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Theoretical infrared signature of OH defects in Fe³⁺, Cr³⁺ and Al³⁺-doped enstatite

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**Theoretical infrared signature of OH defects
in Fe³⁺, Cr³⁺ and Al³⁺-doped enstatite**

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Abstract

The infrared spectroscopic properties of selected defects involving one proton and one nearby M^{3+} ($M=Al, Cr, Fe$) substitution in orthoenstatite are investigated by first-principles calculations. Based on the theoretical results, the absorption bands experimentally observed on synthetic samples with high crystalline quality and low doping levels can be assigned to specific defect configurations. Most of them correspond to Mg vacancies at M2 sites locally compensated by one proton and one M^{3+} cation at a nearby M1 site. This confirms that the $M^{3+} + H^+ = 2 Mg^{2+}$ exchange mechanism is the dominant hydrogen incorporation mechanism at the lowest concentration levels in doped enstatite. At higher concentration levels, more complex incorporation mechanisms could become dominant in Al-bearing samples.

1. Introduction

Enstatite (MgSiO_3) is a major phase of the Earth's upper mantle that is known to incorporate various amounts of OH-bearing defects (Beran and Zemann, 1986; Ingrin and Skogby 2000; Stalder and Skogby 2002; Rauch and Keppler 2002). Although these defects have been extensively studied by infrared spectroscopy and, more recently, by nuclear magnetic resonance (Xue et al. 2024), the corresponding atomic-scale geometries are still debated.

The OH-stretching spectrum of synthetic ortho-enstatite usually displays two bands assigned to doubly protonated M2 vacancies. They are observed at 3070 and 3360 cm^{-1} with maximum intensity for a polarization parallel to [001] and almost no intensity along [100] (Mierdel and Keppler 2004; Prechtel and Stalder 2010). Additional bands dominantly polarized along [100] are observed at 3592 and 3687 cm^{-1} in samples synthesized at lower silica activity and higher pressure (Prechtel and Stalder 2010, 2011) These two bands are most likely related to protons ensuring the charge compensation of Si^{4+} vacancies (Balan et al. 2013; Xue et al. 2024). Assignment to a 4-fold protonated vacancy (“hydrogarnet” defect, Xue et al. 2024) versus a partially protonated vacancy (Balan et al. 2013) remains an open question due to the lack of experimental evidence for the presence of strong OH bands below 3000 cm^{-1} (see, e.g., Stalder et al. 2012).

In natural samples, OH-defects are expected to interact with various impurities, such as aluminum and other trivalent cations. These interactions can lead to rather complex infrared spectra with broadened absorption bands (e.g., Stalder et al. 2015). In comparison, synthetic enstatite samples with low concentration levels of trivalent impurities display narrow peaks not observed in the pure Mg-Si-O-H system (Stalder 2004). Three peaks are observed at 3283, 3322 and 3449 cm^{-1} in Cr-doped samples, while only two peaks are

observed at 3328 and 3461 cm^{-1} in Fe-doped samples (Fig. 1). Five major peaks are observed at 3320, 3381, 3475, 3517 and 3548 cm^{-1} in enstatite doped with 0.25 wt.% Al_2O_3 (Fig. 1). They are also consistently reported for the Al-doped samples investigated by Stalder and Skogby (2002). All these peaks are specifically related to the trivalent impurities and have a dominant polarization parallel to [001] (Stalder 2004), suggesting that they involve M vacancies.

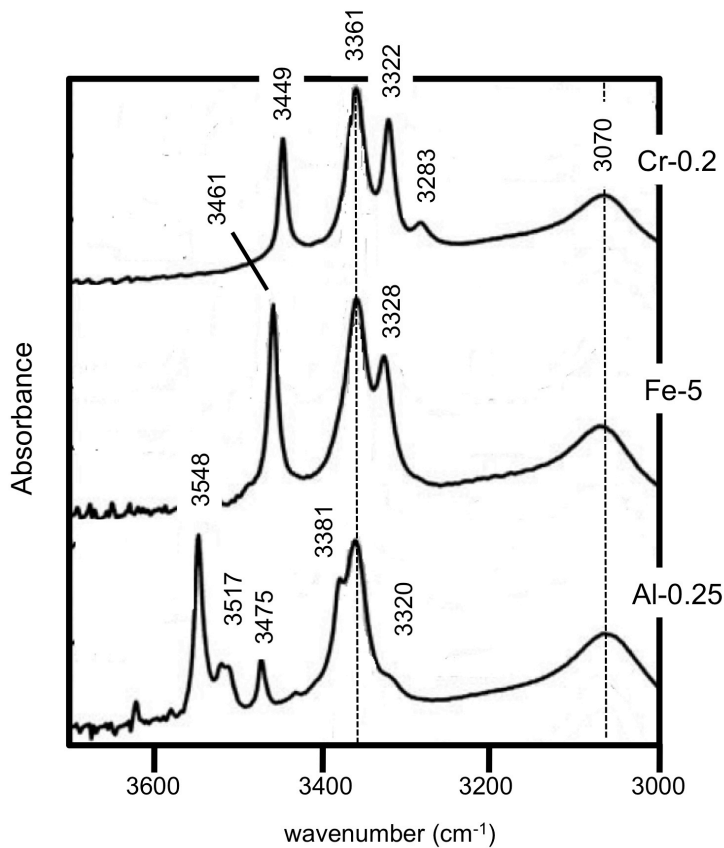


Fig. 1 Experimental IR-spectra of synthetic orthopyroxenes doped with Cr, Fe and Al from Stalder (2004). The dotted lines correspond to the bands associated to doubly protonated M2 vacancies which are also observed in pure enstatite.

In the present study, we theoretically determine the atomic-scale geometry and infrared spectroscopic properties of OH-bearing defects associated with major trivalent impurities in enstatite. The high crystalline quality and chemically well-constrained character of the samples synthesized and investigated by Stalder (2004) facilitate the

comparison of experimental observations with the theoretical properties of OH-bearing defects. The results confirm that most of the bands observed by Stalder (2004) correspond to protonated M2 vacancies associated with trivalent cations and support their one-to-one assignment to a specific defect geometry.

2. Theoretical modeling of OH-defects

The properties of OH-defects have been theoretically investigated within the density functional theory (DFT) framework using the PWscf code of the Quantum Espresso package (Giannozzi et al., 2009; <http://www.quantum-espresso.org>). The modeling scheme used the generalized gradient approximation (GGA) to the exchange-correlation functional as proposed by Perdew, Burke and Ernzerhof (PBE functional; Perdew et al. 1996), and periodic boundary conditions. The ionic cores were described using optimized norm-conserving Vanderbilt (ONCV) pseudopotentials (Hamann 2013; Schlipf and Gygi 2015) with a 80 Ry cut-off on the electronic wave functions. Unit-cell parameters of pure enstatite (space group Pbc₂) were optimized at zero pressure, using a shifted Monkhorst-Pack 2x2x2 k-point grid for the electronic integration. The theoretical cell parameters (a=18.43 Å, b=8.92 Å, c=5.24 Å) overestimate their experimental counterparts (a = 18.21 Å, b=8.81 Å, c=5.18 Å; Morimoto and Koto 1969) as usually observed in GGA calculations. The vibrational properties of OH-bearing defects were determined using 1x2x3 supercells (480 atoms) containing one to two hydrogen atoms equivalent to a hydrogen concentration of 0.093 wt. % H₂O and 0.187 wt. % H₂O, respectively. These relatively large supercells help minimizing the interaction of the defects with their periodic images. The theoretical unit-cell parameters of pure enstatite were used without further relaxation to produce the supercells and the electronic integration was restricted to the Γ point. For all systems, the relaxation of

atomic internal coordinates was performed until the residual forces were $< 10^{-4}$ Ry/a.u.. For models containing isolated paramagnetic cations (Cr^{3+} , Fe^{3+}), spin-polarized calculations have been performed, imposing the high-spin state of the ion to the supercell.

The vibrational modes were calculated at the Brillouin zone center (Γ point), using the linear response theory (Baroni et al., 2001) as implemented in the PHonon code (Giannozzi et al., 2009; <http://www.quantum-espresso.org>; last access:). The high-frequency OH stretching modes that are decoupled from the other vibrational modes occurring at significantly lower frequency were calculated on the $1 \times 2 \times 3$ supercell models by only considering the displacement of the oxygen and hydrogen atoms involved in the OH groups (Balan et al. 2008; Fuchs et al. 2022). The Born effective charge tensors and electronic dielectric tensor were obtained on the equivalent models computed with a smaller $1 \times 1 \times 2$ supercell. The complex low-frequency dielectric permittivity tensor has been calculated for each defect by adding only the ionic contributions related to the OH-stretching modes to the electronic permittivity tensor and using an arbitrary damping parameter of 4 cm^{-1} , accounting for the width of absorption bands (Balan et al., 2008). Theoretical absorption coefficients have then been obtained from the low-frequency dielectric permittivity tensor using the approach detailed in the Appendix.

3. Results and discussion

The enstatite structure displays two types of octahedral sites nominally occupied by Mg^{2+} cations. The Mg^{2+} cations at the M1 site are bound to four O1 and two O2 oxygen atoms, corresponding to apical and equatorial non-bridging oxygen in silicate tetrahedra,

respectively. The more distorted M2 sites involve O1 and O2 oxygen atoms and the silicate-bridging O3 oxygen atoms. Previous theoretical studies consistently indicate that the protonation of vacant M2 sites is significantly favored with respect to that of M1 sites (Gatzemeier and Wright 2006; Balan et al. 2013; Xue et al. 2024). In the fully protonated M2 vacancies, the two non-equivalent O2-H groups (referred to as OaH and ObH) are oriented in the (100) plane, leading to two bands dominantly polarized along the [001] direction. The shorter ObH bond vibrates at $\sim 3360\text{ cm}^{-1}$ and the other OaH bond at $\sim 3070\text{ cm}^{-1}$ (e.g. Rauch and Keppler 2002; Stalder and Skogby 2002; Stalder 2004). The theoretical frequencies obtained in the present modelling are 3425 and 3134 cm^{-1} (Table 1). Differences with the theoretical frequencies previously obtained with the PBE functional by Balan et al. (2013) (3361 and 3034 cm^{-1}) and Xue et al. (2024) (3361 and 3161 cm^{-1}) are mostly due to the use of different sets of pseudopotentials and different size of supercells.

Based on their polarization properties, the peaks observed by Stalder (2004) in the doped enstatite samples can be assumed to be related to M vacancies. Accordingly, a series of models has been built by removing one proton from the previously investigated protonated M2 vacancy and introducing trivalent cations (Al, Cr, Fe) in the neighboring M1 sites (Table 1). The association of one proton and one trivalent impurity compensates for the charge deficit due to the Mg vacancy and ensures the electrostatic neutrality of the defect. In each model, a single M^{3+} for Mg^{2+} substitution was considered and it was assumed that the OH group is not coordinated to the trivalent cation due to the bond valence constraints. Each composition thus leads to four defect configurations (Fig. 2). In configurations 1 and 2, the hydrogen is bonded to the Ob oxygen, while it is bonded to Oa in configurations 3 and 4. The substitution affects the octahedral site almost facing the OH group along the [001] direction in configurations 1 and 4, and the site in a more lateral position in configurations 2 and 3. Only

substitutions at M1 sites have been considered for the Cr and Fe-bearing systems, but two additional defect models were considered in the aluminous system to account for potential Al for Si substitution affecting the two non-equivalent Si sites of enstatite (Table 1).

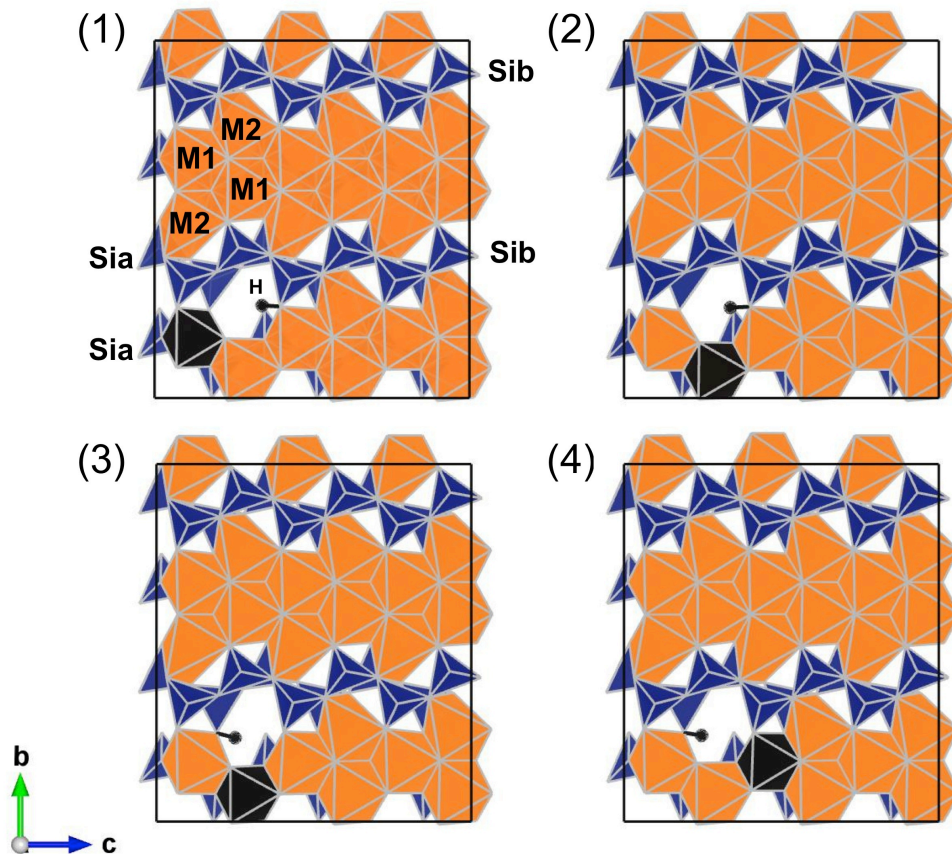


Fig. 2 Configurations of OH-bearing defects associated to M2 vacancies and M³⁺ substitution at M1 site. View along the [100] direction of the 1x2x3 supercell. Tetrahedral Si site: blue, octahedral Mg sites: orange, H atom: black sphere. The substituted octahedral M1 site is in black. Configurations (1) and (2) correspond to protonation of O2b. Configurations (3) and (4) correspond to protonation of O2a. In configurations (1) and (4) the substituted site faces the OH group, while it is in a more lateral position in configurations (2) and (3).

The presence of neighboring impurities has a significant effect on the vibrational properties of the OH group at the vacant M2 site (Table 1). As is usually observed, the

stretching frequency is inversely correlated with the OH bond length (Fig. 3A). The slope of the correlation ($\sim -18000 \text{ cm}^{-1}/\text{\AA}$) is similar to that previously reported for hydrous defects in enstatite and other minerals (e.g., Balan et al. 2013; Balan et al. 2020). The inverse correlation of the absorption coefficient with the stretching frequency (Fig. 3B) is also similar to that inferred from the theoretical modeling of OH groups in minerals (Balan et al. 2008). As previously noted (Balan et al. 2008), the theoretical correlation is steeper than those inferred from experimental data (e.g.; Libowitzky and Rossman 1997; Stalder et al. 2012). This difference is mostly related to the use of observed (anharmonic) stretching frequencies in the experimental correlation. A closer agreement between theoretical and experimental slopes is observed when the experimental frequencies are corrected for anharmonicity (Fig. 3B, see appendix for the estimation of the effect of anharmonicity on frequency).

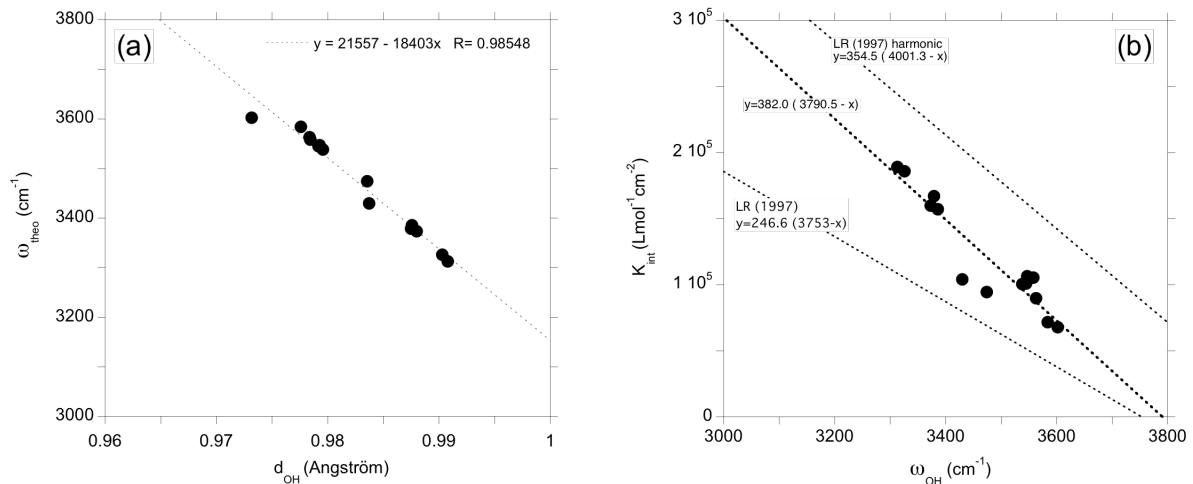


Fig. 3 (a) Relation between the theoretical stretching frequency and OH bond length for the investigated defects. (b) Theoretical integrated molar absorption coefficients of the stretching modes of OH defects as a function of the stretching frequency. The bottom line corresponds to the calibration of Libowitzky and Rossman (1997). When corrected for anharmonicity (top line; Appendix B), the slope of the experimental calibration is significantly closer to the theoretical slope.

For each chemical composition, significant differences in the relative energy and OH stretching frequency are observed between the various configurations of the defects. At equivalent positions of the trivalent cation in M1, the configurations 3 and 4, corresponding to the protonation of Oa, are more stable and lead to lower stretching frequencies than those which involve Ob, configurations 2 and 1, respectively. The position of the substituted site has a significant influence too. In models 1 and 4, the electrostatic charge excess at the substituted site can increase the stretching frequency of the facing OH group by several dozens of cm^{-1} with respect to the model in which the substituted site is in a more lateral position with respect to the OH group (models 2 and 3, respectively). The facing configurations (1 and 4) are also energetically favored with respect to the lateral ones.

Table 1: Theoretical properties of OH-defects in enstatite (structure files are provided in the Supplement).

model	protonated oxygen	rel. energy (kJ/mol)	rel. abundance at 1500K (%) **	d_{OH} (Å)	ω_{OH} (cm^{-1})	$I_x^{\text{***}}$ (%)	$I_y^{\text{***}}$ (%)	$I_z^{\text{***}}$ (%)	K_{int} (cm^{-2} per $\text{molH}_2\text{O/L}$)	$\omega_{\text{exp}}^{\text{****}}$ (cm^{-1})
1	$[(1\text{H}^+)_{\text{M2}}(\text{Al}^{3+})_{\text{M1}}]_{\text{O2b}}^{\text{x}}_1$	7.3	23.5	0.9776	3584	17	8	75	72000	3548
2	$[(1\text{H}^+)_{\text{M2}}(\text{Al}^{3+})_{\text{M1}}]_{\text{O2b}}^{\text{x}}_2$	12.4	15.6	0.9784	3563	3	19	78	89000	3475
3	$[(1\text{H}^+)_{\text{M2}}(\text{Al}^{3+})_{\text{M1}}]_{\text{O2a}}^{\text{x}}_3$	10.1	18.8	0.9880	3373	3	34	63	159000	3320
4	$[(1\text{H}^+)_{\text{M2}}(\text{Al}^{3+})_{\text{M1}}]_{\text{O2a}}^{\text{x}}_4$	0	42.2	0.9836	3474	14	23	63	94000	3381
5	$[(1\text{H}^+)_{\text{M2}}(\text{Fe}^{3+})_{\text{M1}}]_{\text{O2b}}^{\text{x}}_1$	2.0	42.6	0.9784	3558	7	11	82	105000	3461
6	$[(1\text{H}^+)_{\text{M2}}(\text{Fe}^{3+})_{\text{M1}}]_{\text{O2b}}^{\text{x}}_2$	34.2	3.2	0.9792	3545	5	26	69	101000	n.o.
7	$[(1\text{H}^+)_{\text{M2}}(\text{Fe}^{3+})_{\text{M1}}]_{\text{O2a}}^{\text{x}}_3$	31.8	3.9	0.9908	3313	4	43	53	188000	n.o.
8	$[(1\text{H}^+)_{\text{M2}}(\text{Fe}^{3+})_{\text{M1}}]_{\text{O2a}}^{\text{x}}_4$	0	50.2	0.9875	3379	6	21	73	167000	3328
9	$[(1\text{H}^+)_{\text{M2}}(\text{Cr}^{3+})_{\text{M1}}]_{\text{O2b}}^{\text{x}}_1$	7.4	23.3	0.9793	3547	7	13	80	106000	3449
10	$[(1\text{H}^+)_{\text{M2}}(\text{Cr}^{3+})_{\text{M1}}]_{\text{O2b}}^{\text{x}}_2$	12.5	15.5	0.9796	3538	4	25	71	100000	3449
11	$[(1\text{H}^+)_{\text{M2}}(\text{Cr}^{3+})_{\text{M1}}]_{\text{O2a}}^{\text{x}}_3$	9.8	19.2	0.9903	3326	3	41	56	185000	3283
12	$[(1\text{H}^+)_{\text{M2}}(\text{Cr}^{3+})_{\text{M1}}]_{\text{O2a}}^{\text{x}}_4$	0	42.1	0.9876	3386	7	23	70	157000	3322
13	$(\text{Al}^{3+}, \text{H}^+)_{\text{Si}}^{\text{x}}_1$	21	15.5	0.9732	3602	37	56	7	68000	n.o.
14	$(\text{Al}^{3+}, \text{H}^+)_{\text{Si}}^{\text{x}}_2$	0	84.5	0.9837	3430	52	10	38	104000	n.o.
15	$(2\text{H}^+)_{\text{M2}}$	0		0.9994	3134	0	30	70	422000	3070
				0.9845	3425					3361

* The relative energy is defined with respect to the most stable configuration of the model with the same stoichiometry.

** The relative abundances are obtained using a Boltzmann distribution at 1500 K applied to the models with the same stoichiometry.

*** I_x , I_y , I_z correspond to the relative theoretical intensities for polarizations parallel to [100], [010] and [001], respectively.

****Stalder (2004) (n.o.: not observed)

For the Fe-bearing models (Table 1), the energy difference between the configurations can be particularly important (> 30 kJ/mol). The relative abundance of the two less stable configurations (2 and 3) is not expected to exceed a few percent at 1500 K (1227 °C), while that of the two other configurations is above 40% (Table 1). Consistently, the Fe-bearing samples synthesized by slow cooling from 1400 to 1150 °C only display two specific bands at 3461 cm^{-1} and 3328 cm^{-1} (Stalder 2004). These two bands can thus be confidently assigned to the two more stable geometries of the Fe-bearing models, i.e., configurations 1 and 4, respectively (Table 1).

For the Cr-bearing models, the energy difference between the four configurations is smaller and all four configurations are expected to occur in the synthetic Cr-bearing samples (Table 1). The configuration 4 is expected to be dominant (42% at 1500 K), while the relative abundances of the three other configurations range between 15 and 25%. Based on their relative intensities (Fig. 1) and stretching frequencies (Fig. 4), the bands experimentally observed at 3283 and 3322 cm^{-1} (Stalder 2004) can be assigned to configurations 3 and 4, respectively. Considering that the theoretical stretching frequencies of the two other configurations are close to each other, it is likely that these two configurations contribute to the remaining band at 3449 cm^{-1} . This would explain its comparatively strong intensity, similar to that of the band at 3322 cm^{-1} , which is assigned to the more stable configuration 4. Although not frequent, the fortuitous contribution of two different OH-bearing defects to a single infrared band has previously been reported in corundum (e.g., Moon and Philips 1991; Balan 2020). Alternatively, it cannot be fully excluded that the energy difference between the two configurations is larger than theoretically expected (Table 1) and that only the most stable of the two configurations is actually observed.

The relative stabilities of the Al-bearing models are similar to those computed for the Cr-bearing defects (Table 1). On the same criteria as for the Cr-bearing samples, the two bands observed at 3320 and 3381 cm^{-1} are assigned to configurations 3 and 4, respectively. The two major bands at 3475 and 3548 cm^{-1} observed in the Al-doped sample with the lowest Al concentrations (Stalder and Skogby 2002; Stalder 2004) are assigned to the two remaining configurations (configurations 2 and 1, respectively) (Table 1). A minor band at 3520 cm^{-1} is also observed in the spectrum of the Al-0.25 sample with a polarization similar to that of the other bands assigned to M2 vacancies (Fig. 1). This minor band becomes dominant in the Al-rich samples (Stalder 2004) which suggests that it could be related to a medium-range environment of M2 vacancies involving more than a single Al atom. A comparatively more complex speciation of OH groups could thus occur in Al-bearing samples depending on their synthesis conditions (see also Rauch and Keppler 2002).

In the models with tetrahedral Al, the underbonded O2 atom is the most favorable site for the proton location due to bond valence requirements, as in diopside (Balan et al. 2020). The defect involving the larger Sib site is significantly favored ($> 20 \text{ kJ/mol}$) with respect to that involving the smaller Sia site (Table 1). The Sia and Sib models display different OH bond lengths leading to theoretical OH stretching frequencies of 3602 and 3430 cm^{-1} , respectively, with dominant polarizations along [010] and [100], respectively (Table 1). The polarization properties of OH bands associated to tetrahedral substitutions thus markedly differ from those associated to M2 vacancies. It is noteworthy that Grant et al. (2007) report two bands with a different polarization at 3600 and 3390 cm^{-1} in synthetic enstatite with higher Al concentrations. Unfortunately, it was not possible to unambiguously relate these bands to simple models of OH-bearing defects. Even though the stretching frequencies reported by Grant et al. (2007) are close to those obtained for the models with tetrahedral Al

(Table 1), the relative intensities of the experimental bands are more difficult to reconcile with the theoretical expectations.

A plot of the theoretical OH stretching frequencies versus experimentally observed frequencies of the OH bands in enstatite summarizes the results in Figure 4. They show a linear trend similar to the one previously observed for diopside, with a positive shift of theoretical frequencies around 50 to 60 cm^{-1} (Balan et al. 2020).

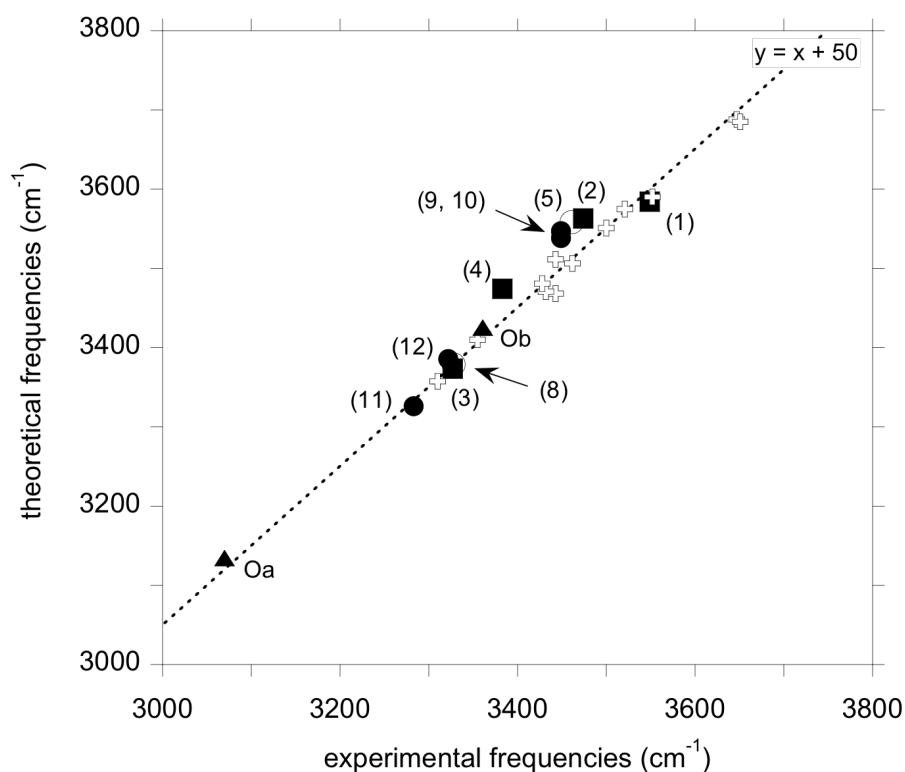


Fig. 4 Comparison of theoretical and observed OH stretching frequencies for the relevant defect models. The labels refer to Table 1. Triangles: doubly protonated M2 vacancy (contribution from protonation of Oa and Ob oxygens are indicated), squares: Al-bearing defects, open circles: Fe-bearing defects, full circles: Cr-bearing defects, open crosses: OH-bearing defects in diopside (Balan et al. 2020).

4. Conclusions

The properties of defects involving a coupled incorporation of trivalent cation and proton in enstatite have been theoretically investigated. The use of large super-cells accounts for the isolated nature of the defects and favors the comparison of the theoretical results with observations made on samples with low levels of doping and low hydrogen content. In this case, it is possible to unambiguously assign most of the experimentally observed bands to specific defect configurations. These bands correspond to neutral defects corresponding to protonated M2 vacancies associated with a trivalent cation substitution at a neighboring M1 site. The theoretical modeling thus confirms that the $M^{3+} + H^+ = 2 Mg^{2+}$ exchange mechanism is the dominant hydrogen incorporation mechanism at the lowest concentration levels in enstatite doped with trivalent cations (Stalder and Skogby 2002; Stalder 2004). For the Al-bearing enstatite, the significant change in the spectra observed when the Al and hydrogen content increase (Stalder 2004) suggests that more complex incorporation mechanisms occur. Their modeling will likely require different strategies accounting for the multiplicity of potential configurations and for the interactions between the defective sites at elevated concentrations.

Code and data availability. Structure drawings have been produced with the Vesta software (Momma and Izumi 2011). PWscf and PHonon codes (Giannozzi et al., 2009) are available at <http://www.quantum-espresso.org/>. Model structures are provided as electronic supplementary files under ".cif" formats.

Author contribution. JI and EB designed the study. EB performed the simulations. All co-authors discussed the results and prepared the manuscript.

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Appendix

A Computation of theoretical absorption coefficients

Considering the propagation of an IR beam through a section of an isotropic medium, the integrated absorbance is defined by :

$$A = \int_{\bar{\nu}} \log_{10}\left(\frac{I_0}{I_t}\right) d\bar{\nu} = \frac{1}{\ln(10)} \int_{\bar{\nu}} \ln\left(\frac{I_0}{I_t}\right) d\bar{\nu} \quad (1)$$

where $\bar{\nu}$ is the frequency in wavenumbers and I_0 and I_t are the intensity of the incident and transmitted light, respectively.

Let $n=n_1+in_2$ be the (frequency dependent) complex refractive index of the medium, the absorbance is related to the imaginary part of the refractive index n_2 by (Bruesch 1986):

$$\ln\left(\frac{I_0}{I_t}\right) = 4\pi \bar{\nu} n_2 \quad (2)$$

The imaginary part of the refractive index is related to the complex (frequency dependent) dielectric function by:

$$2n_2^2 = (\epsilon_1^2 + \epsilon_2^2)^{1/2} - \epsilon_1 \quad (3)$$

where ϵ_1 and ϵ_2 are its real and imaginary parts, respectively. Considering that $\epsilon_1 = 2 n_1 n_2$, Eq. (2) is equivalently expressed as:

$$\ln\left(\frac{I_0}{I_t}\right) = 2\pi \bar{\nu} \frac{\epsilon_2}{n_1} \quad (4)$$

For a dilute species in a non-absorbing medium, the Beer-Lambert law (e.g., Mayerhöfer and Popp 2019) relates the integrated absorbance to the molar concentration C of the absorbing species:

$$A = K C t \quad (5)$$

where K is the absorption coefficient and t the thickness of the sample. When the species of interest is a molecular impurity in a crystal, such as an OH group, it is appropriate to use the total absorbance A_{tot} which is the sum of absorbances in all three orthogonal polarization directions (Libowitzky and Rossman 1996). The total integrated absorption coefficient K_{int} can thus be defined as:

$$A_{\text{tot}} = K_{\text{int}} C t \quad (6)$$

For an isotropic crystal, K_{int} is three times as large as K , which is defined for a single direction. For crystals with orthorhombic symmetry or higher, the principal axes of the refraction and dielectric tensors are determined by the symmetry (Sambridge et al. 2008) and K_{int} can be determined using Eqs. (1), (2) and (3) for each polarization.

It is noteworthy that quantum chemistry codes often provide the infrared absorptivities I_k of vibrational mode k in $(\text{D}/\text{\AA})^2/\text{amu}$, which can be converted to an integrated absorption coefficient. For a non-degenerate mode, the relation of I_k to the absorption coefficient K (in km/mol) of a molecular species in gas phase is (e.g., Monguzi et al. 2009):

$$K = I_k \times 42.256 / \ln(10) \quad (7)$$

In this case, n_1 in Eq. (4) is approximately equal to one. For a weakly absorbing molecular impurity diluted in a condensed phase, n_1 usually differs from one but it can be assumed to be constant and close to the refractive index of the host medium. The theoretical absorptivities of OH stretching modes in $(\text{D}/\text{\AA})^2/\text{amu}$ is then related to the integrated absorption coefficients K_{int} in cm^{-2} per $\text{mol}(\text{H}_2\text{O})\cdot\text{L}^{-1}$ by:

$$K_{\text{int}} \approx I_k \times 4225.6 \times 3 \times 2 / (n_{\text{host}} \times \ln(10)) \quad (8)$$

where n_{host} is the average refractive index of the host. The factor 2 in Eq. (8) is related to the use of H_2O equivalent and the factor 3 accounts for the use of total intensities, instead of considering a single direction as in the definition of K (Wilson et al. 1980). Benchmarking calculations performed on a series of OH bearing defects in corundum previously investigated by Balan (2020) and Jollands and Balan (2022) indicate that the two different approaches provide absorption coefficients differing by less than a few percent (Fig. 5).

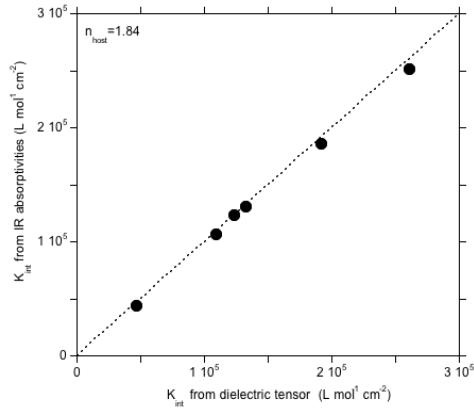


Figure 5: Comparison of absorption coefficients obtained from the theoretical dielectric tensor components with those obtained from theoretical IR absorptivities (Eq. 7) for a series of OH defects in corundum previously investigated by Balan (2020) and Jollands and Balan (2022).

B Effect of OH bond anharmonicity on the IR absorption calibration curves.

The anharmonic shift ($2\omega_e x_e$) related to the anharmonicity of the OH potential increases when the stretching frequency decreases (Wöhlecke and Kovács 2001). An approximate polynomial relation (Fig. 6) between the anharmonicity constant and the observed (anharmonic) stretching frequency can be obtained using the experimental data on solid hydrates reported by Berglund et al. (1978). By combining this relation with the correlation reported by Libowitzky and Rossmann (1997), an experimental relation between the absorption coefficient and the harmonic stretching frequency can be obtained:

$$K_{int} = 354.5 (4001.3 - \omega_{OH})$$

where K_{int} is the integrated absorption coefficients in cm^{-2} per $mol(H_2O) \cdot L^{-1}$ and ω_{OH} is the harmonic stretching frequency. In this case, the theoretical slope is significantly closer to the experimental one (Fig. 3b). This supports the idea that the apparent discrepancy between theoretical and experimental correlations is mostly related to the assumptions made in the calculation of theoretical frequencies.

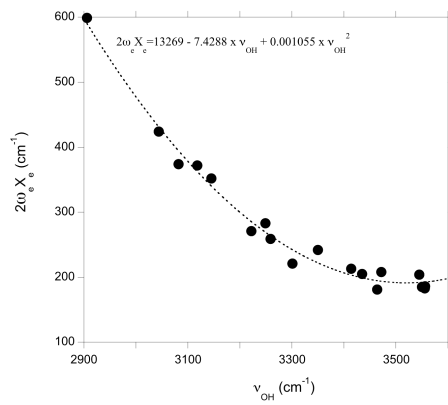


Figure 6: Experimental relation between the anharmonicity parameter and the OH stretching frequency from the Table 1 of Berglund et al. (1978). The value for free hydroxyl (Wöhlecke and Kovács 2001) has also been included. The dotted line corresponds to a quadratic polynomial interpolation which can be used to assess the harmonic stretching frequencies from experimentally observed frequencies.

Supplementary information to:

"Theoretical infrared signature of OH defects
in Fe³⁺, Cr³⁺ and Al³⁺-doped enstatite" by Etienne Balan¹ and Jannick Ingrin²

submitted to Physics and Chemistry of Minerals

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The .cif files correspond to the 14 models of hydrous enstatite doped with trivalent cations and listed in Table 1.

model 1

#=====

CRYSTAL DATA

#-----

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O	1.0	0.436871	0.420174	0.900425	Biso	1.000000	O
O	1.0	0.436342	0.921307	0.233639	Biso	1.000000	O
O	1.0	0.437295	0.920043	0.567203	Biso	1.000000	O
O	1.0	0.436887	0.920432	0.900638	Biso	1.000000	O
O	1.0	0.562311	0.079619	0.099667	Biso	1.000000	O
O	1.0	0.562696	0.079630	0.433006	Biso	1.000000	O
O	1.0	0.562578	0.079732	0.766516	Biso	1.000000	O
O	1.0	0.562735	0.579529	0.099520	Biso	1.000000	O
O	1.0	0.563004	0.579995	0.432878	Biso	1.000000	O
O	1.0	0.562840	0.579702	0.766251	Biso	1.000000	O
O	1.0	0.063773	0.084594	0.068985	Biso	1.000000	O
O	1.0	0.062789	0.079879	0.400704	Biso	1.000000	O
O	1.0	0.062905	0.079565	0.733755	Biso	1.000000	O
O	1.0	0.063395	0.578290	0.067518	Biso	1.000000	O
O	1.0	0.063355	0.579679	0.401212	Biso	1.000000	O
O	1.0	0.062996	0.579232	0.733940	Biso	1.000000	O
O	1.0	0.937198	0.420580	0.266121	Biso	1.000000	O
O	1.0	0.937105	0.419975	0.598657	Biso	1.000000	O
O	1.0	0.936917	0.419343	0.931756	Biso	1.000000	O
O	1.0	0.937863	0.921089	0.266103	Biso	1.000000	O
O	1.0	0.937198	0.920405	0.599348	Biso	1.000000	O
O	1.0	0.937081	0.920195	0.932820	Biso	1.000000	O
O	1.0	0.309740	0.251898	0.014747	Biso	1.000000	O
O	1.0	0.310609	0.250710	0.349197	Biso	1.000000	O
O	1.0	0.311314	0.250558	0.681669	Biso	1.000000	O
O	1.0	0.311097	0.751007	0.014790	Biso	1.000000	O
O	1.0	0.311526	0.751309	0.348579	Biso	1.000000	O
O	1.0	0.311352	0.751074	0.682058	Biso	1.000000	O
O	1.0	0.688630	0.248784	0.318180	Biso	1.000000	O
O	1.0	0.688479	0.248978	0.651600	Biso	1.000000	O
O	1.0	0.688315	0.248912	0.984975	Biso	1.000000	O
O	1.0	0.688740	0.749300	0.318201	Biso	1.000000	O
O	1.0	0.688751	0.749101	0.651717	Biso	1.000000	O

O	1.0	0.688690	0.749163	0.985246	Biso	1.000000	O
O	1.0	0.192751	0.245111	0.172885	Biso	1.000000	O
O	1.0	0.187736	0.249519	0.514038	Biso	1.000000	O
O	1.0	0.188590	0.247750	0.850455	Biso	1.000000	O
O	1.0	0.188557	0.748857	0.181328	Biso	1.000000	O
O	1.0	0.188366	0.749517	0.515283	Biso	1.000000	O
O	1.0	0.188477	0.749209	0.848964	Biso	1.000000	O
O	1.0	0.811408	0.250736	0.152340	Biso	1.000000	O
O	1.0	0.811550	0.250695	0.484212	Biso	1.000000	O
O	1.0	0.811591	0.250541	0.818072	Biso	1.000000	O
O	1.0	0.811730	0.750907	0.151451	Biso	1.000000	O
O	1.0	0.811817	0.750749	0.484745	Biso	1.000000	O
O	1.0	0.811725	0.750676	0.818294	Biso	1.000000	O
O	1.0	0.688568	0.001098	0.151756	Biso	1.000000	O
O	1.0	0.688683	0.000919	0.485049	Biso	1.000000	O
O	1.0	0.688569	0.000865	0.818512	Biso	1.000000	O
O	1.0	0.688869	0.500681	0.151680	Biso	1.000000	O
O	1.0	0.688547	0.500709	0.484702	Biso	1.000000	O
O	1.0	0.688626	0.500777	0.818326	Biso	1.000000	O
O	1.0	0.311511	0.499632	0.181860	Biso	1.000000	O
O	1.0	0.311582	0.499406	0.515370	Biso	1.000000	O
O	1.0	0.311178	0.498928	0.848296	Biso	1.000000	O
O	1.0	0.307521	1.000034	0.181809	Biso	1.000000	O
O	1.0	0.311960	0.998621	0.515234	Biso	1.000000	O
O	1.0	0.311103	1.000219	0.849537	Biso	1.000000	O
O	1.0	0.811280	0.499060	0.317676	Biso	1.000000	O
O	1.0	0.811638	0.498997	0.651376	Biso	1.000000	O
O	1.0	0.811841	0.498893	0.984931	Biso	1.000000	O
O	1.0	0.811845	0.999145	0.317902	Biso	1.000000	O
O	1.0	0.811599	0.999121	0.651323	Biso	1.000000	O
O	1.0	0.812094	0.999518	0.985450	Biso	1.000000	O
O	1.0	0.187563	0.001465	0.016108	Biso	1.000000	O
O	1.0	0.187882	0.000192	0.346233	Biso	1.000000	O
O	1.0	0.188435	0.000913	0.682611	Biso	1.000000	O
O	1.0	0.188229	0.500112	0.015615	Biso	1.000000	O
O	1.0	0.189693	0.502023	0.348927	Biso	1.000000	O
O	1.0	0.188263	0.500143	0.682042	Biso	1.000000	O
O	1.0	0.432131	0.241579	0.229917	Biso	1.000000	O
O	1.0	0.432291	0.241085	0.562994	Biso	1.000000	O
O	1.0	0.432140	0.241271	0.896431	Biso	1.000000	O
O	1.0	0.432379	0.741521	0.229644	Biso	1.000000	O
O	1.0	0.432598	0.741462	0.563119	Biso	1.000000	O
O	1.0	0.432447	0.741418	0.896519	Biso	1.000000	O
O	1.0	0.567159	0.258594	0.103643	Biso	1.000000	O
O	1.0	0.567530	0.258704	0.436958	Biso	1.000000	O
O	1.0	0.567395	0.258711	0.770338	Biso	1.000000	O
O	1.0	0.567413	0.758987	0.103710	Biso	1.000000	O
O	1.0	0.567738	0.759043	0.436871	Biso	1.000000	O
O	1.0	0.567688	0.758816	0.770485	Biso	1.000000	O
O	1.0	0.069984	0.253071	0.070573	Biso	1.000000	O
O	1.0	0.064142	0.256185	0.398426	Biso	1.000000	O
O	1.0	0.067565	0.257365	0.728334	Biso	1.000000	O
O	1.0	0.067625	0.758806	0.063360	Biso	1.000000	O
O	1.0	0.067590	0.758873	0.396318	Biso	1.000000	O
O	1.0	0.067675	0.758711	0.730028	Biso	1.000000	O
O	1.0	0.935918	0.241925	0.269977	Biso	1.000000	O
O	1.0	0.932566	0.241440	0.602935	Biso	1.000000	O
O	1.0	0.932887	0.241237	0.937153	Biso	1.000000	O
O	1.0	0.932457	0.741059	0.269899	Biso	1.000000	O
O	1.0	0.932450	0.741114	0.603638	Biso	1.000000	O
O	1.0	0.932527	0.740878	0.936999	Biso	1.000000	O
O	1.0	0.567485	0.491105	0.270177	Biso	1.000000	O
O	1.0	0.567570	0.491181	0.603581	Biso	1.000000	O
O	1.0	0.567458	0.491123	0.937040	Biso	1.000000	O
O	1.0	0.567216	0.991553	0.270413	Biso	1.000000	O
O	1.0	0.567597	0.991226	0.603857	Biso	1.000000	O
O	1.0	0.567172	0.991413	0.937202	Biso	1.000000	O
O	1.0	0.431185	0.009119	0.063818	Biso	1.000000	O
O	1.0	0.432119	0.008886	0.396113	Biso	1.000000	O
O	1.0	0.432244	0.008699	0.729979	Biso	1.000000	O
O	1.0	0.432027	0.508521	0.063186	Biso	1.000000	O
O	1.0	0.432782	0.508802	0.396468	Biso	1.000000	O
O	1.0	0.432336	0.508735	0.729719	Biso	1.000000	O
O	1.0	0.934387	0.009179	0.103559	Biso	1.000000	O
O	1.0	0.932023	0.009613	0.436140	Biso	1.000000	O
O	1.0	0.932309	0.008894	0.770063	Biso	1.000000	O
O	1.0	0.933262	0.507017	0.103102	Biso	1.000000	O
O	1.0	0.932831	0.508110	0.436806	Biso	1.000000	O
O	1.0	0.932562	0.508135	0.770020	Biso	1.000000	O

O	1.0	0.067473	0.493559	0.231116	Biso	1.000000	O
O	1.0	0.068081	0.490927	0.562446	Biso	1.000000	O
O	1.0	0.067546	0.489734	0.896178	Biso	1.000000	O
O	1.0	0.068790	0.992146	0.230130	Biso	1.000000	O
O	1.0	0.067709	0.991126	0.562666	Biso	1.000000	O
O	1.0	0.067309	0.991753	0.897151	Biso	1.000000	O
O	1.0	0.303597	0.111152	0.279195	Biso	1.000000	O
O	1.0	0.303457	0.109495	0.613044	Biso	1.000000	O
O	1.0	0.299016	0.111981	0.946909	Biso	1.000000	O
O	1.0	0.303528	0.610986	0.279177	Biso	1.000000	O
O	1.0	0.303345	0.610563	0.612681	Biso	1.000000	O
O	1.0	0.302984	0.610071	0.945862	Biso	1.000000	O
O	1.0	0.697026	0.389547	0.054274	Biso	1.000000	O
O	1.0	0.697355	0.389329	0.387414	Biso	1.000000	O
O	1.0	0.696812	0.389609	0.720978	Biso	1.000000	O
O	1.0	0.697213	0.889867	0.054533	Biso	1.000000	O
O	1.0	0.697136	0.889725	0.387733	Biso	1.000000	O
O	1.0	0.697043	0.889660	0.721187	Biso	1.000000	O
O	1.0	0.195479	0.388164	0.111568	Biso	1.000000	O
O	1.0	0.196676	0.390051	0.444351	Biso	1.000000	O
O	1.0	0.196265	0.387861	0.778158	Biso	1.000000	O
O	1.0	0.196307	0.889819	0.112657	Biso	1.000000	O
O	1.0	0.196878	0.890009	0.445551	Biso	1.000000	O
O	1.0	0.196656	0.889656	0.779237	Biso	1.000000	O
O	1.0	0.803000	0.110232	0.220927	Biso	1.000000	O
O	1.0	0.803163	0.110415	0.554263	Biso	1.000000	O
O	1.0	0.803100	0.110238	0.887773	Biso	1.000000	O
O	1.0	0.803260	0.610399	0.220903	Biso	1.000000	O
O	1.0	0.803251	0.610231	0.554314	Biso	1.000000	O
O	1.0	0.803317	0.610102	0.887738	Biso	1.000000	O
O	1.0	0.697133	0.360099	0.220912	Biso	1.000000	O
O	1.0	0.696887	0.360201	0.554223	Biso	1.000000	O
O	1.0	0.696869	0.360109	0.887632	Biso	1.000000	O
O	1.0	0.697346	0.860589	0.221037	Biso	1.000000	O
O	1.0	0.697143	0.860356	0.554437	Biso	1.000000	O
O	1.0	0.697072	0.860299	0.887919	Biso	1.000000	O
O	1.0	0.305169	0.140340	0.112417	Biso	1.000000	O
O	1.0	0.304474	0.139725	0.446701	Biso	1.000000	O
O	1.0	0.302667	0.139840	0.779634	Biso	1.000000	O
O	1.0	0.303371	0.640150	0.112394	Biso	1.000000	O
O	1.0	0.303326	0.640150	0.445914	Biso	1.000000	O
O	1.0	0.302936	0.639777	0.779337	Biso	1.000000	O
O	1.0	0.802530	0.140058	0.054270	Biso	1.000000	O
O	1.0	0.803213	0.139537	0.387385	Biso	1.000000	O
O	1.0	0.803179	0.139537	0.720945	Biso	1.000000	O
O	1.0	0.803286	0.639535	0.054354	Biso	1.000000	O
O	1.0	0.803224	0.639484	0.387629	Biso	1.000000	O
O	1.0	0.803271	0.639500	0.721066	Biso	1.000000	O
O	1.0	0.197744	0.364158	0.275501	Biso	1.000000	O
O	1.0	0.196426	0.360217	0.611177	Biso	1.000000	O
O	1.0	0.196100	0.359957	0.945071	Biso	1.000000	O
O	1.0	0.196723	0.859314	0.279209	Biso	1.000000	O
O	1.0	0.196788	0.860631	0.612384	Biso	1.000000	O
O	1.0	0.196329	0.860902	0.945844	Biso	1.000000	O
O	1.0	0.447606	0.097527	0.201406	Biso	1.000000	O
O	1.0	0.448144	0.097083	0.534725	Biso	1.000000	O
O	1.0	0.447442	0.097413	0.868035	Biso	1.000000	O
O	1.0	0.448086	0.597576	0.201075	Biso	1.000000	O
O	1.0	0.448194	0.597588	0.534432	Biso	1.000000	O
O	1.0	0.448024	0.597557	0.867681	Biso	1.000000	O
O	1.0	0.551799	0.402445	0.132105	Biso	1.000000	O
O	1.0	0.551955	0.402517	0.465411	Biso	1.000000	O
O	1.0	0.551768	0.402580	0.798893	Biso	1.000000	O
O	1.0	0.551458	0.902942	0.132248	Biso	1.000000	O
O	1.0	0.552061	0.902795	0.465545	Biso	1.000000	O
O	1.0	0.551868	0.902687	0.799057	Biso	1.000000	O
O	1.0	0.052925	0.394421	0.029069	Biso	1.000000	O
O	1.0	0.052167	0.400977	0.365486	Biso	1.000000	O
O	1.0	0.051802	0.401187	0.699331	Biso	1.000000	O
O	1.0	0.051843	0.902877	0.034554	Biso	1.000000	O
O	1.0	0.052132	0.903044	0.368053	Biso	1.000000	O
O	1.0	0.051840	0.902626	0.701054	Biso	1.000000	O
O	1.0	0.949769	0.098736	0.297705	Biso	1.000000	O
O	1.0	0.948372	0.097675	0.631897	Biso	1.000000	O
O	1.0	0.948980	0.097187	0.965126	Biso	1.000000	O
O	1.0	0.948362	0.597407	0.299433	Biso	1.000000	O
O	1.0	0.948310	0.597158	0.632353	Biso	1.000000	O
O	1.0	0.948496	0.596801	0.965844	Biso	1.000000	O
O	1.0	0.552004	0.347269	0.298764	Biso	1.000000	O

O	1.0	0.551967	0.347336	0.632167	Biso	1.000000	O
O	1.0	0.551597	0.347247	0.965541	Biso	1.000000	O
O	1.0	0.551377	0.847812	0.298674	Biso	1.000000	O
O	1.0	0.552125	0.847380	0.632362	Biso	1.000000	O
O	1.0	0.551715	0.847544	0.965709	Biso	1.000000	O
O	1.0	0.447770	0.152510	0.034253	Biso	1.000000	O
O	1.0	0.448099	0.152798	0.368079	Biso	1.000000	O
O	1.0	0.447857	0.152609	0.701326	Biso	1.000000	O
O	1.0	0.448049	0.652503	0.034419	Biso	1.000000	O
O	1.0	0.448173	0.652833	0.367805	Biso	1.000000	O
O	1.0	0.448119	0.652660	0.701130	Biso	1.000000	O
O	1.0	0.945267	0.153659	0.130558	Biso	1.000000	O
O	1.0	0.948196	0.153340	0.464841	Biso	1.000000	O
O	1.0	0.948549	0.152646	0.798796	Biso	1.000000	O
O	1.0	0.948408	0.651221	0.132568	Biso	1.000000	O
O	1.0	0.948235	0.652103	0.465862	Biso	1.000000	O
O	1.0	0.948243	0.652011	0.799184	Biso	1.000000	O
O	1.0	0.051439	0.352127	0.196442	Biso	1.000000	O
O	1.0	0.051470	0.347519	0.532069	Biso	1.000000	O
O	1.0	0.051703	0.345882	0.865115	Biso	1.000000	O
O	1.0	0.052193	0.847964	0.201265	Biso	1.000000	O
O	1.0	0.051848	0.847260	0.534495	Biso	1.000000	O
O	1.0	0.051926	0.847806	0.867693	Biso	1.000000	O
Si	1.0	0.270220	0.172133	0.020383	Biso	1.000000	Si
Si	1.0	0.270151	0.170845	0.352308	Biso	1.000000	Si
Si	1.0	0.271948	0.170276	0.684599	Biso	1.000000	Si
Si	1.0	0.271581	0.670751	0.017837	Biso	1.000000	Si
Si	1.0	0.271857	0.671171	0.351338	Biso	1.000000	Si
Si	1.0	0.271707	0.670900	0.684759	Biso	1.000000	Si
Si	1.0	0.728615	0.328757	0.315240	Biso	1.000000	Si
Si	1.0	0.728081	0.329147	0.648811	Biso	1.000000	Si
Si	1.0	0.728202	0.328948	0.982172	Biso	1.000000	Si
Si	1.0	0.728630	0.829356	0.315515	Biso	1.000000	Si
Si	1.0	0.728469	0.829230	0.648983	Biso	1.000000	Si
Si	1.0	0.728536	0.829245	0.982486	Biso	1.000000	Si
Si	1.0	0.226065	0.327283	0.185371	Biso	1.000000	Si
Si	1.0	0.227973	0.329504	0.516147	Biso	1.000000	Si
Si	1.0	0.228069	0.328345	0.851161	Biso	1.000000	Si
Si	1.0	0.228012	0.829067	0.184303	Biso	1.000000	Si
Si	1.0	0.228264	0.829574	0.517805	Biso	1.000000	Si
Si	1.0	0.228077	0.829419	0.851599	Biso	1.000000	Si
Si	1.0	0.771293	0.170858	0.149165	Biso	1.000000	Si
Si	1.0	0.771609	0.170671	0.481948	Biso	1.000000	Si
Si	1.0	0.771582	0.170570	0.815511	Biso	1.000000	Si
Si	1.0	0.771785	0.670858	0.148768	Biso	1.000000	Si
Si	1.0	0.771855	0.670730	0.482119	Biso	1.000000	Si
Si	1.0	0.771849	0.670603	0.815639	Biso	1.000000	Si
Si	1.0	0.728605	0.420528	0.148791	Biso	1.000000	Si
Si	1.0	0.728269	0.420593	0.481968	Biso	1.000000	Si
Si	1.0	0.728282	0.420624	0.815532	Biso	1.000000	Si
Si	1.0	0.728697	0.921173	0.148967	Biso	1.000000	Si
Si	1.0	0.728516	0.920844	0.482254	Biso	1.000000	Si
Si	1.0	0.728384	0.920767	0.815723	Biso	1.000000	Si
Si	1.0	0.271423	0.082066	0.184991	Biso	1.000000	Si
Si	1.0	0.272579	0.078902	0.517859	Biso	1.000000	Si
Si	1.0	0.270612	0.079977	0.851902	Biso	1.000000	Si
Si	1.0	0.272161	0.579810	0.184823	Biso	1.000000	Si
Si	1.0	0.272110	0.579614	0.518047	Biso	1.000000	Si
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Si	1.0	0.771646	0.079122	0.648710	Biso	1.000000	Si
Si	1.0	0.771517	0.079186	0.982332	Biso	1.000000	Si
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Si	1.0	0.771793	0.579105	0.648864	Biso	1.000000	Si
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Si	1.0	0.228063	0.920565	0.350549	Biso	1.000000	Si
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model 2

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CRYSTAL DATA

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_atom_site_fract_y
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_atom_site_B_iso_or_equiv
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O	1.0	0.063048	0.579829	0.733611	Biso	1.000000	O
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O	1.0	0.937186	0.419720	0.598145	Biso	1.000000	O
O	1.0	0.936552	0.420234	0.931049	Biso	1.000000	O
O	1.0	0.938208	0.922679	0.266984	Biso	1.000000	O
O	1.0	0.936805	0.920059	0.599871	Biso	1.000000	O
O	1.0	0.937177	0.920677	0.933008	Biso	1.000000	O
O	1.0	0.311437	0.249383	0.015703	Biso	1.000000	O
O	1.0	0.306857	0.249715	0.348375	Biso	1.000000	O
O	1.0	0.311140	0.250736	0.681616	Biso	1.000000	O
O	1.0	0.311215	0.751480	0.014603	Biso	1.000000	O
O	1.0	0.311173	0.752137	0.348675	Biso	1.000000	O
O	1.0	0.311296	0.751572	0.681716	Biso	1.000000	O
O	1.0	0.688690	0.248727	0.318217	Biso	1.000000	O
O	1.0	0.688431	0.248879	0.651417	Biso	1.000000	O
O	1.0	0.688383	0.249046	0.984886	Biso	1.000000	O
O	1.0	0.688891	0.749054	0.318519	Biso	1.000000	O
O	1.0	0.688630	0.748989	0.651832	Biso	1.000000	O

O	1.0	0.688783	0.749067	0.985234	Biso	1.000000	O
O	1.0	0.199852	0.244991	0.175794	Biso	1.000000	O
O	1.0	0.187572	0.249663	0.512317	Biso	1.000000	O
O	1.0	0.188306	0.248655	0.848688	Biso	1.000000	O
O	1.0	0.188282	0.749448	0.182284	Biso	1.000000	O
O	1.0	0.187625	0.751470	0.513671	Biso	1.000000	O
O	1.0	0.188366	0.749717	0.849008	Biso	1.000000	O
O	1.0	0.812801	0.250038	0.153046	Biso	1.000000	O
O	1.0	0.812023	0.250272	0.484174	Biso	1.000000	O
O	1.0	0.811495	0.250885	0.817637	Biso	1.000000	O
O	1.0	0.811858	0.750855	0.151554	Biso	1.000000	O
O	1.0	0.811610	0.750840	0.484747	Biso	1.000000	O
O	1.0	0.811671	0.750706	0.818364	Biso	1.000000	O
O	1.0	0.688615	0.000962	0.152031	Biso	1.000000	O
O	1.0	0.688563	0.000933	0.485105	Biso	1.000000	O
O	1.0	0.688648	0.000978	0.818522	Biso	1.000000	O
O	1.0	0.688835	0.500687	0.151608	Biso	1.000000	O
O	1.0	0.688532	0.500454	0.484689	Biso	1.000000	O
O	1.0	0.688466	0.500732	0.818000	Biso	1.000000	O
O	1.0	0.312124	0.500791	0.181898	Biso	1.000000	O
O	1.0	0.311481	0.499898	0.515345	Biso	1.000000	O
O	1.0	0.311270	0.499450	0.848059	Biso	1.000000	O
O	1.0	0.310224	0.997138	0.182578	Biso	1.000000	O
O	1.0	0.311685	0.998790	0.515223	Biso	1.000000	O
O	1.0	0.311245	0.999170	0.848478	Biso	1.000000	O
O	1.0	0.811322	0.499119	0.317845	Biso	1.000000	O
O	1.0	0.811659	0.498955	0.651156	Biso	1.000000	O
O	1.0	0.811498	0.498917	0.984667	Biso	1.000000	O
O	1.0	0.810723	0.998560	0.318977	Biso	1.000000	O
O	1.0	0.811444	0.999019	0.651714	Biso	1.000000	O
O	1.0	0.811755	0.999477	0.985246	Biso	1.000000	O
O	1.0	0.189130	0.001829	0.017142	Biso	1.000000	O
O	1.0	0.183945	0.001884	0.344618	Biso	1.000000	O
O	1.0	0.188680	0.001317	0.682283	Biso	1.000000	O
O	1.0	0.188526	0.500705	0.014918	Biso	1.000000	O
O	1.0	0.190317	0.503759	0.349907	Biso	1.000000	O
O	1.0	0.188082	0.500326	0.681014	Biso	1.000000	O
O	1.0	0.430486	0.240944	0.230792	Biso	1.000000	O
O	1.0	0.431391	0.240683	0.562434	Biso	1.000000	O
O	1.0	0.432365	0.241154	0.896234	Biso	1.000000	O
O	1.0	0.432543	0.741501	0.229657	Biso	1.000000	O
O	1.0	0.432260	0.741652	0.563037	Biso	1.000000	O
O	1.0	0.432598	0.741511	0.896397	Biso	1.000000	O
O	1.0	0.567227	0.258564	0.103733	Biso	1.000000	O
O	1.0	0.567131	0.258481	0.436917	Biso	1.000000	O
O	1.0	0.567331	0.258706	0.770214	Biso	1.000000	O
O	1.0	0.567765	0.758705	0.103715	Biso	1.000000	O
O	1.0	0.567351	0.758786	0.437127	Biso	1.000000	O
O	1.0	0.567660	0.758831	0.770503	Biso	1.000000	O
O	1.0	0.067007	0.258034	0.064169	Biso	1.000000	O
O	1.0	0.064299	0.255435	0.398832	Biso	1.000000	O
O	1.0	0.067427	0.257907	0.728301	Biso	1.000000	O
O	1.0	0.067976	0.760149	0.064457	Biso	1.000000	O
O	1.0	0.067398	0.759280	0.396306	Biso	1.000000	O
O	1.0	0.067769	0.759150	0.729888	Biso	1.000000	O
O	1.0	0.937766	0.239705	0.271333	Biso	1.000000	O
O	1.0	0.932809	0.240553	0.601937	Biso	1.000000	O
O	1.0	0.932139	0.241301	0.936493	Biso	1.000000	O
O	1.0	0.932854	0.742080	0.270028	Biso	1.000000	O
O	1.0	0.932402	0.741364	0.603688	Biso	1.000000	O
O	1.0	0.932614	0.741377	0.937060	Biso	1.000000	O
O	1.0	0.568217	0.490869	0.270196	Biso	1.000000	O
O	1.0	0.567425	0.490948	0.603313	Biso	1.000000	O
O	1.0	0.567469	0.491009	0.936905	Biso	1.000000	O
O	1.0	0.567431	0.991213	0.270469	Biso	1.000000	O
O	1.0	0.567647	0.991218	0.603794	Biso	1.000000	O
O	1.0	0.567735	0.991313	0.937168	Biso	1.000000	O
O	1.0	0.432508	0.008286	0.063521	Biso	1.000000	O
O	1.0	0.432963	0.008391	0.396346	Biso	1.000000	O
O	1.0	0.432684	0.008628	0.729662	Biso	1.000000	O
O	1.0	0.432242	0.508746	0.062907	Biso	1.000000	O
O	1.0	0.432958	0.508952	0.396630	Biso	1.000000	O
O	1.0	0.432137	0.508857	0.729653	Biso	1.000000	O
O	1.0	0.932743	0.008617	0.104451	Biso	1.000000	O
O	1.0	0.933870	0.006771	0.437914	Biso	1.000000	O
O	1.0	0.932446	0.008598	0.770297	Biso	1.000000	O
O	1.0	0.932524	0.508443	0.103342	Biso	1.000000	O
O	1.0	0.932794	0.508498	0.436618	Biso	1.000000	O
O	1.0	0.932399	0.508483	0.769604	Biso	1.000000	O

O	1.0	0.067410	0.493725	0.231137	Biso	1.000000	O
O	1.0	0.067975	0.491000	0.562023	Biso	1.000000	O
O	1.0	0.067105	0.491863	0.895039	Biso	1.000000	O
O	1.0	0.070538	0.996091	0.236551	Biso	1.000000	O
O	1.0	0.066757	0.991746	0.563095	Biso	1.000000	O
O	1.0	0.067809	0.992052	0.896676	Biso	1.000000	O
O	1.0	0.305469	0.109063	0.279155	Biso	1.000000	O
O	1.0	0.303031	0.110007	0.612460	Biso	1.000000	O
O	1.0	0.302539	0.110287	0.945888	Biso	1.000000	O
O	1.0	0.303387	0.611948	0.279105	Biso	1.000000	O
O	1.0	0.303372	0.610948	0.612717	Biso	1.000000	O
O	1.0	0.302926	0.610608	0.945822	Biso	1.000000	O
O	1.0	0.696883	0.389660	0.054108	Biso	1.000000	O
O	1.0	0.697692	0.389243	0.387113	Biso	1.000000	O
O	1.0	0.696864	0.389524	0.720580	Biso	1.000000	O
O	1.0	0.697193	0.889696	0.054744	Biso	1.000000	O
O	1.0	0.697020	0.889454	0.388105	Biso	1.000000	O
O	1.0	0.696975	0.889589	0.721462	Biso	1.000000	O
O	1.0	0.195904	0.388983	0.111454	Biso	1.000000	O
O	1.0	0.196486	0.390939	0.444195	Biso	1.000000	O
O	1.0	0.196417	0.388939	0.777996	Biso	1.000000	O
O	1.0	0.196613	0.889709	0.112393	Biso	1.000000	O
O	1.0	0.196668	0.893289	0.445319	Biso	1.000000	O
O	1.0	0.196811	0.889792	0.778858	Biso	1.000000	O
O	1.0	0.802691	0.109586	0.221189	Biso	1.000000	O
O	1.0	0.803263	0.110151	0.554332	Biso	1.000000	O
O	1.0	0.803170	0.110522	0.887810	Biso	1.000000	O
O	1.0	0.803395	0.610460	0.221019	Biso	1.000000	O
O	1.0	0.803190	0.610275	0.554320	Biso	1.000000	O
O	1.0	0.803209	0.610167	0.887686	Biso	1.000000	O
O	1.0	0.697176	0.359842	0.220635	Biso	1.000000	O
O	1.0	0.697028	0.359910	0.553907	Biso	1.000000	O
O	1.0	0.696673	0.360177	0.887327	Biso	1.000000	O
O	1.0	0.697093	0.860330	0.221358	Biso	1.000000	O
O	1.0	0.696960	0.860358	0.554773	Biso	1.000000	O
O	1.0	0.697092	0.860366	0.888142	Biso	1.000000	O
O	1.0	0.301846	0.135436	0.111776	Biso	1.000000	O
O	1.0	0.302451	0.139334	0.445789	Biso	1.000000	O
O	1.0	0.303010	0.139561	0.779104	Biso	1.000000	O
O	1.0	0.303125	0.640997	0.112429	Biso	1.000000	O
O	1.0	0.303223	0.640934	0.446084	Biso	1.000000	O
O	1.0	0.303012	0.640395	0.779267	Biso	1.000000	O
O	1.0	0.803224	0.139895	0.054606	Biso	1.000000	O
O	1.0	0.803101	0.139282	0.387622	Biso	1.000000	O
O	1.0	0.803238	0.139531	0.720973	Biso	1.000000	O
O	1.0	0.803285	0.639543	0.054337	Biso	1.000000	O
O	1.0	0.803300	0.639595	0.387711	Biso	1.000000	O
O	1.0	0.803171	0.639465	0.721059	Biso	1.000000	O
O	1.0	0.198218	0.367341	0.274629	Biso	1.000000	O
O	1.0	0.196287	0.359820	0.610874	Biso	1.000000	O
O	1.0	0.196356	0.360239	0.944932	Biso	1.000000	O
O	1.0	0.196481	0.861038	0.278785	Biso	1.000000	O
O	1.0	0.196552	0.861676	0.611800	Biso	1.000000	O
O	1.0	0.196659	0.861504	0.945663	Biso	1.000000	O
O	1.0	0.447912	0.096973	0.201423	Biso	1.000000	O
O	1.0	0.447851	0.096829	0.534780	Biso	1.000000	O
O	1.0	0.447897	0.097247	0.867752	Biso	1.000000	O
O	1.0	0.448247	0.597643	0.201073	Biso	1.000000	O
O	1.0	0.448135	0.597793	0.534448	Biso	1.000000	O
O	1.0	0.447967	0.597652	0.867668	Biso	1.000000	O
O	1.0	0.551996	0.402400	0.132062	Biso	1.000000	O
O	1.0	0.551252	0.402171	0.465149	Biso	1.000000	O
O	1.0	0.551702	0.402562	0.798668	Biso	1.000000	O
O	1.0	0.552081	0.902523	0.132304	Biso	1.000000	O
O	1.0	0.552142	0.902675	0.465565	Biso	1.000000	O
O	1.0	0.552086	0.902738	0.798976	Biso	1.000000	O
O	1.0	0.051449	0.401581	0.030678	Biso	1.000000	O
O	1.0	0.052151	0.400433	0.365021	Biso	1.000000	O
O	1.0	0.051894	0.401508	0.698885	Biso	1.000000	O
O	1.0	0.051978	0.903916	0.034410	Biso	1.000000	O
O	1.0	0.052362	0.903439	0.369256	Biso	1.000000	O
O	1.0	0.051794	0.902925	0.701218	Biso	1.000000	O
O	1.0	0.944569	0.095031	0.299455	Biso	1.000000	O
O	1.0	0.948703	0.097175	0.632238	Biso	1.000000	O
O	1.0	0.948386	0.097627	0.966253	Biso	1.000000	O
O	1.0	0.948271	0.598259	0.299423	Biso	1.000000	O
O	1.0	0.948360	0.597433	0.632189	Biso	1.000000	O
O	1.0	0.948411	0.597516	0.965916	Biso	1.000000	O
O	1.0	0.551647	0.346997	0.298703	Biso	1.000000	O

O	1.0	0.551722	0.347120	0.631910	Biso	1.000000	O
O	1.0	0.551707	0.347165	0.965452	Biso	1.000000	O
O	1.0	0.552057	0.847339	0.298973	Biso	1.000000	O
O	1.0	0.552109	0.847362	0.632298	Biso	1.000000	O
O	1.0	0.552045	0.847421	0.965602	Biso	1.000000	O
O	1.0	0.447997	0.151830	0.034098	Biso	1.000000	O
O	1.0	0.447537	0.152391	0.368183	Biso	1.000000	O
O	1.0	0.447767	0.152555	0.701102	Biso	1.000000	O
O	1.0	0.448089	0.652769	0.034535	Biso	1.000000	O
O	1.0	0.448205	0.652934	0.367811	Biso	1.000000	O
O	1.0	0.447927	0.652853	0.701155	Biso	1.000000	O
O	1.0	0.949405	0.152144	0.133162	Biso	1.000000	O
O	1.0	0.950258	0.150512	0.464719	Biso	1.000000	O
O	1.0	0.948239	0.152335	0.799120	Biso	1.000000	O
O	1.0	0.948448	0.652467	0.132433	Biso	1.000000	O
O	1.0	0.948188	0.652523	0.465777	Biso	1.000000	O
O	1.0	0.948263	0.652361	0.799115	Biso	1.000000	O
O	1.0	0.050644	0.352244	0.195538	Biso	1.000000	O
O	1.0	0.051682	0.347252	0.531670	Biso	1.000000	O
O	1.0	0.051578	0.347969	0.865103	Biso	1.000000	O
O	1.0	0.053016	0.853202	0.200269	Biso	1.000000	O
O	1.0	0.051818	0.847847	0.534685	Biso	1.000000	O
O	1.0	0.051909	0.848057	0.867919	Biso	1.000000	O
Si	1.0	0.270560	0.169916	0.019207	Biso	1.000000	Si
Si	1.0	0.269470	0.168275	0.350053	Biso	1.000000	Si
Si	1.0	0.271808	0.170491	0.684697	Biso	1.000000	Si
Si	1.0	0.271505	0.671327	0.017682	Biso	1.000000	Si
Si	1.0	0.271761	0.671762	0.351382	Biso	1.000000	Si
Si	1.0	0.271739	0.671371	0.684678	Biso	1.000000	Si
Si	1.0	0.728820	0.328621	0.314897	Biso	1.000000	Si
Si	1.0	0.728237	0.328942	0.648605	Biso	1.000000	Si
Si	1.0	0.728087	0.329176	0.981881	Biso	1.000000	Si
Si	1.0	0.728528	0.829209	0.315832	Biso	1.000000	Si
Si	1.0	0.728316	0.829124	0.649297	Biso	1.000000	Si
Si	1.0	0.728576	0.829162	0.982608	Biso	1.000000	Si
Si	1.0	0.227694	0.328249	0.185706	Biso	1.000000	Si
Si	1.0	0.227633	0.329919	0.515346	Biso	1.000000	Si
Si	1.0	0.227834	0.328950	0.850894	Biso	1.000000	Si
Si	1.0	0.228290	0.829324	0.184294	Biso	1.000000	Si
Si	1.0	0.227935	0.831197	0.517114	Biso	1.000000	Si
Si	1.0	0.228296	0.829733	0.851468	Biso	1.000000	Si
Si	1.0	0.771767	0.170678	0.149313	Biso	1.000000	Si
Si	1.0	0.771578	0.170515	0.482156	Biso	1.000000	Si
Si	1.0	0.771644	0.170853	0.815483	Biso	1.000000	Si
Si	1.0	0.771910	0.670786	0.148768	Biso	1.000000	Si
Si	1.0	0.771740	0.670753	0.482190	Biso	1.000000	Si
Si	1.0	0.771737	0.670649	0.815610	Biso	1.000000	Si
Si	1.0	0.728585	0.420545	0.148634	Biso	1.000000	Si
Si	1.0	0.728414	0.420411	0.481777	Biso	1.000000	Si
Si	1.0	0.728168	0.420591	0.815186	Biso	1.000000	Si
Si	1.0	0.728418	0.920880	0.149260	Biso	1.000000	Si
Si	1.0	0.728261	0.920785	0.482551	Biso	1.000000	Si
Si	1.0	0.728356	0.920835	0.815947	Biso	1.000000	Si
Si	1.0	0.271818	0.077807	0.186216	Biso	1.000000	Si
Si	1.0	0.271927	0.078766	0.518055	Biso	1.000000	Si
Si	1.0	0.271499	0.079348	0.851575	Biso	1.000000	Si
Si	1.0	0.272018	0.580426	0.184794	Biso	1.000000	Si
Si	1.0	0.272074	0.580121	0.518080	Biso	1.000000	Si
Si	1.0	0.271702	0.579602	0.851265	Biso	1.000000	Si
Si	1.0	0.771118	0.078739	0.315791	Biso	1.000000	Si
Si	1.0	0.771612	0.079104	0.648939	Biso	1.000000	Si
Si	1.0	0.771744	0.079469	0.982392	Biso	1.000000	Si
Si	1.0	0.771732	0.579326	0.315374	Biso	1.000000	Si
Si	1.0	0.771726	0.579033	0.648848	Biso	1.000000	Si
Si	1.0	0.771735	0.579020	0.982265	Biso	1.000000	Si
Si	1.0	0.227683	0.420038	0.018186	Biso	1.000000	Si
Si	1.0	0.228615	0.422400	0.348908	Biso	1.000000	Si
Si	1.0	0.227804	0.420111	0.683532	Biso	1.000000	Si
Si	1.0	0.228467	0.921372	0.018221	Biso	1.000000	Si
Si	1.0	0.227290	0.922594	0.349457	Biso	1.000000	Si
Si	1.0	0.228478	0.921251	0.684693	Biso	1.000000	Si
Si	1.0	0.473051	0.168794	0.266053	Biso	1.000000	Si
Si	1.0	0.473436	0.168653	0.599065	Biso	1.000000	Si
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Si	1.0	0.024141	0.334351	0.431422	Biso	1.000000	Si
Si	1.0	0.025841	0.330664	0.764078	Biso	1.000000	Si
Si	1.0	0.026321	0.833044	0.099449	Biso	1.000000	Si
Si	1.0	0.025793	0.831433	0.432981	Biso	1.000000	Si
Si	1.0	0.026099	0.831589	0.766086	Biso	1.000000	Si
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model 3

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CRYSTAL DATA

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_atom_site_fract_y
_atom_site_fract_z
_atom_site_adp_type
_atom_site_B_iso_or_equiv
_atom_site_type_symbol
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O	1.0	0.688793	0.749140	0.318510	Biso	1.000000	O
O	1.0	0.688517	0.749223	0.651817	Biso	1.000000	O

O	1.0	0.688715	0.749139	0.985217	Biso	1.000000	O
O	1.0	0.189827	0.247523	0.190781	Biso	1.000000	O
O	1.0	0.189057	0.249160	0.512024	Biso	1.000000	O
O	1.0	0.188445	0.248225	0.848525	Biso	1.000000	O
O	1.0	0.188325	0.749429	0.181968	Biso	1.000000	O
O	1.0	0.187631	0.751664	0.513277	Biso	1.000000	O
O	1.0	0.188292	0.749665	0.848762	Biso	1.000000	O
O	1.0	0.812511	0.250472	0.152623	Biso	1.000000	O
O	1.0	0.812710	0.250492	0.484421	Biso	1.000000	O
O	1.0	0.811704	0.250883	0.817784	Biso	1.000000	O
O	1.0	0.811757	0.750937	0.151702	Biso	1.000000	O
O	1.0	0.811479	0.751135	0.484795	Biso	1.000000	O
O	1.0	0.811548	0.751020	0.818576	Biso	1.000000	O
O	1.0	0.688617	0.000898	0.151865	Biso	1.000000	O
O	1.0	0.688569	0.000939	0.485067	Biso	1.000000	O
O	1.0	0.688639	0.000973	0.818592	Biso	1.000000	O
O	1.0	0.688782	0.500562	0.151878	Biso	1.000000	O
O	1.0	0.688208	0.500500	0.484843	Biso	1.000000	O
O	1.0	0.688432	0.500822	0.818232	Biso	1.000000	O
O	1.0	0.310896	0.498641	0.181983	Biso	1.000000	O
O	1.0	0.311536	0.499653	0.514976	Biso	1.000000	O
O	1.0	0.311176	0.498908	0.848115	Biso	1.000000	O
O	1.0	0.310776	0.997021	0.180722	Biso	1.000000	O
O	1.0	0.311479	0.998766	0.515564	Biso	1.000000	O
O	1.0	0.311413	0.999509	0.848553	Biso	1.000000	O
O	1.0	0.812118	0.498985	0.318493	Biso	1.000000	O
O	1.0	0.811323	0.499358	0.651777	Biso	1.000000	O
O	1.0	0.811526	0.499108	0.984914	Biso	1.000000	O
O	1.0	0.811082	0.998565	0.318762	Biso	1.000000	O
O	1.0	0.811609	0.999054	0.651534	Biso	1.000000	O
O	1.0	0.811853	0.999518	0.985328	Biso	1.000000	O
O	1.0	0.189271	0.002029	0.016684	Biso	1.000000	O
O	1.0	0.184332	0.002577	0.343727	Biso	1.000000	O
O	1.0	0.188631	0.001863	0.681643	Biso	1.000000	O
O	1.0	0.187429	0.499038	0.017573	Biso	1.000000	O
O	1.0	0.191107	0.505404	0.352070	Biso	1.000000	O
O	1.0	0.188383	0.500660	0.681197	Biso	1.000000	O
O	1.0	0.431444	0.240644	0.230285	Biso	1.000000	O
O	1.0	0.431824	0.240766	0.562669	Biso	1.000000	O
O	1.0	0.431863	0.240953	0.896633	Biso	1.000000	O
O	1.0	0.432531	0.741122	0.229448	Biso	1.000000	O
O	1.0	0.431885	0.741503	0.562917	Biso	1.000000	O
O	1.0	0.432241	0.741148	0.896308	Biso	1.000000	O
O	1.0	0.567164	0.258535	0.103905	Biso	1.000000	O
O	1.0	0.567481	0.258238	0.437043	Biso	1.000000	O
O	1.0	0.567383	0.258657	0.770479	Biso	1.000000	O
O	1.0	0.567711	0.758559	0.103751	Biso	1.000000	O
O	1.0	0.567155	0.758653	0.437029	Biso	1.000000	O
O	1.0	0.567421	0.758799	0.770529	Biso	1.000000	O
O	1.0	0.067832	0.259164	0.064247	Biso	1.000000	O
O	1.0	0.057913	0.251427	0.404227	Biso	1.000000	O
O	1.0	0.067614	0.259256	0.728156	Biso	1.000000	O
O	1.0	0.068108	0.760151	0.063814	Biso	1.000000	O
O	1.0	0.067573	0.759141	0.396264	Biso	1.000000	O
O	1.0	0.067859	0.759375	0.729733	Biso	1.000000	O
O	1.0	0.936535	0.239646	0.269695	Biso	1.000000	O
O	1.0	0.932957	0.240169	0.602288	Biso	1.000000	O
O	1.0	0.932353	0.241234	0.936838	Biso	1.000000	O
O	1.0	0.932961	0.742418	0.270046	Biso	1.000000	O
O	1.0	0.932407	0.742024	0.603774	Biso	1.000000	O
O	1.0	0.932683	0.741650	0.937221	Biso	1.000000	O
O	1.0	0.567497	0.490931	0.270343	Biso	1.000000	O
O	1.0	0.567538	0.491109	0.603469	Biso	1.000000	O
O	1.0	0.567376	0.491112	0.937172	Biso	1.000000	O
O	1.0	0.567461	0.991182	0.270322	Biso	1.000000	O
O	1.0	0.567623	0.991284	0.603741	Biso	1.000000	O
O	1.0	0.567658	0.991224	0.937184	Biso	1.000000	O
O	1.0	0.432457	0.008622	0.063095	Biso	1.000000	O
O	1.0	0.432950	0.008444	0.396324	Biso	1.000000	O
O	1.0	0.432584	0.008743	0.729847	Biso	1.000000	O
O	1.0	0.431905	0.508713	0.062955	Biso	1.000000	O
O	1.0	0.433268	0.508739	0.396442	Biso	1.000000	O
O	1.0	0.432166	0.508868	0.729632	Biso	1.000000	O
O	1.0	0.933088	0.008684	0.104381	Biso	1.000000	O
O	1.0	0.934854	0.005843	0.437024	Biso	1.000000	O
O	1.0	0.932583	0.008644	0.770577	Biso	1.000000	O
O	1.0	0.932543	0.508855	0.103644	Biso	1.000000	O
O	1.0	0.932327	0.509907	0.437318	Biso	1.000000	O
O	1.0	0.932177	0.509388	0.770151	Biso	1.000000	O

O	1.0	0.067900	0.492685	0.233544	Biso	1.000000	O
O	1.0	0.067200	0.492303	0.563330	Biso	1.000000	O
O	1.0	0.067324	0.491505	0.895236	Biso	1.000000	O
O	1.0	0.071064	0.994770	0.235190	Biso	1.000000	O
O	1.0	0.067018	0.991810	0.562881	Biso	1.000000	O
O	1.0	0.067942	0.991791	0.896277	Biso	1.000000	O
O	1.0	0.306115	0.107101	0.279295	Biso	1.000000	O
O	1.0	0.302734	0.110248	0.612583	Biso	1.000000	O
O	1.0	0.301967	0.110543	0.946079	Biso	1.000000	O
O	1.0	0.303260	0.610810	0.278514	Biso	1.000000	O
O	1.0	0.303121	0.610771	0.612131	Biso	1.000000	O
O	1.0	0.302689	0.609907	0.945526	Biso	1.000000	O
O	1.0	0.697080	0.389645	0.054544	Biso	1.000000	O
O	1.0	0.697734	0.389220	0.387446	Biso	1.000000	O
O	1.0	0.696970	0.389628	0.720848	Biso	1.000000	O
O	1.0	0.697205	0.889721	0.054729	Biso	1.000000	O
O	1.0	0.697111	0.889546	0.388089	Biso	1.000000	O
O	1.0	0.696926	0.889728	0.721414	Biso	1.000000	O
O	1.0	0.195249	0.382203	0.108494	Biso	1.000000	O
O	1.0	0.197856	0.391348	0.445066	Biso	1.000000	O
O	1.0	0.196613	0.388565	0.777240	Biso	1.000000	O
O	1.0	0.196750	0.389746	0.111843	Biso	1.000000	O
O	1.0	0.196666	0.893658	0.444717	Biso	1.000000	O
O	1.0	0.196779	0.889915	0.778279	Biso	1.000000	O
O	1.0	0.802829	0.109545	0.221004	Biso	1.000000	O
O	1.0	0.803330	0.110149	0.554266	Biso	1.000000	O
O	1.0	0.803268	0.110490	0.887810	Biso	1.000000	O
O	1.0	0.803443	0.610473	0.221286	Biso	1.000000	O
O	1.0	0.803029	0.610613	0.554549	Biso	1.000000	O
O	1.0	0.803065	0.610406	0.887843	Biso	1.000000	O
O	1.0	0.697416	0.359890	0.221132	Biso	1.000000	O
O	1.0	0.697013	0.359988	0.554162	Biso	1.000000	O
O	1.0	0.696774	0.360324	0.887661	Biso	1.000000	O
O	1.0	0.697160	0.860383	0.221363	Biso	1.000000	O
O	1.0	0.697037	0.860512	0.554686	Biso	1.000000	O
O	1.0	0.697056	0.860426	0.888113	Biso	1.000000	O
O	1.0	0.300071	0.138297	0.113640	Biso	1.000000	O
O	1.0	0.303348	0.138529	0.446165	Biso	1.000000	O
O	1.0	0.302793	0.139928	0.778950	Biso	1.000000	O
O	1.0	0.302919	0.639250	0.112080	Biso	1.000000	O
O	1.0	0.302990	0.640325	0.445560	Biso	1.000000	O
O	1.0	0.302774	0.639835	0.778830	Biso	1.000000	O
O	1.0	0.803402	0.139886	0.054630	Biso	1.000000	O
O	1.0	0.803368	0.139045	0.387718	Biso	1.000000	O
O	1.0	0.803255	0.139508	0.721017	Biso	1.000000	O
O	1.0	0.803257	0.639705	0.054492	Biso	1.000000	O
O	1.0	0.803219	0.639704	0.387838	Biso	1.000000	O
O	1.0	0.803024	0.639897	0.721216	Biso	1.000000	O
O	1.0	0.198635	0.371025	0.275498	Biso	1.000000	O
O	1.0	0.197045	0.360059	0.610682	Biso	1.000000	O
O	1.0	0.196219	0.360400	0.943370	Biso	1.000000	O
O	1.0	0.196514	0.861327	0.278242	Biso	1.000000	O
O	1.0	0.196497	0.862190	0.611172	Biso	1.000000	O
O	1.0	0.196697	0.861647	0.945184	Biso	1.000000	O
O	1.0	0.448056	0.096919	0.201327	Biso	1.000000	O
O	1.0	0.448067	0.096946	0.534814	Biso	1.000000	O
O	1.0	0.447852	0.097211	0.868136	Biso	1.000000	O
O	1.0	0.447997	0.597174	0.201170	Biso	1.000000	O
O	1.0	0.448156	0.597683	0.534400	Biso	1.000000	O
O	1.0	0.447898	0.597386	0.867780	Biso	1.000000	O
O	1.0	0.551850	0.402453	0.132187	Biso	1.000000	O
O	1.0	0.551319	0.402030	0.465364	Biso	1.000000	O
O	1.0	0.551706	0.402565	0.798948	Biso	1.000000	O
O	1.0	0.551993	0.902445	0.132118	Biso	1.000000	O
O	1.0	0.551971	0.902573	0.465528	Biso	1.000000	O
O	1.0	0.552044	0.902687	0.798882	Biso	1.000000	O
O	1.0	0.051693	0.402461	0.031884	Biso	1.000000	O
O	1.0	0.052873	0.400683	0.369036	Biso	1.000000	O
O	1.0	0.051751	0.403873	0.701608	Biso	1.000000	O
O	1.0	0.052130	0.904179	0.034543	Biso	1.000000	O
O	1.0	0.052730	0.902961	0.368644	Biso	1.000000	O
O	1.0	0.051907	0.903211	0.701224	Biso	1.000000	O
O	1.0	0.944949	0.095352	0.299119	Biso	1.000000	O
O	1.0	0.948179	0.096776	0.632250	Biso	1.000000	O
O	1.0	0.948391	0.097379	0.965755	Biso	1.000000	O
O	1.0	0.948086	0.598539	0.299156	Biso	1.000000	O
O	1.0	0.948004	0.598232	0.632206	Biso	1.000000	O
O	1.0	0.948022	0.597729	0.965607	Biso	1.000000	O
O	1.0	0.551618	0.346935	0.298834	Biso	1.000000	O

O	1.0	0.551891	0.347268	0.632227	Biso	1.000000	O
O	1.0	0.551656	0.347232	0.965571	Biso	1.000000	O
O	1.0	0.551968	0.847246	0.298911	Biso	1.000000	O
O	1.0	0.551982	0.847382	0.632219	Biso	1.000000	O
O	1.0	0.552069	0.847253	0.965481	Biso	1.000000	O
O	1.0	0.447570	0.152475	0.034895	Biso	1.000000	O
O	1.0	0.447773	0.152304	0.368051	Biso	1.000000	O
O	1.0	0.447986	0.152629	0.701308	Biso	1.000000	O
O	1.0	0.447949	0.652570	0.034584	Biso	1.000000	O
O	1.0	0.448080	0.652679	0.367699	Biso	1.000000	O
O	1.0	0.447815	0.652831	0.701159	Biso	1.000000	O
O	1.0	0.949935	0.152751	0.132439	Biso	1.000000	O
O	1.0	0.948739	0.148337	0.465776	Biso	1.000000	O
O	1.0	0.948170	0.152533	0.798894	Biso	1.000000	O
O	1.0	0.948180	0.653177	0.132125	Biso	1.000000	O
O	1.0	0.948089	0.653865	0.465417	Biso	1.000000	O
O	1.0	0.948150	0.653216	0.798894	Biso	1.000000	O
O	1.0	0.052035	0.352700	0.196179	Biso	1.000000	O
O	1.0	0.051984	0.347859	0.535896	Biso	1.000000	O
O	1.0	0.051703	0.347253	0.866827	Biso	1.000000	O
O	1.0	0.053174	0.852354	0.199958	Biso	1.000000	O
O	1.0	0.051975	0.847829	0.534637	Biso	1.000000	O
O	1.0	0.051941	0.847916	0.867925	Biso	1.000000	O
Si	1.0	0.270623	0.170313	0.018653	Biso	1.000000	Si
Si	1.0	0.271342	0.166307	0.351088	Biso	1.000000	Si
Si	1.0	0.271256	0.171150	0.684356	Biso	1.000000	Si
Si	1.0	0.271429	0.670468	0.017668	Biso	1.000000	Si
Si	1.0	0.271746	0.671047	0.350832	Biso	1.000000	Si
Si	1.0	0.271579	0.671114	0.684215	Biso	1.000000	Si
Si	1.0	0.729450	0.328535	0.315479	Biso	1.000000	Si
Si	1.0	0.728559	0.329115	0.648755	Biso	1.000000	Si
Si	1.0	0.728319	0.329275	0.982198	Biso	1.000000	Si
Si	1.0	0.728615	0.829232	0.315883	Biso	1.000000	Si
Si	1.0	0.728342	0.829293	0.649201	Biso	1.000000	Si
Si	1.0	0.728574	0.829204	0.982554	Biso	1.000000	Si
Si	1.0	0.228062	0.333035	0.188421	Biso	1.000000	Si
Si	1.0	0.228304	0.329546	0.515754	Biso	1.000000	Si
Si	1.0	0.228000	0.328542	0.849607	Biso	1.000000	Si
Si	1.0	0.228314	0.829307	0.183949	Biso	1.000000	Si
Si	1.0	0.227745	0.831483	0.516592	Biso	1.000000	Si
Si	1.0	0.228111	0.829775	0.850866	Biso	1.000000	Si
Si	1.0	0.772042	0.170835	0.149381	Biso	1.000000	Si
Si	1.0	0.772326	0.170826	0.481880	Biso	1.000000	Si
Si	1.0	0.771848	0.170864	0.815416	Biso	1.000000	Si
Si	1.0	0.771991	0.670725	0.149140	Biso	1.000000	Si
Si	1.0	0.771740	0.670961	0.482243	Biso	1.000000	Si
Si	1.0	0.771663	0.670940	0.815767	Biso	1.000000	Si
Si	1.0	0.728899	0.420551	0.149191	Biso	1.000000	Si
Si	1.0	0.728527	0.420632	0.482056	Biso	1.000000	Si
Si	1.0	0.728271	0.420722	0.815410	Biso	1.000000	Si
Si	1.0	0.728565	0.920886	0.149274	Biso	1.000000	Si
Si	1.0	0.728519	0.920944	0.482525	Biso	1.000000	Si
Si	1.0	0.728397	0.920860	0.815888	Biso	1.000000	Si
Si	1.0	0.271833	0.077008	0.185921	Biso	1.000000	Si
Si	1.0	0.271248	0.078570	0.518626	Biso	1.000000	Si
Si	1.0	0.271379	0.079525	0.851045	Biso	1.000000	Si
Si	1.0	0.271326	0.578977	0.184501	Biso	1.000000	Si
Si	1.0	0.271410	0.579582	0.517587	Biso	1.000000	Si
Si	1.0	0.271432	0.579050	0.850722	Biso	1.000000	Si
Si	1.0	0.771583	0.078871	0.315908	Biso	1.000000	Si
Si	1.0	0.771845	0.079162	0.648744	Biso	1.000000	Si
Si	1.0	0.771906	0.079553	0.982439	Biso	1.000000	Si
Si	1.0	0.772151	0.578957	0.315621	Biso	1.000000	Si
Si	1.0	0.771614	0.579431	0.649025	Biso	1.000000	Si
Si	1.0	0.771767	0.579202	0.982427	Biso	1.000000	Si
Si	1.0	0.227394	0.418956	0.017219	Biso	1.000000	Si
Si	1.0	0.229747	0.424642	0.351842	Biso	1.000000	Si
Si	1.0	0.228046	0.420387	0.683113	Biso	1.000000	Si
Si	1.0	0.228641	0.921423	0.017639	Biso	1.000000	Si
Si	1.0	0.227183	0.922916	0.348993	Biso	1.000000	Si
Si	1.0	0.228331	0.921725	0.684114	Biso	1.000000	Si
Si	1.0	0.473776	0.168467	0.266199	Biso	1.000000	Si
Si	1.0	0.473823	0.168680	0.599194	Biso	1.000000	Si
Si	1.0	0.473696	0.168629	0.932820	Biso	1.000000	Si
Si	1.0	0.474043	0.668580	0.265791	Biso	1.000000	Si
Si	1.0	0.473688	0.669042	0.599143	Biso	1.000000	Si
Si	1.0	0.473824	0.668607	0.932515	Biso	1.000000	Si
Si	1.0	0.525934	0.331200	0.067529	Biso	1.000000	Si
Si	1.0	0.525627	0.330520	0.400762	Biso	1.000000	Si

Si	1.0	0.525985	0.331249	0.734155	Biso	1.000000	Si
Si	1.0	0.526252	0.831043	0.067413	Biso	1.000000	Si
Si	1.0	0.525873	0.831330	0.400854	Biso	1.000000	Si
Si	1.0	0.526058	0.831369	0.734176	Biso	1.000000	Si
Si	1.0	0.025705	0.332665	0.098498	Biso	1.000000	Si
Si	1.0	0.025555	0.328807	0.432973	Biso	1.000000	Si
Si	1.0	0.026043	0.331587	0.764804	Biso	1.000000	Si
Si	1.0	0.026298	0.832790	0.099174	Biso	1.000000	Si
Si	1.0	0.026010	0.831370	0.432889	Biso	1.000000	Si
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Si	1.0	0.973919	0.168766	0.900779	Biso	1.000000	Si
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model 4

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CRYSTAL DATA

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_atom_site_B_iso_or_equiv
_atom_site_type_symbol
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O	1.0	0.811688	0.751086	0.484989	Biso	1.000000	O
O	1.0	0.811639	0.750922	0.818207	Biso	1.000000	O
O	1.0	0.688483	0.000788	0.151789	Biso	1.000000	O
O	1.0	0.688685	0.001060	0.485074	Biso	1.000000	O
O	1.0	0.688603	0.000950	0.818452	Biso	1.000000	O
O	1.0	0.688863	0.500764	0.151710	Biso	1.000000	O
O	1.0	0.688781	0.500649	0.485270	Biso	1.000000	O
O	1.0	0.688432	0.500714	0.818157	Biso	1.000000	O
O	1.0	0.311151	0.498390	0.181930	Biso	1.000000	O
O	1.0	0.311268	0.498848	0.514894	Biso	1.000000	O
O	1.0	0.311209	0.498456	0.847774	Biso	1.000000	O
O	1.0	0.311658	1.000183	0.182184	Biso	1.000000	O
O	1.0	0.308365	0.999774	0.515376	Biso	1.000000	O
O	1.0	0.311274	0.999332	0.848661	Biso	1.000000	O
O	1.0	0.812428	0.499018	0.318761	Biso	1.000000	O
O	1.0	0.811354	0.499045	0.651428	Biso	1.000000	O
O	1.0	0.811538	0.499035	0.984874	Biso	1.000000	O
O	1.0	0.812267	0.999434	0.319072	Biso	1.000000	O
O	1.0	0.812300	0.999304	0.651342	Biso	1.000000	O
O	1.0	0.811490	0.999059	0.984806	Biso	1.000000	O
O	1.0	0.188293	0.001231	0.015372	Biso	1.000000	O
O	1.0	0.187123	0.001230	0.348250	Biso	1.000000	O
O	1.0	0.188856	0.001485	0.681053	Biso	1.000000	O
O	1.0	0.187577	0.499168	0.016908	Biso	1.000000	O
O	1.0	0.191046	0.504923	0.353159	Biso	1.000000	O
O	1.0	0.187733	0.498284	0.679239	Biso	1.000000	O
O	1.0	0.432114	0.241336	0.230144	Biso	1.000000	O
O	1.0	0.432884	0.241231	0.563024	Biso	1.000000	O
O	1.0	0.432551	0.241172	0.896454	Biso	1.000000	O
O	1.0	0.432384	0.741186	0.229543	Biso	1.000000	O
O	1.0	0.432183	0.741370	0.563017	Biso	1.000000	O
O	1.0	0.432156	0.741094	0.896297	Biso	1.000000	O
O	1.0	0.567424	0.258628	0.103824	Biso	1.000000	O
O	1.0	0.567683	0.258574	0.437085	Biso	1.000000	O
O	1.0	0.567549	0.258655	0.770351	Biso	1.000000	O
O	1.0	0.567554	0.758710	0.103725	Biso	1.000000	O
O	1.0	0.567432	0.758947	0.437063	Biso	1.000000	O
O	1.0	0.567446	0.758918	0.770278	Biso	1.000000	O
O	1.0	0.067890	0.259319	0.062145	Biso	1.000000	O
O	1.0	0.062479	0.247642	0.410529	Biso	1.000000	O
O	1.0	0.066923	0.258205	0.728841	Biso	1.000000	O
O	1.0	0.067746	0.758574	0.063271	Biso	1.000000	O
O	1.0	0.067701	0.759106	0.396405	Biso	1.000000	O
O	1.0	0.067742	0.758891	0.729722	Biso	1.000000	O
O	1.0	0.933294	0.240829	0.270000	Biso	1.000000	O
O	1.0	0.935270	0.241915	0.603956	Biso	1.000000	O
O	1.0	0.932319	0.241196	0.936643	Biso	1.000000	O
O	1.0	0.932528	0.741241	0.270275	Biso	1.000000	O
O	1.0	0.932457	0.741477	0.603577	Biso	1.000000	O
O	1.0	0.932537	0.741170	0.936868	Biso	1.000000	O
O	1.0	0.567817	0.491176	0.270389	Biso	1.000000	O
O	1.0	0.567251	0.491326	0.603581	Biso	1.000000	O
O	1.0	0.567488	0.491156	0.937091	Biso	1.000000	O
O	1.0	0.567225	0.991388	0.270487	Biso	1.000000	O
O	1.0	0.567291	0.991497	0.603773	Biso	1.000000	O
O	1.0	0.567363	0.991252	0.937140	Biso	1.000000	O
O	1.0	0.432136	0.008899	0.063223	Biso	1.000000	O
O	1.0	0.431307	0.009257	0.397000	Biso	1.000000	O
O	1.0	0.431888	0.009024	0.729657	Biso	1.000000	O
O	1.0	0.432230	0.508700	0.062845	Biso	1.000000	O
O	1.0	0.433460	0.508769	0.396440	Biso	1.000000	O
O	1.0	0.431903	0.508675	0.729472	Biso	1.000000	O
O	1.0	0.932257	0.008747	0.103590	Biso	1.000000	O
O	1.0	0.935881	0.008448	0.437076	Biso	1.000000	O
O	1.0	0.932820	0.009356	0.769852	Biso	1.000000	O
O	1.0	0.932631	0.508347	0.103710	Biso	1.000000	O
O	1.0	0.932988	0.508590	0.437253	Biso	1.000000	O
O	1.0	0.932229	0.508771	0.769939	Biso	1.000000	O

O	1.0	0.068519	0.491077	0.234347	Biso	1.000000	O
O	1.0	0.067166	0.491407	0.563028	Biso	1.000000	O
O	1.0	0.067467	0.491187	0.894664	Biso	1.000000	O
O	1.0	0.067889	0.991453	0.230743	Biso	1.000000	O
O	1.0	0.068999	0.991429	0.562914	Biso	1.000000	O
O	1.0	0.067599	0.991189	0.896125	Biso	1.000000	O
O	1.0	0.301117	0.111444	0.280187	Biso	1.000000	O
O	1.0	0.302255	0.110525	0.613127	Biso	1.000000	O
O	1.0	0.302294	0.110414	0.946310	Biso	1.000000	O
O	1.0	0.303149	0.610443	0.278473	Biso	1.000000	O
O	1.0	0.303156	0.610024	0.612180	Biso	1.000000	O
O	1.0	0.302797	0.609527	0.945393	Biso	1.000000	O
O	1.0	0.697148	0.389623	0.054577	Biso	1.000000	O
O	1.0	0.697288	0.389596	0.387713	Biso	1.000000	O
O	1.0	0.697102	0.389393	0.720915	Biso	1.000000	O
O	1.0	0.697031	0.889608	0.054559	Biso	1.000000	O
O	1.0	0.697243	0.889882	0.387874	Biso	1.000000	O
O	1.0	0.697151	0.889917	0.721127	Biso	1.000000	O
O	1.0	0.195703	0.382947	0.108011	Biso	1.000000	O
O	1.0	0.197470	0.389283	0.444249	Biso	1.000000	O
O	1.0	0.196646	0.386968	0.776137	Biso	1.000000	O
O	1.0	0.196714	0.889843	0.112400	Biso	1.000000	O
O	1.0	0.196374	0.890033	0.445595	Biso	1.000000	O
O	1.0	0.196713	0.890184	0.778855	Biso	1.000000	O
O	1.0	0.803034	0.110082	0.221127	Biso	1.000000	O
O	1.0	0.803381	0.110280	0.554401	Biso	1.000000	O
O	1.0	0.803118	0.110336	0.887727	Biso	1.000000	O
O	1.0	0.803473	0.610371	0.221234	Biso	1.000000	O
O	1.0	0.803196	0.610465	0.554476	Biso	1.000000	O
O	1.0	0.803110	0.610350	0.887757	Biso	1.000000	O
O	1.0	0.697170	0.360286	0.221197	Biso	1.000000	O
O	1.0	0.697219	0.360042	0.554340	Biso	1.000000	O
O	1.0	0.696781	0.360226	0.887778	Biso	1.000000	O
O	1.0	0.697043	0.860346	0.221258	Biso	1.000000	O
O	1.0	0.697432	0.860666	0.554398	Biso	1.000000	O
O	1.0	0.697166	0.860441	0.887797	Biso	1.000000	O
O	1.0	0.303043	0.140882	0.113286	Biso	1.000000	O
O	1.0	0.305806	0.140835	0.447405	Biso	1.000000	O
O	1.0	0.302589	0.139777	0.779423	Biso	1.000000	O
O	1.0	0.302876	0.638889	0.112020	Biso	1.000000	O
O	1.0	0.302995	0.639529	0.445428	Biso	1.000000	O
O	1.0	0.302990	0.639391	0.778828	Biso	1.000000	O
O	1.0	0.802863	0.139597	0.054432	Biso	1.000000	O
O	1.0	0.802998	0.139814	0.387764	Biso	1.000000	O
O	1.0	0.803428	0.139557	0.720973	Biso	1.000000	O
O	1.0	0.803234	0.639640	0.054429	Biso	1.000000	O
O	1.0	0.803387	0.639730	0.387853	Biso	1.000000	O
O	1.0	0.803137	0.639635	0.721110	Biso	1.000000	O
O	1.0	0.198867	0.371680	0.274692	Biso	1.000000	O
O	1.0	0.196828	0.356222	0.610080	Biso	1.000000	O
O	1.0	0.196625	0.360646	0.942636	Biso	1.000000	O
O	1.0	0.196562	0.860412	0.278864	Biso	1.000000	O
O	1.0	0.196630	0.860596	0.612296	Biso	1.000000	O
O	1.0	0.196643	0.860601	0.945590	Biso	1.000000	O
O	1.0	0.447757	0.097548	0.201510	Biso	1.000000	O
O	1.0	0.447775	0.097303	0.535018	Biso	1.000000	O
O	1.0	0.447804	0.097324	0.868056	Biso	1.000000	O
O	1.0	0.448081	0.597201	0.201194	Biso	1.000000	O
O	1.0	0.448290	0.597569	0.534360	Biso	1.000000	O
O	1.0	0.447823	0.597228	0.867718	Biso	1.000000	O
O	1.0	0.552142	0.402605	0.132095	Biso	1.000000	O
O	1.0	0.551973	0.402488	0.465528	Biso	1.000000	O
O	1.0	0.551944	0.402600	0.798783	Biso	1.000000	O
O	1.0	0.551695	0.902589	0.132272	Biso	1.000000	O
O	1.0	0.551556	0.902882	0.465577	Biso	1.000000	O
O	1.0	0.551721	0.902733	0.798875	Biso	1.000000	O
O	1.0	0.051599	0.402758	0.031793	Biso	1.000000	O
O	1.0	0.053962	0.395180	0.367473	Biso	1.000000	O
O	1.0	0.051911	0.402564	0.701056	Biso	1.000000	O
O	1.0	0.051972	0.902459	0.034410	Biso	1.000000	O
O	1.0	0.052018	0.903223	0.368260	Biso	1.000000	O
O	1.0	0.052318	0.903015	0.701257	Biso	1.000000	O
O	1.0	0.948398	0.097619	0.300019	Biso	1.000000	O
O	1.0	0.950550	0.098240	0.631474	Biso	1.000000	O
O	1.0	0.947783	0.097171	0.964939	Biso	1.000000	O
O	1.0	0.948168	0.597371	0.298996	Biso	1.000000	O
O	1.0	0.948029	0.597558	0.632099	Biso	1.000000	O
O	1.0	0.948114	0.597257	0.965580	Biso	1.000000	O
O	1.0	0.552104	0.347266	0.298812	Biso	1.000000	O

O	1.0	0.552151	0.347367	0.632128	Biso	1.000000	O
O	1.0	0.551906	0.347273	0.965477	Biso	1.000000	O
O	1.0	0.551737	0.847501	0.299005	Biso	1.000000	O
O	1.0	0.551381	0.847710	0.632109	Biso	1.000000	O
O	1.0	0.551804	0.847336	0.965567	Biso	1.000000	O
O	1.0	0.447892	0.152730	0.034772	Biso	1.000000	O
O	1.0	0.447928	0.152967	0.368244	Biso	1.000000	O
O	1.0	0.447938	0.152849	0.701534	Biso	1.000000	O
O	1.0	0.447992	0.652495	0.034447	Biso	1.000000	O
O	1.0	0.448254	0.652667	0.367719	Biso	1.000000	O
O	1.0	0.447910	0.652593	0.701075	Biso	1.000000	O
O	1.0	0.946936	0.153043	0.131482	Biso	1.000000	O
O	1.0	0.945275	0.152145	0.466523	Biso	1.000000	O
O	1.0	0.948453	0.153056	0.798382	Biso	1.000000	O
O	1.0	0.948154	0.652495	0.132187	Biso	1.000000	O
O	1.0	0.948016	0.652775	0.465430	Biso	1.000000	O
O	1.0	0.948277	0.652583	0.798795	Biso	1.000000	O
O	1.0	0.052104	0.351556	0.195222	Biso	1.000000	O
O	1.0	0.052536	0.346909	0.536003	Biso	1.000000	O
O	1.0	0.051801	0.347041	0.866729	Biso	1.000000	O
O	1.0	0.052064	0.847422	0.201278	Biso	1.000000	O
O	1.0	0.052174	0.847602	0.534650	Biso	1.000000	O
O	1.0	0.051977	0.847363	0.867804	Biso	1.000000	O
Si	1.0	0.271368	0.171140	0.018369	Biso	1.000000	Si
Si	1.0	0.270941	0.170852	0.354038	Biso	1.000000	Si
Si	1.0	0.271197	0.171205	0.685300	Biso	1.000000	Si
Si	1.0	0.271498	0.670113	0.017616	Biso	1.000000	Si
Si	1.0	0.271605	0.670696	0.350851	Biso	1.000000	Si
Si	1.0	0.271633	0.670519	0.684249	Biso	1.000000	Si
Si	1.0	0.728885	0.329070	0.315576	Biso	1.000000	Si
Si	1.0	0.728665	0.328895	0.648837	Biso	1.000000	Si
Si	1.0	0.728368	0.329106	0.982347	Biso	1.000000	Si
Si	1.0	0.728633	0.829299	0.315769	Biso	1.000000	Si
Si	1.0	0.728633	0.829479	0.648960	Biso	1.000000	Si
Si	1.0	0.728492	0.829208	0.982337	Biso	1.000000	Si
Si	1.0	0.228759	0.333676	0.187745	Biso	1.000000	Si
Si	1.0	0.227388	0.327074	0.514166	Biso	1.000000	Si
Si	1.0	0.228568	0.328059	0.849421	Biso	1.000000	Si
Si	1.0	0.228075	0.829228	0.184384	Biso	1.000000	Si
Si	1.0	0.227922	0.829569	0.517644	Biso	1.000000	Si
Si	1.0	0.227973	0.829459	0.851081	Biso	1.000000	Si
Si	1.0	0.771788	0.170801	0.149104	Biso	1.000000	Si
Si	1.0	0.771916	0.170879	0.482341	Biso	1.000000	Si
Si	1.0	0.771804	0.170747	0.815481	Biso	1.000000	Si
Si	1.0	0.771975	0.670658	0.149110	Biso	1.000000	Si
Si	1.0	0.771911	0.670946	0.482255	Biso	1.000000	Si
Si	1.0	0.771740	0.670839	0.815608	Biso	1.000000	Si
Si	1.0	0.728876	0.420721	0.149113	Biso	1.000000	Si
Si	1.0	0.728755	0.420605	0.482241	Biso	1.000000	Si
Si	1.0	0.728230	0.420590	0.815519	Biso	1.000000	Si
Si	1.0	0.728480	0.920793	0.149064	Biso	1.000000	Si
Si	1.0	0.728844	0.921167	0.482247	Biso	1.000000	Si
Si	1.0	0.728622	0.920970	0.815722	Biso	1.000000	Si
Si	1.0	0.271432	0.080017	0.185095	Biso	1.000000	Si
Si	1.0	0.271174	0.081192	0.518088	Biso	1.000000	Si
Si	1.0	0.271285	0.079291	0.851636	Biso	1.000000	Si
Si	1.0	0.271353	0.578614	0.184384	Biso	1.000000	Si
Si	1.0	0.271454	0.579057	0.517524	Biso	1.000000	Si
Si	1.0	0.271571	0.578637	0.850659	Biso	1.000000	Si
Si	1.0	0.771851	0.079203	0.315767	Biso	1.000000	Si
Si	1.0	0.771954	0.079086	0.648832	Biso	1.000000	Si
Si	1.0	0.771649	0.079144	0.982274	Biso	1.000000	Si
Si	1.0	0.772360	0.578964	0.315639	Biso	1.000000	Si
Si	1.0	0.771707	0.579221	0.648894	Biso	1.000000	Si
Si	1.0	0.771783	0.579147	0.982361	Biso	1.000000	Si
Si	1.0	0.227805	0.419270	0.016500	Biso	1.000000	Si
Si	1.0	0.229952	0.424357	0.351691	Biso	1.000000	Si
Si	1.0	0.227812	0.418327	0.681965	Biso	1.000000	Si
Si	1.0	0.227930	0.921033	0.017895	Biso	1.000000	Si
Si	1.0	0.227414	0.921293	0.350901	Biso	1.000000	Si
Si	1.0	0.228200	0.921043	0.684210	Biso	1.000000	Si
Si	1.0	0.473914	0.168876	0.266129	Biso	1.000000	Si
Si	1.0	0.474078	0.168657	0.599541	Biso	1.000000	Si
Si	1.0	0.473938	0.168605	0.932757	Biso	1.000000	Si
Si	1.0	0.474074	0.668732	0.265749	Biso	1.000000	Si
Si	1.0	0.473897	0.668873	0.599171	Biso	1.000000	Si
Si	1.0	0.473791	0.668567	0.932437	Biso	1.000000	Si
Si	1.0	0.526173	0.331275	0.067480	Biso	1.000000	Si
Si	1.0	0.526363	0.331171	0.400757	Biso	1.000000	Si

Si	1.0	0.526213	0.331273	0.734047	Biso	1.000000	Si
Si	1.0	0.525917	0.831195	0.067559	Biso	1.000000	Si
Si	1.0	0.525772	0.831445	0.400935	Biso	1.000000	Si
Si	1.0	0.525838	0.831428	0.734133	Biso	1.000000	Si
Si	1.0	0.025632	0.332115	0.097422	Biso	1.000000	Si
Si	1.0	0.026654	0.326378	0.433922	Biso	1.000000	Si
Si	1.0	0.025700	0.331059	0.765180	Biso	1.000000	Si
Si	1.0	0.026224	0.831232	0.099270	Biso	1.000000	Si
Si	1.0	0.026290	0.831622	0.432697	Biso	1.000000	Si
Si	1.0	0.026265	0.831480	0.765845	Biso	1.000000	Si
Si	1.0	0.975905	0.168701	0.233869	Biso	1.000000	Si
Si	1.0	0.975090	0.169235	0.565848	Biso	1.000000	Si
Si	1.0	0.973876	0.168706	0.900731	Biso	1.000000	Si
Si	1.0	0.973979	0.668591	0.234196	Biso	1.000000	Si
Si	1.0	0.973864	0.668849	0.567366	Biso	1.000000	Si
Si	1.0	0.974015	0.668517	0.900848	Biso	1.000000	Si
Si	1.0	0.526349	0.418647	0.234102	Biso	1.000000	Si
Si	1.0	0.526053	0.418574	0.567425	Biso	1.000000	Si
Si	1.0	0.526034	0.418626	0.900770	Biso	1.000000	Si
Si	1.0	0.525901	0.918730	0.234236	Biso	1.000000	Si
Si	1.0	0.525563	0.919121	0.567464	Biso	1.000000	Si
Si	1.0	0.525928	0.918678	0.900913	Biso	1.000000	Si
Si	1.0	0.473770	0.081334	0.099510	Biso	1.000000	Si
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Si	1.0	0.473763	0.081261	0.766073	Biso	1.000000	Si
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Si	1.0	0.973281	0.081676	0.067498	Biso	1.000000	Si
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Si	1.0	0.973933	0.581254	0.733968	Biso	1.000000	Si
Si	1.0	0.028029	0.415783	0.266532	Biso	1.000000	Si
Si	1.0	0.025916	0.418626	0.598961	Biso	1.000000	Si
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Si	1.0	0.026774	0.919080	0.599149	Biso	1.000000	Si
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model 5

#=====

CRYSTAL DATA

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_cell_length_c 15.70671
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_symmetry_Int_Tables_number 1

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_atom_site_fract_y
_atom_site_fract_z
_atom_site_adp_type
_atom_site_B_iso_or_equiv
_atom_site_type_symbol
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O	1.0	0.811579	0.498938	0.651471	Biso	1.000000	O
O	1.0	0.811372	0.498975	0.984693	Biso	1.000000	O
O	1.0	0.811273	0.998887	0.318228	Biso	1.000000	O
O	1.0	0.811504	0.999021	0.651599	Biso	1.000000	O
O	1.0	0.811456	0.999110	0.985009	Biso	1.000000	O
O	1.0	0.188207	0.001280	0.015849	Biso	1.000000	O
O	1.0	0.187942	-0.000402	0.347318	Biso	1.000000	O
O	1.0	0.188520	0.000833	0.682457	Biso	1.000000	O
O	1.0	0.188122	0.500668	0.014793	Biso	1.000000	O
O	1.0	0.190030	0.503050	0.349736	Biso	1.000000	O
O	1.0	0.188333	0.500587	0.681507	Biso	1.000000	O
O	1.0	0.432351	0.241498	0.229899	Biso	1.000000	O
O	1.0	0.432179	0.241054	0.562940	Biso	1.000000	O
O	1.0	0.432300	0.241267	0.896291	Biso	1.000000	O
O	1.0	0.432553	0.741364	0.229613	Biso	1.000000	O
O	1.0	0.432676	0.741400	0.563153	Biso	1.000000	O
O	1.0	0.432447	0.741354	0.896413	Biso	1.000000	O
O	1.0	0.567375	0.258730	0.103647	Biso	1.000000	O
O	1.0	0.567606	0.258723	0.437039	Biso	1.000000	O
O	1.0	0.567374	0.258718	0.770347	Biso	1.000000	O
O	1.0	0.567589	0.758820	0.103776	Biso	1.000000	O
O	1.0	0.567808	0.758825	0.437120	Biso	1.000000	O
O	1.0	0.567632	0.758725	0.770537	Biso	1.000000	O
O	1.0	0.068225	0.257547	0.065629	Biso	1.000000	O
O	1.0	0.063161	0.255535	0.399108	Biso	1.000000	O
O	1.0	0.067606	0.257681	0.728773	Biso	1.000000	O
O	1.0	0.067541	0.758706	0.063346	Biso	1.000000	O
O	1.0	0.067605	0.758773	0.396421	Biso	1.000000	O
O	1.0	0.067590	0.758713	0.729964	Biso	1.000000	O
O	1.0	0.933429	0.241327	0.270311	Biso	1.000000	O
O	1.0	0.932578	0.241334	0.602921	Biso	1.000000	O
O	1.0	0.932593	0.241271	0.936972	Biso	1.000000	O
O	1.0	0.932419	0.741069	0.270166	Biso	1.000000	O
O	1.0	0.932388	0.741073	0.603740	Biso	1.000000	O
O	1.0	0.932388	0.741010	0.936952	Biso	1.000000	O
O	1.0	0.567983	0.491167	0.270319	Biso	1.000000	O
O	1.0	0.567531	0.491197	0.603682	Biso	1.000000	O
O	1.0	0.567483	0.491206	0.937011	Biso	1.000000	O
O	1.0	0.567508	0.991254	0.270462	Biso	1.000000	O
O	1.0	0.567647	0.991118	0.603890	Biso	1.000000	O
O	1.0	0.567390	0.991262	0.937148	Biso	1.000000	O
O	1.0	0.432131	0.008821	0.063212	Biso	1.000000	O
O	1.0	0.432653	0.008505	0.396360	Biso	1.000000	O
O	1.0	0.432393	0.008644	0.729858	Biso	1.000000	O
O	1.0	0.432366	0.508864	0.062881	Biso	1.000000	O
O	1.0	0.433045	0.508822	0.396582	Biso	1.000000	O
O	1.0	0.432299	0.508808	0.729744	Biso	1.000000	O
O	1.0	0.932231	0.008794	0.103577	Biso	1.000000	O
O	1.0	0.931885	0.008698	0.436861	Biso	1.000000	O
O	1.0	0.932362	0.008830	0.770211	Biso	1.000000	O
O	1.0	0.932705	0.507713	0.103173	Biso	1.000000	O
O	1.0	0.932787	0.508189	0.436861	Biso	1.000000	O
O	1.0	0.932431	0.508286	0.769910	Biso	1.000000	O

O	1.0	0.067555	0.493501	0.231083	Biso	1.000000	O
O	1.0	0.067971	0.490912	0.562480	Biso	1.000000	O
O	1.0	0.067226	0.491041	0.895198	Biso	1.000000	O
O	1.0	0.068113	0.991890	0.230317	Biso	1.000000	O
O	1.0	0.067690	0.990993	0.562901	Biso	1.000000	O
O	1.0	0.067437	0.991414	0.896780	Biso	1.000000	O
O	1.0	0.304672	0.110528	0.279140	Biso	1.000000	O
O	1.0	0.303483	0.109547	0.612855	Biso	1.000000	O
O	1.0	0.301485	0.110969	0.946221	Biso	1.000000	O
O	1.0	0.303439	0.611008	0.278961	Biso	1.000000	O
O	1.0	0.303345	0.610663	0.612562	Biso	1.000000	O
O	1.0	0.303018	0.610243	0.945677	Biso	1.000000	O
O	1.0	0.696857	0.389643	0.054314	Biso	1.000000	O
O	1.0	0.697006	0.389596	0.387666	Biso	1.000000	O
O	1.0	0.696743	0.389600	0.721000	Biso	1.000000	O
O	1.0	0.697000	0.889601	0.054665	Biso	1.000000	O
O	1.0	0.697008	0.889515	0.387977	Biso	1.000000	O
O	1.0	0.697019	0.889616	0.721352	Biso	1.000000	O
O	1.0	0.195998	0.388983	0.110763	Biso	1.000000	O
O	1.0	0.196788	0.390348	0.444355	Biso	1.000000	O
O	1.0	0.196542	0.388827	0.778023	Biso	1.000000	O
O	1.0	0.196751	0.889741	0.112658	Biso	1.000000	O
O	1.0	0.196994	0.889377	0.445740	Biso	1.000000	O
O	1.0	0.196760	0.889636	0.779218	Biso	1.000000	O
O	1.0	0.802893	0.110292	0.221167	Biso	1.000000	O
O	1.0	0.803039	0.110327	0.554505	Biso	1.000000	O
O	1.0	0.802992	0.110334	0.887838	Biso	1.000000	O
O	1.0	0.803260	0.610439	0.221065	Biso	1.000000	O
O	1.0	0.803248	0.610193	0.554483	Biso	1.000000	O
O	1.0	0.803197	0.610247	0.887780	Biso	1.000000	O
O	1.0	0.696830	0.360313	0.220985	Biso	1.000000	O
O	1.0	0.696859	0.360205	0.554379	Biso	1.000000	O
O	1.0	0.696695	0.360198	0.887618	Biso	1.000000	O
O	1.0	0.697012	0.860333	0.221310	Biso	1.000000	O
O	1.0	0.696992	0.860231	0.554682	Biso	1.000000	O
O	1.0	0.697022	0.860321	0.888010	Biso	1.000000	O
O	1.0	0.304394	0.139640	0.112290	Biso	1.000000	O
O	1.0	0.304654	0.139842	0.446618	Biso	1.000000	O
O	1.0	0.302856	0.139643	0.779386	Biso	1.000000	O
O	1.0	0.303303	0.640020	0.112199	Biso	1.000000	O
O	1.0	0.303301	0.640025	0.445752	Biso	1.000000	O
O	1.0	0.303042	0.639888	0.779153	Biso	1.000000	O
O	1.0	0.802610	0.139750	0.054363	Biso	1.000000	O
O	1.0	0.802910	0.139551	0.387689	Biso	1.000000	O
O	1.0	0.803118	0.139526	0.721076	Biso	1.000000	O
O	1.0	0.803218	0.639512	0.054455	Biso	1.000000	O
O	1.0	0.803273	0.639514	0.387845	Biso	1.000000	O
O	1.0	0.803217	0.639468	0.721181	Biso	1.000000	O
O	1.0	0.198512	0.366593	0.275074	Biso	1.000000	O
O	1.0	0.196447	0.360394	0.611118	Biso	1.000000	O
O	1.0	0.196442	0.360239	0.944650	Biso	1.000000	O
O	1.0	0.197001	0.859210	0.279193	Biso	1.000000	O
O	1.0	0.196889	0.860433	0.612468	Biso	1.000000	O
O	1.0	0.196618	0.860711	0.945877	Biso	1.000000	O
O	1.0	0.447995	0.097438	0.201171	Biso	1.000000	O
O	1.0	0.448192	0.097056	0.534731	Biso	1.000000	O
O	1.0	0.447695	0.097352	0.867950	Biso	1.000000	O
O	1.0	0.448145	0.597454	0.201232	Biso	1.000000	O
O	1.0	0.448215	0.597527	0.534618	Biso	1.000000	O
O	1.0	0.447966	0.597425	0.867929	Biso	1.000000	O
O	1.0	0.552158	0.402649	0.132082	Biso	1.000000	O
O	1.0	0.551977	0.402563	0.465492	Biso	1.000000	O
O	1.0	0.551862	0.402643	0.798735	Biso	1.000000	O
O	1.0	0.551894	0.902714	0.132215	Biso	1.000000	O
O	1.0	0.552195	0.902645	0.465601	Biso	1.000000	O
O	1.0	0.552001	0.902637	0.798959	Biso	1.000000	O
O	1.0	0.051809	0.399644	0.030335	Biso	1.000000	O
O	1.0	0.052060	0.400556	0.365282	Biso	1.000000	O
O	1.0	0.051857	0.401341	0.699403	Biso	1.000000	O
O	1.0	0.051829	0.902611	0.034581	Biso	1.000000	O
O	1.0	0.051949	0.902776	0.368163	Biso	1.000000	O
O	1.0	0.051854	0.902588	0.701239	Biso	1.000000	O
O	1.0	0.947359	0.097470	0.298679	Biso	1.000000	O
O	1.0	0.948353	0.097546	0.632066	Biso	1.000000	O
O	1.0	0.947942	0.097168	0.964971	Biso	1.000000	O
O	1.0	0.948302	0.597390	0.299329	Biso	1.000000	O
O	1.0	0.948214	0.597110	0.632198	Biso	1.000000	O
O	1.0	0.948282	0.597080	0.965756	Biso	1.000000	O
O	1.0	0.552080	0.347303	0.298837	Biso	1.000000	O

O	1.0	0.551979	0.347284	0.632112	Biso	1.000000	O
O	1.0	0.551925	0.347321	0.965384	Biso	1.000000	O
O	1.0	0.551973	0.847413	0.298839	Biso	1.000000	O
O	1.0	0.552190	0.847248	0.632343	Biso	1.000000	O
O	1.0	0.551949	0.847367	0.965588	Biso	1.000000	O
O	1.0	0.447945	0.152551	0.034331	Biso	1.000000	O
O	1.0	0.448225	0.152550	0.367980	Biso	1.000000	O
O	1.0	0.447855	0.152616	0.701326	Biso	1.000000	O
O	1.0	0.448055	0.652772	0.034606	Biso	1.000000	O
O	1.0	0.448214	0.652807	0.367941	Biso	1.000000	O
O	1.0	0.448081	0.652714	0.701303	Biso	1.000000	O
O	1.0	0.946028	0.152914	0.130965	Biso	1.000000	O
O	1.0	0.947744	0.152612	0.465263	Biso	1.000000	O
O	1.0	0.948328	0.152680	0.798665	Biso	1.000000	O
O	1.0	0.948268	0.651714	0.132546	Biso	1.000000	O
O	1.0	0.948130	0.652191	0.465782	Biso	1.000000	O
O	1.0	0.948123	0.652145	0.799055	Biso	1.000000	O
O	1.0	0.050971	0.352282	0.195961	Biso	1.000000	O
O	1.0	0.051392	0.347448	0.531910	Biso	1.000000	O
O	1.0	0.051703	0.346887	0.865776	Biso	1.000000	O
O	1.0	0.052055	0.847738	0.201353	Biso	1.000000	O
O	1.0	0.051834	0.847134	0.534667	Biso	1.000000	O
O	1.0	0.051871	0.847497	0.867912	Biso	1.000000	O
Si	1.0	0.271668	0.171323	0.019053	Biso	1.000000	Si
Si	1.0	0.270648	0.170371	0.351767	Biso	1.000000	Si
Si	1.0	0.271943	0.170232	0.684504	Biso	1.000000	Si
Si	1.0	0.271552	0.670850	0.017712	Biso	1.000000	Si
Si	1.0	0.271824	0.671161	0.351223	Biso	1.000000	Si
Si	1.0	0.271665	0.671016	0.684612	Biso	1.000000	Si
Si	1.0	0.728203	0.329112	0.315410	Biso	1.000000	Si
Si	1.0	0.728107	0.329088	0.648937	Biso	1.000000	Si
Si	1.0	0.728052	0.329101	0.982146	Biso	1.000000	Si
Si	1.0	0.728504	0.829158	0.315766	Biso	1.000000	Si
Si	1.0	0.728449	0.829153	0.649207	Biso	1.000000	Si
Si	1.0	0.728439	0.829159	0.982516	Biso	1.000000	Si
Si	1.0	0.228633	0.331473	0.185654	Biso	1.000000	Si
Si	1.0	0.227900	0.329594	0.516109	Biso	1.000000	Si
Si	1.0	0.228227	0.328820	0.850507	Biso	1.000000	Si
Si	1.0	0.228321	0.828909	0.184290	Biso	1.000000	Si
Si	1.0	0.228465	0.829180	0.518024	Biso	1.000000	Si
Si	1.0	0.228200	0.829359	0.851524	Biso	1.000000	Si
Si	1.0	0.771302	0.170726	0.149095	Biso	1.000000	Si
Si	1.0	0.771389	0.170562	0.482315	Biso	1.000000	Si
Si	1.0	0.771543	0.170666	0.815579	Biso	1.000000	Si
Si	1.0	0.771763	0.670844	0.148890	Biso	1.000000	Si
Si	1.0	0.771832	0.670715	0.482345	Biso	1.000000	Si
Si	1.0	0.771729	0.670720	0.815642	Biso	1.000000	Si
Si	1.0	0.728332	0.420714	0.148835	Biso	1.000000	Si
Si	1.0	0.728199	0.420696	0.482240	Biso	1.000000	Si
Si	1.0	0.728172	0.420659	0.815518	Biso	1.000000	Si
Si	1.0	0.728395	0.920806	0.149157	Biso	1.000000	Si
Si	1.0	0.728385	0.920669	0.482472	Biso	1.000000	Si
Si	1.0	0.728417	0.920788	0.815852	Biso	1.000000	Si
Si	1.0	0.272799	0.080166	0.185163	Biso	1.000000	Si
Si	1.0	0.272609	0.078923	0.517674	Biso	1.000000	Si
Si	1.0	0.271122	0.079446	0.851550	Biso	1.000000	Si
Si	1.0	0.272053	0.579723	0.184637	Biso	1.000000	Si
Si	1.0	0.272009	0.579663	0.518000	Biso	1.000000	Si
Si	1.0	0.271619	0.579280	0.851124	Biso	1.000000	Si
Si	1.0	0.771436	0.078945	0.315580	Biso	1.000000	Si
Si	1.0	0.771584	0.079046	0.648969	Biso	1.000000	Si
Si	1.0	0.771420	0.079071	0.982268	Biso	1.000000	Si
Si	1.0	0.771655	0.579373	0.315497	Biso	1.000000	Si
Si	1.0	0.771746	0.579053	0.649000	Biso	1.000000	Si
Si	1.0	0.771654	0.579140	0.982303	Biso	1.000000	Si
Si	1.0	0.227939	0.420538	0.017099	Biso	1.000000	Si
Si	1.0	0.228989	0.422177	0.349850	Biso	1.000000	Si
Si	1.0	0.228064	0.420394	0.683642	Biso	1.000000	Si
Si	1.0	0.227974	0.921074	0.018250	Biso	1.000000	Si
Si	1.0	0.228302	0.920106	0.350954	Biso	1.000000	Si
Si	1.0	0.228321	0.920742	0.684728	Biso	1.000000	Si
Si	1.0	0.473653	0.168791	0.265967	Biso	1.000000	Si
Si	1.0	0.473714	0.168596	0.599233	Biso	1.000000	Si
Si	1.0	0.473760	0.168707	0.932566	Biso	1.000000	Si
Si	1.0	0.473988	0.668812	0.265909	Biso	1.000000	Si
Si	1.0	0.474031	0.668786	0.599371	Biso	1.000000	Si
Si	1.0	0.473882	0.668763	0.932619	Biso	1.000000	Si
Si	1.0	0.526025	0.331361	0.067426	Biso	1.000000	Si
Si	1.0	0.525967	0.331188	0.400780	Biso	1.000000	Si

Si	1.0	0.525958	0.331286	0.734039	Biso	1.000000	Si
Si	1.0	0.526024	0.831328	0.067568	Biso	1.000000	Si
Si	1.0	0.526262	0.831325	0.400869	Biso	1.000000	Si
Si	1.0	0.526143	0.831258	0.734276	Biso	1.000000	Si
Si	1.0	0.024917	0.332188	0.098239	Biso	1.000000	Si
Si	1.0	0.023686	0.334445	0.431744	Biso	1.000000	Si
Si	1.0	0.025804	0.330310	0.764206	Biso	1.000000	Si
Si	1.0	0.026196	0.831410	0.099476	Biso	1.000000	Si
Si	1.0	0.026085	0.831290	0.432590	Biso	1.000000	Si
Si	1.0	0.026052	0.831300	0.766005	Biso	1.000000	Si
Si	1.0	0.972940	0.167995	0.232618	Biso	1.000000	Si
Si	1.0	0.974239	0.168638	0.567024	Biso	1.000000	Si
Si	1.0	0.973873	0.168655	0.900618	Biso	1.000000	Si
Si	1.0	0.974162	0.668477	0.234379	Biso	1.000000	Si
Si	1.0	0.973984	0.668559	0.567613	Biso	1.000000	Si
Si	1.0	0.973957	0.668400	0.901007	Biso	1.000000	Si
Si	1.0	0.526256	0.418721	0.234146	Biso	1.000000	Si
Si	1.0	0.526055	0.418638	0.567409	Biso	1.000000	Si
Si	1.0	0.525988	0.418676	0.900738	Biso	1.000000	Si
Si	1.0	0.525951	0.918785	0.234205	Biso	1.000000	Si
Si	1.0	0.526259	0.918545	0.567600	Biso	1.000000	Si
Si	1.0	0.526016	0.918672	0.900896	Biso	1.000000	Si
Si	1.0	0.473717	0.081420	0.099255	Biso	1.000000	Si
Si	1.0	0.473876	0.081201	0.432611	Biso	1.000000	Si
Si	1.0	0.473736	0.081282	0.766021	Biso	1.000000	Si
Si	1.0	0.473871	0.581346	0.099242	Biso	1.000000	Si
Si	1.0	0.474173	0.581519	0.432682	Biso	1.000000	Si
Si	1.0	0.473826	0.581344	0.765972	Biso	1.000000	Si
Si	1.0	0.973445	0.081454	0.067220	Biso	1.000000	Si
Si	1.0	0.973540	0.081117	0.400659	Biso	1.000000	Si
Si	1.0	0.974042	0.081241	0.733992	Biso	1.000000	Si
Si	1.0	0.974227	0.580579	0.067623	Biso	1.000000	Si
Si	1.0	0.974349	0.580987	0.401042	Biso	1.000000	Si
Si	1.0	0.974000	0.580988	0.734163	Biso	1.000000	Si
Si	1.0	0.026228	0.419469	0.263550	Biso	1.000000	Si
Si	1.0	0.025939	0.418654	0.598241	Biso	1.000000	Si
Si	1.0	0.025431	0.418190	0.929956	Biso	1.000000	Si
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Si	1.0	0.025999	0.918710	0.932757	Biso	1.000000	Si

model 6

#=====

CRYSTAL DATA

#-----

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_cell_length_c 15.70671
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_symmetry_Int_Tables_number 1

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'x, y, z'

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_atom_site_fract_y
_atom_site_fract_z
_atom_site_adp_type
_atom_site_B_iso_or_equiv
_atom_site_type_symbol
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O	1.0	0.432655	0.741478	0.896415	Biso	1.000000	O
O	1.0	0.567357	0.258679	0.103690	Biso	1.000000	O
O	1.0	0.567349	0.258743	0.436988	Biso	1.000000	O
O	1.0	0.567351	0.258748	0.770222	Biso	1.000000	O
O	1.0	0.567747	0.758629	0.103725	Biso	1.000000	O
O	1.0	0.567668	0.758741	0.437241	Biso	1.000000	O
O	1.0	0.567693	0.758770	0.770544	Biso	1.000000	O
O	1.0	0.066783	0.258734	0.063077	Biso	1.000000	O
O	1.0	0.063567	0.255253	0.398952	Biso	1.000000	O
O	1.0	0.067380	0.257991	0.728680	Biso	1.000000	O
O	1.0	0.067757	0.759304	0.063703	Biso	1.000000	O
O	1.0	0.067504	0.759158	0.396377	Biso	1.000000	O
O	1.0	0.067676	0.758903	0.730099	Biso	1.000000	O
O	1.0	0.934840	0.240544	0.271064	Biso	1.000000	O
O	1.0	0.932546	0.241083	0.602750	Biso	1.000000	O
O	1.0	0.932069	0.241275	0.936480	Biso	1.000000	O
O	1.0	0.932571	0.741618	0.270110	Biso	1.000000	O
O	1.0	0.932429	0.741262	0.603732	Biso	1.000000	O
O	1.0	0.932525	0.741234	0.936989	Biso	1.000000	O
O	1.0	0.568308	0.491068	0.270270	Biso	1.000000	O
O	1.0	0.567469	0.491175	0.603555	Biso	1.000000	O
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model 7

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CRYSTAL DATA

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'x, y, z'

loop_
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_atom_site_fract_x
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_atom_site_fract_z
_atom_site_adp_type
_atom_site_B_iso_or_equiv
_atom_site_type_symbol
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Fe 1.0 0.123453 0.078645 0.288831 Biso 1.000000 Fe
Mg 1.0 0.375961 0.326835 0.289534 Biso 1.000000 Mg
Mg 1.0 0.375781 0.326832 0.622048 Biso 1.000000 Mg
Mg 1.0 0.375608 0.326567 0.955413 Biso 1.000000 Mg
Mg 1.0 0.376310 0.826216 0.288517 Biso 1.000000 Mg
Mg 1.0 0.375751 0.826876 0.622240 Biso 1.000000 Mg
Mg 1.0 0.375833 0.826347 0.955377 Biso 1.000000 Mg
Mg 1.0 0.624247 0.173489 0.044520 Biso 1.000000 Mg
Mg 1.0 0.624515 0.173429 0.377794 Biso 1.000000 Mg
Mg 1.0 0.624208 0.173440 0.711141 Biso 1.000000 Mg
Mg 1.0 0.624212 0.673058 0.044454 Biso 1.000000 Mg
Mg 1.0 0.624291 0.673180 0.377859 Biso 1.000000 Mg
Mg 1.0 0.624035 0.673379 0.711240 Biso 1.000000 Mg
Mg 1.0 0.119882 0.174679 0.122969 Biso 1.000000 Mg
Mg 1.0 0.123418 0.177864 0.450308 Biso 1.000000 Mg
Mg 1.0 0.123586 0.173943 0.787822 Biso 1.000000 Mg
Mg 1.0 0.123857 0.672833 0.122342 Biso 1.000000 Mg
Mg 1.0 0.124068 0.673224 0.455815 Biso 1.000000 Mg
Mg 1.0 0.123935 0.673238 0.789031 Biso 1.000000 Mg
Mg 1.0 0.877492 0.326567 0.211250 Biso 1.000000 Mg
Mg 1.0 0.876212 0.327113 0.544404 Biso 1.000000 Mg
Mg 1.0 0.875911 0.326710 0.877390 Biso 1.000000 Mg
Mg 1.0 0.875563 0.826506 0.210911 Biso 1.000000 Mg
Mg 1.0 0.875687 0.826821 0.544559 Biso 1.000000 Mg
Mg 1.0 0.875960 0.826757 0.877879 Biso 1.000000 Mg
Mg 1.0 0.624265 0.076770 0.211117 Biso 1.000000 Mg
Mg 1.0 0.624323 0.076779 0.544496 Biso 1.000000 Mg
Mg 1.0 0.624198 0.076747 0.877849 Biso 1.000000 Mg
Mg 1.0 0.624398 0.576413 0.211139 Biso 1.000000 Mg
Mg 1.0 0.624214 0.576751 0.544482 Biso 1.000000 Mg
Mg 1.0 0.624022 0.576555 0.877838 Biso 1.000000 Mg
Mg 1.0 0.375878 0.423376 0.122193 Biso 1.000000 Mg
Mg 1.0 0.376613 0.423916 0.456032 Biso 1.000000 Mg
Mg 1.0 0.375796 0.423241 0.788633 Biso 1.000000 Mg
Mg 1.0 0.376774 0.922358 0.121591 Biso 1.000000 Mg
Mg 1.0 0.376156 0.923475 0.455594 Biso 1.000000 Mg
Mg 1.0 0.375829 0.923392 0.788965 Biso 1.000000 Mg
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Mg 1.0 0.877049 0.423362 0.378436 Biso 1.000000 Mg
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Mg 1.0 0.875097 0.922597 0.377705 Biso 1.000000 Mg
Mg 1.0 0.875883 0.923430 0.711290 Biso 1.000000 Mg
Mg 1.0 0.123919 0.077862 0.621460 Biso 1.000000 Mg

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Mg	1.0	0.123888	0.576943	0.622133	Biso	1.000000	Mg
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Mg	1.0	0.377174	0.244125	0.119990	Biso	1.000000	Mg
Mg	1.0	0.376271	0.244067	0.453623	Biso	1.000000	Mg
Mg	1.0	0.376636	0.243661	0.786314	Biso	1.000000	Mg
Mg	1.0	0.376667	0.742931	0.119641	Biso	1.000000	Mg
Mg	1.0	0.376201	0.743761	0.453355	Biso	1.000000	Mg
Mg	1.0	0.376498	0.743750	0.786526	Biso	1.000000	Mg
Mg	1.0	0.623866	0.256491	0.213412	Biso	1.000000	Mg
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Mg	1.0	0.623595	0.256298	0.879956	Biso	1.000000	Mg
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Mg	1.0	0.623661	0.756242	0.546779	Biso	1.000000	Mg
Mg	1.0	0.623532	0.756177	0.880157	Biso	1.000000	Mg
Mg	1.0	0.121978	0.257047	0.616828	Biso	1.000000	Mg
Mg	1.0	0.122793	0.257330	0.952749	Biso	1.000000	Mg
Mg	1.0	0.123590	0.755682	0.286847	Biso	1.000000	Mg
Mg	1.0	0.123411	0.756491	0.620070	Biso	1.000000	Mg
Mg	1.0	0.123540	0.755735	0.953413	Biso	1.000000	Mg
Mg	1.0	0.876426	0.243993	0.046633	Biso	1.000000	Mg
Mg	1.0	0.878964	0.245155	0.380492	Biso	1.000000	Mg
Mg	1.0	0.876714	0.243712	0.712654	Biso	1.000000	Mg
Mg	1.0	0.876497	0.743543	0.046634	Biso	1.000000	Mg
Mg	1.0	0.876807	0.743207	0.380187	Biso	1.000000	Mg
Mg	1.0	0.876550	0.743815	0.713521	Biso	1.000000	Mg
Mg	1.0	0.623724	0.493479	0.046748	Biso	1.000000	Mg
Mg	1.0	0.623778	0.493799	0.379946	Biso	1.000000	Mg
Mg	1.0	0.623615	0.493897	0.713257	Biso	1.000000	Mg
Mg	1.0	0.623871	0.993801	0.046598	Biso	1.000000	Mg
Mg	1.0	0.623597	0.993832	0.380060	Biso	1.000000	Mg
Mg	1.0	0.623662	0.993825	0.713436	Biso	1.000000	Mg
Mg	1.0	0.378264	0.006049	0.286047	Biso	1.000000	Mg
Mg	1.0	0.376763	0.006305	0.620109	Biso	1.000000	Mg
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Mg	1.0	0.376354	0.506507	0.620088	Biso	1.000000	Mg
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Mg	1.0	0.875824	0.006617	0.213425	Biso	1.000000	Mg
Mg	1.0	0.876493	0.006409	0.546778	Biso	1.000000	Mg
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Mg	1.0	0.877840	0.504989	0.214152	Biso	1.000000	Mg
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Mg	1.0	0.122680	0.492996	0.453382	Biso	1.000000	Mg
Mg	1.0	0.122869	0.493458	0.785537	Biso	1.000000	Mg
Mg	1.0	0.122009	0.992072	0.117680	Biso	1.000000	Mg
Mg	1.0	0.123680	0.993192	0.454949	Biso	1.000000	Mg
Mg	1.0	0.123294	0.994313	0.786394	Biso	1.000000	Mg
O	1.0	0.182739	0.171513	0.014930	Biso	1.000000	O
O	1.0	0.185400	0.162988	0.342472	Biso	1.000000	O
O	1.0	0.183094	0.170840	0.677742	Biso	1.000000	O
O	1.0	0.183091	0.669628	0.012009	Biso	1.000000	O
O	1.0	0.183322	0.671072	0.345237	Biso	1.000000	O
O	1.0	0.183199	0.670616	0.678603	Biso	1.000000	O
O	1.0	0.817276	0.329469	0.321069	Biso	1.000000	O
O	1.0	0.816797	0.329856	0.654620	Biso	1.000000	O
O	1.0	0.816580	0.329806	0.987680	Biso	1.000000	O
O	1.0	0.816771	0.829705	0.321436	Biso	1.000000	O
O	1.0	0.816677	0.829926	0.655009	Biso	1.000000	O
O	1.0	0.816826	0.829928	0.988236	Biso	1.000000	O
O	1.0	0.316409	0.329126	0.179108	Biso	1.000000	O
O	1.0	0.317083	0.329947	0.511344	Biso	1.000000	O
O	1.0	0.316607	0.329467	0.844909	Biso	1.000000	O
O	1.0	0.316711	0.829509	0.178339	Biso	1.000000	O
O	1.0	0.316365	0.830499	0.511492	Biso	1.000000	O
O	1.0	0.316581	0.830021	0.845182	Biso	1.000000	O
O	1.0	0.683430	0.170260	0.154800	Biso	1.000000	O
O	1.0	0.683697	0.170173	0.488130	Biso	1.000000	O
O	1.0	0.683385	0.170142	0.821516	Biso	1.000000	O
O	1.0	0.683395	0.669925	0.154778	Biso	1.000000	O
O	1.0	0.683382	0.670298	0.488223	Biso	1.000000	O
O	1.0	0.683254	0.670220	0.821610	Biso	1.000000	O
O	1.0	0.817049	0.420104	0.154768	Biso	1.000000	O
O	1.0	0.816520	0.420802	0.488460	Biso	1.000000	O
O	1.0	0.816562	0.420130	0.821187	Biso	1.000000	O
O	1.0	0.816780	0.920094	0.154874	Biso	1.000000	O

O	1.0	0.816541	0.919989	0.488362	Biso	1.000000	O
O	1.0	0.816771	0.920248	0.821700	Biso	1.000000	O
O	1.0	0.183946	0.078661	0.180545	Biso	1.000000	O
O	1.0	0.183412	0.079244	0.510576	Biso	1.000000	O
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O	1.0	0.182972	0.579721	0.178878	Biso	1.000000	O
O	1.0	0.183126	0.580741	0.512635	Biso	1.000000	O
O	1.0	0.183112	0.579454	0.845411	Biso	1.000000	O
O	1.0	0.683144	0.079834	0.321471	Biso	1.000000	O
O	1.0	0.683325	0.079832	0.654904	Biso	1.000000	O
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O	1.0	0.683667	0.579715	0.321442	Biso	1.000000	O
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O	1.0	0.683260	0.579835	0.988175	Biso	1.000000	O
O	1.0	0.315999	0.419515	0.012104	Biso	1.000000	O
O	1.0	0.318540	0.421565	0.346471	Biso	1.000000	O
O	1.0	0.316718	0.420201	0.678229	Biso	1.000000	O
O	1.0	0.316989	0.920109	0.011714	Biso	1.000000	O
O	1.0	0.316345	0.921388	0.344894	Biso	1.000000	O
O	1.0	0.316630	0.920417	0.678630	Biso	1.000000	O
O	1.0	0.562954	0.170249	0.266264	Biso	1.000000	O
O	1.0	0.562923	0.170258	0.599688	Biso	1.000000	O
O	1.0	0.562712	0.170242	0.933079	Biso	1.000000	O
O	1.0	0.562931	0.670022	0.266261	Biso	1.000000	O
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O	1.0	0.437365	0.329265	0.400338	Biso	1.000000	O
O	1.0	0.437171	0.329774	0.733658	Biso	1.000000	O
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O	1.0	0.437134	0.829880	0.733755	Biso	1.000000	O
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O	1.0	0.062384	0.157425	0.231868	Biso	1.000000	O
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O	1.0	0.062876	0.170490	0.900460	Biso	1.000000	O
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O	1.0	0.563005	0.079746	0.099571	Biso	1.000000	O
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O	1.0	0.062032	0.077053	0.397479	Biso	1.000000	O
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O	1.0	0.062833	0.580573	0.401107	Biso	1.000000	O
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O	1.0	0.932332	0.241210	0.936850	Biso	1.000000	O
O	1.0	0.932582	0.741853	0.270120	Biso	1.000000	O
O	1.0	0.932407	0.741901	0.603819	Biso	1.000000	O
O	1.0	0.932569	0.741481	0.937147	Biso	1.000000	O
O	1.0	0.567657	0.491175	0.270406	Biso	1.000000	O
O	1.0	0.567604	0.491364	0.603716	Biso	1.000000	O
O	1.0	0.567350	0.491230	0.937196	Biso	1.000000	O
O	1.0	0.567553	0.991109	0.270334	Biso	1.000000	O
O	1.0	0.567605	0.991256	0.603799	Biso	1.000000	O
O	1.0	0.567612	0.991186	0.937171	Biso	1.000000	O
O	1.0	0.432598	0.008673	0.062968	Biso	1.000000	O
O	1.0	0.432877	0.008548	0.396424	Biso	1.000000	O
O	1.0	0.432489	0.008717	0.729807	Biso	1.000000	O
O	1.0	0.431960	0.508781	0.062924	Biso	1.000000	O
O	1.0	0.433433	0.508908	0.396399	Biso	1.000000	O
O	1.0	0.432316	0.508893	0.729670	Biso	1.000000	O
O	1.0	0.932778	0.008615	0.104158	Biso	1.000000	O
O	1.0	0.932772	0.006197	0.436826	Biso	1.000000	O
O	1.0	0.932615	0.008637	0.770674	Biso	1.000000	O
O	1.0	0.932424	0.508757	0.103605	Biso	1.000000	O
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O	1.0	0.068871	0.991395	0.230915	Biso	1.000000	O
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O	1.0	0.551960	0.902553	0.465593	Biso	1.000000	O
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model 8

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CRYSTAL DATA

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_symmetry_Int_Tables_number 1

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'x, y, z'

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_atom_site_fract_y
_atom_site_fract_z
_atom_site_adp_type
_atom_site_B_iso_or_equiv
_atom_site_type_symbol
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Mg 1.0 0.875949 0.826693 0.211071 Biso 1.000000 Mg
Mg 1.0 0.876010 0.826749 0.544503 Biso 1.000000 Mg
Mg 1.0 0.876080 0.826818 0.877884 Biso 1.000000 Mg
Mg 1.0 0.624202 0.076617 0.211130 Biso 1.000000 Mg
Mg 1.0 0.624257 0.076539 0.544525 Biso 1.000000 Mg
Mg 1.0 0.624133 0.076600 0.877894 Biso 1.000000 Mg
Mg 1.0 0.624425 0.576636 0.211051 Biso 1.000000 Mg
Mg 1.0 0.624254 0.576843 0.544550 Biso 1.000000 Mg
Mg 1.0 0.624026 0.576617 0.877892 Biso 1.000000 Mg
Mg 1.0 0.376032 0.423341 0.122056 Biso 1.000000 Mg
Mg 1.0 0.377107 0.424082 0.455712 Biso 1.000000 Mg
Mg 1.0 0.375752 0.423001 0.788613 Biso 1.000000 Mg
Mg 1.0 0.376014 0.922984 0.122115 Biso 1.000000 Mg
Mg 1.0 0.375717 0.923218 0.455500 Biso 1.000000 Mg
Mg 1.0 0.375797 0.923335 0.789121 Biso 1.000000 Mg
Mg 1.0 0.875982 0.422879 0.044185 Biso 1.000000 Mg
Mg 1.0 0.876206 0.423350 0.377744 Biso 1.000000 Mg
Mg 1.0 0.875686 0.423452 0.711080 Biso 1.000000 Mg
Mg 1.0 0.875981 0.923426 0.044610 Biso 1.000000 Mg
Mg 1.0 0.875985 0.923042 0.377645 Biso 1.000000 Mg
Mg 1.0 0.876168 0.923475 0.711206 Biso 1.000000 Mg
Mg 1.0 0.124294 0.076839 0.621546 Biso 1.000000 Mg

Mg	1.0	0.123669	0.076826	0.955882	Biso	1.000000	Mg
Mg	1.0	0.124374	0.577382	0.289921	Biso	1.000000	Mg
Mg	1.0	0.123918	0.577177	0.622416	Biso	1.000000	Mg
Mg	1.0	0.124084	0.575612	0.955921	Biso	1.000000	Mg
Mg	1.0	0.376978	0.243606	0.119996	Biso	1.000000	Mg
Mg	1.0	0.378157	0.243536	0.452987	Biso	1.000000	Mg
Mg	1.0	0.376886	0.243517	0.786499	Biso	1.000000	Mg
Mg	1.0	0.376341	0.743480	0.119937	Biso	1.000000	Mg
Mg	1.0	0.376407	0.743811	0.453370	Biso	1.000000	Mg
Mg	1.0	0.376426	0.743798	0.786701	Biso	1.000000	Mg
Mg	1.0	0.623879	0.256236	0.213272	Biso	1.000000	Mg
Mg	1.0	0.623816	0.256026	0.546678	Biso	1.000000	Mg
Mg	1.0	0.623587	0.256198	0.880065	Biso	1.000000	Mg
Mg	1.0	0.623750	0.756172	0.213297	Biso	1.000000	Mg
Mg	1.0	0.623734	0.756327	0.546790	Biso	1.000000	Mg
Mg	1.0	0.623555	0.756268	0.880145	Biso	1.000000	Mg
Mg	1.0	0.122708	0.256920	0.619778	Biso	1.000000	Mg
Mg	1.0	0.123398	0.256345	0.953261	Biso	1.000000	Mg
Mg	1.0	0.123221	0.756598	0.286400	Biso	1.000000	Mg
Mg	1.0	0.123516	0.756402	0.620164	Biso	1.000000	Mg
Mg	1.0	0.123529	0.755827	0.953532	Biso	1.000000	Mg
Mg	1.0	0.876940	0.243066	0.047096	Biso	1.000000	Mg
Mg	1.0	0.876634	0.243803	0.379230	Biso	1.000000	Mg
Mg	1.0	0.876487	0.243692	0.713136	Biso	1.000000	Mg
Mg	1.0	0.876564	0.743761	0.046660	Biso	1.000000	Mg
Mg	1.0	0.876685	0.743629	0.380079	Biso	1.000000	Mg
Mg	1.0	0.876612	0.743902	0.713474	Biso	1.000000	Mg
Mg	1.0	0.623721	0.493562	0.046740	Biso	1.000000	Mg
Mg	1.0	0.623913	0.494073	0.379930	Biso	1.000000	Mg
Mg	1.0	0.623585	0.493902	0.713378	Biso	1.000000	Mg
Mg	1.0	0.623657	0.993666	0.046713	Biso	1.000000	Mg
Mg	1.0	0.623616	0.993660	0.380035	Biso	1.000000	Mg
Mg	1.0	0.623657	0.993655	0.713479	Biso	1.000000	Mg
Mg	1.0	0.376738	0.005792	0.286530	Biso	1.000000	Mg
Mg	1.0	0.376673	0.005922	0.620241	Biso	1.000000	Mg
Mg	1.0	0.376455	0.006046	0.953492	Biso	1.000000	Mg
Mg	1.0	0.377635	0.507008	0.286389	Biso	1.000000	Mg
Mg	1.0	0.376263	0.506328	0.620085	Biso	1.000000	Mg
Mg	1.0	0.376022	0.505932	0.953273	Biso	1.000000	Mg
Mg	1.0	0.876947	0.006660	0.213746	Biso	1.000000	Mg
Mg	1.0	0.876523	0.006094	0.546425	Biso	1.000000	Mg
Mg	1.0	0.876925	0.006537	0.880299	Biso	1.000000	Mg
Mg	1.0	0.877575	0.505282	0.213847	Biso	1.000000	Mg
Mg	1.0	0.876264	0.506501	0.546549	Biso	1.000000	Mg
Mg	1.0	0.876109	0.506270	0.879714	Biso	1.000000	Mg
Mg	1.0	0.121390	0.492970	0.121588	Biso	1.000000	Mg
Mg	1.0	0.123540	0.494797	0.454093	Biso	1.000000	Mg
Mg	1.0	0.123133	0.493431	0.785698	Biso	1.000000	Mg
Mg	1.0	0.123263	0.994387	0.120033	Biso	1.000000	Mg
Mg	1.0	0.123368	0.994357	0.452650	Biso	1.000000	Mg
Mg	1.0	0.123387	0.993772	0.786618	Biso	1.000000	Mg
O	1.0	0.182940	0.171392	0.014729	Biso	1.000000	O
O	1.0	0.185321	0.166711	0.347267	Biso	1.000000	O
O	1.0	0.183176	0.171028	0.677591	Biso	1.000000	O
O	1.0	0.183171	0.669405	0.011877	Biso	1.000000	O
O	1.0	0.183289	0.671013	0.345271	Biso	1.000000	O
O	1.0	0.183269	0.670010	0.678837	Biso	1.000000	O
O	1.0	0.816939	0.329783	0.321134	Biso	1.000000	O
O	1.0	0.816639	0.329759	0.654722	Biso	1.000000	O
O	1.0	0.816644	0.329545	0.987886	Biso	1.000000	O
O	1.0	0.816794	0.829759	0.321531	Biso	1.000000	O
O	1.0	0.816871	0.830018	0.654879	Biso	1.000000	O
O	1.0	0.816829	0.829868	0.988147	Biso	1.000000	O
O	1.0	0.316728	0.329524	0.178989	Biso	1.000000	O
O	1.0	0.316675	0.328469	0.511355	Biso	1.000000	O
O	1.0	0.316717	0.329336	0.844753	Biso	1.000000	O
O	1.0	0.316667	0.829669	0.178448	Biso	1.000000	O
O	1.0	0.316623	0.830080	0.511912	Biso	1.000000	O
O	1.0	0.316553	0.829939	0.845232	Biso	1.000000	O
O	1.0	0.683231	0.170114	0.154848	Biso	1.000000	O
O	1.0	0.683378	0.169964	0.488220	Biso	1.000000	O
O	1.0	0.683333	0.170085	0.821464	Biso	1.000000	O
O	1.0	0.683403	0.670054	0.154771	Biso	1.000000	O
O	1.0	0.683468	0.670294	0.488253	Biso	1.000000	O
O	1.0	0.683335	0.670187	0.821571	Biso	1.000000	O
O	1.0	0.817017	0.420065	0.154851	Biso	1.000000	O
O	1.0	0.816601	0.420430	0.488229	Biso	1.000000	O
O	1.0	0.816511	0.420109	0.821264	Biso	1.000000	O
O	1.0	0.816825	0.920197	0.154940	Biso	1.000000	O

O	1.0	0.816821	0.920124	0.488137	Biso	1.000000	O
O	1.0	0.816941	0.920350	0.821504	Biso	1.000000	O
O	1.0	0.183914	0.080242	0.178474	Biso	1.000000	O
O	1.0	0.183566	0.081283	0.511079	Biso	1.000000	O
O	1.0	0.182991	0.079975	0.845436	Biso	1.000000	O
O	1.0	0.183029	0.579371	0.178885	Biso	1.000000	O
O	1.0	0.183213	0.580656	0.512960	Biso	1.000000	O
O	1.0	0.183192	0.579146	0.845124	Biso	1.000000	O
O	1.0	0.683219	0.079681	0.321556	Biso	1.000000	O
O	1.0	0.683449	0.079725	0.654889	Biso	1.000000	O
O	1.0	0.683227	0.079743	0.988114	Biso	1.000000	O
O	1.0	0.683644	0.579890	0.321436	Biso	1.000000	O
O	1.0	0.683279	0.580055	0.654922	Biso	1.000000	O
O	1.0	0.683301	0.579836	0.988176	Biso	1.000000	O
O	1.0	0.316161	0.419633	0.011879	Biso	1.000000	O
O	1.0	0.318506	0.421767	0.346671	Biso	1.000000	O
O	1.0	0.316402	0.419399	0.677722	Biso	1.000000	O
O	1.0	0.316594	0.920038	0.011879	Biso	1.000000	O
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O	1.0	0.562939	0.170270	0.266427	Biso	1.000000	O
O	1.0	0.562986	0.170048	0.599810	Biso	1.000000	O
O	1.0	0.562767	0.170167	0.933019	Biso	1.000000	O
O	1.0	0.562934	0.670186	0.266242	Biso	1.000000	O
O	1.0	0.562858	0.670466	0.599815	Biso	1.000000	O
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O	1.0	0.437143	0.329857	0.067124	Biso	1.000000	O
O	1.0	0.437661	0.329838	0.400493	Biso	1.000000	O
O	1.0	0.437210	0.329692	0.733615	Biso	1.000000	O
O	1.0	0.437134	0.829557	0.066988	Biso	1.000000	O
O	1.0	0.437173	0.829859	0.400379	Biso	1.000000	O
O	1.0	0.437139	0.829775	0.733759	Biso	1.000000	O
O	1.0	0.936604	0.329661	0.097874	Biso	1.000000	O
O	1.0	0.935681	0.330947	0.433556	Biso	1.000000	O
O	1.0	0.936876	0.329738	0.765754	Biso	1.000000	O
O	1.0	0.937231	0.829649	0.099592	Biso	1.000000	O
O	1.0	0.937178	0.829767	0.433090	Biso	1.000000	O
O	1.0	0.937278	0.829990	0.766274	Biso	1.000000	O
O	1.0	0.062017	0.162073	0.230666	Biso	1.000000	O
O	1.0	0.063485	0.169719	0.565248	Biso	1.000000	O
O	1.0	0.062836	0.170177	0.900320	Biso	1.000000	O
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O	1.0	0.062906	0.669994	0.900497	Biso	1.000000	O
O	1.0	0.437492	0.420285	0.233558	Biso	1.000000	O
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O	1.0	0.436959	0.420083	0.900374	Biso	1.000000	O
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O	1.0	0.062179	0.079544	0.066173	Biso	1.000000	O
O	1.0	0.062422	0.081389	0.401079	Biso	1.000000	O
O	1.0	0.063149	0.080075	0.733338	Biso	1.000000	O
O	1.0	0.062664	0.579379	0.067291	Biso	1.000000	O
O	1.0	0.062867	0.580323	0.401144	Biso	1.000000	O
O	1.0	0.062802	0.579901	0.733561	Biso	1.000000	O
O	1.0	0.937982	0.419747	0.267280	Biso	1.000000	O
O	1.0	0.936904	0.420688	0.599761	Biso	1.000000	O
O	1.0	0.936690	0.420357	0.931733	Biso	1.000000	O
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O	1.0	0.937264	0.920241	0.933028	Biso	1.000000	O
O	1.0	0.311235	0.251040	0.015481	Biso	1.000000	O
O	1.0	0.311597	0.250522	0.348343	Biso	1.000000	O
O	1.0	0.311464	0.250817	0.681464	Biso	1.000000	O
O	1.0	0.311271	0.750340	0.014809	Biso	1.000000	O
O	1.0	0.311610	0.750885	0.348347	Biso	1.000000	O
O	1.0	0.311333	0.750862	0.681720	Biso	1.000000	O
O	1.0	0.688711	0.249142	0.318495	Biso	1.000000	O
O	1.0	0.688603	0.249028	0.651854	Biso	1.000000	O
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O	1.0	0.688677	0.749068	0.318439	Biso	1.000000	O
O	1.0	0.688724	0.749192	0.651994	Biso	1.000000	O

O	1.0	0.688624	0.749123	0.985129	Biso	1.000000	O
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O	1.0	0.187272	0.249020	0.511400	Biso	1.000000	O
O	1.0	0.188674	0.248015	0.848055	Biso	1.000000	O
O	1.0	0.188514	0.748933	0.181376	Biso	1.000000	O
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O	1.0	0.188463	0.749112	0.848410	Biso	1.000000	O
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O	1.0	0.811808	0.999160	0.651686	Biso	1.000000	O
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O	1.0	0.190956	0.505241	0.352378	Biso	1.000000	O
O	1.0	0.187929	0.499518	0.680294	Biso	1.000000	O
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O	1.0	0.567390	0.258668	0.103832	Biso	1.000000	O
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O	1.0	0.567568	0.758617	0.103745	Biso	1.000000	O
O	1.0	0.567600	0.758781	0.437178	Biso	1.000000	O
O	1.0	0.567515	0.758768	0.770505	Biso	1.000000	O
O	1.0	0.068049	0.259550	0.062706	Biso	1.000000	O
O	1.0	0.059514	0.251797	0.406568	Biso	1.000000	O
O	1.0	0.067241	0.258673	0.728965	Biso	1.000000	O
O	1.0	0.067639	0.758435	0.063015	Biso	1.000000	O
O	1.0	0.067575	0.758946	0.396392	Biso	1.000000	O
O	1.0	0.067722	0.758940	0.729783	Biso	1.000000	O
O	1.0	0.933185	0.240715	0.270068	Biso	1.000000	O
O	1.0	0.933082	0.241516	0.603435	Biso	1.000000	O
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O	1.0	0.932339	0.741270	0.270302	Biso	1.000000	O
O	1.0	0.932406	0.741496	0.603806	Biso	1.000000	O
O	1.0	0.932512	0.741268	0.937009	Biso	1.000000	O
O	1.0	0.567795	0.491308	0.270411	Biso	1.000000	O
O	1.0	0.567481	0.491421	0.603817	Biso	1.000000	O
O	1.0	0.567374	0.491215	0.937189	Biso	1.000000	O
O	1.0	0.567441	0.991196	0.270435	Biso	1.000000	O
O	1.0	0.567557	0.991244	0.603837	Biso	1.000000	O
O	1.0	0.567476	0.991200	0.937140	Biso	1.000000	O
O	1.0	0.432418	0.008747	0.063048	Biso	1.000000	O
O	1.0	0.432182	0.008909	0.396456	Biso	1.000000	O
O	1.0	0.432431	0.008711	0.729818	Biso	1.000000	O
O	1.0	0.432059	0.508776	0.062935	Biso	1.000000	O
O	1.0	0.433502	0.508992	0.396378	Biso	1.000000	O
O	1.0	0.432092	0.508736	0.729636	Biso	1.000000	O
O	1.0	0.932217	0.008768	0.103648	Biso	1.000000	O
O	1.0	0.933099	0.008020	0.437087	Biso	1.000000	O
O	1.0	0.932690	0.009021	0.770277	Biso	1.000000	O
O	1.0	0.932532	0.508456	0.103621	Biso	1.000000	O
O	1.0	0.932687	0.508856	0.437280	Biso	1.000000	O
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O	1.0	0.068064	0.492263	0.233617	Biso	1.000000	O
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O	1.0	0.067827	0.990245	0.229471	Biso	1.000000	O
O	1.0	0.068089	0.991352	0.562754	Biso	1.000000	O
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O	1.0	0.302961	0.110121	0.612863	Biso	1.000000	O
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O	1.0	0.303142	0.610584	0.278462	Biso	1.000000	O
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O	1.0	0.697105	0.389683	0.387810	Biso	1.000000	O
O	1.0	0.696782	0.389629	0.721216	Biso	1.000000	O
O	1.0	0.697018	0.889608	0.054702	Biso	1.000000	O
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O	1.0	0.197539	0.390277	0.444192	Biso	1.000000	O
O	1.0	0.196545	0.387664	0.776668	Biso	1.000000	O
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O	1.0	0.696918	0.360246	0.554526	Biso	1.000000	O
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O	1.0	0.448156	0.097421	0.201311	Biso	1.000000	O
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O	1.0	0.448263	0.597520	0.534552	Biso	1.000000	O
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O	1.0	0.551924	0.902507	0.132163	Biso	1.000000	O
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O	1.0	0.447962	0.652578	0.034619	Biso	1.000000	O
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O	1.0	0.447940	0.652634	0.701248	Biso	1.000000	O
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model 9

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CRYSTAL DATA

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Mg 1.0 0.876008 0.923315 0.377635 Biso 1.000000 Mg
Mg 1.0 0.875971 0.923256 0.710993 Biso 1.000000 Mg
Mg 1.0 0.124370 0.075885 0.622382 Biso 1.000000 Mg

Mg	1.0	0.123773	0.077171	0.956205	Biso	1.000000	Mg
Mg	1.0	0.124666	0.577159	0.289727	Biso	1.000000	Mg
Mg	1.0	0.124123	0.576715	0.622446	Biso	1.000000	Mg
Mg	1.0	0.123949	0.575724	0.955989	Biso	1.000000	Mg
Mg	1.0	0.375104	0.245445	0.121286	Biso	1.000000	Mg
Mg	1.0	0.375975	0.243216	0.453194	Biso	1.000000	Mg
Mg	1.0	0.376737	0.243794	0.786521	Biso	1.000000	Mg
Mg	1.0	0.376335	0.743775	0.119987	Biso	1.000000	Mg
Mg	1.0	0.376587	0.743819	0.453421	Biso	1.000000	Mg
Mg	1.0	0.376439	0.743924	0.786927	Biso	1.000000	Mg
Mg	1.0	0.622948	0.256405	0.213473	Biso	1.000000	Mg
Mg	1.0	0.623146	0.256178	0.546654	Biso	1.000000	Mg
Mg	1.0	0.623368	0.256179	0.879979	Biso	1.000000	Mg
Mg	1.0	0.623448	0.756310	0.213349	Biso	1.000000	Mg
Mg	1.0	0.623578	0.756189	0.546731	Biso	1.000000	Mg
Mg	1.0	0.623638	0.756186	0.880198	Biso	1.000000	Mg
Mg	1.0	0.124860	0.255115	0.620144	Biso	1.000000	Mg
Mg	1.0	0.123652	0.257634	0.953515	Biso	1.000000	Mg
Mg	1.0	0.123738	0.756401	0.286783	Biso	1.000000	Mg
Mg	1.0	0.123528	0.756268	0.620327	Biso	1.000000	Mg
Mg	1.0	0.123602	0.755775	0.953870	Biso	1.000000	Mg
Mg	1.0	0.875436	0.243121	0.046269	Biso	1.000000	Mg
Mg	1.0	0.875303	0.243130	0.378966	Biso	1.000000	Mg
Mg	1.0	0.875967	0.243529	0.712515	Biso	1.000000	Mg
Mg	1.0	0.876692	0.743809	0.046648	Biso	1.000000	Mg
Mg	1.0	0.876662	0.743640	0.379786	Biso	1.000000	Mg
Mg	1.0	0.876529	0.743730	0.713284	Biso	1.000000	Mg
Mg	1.0	0.623327	0.493656	0.046769	Biso	1.000000	Mg
Mg	1.0	0.623154	0.493764	0.379919	Biso	1.000000	Mg
Mg	1.0	0.623315	0.493747	0.713315	Biso	1.000000	Mg
Mg	1.0	0.623397	0.993715	0.046936	Biso	1.000000	Mg
Mg	1.0	0.623405	0.993716	0.380112	Biso	1.000000	Mg
Mg	1.0	0.623503	0.993734	0.713516	Biso	1.000000	Mg
Mg	1.0	0.375636	0.006671	0.287217	Biso	1.000000	Mg
Mg	1.0	0.376807	0.005920	0.620138	Biso	1.000000	Mg
Mg	1.0	0.376591	0.006216	0.953606	Biso	1.000000	Mg
Mg	1.0	0.376182	0.505668	0.287044	Biso	1.000000	Mg
Mg	1.0	0.376501	0.506011	0.620025	Biso	1.000000	Mg
Mg	1.0	0.375795	0.505745	0.953799	Biso	1.000000	Mg
Mg	1.0	0.877075	0.006654	0.213522	Biso	1.000000	Mg
Mg	1.0	0.876363	0.006072	0.546419	Biso	1.000000	Mg
Mg	1.0	0.876258	0.006013	0.879756	Biso	1.000000	Mg
Mg	1.0	0.876365	0.506196	0.212748	Biso	1.000000	Mg
Mg	1.0	0.876277	0.506310	0.546199	Biso	1.000000	Mg
Mg	1.0	0.876191	0.506122	0.879491	Biso	1.000000	Mg
Mg	1.0	0.125444	0.493381	0.122422	Biso	1.000000	Mg
Mg	1.0	0.125962	0.494408	0.453806	Biso	1.000000	Mg
Mg	1.0	0.124072	0.493843	0.786839	Biso	1.000000	Mg
Mg	1.0	0.123586	0.994545	0.121302	Biso	1.000000	Mg
Mg	1.0	0.123540	0.993343	0.452547	Biso	1.000000	Mg
Mg	1.0	0.123468	0.993560	0.787282	Biso	1.000000	Mg
O	1.0	0.182389	0.170759	0.016267	Biso	1.000000	O
O	1.0	0.183995	0.163296	0.349317	Biso	1.000000	O
O	1.0	0.183646	0.169540	0.678620	Biso	1.000000	O
O	1.0	0.183179	0.669823	0.012108	Biso	1.000000	O
O	1.0	0.183422	0.670572	0.345573	Biso	1.000000	O
O	1.0	0.183265	0.670169	0.678977	Biso	1.000000	O
O	1.0	0.816660	0.329680	0.320899	Biso	1.000000	O
O	1.0	0.816465	0.329791	0.654487	Biso	1.000000	O
O	1.0	0.816502	0.329563	0.987689	Biso	1.000000	O
O	1.0	0.816940	0.829936	0.321334	Biso	1.000000	O
O	1.0	0.816823	0.829840	0.654758	Biso	1.000000	O
O	1.0	0.816936	0.829975	0.988145	Biso	1.000000	O
O	1.0	0.315476	0.329828	0.178680	Biso	1.000000	O
O	1.0	0.316287	0.329835	0.511788	Biso	1.000000	O
O	1.0	0.316718	0.329766	0.844962	Biso	1.000000	O
O	1.0	0.316535	0.830062	0.178466	Biso	1.000000	O
O	1.0	0.316703	0.829799	0.512096	Biso	1.000000	O
O	1.0	0.316561	0.830161	0.845583	Biso	1.000000	O
O	1.0	0.683048	0.170202	0.154836	Biso	1.000000	O
O	1.0	0.683103	0.169977	0.488106	Biso	1.000000	O
O	1.0	0.683411	0.170010	0.821421	Biso	1.000000	O
O	1.0	0.683321	0.670244	0.154731	Biso	1.000000	O
O	1.0	0.683385	0.670165	0.488099	Biso	1.000000	O
O	1.0	0.683415	0.670080	0.821526	Biso	1.000000	O
O	1.0	0.816819	0.419874	0.154291	Biso	1.000000	O
O	1.0	0.816527	0.420170	0.487782	Biso	1.000000	O
O	1.0	0.816580	0.419904	0.821000	Biso	1.000000	O
O	1.0	0.817170	0.920771	0.154716	Biso	1.000000	O

O	1.0	0.816781	0.920004	0.488046	Biso	1.000000	O
O	1.0	0.816772	0.920119	0.821473	Biso	1.000000	O
O	1.0	0.183165	0.084405	0.177440	Biso	1.000000	O
O	1.0	0.184183	0.078430	0.512874	Biso	1.000000	O
O	1.0	0.182858	0.080065	0.845994	Biso	1.000000	O
O	1.0	0.183623	0.580450	0.178930	Biso	1.000000	O
O	1.0	0.183604	0.580502	0.512560	Biso	1.000000	O
O	1.0	0.183209	0.579778	0.845500	Biso	1.000000	O
O	1.0	0.683215	0.079774	0.321473	Biso	1.000000	O
O	1.0	0.683339	0.079810	0.654869	Biso	1.000000	O
O	1.0	0.683420	0.079670	0.988158	Biso	1.000000	O
O	1.0	0.683136	0.580034	0.321324	Biso	1.000000	O
O	1.0	0.683347	0.579763	0.654749	Biso	1.000000	O
O	1.0	0.683353	0.579792	0.988126	Biso	1.000000	O
O	1.0	0.316063	0.419695	0.011770	Biso	1.000000	O
O	1.0	0.316963	0.420380	0.345709	Biso	1.000000	O
O	1.0	0.316456	0.419825	0.678399	Biso	1.000000	O
O	1.0	0.316136	0.920719	0.012171	Biso	1.000000	O
O	1.0	0.316564	0.919934	0.345175	Biso	1.000000	O
O	1.0	0.316689	0.920041	0.678962	Biso	1.000000	O
O	1.0	0.562580	0.170323	0.266236	Biso	1.000000	O
O	1.0	0.562729	0.170173	0.599768	Biso	1.000000	O
O	1.0	0.562893	0.170102	0.932775	Biso	1.000000	O
O	1.0	0.562749	0.670374	0.266249	Biso	1.000000	O
O	1.0	0.562882	0.670240	0.599689	Biso	1.000000	O
O	1.0	0.562819	0.670264	0.933005	Biso	1.000000	O
O	1.0	0.436885	0.329894	0.067056	Biso	1.000000	O
O	1.0	0.436911	0.329560	0.400428	Biso	1.000000	O
O	1.0	0.437130	0.329771	0.733520	Biso	1.000000	O
O	1.0	0.436937	0.829956	0.067125	Biso	1.000000	O
O	1.0	0.437235	0.829831	0.400449	Biso	1.000000	O
O	1.0	0.437251	0.829773	0.733900	Biso	1.000000	O
O	1.0	0.936897	0.327834	0.098018	Biso	1.000000	O
O	1.0	0.935812	0.329948	0.432059	Biso	1.000000	O
O	1.0	0.936892	0.329094	0.765244	Biso	1.000000	O
O	1.0	0.937332	0.830006	0.099685	Biso	1.000000	O
O	1.0	0.937197	0.829772	0.432838	Biso	1.000000	O
O	1.0	0.937171	0.829747	0.766368	Biso	1.000000	O
O	1.0	0.062923	0.167652	0.230207	Biso	1.000000	O
O	1.0	0.063230	0.170243	0.566293	Biso	1.000000	O
O	1.0	0.063449	0.171107	0.901129	Biso	1.000000	O
O	1.0	0.063012	0.670614	0.233921	Biso	1.000000	O
O	1.0	0.062911	0.670238	0.567365	Biso	1.000000	O
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O	1.0	0.437073	0.420084	0.567045	Biso	1.000000	O
O	1.0	0.437001	0.420262	0.900313	Biso	1.000000	O
O	1.0	0.436761	0.920781	0.233705	Biso	1.000000	O
O	1.0	0.437378	0.919928	0.567216	Biso	1.000000	O
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O	1.0	0.562812	0.079617	0.433044	Biso	1.000000	O
O	1.0	0.562773	0.079729	0.766451	Biso	1.000000	O
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O	1.0	0.562821	0.579931	0.432953	Biso	1.000000	O
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O	1.0	0.062379	0.079529	0.401021	Biso	1.000000	O
O	1.0	0.063049	0.079515	0.733969	Biso	1.000000	O
O	1.0	0.063209	0.578631	0.067366	Biso	1.000000	O
O	1.0	0.063253	0.579657	0.401093	Biso	1.000000	O
O	1.0	0.062941	0.579431	0.733760	Biso	1.000000	O
O	1.0	0.937030	0.420792	0.266187	Biso	1.000000	O
O	1.0	0.937100	0.419973	0.598703	Biso	1.000000	O
O	1.0	0.936693	0.419757	0.931581	Biso	1.000000	O
O	1.0	0.937641	0.920876	0.266311	Biso	1.000000	O
O	1.0	0.937176	0.920289	0.599549	Biso	1.000000	O
O	1.0	0.937156	0.920406	0.933027	Biso	1.000000	O
O	1.0	0.311320	0.251458	0.014318	Biso	1.000000	O
O	1.0	0.310702	0.250515	0.349076	Biso	1.000000	O
O	1.0	0.311352	0.250570	0.681657	Biso	1.000000	O
O	1.0	0.311124	0.751048	0.014751	Biso	1.000000	O
O	1.0	0.311493	0.751208	0.348474	Biso	1.000000	O
O	1.0	0.311350	0.751093	0.681961	Biso	1.000000	O
O	1.0	0.688528	0.248980	0.318269	Biso	1.000000	O
O	1.0	0.688527	0.248989	0.651608	Biso	1.000000	O
O	1.0	0.688446	0.249007	0.985014	Biso	1.000000	O
O	1.0	0.688689	0.749222	0.318279	Biso	1.000000	O
O	1.0	0.688735	0.749004	0.651820	Biso	1.000000	O

O	1.0	0.688708	0.749170	0.985346	Biso	1.000000	O
O	1.0	0.194849	0.244238	0.171895	Biso	1.000000	O
O	1.0	0.187659	0.249518	0.514213	Biso	1.000000	O
O	1.0	0.188912	0.248258	0.848990	Biso	1.000000	O
O	1.0	0.188479	0.748906	0.181195	Biso	1.000000	O
O	1.0	0.188431	0.749270	0.515354	Biso	1.000000	O
O	1.0	0.188473	0.749230	0.848927	Biso	1.000000	O
O	1.0	0.811315	0.250996	0.152222	Biso	1.000000	O
O	1.0	0.811143	0.250835	0.484659	Biso	1.000000	O
O	1.0	0.811694	0.250625	0.818181	Biso	1.000000	O
O	1.0	0.811650	0.750987	0.151505	Biso	1.000000	O
O	1.0	0.811706	0.750752	0.484871	Biso	1.000000	O
O	1.0	0.811662	0.750744	0.818336	Biso	1.000000	O
O	1.0	0.688681	0.001138	0.151860	Biso	1.000000	O
O	1.0	0.688707	0.000881	0.485153	Biso	1.000000	O
O	1.0	0.688703	0.000863	0.818533	Biso	1.000000	O
O	1.0	0.688718	0.500891	0.151674	Biso	1.000000	O
O	1.0	0.688446	0.500887	0.484855	Biso	1.000000	O
O	1.0	0.688580	0.500862	0.818330	Biso	1.000000	O
O	1.0	0.311394	0.499578	0.181673	Biso	1.000000	O
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O	1.0	0.311212	0.499026	0.848189	Biso	1.000000	O
O	1.0	0.309333	0.999552	0.181936	Biso	1.000000	O
O	1.0	0.312034	0.998516	0.515215	Biso	1.000000	O
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O	1.0	0.811080	0.499156	0.317771	Biso	1.000000	O
O	1.0	0.811570	0.499012	0.651434	Biso	1.000000	O
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O	1.0	0.811608	0.999156	0.318182	Biso	1.000000	O
O	1.0	0.811603	0.999093	0.651592	Biso	1.000000	O
O	1.0	0.812279	0.999624	0.985621	Biso	1.000000	O
O	1.0	0.187620	0.001337	0.016048	Biso	1.000000	O
O	1.0	0.187815	-0.000135	0.346684	Biso	1.000000	O
O	1.0	0.188537	0.000807	0.682517	Biso	1.000000	O
O	1.0	0.188136	0.500228	0.015171	Biso	1.000000	O
O	1.0	0.189520	0.501881	0.348724	Biso	1.000000	O
O	1.0	0.188317	0.500538	0.681634	Biso	1.000000	O
O	1.0	0.432125	0.241504	0.229937	Biso	1.000000	O
O	1.0	0.432243	0.241028	0.562986	Biso	1.000000	O
O	1.0	0.432610	0.241303	0.896144	Biso	1.000000	O
O	1.0	0.432367	0.741416	0.229606	Biso	1.000000	O
O	1.0	0.432572	0.741363	0.563052	Biso	1.000000	O
O	1.0	0.432446	0.741388	0.896455	Biso	1.000000	O
O	1.0	0.567288	0.258739	0.103610	Biso	1.000000	O
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O	1.0	0.567561	0.258790	0.770313	Biso	1.000000	O
O	1.0	0.567429	0.758876	0.103755	Biso	1.000000	O
O	1.0	0.567702	0.758875	0.436998	Biso	1.000000	O
O	1.0	0.567708	0.758758	0.770543	Biso	1.000000	O
O	1.0	0.069258	0.255920	0.067043	Biso	1.000000	O
O	1.0	0.063451	0.255690	0.398916	Biso	1.000000	O
O	1.0	0.067596	0.257549	0.728677	Biso	1.000000	O
O	1.0	0.067610	0.759008	0.063273	Biso	1.000000	O
O	1.0	0.067601	0.758832	0.396381	Biso	1.000000	O
O	1.0	0.067664	0.758823	0.730097	Biso	1.000000	O
O	1.0	0.934169	0.242152	0.270824	Biso	1.000000	O
O	1.0	0.932584	0.241508	0.603110	Biso	1.000000	O
O	1.0	0.932866	0.241456	0.937192	Biso	1.000000	O
O	1.0	0.932420	0.741180	0.270010	Biso	1.000000	O
O	1.0	0.932416	0.741106	0.603719	Biso	1.000000	O
O	1.0	0.932509	0.741020	0.937021	Biso	1.000000	O
O	1.0	0.567390	0.491165	0.270263	Biso	1.000000	O
O	1.0	0.567463	0.491156	0.603615	Biso	1.000000	O
O	1.0	0.567485	0.491211	0.937010	Biso	1.000000	O
O	1.0	0.567431	0.991374	0.270425	Biso	1.000000	O
O	1.0	0.567705	0.991098	0.603864	Biso	1.000000	O
O	1.0	0.567480	0.991289	0.937177	Biso	1.000000	O
O	1.0	0.431858	0.008930	0.063414	Biso	1.000000	O
O	1.0	0.432493	0.008580	0.396296	Biso	1.000000	O
O	1.0	0.432514	0.008587	0.729864	Biso	1.000000	O
O	1.0	0.431979	0.508620	0.063084	Biso	1.000000	O
O	1.0	0.432537	0.508799	0.396430	Biso	1.000000	O
O	1.0	0.432325	0.508802	0.729643	Biso	1.000000	O
O	1.0	0.934275	0.009442	0.104039	Biso	1.000000	O
O	1.0	0.931906	0.009015	0.436720	Biso	1.000000	O
O	1.0	0.932427	0.008782	0.770318	Biso	1.000000	O
O	1.0	0.932820	0.507597	0.103196	Biso	1.000000	O
O	1.0	0.932684	0.508278	0.436813	Biso	1.000000	O
O	1.0	0.932467	0.508300	0.769986	Biso	1.000000	O

O	1.0	0.067302	0.493574	0.230975	Biso	1.000000	O
O	1.0	0.068048	0.490824	0.562323	Biso	1.000000	O
O	1.0	0.067329	0.490500	0.895568	Biso	1.000000	O
O	1.0	0.068345	0.992134	0.230255	Biso	1.000000	O
O	1.0	0.067701	0.991075	0.562851	Biso	1.000000	O
O	1.0	0.067448	0.991943	0.897345	Biso	1.000000	O
O	1.0	0.304380	0.110906	0.279132	Biso	1.000000	O
O	1.0	0.303569	0.109470	0.612947	Biso	1.000000	O
O	1.0	0.301094	0.111018	0.946258	Biso	1.000000	O
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O	1.0	0.696969	0.389577	0.387607	Biso	1.000000	O
O	1.0	0.696732	0.389635	0.721016	Biso	1.000000	O
O	1.0	0.697278	0.889905	0.054639	Biso	1.000000	O
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O	1.0	0.196562	0.388630	0.777954	Biso	1.000000	O
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O	1.0	0.803335	0.110314	0.887935	Biso	1.000000	O
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model 10

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CRYSTAL DATA

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_atom_site_B_iso_or_equiv
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Mg	1.0	0.623051	0.256255	0.880052	Biso	1.000000	Mg
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Mg	1.0	0.623607	0.756124	0.546868	Biso	1.000000	Mg
Mg	1.0	0.623603	0.756102	0.880197	Biso	1.000000	Mg
Mg	1.0	0.124961	0.255684	0.620312	Biso	1.000000	Mg
Mg	1.0	0.124669	0.255372	0.955432	Biso	1.000000	Mg
Mg	1.0	0.124005	0.755734	0.287222	Biso	1.000000	Mg
Mg	1.0	0.123690	0.756504	0.620299	Biso	1.000000	Mg
Mg	1.0	0.123533	0.756235	0.953896	Biso	1.000000	Mg
Mg	1.0	0.875991	0.243804	0.045990	Biso	1.000000	Mg
Mg	1.0	0.875112	0.243211	0.378267	Biso	1.000000	Mg
Mg	1.0	0.876314	0.243364	0.712625	Biso	1.000000	Mg
Mg	1.0	0.876869	0.743592	0.046662	Biso	1.000000	Mg
Mg	1.0	0.876637	0.743332	0.379795	Biso	1.000000	Mg
Mg	1.0	0.876622	0.743618	0.713460	Biso	1.000000	Mg
Mg	1.0	0.623259	0.493388	0.046723	Biso	1.000000	Mg
Mg	1.0	0.623525	0.493854	0.379893	Biso	1.000000	Mg
Mg	1.0	0.623182	0.493645	0.713277	Biso	1.000000	Mg
Mg	1.0	0.623539	0.993926	0.046836	Biso	1.000000	Mg
Mg	1.0	0.623215	0.993796	0.380265	Biso	1.000000	Mg
Mg	1.0	0.623403	0.993759	0.713643	Biso	1.000000	Mg
Mg	1.0	0.378129	0.006612	0.286263	Biso	1.000000	Mg
Mg	1.0	0.376982	0.006170	0.620061	Biso	1.000000	Mg
Mg	1.0	0.376472	0.006826	0.953638	Biso	1.000000	Mg
Mg	1.0	0.376780	0.506237	0.287005	Biso	1.000000	Mg
Mg	1.0	0.376302	0.506073	0.620337	Biso	1.000000	Mg
Mg	1.0	0.375732	0.505373	0.953855	Biso	1.000000	Mg
Mg	1.0	0.875498	0.006614	0.213250	Biso	1.000000	Mg
Mg	1.0	0.875976	0.005673	0.547056	Biso	1.000000	Mg
Mg	1.0	0.876486	0.006462	0.880072	Biso	1.000000	Mg
Mg	1.0	0.876254	0.505874	0.212597	Biso	1.000000	Mg
Mg	1.0	0.876307	0.506202	0.546059	Biso	1.000000	Mg
Mg	1.0	0.875955	0.506084	0.879180	Biso	1.000000	Mg
Mg	1.0	0.125122	0.492474	0.121768	Biso	1.000000	Mg
Mg	1.0	0.126171	0.494931	0.453966	Biso	1.000000	Mg
Mg	1.0	0.124256	0.494087	0.786870	Biso	1.000000	Mg
Mg	1.0	0.122685	0.993768	0.119233	Biso	1.000000	Mg
Mg	1.0	0.123578	0.991683	0.455031	Biso	1.000000	Mg
Mg	1.0	0.124036	0.994210	0.787712	Biso	1.000000	Mg
O	1.0	0.182462	0.168921	0.013305	Biso	1.000000	O
O	1.0	0.182829	0.158535	0.347459	Biso	1.000000	O
O	1.0	0.183416	0.169810	0.678362	Biso	1.000000	O
O	1.0	0.183169	0.670467	0.012147	Biso	1.000000	O
O	1.0	0.183372	0.671065	0.345863	Biso	1.000000	O
O	1.0	0.183358	0.670635	0.678703	Biso	1.000000	O
O	1.0	0.817001	0.329287	0.320357	Biso	1.000000	O
O	1.0	0.816575	0.329510	0.654178	Biso	1.000000	O
O	1.0	0.816343	0.329667	0.987473	Biso	1.000000	O
O	1.0	0.816873	0.829890	0.321351	Biso	1.000000	O
O	1.0	0.816726	0.829749	0.654927	Biso	1.000000	O
O	1.0	0.816912	0.829874	0.988252	Biso	1.000000	O
O	1.0	0.317671	0.333891	0.179153	Biso	1.000000	O
O	1.0	0.316140	0.329960	0.511571	Biso	1.000000	O
O	1.0	0.316347	0.329768	0.845204	Biso	1.000000	O
O	1.0	0.316676	0.829634	0.178615	Biso	1.000000	O
O	1.0	0.316476	0.830635	0.511691	Biso	1.000000	O
O	1.0	0.316729	0.830143	0.845345	Biso	1.000000	O
O	1.0	0.683316	0.170345	0.154875	Biso	1.000000	O
O	1.0	0.683175	0.170031	0.488105	Biso	1.000000	O
O	1.0	0.683242	0.170120	0.821350	Biso	1.000000	O
O	1.0	0.683478	0.670063	0.154725	Biso	1.000000	O
O	1.0	0.683454	0.670136	0.488180	Biso	1.000000	O
O	1.0	0.683380	0.670028	0.821486	Biso	1.000000	O
O	1.0	0.816780	0.419872	0.154300	Biso	1.000000	O
O	1.0	0.816722	0.419950	0.487560	Biso	1.000000	O
O	1.0	0.816478	0.419922	0.820685	Biso	1.000000	O
O	1.0	0.816748	0.920099	0.154986	Biso	1.000000	O

O	1.0	0.816511	0.919908	0.488332	Biso	1.000000	O
O	1.0	0.816760	0.920166	0.821665	Biso	1.000000	O
O	1.0	0.183169	0.077954	0.183716	Biso	1.000000	O
O	1.0	0.183537	0.078207	0.512426	Biso	1.000000	O
O	1.0	0.183141	0.080030	0.845683	Biso	1.000000	O
O	1.0	0.183653	0.580648	0.178913	Biso	1.000000	O
O	1.0	0.183663	0.581205	0.512880	Biso	1.000000	O
O	1.0	0.183346	0.580246	0.845269	Biso	1.000000	O
O	1.0	0.682842	0.079966	0.321570	Biso	1.000000	O
O	1.0	0.683219	0.079842	0.654812	Biso	1.000000	O
O	1.0	0.683330	0.079903	0.988231	Biso	1.000000	O
O	1.0	0.683405	0.580117	0.321392	Biso	1.000000	O
O	1.0	0.683373	0.579686	0.654701	Biso	1.000000	O
O	1.0	0.683303	0.579736	0.988061	Biso	1.000000	O
O	1.0	0.316294	0.419824	0.011681	Biso	1.000000	O
O	1.0	0.317507	0.421535	0.346553	Biso	1.000000	O
O	1.0	0.316301	0.419815	0.678334	Biso	1.000000	O
O	1.0	0.316856	0.920264	0.012068	Biso	1.000000	O
O	1.0	0.316204	0.921739	0.345214	Biso	1.000000	O
O	1.0	0.316799	0.920281	0.678677	Biso	1.000000	O
O	1.0	0.562203	0.170572	0.266303	Biso	1.000000	O
O	1.0	0.562489	0.170281	0.599587	Biso	1.000000	O
O	1.0	0.562770	0.170116	0.932792	Biso	1.000000	O
O	1.0	0.562989	0.670306	0.266329	Biso	1.000000	O
O	1.0	0.562840	0.670395	0.599777	Biso	1.000000	O
O	1.0	0.562852	0.670173	0.933001	Biso	1.000000	O
O	1.0	0.436906	0.329666	0.067109	Biso	1.000000	O
O	1.0	0.436617	0.329215	0.400321	Biso	1.000000	O
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O	1.0	0.437329	0.829630	0.067144	Biso	1.000000	O
O	1.0	0.437231	0.830095	0.400347	Biso	1.000000	O
O	1.0	0.437294	0.829890	0.733825	Biso	1.000000	O
O	1.0	0.936152	0.329651	0.097365	Biso	1.000000	O
O	1.0	0.935934	0.329568	0.431712	Biso	1.000000	O
O	1.0	0.936842	0.329278	0.764858	Biso	1.000000	O
O	1.0	0.937308	0.830119	0.099931	Biso	1.000000	O
O	1.0	0.937014	0.829819	0.432881	Biso	1.000000	O
O	1.0	0.937180	0.829733	0.766420	Biso	1.000000	O
O	1.0	0.063092	0.160430	0.237110	Biso	1.000000	O
O	1.0	0.063500	0.169907	0.565831	Biso	1.000000	O
O	1.0	0.062867	0.170527	0.900580	Biso	1.000000	O
O	1.0	0.062993	0.671068	0.234003	Biso	1.000000	O
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O	1.0	0.062969	0.670519	0.900681	Biso	1.000000	O
O	1.0	0.437603	0.421071	0.233991	Biso	1.000000	O
O	1.0	0.436945	0.420169	0.567140	Biso	1.000000	O
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O	1.0	0.562789	0.079831	0.766292	Biso	1.000000	O
O	1.0	0.562823	0.579652	0.099569	Biso	1.000000	O
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O	1.0	0.562711	0.579742	0.766200	Biso	1.000000	O
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O	1.0	0.062721	0.077504	0.397693	Biso	1.000000	O
O	1.0	0.063007	0.079629	0.733922	Biso	1.000000	O
O	1.0	0.063251	0.579310	0.067537	Biso	1.000000	O
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O	1.0	0.937142	0.419767	0.598272	Biso	1.000000	O
O	1.0	0.936519	0.420309	0.931099	Biso	1.000000	O
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O	1.0	0.936852	0.920082	0.599878	Biso	1.000000	O
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O	1.0	0.311501	0.249774	0.015329	Biso	1.000000	O
O	1.0	0.308541	0.250313	0.348747	Biso	1.000000	O
O	1.0	0.311161	0.250728	0.681576	Biso	1.000000	O
O	1.0	0.311255	0.751418	0.014559	Biso	1.000000	O
O	1.0	0.311221	0.752031	0.348711	Biso	1.000000	O
O	1.0	0.311312	0.751491	0.681745	Biso	1.000000	O
O	1.0	0.688653	0.248909	0.318268	Biso	1.000000	O
O	1.0	0.688434	0.248905	0.651484	Biso	1.000000	O
O	1.0	0.688376	0.249035	0.984918	Biso	1.000000	O
O	1.0	0.688843	0.748945	0.318508	Biso	1.000000	O
O	1.0	0.688703	0.748925	0.651965	Biso	1.000000	O

O	1.0	0.688762	0.749004	0.985239	Biso	1.000000	O
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O	1.0	0.187558	0.249847	0.512939	Biso	1.000000	O
O	1.0	0.188322	0.248790	0.848464	Biso	1.000000	O
O	1.0	0.188230	0.749291	0.181949	Biso	1.000000	O
O	1.0	0.187792	0.750848	0.514123	Biso	1.000000	O
O	1.0	0.188461	0.749457	0.848813	Biso	1.000000	O
O	1.0	0.812418	0.250281	0.152670	Biso	1.000000	O
O	1.0	0.811633	0.250410	0.484421	Biso	1.000000	O
O	1.0	0.811393	0.250904	0.817789	Biso	1.000000	O
O	1.0	0.811688	0.750815	0.151455	Biso	1.000000	O
O	1.0	0.811661	0.750800	0.484846	Biso	1.000000	O
O	1.0	0.811650	0.750711	0.818362	Biso	1.000000	O
O	1.0	0.688642	0.000914	0.152022	Biso	1.000000	O
O	1.0	0.688554	0.000856	0.485155	Biso	1.000000	O
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O	1.0	0.688807	0.500838	0.151540	Biso	1.000000	O
O	1.0	0.688584	0.500664	0.484867	Biso	1.000000	O
O	1.0	0.688481	0.500786	0.818107	Biso	1.000000	O
O	1.0	0.312225	0.500807	0.181840	Biso	1.000000	O
O	1.0	0.311535	0.499861	0.515425	Biso	1.000000	O
O	1.0	0.311306	0.499417	0.848048	Biso	1.000000	O
O	1.0	0.311075	0.997447	0.182705	Biso	1.000000	O
O	1.0	0.311734	0.998745	0.515040	Biso	1.000000	O
O	1.0	0.311243	0.999124	0.848433	Biso	1.000000	O
O	1.0	0.811260	0.499171	0.317886	Biso	1.000000	O
O	1.0	0.811617	0.498931	0.651237	Biso	1.000000	O
O	1.0	0.811384	0.498883	0.984651	Biso	1.000000	O
O	1.0	0.810663	0.998631	0.318690	Biso	1.000000	O
O	1.0	0.811333	0.998973	0.651891	Biso	1.000000	O
O	1.0	0.811652	0.999355	0.985197	Biso	1.000000	O
O	1.0	0.189018	0.001457	0.016184	Biso	1.000000	O
O	1.0	0.186195	0.001170	0.346451	Biso	1.000000	O
O	1.0	0.188649	0.001130	0.682250	Biso	1.000000	O
O	1.0	0.188501	0.500742	0.014787	Biso	1.000000	O
O	1.0	0.190154	0.503428	0.349717	Biso	1.000000	O
O	1.0	0.188193	0.500530	0.681142	Biso	1.000000	O
O	1.0	0.430770	0.241013	0.230540	Biso	1.000000	O
O	1.0	0.431699	0.240870	0.562695	Biso	1.000000	O
O	1.0	0.432455	0.241167	0.896169	Biso	1.000000	O
O	1.0	0.432617	0.741404	0.229605	Biso	1.000000	O
O	1.0	0.432451	0.741612	0.563083	Biso	1.000000	O
O	1.0	0.432638	0.741479	0.896399	Biso	1.000000	O
O	1.0	0.567300	0.258620	0.103724	Biso	1.000000	O
O	1.0	0.567251	0.258632	0.436981	Biso	1.000000	O
O	1.0	0.567337	0.258715	0.770231	Biso	1.000000	O
O	1.0	0.567762	0.758648	0.103731	Biso	1.000000	O
O	1.0	0.567577	0.758749	0.437215	Biso	1.000000	O
O	1.0	0.567688	0.758785	0.770534	Biso	1.000000	O
O	1.0	0.066910	0.258470	0.063490	Biso	1.000000	O
O	1.0	0.063642	0.255187	0.399001	Biso	1.000000	O
O	1.0	0.067375	0.257952	0.728547	Biso	1.000000	O
O	1.0	0.067831	0.759661	0.063974	Biso	1.000000	O
O	1.0	0.067479	0.759249	0.396291	Biso	1.000000	O
O	1.0	0.067729	0.758987	0.729958	Biso	1.000000	O
O	1.0	0.935667	0.240191	0.271169	Biso	1.000000	O
O	1.0	0.932614	0.240834	0.602444	Biso	1.000000	O
O	1.0	0.932094	0.241290	0.936468	Biso	1.000000	O
O	1.0	0.932713	0.741840	0.270066	Biso	1.000000	O
O	1.0	0.932445	0.741308	0.603715	Biso	1.000000	O
O	1.0	0.932570	0.741292	0.937010	Biso	1.000000	O
O	1.0	0.568316	0.490988	0.270258	Biso	1.000000	O
O	1.0	0.567447	0.491082	0.603482	Biso	1.000000	O
O	1.0	0.567444	0.491066	0.936934	Biso	1.000000	O
O	1.0	0.567550	0.991130	0.270478	Biso	1.000000	O
O	1.0	0.567669	0.991184	0.603828	Biso	1.000000	O
O	1.0	0.567723	0.991262	0.937165	Biso	1.000000	O
O	1.0	0.432653	0.008256	0.063405	Biso	1.000000	O
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O	1.0	0.432665	0.008580	0.729652	Biso	1.000000	O
O	1.0	0.432317	0.508788	0.062875	Biso	1.000000	O
O	1.0	0.433015	0.509019	0.396635	Biso	1.000000	O
O	1.0	0.432226	0.508855	0.729692	Biso	1.000000	O
O	1.0	0.932528	0.008627	0.104292	Biso	1.000000	O
O	1.0	0.932649	0.007144	0.437793	Biso	1.000000	O
O	1.0	0.932455	0.008569	0.770349	Biso	1.000000	O
O	1.0	0.932419	0.508447	0.103331	Biso	1.000000	O
O	1.0	0.932766	0.508484	0.436727	Biso	1.000000	O
O	1.0	0.932369	0.508472	0.769648	Biso	1.000000	O

O	1.0	0.067341	0.493620	0.231047	Biso	1.000000	O
O	1.0	0.067984	0.490930	0.562028	Biso	1.000000	O
O	1.0	0.067038	0.491968	0.894972	Biso	1.000000	O
O	1.0	0.069140	0.993898	0.233335	Biso	1.000000	O
O	1.0	0.067037	0.991536	0.563330	Biso	1.000000	O
O	1.0	0.067790	0.991882	0.896790	Biso	1.000000	O
O	1.0	0.305056	0.109616	0.278944	Biso	1.000000	O
O	1.0	0.303129	0.109949	0.612443	Biso	1.000000	O
O	1.0	0.302641	0.110402	0.945655	Biso	1.000000	O
O	1.0	0.303354	0.611890	0.279065	Biso	1.000000	O
O	1.0	0.303382	0.610943	0.612672	Biso	1.000000	O
O	1.0	0.302983	0.610565	0.945785	Biso	1.000000	O
O	1.0	0.696819	0.389673	0.054160	Biso	1.000000	O
O	1.0	0.697349	0.389472	0.387327	Biso	1.000000	O
O	1.0	0.696769	0.389564	0.720719	Biso	1.000000	O
O	1.0	0.697106	0.889612	0.054723	Biso	1.000000	O
O	1.0	0.696945	0.889388	0.388125	Biso	1.000000	O
O	1.0	0.697001	0.889563	0.721498	Biso	1.000000	O
O	1.0	0.196091	0.389246	0.111550	Biso	1.000000	O
O	1.0	0.196603	0.390829	0.444221	Biso	1.000000	O
O	1.0	0.196503	0.389147	0.778107	Biso	1.000000	O
O	1.0	0.196783	0.889669	0.112218	Biso	1.000000	O
O	1.0	0.196894	0.892121	0.445385	Biso	1.000000	O
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O	1.0	0.696951	0.360036	0.554069	Biso	1.000000	O
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model 11

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CRYSTAL DATA

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Mg	1.0	0.876552	0.743861	0.713501	Biso	1.000000	Mg
Mg	1.0	0.623789	0.493417	0.046699	Biso	1.000000	Mg
Mg	1.0	0.623754	0.493714	0.379841	Biso	1.000000	Mg
Mg	1.0	0.623583	0.493847	0.713179	Biso	1.000000	Mg
Mg	1.0	0.623888	0.993787	0.046594	Biso	1.000000	Mg
Mg	1.0	0.623583	0.993786	0.380081	Biso	1.000000	Mg
Mg	1.0	0.623675	0.993838	0.713409	Biso	1.000000	Mg
Mg	1.0	0.378346	0.006013	0.286022	Biso	1.000000	Mg
Mg	1.0	0.376867	0.006329	0.620079	Biso	1.000000	Mg
Mg	1.0	0.376930	0.006226	0.953051	Biso	1.000000	Mg
Mg	1.0	0.377277	0.506442	0.286683	Biso	1.000000	Mg
Mg	1.0	0.376251	0.506398	0.620109	Biso	1.000000	Mg
Mg	1.0	0.375798	0.505801	0.953403	Biso	1.000000	Mg
Mg	1.0	0.875879	0.007040	0.213527	Biso	1.000000	Mg
Mg	1.0	0.876770	0.006572	0.546721	Biso	1.000000	Mg
Mg	1.0	0.876428	0.006516	0.879974	Biso	1.000000	Mg
Mg	1.0	0.877772	0.504909	0.214074	Biso	1.000000	Mg
Mg	1.0	0.876323	0.506358	0.546699	Biso	1.000000	Mg
Mg	1.0	0.876028	0.506275	0.879559	Biso	1.000000	Mg
Mg	1.0	0.121168	0.493222	0.121889	Biso	1.000000	Mg
Mg	1.0	0.122588	0.493048	0.453392	Biso	1.000000	Mg
Mg	1.0	0.122820	0.493460	0.785519	Biso	1.000000	Mg
Mg	1.0	0.121997	0.992160	0.118119	Biso	1.000000	Mg
Mg	1.0	0.123738	0.993284	0.454906	Biso	1.000000	Mg
Mg	1.0	0.123320	0.994350	0.786293	Biso	1.000000	Mg
O	1.0	0.182539	0.171286	0.015102	Biso	1.000000	O
O	1.0	0.184393	0.161331	0.341702	Biso	1.000000	O
O	1.0	0.183087	0.170824	0.677787	Biso	1.000000	O
O	1.0	0.183051	0.669759	0.012079	Biso	1.000000	O
O	1.0	0.183398	0.671024	0.345337	Biso	1.000000	O
O	1.0	0.183215	0.670713	0.678541	Biso	1.000000	O
O	1.0	0.817412	0.329192	0.320975	Biso	1.000000	O
O	1.0	0.816805	0.329795	0.654515	Biso	1.000000	O
O	1.0	0.816590	0.329739	0.987679	Biso	1.000000	O
O	1.0	0.816896	0.829871	0.321397	Biso	1.000000	O
O	1.0	0.816676	0.829932	0.655001	Biso	1.000000	O
O	1.0	0.816888	0.829978	0.988284	Biso	1.000000	O
O	1.0	0.316237	0.329048	0.179122	Biso	1.000000	O
O	1.0	0.316920	0.329787	0.511245	Biso	1.000000	O
O	1.0	0.316526	0.329410	0.844985	Biso	1.000000	O
O	1.0	0.316741	0.829485	0.178345	Biso	1.000000	O
O	1.0	0.316372	0.830638	0.511392	Biso	1.000000	O
O	1.0	0.316573	0.830034	0.845199	Biso	1.000000	O
O	1.0	0.683466	0.170304	0.154802	Biso	1.000000	O
O	1.0	0.683750	0.170223	0.488102	Biso	1.000000	O
O	1.0	0.683383	0.170150	0.821496	Biso	1.000000	O
O	1.0	0.683480	0.669948	0.154753	Biso	1.000000	O
O	1.0	0.683391	0.670270	0.488164	Biso	1.000000	O
O	1.0	0.683268	0.670196	0.821579	Biso	1.000000	O
O	1.0	0.817086	0.420018	0.154749	Biso	1.000000	O
O	1.0	0.816531	0.420788	0.488407	Biso	1.000000	O
O	1.0	0.816554	0.420106	0.821150	Biso	1.000000	O
O	1.0	0.816869	0.920253	0.154957	Biso	1.000000	O

O	1.0	0.816668	0.920174	0.488318	Biso	1.000000	O
O	1.0	0.816761	0.920256	0.821673	Biso	1.000000	O
O	1.0	0.183376	0.078222	0.182471	Biso	1.000000	O
O	1.0	0.183330	0.079075	0.510811	Biso	1.000000	O
O	1.0	0.183089	0.080105	0.845427	Biso	1.000000	O
O	1.0	0.182976	0.579816	0.178923	Biso	1.000000	O
O	1.0	0.183111	0.580823	0.512669	Biso	1.000000	O
O	1.0	0.183081	0.579498	0.845390	Biso	1.000000	O
O	1.0	0.683115	0.079812	0.321482	Biso	1.000000	O
O	1.0	0.683346	0.079845	0.654855	Biso	1.000000	O
O	1.0	0.683419	0.079937	0.988169	Biso	1.000000	O
O	1.0	0.683674	0.579670	0.321392	Biso	1.000000	O
O	1.0	0.683199	0.580125	0.654814	Biso	1.000000	O
O	1.0	0.683306	0.579806	0.988154	Biso	1.000000	O
O	1.0	0.315937	0.419435	0.012142	Biso	1.000000	O
O	1.0	0.318412	0.421376	0.346493	Biso	1.000000	O
O	1.0	0.316608	0.420096	0.678209	Biso	1.000000	O
O	1.0	0.316994	0.920086	0.011712	Biso	1.000000	O
O	1.0	0.316197	0.921728	0.344841	Biso	1.000000	O
O	1.0	0.316679	0.920432	0.678622	Biso	1.000000	O
O	1.0	0.562803	0.170225	0.266267	Biso	1.000000	O
O	1.0	0.562843	0.170270	0.599660	Biso	1.000000	O
O	1.0	0.562636	0.170239	0.933132	Biso	1.000000	O
O	1.0	0.562975	0.669991	0.266220	Biso	1.000000	O
O	1.0	0.562712	0.670547	0.599756	Biso	1.000000	O
O	1.0	0.562739	0.670175	0.933082	Biso	1.000000	O
O	1.0	0.437030	0.329835	0.067096	Biso	1.000000	O
O	1.0	0.437043	0.328828	0.400272	Biso	1.000000	O
O	1.0	0.437095	0.329703	0.733645	Biso	1.000000	O
O	1.0	0.437333	0.829365	0.066915	Biso	1.000000	O
O	1.0	0.437064	0.829964	0.400210	Biso	1.000000	O
O	1.0	0.437149	0.829873	0.733747	Biso	1.000000	O
O	1.0	0.936596	0.329933	0.097939	Biso	1.000000	O
O	1.0	0.935571	0.332980	0.433921	Biso	1.000000	O
O	1.0	0.937070	0.329749	0.765638	Biso	1.000000	O
O	1.0	0.937327	0.830230	0.099773	Biso	1.000000	O
O	1.0	0.937178	0.829886	0.432858	Biso	1.000000	O
O	1.0	0.937189	0.829997	0.766492	Biso	1.000000	O
O	1.0	0.063302	0.156594	0.232395	Biso	1.000000	O
O	1.0	0.063447	0.168242	0.566895	Biso	1.000000	O
O	1.0	0.062874	0.170483	0.900455	Biso	1.000000	O
O	1.0	0.062846	0.671142	0.233689	Biso	1.000000	O
O	1.0	0.062763	0.671146	0.567173	Biso	1.000000	O
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O	1.0	0.437198	0.419977	0.233506	Biso	1.000000	O
O	1.0	0.437195	0.420293	0.567257	Biso	1.000000	O
O	1.0	0.436853	0.420051	0.900481	Biso	1.000000	O
O	1.0	0.437479	0.919644	0.233535	Biso	1.000000	O
O	1.0	0.437263	0.920190	0.567091	Biso	1.000000	O
O	1.0	0.437290	0.920112	0.900414	Biso	1.000000	O
O	1.0	0.562968	0.079726	0.099598	Biso	1.000000	O
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O	1.0	0.562826	0.079791	0.766501	Biso	1.000000	O
O	1.0	0.562737	0.579397	0.099614	Biso	1.000000	O
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O	1.0	0.062887	0.077043	0.396082	Biso	1.000000	O
O	1.0	0.062877	0.079999	0.733790	Biso	1.000000	O
O	1.0	0.062603	0.579842	0.067331	Biso	1.000000	O
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O	1.0	0.938147	0.419721	0.267221	Biso	1.000000	O
O	1.0	0.936955	0.421093	0.600119	Biso	1.000000	O
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O	1.0	0.937268	0.920601	0.933167	Biso	1.000000	O
O	1.0	0.311256	0.250442	0.016162	Biso	1.000000	O
O	1.0	0.309723	0.248815	0.347137	Biso	1.000000	O
O	1.0	0.311502	0.250935	0.681488	Biso	1.000000	O
O	1.0	0.311208	0.750576	0.014892	Biso	1.000000	O
O	1.0	0.311389	0.751272	0.348076	Biso	1.000000	O
O	1.0	0.311292	0.751193	0.681639	Biso	1.000000	O
O	1.0	0.688765	0.248968	0.318363	Biso	1.000000	O
O	1.0	0.688655	0.249075	0.651854	Biso	1.000000	O
O	1.0	0.688433	0.249160	0.985043	Biso	1.000000	O
O	1.0	0.688747	0.748995	0.318460	Biso	1.000000	O
O	1.0	0.688584	0.749127	0.651969	Biso	1.000000	O

O	1.0	0.688703	0.749061	0.985212	Biso	1.000000	O
O	1.0	0.190486	0.247532	0.190375	Biso	1.000000	O
O	1.0	0.188820	0.249519	0.512142	Biso	1.000000	O
O	1.0	0.188479	0.248356	0.848228	Biso	1.000000	O
O	1.0	0.188253	0.749275	0.181595	Biso	1.000000	O
O	1.0	0.187823	0.750876	0.513862	Biso	1.000000	O
O	1.0	0.188332	0.749450	0.848632	Biso	1.000000	O
O	1.0	0.812063	0.250748	0.152222	Biso	1.000000	O
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O	1.0	0.811641	0.250874	0.817915	Biso	1.000000	O
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O	1.0	0.688531	0.000833	0.485111	Biso	1.000000	O
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O	1.0	0.688771	0.500675	0.151784	Biso	1.000000	O
O	1.0	0.688213	0.500685	0.484986	Biso	1.000000	O
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O	1.0	0.310945	0.498644	0.181938	Biso	1.000000	O
O	1.0	0.311599	0.499625	0.515056	Biso	1.000000	O
O	1.0	0.311196	0.498870	0.848093	Biso	1.000000	O
O	1.0	0.311581	0.997237	0.180869	Biso	1.000000	O
O	1.0	0.311504	0.998736	0.515315	Biso	1.000000	O
O	1.0	0.311422	0.999461	0.848528	Biso	1.000000	O
O	1.0	0.812061	0.499039	0.318476	Biso	1.000000	O
O	1.0	0.811243	0.499327	0.651892	Biso	1.000000	O
O	1.0	0.811433	0.499054	0.984897	Biso	1.000000	O
O	1.0	0.810862	0.998602	0.318476	Biso	1.000000	O
O	1.0	0.811453	0.998990	0.651703	Biso	1.000000	O
O	1.0	0.811754	0.999413	0.985285	Biso	1.000000	O
O	1.0	0.189140	0.001698	0.015866	Biso	1.000000	O
O	1.0	0.186662	0.001573	0.345836	Biso	1.000000	O
O	1.0	0.188531	0.001585	0.681489	Biso	1.000000	O
O	1.0	0.187415	0.499047	0.017464	Biso	1.000000	O
O	1.0	0.191070	0.505382	0.351916	Biso	1.000000	O
O	1.0	0.188460	0.500816	0.681216	Biso	1.000000	O
O	1.0	0.431963	0.240821	0.229966	Biso	1.000000	O
O	1.0	0.432191	0.240977	0.562884	Biso	1.000000	O
O	1.0	0.431960	0.240978	0.896529	Biso	1.000000	O
O	1.0	0.432617	0.741006	0.229378	Biso	1.000000	O
O	1.0	0.432141	0.741460	0.562973	Biso	1.000000	O
O	1.0	0.432301	0.741114	0.896328	Biso	1.000000	O
O	1.0	0.567246	0.258594	0.103861	Biso	1.000000	O
O	1.0	0.567631	0.258411	0.437075	Biso	1.000000	O
O	1.0	0.567379	0.258667	0.770482	Biso	1.000000	O
O	1.0	0.567706	0.758475	0.103749	Biso	1.000000	O
O	1.0	0.567400	0.758580	0.437113	Biso	1.000000	O
O	1.0	0.567443	0.758730	0.770566	Biso	1.000000	O
O	1.0	0.067790	0.259573	0.063524	Biso	1.000000	O
O	1.0	0.056776	0.251110	0.404505	Biso	1.000000	O
O	1.0	0.067609	0.259317	0.728281	Biso	1.000000	O
O	1.0	0.067958	0.759823	0.063532	Biso	1.000000	O
O	1.0	0.067659	0.759169	0.396282	Biso	1.000000	O
O	1.0	0.067771	0.759206	0.729870	Biso	1.000000	O
O	1.0	0.934690	0.240082	0.269601	Biso	1.000000	O
O	1.0	0.932798	0.240476	0.602716	Biso	1.000000	O
O	1.0	0.932335	0.241218	0.936816	Biso	1.000000	O
O	1.0	0.932781	0.742218	0.270070	Biso	1.000000	O
O	1.0	0.932399	0.741985	0.603807	Biso	1.000000	O
O	1.0	0.932619	0.741585	0.937194	Biso	1.000000	O
O	1.0	0.567579	0.491068	0.270376	Biso	1.000000	O
O	1.0	0.567534	0.491243	0.603626	Biso	1.000000	O
O	1.0	0.567346	0.491162	0.937181	Biso	1.000000	O
O	1.0	0.567547	0.991092	0.270332	Biso	1.000000	O
O	1.0	0.567621	0.991246	0.603779	Biso	1.000000	O
O	1.0	0.567617	0.991186	0.937172	Biso	1.000000	O
O	1.0	0.432571	0.008599	0.062999	Biso	1.000000	O
O	1.0	0.432967	0.008422	0.396422	Biso	1.000000	O
O	1.0	0.432548	0.008687	0.729814	Biso	1.000000	O
O	1.0	0.431933	0.508729	0.062918	Biso	1.000000	O
O	1.0	0.433350	0.508802	0.396417	Biso	1.000000	O
O	1.0	0.432247	0.508845	0.729662	Biso	1.000000	O
O	1.0	0.932891	0.008736	0.104281	Biso	1.000000	O
O	1.0	0.933477	0.006161	0.436893	Biso	1.000000	O
O	1.0	0.932593	0.008651	0.770629	Biso	1.000000	O
O	1.0	0.932458	0.508843	0.103631	Biso	1.000000	O
O	1.0	0.932244	0.509940	0.437416	Biso	1.000000	O
O	1.0	0.932121	0.509385	0.770187	Biso	1.000000	O

O	1.0	0.067868	0.492543	0.233509	Biso	1.000000	O
O	1.0	0.067158	0.492303	0.563326	Biso	1.000000	O
O	1.0	0.067267	0.491580	0.895163	Biso	1.000000	O
O	1.0	0.069669	0.993086	0.232678	Biso	1.000000	O
O	1.0	0.067231	0.991597	0.563101	Biso	1.000000	O
O	1.0	0.067898	0.991673	0.896362	Biso	1.000000	O
O	1.0	0.305928	0.107475	0.279133	Biso	1.000000	O
O	1.0	0.302822	0.110170	0.612516	Biso	1.000000	O
O	1.0	0.302117	0.110635	0.945858	Biso	1.000000	O
O	1.0	0.303236	0.610792	0.278454	Biso	1.000000	O
O	1.0	0.303117	0.610754	0.612113	Biso	1.000000	O
O	1.0	0.302703	0.609858	0.945504	Biso	1.000000	O
O	1.0	0.697040	0.389640	0.054549	Biso	1.000000	O
O	1.0	0.697426	0.389419	0.387611	Biso	1.000000	O
O	1.0	0.696863	0.389655	0.720969	Biso	1.000000	O
O	1.0	0.697105	0.889619	0.054730	Biso	1.000000	O
O	1.0	0.696989	0.889424	0.388130	Biso	1.000000	O
O	1.0	0.696921	0.889689	0.721473	Biso	1.000000	O
O	1.0	0.195372	0.382375	0.108557	Biso	1.000000	O
O	1.0	0.198058	0.391593	0.445172	Biso	1.000000	O
O	1.0	0.196719	0.388817	0.777340	Biso	1.000000	O
O	1.0	0.196913	0.889788	0.111856	Biso	1.000000	O
O	1.0	0.196910	0.892297	0.445056	Biso	1.000000	O
O	1.0	0.196826	0.889886	0.778518	Biso	1.000000	O
O	1.0	0.802842	0.109809	0.221054	Biso	1.000000	O
O	1.0	0.803174	0.110118	0.554425	Biso	1.000000	O
O	1.0	0.803189	0.110431	0.887839	Biso	1.000000	O
O	1.0	0.803407	0.610506	0.221302	Biso	1.000000	O
O	1.0	0.803065	0.610575	0.554633	Biso	1.000000	O
O	1.0	0.803058	0.610394	0.887872	Biso	1.000000	O
O	1.0	0.697230	0.360095	0.221165	Biso	1.000000	O
O	1.0	0.696922	0.360089	0.554295	Biso	1.000000	O
O	1.0	0.696737	0.360307	0.887723	Biso	1.000000	O
O	1.0	0.697071	0.860319	0.221385	Biso	1.000000	O
O	1.0	0.696880	0.860362	0.554802	Biso	1.000000	O
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O	1.0	0.301559	0.138760	0.113068	Biso	1.000000	O
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O	1.0	0.551675	0.402270	0.465494	Biso	1.000000	O
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model 12

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CRYSTAL DATA

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Mg	1.0	0.876860	0.006542	0.880281	Biso	1.000000	Mg
Mg	1.0	0.878155	0.504947	0.214293	Biso	1.000000	Mg
Mg	1.0	0.876498	0.506305	0.546526	Biso	1.000000	Mg
Mg	1.0	0.876125	0.506217	0.879659	Biso	1.000000	Mg
Mg	1.0	0.121287	0.492649	0.121785	Biso	1.000000	Mg
Mg	1.0	0.123369	0.494198	0.453991	Biso	1.000000	Mg
Mg	1.0	0.123215	0.493099	0.785387	Biso	1.000000	Mg
Mg	1.0	0.123304	0.994870	0.120532	Biso	1.000000	Mg
Mg	1.0	0.122579	0.993032	0.452005	Biso	1.000000	Mg
Mg	1.0	0.123494	0.993662	0.786800	Biso	1.000000	Mg
O	1.0	0.182944	0.171564	0.014559	Biso	1.000000	O
O	1.0	0.183936	0.167222	0.349642	Biso	1.000000	O
O	1.0	0.182815	0.171170	0.677445	Biso	1.000000	O
O	1.0	0.183150	0.669384	0.011851	Biso	1.000000	O
O	1.0	0.183282	0.670991	0.345250	Biso	1.000000	O
O	1.0	0.183257	0.669845	0.678803	Biso	1.000000	O
O	1.0	0.817144	0.329687	0.321307	Biso	1.000000	O
O	1.0	0.816765	0.329711	0.654634	Biso	1.000000	O
O	1.0	0.816633	0.329575	0.987873	Biso	1.000000	O
O	1.0	0.816882	0.829860	0.321508	Biso	1.000000	O
O	1.0	0.816915	0.830087	0.654786	Biso	1.000000	O
O	1.0	0.816835	0.829822	0.988135	Biso	1.000000	O
O	1.0	0.316662	0.329460	0.178809	Biso	1.000000	O
O	1.0	0.316156	0.327615	0.511092	Biso	1.000000	O
O	1.0	0.316813	0.329314	0.844665	Biso	1.000000	O
O	1.0	0.316600	0.829883	0.178511	Biso	1.000000	O
O	1.0	0.316497	0.830250	0.511874	Biso	1.000000	O
O	1.0	0.316444	0.829997	0.845232	Biso	1.000000	O
O	1.0	0.683240	0.170074	0.154882	Biso	1.000000	O
O	1.0	0.683448	0.170063	0.488210	Biso	1.000000	O
O	1.0	0.683268	0.170066	0.821436	Biso	1.000000	O
O	1.0	0.683490	0.670054	0.154772	Biso	1.000000	O
O	1.0	0.683508	0.670299	0.488179	Biso	1.000000	O
O	1.0	0.683332	0.670207	0.821473	Biso	1.000000	O
O	1.0	0.817155	0.420079	0.154965	Biso	1.000000	O
O	1.0	0.816935	0.420182	0.488127	Biso	1.000000	O
O	1.0	0.816515	0.420106	0.821208	Biso	1.000000	O
O	1.0	0.816808	0.920229	0.154967	Biso	1.000000	O

O	1.0	0.817025	0.920469	0.488009	Biso	1.000000	O
O	1.0	0.816915	0.920381	0.821434	Biso	1.000000	O
O	1.0	0.183729	0.080600	0.178460	Biso	1.000000	O
O	1.0	0.182922	0.083377	0.510081	Biso	1.000000	O
O	1.0	0.182910	0.079911	0.845389	Biso	1.000000	O
O	1.0	0.182998	0.579276	0.178924	Biso	1.000000	O
O	1.0	0.183147	0.580560	0.512895	Biso	1.000000	O
O	1.0	0.183206	0.578997	0.844968	Biso	1.000000	O
O	1.0	0.683327	0.079640	0.321540	Biso	1.000000	O
O	1.0	0.683471	0.079704	0.654847	Biso	1.000000	O
O	1.0	0.683163	0.079720	0.988126	Biso	1.000000	O
O	1.0	0.683858	0.579721	0.321436	Biso	1.000000	O
O	1.0	0.683328	0.580035	0.654831	Biso	1.000000	O
O	1.0	0.683334	0.579838	0.988125	Biso	1.000000	O
O	1.0	0.316192	0.419673	0.011770	Biso	1.000000	O
O	1.0	0.318529	0.421811	0.346592	Biso	1.000000	O
O	1.0	0.316394	0.419162	0.677411	Biso	1.000000	O
O	1.0	0.316447	0.920177	0.011995	Biso	1.000000	O
O	1.0	0.316210	0.920695	0.345205	Biso	1.000000	O
O	1.0	0.316629	0.920233	0.678595	Biso	1.000000	O
O	1.0	0.562900	0.170337	0.266439	Biso	1.000000	O
O	1.0	0.562941	0.170079	0.599761	Biso	1.000000	O
O	1.0	0.562741	0.170143	0.933019	Biso	1.000000	O
O	1.0	0.562996	0.670218	0.266211	Biso	1.000000	O
O	1.0	0.562864	0.670532	0.599732	Biso	1.000000	O
O	1.0	0.562718	0.670205	0.932937	Biso	1.000000	O
O	1.0	0.437179	0.329885	0.067061	Biso	1.000000	O
O	1.0	0.437635	0.329833	0.400408	Biso	1.000000	O
O	1.0	0.437211	0.329700	0.733426	Biso	1.000000	O
O	1.0	0.437050	0.829643	0.067035	Biso	1.000000	O
O	1.0	0.437046	0.829962	0.400417	Biso	1.000000	O
O	1.0	0.437007	0.829822	0.733759	Biso	1.000000	O
O	1.0	0.936598	0.329678	0.097817	Biso	1.000000	O
O	1.0	0.937045	0.329748	0.433712	Biso	1.000000	O
O	1.0	0.936812	0.329758	0.765910	Biso	1.000000	O
O	1.0	0.937280	0.829667	0.099654	Biso	1.000000	O
O	1.0	0.937227	0.829862	0.433036	Biso	1.000000	O
O	1.0	0.937294	0.830011	0.766176	Biso	1.000000	O
O	1.0	0.062233	0.162608	0.230112	Biso	1.000000	O
O	1.0	0.063604	0.169736	0.564194	Biso	1.000000	O
O	1.0	0.062796	0.170172	0.900263	Biso	1.000000	O
O	1.0	0.062849	0.670314	0.233813	Biso	1.000000	O
O	1.0	0.062767	0.670567	0.567136	Biso	1.000000	O
O	1.0	0.062927	0.669931	0.900508	Biso	1.000000	O
O	1.0	0.437515	0.420330	0.233480	Biso	1.000000	O
O	1.0	0.437168	0.420021	0.567009	Biso	1.000000	O
O	1.0	0.437000	0.420084	0.900262	Biso	1.000000	O
O	1.0	0.437107	0.920171	0.233803	Biso	1.000000	O
O	1.0	0.436905	0.920600	0.566928	Biso	1.000000	O
O	1.0	0.437018	0.920194	0.900470	Biso	1.000000	O
O	1.0	0.562718	0.079724	0.099747	Biso	1.000000	O
O	1.0	0.562705	0.079689	0.433084	Biso	1.000000	O
O	1.0	0.562700	0.079691	0.766374	Biso	1.000000	O
O	1.0	0.562794	0.579568	0.099649	Biso	1.000000	O
O	1.0	0.563406	0.580220	0.432974	Biso	1.000000	O
O	1.0	0.562639	0.579655	0.766281	Biso	1.000000	O
O	1.0	0.062145	0.079586	0.066136	Biso	1.000000	O
O	1.0	0.063200	0.083521	0.402833	Biso	1.000000	O
O	1.0	0.063180	0.080029	0.733404	Biso	1.000000	O
O	1.0	0.062698	0.579242	0.067365	Biso	1.000000	O
O	1.0	0.062932	0.580220	0.401151	Biso	1.000000	O
O	1.0	0.062863	0.579754	0.733451	Biso	1.000000	O
O	1.0	0.938450	0.419322	0.267622	Biso	1.000000	O
O	1.0	0.937033	0.420376	0.599713	Biso	1.000000	O
O	1.0	0.936726	0.420355	0.931734	Biso	1.000000	O
O	1.0	0.937319	0.920034	0.266303	Biso	1.000000	O
O	1.0	0.937602	0.920809	0.599611	Biso	1.000000	O
O	1.0	0.937209	0.920230	0.932964	Biso	1.000000	O
O	1.0	0.311259	0.251162	0.015246	Biso	1.000000	O
O	1.0	0.311043	0.251214	0.348241	Biso	1.000000	O
O	1.0	0.311375	0.250863	0.681622	Biso	1.000000	O
O	1.0	0.311231	0.750354	0.014812	Biso	1.000000	O
O	1.0	0.311568	0.750916	0.348320	Biso	1.000000	O
O	1.0	0.311254	0.750843	0.681628	Biso	1.000000	O
O	1.0	0.688793	0.249156	0.318480	Biso	1.000000	O
O	1.0	0.688631	0.249045	0.651811	Biso	1.000000	O
O	1.0	0.688375	0.249082	0.985072	Biso	1.000000	O
O	1.0	0.688711	0.749149	0.318485	Biso	1.000000	O
O	1.0	0.688694	0.749304	0.651853	Biso	1.000000	O

O	1.0	0.688599	0.749119	0.985061	Biso	1.000000	O
O	1.0	0.191039	0.248095	0.190658	Biso	1.000000	O
O	1.0	0.186016	0.248174	0.510987	Biso	1.000000	O
O	1.0	0.188764	0.247933	0.847975	Biso	1.000000	O
O	1.0	0.188519	0.749018	0.181441	Biso	1.000000	O
O	1.0	0.188398	0.749433	0.515143	Biso	1.000000	O
O	1.0	0.188330	0.749219	0.848378	Biso	1.000000	O
O	1.0	0.811270	0.251017	0.151835	Biso	1.000000	O
O	1.0	0.811760	0.250819	0.485054	Biso	1.000000	O
O	1.0	0.811364	0.250901	0.818168	Biso	1.000000	O
O	1.0	0.811563	0.750901	0.151633	Biso	1.000000	O
O	1.0	0.811606	0.751059	0.485036	Biso	1.000000	O
O	1.0	0.811614	0.750950	0.818356	Biso	1.000000	O
O	1.0	0.688507	0.000808	0.151818	Biso	1.000000	O
O	1.0	0.688675	0.000946	0.485140	Biso	1.000000	O
O	1.0	0.688588	0.000949	0.818514	Biso	1.000000	O
O	1.0	0.688864	0.500821	0.151728	Biso	1.000000	O
O	1.0	0.688744	0.500824	0.485262	Biso	1.000000	O
O	1.0	0.688455	0.500853	0.818374	Biso	1.000000	O
O	1.0	0.311118	0.498531	0.181916	Biso	1.000000	O
O	1.0	0.311321	0.499007	0.514970	Biso	1.000000	O
O	1.0	0.311179	0.498540	0.847774	Biso	1.000000	O
O	1.0	0.311695	0.999511	0.181828	Biso	1.000000	O
O	1.0	0.309992	0.999423	0.515172	Biso	1.000000	O
O	1.0	0.311272	0.999395	0.848526	Biso	1.000000	O
O	1.0	0.812335	0.499081	0.318735	Biso	1.000000	O
O	1.0	0.811374	0.499130	0.651560	Biso	1.000000	O
O	1.0	0.811499	0.499026	0.984963	Biso	1.000000	O
O	1.0	0.811888	0.999187	0.318829	Biso	1.000000	O
O	1.0	0.811976	0.999252	0.651552	Biso	1.000000	O
O	1.0	0.811407	0.999045	0.984958	Biso	1.000000	O
O	1.0	0.188349	0.001198	0.015173	Biso	1.000000	O
O	1.0	0.187338	0.001123	0.347931	Biso	1.000000	O
O	1.0	0.188779	0.001333	0.681261	Biso	1.000000	O
O	1.0	0.187522	0.499082	0.017043	Biso	1.000000	O
O	1.0	0.191094	0.505318	0.352700	Biso	1.000000	O
O	1.0	0.187884	0.498930	0.679698	Biso	1.000000	O
O	1.0	0.432484	0.241476	0.229915	Biso	1.000000	O
O	1.0	0.432846	0.241276	0.563043	Biso	1.000000	O
O	1.0	0.432382	0.241159	0.896363	Biso	1.000000	O
O	1.0	0.432476	0.741189	0.229491	Biso	1.000000	O
O	1.0	0.432309	0.741355	0.562998	Biso	1.000000	O
O	1.0	0.432218	0.741130	0.896311	Biso	1.000000	O
O	1.0	0.567435	0.258707	0.103827	Biso	1.000000	O
O	1.0	0.567797	0.258738	0.437087	Biso	1.000000	O
O	1.0	0.567477	0.258704	0.770389	Biso	1.000000	O
O	1.0	0.567562	0.758678	0.103740	Biso	1.000000	O
O	1.0	0.567557	0.758861	0.437106	Biso	1.000000	O
O	1.0	0.567475	0.758850	0.770408	Biso	1.000000	O
O	1.0	0.067941	0.259521	0.062313	Biso	1.000000	O
O	1.0	0.060958	0.248562	0.408288	Biso	1.000000	O
O	1.0	0.066982	0.258531	0.728906	Biso	1.000000	O
O	1.0	0.067711	0.758532	0.063211	Biso	1.000000	O
O	1.0	0.067631	0.759103	0.396327	Biso	1.000000	O
O	1.0	0.067733	0.758922	0.729739	Biso	1.000000	O
O	1.0	0.933078	0.240730	0.269868	Biso	1.000000	O
O	1.0	0.933417	0.241651	0.603944	Biso	1.000000	O
O	1.0	0.932297	0.241153	0.936701	Biso	1.000000	O
O	1.0	0.932443	0.741251	0.270311	Biso	1.000000	O
O	1.0	0.932429	0.741503	0.603691	Biso	1.000000	O
O	1.0	0.932532	0.741216	0.936957	Biso	1.000000	O
O	1.0	0.567870	0.491295	0.270398	Biso	1.000000	O
O	1.0	0.567400	0.491413	0.603718	Biso	1.000000	O
O	1.0	0.567414	0.491201	0.937152	Biso	1.000000	O
O	1.0	0.567358	0.991312	0.270464	Biso	1.000000	O
O	1.0	0.567425	0.991390	0.603792	Biso	1.000000	O
O	1.0	0.567365	0.991250	0.937144	Biso	1.000000	O
O	1.0	0.432244	0.008873	0.063126	Biso	1.000000	O
O	1.0	0.431821	0.009150	0.396648	Biso	1.000000	O
O	1.0	0.432154	0.008871	0.729719	Biso	1.000000	O
O	1.0	0.432126	0.508785	0.062866	Biso	1.000000	O
O	1.0	0.433527	0.508942	0.396371	Biso	1.000000	O
O	1.0	0.432020	0.508742	0.729539	Biso	1.000000	O
O	1.0	0.932264	0.008710	0.103640	Biso	1.000000	O
O	1.0	0.934519	0.008054	0.437119	Biso	1.000000	O
O	1.0	0.932659	0.009063	0.770199	Biso	1.000000	O
O	1.0	0.932605	0.508431	0.103733	Biso	1.000000	O
O	1.0	0.932895	0.508797	0.437346	Biso	1.000000	O
O	1.0	0.932225	0.508893	0.770053	Biso	1.000000	O

O	1.0	0.068380	0.491455	0.234249	Biso	1.000000	O
O	1.0	0.067273	0.491439	0.563036	Biso	1.000000	O
O	1.0	0.067414	0.491313	0.894820	Biso	1.000000	O
O	1.0	0.067940	0.990954	0.230272	Biso	1.000000	O
O	1.0	0.068540	0.991348	0.562781	Biso	1.000000	O
O	1.0	0.067593	0.991157	0.896257	Biso	1.000000	O
O	1.0	0.302844	0.110827	0.279386	Biso	1.000000	O
O	1.0	0.302433	0.110411	0.612754	Biso	1.000000	O
O	1.0	0.302245	0.110588	0.945986	Biso	1.000000	O
O	1.0	0.303146	0.610613	0.278408	Biso	1.000000	O
O	1.0	0.303169	0.610209	0.612146	Biso	1.000000	O
O	1.0	0.302797	0.609576	0.945393	Biso	1.000000	O
O	1.0	0.697132	0.389618	0.054647	Biso	1.000000	O
O	1.0	0.697261	0.389671	0.387784	Biso	1.000000	O
O	1.0	0.696856	0.389605	0.721118	Biso	1.000000	O
O	1.0	0.697022	0.889587	0.054660	Biso	1.000000	O
O	1.0	0.697108	0.889696	0.387970	Biso	1.000000	O
O	1.0	0.697091	0.889822	0.721292	Biso	1.000000	O
O	1.0	0.195659	0.382584	0.107972	Biso	1.000000	O
O	1.0	0.197558	0.390051	0.444014	Biso	1.000000	O
O	1.0	0.196620	0.387297	0.776239	Biso	1.000000	O
O	1.0	0.196799	0.889764	0.112249	Biso	1.000000	O
O	1.0	0.196608	0.890047	0.445418	Biso	1.000000	O
O	1.0	0.196769	0.890000	0.778797	Biso	1.000000	O
O	1.0	0.802865	0.110104	0.221127	Biso	1.000000	O
O	1.0	0.803282	0.110349	0.554517	Biso	1.000000	O
O	1.0	0.803003	0.110332	0.887842	Biso	1.000000	O
O	1.0	0.803452	0.610444	0.221295	Biso	1.000000	O
O	1.0	0.803218	0.610491	0.554593	Biso	1.000000	O
O	1.0	0.803106	0.610363	0.887879	Biso	1.000000	O
O	1.0	0.697144	0.360373	0.221254	Biso	1.000000	O
O	1.0	0.697072	0.360232	0.554438	Biso	1.000000	O
O	1.0	0.696765	0.360301	0.887905	Biso	1.000000	O
O	1.0	0.697010	0.860354	0.221324	Biso	1.000000	O
O	1.0	0.697201	0.860512	0.554597	Biso	1.000000	O
O	1.0	0.697095	0.860423	0.887947	Biso	1.000000	O
O	1.0	0.303329	0.140450	0.112865	Biso	1.000000	O
O	1.0	0.305294	0.140529	0.446880	Biso	1.000000	O
O	1.0	0.302500	0.139767	0.779059	Biso	1.000000	O
O	1.0	0.302896	0.638986	0.111975	Biso	1.000000	O
O	1.0	0.302997	0.639620	0.445372	Biso	1.000000	O
O	1.0	0.302965	0.639451	0.778810	Biso	1.000000	O
O	1.0	0.802724	0.139635	0.054475	Biso	1.000000	O
O	1.0	0.802992	0.139591	0.387833	Biso	1.000000	O
O	1.0	0.803243	0.139632	0.721159	Biso	1.000000	O
O	1.0	0.803210	0.639627	0.054510	Biso	1.000000	O
O	1.0	0.803380	0.639717	0.387937	Biso	1.000000	O
O	1.0	0.803166	0.639679	0.721255	Biso	1.000000	O
O	1.0	0.199035	0.371695	0.274704	Biso	1.000000	O
O	1.0	0.196994	0.357474	0.610030	Biso	1.000000	O
O	1.0	0.196529	0.360618	0.942646	Biso	1.000000	O
O	1.0	0.196781	0.860349	0.278755	Biso	1.000000	O
O	1.0	0.196757	0.860665	0.612145	Biso	1.000000	O
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model 13

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CRYSTAL DATA

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O	1.0	0.816817	0.329900	0.321553	Biso	1.000000	O
O	1.0	0.816900	0.329770	0.654914	Biso	1.000000	O
O	1.0	0.816603	0.330004	0.988174	Biso	1.000000	O
O	1.0	0.816818	0.830004	0.321392	Biso	1.000000	O
O	1.0	0.816807	0.829860	0.654705	Biso	1.000000	O
O	1.0	0.816727	0.829879	0.988113	Biso	1.000000	O
O	1.0	0.316234	0.329504	0.178180	Biso	1.000000	O
O	1.0	0.316468	0.330006	0.512241	Biso	1.000000	O
O	1.0	0.317122	0.329842	0.845644	Biso	1.000000	O
O	1.0	0.316630	0.830116	0.178484	Biso	1.000000	O
O	1.0	0.316652	0.829525	0.511565	Biso	1.000000	O
O	1.0	0.316680	0.828740	0.844933	Biso	1.000000	O
O	1.0	0.683346	0.169984	0.154793	Biso	1.000000	O
O	1.0	0.683500	0.170174	0.488191	Biso	1.000000	O
O	1.0	0.683206	0.169967	0.821419	Biso	1.000000	O
O	1.0	0.683394	0.670281	0.154911	Biso	1.000000	O
O	1.0	0.683381	0.670158	0.488206	Biso	1.000000	O
O	1.0	0.683467	0.670166	0.821478	Biso	1.000000	O
O	1.0	0.816602	0.420336	0.154973	Biso	1.000000	O
O	1.0	0.816822	0.420179	0.488279	Biso	1.000000	O
O	1.0	0.816819	0.420107	0.821580	Biso	1.000000	O

O	1.0	0.816519	0.920038	0.154827	Biso	1.000000	O
O	1.0	0.816924	0.920201	0.488047	Biso	1.000000	O
O	1.0	0.816780	0.919991	0.821338	Biso	1.000000	O
O	1.0	0.185126	0.081115	0.178905	Biso	1.000000	O
O	1.0	0.183194	0.079910	0.511812	Biso	1.000000	O
O	1.0	0.183822	0.079056	0.844469	Biso	1.000000	O
O	1.0	0.183163	0.579729	0.178382	Biso	1.000000	O
O	1.0	0.183095	0.579817	0.511967	Biso	1.000000	O
O	1.0	0.183078	0.579955	0.845154	Biso	1.000000	O
O	1.0	0.683377	0.079828	0.321447	Biso	1.000000	O
O	1.0	0.683413	0.079777	0.654619	Biso	1.000000	O
O	1.0	0.683082	0.079912	0.988061	Biso	1.000000	O
O	1.0	0.683317	0.579927	0.321595	Biso	1.000000	O
O	1.0	0.683444	0.579906	0.654846	Biso	1.000000	O
O	1.0	0.683589	0.580156	0.988228	Biso	1.000000	O
O	1.0	0.317476	0.420966	0.012071	Biso	1.000000	O
O	1.0	0.316638	0.420297	0.345392	Biso	1.000000	O
O	1.0	0.316514	0.420343	0.678747	Biso	1.000000	O
O	1.0	0.316596	0.919867	0.011549	Biso	1.000000	O
O	1.0	0.316633	0.919784	0.345363	Biso	1.000000	O
O	1.0	0.316762	0.919209	0.677289	Biso	1.000000	O
O	1.0	0.562327	0.170145	0.266571	Biso	1.000000	O
O	1.0	0.562953	0.170284	0.599559	Biso	1.000000	O
O	1.0	0.562701	0.170345	0.933102	Biso	1.000000	O
O	1.0	0.562804	0.670329	0.266366	Biso	1.000000	O
O	1.0	0.562867	0.670169	0.599677	Biso	1.000000	O
O	1.0	0.562996	0.670213	0.932967	Biso	1.000000	O
O	1.0	0.436963	0.328462	0.067274	Biso	1.000000	O
O	1.0	0.437140	0.329908	0.400826	Biso	1.000000	O
O	1.0	0.437134	0.329698	0.734230	Biso	1.000000	O
O	1.0	0.437173	0.829849	0.066929	Biso	1.000000	O
O	1.0	0.437260	0.829610	0.400229	Biso	1.000000	O
O	1.0	0.437377	0.829195	0.733342	Biso	1.000000	O
O	1.0	0.936432	0.330803	0.099729	Biso	1.000000	O
O	1.0	0.937200	0.329904	0.433003	Biso	1.000000	O
O	1.0	0.937317	0.329665	0.766578	Biso	1.000000	O
O	1.0	0.937125	0.829868	0.099656	Biso	1.000000	O
O	1.0	0.937195	0.829884	0.432824	Biso	1.000000	O
O	1.0	0.937152	0.829725	0.766192	Biso	1.000000	O
O	1.0	0.062796	0.170186	0.233316	Biso	1.000000	O
O	1.0	0.062712	0.170121	0.566975	Biso	1.000000	O
O	1.0	0.060898	0.169296	0.897648	Biso	1.000000	O
O	1.0	0.062808	0.670349	0.233680	Biso	1.000000	O
O	1.0	0.062773	0.670268	0.567019	Biso	1.000000	O
O	1.0	0.062613	0.670418	0.900306	Biso	1.000000	O
O	1.0	0.437013	0.420241	0.233993	Biso	1.000000	O
O	1.0	0.437141	0.420306	0.567330	Biso	1.000000	O
O	1.0	0.438007	0.421323	0.899959	Biso	1.000000	O
O	1.0	0.437219	0.920208	0.233705	Biso	1.000000	O
O	1.0	0.437295	0.919987	0.566871	Biso	1.000000	O
O	1.0	0.437085	0.919947	0.899976	Biso	1.000000	O
O	1.0	0.562349	0.080046	0.099318	Biso	1.000000	O
O	1.0	0.563059	0.079641	0.433077	Biso	1.000000	O
O	1.0	0.563318	0.079610	0.765795	Biso	1.000000	O
O	1.0	0.563083	0.579942	0.099711	Biso	1.000000	O
O	1.0	0.562849	0.579755	0.433043	Biso	1.000000	O
O	1.0	0.562913	0.579691	0.766435	Biso	1.000000	O
O	1.0	0.061819	0.078340	0.067310	Biso	1.000000	O
O	1.0	0.062952	0.080089	0.400120	Biso	1.000000	O
O	1.0	0.062464	0.079631	0.733368	Biso	1.000000	O
O	1.0	0.062574	0.580164	0.066939	Biso	1.000000	O
O	1.0	0.062706	0.579917	0.400419	Biso	1.000000	O
O	1.0	0.062651	0.580000	0.733753	Biso	1.000000	O
O	1.0	0.937059	0.420559	0.266501	Biso	1.000000	O
O	1.0	0.937225	0.420178	0.599828	Biso	1.000000	O
O	1.0	0.937179	0.420239	0.933064	Biso	1.000000	O
O	1.0	0.937398	0.920589	0.266183	Biso	1.000000	O
O	1.0	0.937167	0.920126	0.599459	Biso	1.000000	O
O	1.0	0.937067	0.920202	0.932842	Biso	1.000000	O
O	1.0	0.309572	0.255091	0.012321	Biso	1.000000	O
O	1.0	0.311551	0.250988	0.348155	Biso	1.000000	O
O	1.0	0.311195	0.250609	0.681616	Biso	1.000000	O
O	1.0	0.311402	0.751003	0.014929	Biso	1.000000	O
O	1.0	0.311376	0.750788	0.348020	Biso	1.000000	O
O	1.0	0.311430	0.750589	0.681285	Biso	1.000000	O
O	1.0	0.688767	0.249066	0.318680	Biso	1.000000	O
O	1.0	0.688640	0.249099	0.651968	Biso	1.000000	O
O	1.0	0.688490	0.249176	0.985149	Biso	1.000000	O
O	1.0	0.688739	0.749121	0.318493	Biso	1.000000	O

O	1.0	0.688723	0.749079	0.651683	Biso	1.000000	O
O	1.0	0.688708	0.749063	0.985089	Biso	1.000000	O
O	1.0	0.187201	0.251212	0.180215	Biso	1.000000	O
O	1.0	0.188001	0.249594	0.515129	Biso	1.000000	O
O	1.0	0.187866	0.249847	0.848457	Biso	1.000000	O
O	1.0	0.188542	0.749195	0.181568	Biso	1.000000	O
O	1.0	0.188531	0.748760	0.514728	Biso	1.000000	O
O	1.0	0.188300	0.748920	0.848444	Biso	1.000000	O
O	1.0	0.811398	0.250840	0.151562	Biso	1.000000	O
O	1.0	0.811669	0.250903	0.484940	Biso	1.000000	O
O	1.0	0.811075	0.251014	0.818129	Biso	1.000000	O
O	1.0	0.811552	0.751044	0.151840	Biso	1.000000	O
O	1.0	0.811539	0.750987	0.485012	Biso	1.000000	O
O	1.0	0.811540	0.751029	0.818285	Biso	1.000000	O
O	1.0	0.688403	0.000915	0.151605	Biso	1.000000	O
O	1.0	0.688809	0.000944	0.485068	Biso	1.000000	O
O	1.0	0.688732	0.000824	0.818377	Biso	1.000000	O
O	1.0	0.688565	0.500966	0.152087	Biso	1.000000	O
O	1.0	0.688663	0.500912	0.485273	Biso	1.000000	O
O	1.0	0.688820	0.501009	0.818437	Biso	1.000000	O
O	1.0	0.311481	0.499151	0.181357	Biso	1.000000	O
O	1.0	0.311304	0.499032	0.514756	Biso	1.000000	O
O	1.0	0.311443	0.499199	0.848654	Biso	1.000000	O
O	1.0	0.311956	0.999832	0.182151	Biso	1.000000	O
O	1.0	0.311443	0.999281	0.514253	Biso	1.000000	O
O	1.0	0.310239	0.995110	0.843090	Biso	1.000000	O
O	1.0	0.811434	0.499152	0.318469	Biso	1.000000	O
O	1.0	0.811613	0.499130	0.651777	Biso	1.000000	O
O	1.0	0.811571	0.499269	0.985020	Biso	1.000000	O
O	1.0	0.811503	0.999079	0.318380	Biso	1.000000	O
O	1.0	0.811545	0.999035	0.651533	Biso	1.000000	O
O	1.0	0.810972	0.998832	0.984648	Biso	1.000000	O
O	1.0	0.188934	0.001240	0.014957	Biso	1.000000	O
O	1.0	0.188343	0.000752	0.348506	Biso	1.000000	O
O	1.0	0.188342	0.000299	0.681065	Biso	1.000000	O
O	1.0	0.188143	0.502243	0.014073	Biso	1.000000	O
O	1.0	0.188556	0.501398	0.348781	Biso	1.000000	O
O	1.0	0.188231	0.500986	0.681939	Biso	1.000000	O
O	1.0	0.433410	0.241884	0.230863	Biso	1.000000	O
O	1.0	0.432541	0.241370	0.563196	Biso	1.000000	O
O	1.0	0.431804	0.240672	0.896522	Biso	1.000000	O
O	1.0	0.432305	0.741164	0.229575	Biso	1.000000	O
O	1.0	0.432442	0.741004	0.562755	Biso	1.000000	O
O	1.0	0.432549	0.741074	0.896167	Biso	1.000000	O
O	1.0	0.567876	0.258626	0.103952	Biso	1.000000	O
O	1.0	0.567627	0.258747	0.437214	Biso	1.000000	O
O	1.0	0.567459	0.258616	0.770565	Biso	1.000000	O
O	1.0	0.567537	0.758836	0.103759	Biso	1.000000	O
O	1.0	0.567588	0.758668	0.437026	Biso	1.000000	O
O	1.0	0.567766	0.758581	0.770353	Biso	1.000000	O
O	1.0	0.065271	0.259173	0.062782	Biso	1.000000	O
O	1.0	0.067546	0.259037	0.396227	Biso	1.000000	O
O	1.0	0.067745	0.258758	0.729931	Biso	1.000000	O
O	1.0	0.067446	0.758763	0.063053	Biso	1.000000	O
O	1.0	0.067557	0.758810	0.396173	Biso	1.000000	O
O	1.0	0.067502	0.758730	0.729483	Biso	1.000000	O
O	1.0	0.932419	0.241236	0.269952	Biso	1.000000	O
O	1.0	0.932387	0.241022	0.603683	Biso	1.000000	O
O	1.0	0.931549	0.240777	0.936497	Biso	1.000000	O
O	1.0	0.932403	0.741400	0.270359	Biso	1.000000	O
O	1.0	0.932356	0.741305	0.603609	Biso	1.000000	O
O	1.0	0.932242	0.741332	0.937017	Biso	1.000000	O
O	1.0	0.567465	0.491372	0.270483	Biso	1.000000	O
O	1.0	0.567606	0.491310	0.603912	Biso	1.000000	O
O	1.0	0.568461	0.491442	0.937137	Biso	1.000000	O
O	1.0	0.567666	0.991149	0.270406	Biso	1.000000	O
O	1.0	0.567796	0.990999	0.603563	Biso	1.000000	O
O	1.0	0.567552	0.991069	0.936837	Biso	1.000000	O
O	1.0	0.432080	0.009146	0.062209	Biso	1.000000	O
O	1.0	0.432894	0.008366	0.396607	Biso	1.000000	O
O	1.0	0.433170	0.008300	0.728938	Biso	1.000000	O
O	1.0	0.433040	0.508619	0.062922	Biso	1.000000	O
O	1.0	0.432478	0.508706	0.396333	Biso	1.000000	O
O	1.0	0.432430	0.508850	0.729576	Biso	1.000000	O
O	1.0	0.931333	0.008593	0.103512	Biso	1.000000	O
O	1.0	0.932540	0.008987	0.436857	Biso	1.000000	O
O	1.0	0.932287	0.008437	0.770052	Biso	1.000000	O
O	1.0	0.932273	0.509014	0.103721	Biso	1.000000	O
O	1.0	0.932360	0.508906	0.437040	Biso	1.000000	O

O	1.0	0.932389	0.508834	0.770348	Biso	1.000000	O
O	1.0	0.067524	0.491580	0.229920	Biso	1.000000	O
O	1.0	0.067541	0.491274	0.563372	Biso	1.000000	O
O	1.0	0.067647	0.491307	0.896514	Biso	1.000000	O
O	1.0	0.068209	0.991454	0.229716	Biso	1.000000	O
O	1.0	0.067461	0.991142	0.562704	Biso	1.000000	O
O	1.0	0.067567	0.991171	0.896104	Biso	1.000000	O
O	1.0	0.303465	0.108172	0.283489	Biso	1.000000	O
O	1.0	0.303037	0.109616	0.612601	Biso	1.000000	O
O	1.0	0.307449	0.103635	0.941973	Biso	1.000000	O
O	1.0	0.302936	0.610224	0.278692	Biso	1.000000	O
O	1.0	0.302931	0.610082	0.612013	Biso	1.000000	O
O	1.0	0.302949	0.610529	0.945370	Biso	1.000000	O
O	1.0	0.696813	0.389736	0.054809	Biso	1.000000	O
O	1.0	0.697019	0.389660	0.388130	Biso	1.000000	O
O	1.0	0.697091	0.389647	0.721387	Biso	1.000000	O
O	1.0	0.696815	0.889542	0.054594	Biso	1.000000	O
O	1.0	0.697042	0.889684	0.387928	Biso	1.000000	O
O	1.0	0.696986	0.889588	0.721211	Biso	1.000000	O
O	1.0	0.198073	0.391840	0.112883	Biso	1.000000	O
O	1.0	0.196821	0.390279	0.446393	Biso	1.000000	O
O	1.0	0.197146	0.390551	0.780240	Biso	1.000000	O
O	1.0	0.196834	0.889716	0.111903	Biso	1.000000	O
O	1.0	0.196795	0.889376	0.445347	Biso	1.000000	O
O	1.0	0.196650	0.888840	0.778171	Biso	1.000000	O
O	1.0	0.803148	0.110300	0.221164	Biso	1.000000	O
O	1.0	0.803292	0.110361	0.554435	Biso	1.000000	O
O	1.0	0.802958	0.110382	0.887780	Biso	1.000000	O
O	1.0	0.803132	0.610419	0.221314	Biso	1.000000	O
O	1.0	0.803215	0.610418	0.554590	Biso	1.000000	O
O	1.0	0.803323	0.610529	0.887922	Biso	1.000000	O
O	1.0	0.696919	0.360330	0.221491	Biso	1.000000	O
O	1.0	0.697068	0.360334	0.554788	Biso	1.000000	O
O	1.0	0.696793	0.360555	0.888121	Biso	1.000000	O
O	1.0	0.696809	0.860373	0.221303	Biso	1.000000	O
O	1.0	0.697086	0.860383	0.554526	Biso	1.000000	O
O	1.0	0.696964	0.860259	0.887879	Biso	1.000000	O
O	1.0	0.307422	0.143484	0.119295	Biso	1.000000	O
O	1.0	0.302837	0.141376	0.447616	Biso	1.000000	O
O	1.0	0.303214	0.138892	0.778254	Biso	1.000000	O
O	1.0	0.302899	0.639608	0.111936	Biso	1.000000	O
O	1.0	0.302923	0.639508	0.445274	Biso	1.000000	O
O	1.0	0.302987	0.639413	0.778582	Biso	1.000000	O
O	1.0	0.802964	0.139474	0.054413	Biso	1.000000	O
O	1.0	0.803222	0.139660	0.387778	Biso	1.000000	O
O	1.0	0.802943	0.139625	0.721048	Biso	1.000000	O
O	1.0	0.803346	0.639764	0.054725	Biso	1.000000	O
O	1.0	0.803176	0.639681	0.387955	Biso	1.000000	O
O	1.0	0.803253	0.639659	0.721251	Biso	1.000000	O
O	1.0	0.196642	0.360958	0.279917	Biso	1.000000	O
O	1.0	0.196795	0.360268	0.613123	Biso	1.000000	O
O	1.0	0.200169	0.358500	0.948780	Biso	1.000000	O
O	1.0	0.196778	0.860420	0.278659	Biso	1.000000	O
O	1.0	0.196690	0.859922	0.611835	Biso	1.000000	O
O	1.0	0.196788	0.860450	0.945102	Biso	1.000000	O
O	1.0	0.448410	0.097764	0.201329	Biso	1.000000	O
O	1.0	0.448162	0.097359	0.534580	Biso	1.000000	O
O	1.0	0.448996	0.097182	0.867087	Biso	1.000000	O
O	1.0	0.448125	0.597284	0.201220	Biso	1.000000	O
O	1.0	0.448045	0.597146	0.534642	Biso	1.000000	O
O	1.0	0.448124	0.597058	0.868110	Biso	1.000000	O
O	1.0	0.551484	0.402441	0.132516	Biso	1.000000	O
O	1.0	0.552001	0.402650	0.465836	Biso	1.000000	O
O	1.0	0.552368	0.402595	0.798861	Biso	1.000000	O
O	1.0	0.551985	0.902763	0.132025	Biso	1.000000	O
O	1.0	0.552145	0.902519	0.465346	Biso	1.000000	O
O	1.0	0.552004	0.902424	0.798684	Biso	1.000000	O
O	1.0	0.051932	0.403550	0.035105	Biso	1.000000	O
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model 14

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CRYSTAL DATA

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_atom_site_fract_x
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_atom_site_B_iso_or_equiv
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O	1.0	0.682385	0.171593	0.822975	Biso	1.000000	O
O	1.0	0.683288	0.670178	0.155283	Biso	1.000000	O
O	1.0	0.683343	0.670352	0.488606	Biso	1.000000	O
O	1.0	0.683132	0.669956	0.821935	Biso	1.000000	O
O	1.0	0.816847	0.419992	0.155431	Biso	1.000000	O
O	1.0	0.817141	0.420465	0.488677	Biso	1.000000	O
O	1.0	0.817099	0.420274	0.821691	Biso	1.000000	O

O	1.0	0.816804	0.920063	0.155010	Biso	1.000000	O
O	1.0	0.816789	0.920287	0.488530	Biso	1.000000	O
O	1.0	0.816656	0.920210	0.821723	Biso	1.000000	O
O	1.0	0.183080	0.079659	0.178443	Biso	1.000000	O
O	1.0	0.183254	0.079974	0.511707	Biso	1.000000	O
O	1.0	0.182927	0.079561	0.844999	Biso	1.000000	O
O	1.0	0.183331	0.579604	0.178535	Biso	1.000000	O
O	1.0	0.183114	0.579912	0.511864	Biso	1.000000	O
O	1.0	0.182984	0.579889	0.845100	Biso	1.000000	O
O	1.0	0.683368	0.079734	0.321896	Biso	1.000000	O
O	1.0	0.683028	0.079899	0.655333	Biso	1.000000	O
O	1.0	0.683245	0.079182	0.988446	Biso	1.000000	O
O	1.0	0.683490	0.580244	0.322335	Biso	1.000000	O
O	1.0	0.683002	0.579531	0.655379	Biso	1.000000	O
O	1.0	0.682910	0.579170	0.988961	Biso	1.000000	O
O	1.0	0.315751	0.421740	0.010560	Biso	1.000000	O
O	1.0	0.316880	0.419786	0.344706	Biso	1.000000	O
O	1.0	0.316613	0.420174	0.677929	Biso	1.000000	O
O	1.0	0.316344	0.919806	0.011669	Biso	1.000000	O
O	1.0	0.316535	0.920046	0.345040	Biso	1.000000	O
O	1.0	0.316507	0.920052	0.678352	Biso	1.000000	O
O	1.0	0.563341	0.170105	0.266019	Biso	1.000000	O
O	1.0	0.562576	0.170290	0.599886	Biso	1.000000	O
O	1.0	0.562001	0.169750	0.934239	Biso	1.000000	O
O	1.0	0.562681	0.670410	0.266732	Biso	1.000000	O
O	1.0	0.562618	0.670289	0.600016	Biso	1.000000	O
O	1.0	0.562607	0.670062	0.933307	Biso	1.000000	O
O	1.0	0.431211	0.330933	0.065607	Biso	1.000000	O
O	1.0	0.437994	0.329428	0.398815	Biso	1.000000	O
O	1.0	0.437306	0.330089	0.732404	Biso	1.000000	O
O	1.0	0.437084	0.829525	0.067060	Biso	1.000000	O
O	1.0	0.437106	0.829784	0.400376	Biso	1.000000	O
O	1.0	0.437123	0.829759	0.733640	Biso	1.000000	O
O	1.0	0.937111	0.329851	0.099863	Biso	1.000000	O
O	1.0	0.937497	0.329817	0.433390	Biso	1.000000	O
O	1.0	0.937138	0.329656	0.766527	Biso	1.000000	O
O	1.0	0.937081	0.829651	0.099790	Biso	1.000000	O
O	1.0	0.937145	0.829763	0.433184	Biso	1.000000	O
O	1.0	0.937015	0.829706	0.766429	Biso	1.000000	O
O	1.0	0.062763	0.169934	0.233821	Biso	1.000000	O
O	1.0	0.062872	0.170195	0.567012	Biso	1.000000	O
O	1.0	0.062496	0.170123	0.900260	Biso	1.000000	O
O	1.0	0.062756	0.670151	0.233765	Biso	1.000000	O
O	1.0	0.062761	0.670223	0.567130	Biso	1.000000	O
O	1.0	0.062613	0.670180	0.900411	Biso	1.000000	O
O	1.0	0.438382	0.419858	0.233116	Biso	1.000000	O
O	1.0	0.437276	0.420146	0.565980	Biso	1.000000	O
O	1.0	0.438152	0.420977	0.897391	Biso	1.000000	O
O	1.0	0.437139	0.919921	0.233615	Biso	1.000000	O
O	1.0	0.437075	0.920272	0.566957	Biso	1.000000	O
O	1.0	0.437001	0.919954	0.900274	Biso	1.000000	O
O	1.0	0.562718	0.079298	0.100007	Biso	1.000000	O
O	1.0	0.562684	0.079812	0.433073	Biso	1.000000	O
O	1.0	0.562513	0.080022	0.766606	Biso	1.000000	O
O	1.0	0.562667	0.580496	0.100189	Biso	1.000000	O
O	1.0	0.562635	0.580355	0.433928	Biso	1.000000	O
O	1.0	0.562426	0.580041	0.766613	Biso	1.000000	O
O	1.0	0.062448	0.079470	0.067106	Biso	1.000000	O
O	1.0	0.062901	0.079849	0.400368	Biso	1.000000	O
O	1.0	0.062682	0.079797	0.733692	Biso	1.000000	O
O	1.0	0.062548	0.579965	0.067182	Biso	1.000000	O
O	1.0	0.062919	0.579815	0.400440	Biso	1.000000	O
O	1.0	0.062725	0.579789	0.733731	Biso	1.000000	O
O	1.0	0.937360	0.420376	0.266575	Biso	1.000000	O
O	1.0	0.937326	0.420196	0.599854	Biso	1.000000	O
O	1.0	0.936916	0.419984	0.933307	Biso	1.000000	O
O	1.0	0.937157	0.920084	0.266520	Biso	1.000000	O
O	1.0	0.937123	0.920293	0.599818	Biso	1.000000	O
O	1.0	0.937038	0.920066	0.933093	Biso	1.000000	O
O	1.0	0.308369	0.250834	0.012583	Biso	1.000000	O
O	1.0	0.313878	0.249758	0.345973	Biso	1.000000	O
O	1.0	0.311295	0.250861	0.681345	Biso	1.000000	O
O	1.0	0.311189	0.750778	0.014893	Biso	1.000000	O
O	1.0	0.311250	0.750848	0.348119	Biso	1.000000	O
O	1.0	0.311207	0.750980	0.681264	Biso	1.000000	O
O	1.0	0.690380	0.249087	0.321240	Biso	1.000000	O
O	1.0	0.688679	0.249014	0.651791	Biso	1.000000	O
O	1.0	0.684777	0.251047	0.988964	Biso	1.000000	O
O	1.0	0.688597	0.749181	0.318834	Biso	1.000000	O

O	1.0	0.688569	0.749063	0.652266	Biso	1.000000	O
O	1.0	0.688518	0.748969	0.985372	Biso	1.000000	O
O	1.0	0.187620	0.249417	0.181228	Biso	1.000000	O
O	1.0	0.188649	0.249068	0.514934	Biso	1.000000	O
O	1.0	0.188338	0.249092	0.848342	Biso	1.000000	O
O	1.0	0.188333	0.748943	0.181766	Biso	1.000000	O
O	1.0	0.188347	0.749106	0.514982	Biso	1.000000	O
O	1.0	0.188186	0.748991	0.848176	Biso	1.000000	O
O	1.0	0.812113	0.250618	0.152654	Biso	1.000000	O
O	1.0	0.811714	0.250894	0.485268	Biso	1.000000	O
O	1.0	0.811392	0.251082	0.818761	Biso	1.000000	O
O	1.0	0.811465	0.750829	0.151857	Biso	1.000000	O
O	1.0	0.811582	0.750970	0.485534	Biso	1.000000	O
O	1.0	0.811396	0.750657	0.818762	Biso	1.000000	O
O	1.0	0.688708	0.000884	0.151765	Biso	1.000000	O
O	1.0	0.688586	0.000973	0.485581	Biso	1.000000	O
O	1.0	0.688496	0.001071	0.818779	Biso	1.000000	O
O	1.0	0.689092	0.501188	0.153676	Biso	1.000000	O
O	1.0	0.688824	0.501282	0.485999	Biso	1.000000	O
O	1.0	0.688713	0.500732	0.818569	Biso	1.000000	O
O	1.0	0.311724	0.498766	0.181261	Biso	1.000000	O
O	1.0	0.311178	0.499079	0.514540	Biso	1.000000	O
O	1.0	0.311197	0.499302	0.847406	Biso	1.000000	O
O	1.0	0.311334	0.998938	0.180669	Biso	1.000000	O
O	1.0	0.311341	0.999212	0.514589	Biso	1.000000	O
O	1.0	0.311085	0.998637	0.847618	Biso	1.000000	O
O	1.0	0.811738	0.499256	0.318930	Biso	1.000000	O
O	1.0	0.811521	0.498972	0.652022	Biso	1.000000	O
O	1.0	0.811391	0.498744	0.985434	Biso	1.000000	O
O	1.0	0.811569	0.998880	0.318722	Biso	1.000000	O
O	1.0	0.811448	0.999282	0.652209	Biso	1.000000	O
O	1.0	0.811663	0.999057	0.985155	Biso	1.000000	O
O	1.0	0.188074	0.000534	0.014892	Biso	1.000000	O
O	1.0	0.188461	0.000908	0.348331	Biso	1.000000	O
O	1.0	0.188358	0.000856	0.681621	Biso	1.000000	O
O	1.0	0.187354	0.501154	0.014722	Biso	1.000000	O
O	1.0	0.188780	0.501018	0.348464	Biso	1.000000	O
O	1.0	0.188351	0.500913	0.681560	Biso	1.000000	O
O	1.0	0.436304	0.239327	0.223889	Biso	1.000000	O
O	1.0	0.432135	0.240972	0.562702	Biso	1.000000	O
O	1.0	0.430960	0.239840	0.896421	Biso	1.000000	O
O	1.0	0.432325	0.741109	0.229571	Biso	1.000000	O
O	1.0	0.432386	0.741401	0.562816	Biso	1.000000	O
O	1.0	0.432399	0.741276	0.896214	Biso	1.000000	O
O	1.0	0.562240	0.254350	0.109603	Biso	1.000000	O
O	1.0	0.568103	0.259171	0.436480	Biso	1.000000	O
O	1.0	0.567204	0.260208	0.769661	Biso	1.000000	O
O	1.0	0.567672	0.758857	0.103952	Biso	1.000000	O
O	1.0	0.567600	0.758962	0.437440	Biso	1.000000	O
O	1.0	0.567600	0.758890	0.770587	Biso	1.000000	O
O	1.0	0.067291	0.258753	0.062954	Biso	1.000000	O
O	1.0	0.067744	0.258739	0.396499	Biso	1.000000	O
O	1.0	0.067568	0.258761	0.729701	Biso	1.000000	O
O	1.0	0.067523	0.758703	0.063090	Biso	1.000000	O
O	1.0	0.067573	0.758774	0.396469	Biso	1.000000	O
O	1.0	0.067447	0.758753	0.729668	Biso	1.000000	O
O	1.0	0.932625	0.241083	0.270705	Biso	1.000000	O
O	1.0	0.932465	0.241149	0.603930	Biso	1.000000	O
O	1.0	0.932200	0.241182	0.937183	Biso	1.000000	O
O	1.0	0.932390	0.741167	0.270625	Biso	1.000000	O
O	1.0	0.932349	0.741177	0.603967	Biso	1.000000	O
O	1.0	0.932264	0.741174	0.937177	Biso	1.000000	O
O	1.0	0.566874	0.492793	0.273108	Biso	1.000000	O
O	1.0	0.567460	0.490768	0.603390	Biso	1.000000	O
O	1.0	0.567848	0.489964	0.936478	Biso	1.000000	O
O	1.0	0.567694	0.990937	0.270674	Biso	1.000000	O
O	1.0	0.567374	0.991334	0.603873	Biso	1.000000	O
O	1.0	0.567390	0.991203	0.937212	Biso	1.000000	O
O	1.0	0.432339	0.007597	0.062514	Biso	1.000000	O
O	1.0	0.432249	0.008761	0.396070	Biso	1.000000	O
O	1.0	0.432313	0.008589	0.729501	Biso	1.000000	O
O	1.0	0.432698	0.508997	0.062352	Biso	1.000000	O
O	1.0	0.432165	0.509125	0.396349	Biso	1.000000	O
O	1.0	0.431752	0.509685	0.728927	Biso	1.000000	O
O	1.0	0.932088	0.008705	0.103807	Biso	1.000000	O
O	1.0	0.932451	0.008831	0.437321	Biso	1.000000	O
O	1.0	0.932359	0.008743	0.770408	Biso	1.000000	O
O	1.0	0.932263	0.508797	0.103919	Biso	1.000000	O
O	1.0	0.932649	0.508919	0.437455	Biso	1.000000	O

O	1.0	0.932392	0.508768	0.770559	Biso	1.000000	O
O	1.0	0.067731	0.491237	0.229883	Biso	1.000000	O
O	1.0	0.067674	0.491161	0.563084	Biso	1.000000	O
O	1.0	0.067128	0.491193	0.896186	Biso	1.000000	O
O	1.0	0.067532	0.991110	0.229792	Biso	1.000000	O
O	1.0	0.067612	0.991211	0.563109	Biso	1.000000	O
O	1.0	0.067307	0.991037	0.896261	Biso	1.000000	O
O	1.0	0.303195	0.109770	0.278146	Biso	1.000000	O
O	1.0	0.302966	0.110406	0.611821	Biso	1.000000	O
O	1.0	0.302509	0.109427	0.945255	Biso	1.000000	O
O	1.0	0.303011	0.610283	0.278530	Biso	1.000000	O
O	1.0	0.302855	0.610385	0.611908	Biso	1.000000	O
O	1.0	0.302793	0.610404	0.945140	Biso	1.000000	O
O	1.0	0.696857	0.390020	0.055715	Biso	1.000000	O
O	1.0	0.697642	0.390177	0.388675	Biso	1.000000	O
O	1.0	0.697372	0.389266	0.721724	Biso	1.000000	O
O	1.0	0.696938	0.889568	0.054920	Biso	1.000000	O
O	1.0	0.697015	0.889746	0.388363	Biso	1.000000	O
O	1.0	0.696900	0.889725	0.721613	Biso	1.000000	O
O	1.0	0.196626	0.390010	0.111900	Biso	1.000000	O
O	1.0	0.197012	0.389630	0.445325	Biso	1.000000	O
O	1.0	0.196669	0.389580	0.778510	Biso	1.000000	O
O	1.0	0.196674	0.889396	0.112118	Biso	1.000000	O
O	1.0	0.196741	0.889645	0.445440	Biso	1.000000	O
O	1.0	0.196674	0.889526	0.778712	Biso	1.000000	O
O	1.0	0.802958	0.110113	0.221675	Biso	1.000000	O
O	1.0	0.803039	0.110514	0.555229	Biso	1.000000	O
O	1.0	0.802386	0.110676	0.888175	Biso	1.000000	O
O	1.0	0.803264	0.610535	0.221829	Biso	1.000000	O
O	1.0	0.802992	0.610420	0.555221	Biso	1.000000	O
O	1.0	0.802793	0.610162	0.888550	Biso	1.000000	O
O	1.0	0.697889	0.359283	0.222190	Biso	1.000000	O
O	1.0	0.697334	0.360544	0.555043	Biso	1.000000	O
O	1.0	0.697952	0.360213	0.888344	Biso	1.000000	O
O	1.0	0.696971	0.860515	0.221708	Biso	1.000000	O
O	1.0	0.696971	0.860397	0.555025	Biso	1.000000	O
O	1.0	0.696893	0.860496	0.888310	Biso	1.000000	O
O	1.0	0.302391	0.139870	0.111450	Biso	1.000000	O
O	1.0	0.303141	0.139802	0.445031	Biso	1.000000	O
O	1.0	0.302793	0.139347	0.778519	Biso	1.000000	O
O	1.0	0.302919	0.639460	0.111934	Biso	1.000000	O
O	1.0	0.302920	0.639708	0.445314	Biso	1.000000	O
O	1.0	0.302766	0.639944	0.778656	Biso	1.000000	O
O	1.0	0.802518	0.139717	0.054758	Biso	1.000000	O
O	1.0	0.803200	0.139336	0.388555	Biso	1.000000	O
O	1.0	0.802300	0.139828	0.721952	Biso	1.000000	O
O	1.0	0.802870	0.639317	0.054993	Biso	1.000000	O
O	1.0	0.803369	0.639716	0.388536	Biso	1.000000	O
O	1.0	0.802896	0.639383	0.721749	Biso	1.000000	O
O	1.0	0.196277	0.360448	0.279013	Biso	1.000000	O
O	1.0	0.196940	0.360370	0.611946	Biso	1.000000	O
O	1.0	0.196249	0.360665	0.945107	Biso	1.000000	O
O	1.0	0.196711	0.860338	0.278748	Biso	1.000000	O
O	1.0	0.196668	0.860380	0.612054	Biso	1.000000	O
O	1.0	0.196554	0.860133	0.945335	Biso	1.000000	O
O	1.0	0.448704	0.094711	0.202200	Biso	1.000000	O
O	1.0	0.447871	0.097216	0.534611	Biso	1.000000	O
O	1.0	0.447704	0.096340	0.868350	Biso	1.000000	O
O	1.0	0.447777	0.597237	0.201437	Biso	1.000000	O
O	1.0	0.447654	0.597411	0.534930	Biso	1.000000	O
O	1.0	0.447643	0.597409	0.868067	Biso	1.000000	O
O	1.0	0.556194	0.407150	0.133041	Biso	1.000000	O
O	1.0	0.552349	0.403338	0.463817	Biso	1.000000	O
O	1.0	0.552118	0.406412	0.791799	Biso	1.000000	O
O	1.0	0.551939	0.902769	0.132108	Biso	1.000000	O
O	1.0	0.551884	0.902901	0.465445	Biso	1.000000	O
O	1.0	0.551865	0.902789	0.798835	Biso	1.000000	O
O	1.0	0.051750	0.402747	0.034684	Biso	1.000000	O
O	1.0	0.052082	0.402699	0.368146	Biso	1.000000	O
O	1.0	0.051933	0.402682	0.701500	Biso	1.000000	O
O	1.0	0.051758	0.902622	0.034702	Biso	1.000000	O
O	1.0	0.051887	0.902679	0.368091	Biso	1.000000	O
O	1.0	0.051812	0.902721	0.701446	Biso	1.000000	O
O	1.0	0.947982	0.097113	0.298895	Biso	1.000000	O
O	1.0	0.948001	0.097240	0.632065	Biso	1.000000	O
O	1.0	0.947721	0.097269	0.965480	Biso	1.000000	O
O	1.0	0.948092	0.597259	0.298954	Biso	1.000000	O
O	1.0	0.948002	0.597212	0.632142	Biso	1.000000	O
O	1.0	0.947856	0.597269	0.965551	Biso	1.000000	O

O	1.0	0.553370	0.347403	0.297394	Biso	1.000000	O
O	1.0	0.552006	0.346077	0.628831	Biso	1.000000	O
O	1.0	0.553831	0.343830	0.952336	Biso	1.000000	O
O	1.0	0.551965	0.847214	0.298930	Biso	1.000000	O
O	1.0	0.551936	0.847394	0.632191	Biso	1.000000	O
O	1.0	0.551939	0.847407	0.965638	Biso	1.000000	O
O	1.0	0.448011	0.152075	0.035744	Biso	1.000000	O
O	1.0	0.448026	0.152509	0.367655	Biso	1.000000	O
O	1.0	0.447707	0.152567	0.701390	Biso	1.000000	O
O	1.0	0.447755	0.653052	0.034864	Biso	1.000000	O
O	1.0	0.447882	0.652929	0.368166	Biso	1.000000	O
O	1.0	0.447788	0.653452	0.701587	Biso	1.000000	O
O	1.0	0.947869	0.152595	0.132239	Biso	1.000000	O
O	1.0	0.948114	0.152820	0.465423	Biso	1.000000	O
O	1.0	0.947765	0.152665	0.798740	Biso	1.000000	O
O	1.0	0.947847	0.652734	0.132287	Biso	1.000000	O
O	1.0	0.948115	0.652830	0.465535	Biso	1.000000	O
O	1.0	0.947913	0.652691	0.798832	Biso	1.000000	O
O	1.0	0.051850	0.347300	0.201370	Biso	1.000000	O
O	1.0	0.052194	0.347222	0.534891	Biso	1.000000	O
O	1.0	0.051767	0.347161	0.868123	Biso	1.000000	O
O	1.0	0.051847	0.847208	0.201362	Biso	1.000000	O
O	1.0	0.051850	0.847305	0.534764	Biso	1.000000	O
O	1.0	0.051762	0.847124	0.868024	Biso	1.000000	O
Si	1.0	0.270307	0.170119	0.016635	Biso	1.000000	Si
Si	1.0	0.272245	0.170636	0.350170	Biso	1.000000	Si
Si	1.0	0.271511	0.170763	0.684121	Biso	1.000000	Si
Si	1.0	0.271428	0.670620	0.017459	Biso	1.000000	Si
Si	1.0	0.271573	0.670651	0.350667	Biso	1.000000	Si
Si	1.0	0.271438	0.670860	0.684066	Biso	1.000000	Si
Si	1.0	0.729702	0.329596	0.317554	Biso	1.000000	Si
Si	1.0	0.728650	0.329044	0.649471	Biso	1.000000	Si
Si	1.0	0.727708	0.329490	0.983329	Biso	1.000000	Si
Si	1.0	0.728416	0.829229	0.316197	Biso	1.000000	Si
Si	1.0	0.728341	0.829162	0.649542	Biso	1.000000	Si
Si	1.0	0.728323	0.829033	0.982643	Biso	1.000000	Si
Si	1.0	0.227382	0.329531	0.184342	Biso	1.000000	Si
Si	1.0	0.228337	0.329229	0.517508	Biso	1.000000	Si
Si	1.0	0.228129	0.329266	0.850899	Biso	1.000000	Si
Si	1.0	0.228158	0.828995	0.184298	Biso	1.000000	Si
Si	1.0	0.228169	0.829168	0.517611	Biso	1.000000	Si
Si	1.0	0.228095	0.829003	0.850824	Biso	1.000000	Si
Si	1.0	0.772102	0.170773	0.149634	Biso	1.000000	Si
Si	1.0	0.771692	0.170892	0.482948	Biso	1.000000	Si
Si	1.0	0.770722	0.171470	0.816262	Biso	1.000000	Si
Si	1.0	0.771632	0.670691	0.149465	Biso	1.000000	Si
Si	1.0	0.771715	0.670871	0.482993	Biso	1.000000	Si
Si	1.0	0.771497	0.670554	0.816254	Biso	1.000000	Si
Si	1.0	0.728460	0.421040	0.150173	Biso	1.000000	Si
Si	1.0	0.728800	0.421316	0.483364	Biso	1.000000	Si
Si	1.0	0.728734	0.420756	0.816041	Biso	1.000000	Si
Si	1.0	0.728503	0.920691	0.149430	Biso	1.000000	Si
Si	1.0	0.728440	0.920865	0.482937	Biso	1.000000	Si
Si	1.0	0.728287	0.920923	0.816085	Biso	1.000000	Si
Si	1.0	0.271443	0.078990	0.183565	Biso	1.000000	Si
Si	1.0	0.271621	0.079357	0.517275	Biso	1.000000	Si
Si	1.0	0.271282	0.078734	0.850414	Biso	1.000000	Si
Si	1.0	0.271754	0.578783	0.184099	Biso	1.000000	Si
Si	1.0	0.271471	0.579226	0.517405	Biso	1.000000	Si
Si	1.0	0.271383	0.579278	0.850705	Biso	1.000000	Si
Si	1.0	0.771810	0.078975	0.316408	Biso	1.000000	Si
Si	1.0	0.771407	0.079288	0.649667	Biso	1.000000	Si
Si	1.0	0.771739	0.078968	0.982469	Biso	1.000000	Si
Si	1.0	0.771803	0.579331	0.316319	Biso	1.000000	Si
Si	1.0	0.771361	0.578911	0.649591	Biso	1.000000	Si
Si	1.0	0.771234	0.578705	0.982993	Biso	1.000000	Si
Si	1.0	0.227705	0.421399	0.017069	Biso	1.000000	Si
Si	1.0	0.228507	0.420870	0.350820	Biso	1.000000	Si
Si	1.0	0.228269	0.420884	0.684163	Biso	1.000000	Si
Si	1.0	0.227970	0.920498	0.017546	Biso	1.000000	Si
Si	1.0	0.228153	0.920733	0.350918	Biso	1.000000	Si
Si	1.0	0.228140	0.920744	0.684270	Biso	1.000000	Si
Si	1.0	0.474253	0.166485	0.266291	Biso	1.000000	Si
Si	1.0	0.473673	0.168657	0.599424	Biso	1.000000	Si
Si	1.0	0.473025	0.167952	0.932964	Biso	1.000000	Si
Si	1.0	0.473771	0.668640	0.266100	Biso	1.000000	Si
Si	1.0	0.473689	0.668900	0.599459	Biso	1.000000	Si
Si	1.0	0.473688	0.668722	0.932776	Biso	1.000000	Si
Al	1.0	0.524427	0.337917	0.060411	Biso	1.000000	Al

Si	1.0	0.526982	0.331639	0.399234	Biso	1.000000	Si
Si	1.0	0.526227	0.332150	0.731306	Biso	1.000000	Si
Si	1.0	0.525988	0.831149	0.067544	Biso	1.000000	Si
Si	1.0	0.526022	0.831300	0.400961	Biso	1.000000	Si
Si	1.0	0.526054	0.831309	0.734212	Biso	1.000000	Si
Si	1.0	0.026049	0.331385	0.099319	Biso	1.000000	Si
Si	1.0	0.026382	0.331315	0.432873	Biso	1.000000	Si
Si	1.0	0.026034	0.331227	0.766079	Biso	1.000000	Si
Si	1.0	0.026001	0.831172	0.099364	Biso	1.000000	Si
Si	1.0	0.026064	0.831268	0.432756	Biso	1.000000	Si
Si	1.0	0.025934	0.831215	0.765998	Biso	1.000000	Si
Si	1.0	0.973859	0.168493	0.234258	Biso	1.000000	Si
Si	1.0	0.973963	0.168714	0.567534	Biso	1.000000	Si
Si	1.0	0.973627	0.168693	0.900763	Biso	1.000000	Si
Si	1.0	0.973848	0.668654	0.234260	Biso	1.000000	Si
Si	1.0	0.973864	0.668713	0.567599	Biso	1.000000	Si
Si	1.0	0.973712	0.668647	0.900864	Biso	1.000000	Si
Si	1.0	0.527816	0.420213	0.232752	Biso	1.000000	Si
Si	1.0	0.526204	0.418682	0.565825	Biso	1.000000	Si
Si	1.0	0.527396	0.418287	0.895589	Biso	1.000000	Si
Si	1.0	0.526056	0.918477	0.234259	Biso	1.000000	Si
Si	1.0	0.525995	0.918750	0.567561	Biso	1.000000	Si
Si	1.0	0.525917	0.918645	0.900825	Biso	1.000000	Si
Si	1.0	0.473594	0.079738	0.099360	Biso	1.000000	Si
Si	1.0	0.473770	0.080949	0.432929	Biso	1.000000	Si
Si	1.0	0.473564	0.081125	0.766074	Biso	1.000000	Si
Si	1.0	0.473740	0.581446	0.099319	Biso	1.000000	Si
Si	1.0	0.473715	0.581520	0.432844	Biso	1.000000	Si
Si	1.0	0.473507	0.581699	0.765945	Biso	1.000000	Si
Si	1.0	0.973609	0.081165	0.067475	Biso	1.000000	Si
Si	1.0	0.973965	0.081278	0.400918	Biso	1.000000	Si
Si	1.0	0.973789	0.081295	0.734119	Biso	1.000000	Si
Si	1.0	0.973673	0.581352	0.067598	Biso	1.000000	Si
Si	1.0	0.974021	0.581400	0.400949	Biso	1.000000	Si
Si	1.0	0.973827	0.581265	0.734223	Biso	1.000000	Si
Si	1.0	0.026254	0.418744	0.266133	Biso	1.000000	Si
Si	1.0	0.026225	0.418673	0.599477	Biso	1.000000	Si
Si	1.0	0.025867	0.418620	0.932658	Biso	1.000000	Si
Si	1.0	0.026077	0.918567	0.266067	Biso	1.000000	Si
Si	1.0	0.026044	0.918726	0.599398	Biso	1.000000	Si
Si	1.0	0.025952	0.918493	0.932657	Biso	1.000000	Si