99319	0.27635	0.00000	Uiso	1.00
O187	O	0.39073	0.67864	0.17219	0.00000	Uiso	1.00
O188	O	0.36430	0.98319	0.23745	0.00000	Uiso	1.00
O189	O	0.44331	0.79116	0.56053	0.00000	Uiso	1.00
O190	O	0.42537	0.77256	0.00979	0.00000	Uiso	1.00
Si191	Si	0.39217	0.96089	0.77235	0.00000	Uiso	1.00
Si192	Si	0.41387	0.34024	0.76432	0.00000	Uiso	1.00
Si193	Si	0.43396	0.48376	0.62076	0.00000	Uiso	1.00
Si194	Si	0.39310	0.48613	0.18798	0.00000	Uiso	1.00
Si195	Si	0.39620	0.15848	0.04840	0.00000	Uiso	1.00
Si196	Si	0.39414	0.63980	0.31150	0.00000	Uiso	1.00
Si197	Si	0.37545	0.30901	0.15308	0.00000	Uiso	1.00
Si198	Si	0.41611	0.64204	0.72969	0.00000	Uiso	1.00
Si199	Si	0.41207	0.94844	0.50176	0.00000	Uiso	1.00
Si200	Si	0.40529	0.12660	0.52335	0.00000	Uiso	1.00
Si201	Si	0.40051	0.99145	0.17879	0.00000	Uiso	1.00
Si202	Si	0.40093	0.84611	0.00183	0.00000	Uiso	1.00
H203	H	0.46891	0.44902	0.76112	0.00000	Uiso	1.00
H204	H	0.45153	0.29286	0.88004	0.00000	Uiso	1.00
H205	H	0.46790	0.62739	0.70459	0.00000	Uiso	1.00
H206	H	0.43202	0.51170	0.41912	0.00000	Uiso	1.00
H207	H	0.43810	0.21676	0.43839	0.00000	Uiso	1.00
H208	H	0.45666	0.94718	0.40601	0.00000	Uiso	1.00
H209	H	0.43402	0.04788	0.30142	0.00000	Uiso	1.00
H210	H	0.45421	0.84221	0.54703	0.00000	Uiso	1.00
H211	H	0.45324	0.75188	0.61708	0.00000	Uiso	1.00
H212	H	0.46507	0.89749	0.97557	0.00000	Uiso	1.00
H213	H	0.46047	0.64815	0.07452	0.00000	Uiso	1.00
H214	H	0.46703	0.67538	0.92080	0.00000	Uiso	1.00
H215	H	0.49652	0.69097	0.03204	0.00000	Uiso	1.00
H216	H	0.45597	0.85863	0.19037	0.00000	Uiso	1.00
H217	H	0.48771	0.79006	0.19622	0.00000	Uiso	1.00
H218	H	0.44923	0.75678	0.22952	0.00000	Uiso	1.00
H219	H	0.47012	0.82205	0.86278	0.00000	Uiso	1.00
H220	H	0.49945	0.83873	0.97371	0.00000	Uiso	1.00
C221	C	0.46301	0.79688	0.17236	0.00000	Uiso	1.00
C222	C	0.45899	0.77577	0.03972	0.00000	Uiso	1.00
C223	C	0.47137	0.69232	0.01439	0.00000	Uiso	1.00
C224	C	0.47424	0.83736	0.95747	0.00000	Uiso	1.00

File n°19:

Al2	Al	0.35106	0.05704	0.89485	0.00000	Uiso	1.00
Al3	Al	0.35054	0.03695	0.37821	0.00000	Uiso	1.00
Al4	Al	0.34547	0.56788	0.89902	0.00000	Uiso	1.00
Al5	Al	0.34398	0.53289	0.38506	0.00000	Uiso	1.00
Al6	Al	0.34407	0.87503	0.89630	0.00000	Uiso	1.00
Al7	Al	0.34964	0.85227	0.41145	0.00000	Uiso	1.00
Al8	Al	0.35372	0.40171	0.88490	0.00000	Uiso	1.00
Al9	Al	0.32881	0.38561	0.51921	0.00000	Uiso	1.00
Al10	Al	0.30448	0.80312	0.26359	0.00000	Uiso	1.00
Al11	Al	0.30076	0.80704	0.76466	0.00000	Uiso	1.00
Al12	Al	0.30462	0.30714	0.25973	0.00000	Uiso	1.00
Al13	Al	0.30169	0.31470	0.77347	0.00000	Uiso	1.00
Al14	Al	0.30645	0.13425	0.26047	0.00000	Uiso	1.00
Al15	Al	0.30314	0.13599	0.75825	0.00000	Uiso	1.00
Al16	Al	0.29741	0.63529	0.26723	0.00000	Uiso	1.00
Al17	Al	0.29911	0.64085	0.76108	0.00000	Uiso	1.00
Al18	Al	0.21191	0.97110	0.25381	0.00000	Uiso	1.00
Al19	Al	0.21176	0.97245	0.75450	0.00000	Uiso	1.00
Al20	Al	0.20935	0.47056	0.25063	0.00000	Uiso	1.00
Al21	Al	0.21015	0.47068	0.75172	0.00000	Uiso	1.00
Al22	Al	0.32933	0.96982	0.12964	0.00000	Uiso	1.00
Al23	Al	0.32691	0.96650	0.62730	0.00000	Uiso	1.00
Al24	Al	0.32455	0.47629	0.12602	0.00000	Uiso	1.00
Al25	Al	0.33985	0.53460	0.65890	0.00000	Uiso	1.00
Al26	Al	0.28082	0.22011	0.02345	0.00000	Uiso	1.00
Al27	Al	0.28198	0.22130	0.51625	0.00000	Uiso	1.00
Al28	Al	0.28096	0.71866	0.00720	0.00000	Uiso	1.00
Al29	Al	0.28102	0.72094	0.50718	0.00000	Uiso	1.00
Al30	Al	0.34597	0.23236	0.91631	0.00000	Uiso	1.00
Al31	Al	0.35605	0.23937	0.65561	0.00000	Uiso	1.00
Al32	Al	0.35168	0.73338	0.12747	0.00000	Uiso	1.00
Al33	Al	0.35157	0.73102	0.66501	0.00000	Uiso	1.00
Al34	Al	0.21198	0.97156	0.00634	0.00000	Uiso	1.00
Al35	Al	0.21143	0.97204	0.50418	0.00000	Uiso	1.00
Al36	Al	0.21023	0.46983	0.00295	0.00000	Uiso	1.00
Al37	Al	0.20960	0.47001	0.50306	0.00000	Uiso	1.00
Al38	Al	0.28281	0.96215	0.37883	0.00000	Uiso	1.00

AI39	AI	0.28186	0.97623	0.87925	0.00000	Uiso	1.00
AI40	AI	0.27849	0.46766	0.37672	0.00000	Uiso	1.00
AI41	AI	0.28099	0.47534	0.87730	0.00000	Uiso	1.00
AI42	AI	0.23655	0.21902	0.25537	0.00000	Uiso	1.00
AI43	AI	0.23539	0.22002	0.75396	0.00000	Uiso	1.00
AI44	AI	0.23490	0.72406	0.25056	0.00000	Uiso	1.00
AI45	AI	0.23417	0.72320	0.74999	0.00000	Uiso	1.00
AI46	AI	0.26186	0.05810	0.13329	0.00000	Uiso	1.00
AI47	AI	0.26127	0.05827	0.62615	0.00000	Uiso	1.00
AI48	AI	0.25841	0.55813	0.12481	0.00000	Uiso	1.00
AI49	AI	0.25901	0.55861	0.62456	0.00000	Uiso	1.00
AI50	AI	0.26183	0.88315	0.12666	0.00000	Uiso	1.00
AI51	AI	0.25962	0.88322	0.62709	0.00000	Uiso	1.00
AI52	AI	0.25952	0.38232	0.13199	0.00000	Uiso	1.00
AI53	AI	0.25925	0.38332	0.63006	0.00000	Uiso	1.00
AI54	AI	0.21396	0.80723	0.00144	0.00000	Uiso	1.00
AI55	AI	0.21308	0.80675	0.50080	0.00000	Uiso	1.00
AI56	AI	0.21299	0.30593	0.00341	0.00000	Uiso	1.00
AI57	AI	0.21299	0.30600	0.50084	0.00000	Uiso	1.00
AI58	AI	0.21369	0.13512	0.00596	0.00000	Uiso	1.00
AI59	AI	0.21368	0.13572	0.50169	0.00000	Uiso	1.00
AI60	AI	0.21270	0.63517	0.99915	0.00000	Uiso	1.00
AI61	AI	0.21272	0.63523	0.49872	0.00000	Uiso	1.00
AI62	AI	0.40248	0.14924	0.78414	0.00000	Uiso	1.00
AI63	AI	0.35143	0.22625	0.39786	0.00000	Uiso	1.00
AI64	AI	0.39864	0.64582	0.01025	0.00000	Uiso	1.00
AI65	AI	0.40211	0.76637	0.50642	0.00000	Uiso	1.00
O66	O	0.30820	0.87818	0.38325	0.00000	Uiso	1.00
O67	O	0.30368	0.88787	0.88183	0.00000	Uiso	1.00
O68	O	0.30659	0.38898	0.38474	0.00000	Uiso	1.00
O69	O	0.30692	0.39436	0.88160	0.00000	Uiso	1.00
O70	O	0.30867	0.04425	0.36903	0.00000	Uiso	1.00
O71	O	0.30924	0.05839	0.87206	0.00000	Uiso	1.00
O72	O	0.30400	0.55081	0.37088	0.00000	Uiso	1.00
O73	O	0.30376	0.56322	0.87996	0.00000	Uiso	1.00
O74	O	0.30765	0.22405	0.38672	0.00000	Uiso	1.00
O75	O	0.30457	0.22042	0.88834	0.00000	Uiso	1.00
O76	O	0.30186	0.71585	0.37074	0.00000	Uiso	1.00
O77	O	0.30045	0.72192	0.87073	0.00000	Uiso	1.00
O78	O	0.35184	0.13474	0.31158	0.00000	Uiso	1.00
O79	O	0.35588	0.15297	0.78258	0.00000	Uiso	1.00
O80	O	0.36075	0.62565	0.38754	0.00000	Uiso	1.00
O81	O	0.34619	0.63137	0.73521	0.00000	Uiso	1.00
O82	O	0.34873	0.79974	0.26495	0.00000	Uiso	1.00
O83	O	0.34543	0.80563	0.77462	0.00000	Uiso	1.00
O84	O	0.35600	0.31170	0.02169	0.00000	Uiso	1.00
O85	O	0.41561	0.39459	0.64045	0.00000	Uiso	1.00
O86	O	0.35341	0.96393	0.75681	0.00000	Uiso	1.00
O87	O	0.35512	0.49328	0.23794	0.00000	Uiso	1.00
O88	O	0.35456	0.48736	0.78446	0.00000	Uiso	1.00
O89	O	0.30465	0.88706	0.14401	0.00000	Uiso	1.00
O90	O	0.30159	0.88666	0.64303	0.00000	Uiso	1.00
O91	O	0.30251	0.38997	0.14981	0.00000	Uiso	1.00
O92	O	0.30227	0.38135	0.63812	0.00000	Uiso	1.00
O93	O	0.30549	0.05555	0.13900	0.00000	Uiso	1.00
O94	O	0.30482	0.05578	0.63905	0.00000	Uiso	1.00
O95	O	0.30093	0.56012	0.14273	0.00000	Uiso	1.00
O96	O	0.30061	0.55891	0.64001	0.00000	Uiso	1.00
O97	O	0.30668	0.22116	0.14985	0.00000	Uiso	1.00
O98	O	0.31021	0.21850	0.64608	0.00000	Uiso	1.00
O99	O	0.30939	0.71730	0.13757	0.00000	Uiso	1.00
O100	O	0.30657	0.72383	0.63814	0.00000	Uiso	1.00
O101	O	0.35931	0.14384	0.00358	0.00000	Uiso	1.00
O102	O	0.35754	0.65028	0.99276	0.00000	Uiso	1.00
O103	O	0.36173	0.81422	0.01961	0.00000	Uiso	1.00
O104	O	0.35976	0.77935	0.52266	0.00000	Uiso	1.00
O105	O	0.34512	0.30476	0.78691	0.00000	Uiso	1.00
O106	O	0.35350	0.30297	0.51961	0.00000	Uiso	1.00
O107	O	0.35064	0.96883	0.99163	0.00000	Uiso	1.00
O108	O	0.34998	0.95783	0.49368	0.00000	Uiso	1.00
O109	O	0.35020	0.48024	0.00456	0.00000	Uiso	1.00
O110	O	0.34927	0.48011	0.52196	0.00000	Uiso	1.00
O111	O	0.20714	0.89410	0.88748	0.00000	Uiso	1.00
O112	O	0.20694	0.89349	0.38613	0.00000	Uiso	1.00
O113	O	0.20580	0.39218	0.88554	0.00000	Uiso	1.00
O114	O	0.20555	0.39232	0.38447	0.00000	Uiso	1.00
O115	O	0.20727	0.05009	0.88889	0.00000	Uiso	1.00
O116	O	0.20705	0.04986	0.38642	0.00000	Uiso	1.00
O117	O	0.20574	0.54782	0.88445	0.00000	Uiso	1.00
O118	O	0.20531	0.54773	0.38375	0.00000	Uiso	1.00
O119	O	0.21095	0.22046	0.88651	0.00000	Uiso	1.00
O120	O	0.21090	0.22066	0.38494	0.00000	Uiso	1.00
O121	O	0.21040	0.72146	0.88361	0.00000	Uiso	1.00
O122	O	0.21029	0.72184	0.38227	0.00000	Uiso	1.00
O123	O	0.26215	0.13521	0.25359	0.00000	Uiso	1.00
O124	O	0.26141	0.13781	0.74601	0.00000	Uiso	1.00
O125	O	0.25707	0.63595	0.24359	0.00000	Uiso	1.00
O126	O	0.25710	0.63729	0.74183	0.00000	Uiso	1.00
O127	O	0.26170	0.80403	0.24292	0.00000	Uiso	1.00
O128	O	0.25846	0.80743	0.74601	0.00000	Uiso	1.00
O129	O	0.26074	0.30527	0.25416	0.00000	Uiso	1.00
O130	O	0.25984	0.30508	0.75079	0.00000	Uiso	1.00
O131	O	0.25642	0.96842	0.25014	0.00000	Uiso	1.00
O132	O	0.25571	0.97390	0.75027	0.00000	Uiso	1.00
O133	O	0.25338	0.47022	0.24795	0.00000	Uiso	1.00
O134	O	0.25437	0.47040	0.74746	0.00000	Uiso	1.00
O135	O	0.21592	0.89300	0.12150	0.00000	Uiso	1.00
O136	O	0.21497	0.89461	0.62121	0.00000	Uiso	1.00
O137	O	0.21420	0.39217	0.12082	0.00000	Uiso	1.00
O138	O	0.21407	0.39200	0.62043	0.00000	Uiso	1.00
O139	O	0.21590	0.04853	0.12485	0.00000	Uiso	1.00

O140	O	0.21583	0.04998	0.62089	0.00000	Uiso	1.00
O141	O	0.21366	0.54798	0.11865	0.00000	Uiso	1.00
O142	O	0.21380	0.54805	0.61841	0.00000	Uiso	1.00
O143	O	0.20848	0.21991	0.12777	0.00000	Uiso	1.00
O144	O	0.20818	0.22101	0.62578	0.00000	Uiso	1.00
O145	O	0.20815	0.72182	0.12286	0.00000	Uiso	1.00
O146	O	0.20752	0.72170	0.62177	0.00000	Uiso	1.00
O147	O	0.25600	0.13646	0.01719	0.00000	Uiso	1.00
O148	O	0.25648	0.13831	0.51274	0.00000	Uiso	1.00
O149	O	0.25471	0.63737	0.01157	0.00000	Uiso	1.00
O150	O	0.25487	0.63733	0.50809	0.00000	Uiso	1.00
O151	O	0.25632	0.80362	0.01316	0.00000	Uiso	1.00
O152	O	0.25525	0.80440	0.51081	0.00000	Uiso	1.00
O153	O	0.25541	0.30358	0.01769	0.00000	Uiso	1.00
O154	O	0.25553	0.30338	0.51503	0.00000	Uiso	1.00
O155	O	0.25884	0.97248	0.01255	0.00000	Uiso	1.00
O156	O	0.25840	0.97017	0.50951	0.00000	Uiso	1.00
O157	O	0.25710	0.47055	0.01117	0.00000	Uiso	1.00
O158	O	0.25616	0.46930	0.51001	0.00000	Uiso	1.00
O159	O	0.35312	0.29972	0.26951	0.00000	Uiso	1.00
O160	O	0.39613	0.71123	0.65493	0.00000	Uiso	1.00
O161	O	0.41563	0.18074	0.92827	0.00000	Uiso	1.00
O162	O	0.39825	0.88274	0.86795	0.00000	Uiso	1.00
O163	O	0.39689	0.39511	0.16662	0.00000	Uiso	1.00
O164	O	0.39495	0.37896	0.87018	0.00000	Uiso	1.00
O165	O	0.39798	0.25221	0.71381	0.00000	Uiso	1.00
O166	O	0.40975	0.55629	0.64065	0.00000	Uiso	1.00
O167	O	0.46407	0.48903	0.69514	0.00000	Uiso	1.00
O168	O	0.40808	0.54624	0.29485	0.00000	Uiso	1.00
O169	O	0.40708	0.54476	0.06865	0.00000	Uiso	1.00
O170	O	0.39868	0.23187	0.14421	0.00000	Uiso	1.00
O171	O	0.39533	0.04323	0.84411	0.00000	Uiso	1.00
O172	O	0.40557	0.07081	0.10610	0.00000	Uiso	1.00
O173	O	0.41508	0.69778	0.39666	0.00000	Uiso	1.00
O174	O	0.45050	0.32167	0.79843	0.00000	Uiso	1.00
O175	O	0.45344	0.66641	0.69054	0.00000	Uiso	1.00
O176	O	0.41181	0.62520	0.85993	0.00000	Uiso	1.00
O177	O	0.44366	0.48282	0.47067	0.00000	Uiso	1.00
O178	O	0.36990	0.16632	0.53182	0.00000	Uiso	1.00
O179	O	0.42055	0.11279	0.65187	0.00000	Uiso	1.00
O180	O	0.40877	0.94027	0.64934	0.00000	Uiso	1.00
O181	O	0.39776	0.87078	0.43219	0.00000	Uiso	1.00
O182	O	0.42636	0.17196	0.42070	0.00000	Uiso	1.00
O183	O	0.39783	0.03822	0.45676	0.00000	Uiso	1.00
O184	O	0.45029	0.94636	0.49002	0.00000	Uiso	1.00
O185	O	0.40932	0.90455	0.09827	0.00000	Uiso	1.00
O186	O	0.41756	0.75207	0.00716	0.00000	Uiso	1.00
O187	O	0.42996	0.98836	0.27056	0.00000	Uiso	1.00
O188	O	0.38641	0.67785	0.18123	0.00000	Uiso	1.00
O189	O	0.36463	0.98073	0.23547	0.00000	Uiso	1.00
O190	O	0.44298	0.79326	0.56105	0.00000	Uiso	1.00
Si191	Si	0.39186	0.95783	0.77484	0.00000	Uiso	1.00
Si192	Si	0.41341	0.33861	0.76232	0.00000	Uiso	1.00
Si193	Si	0.43238	0.47933	0.60997	0.00000	Uiso	1.00
Si194	Si	0.39205	0.49316	0.17862	0.00000	Uiso	1.00
Si195	Si	0.39633	0.15717	0.04899	0.00000	Uiso	1.00
Si196	Si	0.39335	0.64066	0.31714	0.00000	Uiso	1.00
Si197	Si	0.37592	0.31155	0.15007	0.00000	Uiso	1.00
Si198	Si	0.41619	0.63838	0.71865	0.00000	Uiso	1.00
Si199	Si	0.41156	0.94883	0.50256	0.00000	Uiso	1.00
Si200	Si	0.40512	0.12670	0.52301	0.00000	Uiso	1.00
Si201	Si	0.40082	0.98521	0.17312	0.00000	Uiso	1.00
Si202	Si	0.39923	0.83586	0.00128	0.00000	Uiso	1.00
H203	H	0.46801	0.44184	0.74450	0.00000	Uiso	1.00
H204	H	0.45218	0.29179	0.87323	0.00000	Uiso	1.00
H205	H	0.46732	0.62090	0.67985	0.00000	Uiso	1.00
H206	H	0.42986	0.50638	0.40898	0.00000	Uiso	1.00
H207	H	0.43667	0.22119	0.44366	0.00000	Uiso	1.00
H208	H	0.45537	0.94733	0.40426	0.00000	Uiso	1.00
H209	H	0.43387	0.04350	0.29444	0.00000	Uiso	1.00
H210	H	0.45392	0.84424	0.54688	0.00000	Uiso	1.00
H211	H	0.45340	0.75210	0.61251	0.00000	Uiso	1.00
H212	H	0.49448	0.75625	0.03787	0.00000	Uiso	1.00
H213	H	0.46225	0.60740	0.89975	0.00000	Uiso	1.00
H214	H	0.49603	0.55049	0.92852	0.00000	Uiso	1.00
H215	H	0.47189	0.59308	0.24322	0.00000	Uiso	1.00
H216	H	0.48000	0.73164	0.18904	0.00000	Uiso	1.00
H217	H	0.45456	0.73555	0.06002	0.00000	Uiso	1.00
H218	H	0.48363	0.51643	0.13471	0.00000	Uiso	1.00
H219	H	0.44695	0.56102	0.12162	0.00000	Uiso	1.00
H220	H	0.49884	0.65503	0.88452	0.00000	Uiso	1.00
C221	C	0.48629	0.61062	0.93809	0.00000	Uiso	1.00
C222	C	0.48135	0.63458	0.06342	0.00000	Uiso	1.00
C223	C	0.47932	0.71816	0.09275	0.00000	Uiso	1.00
C224	C	0.47224	0.57429	0.14904	0.00000	Uiso	1.00

File n°20 :

H1	H	0.44235	0.77376	0.03235	0.00000	Uiso	1.00
H2	H	0.46867	0.44769	0.37987	0.00000	Uiso	1.00
H3	H	0.45171	0.29409	0.43981	0.00000	Uiso	1.00
H4	H	0.46832	0.62850	0.35344	0.00000	Uiso	1.00
H5	H	0.43167	0.51175	0.20972	0.00000	Uiso	1.00
H6	H	0.43831	0.21583	0.21856	0.00000	Uiso	1.00
H7	H	0.45662	0.94840	0.20317	0.00000	Uiso	1.00
H8	H	0.43379	0.04890	0.15085	0.00000	Uiso	1.00
H9	H	0.45424	0.84226	0.27356	0.00000	Uiso	1.00
H10	H	0.45348	0.75202	0.30830	0.00000	Uiso	1.00
Al11	Al	0.35125	0.05697	0.44702	0.00000	Uiso	1.00
Al12	Al	0.35014	0.03644	0.19026	0.00000	Uiso	1.00

AI13	AI	0.34387	0.56554	0.45015	0.00000	Uiso	1.00
AI14	AI	0.34381	0.53288	0.19082	0.00000	Uiso	1.00
AI15	AI	0.34466	0.87468	0.44839	0.00000	Uiso	1.00
AI16	AI	0.34995	0.85057	0.20542	0.00000	Uiso	1.00
AI17	AI	0.35317	0.40132	0.44196	0.00000	Uiso	1.00
AI18	AI	0.32886	0.38701	0.25958	0.00000	Uiso	1.00
AI19	AI	0.30476	0.80220	0.13084	0.00000	Uiso	1.00
AI20	AI	0.30078	0.80741	0.38246	0.00000	Uiso	1.00
AI21	AI	0.30451	0.30659	0.13017	0.00000	Uiso	1.00
AI22	AI	0.30163	0.31399	0.38617	0.00000	Uiso	1.00
AI23	AI	0.30633	0.13400	0.13070	0.00000	Uiso	1.00
AI24	AI	0.30315	0.13613	0.37925	0.00000	Uiso	1.00
AI25	AI	0.29763	0.63498	0.13379	0.00000	Uiso	1.00
AI26	AI	0.29900	0.64138	0.38019	0.00000	Uiso	1.00
AI27	AI	0.21191	0.97110	0.12691	0.00000	Uiso	1.00
AI28	AI	0.21176	0.97245	0.37725	0.00000	Uiso	1.00
AI29	AI	0.20935	0.47056	0.12532	0.00000	Uiso	1.00
AI30	AI	0.21015	0.47068	0.37586	0.00000	Uiso	1.00
AI31	AI	0.32937	0.97028	0.06496	0.00000	Uiso	1.00
AI32	AI	0.32684	0.96669	0.31355	0.00000	Uiso	1.00
AI33	AI	0.32451	0.47491	0.06382	0.00000	Uiso	1.00
AI34	AI	0.33980	0.53552	0.32944	0.00000	Uiso	1.00
AI35	AI	0.28083	0.22009	0.01185	0.00000	Uiso	1.00
AI36	AI	0.28185	0.22139	0.25848	0.00000	Uiso	1.00
AI37	AI	0.28101	0.71862	0.00362	0.00000	Uiso	1.00
AI38	AI	0.28101	0.72101	0.25350	0.00000	Uiso	1.00
AI39	AI	0.34596	0.23201	0.45830	0.00000	Uiso	1.00
AI40	AI	0.35641	0.24076	0.32813	0.00000	Uiso	1.00
AI41	AI	0.35277	0.73172	0.06240	0.00000	Uiso	1.00
AI42	AI	0.35174	0.73137	0.33319	0.00000	Uiso	1.00
AI43	AI	0.21198	0.97156	0.00317	0.00000	Uiso	1.00
AI44	AI	0.21143	0.97204	0.25209	0.00000	Uiso	1.00
AI45	AI	0.21023	0.46983	0.00148	0.00000	Uiso	1.00
AI46	AI	0.20960	0.47001	0.25153	0.00000	Uiso	1.00
AI47	AI	0.28282	0.96087	0.18939	0.00000	Uiso	1.00
AI48	AI	0.28195	0.97604	0.43965	0.00000	Uiso	1.00
AI49	AI	0.27837	0.46745	0.18842	0.00000	Uiso	1.00
AI50	AI	0.28071	0.47437	0.43859	0.00000	Uiso	1.00
AI51	AI	0.23655	0.21902	0.12768	0.00000	Uiso	1.00
AI52	AI	0.23539	0.22002	0.37698	0.00000	Uiso	1.00
AI53	AI	0.23490	0.72406	0.12528	0.00000	Uiso	1.00
AI54	AI	0.23417	0.72320	0.37500	0.00000	Uiso	1.00
AI55	AI	0.26186	0.05810	0.06665	0.00000	Uiso	1.00
AI56	AI	0.26127	0.05827	0.31307	0.00000	Uiso	1.00
AI57	AI	0.25841	0.55813	0.06240	0.00000	Uiso	1.00
AI58	AI	0.25901	0.55861	0.31228	0.00000	Uiso	1.00
AI59	AI	0.26183	0.88315	0.06333	0.00000	Uiso	1.00
AI60	AI	0.25962	0.88322	0.31355	0.00000	Uiso	1.00
AI61	AI	0.25952	0.38232	0.06600	0.00000	Uiso	1.00
AI62	AI	0.25925	0.38332	0.31503	0.00000	Uiso	1.00
AI63	AI	0.21396	0.80723	0.00072	0.00000	Uiso	1.00
AI64	AI	0.21308	0.80675	0.25040	0.00000	Uiso	1.00
AI65	AI	0.21299	0.30593	0.00170	0.00000	Uiso	1.00
AI66	AI	0.21299	0.30600	0.25042	0.00000	Uiso	1.00
AI67	AI	0.21369	0.13512	0.00298	0.00000	Uiso	1.00
AI68	AI	0.21368	0.13572	0.25084	0.00000	Uiso	1.00
AI69	AI	0.21270	0.63517	0.49958	0.00000	Uiso	1.00
AI70	AI	0.21272	0.63523	0.24936	0.00000	Uiso	1.00
AI71	AI	0.40273	0.15173	0.39193	0.00000	Uiso	1.00
AI72	AI	0.35104	0.22616	0.19981	0.00000	Uiso	1.00
AI73	AI	0.39708	0.62691	0.00979	0.00000	Uiso	1.00
AI74	AI	0.40242	0.76507	0.25422	0.00000	Uiso	1.00
O75	O	0.30862	0.87706	0.19065	0.00000	Uiso	1.00
O76	O	0.30414	0.88795	0.44114	0.00000	Uiso	1.00
O77	O	0.30659	0.38926	0.19252	0.00000	Uiso	1.00
O78	O	0.30644	0.39326	0.44030	0.00000	Uiso	1.00
O79	O	0.30839	0.04341	0.18480	0.00000	Uiso	1.00
O80	O	0.30939	0.05815	0.43595	0.00000	Uiso	1.00
O81	O	0.30380	0.55065	0.18583	0.00000	Uiso	1.00
O82	O	0.30274	0.56335	0.43938	0.00000	Uiso	1.00
O83	O	0.30736	0.22377	0.19389	0.00000	Uiso	1.00
O84	O	0.30457	0.21993	0.44428	0.00000	Uiso	1.00
O85	O	0.30178	0.71602	0.18520	0.00000	Uiso	1.00
O86	O	0.30068	0.72217	0.43548	0.00000	Uiso	1.00
O87	O	0.35148	0.13431	0.15713	0.00000	Uiso	1.00
O88	O	0.35607	0.15416	0.39112	0.00000	Uiso	1.00
O89	O	0.35910	0.62717	0.18058	0.00000	Uiso	1.00
O90	O	0.34601	0.63194	0.36837	0.00000	Uiso	1.00
O91	O	0.34958	0.79774	0.13132	0.00000	Uiso	1.00
O92	O	0.34563	0.80667	0.38720	0.00000	Uiso	1.00
O93	O	0.35619	0.30976	0.01187	0.00000	Uiso	1.00
O94	O	0.41655	0.39866	0.32266	0.00000	Uiso	1.00
O95	O	0.35367	0.96649	0.37762	0.00000	Uiso	1.00
O96	O	0.35539	0.48658	0.12002	0.00000	Uiso	1.00
O97	O	0.35400	0.48738	0.39202	0.00000	Uiso	1.00
O98	O	0.30494	0.88681	0.07164	0.00000	Uiso	1.00
O99	O	0.30155	0.88690	0.32173	0.00000	Uiso	1.00
O100	O	0.30230	0.38909	0.07511	0.00000	Uiso	1.00
O101	O	0.30229	0.38189	0.31891	0.00000	Uiso	1.00
O102	O	0.30546	0.05549	0.06965	0.00000	Uiso	1.00
O103	O	0.30483	0.05611	0.31940	0.00000	Uiso	1.00
O104	O	0.30112	0.55957	0.07192	0.00000	Uiso	1.00
O105	O	0.30064	0.55976	0.31956	0.00000	Uiso	1.00
O106	O	0.30655	0.22059	0.07516	0.00000	Uiso	1.00
O107	O	0.31015	0.21905	0.32337	0.00000	Uiso	1.00
O108	O	0.30991	0.71783	0.06809	0.00000	Uiso	1.00
O109	O	0.30663	0.72444	0.31913	0.00000	Uiso	1.00
O110	O	0.35924	0.14289	0.00165	0.00000	Uiso	1.00
O111	O	0.35660	0.64474	0.00034	0.00000	Uiso	1.00
O112	O	0.36490	0.81138	0.00819	0.00000	Uiso	1.00
O113	O	0.35994	0.77690	0.26087	0.00000	Uiso	1.00

O114	O	0.34501	0.30495	0.39382	0.00000	Uiso	1.00
O115	O	0.35333	0.30397	0.26015	0.00000	Uiso	1.00
O116	O	0.35086	0.96802	0.49593	0.00000	Uiso	1.00
O117	O	0.34963	0.95617	0.24681	0.00000	Uiso	1.00
O118	O	0.34826	0.47821	0.00110	0.00000	Uiso	1.00
O119	O	0.34948	0.48263	0.26033	0.00000	Uiso	1.00
O120	O	0.20714	0.89410	0.44374	0.00000	Uiso	1.00
O121	O	0.20694	0.89349	0.19307	0.00000	Uiso	1.00
O122	O	0.20580	0.39218	0.44277	0.00000	Uiso	1.00
O123	O	0.20555	0.39232	0.19223	0.00000	Uiso	1.00
O124	O	0.20727	0.05009	0.44444	0.00000	Uiso	1.00
O125	O	0.20705	0.04986	0.19321	0.00000	Uiso	1.00
O126	O	0.20574	0.54782	0.44223	0.00000	Uiso	1.00
O127	O	0.20531	0.54773	0.19188	0.00000	Uiso	1.00
O128	O	0.21095	0.22046	0.44326	0.00000	Uiso	1.00
O129	O	0.21090	0.22066	0.19247	0.00000	Uiso	1.00
O130	O	0.21040	0.72146	0.44180	0.00000	Uiso	1.00
O131	O	0.21029	0.72184	0.19113	0.00000	Uiso	1.00
O132	O	0.26215	0.13521	0.12680	0.00000	Uiso	1.00
O133	O	0.26141	0.13781	0.37300	0.00000	Uiso	1.00
O134	O	0.25707	0.63595	0.12179	0.00000	Uiso	1.00
O135	O	0.25710	0.63729	0.37091	0.00000	Uiso	1.00
O136	O	0.26170	0.80403	0.12146	0.00000	Uiso	1.00
O137	O	0.25846	0.80743	0.37301	0.00000	Uiso	1.00
O138	O	0.26074	0.30527	0.12708	0.00000	Uiso	1.00
O139	O	0.25984	0.30508	0.37539	0.00000	Uiso	1.00
O140	O	0.25642	0.96842	0.12507	0.00000	Uiso	1.00
O141	O	0.25571	0.97390	0.37513	0.00000	Uiso	1.00
O142	O	0.25338	0.47022	0.12398	0.00000	Uiso	1.00
O143	O	0.25437	0.47040	0.37373	0.00000	Uiso	1.00
O144	O	0.21592	0.89300	0.06075	0.00000	Uiso	1.00
O145	O	0.21497	0.89461	0.31060	0.00000	Uiso	1.00
O146	O	0.21420	0.39217	0.06041	0.00000	Uiso	1.00
O147	O	0.21407	0.39200	0.31022	0.00000	Uiso	1.00
O148	O	0.21590	0.04853	0.06243	0.00000	Uiso	1.00
O149	O	0.21583	0.04998	0.31045	0.00000	Uiso	1.00
O150	O	0.21366	0.54798	0.05933	0.00000	Uiso	1.00
O151	O	0.21380	0.54805	0.30921	0.00000	Uiso	1.00
O152	O	0.20848	0.21991	0.06388	0.00000	Uiso	1.00
O153	O	0.20818	0.22101	0.31289	0.00000	Uiso	1.00
O154	O	0.20815	0.72182	0.06143	0.00000	Uiso	1.00
O155	O	0.20752	0.72170	0.31089	0.00000	Uiso	1.00
O156	O	0.25600	0.13646	0.00859	0.00000	Uiso	1.00
O157	O	0.25648	0.13831	0.25637	0.00000	Uiso	1.00
O158	O	0.25471	0.63737	0.00579	0.00000	Uiso	1.00
O159	O	0.25487	0.63733	0.25404	0.00000	Uiso	1.00
O160	O	0.25632	0.80362	0.00658	0.00000	Uiso	1.00
O161	O	0.25525	0.80440	0.25541	0.00000	Uiso	1.00
O162	O	0.25541	0.30358	0.00884	0.00000	Uiso	1.00
O163	O	0.25553	0.30338	0.25751	0.00000	Uiso	1.00
O164	O	0.25884	0.97248	0.00628	0.00000	Uiso	1.00
O165	O	0.25840	0.97017	0.25476	0.00000	Uiso	1.00
O166	O	0.25710	0.47055	0.00558	0.00000	Uiso	1.00
O167	O	0.25616	0.46930	0.25501	0.00000	Uiso	1.00
O168	O	0.35221	0.29808	0.13546	0.00000	Uiso	1.00
O169	O	0.39636	0.71351	0.33001	0.00000	Uiso	1.00
O170	O	0.41534	0.18300	0.46432	0.00000	Uiso	1.00
O171	O	0.39821	0.88752	0.43360	0.00000	Uiso	1.00
O172	O	0.39775	0.38819	0.08848	0.00000	Uiso	1.00
O173	O	0.39437	0.37958	0.43585	0.00000	Uiso	1.00
O174	O	0.39820	0.25452	0.35681	0.00000	Uiso	1.00
O175	O	0.41027	0.55966	0.32768	0.00000	Uiso	1.00
O176	O	0.46470	0.49370	0.35410	0.00000	Uiso	1.00
O177	O	0.40835	0.54445	0.14866	0.00000	Uiso	1.00
O178	O	0.40535	0.53068	0.03513	0.00000	Uiso	1.00
O179	O	0.39823	0.22926	0.07406	0.00000	Uiso	1.00
O180	O	0.39560	0.04554	0.42170	0.00000	Uiso	1.00
O181	O	0.40608	0.07263	0.05296	0.00000	Uiso	1.00
O182	O	0.41387	0.69542	0.19891	0.00000	Uiso	1.00
O183	O	0.45036	0.32257	0.40178	0.00000	Uiso	1.00
O184	O	0.45343	0.67249	0.35267	0.00000	Uiso	1.00
O185	O	0.41090	0.63368	0.43607	0.00000	Uiso	1.00
O186	O	0.44533	0.49103	0.24153	0.00000	Uiso	1.00
O187	O	0.37047	0.16813	0.26594	0.00000	Uiso	1.00
O188	O	0.42082	0.11432	0.32609	0.00000	Uiso	1.00
O189	O	0.40927	0.94017	0.32440	0.00000	Uiso	1.00
O190	O	0.39800	0.86985	0.21658	0.00000	Uiso	1.00
O191	O	0.42690	0.16749	0.20899	0.00000	Uiso	1.00
O192	O	0.39710	0.03746	0.23037	0.00000	Uiso	1.00
O193	O	0.45071	0.94614	0.24552	0.00000	Uiso	1.00
O194	O	0.40939	0.91105	0.05180	0.00000	Uiso	1.00
O195	O	0.42572	0.77391	0.00122	0.00000	Uiso	1.00
O196	O	0.42960	0.99392	0.13861	0.00000	Uiso	1.00
O197	O	0.39134	0.67940	0.08524	0.00000	Uiso	1.00
O198	O	0.36447	0.98277	0.11866	0.00000	Uiso	1.00
O199	O	0.44383	0.79024	0.27878	0.00000	Uiso	1.00
Si200	Si	0.39211	0.96113	0.38606	0.00000	Uiso	1.00
Si201	Si	0.41367	0.34069	0.38236	0.00000	Uiso	1.00
Si202	Si	0.43358	0.48430	0.31065	0.00000	Uiso	1.00
Si203	Si	0.39296	0.48532	0.09379	0.00000	Uiso	1.00
Si204	Si	0.39620	0.15780	0.02426	0.00000	Uiso	1.00
Si205	Si	0.39419	0.63960	0.15482	0.00000	Uiso	1.00
Si206	Si	0.37551	0.30841	0.07658	0.00000	Uiso	1.00
Si207	Si	0.41649	0.64293	0.36524	0.00000	Uiso	1.00
Si208	Si	0.41207	0.94837	0.25092	0.00000	Uiso	1.00
Si209	Si	0.40530	0.12653	0.26160	0.00000	Uiso	1.00
Si210	Si	0.40080	0.99058	0.08950	0.00000	Uiso	1.00
Si211	Si	0.40079	0.84635	0.00082	0.00000	Uiso	1.00
C212	C	0.47330	0.63277	0.54782	0.00000	Uiso	1.00
C213	C	0.48466	0.71647	0.55759	0.00000	Uiso	1.00
C214	C	0.47327	0.76342	0.60154	0.00000	Uiso	1.00

C215	C	0.50870	0.74529	0.51367	0.00000	Uiso	1.00
H216	H	0.45595	0.74179	0.63358	0.00000	Uiso	1.00
H217	H	0.48182	0.82438	0.60706	0.00000	Uiso	1.00
H218	H	0.44235	0.77376	0.53235	0.00000	Uiso	1.00
H219	H	0.45605	0.61429	0.58143	0.00000	Uiso	1.00
H220	H	0.49280	0.59015	0.54964	0.00000	Uiso	1.00
H221	H	0.46326	0.62668	0.50236	0.00000	Uiso	1.00
H222	H	0.49958	0.74186	0.46742	0.00000	Uiso	1.00
H223	H	0.52938	0.70644	0.51519	0.00000	Uiso	1.00
H224	H	0.46867	0.44769	0.87987	0.00000	Uiso	1.00
H225	H	0.45171	0.29409	0.93981	0.00000	Uiso	1.00
H226	H	0.46832	0.62850	0.85344	0.00000	Uiso	1.00
H227	H	0.43167	0.51175	0.70972	0.00000	Uiso	1.00
H228	H	0.43831	0.21583	0.71856	0.00000	Uiso	1.00
H229	H	0.45662	0.94840	0.70317	0.00000	Uiso	1.00
H230	H	0.51594	0.80689	0.52295	0.00000	Uiso	1.00
H231	H	0.43379	0.04890	0.65085	0.00000	Uiso	1.00
H232	H	0.45424	0.84226	0.77356	0.00000	Uiso	1.00
H233	H	0.45348	0.75202	0.80830	0.00000	Uiso	1.00
AI234	AI	0.35125	0.05697	0.94702	0.00000	Uiso	1.00
AI235	AI	0.35014	0.03644	0.69026	0.00000	Uiso	1.00
AI236	AI	0.34387	0.56554	0.95015	0.00000	Uiso	1.00
AI237	AI	0.34381	0.53288	0.69082	0.00000	Uiso	1.00
AI238	AI	0.34466	0.87468	0.94839	0.00000	Uiso	1.00
AI239	AI	0.34995	0.85057	0.70542	0.00000	Uiso	1.00
AI240	AI	0.35317	0.40132	0.94196	0.00000	Uiso	1.00
AI241	AI	0.32886	0.38701	0.75958	0.00000	Uiso	1.00
AI242	AI	0.30476	0.80220	0.63084	0.00000	Uiso	1.00
AI243	AI	0.30078	0.80741	0.88246	0.00000	Uiso	1.00
AI244	AI	0.30451	0.30659	0.63017	0.00000	Uiso	1.00
AI245	AI	0.30163	0.31399	0.88617	0.00000	Uiso	1.00
AI246	AI	0.30633	0.13400	0.63070	0.00000	Uiso	1.00
AI247	AI	0.30315	0.13613	0.87925	0.00000	Uiso	1.00
AI248	AI	0.29763	0.63498	0.63379	0.00000	Uiso	1.00
AI249	AI	0.29900	0.64138	0.88019	0.00000	Uiso	1.00
AI250	AI	0.21191	0.97110	0.62691	0.00000	Uiso	1.00
AI251	AI	0.21176	0.97245	0.87725	0.00000	Uiso	1.00
AI252	AI	0.20935	0.47056	0.62532	0.00000	Uiso	1.00
AI253	AI	0.21015	0.47068	0.87586	0.00000	Uiso	1.00
AI254	AI	0.32937	0.97028	0.56496	0.00000	Uiso	1.00
AI255	AI	0.32684	0.96669	0.81355	0.00000	Uiso	1.00
AI256	AI	0.32451	0.47491	0.56382	0.00000	Uiso	1.00
AI257	AI	0.33980	0.53552	0.82944	0.00000	Uiso	1.00
AI258	AI	0.28083	0.22009	0.51185	0.00000	Uiso	1.00
AI259	AI	0.28185	0.22139	0.75848	0.00000	Uiso	1.00
AI260	AI	0.28101	0.71862	0.50362	0.00000	Uiso	1.00
AI261	AI	0.28101	0.72101	0.75350	0.00000	Uiso	1.00
AI262	AI	0.34596	0.23201	0.95830	0.00000	Uiso	1.00
AI263	AI	0.35641	0.24076	0.82813	0.00000	Uiso	1.00
AI264	AI	0.35277	0.73172	0.56240	0.00000	Uiso	1.00
AI265	AI	0.35174	0.73137	0.83319	0.00000	Uiso	1.00
AI266	AI	0.21198	0.97156	0.50317	0.00000	Uiso	1.00
AI267	AI	0.21143	0.97204	0.75209	0.00000	Uiso	1.00
AI268	AI	0.21023	0.46983	0.50148	0.00000	Uiso	1.00
AI269	AI	0.20960	0.47001	0.75153	0.00000	Uiso	1.00
AI270	AI	0.28282	0.96087	0.68939	0.00000	Uiso	1.00
AI271	AI	0.28195	0.97604	0.93965	0.00000	Uiso	1.00
AI272	AI	0.27837	0.46745	0.68842	0.00000	Uiso	1.00
AI273	AI	0.28071	0.47437	0.93859	0.00000	Uiso	1.00
AI274	AI	0.23655	0.21902	0.62768	0.00000	Uiso	1.00
AI275	AI	0.23539	0.22002	0.87698	0.00000	Uiso	1.00
AI276	AI	0.23490	0.72406	0.62528	0.00000	Uiso	1.00
AI277	AI	0.23417	0.72320	0.87500	0.00000	Uiso	1.00
AI278	AI	0.26186	0.05810	0.56665	0.00000	Uiso	1.00
AI279	AI	0.26127	0.05827	0.81307	0.00000	Uiso	1.00
AI280	AI	0.25841	0.55813	0.56240	0.00000	Uiso	1.00
AI281	AI	0.25901	0.55861	0.81228	0.00000	Uiso	1.00
AI282	AI	0.26183	0.88315	0.56333	0.00000	Uiso	1.00
AI283	AI	0.25962	0.88322	0.81355	0.00000	Uiso	1.00
AI284	AI	0.25952	0.38232	0.56600	0.00000	Uiso	1.00
AI285	AI	0.25925	0.38332	0.81503	0.00000	Uiso	1.00
AI286	AI	0.21396	0.80723	0.50072	0.00000	Uiso	1.00
AI287	AI	0.21308	0.80675	0.75040	0.00000	Uiso	1.00
AI288	AI	0.21299	0.30593	0.50170	0.00000	Uiso	1.00
AI289	AI	0.21299	0.30600	0.75042	0.00000	Uiso	1.00
AI290	AI	0.21369	0.13512	0.50298	0.00000	Uiso	1.00
AI291	AI	0.21368	0.13572	0.75084	0.00000	Uiso	1.00
AI292	AI	0.21270	0.63517	0.99958	0.00000	Uiso	1.00
AI293	AI	0.21272	0.63523	0.74936	0.00000	Uiso	1.00
AI294	AI	0.40273	0.15173	0.89193	0.00000	Uiso	1.00
AI295	AI	0.35104	0.22616	0.69981	0.00000	Uiso	1.00
AI296	AI	0.39708	0.62691	0.50979	0.00000	Uiso	1.00
AI297	AI	0.40242	0.76507	0.75422	0.00000	Uiso	1.00
O298	O	0.30862	0.87706	0.69065	0.00000	Uiso	1.00
O299	O	0.30414	0.88795	0.94114	0.00000	Uiso	1.00
O300	O	0.30659	0.38926	0.69252	0.00000	Uiso	1.00
O301	O	0.30644	0.39326	0.94030	0.00000	Uiso	1.00
O302	O	0.30839	0.04341	0.68480	0.00000	Uiso	1.00
O303	O	0.30939	0.05815	0.93595	0.00000	Uiso	1.00
O304	O	0.30380	0.55065	0.68583	0.00000	Uiso	1.00
O305	O	0.30274	0.56335	0.93938	0.00000	Uiso	1.00
O306	O	0.30736	0.22377	0.69389	0.00000	Uiso	1.00
O307	O	0.30457	0.21993	0.94428	0.00000	Uiso	1.00
O308	O	0.30178	0.71602	0.68520	0.00000	Uiso	1.00
O309	O	0.30068	0.72217	0.93548	0.00000	Uiso	1.00
O310	O	0.35148	0.13431	0.65713	0.00000	Uiso	1.00
O311	O	0.35607	0.15416	0.89112	0.00000	Uiso	1.00
O312	O	0.35910	0.62717	0.68058	0.00000	Uiso	1.00
O313	O	0.34601	0.63194	0.86837	0.00000	Uiso	1.00
O314	O	0.34958	0.79774	0.63132	0.00000	Uiso	1.00
O315	O	0.34563	0.80667	0.88720	0.00000	Uiso	1.00

O316	O	0.35619	0.30976	0.51187	0.00000	Uiso	1.00
O317	O	0.41655	0.39866	0.82266	0.00000	Uiso	1.00
O318	O	0.35367	0.96649	0.87762	0.00000	Uiso	1.00
O319	O	0.35539	0.48658	0.62002	0.00000	Uiso	1.00
O320	O	0.35400	0.48738	0.89202	0.00000	Uiso	1.00
O321	O	0.30494	0.88681	0.57164	0.00000	Uiso	1.00
O322	O	0.30155	0.88690	0.82173	0.00000	Uiso	1.00
O323	O	0.30230	0.38909	0.57511	0.00000	Uiso	1.00
O324	O	0.30229	0.38189	0.81891	0.00000	Uiso	1.00
O325	O	0.30546	0.05549	0.56965	0.00000	Uiso	1.00
O326	O	0.30483	0.05611	0.81940	0.00000	Uiso	1.00
O327	O	0.30112	0.55957	0.57192	0.00000	Uiso	1.00
O328	O	0.30064	0.55976	0.81956	0.00000	Uiso	1.00
O329	O	0.30655	0.22059	0.57516	0.00000	Uiso	1.00
O330	O	0.31015	0.21905	0.82337	0.00000	Uiso	1.00
O331	O	0.30991	0.71783	0.56809	0.00000	Uiso	1.00
O332	O	0.30663	0.72444	0.81913	0.00000	Uiso	1.00
O333	O	0.35924	0.14289	0.50165	0.00000	Uiso	1.00
O334	O	0.35660	0.64474	0.50034	0.00000	Uiso	1.00
O335	O	0.36490	0.81138	0.50819	0.00000	Uiso	1.00
O336	O	0.35994	0.77690	0.76087	0.00000	Uiso	1.00
O337	O	0.34501	0.30495	0.89382	0.00000	Uiso	1.00
O338	O	0.35333	0.30397	0.76015	0.00000	Uiso	1.00
O339	O	0.35086	0.96802	0.99593	0.00000	Uiso	1.00
O340	O	0.34963	0.95617	0.74681	0.00000	Uiso	1.00
O341	O	0.34826	0.47821	0.50110	0.00000	Uiso	1.00
O342	O	0.34948	0.48263	0.76033	0.00000	Uiso	1.00
O343	O	0.20714	0.89410	0.94374	0.00000	Uiso	1.00
O344	O	0.20694	0.89349	0.69307	0.00000	Uiso	1.00
O345	O	0.20580	0.39218	0.94277	0.00000	Uiso	1.00
O346	O	0.20555	0.39232	0.69223	0.00000	Uiso	1.00
O347	O	0.20727	0.05009	0.94444	0.00000	Uiso	1.00
O348	O	0.20705	0.04986	0.69321	0.00000	Uiso	1.00
O349	O	0.20574	0.54782	0.94223	0.00000	Uiso	1.00
O350	O	0.20531	0.54773	0.69188	0.00000	Uiso	1.00
O351	O	0.21095	0.22046	0.94326	0.00000	Uiso	1.00
O352	O	0.21090	0.22066	0.69247	0.00000	Uiso	1.00
O353	O	0.21040	0.72146	0.94180	0.00000	Uiso	1.00
O354	O	0.21029	0.72184	0.69113	0.00000	Uiso	1.00
O355	O	0.26215	0.13521	0.62680	0.00000	Uiso	1.00
O356	O	0.26141	0.13781	0.87300	0.00000	Uiso	1.00
O357	O	0.25707	0.63595	0.62179	0.00000	Uiso	1.00
O358	O	0.25710	0.63729	0.87091	0.00000	Uiso	1.00
O359	O	0.26170	0.80403	0.62146	0.00000	Uiso	1.00
O360	O	0.25846	0.80743	0.87301	0.00000	Uiso	1.00
O361	O	0.26074	0.30527	0.62708	0.00000	Uiso	1.00
O362	O	0.25984	0.30508	0.87539	0.00000	Uiso	1.00
O363	O	0.25642	0.96842	0.62507	0.00000	Uiso	1.00
O364	O	0.25571	0.97390	0.87513	0.00000	Uiso	1.00
O365	O	0.25338	0.47022	0.62398	0.00000	Uiso	1.00
O366	O	0.25437	0.47040	0.87373	0.00000	Uiso	1.00
O367	O	0.21592	0.89300	0.56075	0.00000	Uiso	1.00
O368	O	0.21497	0.89461	0.81060	0.00000	Uiso	1.00
O369	O	0.21420	0.39217	0.56041	0.00000	Uiso	1.00
O370	O	0.21407	0.39200	0.81022	0.00000	Uiso	1.00
O371	O	0.21590	0.04853	0.56243	0.00000	Uiso	1.00
O372	O	0.21583	0.04998	0.81045	0.00000	Uiso	1.00
O373	O	0.21366	0.54798	0.55933	0.00000	Uiso	1.00
O374	O	0.21380	0.54805	0.80921	0.00000	Uiso	1.00
O375	O	0.20848	0.21991	0.56388	0.00000	Uiso	1.00
O376	O	0.20818	0.22101	0.81289	0.00000	Uiso	1.00
O377	O	0.20815	0.72182	0.56143	0.00000	Uiso	1.00
O378	O	0.20752	0.72170	0.81089	0.00000	Uiso	1.00
O379	O	0.25600	0.13646	0.50859	0.00000	Uiso	1.00
O380	O	0.25648	0.13831	0.75637	0.00000	Uiso	1.00
O381	O	0.25471	0.63737	0.50579	0.00000	Uiso	1.00
O382	O	0.25487	0.63733	0.75404	0.00000	Uiso	1.00
O383	O	0.25632	0.80362	0.50658	0.00000	Uiso	1.00
O384	O	0.25525	0.80440	0.75541	0.00000	Uiso	1.00
O385	O	0.25541	0.30358	0.50884	0.00000	Uiso	1.00
O386	O	0.25553	0.30338	0.75751	0.00000	Uiso	1.00
O387	O	0.25884	0.97248	0.50628	0.00000	Uiso	1.00
O388	O	0.25840	0.97017	0.75476	0.00000	Uiso	1.00
O389	O	0.25710	0.47055	0.50558	0.00000	Uiso	1.00
O390	O	0.25616	0.46930	0.75501	0.00000	Uiso	1.00
O391	O	0.35221	0.29808	0.63546	0.00000	Uiso	1.00
O392	O	0.39636	0.71351	0.83001	0.00000	Uiso	1.00
O393	O	0.41534	0.18300	0.96432	0.00000	Uiso	1.00
O394	O	0.39821	0.88752	0.93360	0.00000	Uiso	1.00
O395	O	0.39775	0.38819	0.58848	0.00000	Uiso	1.00
O396	O	0.39437	0.37958	0.93585	0.00000	Uiso	1.00
O397	O	0.39820	0.25452	0.85681	0.00000	Uiso	1.00
O398	O	0.41027	0.55966	0.82768	0.00000	Uiso	1.00
O399	O	0.46470	0.49370	0.85410	0.00000	Uiso	1.00
O400	O	0.40835	0.54445	0.64866	0.00000	Uiso	1.00
O401	O	0.40535	0.53068	0.53513	0.00000	Uiso	1.00
O402	O	0.39823	0.22926	0.57406	0.00000	Uiso	1.00
O403	O	0.39560	0.04554	0.92170	0.00000	Uiso	1.00
O404	O	0.40608	0.07263	0.55296	0.00000	Uiso	1.00
O405	O	0.41387	0.69542	0.69891	0.00000	Uiso	1.00
O406	O	0.45036	0.32257	0.90178	0.00000	Uiso	1.00
O407	O	0.45343	0.67249	0.85267	0.00000	Uiso	1.00
O408	O	0.41090	0.63368	0.93607	0.00000	Uiso	1.00
O409	O	0.44533	0.49103	0.74153	0.00000	Uiso	1.00
O410	O	0.37047	0.16813	0.76594	0.00000	Uiso	1.00
O411	O	0.42082	0.11432	0.82609	0.00000	Uiso	1.00
O412	O	0.40927	0.94017	0.82440	0.00000	Uiso	1.00
O413	O	0.39800	0.86985	0.71658	0.00000	Uiso	1.00
O414	O	0.42690	0.16749	0.70899	0.00000	Uiso	1.00
O415	O	0.39710	0.03746	0.73037	0.00000	Uiso	1.00
O416	O	0.45071	0.94614	0.74552	0.00000	Uiso	1.00

O417	O	0.40939	0.91105	0.55180	0.00000	Uiso	1.00
O418	O	0.42572	0.77391	0.50122	0.00000	Uiso	1.00
O419	O	0.42960	0.99392	0.63861	0.00000	Uiso	1.00
O420	O	0.39134	0.67940	0.58524	0.00000	Uiso	1.00
O421	O	0.36447	0.98277	0.61866	0.00000	Uiso	1.00
O422	O	0.44383	0.79024	0.77878	0.00000	Uiso	1.00
Si423	Si	0.39211	0.96113	0.88606	0.00000	Uiso	1.00
Si424	Si	0.41367	0.34069	0.88236	0.00000	Uiso	1.00
Si425	Si	0.43358	0.48430	0.81065	0.00000	Uiso	1.00
Si426	Si	0.39296	0.48532	0.59379	0.00000	Uiso	1.00
Si427	Si	0.39620	0.15780	0.52426	0.00000	Uiso	1.00
Si428	Si	0.39419	0.63960	0.65482	0.00000	Uiso	1.00
Si429	Si	0.37551	0.30841	0.57658	0.00000	Uiso	1.00
Si430	Si	0.41649	0.64293	0.86524	0.00000	Uiso	1.00
Si431	Si	0.41207	0.94837	0.75092	0.00000	Uiso	1.00
Si432	Si	0.40530	0.12653	0.76160	0.00000	Uiso	1.00
Si433	Si	0.40080	0.99058	0.58950	0.00000	Uiso	1.00
Si434	Si	0.40079	0.84635	0.50082	0.00000	Uiso	1.00

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