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"Theoretical infrared signature of OH defects in Fe<sup>3+</sup>, Cr<sup>3+</sup> and Al<sup>3+</sup>-doped enstatite"

by Etienne Balan<sup>1</sup>, Jannick Ingrin<sup>2</sup>

<sup>1</sup> Sorbonne Université, CNRS, MNHN, Institut de Minéralogie, de Physique des Matériaux et de Cosmochimie (IMPMC), 4 place Jussieu, 75252 Paris cedex 05, France

<sup>2</sup> Univ. Lille, CNRS, INRAE, ENSCL, UMR 8207 - UMET - Unité Matériaux et Transformations, F-59000 Lille, France

Corresponding author:

Etienne Balan (Sorbonne Université - Institut de Minéralogie, de Physique des Matériaux et de Cosmochimie (IMPMC), UMR CNRS 7590, MNHN, 4 place Jussieu, 75252 Paris cedex 05, France.) Email: Etienne.Balan@sorbonne-universite.fr

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1 **Theoretical infrared signature of OH defects**  
2 **in Fe<sup>3+</sup>, Cr<sup>3+</sup> and Al<sup>3+</sup>-doped enstatite**

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6 Etienne Balan<sup>1</sup>, Jannick Ingrin<sup>2</sup>

7  
8 <sup>1</sup> Sorbonne Université, CNRS, MNHN, Institut de Minéralogie, de Physique des Matériaux et  
9 de Cosmochimie (IMPMC), 4 place Jussieu, 75252 Paris cedex 05, France

10 <sup>2</sup> Univ. Lille, CNRS, INRAE, Centrale Lille, UMR 8207 - UMET - Unité Matériaux et  
11 Transformations, F-59000 Lille, France

12  
13  
14  
15  
16 Corresponding author:

17 Etienne Balan (Sorbonne Université - Institut de Minéralogie, de Physique des Matériaux et  
18 de Cosmochimie (IMPMC), UMR CNRS 7590, MNHN, 4 place Jussieu, 75252 Paris cedex  
19 05, France.) Email: Etienne.Balan@sorbonne-universite.fr

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20

21 **Abstract**

22

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

## 32 **1. Introduction**

33 Enstatite ( $\text{Mg}_2(\text{Si}_2\text{O}_6)$ ) is a major phase of the Earth's upper mantle that is known to  
34 incorporate various amounts of OH-bearing defects (Beran and Zemann, 1986; Ingrin and  
35 Skogby 2000; Stalder and Skogby 2002; Rauch and Keppler 2002). Although these defects  
36 have been extensively studied by infrared spectroscopy and, more recently, by nuclear  
37 magnetic resonance (Xue et al. 2024), the corresponding atomic-scale geometries are still  
38 debated.

39 The OH-stretching spectrum of synthetic ortho-enstatite usually displays two bands  
40 assigned to doubly protonated M2 vacancies. They are observed at 3070 and 3360  $\text{cm}^{-1}$  with  
41 maximum absorbance for a polarization parallel to [001] and almost no absorbance along  
42 [100] (Mierdel and Keppler 2004; Prechtel and Stalder 2010). Additional bands dominantly  
43 polarized along [100] are observed at 3592 and 3687  $\text{cm}^{-1}$  in samples synthesized at lower  
44 silica activity and higher pressure (Prechtel and Stalder 2010, 2011) These two bands are  
45 most likely related to protons ensuring the charge compensation of  $\text{Si}^{4+}$  vacancies (Balan et al.  
46 2013; Xue et al. 2024). Assignment to a 4-fold protonated vacancy (“hydrogarnet” defect,  
47 Xue et al. 2024) versus a partially protonated vacancy (Balan et al. 2013) remains an open  
48 question due to the lack of experimental evidence for the presence of strong OH bands below  
49 3000  $\text{cm}^{-1}$  (see, e.g., Stalder et al. 2012).

50 In natural samples, OH-defects are expected to interact with various impurities, such  
51 as aluminum and other trivalent cations. These interactions can lead to rather complex  
52 infrared spectra with broadened absorption bands (e.g., Stalder et al. 2015). In comparison,  
53 synthetic enstatite samples with low concentration levels of trivalent impurities display  
54 narrow bands not observed in the pure Mg-Si-O-H system (Stalder 2004). Three bands are  
55 observed at 3283, 3322 and 3449  $\text{cm}^{-1}$  in Cr-doped samples, while only two bands are  
56 observed at 3328 and 3461  $\text{cm}^{-1}$  in Fe-doped samples (Fig. 1). Five major bands are observed

57 at 3320, 3381, 3475, 3517 and 3548  $\text{cm}^{-1}$  in enstatite doped with 0.25 wt.%  $\text{Al}_2\text{O}_3$  (Fig. 1).  
58 They are also consistently reported for the Al-doped samples investigated by Stalder and  
59 Skogby (2002). All these bands are specifically related to the trivalent impurities and have a  
60 dominant polarization parallel to [001] (Stalder 2004), suggesting that they involve M  
61 vacancies.

62 In the present study, we theoretically determine the atomic-scale geometry and  
63 infrared spectroscopic properties of OH-bearing defects associated with major trivalent  
64 impurities in enstatite. The high crystalline quality and chemically well-constrained character  
65 of the samples synthesized and investigated by Stalder (2004) facilitate the comparison of  
66 experimental observations with the theoretical properties of OH-bearing defects. The results  
67 confirm that most of the bands observed by Stalder (2004) correspond to protonated M2  
68 vacancies associated with trivalent cations and support their one-to-one assignment to a  
69 specific defect geometry.

70

## 71 **2. Theoretical modeling of OH-defects**

72 The properties of OH-defects were theoretically investigated within the density  
73 functional theory (DFT) framework using the PWscf code of the Quantum Espresso package  
74 (Giannozzi et al., 2009; <http://www.quantum-espresso.org>). The modeling scheme used the  
75 generalized gradient approximation (GGA) to the exchange-correlation functional as  
76 proposed by Perdew, Burke and Ernzerhof (PBE functional; Perdew et al. 1996), and periodic  
77 boundary conditions. The ionic cores were described using optimized norm-conserving  
78 Vanderbilt (ONCV) pseudopotentials (Hamann 2013; Schlipf and Gygi 2015) with a 80 Ry  
79 cut-off on the electronic wave functions. Unit-cell parameters of pure enstatite (space group  
80 Pbc<sub>a</sub>) were optimized at zero pressure, using a shifted Monkhorst-Pack 2x2x2 k-point grid for  
81 the electronic integration. The theoretical cell parameters ( $a=18.43 \text{ \AA}$ ,  $b=8.92 \text{ \AA}$ ,  $c=5.24 \text{ \AA}$ )

82 overestimate their experimental counterparts ( $a = 18.21 \text{ \AA}$ ,  $b=8.81 \text{ \AA}$ ,  $c=5.18 \text{ \AA}$ ; Morimoto  
83 and Koto 1969) as usually observed in GGA calculations. The vibrational properties of OH-  
84 bearing defects were determined using  $1 \times 2 \times 3$  supercells (480 atoms) containing one to two  
85 hydrogen atoms equivalent to a hydrogen concentration of 0.093 wt. %  $\text{H}_2\text{O}$  and 0.187 wt. %  
86  $\text{H}_2\text{O}$ , respectively. These relatively large supercells help minimizing the interaction of the  
87 defects with their periodic images. The theoretical unit-cell parameters of pure enstatite were  
88 used without further relaxation to produce the supercells and the electronic integration was  
89 restricted to the  $\Gamma$  point. For all systems, the relaxation of atomic internal coordinates was  
90 performed until the residual forces were  $< 10^{-4} \text{ Ry/a.u.}$ . For models containing isolated  
91 paramagnetic cations ( $\text{Cr}^{3+}$ ,  $\text{Fe}^{3+}$ ), spin-polarized calculations have been performed, imposing  
92 the high-spin state of the ion to the supercell.

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

106

### 107 3. Results and discussion

108

109 The enstatite structure displays two types of octahedral sites nominally occupied by  
110  $\text{Mg}^{2+}$  cations. The  $\text{Mg}^{2+}$  cations at the M1 site are bound to four O1 and two O2 oxygen  
111 atoms, corresponding to apical and equatorial non-bridging oxygen in silicate tetrahedra,  
112 respectively. The more distorted M2 sites involve O1 and O2 oxygen atoms and the silicate-  
113 bridging O3 oxygen atoms. Previous theoretical studies consistently indicate that the  
114 protonation of vacant M2 sites is significantly favored with respect to that of M1 sites  
115 (Gatzemeier and Wright 2006; Balan et al. 2013; Xue et al. 2024). In the fully protonated M2  
116 vacancies, the two non-equivalent O2-H groups (referred to as OaH and ObH) are oriented in  
117 the (100) plane, leading to two bands dominantly polarized along the [001] direction. The  
118 shorter ObH bond vibrates at  $\sim 3360 \text{ cm}^{-1}$  and the other OaH bond at  $\sim 3070 \text{ cm}^{-1}$  (e.g. Rauch  
119 and Keppler 2002; Stalder and Skogby 2002; Stalder 2004). The theoretical frequencies  
120 obtained in the present modelling are  $3425$  and  $3134 \text{ cm}^{-1}$  (Table 1). Differences with the  
121 theoretical frequencies previously obtained with the PBE functional by Balan et al. (2013)  
122 ( $3361$  and  $3034 \text{ cm}^{-1}$ ) and Xue et al. (2024) ( $3361$  and  $3161 \text{ cm}^{-1}$ ) are mostly due to the use of  
123 different sets of pseudopotentials and different size of supercells.

124 Based on their polarization properties, the bands observed by Stalder (2004) in the  
125 doped enstatite samples can be assumed to be related to M vacancies. Accordingly, a series of  
126 models was built by removing one proton from the previously investigated protonated M2  
127 vacancy and introducing trivalent cations (Al, Cr, Fe) in the neighboring M1 sites (Table 1).  
128 The association of one proton and one trivalent impurity compensates for the charge deficit  
129 due to the Mg vacancy and ensures the electrostatic neutrality of the defect. In each model, a  
130 single  $\text{M}^{3+}$  for  $\text{Mg}^{2+}$  substitution was considered and it was assumed that the OH group is not  
131 coordinated to the trivalent cation due to the bond valence constraints. Each composition thus

132 leads to four defect configurations (Fig. 2). In configurations 1 and 2, the hydrogen is bonded  
133 to the Ob oxygen, while it is bonded to Oa in configurations 3 and 4. The substitution affects  
134 the octahedral site almost facing the OH group along the [001] direction in configurations 1  
135 and 4, and the site in a more lateral position in configurations 2 and 3. Only substitutions at  
136 M1 sites were considered for the Cr and Fe-bearing systems, but two additional defect models  
137 were considered in the aluminous system to account for potential Al for Si substitution  
138 affecting the two non-equivalent Si sites of enstatite (Table 1).

139 The presence of neighboring impurities has a significant effect on the vibrational  
140 properties of the OH group at the vacant M2 site (Table 1). As is usually observed, the  
141 stretching frequency is inversely correlated with the OH bond length (Fig. 3A). The slope of  
142 the correlation ( $\sim -19000 \text{ cm}^{-1}/\text{\AA}$ ) is similar to that previously reported for hydrous defects in  
143 enstatite and other minerals (e.g., Balan et al. 2013; Balan et al. 2020). For the OH defects  
144 associated with M2 vacancies, the OH bond length appears to be mostly controlled by the  
145 strength of H-bonding, as attested by its regular decrease as a function of the oxygen-oxygen  
146 distance (Fig. 3B). Compared with the fully protonated vacancy, the presence of a trivalent  
147 cation in the coordination sphere of the H-bond accepting oxygen contributes to the local  
148 charge compensation, leading to a weakening of the H-bond and a shortening of the OH bond.  
149 The relation of the theoretical harmonic OH stretching frequency as a function of oxygen-  
150 oxygen distance is consistent with its experimental counterpart (Libowitzky 1999) when the  
151 experimentally observed frequencies are corrected for anharmonicity (Fig. 3C, see the  
152 appendix for the estimation of the effect of anharmonicity on frequency). The inverse linear  
153 correlation of the absorption coefficient with the stretching frequency (Fig. 3D) is similar to  
154 that inferred from the theoretical modeling of OH groups in minerals (Balan et al. 2008). Its  
155 slope is consistent with that inferred from experimental data (e.g.; Libowitzky and Rossman



156 1997; Stalder et al. 2012) when the experimental frequencies are corrected for anharmonicity  
157 (Fig. 3D).

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

168 For the Fe-bearing models (Table 1), the energy difference between the configurations  
169 can be particularly important ( $> 30$  kJ/mol). The relative abundance of the two less stable  
170 configurations (2 and 3) is not expected to exceed a few percent at 1500 K (1227 °C), while  
171 that of the two other configurations is above 40% (Table 1). Consistently, the Fe-bearing  
172 samples synthesized by slow cooling from 1400 to 1150 °C only display two specific bands at  
173  $3461 \text{ cm}^{-1}$  and  $3328 \text{ cm}^{-1}$  (Stalder 2004). These two bands can thus be confidently assigned to  
174 the two more stable geometries of the Fe-bearing models, i.e., configurations 1 and 4,  
175 respectively (Table 1).

176 For the Cr-bearing models, the energy difference between the four configurations is  
177 smaller and all four configurations are expected to occur in the synthetic Cr-bearing samples  
178 (Table 1). The configuration 4 is expected to be dominant (42% at 1500 K), while the relative  
179 abundances of the three other configurations range between 15 and 25%. Based on their  
180 relative intensities (Fig. 1) and stretching frequencies (Table 1), the bands experimentally

181 observed at 3283 and 3322  $\text{cm}^{-1}$  (Stalder 2004) can be assigned to configurations 3 and 4,  
182 respectively. Considering that the theoretical stretching frequencies of the two other  
183 configurations are close to each other, it is possible that these two configurations contribute to  
184 the remaining band at 3449  $\text{cm}^{-1}$ . This would explain its comparatively strong absorbance,  
185 similar to that of the band at 3322  $\text{cm}^{-1}$ , which is assigned to the more stable configuration 4.  
186 Alternatively, it cannot be fully excluded that the energy difference between the  
187 configurations 1 and 2 is larger than theoretically expected (Table 1) and that only the most  
188 stable of the two configurations is actually observed.

189         The relative stabilities of the Al-bearing models are similar to those computed for the  
190 Cr-bearing defects (Table 1). On the same criteria as for the Cr-bearing samples, the two  
191 bands observed at 3320 and 3381  $\text{cm}^{-1}$  are assigned to configurations 3 and 4, respectively.  
192 The two major bands at 3475 and 3548  $\text{cm}^{-1}$  observed in the Al-doped sample with the lowest  
193 Al concentrations (Stalder and Skogby 2002; Stalder 2004) are assigned to the two remaining  
194 configurations (configurations 2 and 1, respectively) (Table 1). A minor band at 3517  $\text{cm}^{-1}$  is  
195 also observed in the spectrum of the Al-0.25 sample with a polarization similar to that of the  
196 other bands assigned to M2 vacancies (Fig. 1). This minor band becomes dominant in the Al-  
197 rich samples (Stalder 2004) which suggests that it could be related to a medium-range  
198 environment of M2 vacancies involving more than a single Al atom. A comparatively more  
199 complex speciation of OH groups could thus occur in Al-bearing samples depending on their  
200 synthesis conditions (see also Rauch and Keppler 2002).

201         In the models with tetrahedral Al, the underbonded O2 atom is the most favorable site  
202 for the proton location due to bond valence requirements, as in diopside (Balan et al. 2020).  
203 The defect involving the larger Sib site is significantly favored ( $> 20$  kJ/mol) with respect to  
204 that involving the smaller Sia site (Table 1). The Sia and Sib models display different OH  
205 bond lengths leading to theoretical OH stretching frequencies of 3602 and 3430  $\text{cm}^{-1}$ ,

206 respectively, with dominant polarizations along [010] and [100], respectively (Table 1). The  
207 polarization properties of OH bands associated to tetrahedral substitutions thus markedly  
208 differ from those associated to M2 vacancies. It is noteworthy that Grant et al. (2007) report  
209 two bands with a different polarization at 3600 and 3390  $\text{cm}^{-1}$  in synthetic enstatite with  
210 higher Al concentrations. Unfortunately, it was not possible to unambiguously relate these  
211 bands to simple models of OH-bearing defects. Even though the stretching frequencies  
212 reported by Grant et al. (2007) are close to those obtained for the models with tetrahedral Al  
213 (Table 1), the relative intensities of the experimental bands are more difficult to reconcile  
214 with the theoretical expectations.

215 A plot of the theoretical (harmonic) OH stretching frequencies versus experimentally  
216 observed (anharmonic) frequencies of the OH bands in enstatite summarizes the results in  
217 Figure 4. They show a linear trend similar to the one previously observed for diopside, with a  
218 positive offset of theoretical frequencies around 50 to 70  $\text{cm}^{-1}$  (Balan et al. 2020). This  
219 modest offset is consistent with the opposite effects of the neglect of anharmonicity and the  
220 use of the PBE functional in the calculation of theoretical frequencies (Balan et al. 2007).

221

#### 222 **4. Conclusions**

223 Isolated defects involving a coupled incorporation of trivalent cation and proton in  
224 enstatite can be theoretically investigated using periodic models based on large super-cells.  
225 This facilitates the comparison of the theoretical results with observations made on samples  
226 with low levels of doping and low hydrogen content. In this case, it is possible to  
227 unambiguously assign most of the experimentally observed bands to specific defect  
228 configurations. These bands correspond to neutral defects corresponding to protonated M2  
229 vacancies associated with a trivalent cation substitution at a neighboring M1 site. The  
230 theoretical modeling thus confirms that the  $\text{M}^{3+} + \text{H}^+ = 2 \text{Mg}^{2+}$  exchange mechanism is the

231 dominant hydrogen incorporation mechanism at the lowest concentration levels in enstatite  
232 doped with trivalent cations (Stalder and Skogby 2002; Stalder 2004). For the Fe- and Al-  
233 bearing enstatite, the appearance of additional bands and the significant broadening of the  
234 bands observed when the trivalent cation and hydrogen contents increase (Stalder 2004)  
235 suggests that more complex incorporation mechanisms occur. These changes potentially  
236 involve substitutions affecting tetrahedral sites and more significant electrostatic or elastic  
237 interactions between the defects at elevated concentrations. Their modeling will require  
238 different strategies accounting for these interactions and for the multiplicity of potential  
239 configurations.

240

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

245

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

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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)	$d_{O(H)O}$ (Å)	$\omega_{OH}$ (cm <sup>-1</sup> )	$I_x^{***}$ (%)	$I_y^{***}$ (%)	$I_z^{***}$ (%)	$K_{int}$ (cm <sup>-2</sup> per molH <sub>2</sub> O/L)	$\omega_{exp}^{****}$ (cm <sup>-1</sup> )	
1	[(1H <sup>+</sup> ) <sub>M2</sub> (Al <sup>3+</sup> ) <sub>M1</sub> ] <sup>x</sup> _1	O2b	7.3	23.5	0.9776	3.1797	3584	17	8	75	72000	3548
2	[(1H <sup>+</sup> ) <sub>M2</sub> (Al <sup>3+</sup> ) <sub>M1</sub> ] <sup>x</sup> _2	O2b	12.4	15.6	0.9784	3.0836	3563	3	19	78	89000	3475
3	[(1H <sup>+</sup> ) <sub>M2</sub> (Al <sup>3+</sup> ) <sub>M1</sub> ] <sup>x</sup> _3	O2a	10.1	18.8	0.9880	2.8649	3373	3	34	63	159000	3320
4	[(1H <sup>+</sup> ) <sub>M2</sub> (Al <sup>3+</sup> ) <sub>M1</sub> ] <sup>x</sup> _4	O2a	0	42.2	0.9836	2.9820	3474	14	23	63	94000	3381
5	[(1H <sup>+</sup> ) <sub>M2</sub> (Fe <sup>3+</sup> ) <sub>M1</sub> ] <sup>x</sup> _1	O2b	2.0	42.6	0.9784	3.0800	3558	7	11	82	105000	3461
6	[(1H <sup>+</sup> ) <sub>M2</sub> (Fe <sup>3+</sup> ) <sub>M1</sub> ] <sup>x</sup> _2	O2b	34.2	3.2	0.9792	3.0575	3545	5	26	69	101000	n.o.
7	[(1H <sup>+</sup> ) <sub>M2</sub> (Fe <sup>3+</sup> ) <sub>M1</sub> ] <sup>x</sup> _3	O2a	31.8	3.9	0.9908	2.8265	3313	4	43	53	188000	n.o.
8	[(1H <sup>+</sup> ) <sub>M2</sub> (Fe <sup>3+</sup> ) <sub>M1</sub> ] <sup>x</sup> _4	O2a	0	50.2	0.9875	2.8661	3379	6	21	73	167000	3328
9	[(1H <sup>+</sup> ) <sub>M2</sub> (Cr <sup>3+</sup> ) <sub>M1</sub> ] <sup>x</sup> _1	O2b	7.4	23.3	0.9793	3.0801	3547	7	13	80	106000	3449
10	[(1H <sup>+</sup> ) <sub>M2</sub> (Cr <sup>3+</sup> ) <sub>M1</sub> ] <sup>x</sup> _2	O2b	12.5	15.5	0.9796	3.0531	3538	4	25	71	100000	3449
11	[(1H <sup>+</sup> ) <sub>M2</sub> (Cr <sup>3+</sup> ) <sub>M1</sub> ] <sup>x</sup> _3	O2a	9.8	19.2	0.9903	2.8329	3326	3	41	56	185000	3283
12	[(1H <sup>+</sup> ) <sub>M2</sub> (Cr <sup>3+</sup> ) <sub>M1</sub> ] <sup>x</sup> _4	O2a	0	42.1	0.9876	2.8867	3386	7	23	70	157000	3322
13	(Al <sup>3+</sup> ,H <sup>+</sup> ) <sub>Si</sub> <sup>x</sup> _1	O2a	21	15.5	0.9732	2.9091	3602	37	56	7	68000	n.o.
14	(Al <sup>3+</sup> ,H <sup>+</sup> ) <sub>Si</sub> <sup>x</sup> _2	O2b	0	84.5	0.9837	2.9464	3430	52	10	38	104000	n.o.
15	(2H <sup>+</sup> ) <sub>M2</sub>	O2a			0.9994	2.7890	3134	0	33	67	260000	3070
		O2b			0.9845	3.0035	3425	0	25	75	163000	3361

n.o.: not observed

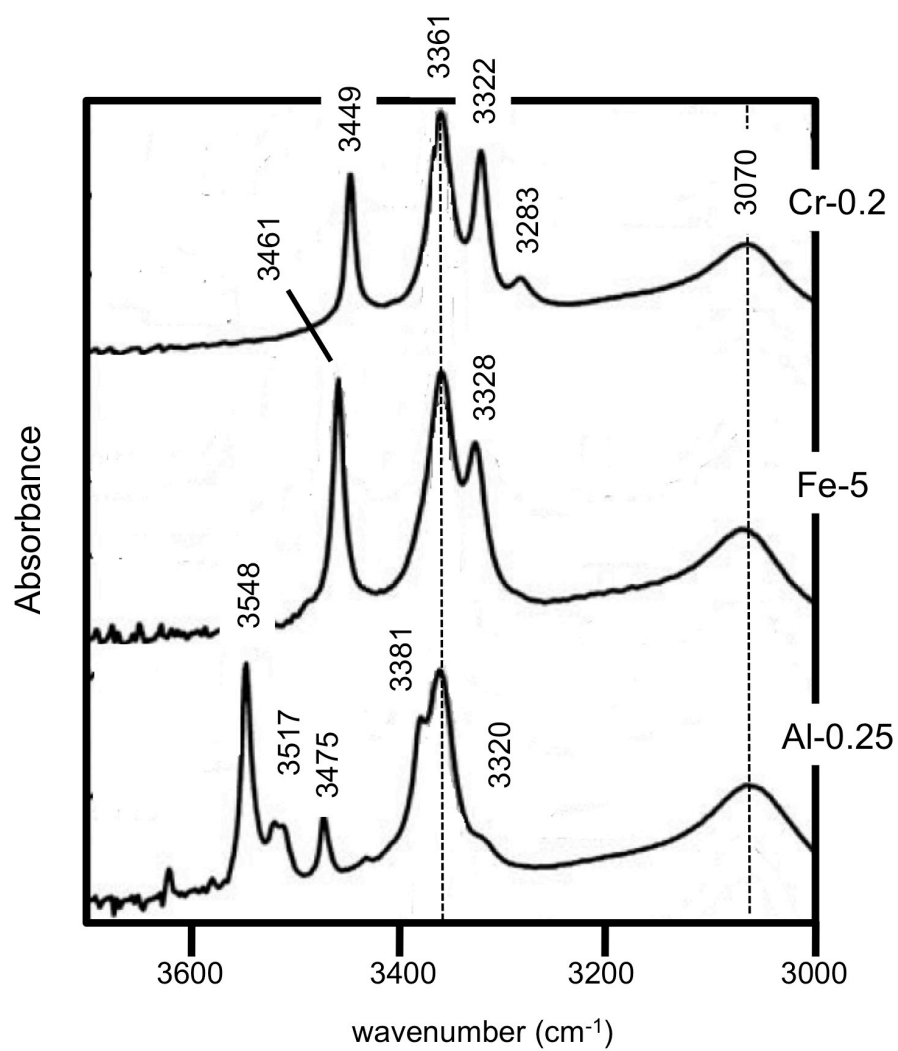
\* The relative energy is defined with respect to the most stable configuration of the model with the same stoichiometry.

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

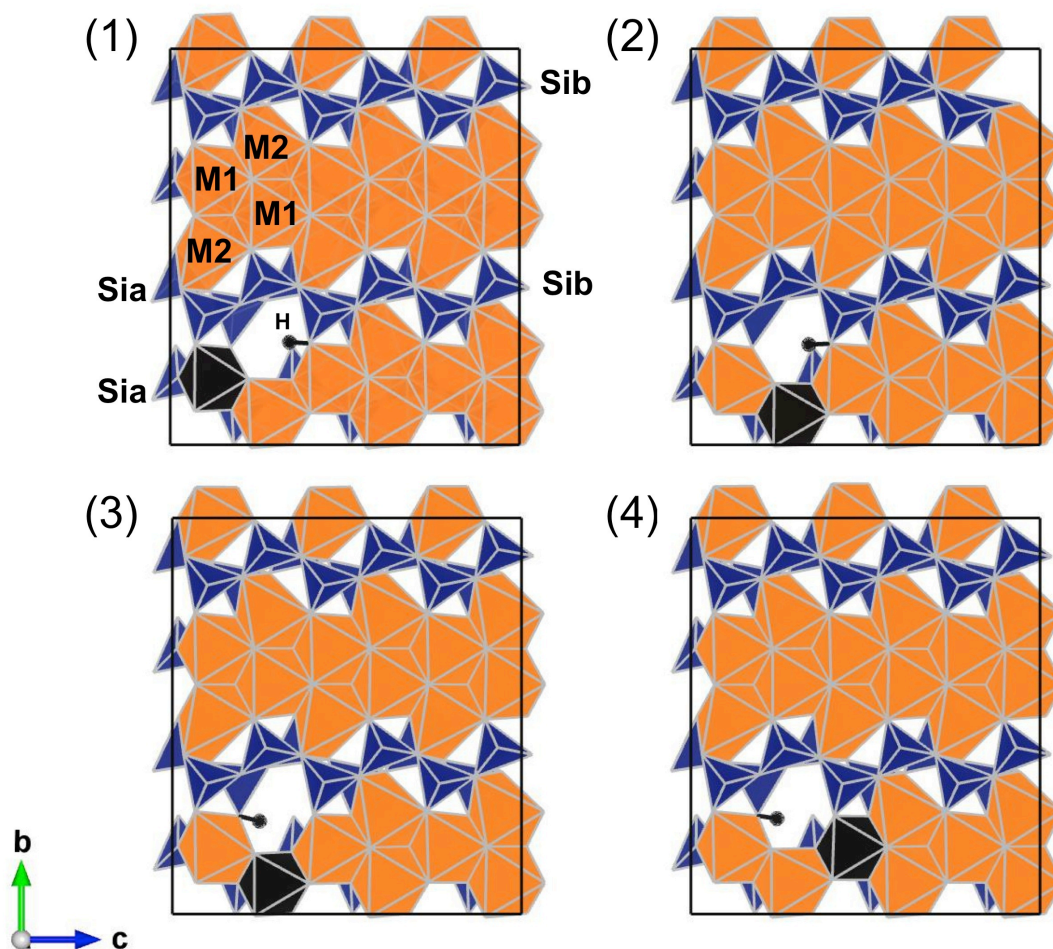
\*\*\*  $I_x$ ,  $I_y$ ,  $I_z$  correspond to the relative theoretical intensities for polarizations parallel to [100], [010] and [001], respectively.

\*\*\*\* Stalder (2004)

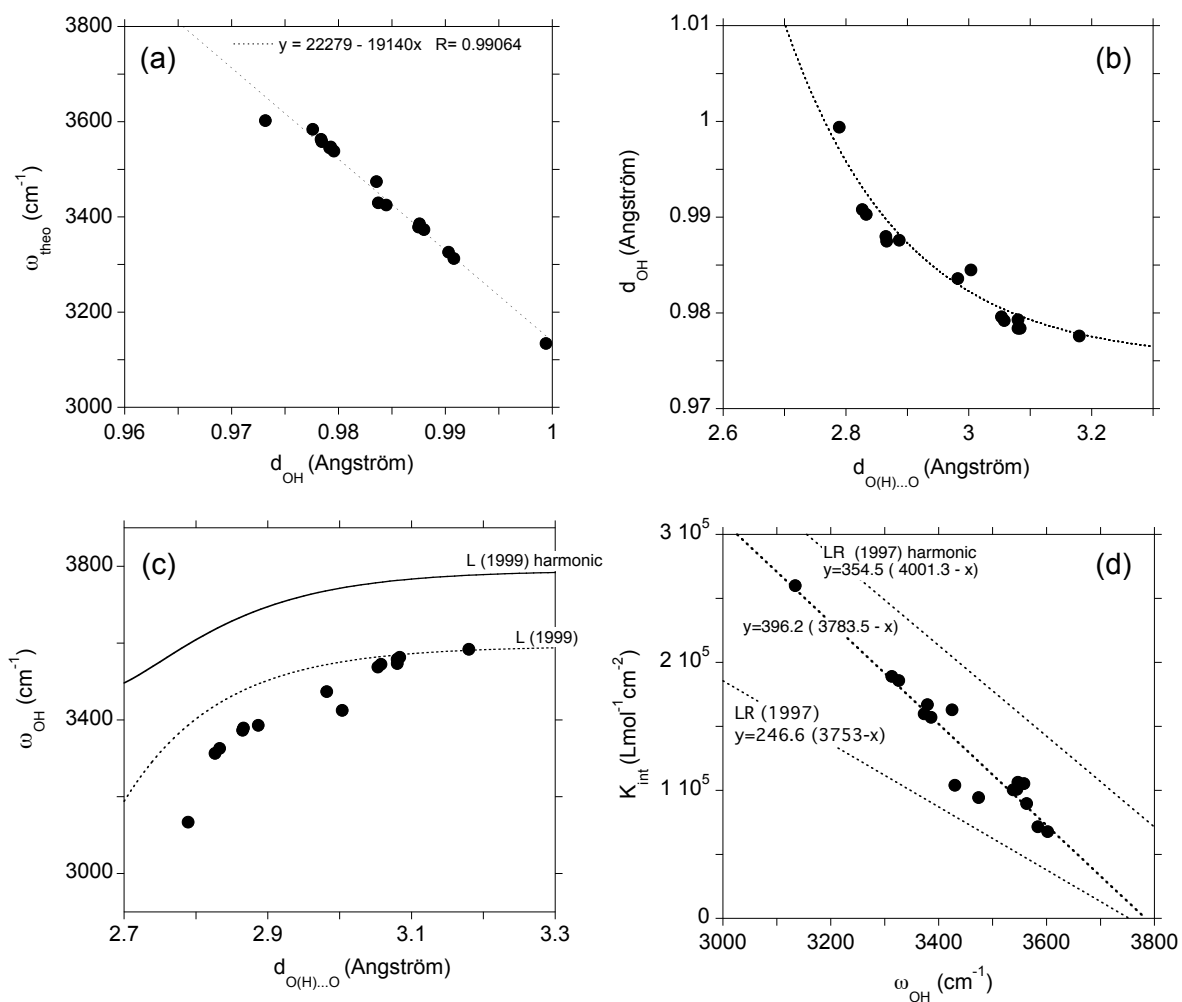
**Fig. 1** Experimental IR-spectra of synthetic orthopyroxenes doped with Cr, Fe and Al from Stalder (2004). The dotted lines correspond to the bands related to doubly protonated M2 vacancies, which are also observed in pure enstatite.



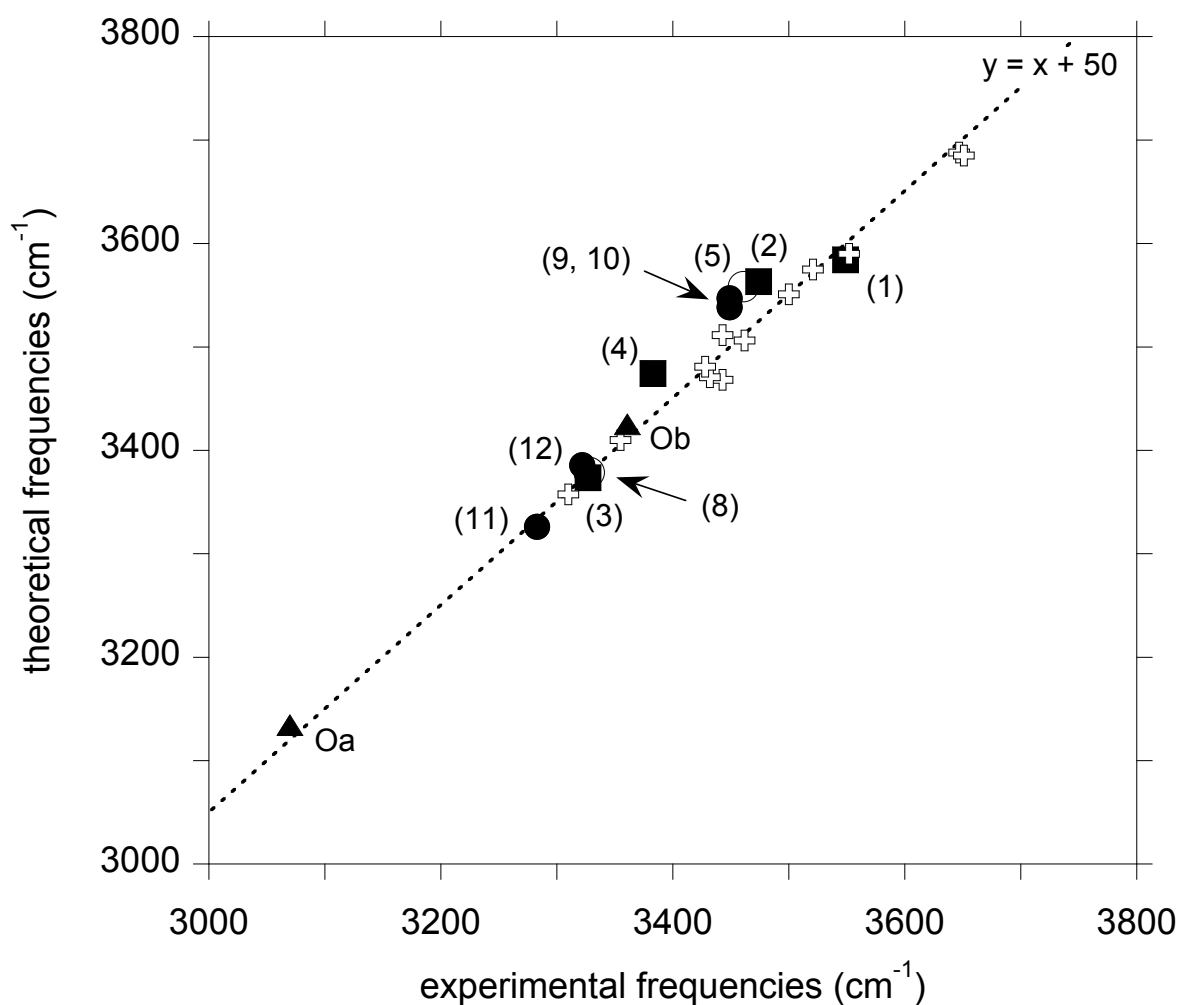
**Fig. 2** Configurations of OH-bearing defects associated to M2 vacancies and  $M^{3+}$  substitution at M1 site. View along the [100] direction of the 1x2x3 supercell. Tetrahedral Si site: blue, octahedral Mg sites: orange, H atom: black sphere. The substituted octahedral M1 site is in black. Configurations (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).



**Fig. 3** (a) Relation between the theoretical stretching frequency and OH bond length for the investigated defects. (b) Relation between the OH bond length and the oxygen-oxygen distance describing the hydrogen bond in protonated M2 vacancies. The dotted line is a guide for the eye. (c) Relation between the harmonic OH stretching frequency and the OH bond length in protonated M2 vacancies. The dotted line corresponds to the experimental relation of Libowitzky (1999) and the solid line is the same relation corrected for anharmonicity (Appendix B) (d) 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 closer to the theoretical slope.



**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 is 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).



## 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:

$$2n_2^2 = (\varepsilon_1^2 + \varepsilon_2^2)^{1/2} - \varepsilon_1 \quad (3)$$

where  $\varepsilon_1$  and  $\varepsilon_2$  are its real and imaginary parts, respectively. Considering that  $\varepsilon_2 = 2 n_1 n_2$ , Eq. (2) is equivalently expressed as:

$$\ln\left(\frac{I_0}{I_t}\right) = 2\pi \bar{\nu} \frac{\varepsilon_2}{n_1} \quad (4)$$

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  $A_{\text{tot}}$  which is the sum of absorbances normalized to thickness in all three orthogonal polarization directions (Libowitzky and Rossman 1996, 1997). The total integrated absorption coefficient  $K_{\text{int}}$  can thus be defined as:

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

For an isotropic crystal,  $K_{\text{int}}$  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  $K_{\text{int}}$  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  $(D/\text{\AA})^2/\text{amu}$ , 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  $\text{km/mol}$ ) of a molecular species in gas phase is (e.g., Monguzi et al. 2009):

$$K = I_k \times 42.256 / \ln(10) \quad (6)$$

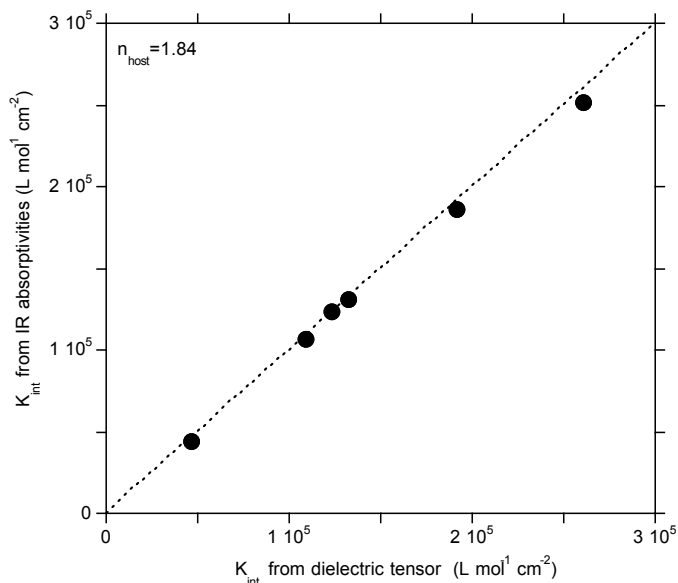
In this case,  $n_1$  in Eq. (4) is approximately equal to one. For a weakly absorbing molecular impurity diluted in a condensed phase,  $n_1$  usually differs from one but it can be assumed to be constant and close to the refractive index of the host medium. The theoretical absorptivities of OH stretching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

$$K_{\text{int}} \approx I_k \times 4225.6 \times 3 \times 2 / (n_{\text{host}} \times \ln(10)) \quad (7)$$

where  $n_{\text{host}}$  is the average refractive index of the host. The factor 2 in Eq. (7) is related to the use of  $\text{H}_2\text{O}$  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).





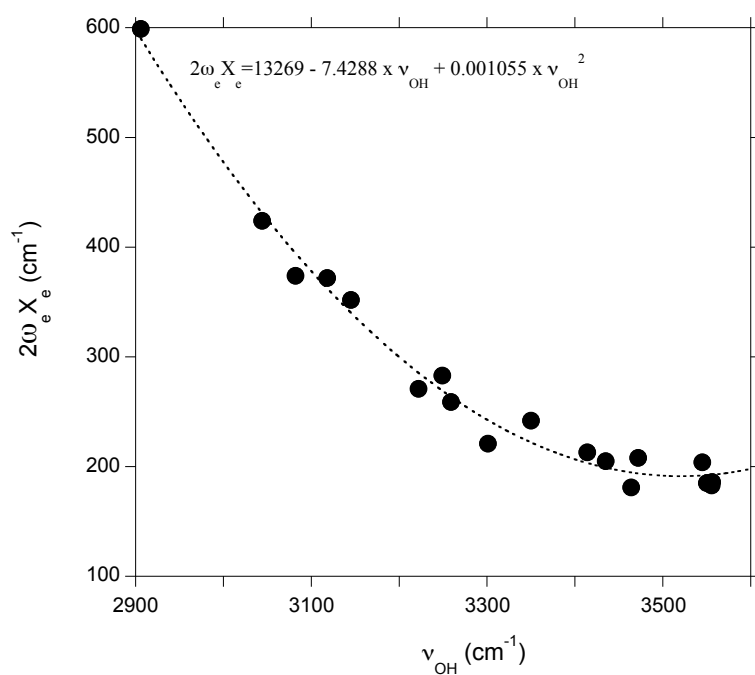
### **B Effect of OH bond anharmonicity on the IR absorption calibration curves.**

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  $mol(H_2O).L^{-1}$  and  $\omega_{OH}$  is the harmonic stretching frequency. In this case, the theoretical slope is significantly closer to the experimental one (Fig. 3d). The anharmonicity correction also improves the comparison of the theoretical and experimental relations between the OH stretching frequency and the oxygen-oxygen distance (Fig. 3c). This supports the idea that the apparent discrepancies between theoretical and experimental correlations are 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 Fe<sup>3+</sup>, Cr<sup>3+</sup> and Al<sup>3+</sup>-doped enstatite" by Etienne Balan<sup>1</sup> and Jannick Ingrin<sup>2</sup>

submitted to Physics and Chemistry of Minerals

Corresponding author: Etienne.Balan@sorbonne-universite.fr

<sup>1</sup> Sorbonne Université, CNRS, MNHN, Institut de Minéralogie, de Physique des Matériaux et de Cosmochimie (IMPMC), 4 place Jussieu, 75252 Paris cedex 05, France  
<sup>2</sup> Univ. Lille, CNRS, INRAE, ENSCL, UMR 8207 - UMET - Unité Matériaux et Transformations, F-59000 Lille, France

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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Mg	1.0	0.126048	0.493508	0.123089	Biso	1.000000	Mg
Mg	1.0	0.126070	0.494545	0.453980	Biso	1.000000	Mg
Mg	1.0	0.123950	0.493582	0.787145	Biso	1.000000	Mg
Mg	1.0	0.123183	0.996471	0.120860	Biso	1.000000	Mg
Mg	1.0	0.123565	0.993400	0.452313	Biso	1.000000	Mg
Mg	1.0	0.123294	0.993703	0.787343	Biso	1.000000	Mg
O	1.0	0.180303	0.170679	0.021773	Biso	1.000000	O
O	1.0	0.183530	0.164081	0.349067	Biso	1.000000	O
O	1.0	0.183557	0.169643	0.678713	Biso	1.000000	O
O	1.0	0.183224	0.669696	0.012214	Biso	1.000000	O
O	1.0	0.183491	0.670614	0.345702	Biso	1.000000	O
O	1.0	0.183324	0.670070	0.679056	Biso	1.000000	O
O	1.0	0.817091	0.329097	0.320659	Biso	1.000000	O
O	1.0	0.816479	0.329692	0.654329	Biso	1.000000	O
O	1.0	0.816577	0.329200	0.987755	Biso	1.000000	O
O	1.0	0.817023	0.830001	0.321172	Biso	1.000000	O
O	1.0	0.816849	0.829901	0.654622	Biso	1.000000	O
O	1.0	0.816917	0.829920	0.988058	Biso	1.000000	O
O	1.0	0.315320	0.329434	0.178956	Biso	1.000000	O
O	1.0	0.316382	0.329866	0.511862	Biso	1.000000	O
O	1.0	0.316366	0.329525	0.845200	Biso	1.000000	O
O	1.0	0.316406	0.830256	0.178574	Biso	1.000000	O
O	1.0	0.316626	0.830007	0.512139	Biso	1.000000	O
O	1.0	0.316454	0.830329	0.845694	Biso	1.000000	O
O	1.0	0.682955	0.170118	0.154811	Biso	1.000000	O
O	1.0	0.683289	0.169998	0.487939	Biso	1.000000	O
O	1.0	0.683250	0.169996	0.821354	Biso	1.000000	O
O	1.0	0.683410	0.670193	0.154642	Biso	1.000000	O
O	1.0	0.683500	0.670179	0.487990	Biso	1.000000	O
O	1.0	0.683483	0.670030	0.821449	Biso	1.000000	O
O	1.0	0.817045	0.419602	0.154179	Biso	1.000000	O
O	1.0	0.816674	0.420029	0.487649	Biso	1.000000	O
O	1.0	0.816657	0.419804	0.821033	Biso	1.000000	O
O	1.0	0.817148	0.920743	0.154554	Biso	1.000000	O

O	1.0	0.816899	0.920186	0.487800	Biso	1.000000	O
O	1.0	0.816762	0.920203	0.821362	Biso	1.000000	O
O	1.0	0.182137	0.088340	0.176048	Biso	1.000000	O
O	1.0	0.184099	0.078458	0.512846	Biso	1.000000	O
O	1.0	0.182250	0.080299	0.846167	Biso	1.000000	O
O	1.0	0.183810	0.580585	0.179226	Biso	1.000000	O
O	1.0	0.183719	0.580549	0.512778	Biso	1.000000	O
O	1.0	0.183176	0.579597	0.845678	Biso	1.000000	O
O	1.0	0.683269	0.079643	0.321419	Biso	1.000000	O
O	1.0	0.683311	0.079815	0.654755	Biso	1.000000	O
O	1.0	0.683179	0.079563	0.988097	Biso	1.000000	O
O	1.0	0.683302	0.579978	0.321225	Biso	1.000000	O
O	1.0	0.683439	0.579769	0.654659	Biso	1.000000	O
O	1.0	0.683488	0.579623	0.988084	Biso	1.000000	O
O	1.0	0.316029	0.419601	0.012007	Biso	1.000000	O
O	1.0	0.317143	0.420509	0.345833	Biso	1.000000	O
O	1.0	0.316375	0.419639	0.678636	Biso	1.000000	O
O	1.0	0.315861	0.920686	0.012264	Biso	1.000000	O
O	1.0	0.316458	0.920132	0.345073	Biso	1.000000	O
O	1.0	0.316565	0.920176	0.679091	Biso	1.000000	O
O	1.0	0.562520	0.170283	0.266262	Biso	1.000000	O
O	1.0	0.562718	0.170153	0.599724	Biso	1.000000	O
O	1.0	0.562628	0.170156	0.932825	Biso	1.000000	O
O	1.0	0.562847	0.670458	0.266161	Biso	1.000000	O
O	1.0	0.562963	0.670325	0.599621	Biso	1.000000	O
O	1.0	0.562870	0.670254	0.932950	Biso	1.000000	O
O	1.0	0.436668	0.329613	0.067086	Biso	1.000000	O
O	1.0	0.437006	0.329576	0.400437	Biso	1.000000	O
O	1.0	0.437023	0.329733	0.733649	Biso	1.000000	O
O	1.0	0.436768	0.830015	0.067208	Biso	1.000000	O
O	1.0	0.437139	0.829978	0.400520	Biso	1.000000	O
O	1.0	0.437161	0.829861	0.733944	Biso	1.000000	O
O	1.0	0.937340	0.326874	0.098042	Biso	1.000000	O
O	1.0	0.936164	0.329620	0.431953	Biso	1.000000	O
O	1.0	0.936795	0.328910	0.765044	Biso	1.000000	O
O	1.0	0.937374	0.829857	0.099626	Biso	1.000000	O
O	1.0	0.937250	0.829935	0.432669	Biso	1.000000	O
O	1.0	0.937149	0.829711	0.766207	Biso	1.000000	O
O	1.0	0.064297	0.166582	0.223409	Biso	1.000000	O
O	1.0	0.063234	0.170291	0.566068	Biso	1.000000	O
O	1.0	0.063201	0.171139	0.901169	Biso	1.000000	O
O	1.0	0.063080	0.670530	0.233977	Biso	1.000000	O
O	1.0	0.062992	0.670227	0.567435	Biso	1.000000	O
O	1.0	0.062978	0.669800	0.900766	Biso	1.000000	O
O	1.0	0.436969	0.420115	0.233686	Biso	1.000000	O
O	1.0	0.437122	0.420125	0.567126	Biso	1.000000	O
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
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model 2

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# CRYSTAL DATA

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O	1.0	0.816666	0.329387	0.653969	Biso	1.000000	O
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O	1.0	0.817005	0.830048	0.321289	Biso	1.000000	O
O	1.0	0.816692	0.829761	0.654903	Biso	1.000000	O
O	1.0	0.816974	0.829948	0.988306	Biso	1.000000	O
O	1.0	0.317306	0.333631	0.179162	Biso	1.000000	O
O	1.0	0.316028	0.329830	0.511364	Biso	1.000000	O
O	1.0	0.316271	0.329701	0.845276	Biso	1.000000	O
O	1.0	0.316580	0.829781	0.178724	Biso	1.000000	O
O	1.0	0.316243	0.831022	0.511490	Biso	1.000000	O
O	1.0	0.316644	0.830283	0.845430	Biso	1.000000	O
O	1.0	0.683399	0.170431	0.154855	Biso	1.000000	O
O	1.0	0.683286	0.170122	0.488059	Biso	1.000000	O
O	1.0	0.683302	0.170134	0.821297	Biso	1.000000	O
O	1.0	0.683558	0.670119	0.154698	Biso	1.000000	O
O	1.0	0.683399	0.670140	0.488091	Biso	1.000000	O
O	1.0	0.683380	0.670035	0.821426	Biso	1.000000	O
O	1.0	0.816898	0.419747	0.154275	Biso	1.000000	O
O	1.0	0.816824	0.419877	0.487452	Biso	1.000000	O
O	1.0	0.816517	0.419893	0.820594	Biso	1.000000	O
O	1.0	0.816849	0.920306	0.155113	Biso	1.000000	O

O	1.0	0.816662	0.920139	0.488230	Biso	1.000000	O
O	1.0	0.816735	0.920204	0.821625	Biso	1.000000	O
O	1.0	0.182116	0.077687	0.188150	Biso	1.000000	O
O	1.0	0.183303	0.077886	0.512402	Biso	1.000000	O
O	1.0	0.183143	0.080036	0.845845	Biso	1.000000	O
O	1.0	0.183669	0.580770	0.178994	Biso	1.000000	O
O	1.0	0.183664	0.581379	0.512969	Biso	1.000000	O
O	1.0	0.183330	0.580293	0.845270	Biso	1.000000	O
O	1.0	0.682832	0.079897	0.321583	Biso	1.000000	O
O	1.0	0.683287	0.079873	0.654720	Biso	1.000000	O
O	1.0	0.683409	0.079979	0.988230	Biso	1.000000	O
O	1.0	0.683415	0.580064	0.321322	Biso	1.000000	O
O	1.0	0.683351	0.579653	0.654594	Biso	1.000000	O
O	1.0	0.683363	0.579705	0.988043	Biso	1.000000	O
O	1.0	0.316222	0.419674	0.011739	Biso	1.000000	O
O	1.0	0.317433	0.421360	0.346560	Biso	1.000000	O
O	1.0	0.316203	0.419696	0.678253	Biso	1.000000	O
O	1.0	0.316748	0.920289	0.012126	Biso	1.000000	O
O	1.0	0.315406	0.922911	0.345214	Biso	1.000000	O
O	1.0	0.316774	0.920368	0.678690	Biso	1.000000	O
O	1.0	0.562080	0.170583	0.266321	Biso	1.000000	O
O	1.0	0.562409	0.170334	0.599515	Biso	1.000000	O
O	1.0	0.562724	0.170141	0.932850	Biso	1.000000	O
O	1.0	0.562982	0.670366	0.266249	Biso	1.000000	O
O	1.0	0.562758	0.670456	0.599684	Biso	1.000000	O
O	1.0	0.562866	0.670196	0.932949	Biso	1.000000	O
O	1.0	0.436808	0.329553	0.067165	Biso	1.000000	O
O	1.0	0.436238	0.328692	0.400188	Biso	1.000000	O
O	1.0	0.436873	0.329683	0.733431	Biso	1.000000	O
O	1.0	0.437254	0.829655	0.067183	Biso	1.000000	O
O	1.0	0.436992	0.830333	0.400309	Biso	1.000000	O
O	1.0	0.437239	0.829969	0.733805	Biso	1.000000	O
O	1.0	0.936262	0.329529	0.097403	Biso	1.000000	O
O	1.0	0.936194	0.329357	0.431574	Biso	1.000000	O
O	1.0	0.936872	0.329157	0.764637	Biso	1.000000	O
O	1.0	0.937475	0.830392	0.100127	Biso	1.000000	O
O	1.0	0.937007	0.829863	0.432861	Biso	1.000000	O
O	1.0	0.937178	0.829808	0.766387	Biso	1.000000	O
O	1.0	0.064350	0.155475	0.238643	Biso	1.000000	O
O	1.0	0.063837	0.169650	0.565419	Biso	1.000000	O
O	1.0	0.062927	0.170552	0.900673	Biso	1.000000	O
O	1.0	0.063059	0.671330	0.234077	Biso	1.000000	O
O	1.0	0.062969	0.670804	0.567270	Biso	1.000000	O
O	1.0	0.062990	0.670651	0.900774	Biso	1.000000	O
O	1.0	0.437434	0.420942	0.233973	Biso	1.000000	O
O	1.0	0.436827	0.420078	0.567120	Biso	1.000000	O
O	1.0	0.436872	0.420058	0.900261	Biso	1.000000	O
O	1.0	0.437192	0.920016	0.233891	Biso	1.000000	O
O	1.0	0.437303	0.920133	0.567006	Biso	1.000000	O
O	1.0	0.437239	0.920510	0.900591	Biso	1.000000	O
O	1.0	0.562784	0.079717	0.099839	Biso	1.000000	O
O	1.0	0.562752	0.079901	0.433122	Biso	1.000000	O
O	1.0	0.562810	0.079900	0.766269	Biso	1.000000	O
O	1.0	0.562834	0.579589	0.099521	Biso	1.000000	O
O	1.0	0.563089	0.580042	0.432932	Biso	1.000000	O
O	1.0	0.562680	0.579717	0.766105	Biso	1.000000	O
O	1.0	0.063280	0.078243	0.068025	Biso	1.000000	O
O	1.0	0.063882	0.077018	0.393582	Biso	1.000000	O
O	1.0	0.063044	0.079701	0.733898	Biso	1.000000	O
O	1.0	0.063309	0.579377	0.067602	Biso	1.000000	O
O	1.0	0.063299	0.580116	0.401126	Biso	1.000000	O
O	1.0	0.063048	0.579829	0.733611	Biso	1.000000	O
O	1.0	0.937183	0.420601	0.266227	Biso	1.000000	O
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
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O	1.0	0.053016	0.853202	0.200269	Biso	1.000000	O
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Si	1.0	0.271761	0.671762	0.351382	Biso	1.000000	Si
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model 3

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# CRYSTAL DATA

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\_symmetry\_space\_group\_name\_H-M 'P 1'  
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loop\_  
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'x, y, z'

loop\_  
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\_atom\_site\_occupancy  
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\_atom\_site\_fract\_y  
\_atom\_site\_fract\_z  
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O	1.0	0.683562	0.670037	0.154764	Biso	1.000000	O
O	1.0	0.683347	0.670325	0.488096	Biso	1.000000	O
O	1.0	0.683272	0.670234	0.821521	Biso	1.000000	O
O	1.0	0.817181	0.419924	0.154762	Biso	1.000000	O
O	1.0	0.816670	0.420676	0.488310	Biso	1.000000	O
O	1.0	0.816590	0.420120	0.821077	Biso	1.000000	O
O	1.0	0.816976	0.920436	0.155063	Biso	1.000000	O

O	1.0	0.816878	0.920451	0.488187	Biso	1.000000	O
O	1.0	0.816756	0.920276	0.821610	Biso	1.000000	O
O	1.0	0.182199	0.077781	0.186882	Biso	1.000000	O
O	1.0	0.183150	0.078673	0.510874	Biso	1.000000	O
O	1.0	0.183081	0.080122	0.845552	Biso	1.000000	O
O	1.0	0.183012	0.579923	0.179000	Biso	1.000000	O
O	1.0	0.183122	0.580988	0.512705	Biso	1.000000	O
O	1.0	0.183091	0.579565	0.845393	Biso	1.000000	O
O	1.0	0.683172	0.079733	0.321484	Biso	1.000000	O
O	1.0	0.683438	0.079876	0.654756	Biso	1.000000	O
O	1.0	0.683510	0.080035	0.988192	Biso	1.000000	O
O	1.0	0.683683	0.579636	0.321354	Biso	1.000000	O
O	1.0	0.683195	0.580115	0.654705	Biso	1.000000	O
O	1.0	0.683352	0.579810	0.988149	Biso	1.000000	O
O	1.0	0.315892	0.419317	0.012225	Biso	1.000000	O
O	1.0	0.318274	0.421121	0.346501	Biso	1.000000	O
O	1.0	0.316521	0.419998	0.678183	Biso	1.000000	O
O	1.0	0.316918	0.920103	0.011721	Biso	1.000000	O
O	1.0	0.315363	0.923090	0.344691	Biso	1.000000	O
O	1.0	0.316689	0.920528	0.678610	Biso	1.000000	O
O	1.0	0.562636	0.170283	0.266290	Biso	1.000000	O
O	1.0	0.562749	0.170343	0.599608	Biso	1.000000	O
O	1.0	0.562587	0.170261	0.933227	Biso	1.000000	O
O	1.0	0.562961	0.670081	0.266171	Biso	1.000000	O
O	1.0	0.562606	0.670658	0.599669	Biso	1.000000	O
O	1.0	0.562744	0.670225	0.933042	Biso	1.000000	O
O	1.0	0.436902	0.329690	0.067182	Biso	1.000000	O
O	1.0	0.436620	0.328252	0.400161	Biso	1.000000	O
O	1.0	0.437063	0.329665	0.733631	Biso	1.000000	O
O	1.0	0.437260	0.829409	0.066951	Biso	1.000000	O
O	1.0	0.436811	0.830249	0.400136	Biso	1.000000	O
O	1.0	0.437109	0.829974	0.733679	Biso	1.000000	O
O	1.0	0.936684	0.329864	0.097991	Biso	1.000000	O
O	1.0	0.935960	0.332625	0.433758	Biso	1.000000	O
O	1.0	0.937093	0.329666	0.765493	Biso	1.000000	O
O	1.0	0.937506	0.830410	0.099901	Biso	1.000000	O
O	1.0	0.937214	0.829941	0.432812	Biso	1.000000	O
O	1.0	0.937218	0.830063	0.766421	Biso	1.000000	O
O	1.0	0.064649	0.152367	0.234610	Biso	1.000000	O
O	1.0	0.063766	0.168033	0.566647	Biso	1.000000	O
O	1.0	0.062888	0.170498	0.900546	Biso	1.000000	O
O	1.0	0.062925	0.671323	0.233721	Biso	1.000000	O
O	1.0	0.062821	0.671250	0.567166	Biso	1.000000	O
O	1.0	0.062901	0.670443	0.900682	Biso	1.000000	O
O	1.0	0.437007	0.419855	0.233558	Biso	1.000000	O
O	1.0	0.437084	0.420226	0.567267	Biso	1.000000	O
O	1.0	0.436806	0.420022	0.900496	Biso	1.000000	O
O	1.0	0.437276	0.919871	0.233559	Biso	1.000000	O
O	1.0	0.437219	0.920245	0.566987	Biso	1.000000	O
O	1.0	0.437278	0.920196	0.900438	Biso	1.000000	O
O	1.0	0.562929	0.079761	0.099612	Biso	1.000000	O
O	1.0	0.562943	0.079831	0.433062	Biso	1.000000	O
O	1.0	0.562853	0.079864	0.766497	Biso	1.000000	O
O	1.0	0.562758	0.579393	0.099593	Biso	1.000000	O
O	1.0	0.563158	0.580066	0.432862	Biso	1.000000	O
O	1.0	0.562677	0.579786	0.766207	Biso	1.000000	O
O	1.0	0.063298	0.078535	0.066821	Biso	1.000000	O
O	1.0	0.064165	0.076578	0.391818	Biso	1.000000	O
O	1.0	0.062893	0.080044	0.733805	Biso	1.000000	O
O	1.0	0.062656	0.579906	0.067366	Biso	1.000000	O
O	1.0	0.062876	0.580755	0.401145	Biso	1.000000	O
O	1.0	0.062805	0.580439	0.733651	Biso	1.000000	O
O	1.0	0.938255	0.419651	0.267236	Biso	1.000000	O
O	1.0	0.937035	0.421000	0.600002	Biso	1.000000	O
O	1.0	0.936704	0.420415	0.931774	Biso	1.000000	O
O	1.0	0.938391	0.922381	0.266464	Biso	1.000000	O
O	1.0	0.937005	0.920264	0.599800	Biso	1.000000	O
O	1.0	0.937269	0.920693	0.933110	Biso	1.000000	O
O	1.0	0.311101	0.250029	0.016506	Biso	1.000000	O
O	1.0	0.307589	0.248343	0.346980	Biso	1.000000	O
O	1.0	0.311456	0.250971	0.681570	Biso	1.000000	O
O	1.0	0.311170	0.750648	0.014940	Biso	1.000000	O
O	1.0	0.311318	0.751397	0.347978	Biso	1.000000	O
O	1.0	0.311244	0.751318	0.681577	Biso	1.000000	O
O	1.0	0.688814	0.248816	0.318340	Biso	1.000000	O
O	1.0	0.688668	0.249059	0.651795	Biso	1.000000	O
O	1.0	0.688434	0.249195	0.985029	Biso	1.000000	O
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
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O	1.0	0.552069	0.847253	0.965481	Biso	1.000000	O
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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
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Si	1.0	0.228304	0.329546	0.515754	Biso	1.000000	Si
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Si	1.0	0.227745	0.831483	0.516592	Biso	1.000000	Si
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model 4

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# CRYSTAL DATA

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\_symmetry\_space\_group\_name\_H-M 'P 1'  
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'x, y, z'

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O	1.0	0.183027	0.579112	0.179028	Biso	1.000000	O
O	1.0	0.183136	0.580502	0.512947	Biso	1.000000	O
O	1.0	0.183240	0.578869	0.844849	Biso	1.000000	O
O	1.0	0.683413	0.079567	0.321511	Biso	1.000000	O
O	1.0	0.683578	0.079565	0.654799	Biso	1.000000	O
O	1.0	0.683245	0.079729	0.988092	Biso	1.000000	O
O	1.0	0.683893	0.579649	0.321399	Biso	1.000000	O
O	1.0	0.683296	0.580006	0.654712	Biso	1.000000	O
O	1.0	0.683371	0.579840	0.988023	Biso	1.000000	O
O	1.0	0.316278	0.419677	0.011774	Biso	1.000000	O
O	1.0	0.318403	0.421501	0.346697	Biso	1.000000	O
O	1.0	0.316232	0.418818	0.677157	Biso	1.000000	O
O	1.0	0.316359	0.920195	0.012166	Biso	1.000000	O
O	1.0	0.315872	0.920763	0.345328	Biso	1.000000	O
O	1.0	0.316537	0.920227	0.678615	Biso	1.000000	O
O	1.0	0.562786	0.170318	0.266443	Biso	1.000000	O
O	1.0	0.562955	0.170016	0.599770	Biso	1.000000	O
O	1.0	0.562816	0.170054	0.933047	Biso	1.000000	O
O	1.0	0.562996	0.670255	0.266160	Biso	1.000000	O
O	1.0	0.562820	0.670594	0.599636	Biso	1.000000	O
O	1.0	0.562718	0.670200	0.932832	Biso	1.000000	O
O	1.0	0.437188	0.329806	0.067103	Biso	1.000000	O
O	1.0	0.437363	0.329423	0.400411	Biso	1.000000	O
O	1.0	0.437277	0.329688	0.733386	Biso	1.000000	O
O	1.0	0.436963	0.829660	0.067090	Biso	1.000000	O
O	1.0	0.436818	0.830038	0.400502	Biso	1.000000	O
O	1.0	0.436889	0.829847	0.733799	Biso	1.000000	O
O	1.0	0.936573	0.329616	0.097692	Biso	1.000000	O
O	1.0	0.937443	0.328915	0.433477	Biso	1.000000	O
O	1.0	0.936879	0.329693	0.765817	Biso	1.000000	O
O	1.0	0.937293	0.829701	0.099587	Biso	1.000000	O
O	1.0	0.937369	0.830005	0.433014	Biso	1.000000	O
O	1.0	0.937343	0.830064	0.766053	Biso	1.000000	O
O	1.0	0.062995	0.163830	0.230684	Biso	1.000000	O
O	1.0	0.065392	0.169389	0.560672	Biso	1.000000	O
O	1.0	0.062859	0.170155	0.900316	Biso	1.000000	O
O	1.0	0.062892	0.670227	0.233840	Biso	1.000000	O
O	1.0	0.062777	0.670467	0.567145	Biso	1.000000	O
O	1.0	0.062950	0.669862	0.900515	Biso	1.000000	O
O	1.0	0.437388	0.420158	0.233531	Biso	1.000000	O
O	1.0	0.437001	0.419775	0.566983	Biso	1.000000	O
O	1.0	0.437068	0.420034	0.900191	Biso	1.000000	O
O	1.0	0.436929	0.920314	0.233917	Biso	1.000000	O
O	1.0	0.436532	0.921020	0.566921	Biso	1.000000	O
O	1.0	0.436977	0.920202	0.900498	Biso	1.000000	O
O	1.0	0.562652	0.079692	0.099825	Biso	1.000000	O
O	1.0	0.562527	0.079601	0.433074	Biso	1.000000	O
O	1.0	0.562662	0.079612	0.766366	Biso	1.000000	O
O	1.0	0.562851	0.579566	0.099596	Biso	1.000000	O
O	1.0	0.563389	0.580128	0.432902	Biso	1.000000	O
O	1.0	0.562595	0.579581	0.766174	Biso	1.000000	O
O	1.0	0.062243	0.079491	0.066236	Biso	1.000000	O
O	1.0	0.064429	0.086802	0.404781	Biso	1.000000	O
O	1.0	0.063543	0.080281	0.733436	Biso	1.000000	O
O	1.0	0.062733	0.579123	0.067382	Biso	1.000000	O
O	1.0	0.062957	0.580036	0.401144	Biso	1.000000	O
O	1.0	0.062907	0.579606	0.733434	Biso	1.000000	O
O	1.0	0.938555	0.419164	0.267590	Biso	1.000000	O
O	1.0	0.937048	0.420219	0.599570	Biso	1.000000	O
O	1.0	0.936748	0.420274	0.931605	Biso	1.000000	O
O	1.0	0.937355	0.920141	0.266188	Biso	1.000000	O
O	1.0	0.937887	0.921059	0.599484	Biso	1.000000	O
O	1.0	0.937218	0.920293	0.932810	Biso	1.000000	O
O	1.0	0.311310	0.251143	0.015152	Biso	1.000000	O
O	1.0	0.309590	0.251441	0.348592	Biso	1.000000	O
O	1.0	0.311494	0.250861	0.681984	Biso	1.000000	O
O	1.0	0.311206	0.750296	0.014895	Biso	1.000000	O
O	1.0	0.311471	0.750824	0.348338	Biso	1.000000	O
O	1.0	0.311202	0.750751	0.681600	Biso	1.000000	O
O	1.0	0.688745	0.249093	0.318444	Biso	1.000000	O
O	1.0	0.688703	0.248874	0.651716	Biso	1.000000	O
O	1.0	0.688405	0.249070	0.985060	Biso	1.000000	O
O	1.0	0.688715	0.749258	0.318519	Biso	1.000000	O
O	1.0	0.688661	0.749465	0.651694	Biso	1.000000	O

O	1.0	0.688567	0.749162	0.984941	Biso	1.000000	O
O	1.0	0.190442	0.248369	0.190979	Biso	1.000000	O
O	1.0	0.184626	0.246944	0.509732	Biso	1.000000	O
O	1.0	0.188921	0.247830	0.848184	Biso	1.000000	O
O	1.0	0.188525	0.749021	0.181557	Biso	1.000000	O
O	1.0	0.188421	0.749355	0.515221	Biso	1.000000	O
O	1.0	0.188251	0.749306	0.848344	Biso	1.000000	O
O	1.0	0.811392	0.250932	0.151800	Biso	1.000000	O
O	1.0	0.811961	0.250747	0.485387	Biso	1.000000	O
O	1.0	0.811593	0.250811	0.817913	Biso	1.000000	O
O	1.0	0.811648	0.750862	0.151619	Biso	1.000000	O
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
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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
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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
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Si	1.0	0.227922	0.829569	0.517644	Biso	1.000000	Si
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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
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model 5

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# CRYSTAL DATA

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\_symmetry\_space\_group\_name\_H-M 'P 1'  
\_symmetry\_Int\_Tables\_number 1

loop\_  
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'x, y, z'

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\_atom\_site\_occupancy  
\_atom\_site\_fract\_x  
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\_atom\_site\_type\_symbol  
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O	1.0	0.316705	0.919807	0.345268	Biso	1.000000	O
O	1.0	0.316672	0.920092	0.678911	Biso	1.000000	O
O	1.0	0.562647	0.170243	0.266292	Biso	1.000000	O
O	1.0	0.562662	0.170189	0.599775	Biso	1.000000	O
O	1.0	0.562688	0.170182	0.932850	Biso	1.000000	O
O	1.0	0.562919	0.670318	0.266310	Biso	1.000000	O
O	1.0	0.562966	0.670252	0.599790	Biso	1.000000	O
O	1.0	0.562818	0.670242	0.933003	Biso	1.000000	O
O	1.0	0.437142	0.330000	0.066882	Biso	1.000000	O
O	1.0	0.437133	0.329539	0.400574	Biso	1.000000	O
O	1.0	0.437043	0.329768	0.733570	Biso	1.000000	O
O	1.0	0.437106	0.829821	0.067103	Biso	1.000000	O
O	1.0	0.437366	0.829768	0.400494	Biso	1.000000	O
O	1.0	0.437232	0.829797	0.733899	Biso	1.000000	O
O	1.0	0.936286	0.328505	0.097678	Biso	1.000000	O
O	1.0	0.935729	0.329931	0.431909	Biso	1.000000	O
O	1.0	0.936914	0.329107	0.765292	Biso	1.000000	O
O	1.0	0.937243	0.829707	0.099698	Biso	1.000000	O
O	1.0	0.937167	0.829664	0.432922	Biso	1.000000	O
O	1.0	0.937134	0.829694	0.766311	Biso	1.000000	O
O	1.0	0.061777	0.167182	0.230626	Biso	1.000000	O
O	1.0	0.063208	0.170185	0.566037	Biso	1.000000	O
O	1.0	0.062865	0.170700	0.900853	Biso	1.000000	O
O	1.0	0.063035	0.670539	0.233951	Biso	1.000000	O
O	1.0	0.062891	0.670271	0.567339	Biso	1.000000	O
O	1.0	0.062868	0.670076	0.900617	Biso	1.000000	O
O	1.0	0.437487	0.420603	0.233731	Biso	1.000000	O
O	1.0	0.437146	0.420173	0.567199	Biso	1.000000	O
O	1.0	0.437057	0.420220	0.900285	Biso	1.000000	O
O	1.0	0.437028	0.920420	0.233772	Biso	1.000000	O
O	1.0	0.437373	0.919952	0.567231	Biso	1.000000	O
O	1.0	0.437081	0.920244	0.900513	Biso	1.000000	O
O	1.0	0.562663	0.079702	0.099611	Biso	1.000000	O
O	1.0	0.562833	0.079638	0.433094	Biso	1.000000	O
O	1.0	0.562666	0.079724	0.766434	Biso	1.000000	O
O	1.0	0.562818	0.579765	0.099622	Biso	1.000000	O
O	1.0	0.563100	0.580069	0.433059	Biso	1.000000	O
O	1.0	0.562763	0.579715	0.766359	Biso	1.000000	O
O	1.0	0.062329	0.080254	0.067342	Biso	1.000000	O
O	1.0	0.062267	0.079317	0.400733	Biso	1.000000	O
O	1.0	0.062953	0.079575	0.733793	Biso	1.000000	O
O	1.0	0.063116	0.578891	0.067291	Biso	1.000000	O
O	1.0	0.063244	0.579718	0.401130	Biso	1.000000	O
O	1.0	0.062916	0.579515	0.733708	Biso	1.000000	O
O	1.0	0.937063	0.420713	0.266134	Biso	1.000000	O
O	1.0	0.937090	0.419891	0.598712	Biso	1.000000	O
O	1.0	0.936568	0.419957	0.931416	Biso	1.000000	O
O	1.0	0.937453	0.920519	0.266329	Biso	1.000000	O
O	1.0	0.937157	0.920207	0.599604	Biso	1.000000	O
O	1.0	0.937069	0.920199	0.932956	Biso	1.000000	O
O	1.0	0.311064	0.251364	0.015007	Biso	1.000000	O
O	1.0	0.310812	0.250528	0.348430	Biso	1.000000	O
O	1.0	0.311264	0.250564	0.681634	Biso	1.000000	O
O	1.0	0.311233	0.751004	0.014782	Biso	1.000000	O
O	1.0	0.311645	0.751217	0.348582	Biso	1.000000	O
O	1.0	0.311368	0.751145	0.681915	Biso	1.000000	O
O	1.0	0.688550	0.248969	0.318305	Biso	1.000000	O
O	1.0	0.688472	0.248939	0.651691	Biso	1.000000	O
O	1.0	0.688355	0.248979	0.984995	Biso	1.000000	O
O	1.0	0.688780	0.749031	0.318427	Biso	1.000000	O
O	1.0	0.688765	0.749003	0.651956	Biso	1.000000	O

O	1.0	0.688685	0.749038	0.985170	Biso	1.000000	O
O	1.0	0.196442	0.247564	0.174373	Biso	1.000000	O
O	1.0	0.187504	0.249729	0.513876	Biso	1.000000	O
O	1.0	0.188566	0.248441	0.848830	Biso	1.000000	O
O	1.0	0.188603	0.748812	0.181298	Biso	1.000000	O
O	1.0	0.188600	0.749119	0.515530	Biso	1.000000	O
O	1.0	0.188452	0.749232	0.848852	Biso	1.000000	O
O	1.0	0.811282	0.250731	0.151877	Biso	1.000000	O
O	1.0	0.811113	0.250742	0.484600	Biso	1.000000	O
O	1.0	0.811516	0.250667	0.818050	Biso	1.000000	O
O	1.0	0.811656	0.750881	0.151523	Biso	1.000000	O
O	1.0	0.811738	0.750738	0.484980	Biso	1.000000	O
O	1.0	0.811580	0.750786	0.818291	Biso	1.000000	O
O	1.0	0.688593	0.000910	0.151831	Biso	1.000000	O
O	1.0	0.688686	0.000819	0.485183	Biso	1.000000	O
O	1.0	0.688611	0.000889	0.818551	Biso	1.000000	O
O	1.0	0.688763	0.500922	0.151601	Biso	1.000000	O
O	1.0	0.688573	0.500847	0.485023	Biso	1.000000	O
O	1.0	0.688569	0.500836	0.818351	Biso	1.000000	O
O	1.0	0.311655	0.499615	0.181800	Biso	1.000000	O
O	1.0	0.311509	0.499438	0.515364	Biso	1.000000	O
O	1.0	0.311217	0.499087	0.848152	Biso	1.000000	O
O	1.0	0.310551	0.999101	0.181765	Biso	1.000000	O
O	1.0	0.312027	0.998642	0.515080	Biso	1.000000	O
O	1.0	0.311199	0.999504	0.848950	Biso	1.000000	O
O	1.0	0.811200	0.499141	0.317841	Biso	1.000000	O
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
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Si	1.0	0.728332	0.420714	0.148835	Biso	1.000000	Si
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model 6

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# CRYSTAL DATA

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\_cell\_length\_c 15.70671  
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\_cell\_angle\_gamma 90  
\_symmetry\_space\_group\_name\_H-M 'P 1'  
\_symmetry\_Int\_Tables\_number 1

loop\_  
\_symmetry\_equiv\_pos\_as\_xyz  
'x, y, z'

loop\_  
\_atom\_site\_label  
\_atom\_site\_occupancy  
\_atom\_site\_fract\_x  
\_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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Fe 1.0 0.125329 0.079887 0.289545 Biso 1.000000 Fe  
Mg 1.0 0.374366 0.327703 0.289374 Biso 1.000000 Mg  
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O	1.0	0.437306	0.829862	0.733852	Biso	1.000000	O
O	1.0	0.936077	0.329741	0.097367	Biso	1.000000	O
O	1.0	0.935857	0.329610	0.431818	Biso	1.000000	O
O	1.0	0.936844	0.329351	0.764998	Biso	1.000000	O
O	1.0	0.937234	0.829921	0.099868	Biso	1.000000	O
O	1.0	0.936984	0.829751	0.432935	Biso	1.000000	O
O	1.0	0.937167	0.829714	0.766487	Biso	1.000000	O
O	1.0	0.062192	0.161428	0.236038	Biso	1.000000	O
O	1.0	0.063335	0.170146	0.566010	Biso	1.000000	O
O	1.0	0.062846	0.170522	0.900537	Biso	1.000000	O
O	1.0	0.062944	0.670871	0.233990	Biso	1.000000	O
O	1.0	0.062895	0.670570	0.567287	Biso	1.000000	O
O	1.0	0.062957	0.670426	0.900664	Biso	1.000000	O
O	1.0	0.437659	0.421069	0.233937	Biso	1.000000	O
O	1.0	0.437025	0.420237	0.567114	Biso	1.000000	O
O	1.0	0.436940	0.420123	0.900267	Biso	1.000000	O
O	1.0	0.437485	0.919744	0.233834	Biso	1.000000	O
O	1.0	0.437380	0.920069	0.567117	Biso	1.000000	O
O	1.0	0.437273	0.920424	0.900533	Biso	1.000000	O
O	1.0	0.562875	0.079709	0.099810	Biso	1.000000	O
O	1.0	0.562797	0.079874	0.433118	Biso	1.000000	O
O	1.0	0.562785	0.079820	0.766295	Biso	1.000000	O
O	1.0	0.562791	0.579655	0.099571	Biso	1.000000	O
O	1.0	0.563137	0.580159	0.433044	Biso	1.000000	O
O	1.0	0.562733	0.579770	0.766237	Biso	1.000000	O
O	1.0	0.062774	0.078972	0.067761	Biso	1.000000	O
O	1.0	0.061967	0.077786	0.399381	Biso	1.000000	O
O	1.0	0.062997	0.079599	0.733927	Biso	1.000000	O
O	1.0	0.063223	0.579241	0.067516	Biso	1.000000	O
O	1.0	0.063272	0.579953	0.401098	Biso	1.000000	O
O	1.0	0.062996	0.579715	0.733560	Biso	1.000000	O
O	1.0	0.937029	0.420757	0.266269	Biso	1.000000	O
O	1.0	0.937124	0.419811	0.598357	Biso	1.000000	O
O	1.0	0.936511	0.420350	0.931126	Biso	1.000000	O
O	1.0	0.937301	0.921259	0.266737	Biso	1.000000	O
O	1.0	0.936865	0.920096	0.599902	Biso	1.000000	O
O	1.0	0.937229	0.920459	0.933149	Biso	1.000000	O
O	1.0	0.311439	0.250154	0.015030	Biso	1.000000	O
O	1.0	0.309730	0.250520	0.348776	Biso	1.000000	O
O	1.0	0.311189	0.250707	0.681484	Biso	1.000000	O
O	1.0	0.311277	0.751360	0.014546	Biso	1.000000	O
O	1.0	0.311275	0.751961	0.348722	Biso	1.000000	O
O	1.0	0.311311	0.751443	0.681789	Biso	1.000000	O
O	1.0	0.688649	0.249001	0.318279	Biso	1.000000	O
O	1.0	0.688435	0.248949	0.651516	Biso	1.000000	O
O	1.0	0.688381	0.249054	0.984919	Biso	1.000000	O
O	1.0	0.688803	0.748899	0.318470	Biso	1.000000	O
O	1.0	0.688729	0.748909	0.652025	Biso	1.000000	O

O	1.0	0.688747	0.748988	0.985235	Biso	1.000000	O
O	1.0	0.200431	0.244836	0.174851	Biso	1.000000	O
O	1.0	0.187582	0.249940	0.513185	Biso	1.000000	O
O	1.0	0.188347	0.248832	0.848266	Biso	1.000000	O
O	1.0	0.188240	0.749189	0.181777	Biso	1.000000	O
O	1.0	0.187960	0.750232	0.514756	Biso	1.000000	O
O	1.0	0.188513	0.749361	0.848769	Biso	1.000000	O
O	1.0	0.812238	0.250414	0.152504	Biso	1.000000	O
O	1.0	0.811410	0.250513	0.484526	Biso	1.000000	O
O	1.0	0.811362	0.250929	0.817878	Biso	1.000000	O
O	1.0	0.811571	0.750814	0.151407	Biso	1.000000	O
O	1.0	0.811649	0.750783	0.484902	Biso	1.000000	O
O	1.0	0.811622	0.750735	0.818361	Biso	1.000000	O
O	1.0	0.688653	0.000897	0.152002	Biso	1.000000	O
O	1.0	0.688544	0.000813	0.485174	Biso	1.000000	O
O	1.0	0.688658	0.000956	0.818565	Biso	1.000000	O
O	1.0	0.688781	0.500909	0.151510	Biso	1.000000	O
O	1.0	0.688607	0.500774	0.484926	Biso	1.000000	O
O	1.0	0.688494	0.500833	0.818165	Biso	1.000000	O
O	1.0	0.312218	0.500739	0.181840	Biso	1.000000	O
O	1.0	0.311571	0.499865	0.515443	Biso	1.000000	O
O	1.0	0.311318	0.499385	0.848033	Biso	1.000000	O
O	1.0	0.311531	0.997713	0.182544	Biso	1.000000	O
O	1.0	0.311699	0.998608	0.514978	Biso	1.000000	O
O	1.0	0.311256	0.999132	0.848432	Biso	1.000000	O
O	1.0	0.811223	0.499202	0.317902	Biso	1.000000	O
O	1.0	0.811589	0.498932	0.651282	Biso	1.000000	O
O	1.0	0.811334	0.498888	0.984640	Biso	1.000000	O
O	1.0	0.810618	0.998640	0.318551	Biso	1.000000	O
O	1.0	0.811283	0.998976	0.651977	Biso	1.000000	O
O	1.0	0.811642	0.999327	0.985194	Biso	1.000000	O
O	1.0	0.188835	0.001264	0.015881	Biso	1.000000	O
O	1.0	0.186780	0.000510	0.346867	Biso	1.000000	O
O	1.0	0.188628	0.001041	0.682256	Biso	1.000000	O
O	1.0	0.188440	0.500609	0.014852	Biso	1.000000	O
O	1.0	0.190140	0.503368	0.349671	Biso	1.000000	O
O	1.0	0.188263	0.500636	0.681198	Biso	1.000000	O
O	1.0	0.431075	0.241095	0.230278	Biso	1.000000	O
O	1.0	0.431942	0.241018	0.562825	Biso	1.000000	O
O	1.0	0.432488	0.241199	0.896116	Biso	1.000000	O
O	1.0	0.432647	0.741369	0.229566	Biso	1.000000	O
O	1.0	0.432554	0.741606	0.563106	Biso	1.000000	O
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
O	1.0	0.567424	0.491114	0.936936	Biso	1.000000	O
O	1.0	0.567580	0.991113	0.270479	Biso	1.000000	O
O	1.0	0.567663	0.991181	0.603843	Biso	1.000000	O
O	1.0	0.567720	0.991266	0.937146	Biso	1.000000	O
O	1.0	0.432725	0.008291	0.063308	Biso	1.000000	O
O	1.0	0.432941	0.008432	0.396451	Biso	1.000000	O
O	1.0	0.432648	0.008572	0.729646	Biso	1.000000	O
O	1.0	0.432289	0.508786	0.062884	Biso	1.000000	O
O	1.0	0.433061	0.509070	0.396605	Biso	1.000000	O
O	1.0	0.432276	0.508866	0.729693	Biso	1.000000	O
O	1.0	0.932465	0.008589	0.104206	Biso	1.000000	O
O	1.0	0.931992	0.007408	0.437753	Biso	1.000000	O
O	1.0	0.932459	0.008606	0.770379	Biso	1.000000	O
O	1.0	0.932386	0.508420	0.103333	Biso	1.000000	O
O	1.0	0.932765	0.508426	0.436793	Biso	1.000000	O
O	1.0	0.932349	0.508466	0.769682	Biso	1.000000	O

O	1.0	0.067336	0.493579	0.231060	Biso	1.000000	O
O	1.0	0.067999	0.490909	0.562068	Biso	1.000000	O
O	1.0	0.067031	0.491987	0.894933	Biso	1.000000	O
O	1.0	0.068591	0.992766	0.232314	Biso	1.000000	O
O	1.0	0.067179	0.991363	0.563454	Biso	1.000000	O
O	1.0	0.067790	0.991752	0.896959	Biso	1.000000	O
O	1.0	0.304977	0.109931	0.278601	Biso	1.000000	O
O	1.0	0.303135	0.109875	0.612388	Biso	1.000000	O
O	1.0	0.302667	0.110521	0.945497	Biso	1.000000	O
O	1.0	0.303331	0.611848	0.279035	Biso	1.000000	O
O	1.0	0.303374	0.610953	0.612657	Biso	1.000000	O
O	1.0	0.303023	0.610502	0.945785	Biso	1.000000	O
O	1.0	0.696801	0.389705	0.054170	Biso	1.000000	O
O	1.0	0.697215	0.389589	0.387401	Biso	1.000000	O
O	1.0	0.696722	0.389618	0.720779	Biso	1.000000	O
O	1.0	0.697064	0.889589	0.054710	Biso	1.000000	O
O	1.0	0.696885	0.889350	0.388128	Biso	1.000000	O
O	1.0	0.697011	0.889573	0.721513	Biso	1.000000	O
O	1.0	0.196098	0.389016	0.111541	Biso	1.000000	O
O	1.0	0.196711	0.390799	0.444218	Biso	1.000000	O
O	1.0	0.196548	0.389225	0.778103	Biso	1.000000	O
O	1.0	0.196844	0.889679	0.112265	Biso	1.000000	O
O	1.0	0.196773	0.890960	0.445472	Biso	1.000000	O
O	1.0	0.196880	0.889662	0.779024	Biso	1.000000	O
O	1.0	0.802774	0.109965	0.221238	Biso	1.000000	O
O	1.0	0.803045	0.110161	0.554561	Biso	1.000000	O
O	1.0	0.803078	0.110460	0.887854	Biso	1.000000	O
O	1.0	0.803323	0.610503	0.221073	Biso	1.000000	O
O	1.0	0.803257	0.610254	0.554441	Biso	1.000000	O
O	1.0	0.803190	0.610203	0.887745	Biso	1.000000	O
O	1.0	0.696901	0.360195	0.220728	Biso	1.000000	O
O	1.0	0.696910	0.360120	0.554133	Biso	1.000000	O
O	1.0	0.696605	0.360231	0.887443	Biso	1.000000	O
O	1.0	0.696979	0.860251	0.221379	Biso	1.000000	O
O	1.0	0.696791	0.860186	0.554900	Biso	1.000000	O
O	1.0	0.697055	0.860327	0.888122	Biso	1.000000	O
O	1.0	0.303869	0.136399	0.110708	Biso	1.000000	O
O	1.0	0.303732	0.139327	0.445910	Biso	1.000000	O
O	1.0	0.303012	0.139497	0.778901	Biso	1.000000	O
O	1.0	0.303142	0.640873	0.112386	Biso	1.000000	O
O	1.0	0.303223	0.640716	0.445972	Biso	1.000000	O
O	1.0	0.303084	0.640259	0.779244	Biso	1.000000	O
O	1.0	0.802998	0.139807	0.054553	Biso	1.000000	O
O	1.0	0.802929	0.139360	0.387782	Biso	1.000000	O
O	1.0	0.803130	0.139571	0.721138	Biso	1.000000	O
O	1.0	0.803194	0.639485	0.054352	Biso	1.000000	O
O	1.0	0.803303	0.639617	0.387802	Biso	1.000000	O
O	1.0	0.803218	0.639463	0.721146	Biso	1.000000	O
O	1.0	0.198624	0.366612	0.274805	Biso	1.000000	O
O	1.0	0.196400	0.360227	0.611085	Biso	1.000000	O
O	1.0	0.196435	0.360238	0.944886	Biso	1.000000	O
O	1.0	0.196701	0.860426	0.278610	Biso	1.000000	O
O	1.0	0.196752	0.861080	0.612164	Biso	1.000000	O
O	1.0	0.196885	0.860841	0.945676	Biso	1.000000	O
O	1.0	0.448081	0.097007	0.201347	Biso	1.000000	O
O	1.0	0.447946	0.097051	0.534703	Biso	1.000000	O
O	1.0	0.447908	0.097223	0.867745	Biso	1.000000	O
O	1.0	0.448236	0.597544	0.201200	Biso	1.000000	O
O	1.0	0.448199	0.597768	0.534565	Biso	1.000000	O
O	1.0	0.447972	0.597611	0.867779	Biso	1.000000	O
O	1.0	0.552143	0.402544	0.132020	Biso	1.000000	O
O	1.0	0.551793	0.402543	0.465348	Biso	1.000000	O
O	1.0	0.551764	0.402627	0.798702	Biso	1.000000	O
O	1.0	0.552255	0.902456	0.132245	Biso	1.000000	O
O	1.0	0.552200	0.902639	0.465610	Biso	1.000000	O
O	1.0	0.552131	0.902702	0.798947	Biso	1.000000	O
O	1.0	0.051299	0.402276	0.030977	Biso	1.000000	O
O	1.0	0.052006	0.400281	0.365003	Biso	1.000000	O
O	1.0	0.051886	0.401505	0.699014	Biso	1.000000	O
O	1.0	0.051953	0.903327	0.034926	Biso	1.000000	O
O	1.0	0.052026	0.903175	0.368758	Biso	1.000000	O
O	1.0	0.051794	0.902666	0.701413	Biso	1.000000	O
O	1.0	0.945148	0.096031	0.299664	Biso	1.000000	O
O	1.0	0.948469	0.097357	0.632410	Biso	1.000000	O
O	1.0	0.948097	0.097456	0.965778	Biso	1.000000	O
O	1.0	0.948193	0.597902	0.299406	Biso	1.000000	O
O	1.0	0.948275	0.597301	0.632163	Biso	1.000000	O
O	1.0	0.948327	0.597418	0.965856	Biso	1.000000	O
O	1.0	0.551998	0.347234	0.298707	Biso	1.000000	O

O	1.0	0.551847	0.347272	0.631995	Biso	1.000000	O
O	1.0	0.551816	0.347236	0.965421	Biso	1.000000	O
O	1.0	0.552316	0.847199	0.298989	Biso	1.000000	O
O	1.0	0.552175	0.847302	0.632339	Biso	1.000000	O
O	1.0	0.552108	0.847355	0.965546	Biso	1.000000	O
O	1.0	0.448248	0.151920	0.033993	Biso	1.000000	O
O	1.0	0.447809	0.152433	0.367968	Biso	1.000000	O
O	1.0	0.447811	0.152515	0.701140	Biso	1.000000	O
O	1.0	0.448055	0.652825	0.034649	Biso	1.000000	O
O	1.0	0.448235	0.653034	0.367948	Biso	1.000000	O
O	1.0	0.448002	0.652852	0.701272	Biso	1.000000	O
O	1.0	0.947645	0.152310	0.132386	Biso	1.000000	O
O	1.0	0.948384	0.151589	0.465576	Biso	1.000000	O
O	1.0	0.948170	0.152447	0.798990	Biso	1.000000	O
O	1.0	0.948327	0.652319	0.132415	Biso	1.000000	O
O	1.0	0.948173	0.652450	0.465726	Biso	1.000000	O
O	1.0	0.948223	0.652322	0.799043	Biso	1.000000	O
O	1.0	0.050441	0.352167	0.195501	Biso	1.000000	O
O	1.0	0.051520	0.347267	0.531717	Biso	1.000000	O
O	1.0	0.051605	0.348032	0.865444	Biso	1.000000	O
O	1.0	0.052213	0.849629	0.201057	Biso	1.000000	O
O	1.0	0.051803	0.847696	0.534701	Biso	1.000000	O
O	1.0	0.051942	0.847770	0.868157	Biso	1.000000	O
Si	1.0	0.270908	0.170549	0.018500	Biso	1.000000	Si
Si	1.0	0.271676	0.169682	0.350624	Biso	1.000000	Si
Si	1.0	0.271833	0.170458	0.684517	Biso	1.000000	Si
Si	1.0	0.271559	0.671200	0.017641	Biso	1.000000	Si
Si	1.0	0.271710	0.671656	0.351338	Biso	1.000000	Si
Si	1.0	0.271703	0.671255	0.684711	Biso	1.000000	Si
Si	1.0	0.728382	0.329114	0.315088	Biso	1.000000	Si
Si	1.0	0.728122	0.329081	0.648784	Biso	1.000000	Si
Si	1.0	0.728048	0.329201	0.981976	Biso	1.000000	Si
Si	1.0	0.728358	0.829072	0.315856	Biso	1.000000	Si
Si	1.0	0.728356	0.829067	0.649417	Biso	1.000000	Si
Si	1.0	0.728494	0.829098	0.982574	Biso	1.000000	Si
Si	1.0	0.228080	0.328141	0.185531	Biso	1.000000	Si
Si	1.0	0.227817	0.330086	0.515726	Biso	1.000000	Si
Si	1.0	0.227980	0.329073	0.850810	Biso	1.000000	Si
Si	1.0	0.228412	0.828976	0.183930	Biso	1.000000	Si
Si	1.0	0.228296	0.829910	0.517901	Biso	1.000000	Si
Si	1.0	0.228413	0.829380	0.851349	Biso	1.000000	Si
Si	1.0	0.771627	0.170808	0.149158	Biso	1.000000	Si
Si	1.0	0.771394	0.170499	0.482387	Biso	1.000000	Si
Si	1.0	0.771565	0.170859	0.815647	Biso	1.000000	Si
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Si	1.0	0.771782	0.670712	0.482324	Biso	1.000000	Si
Si	1.0	0.771723	0.670669	0.815652	Biso	1.000000	Si
Si	1.0	0.728419	0.420732	0.148634	Biso	1.000000	Si
Si	1.0	0.728280	0.420637	0.482031	Biso	1.000000	Si
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Si	1.0	0.728298	0.920738	0.149214	Biso	1.000000	Si
Si	1.0	0.728060	0.920571	0.482647	Biso	1.000000	Si
Si	1.0	0.728396	0.920830	0.815996	Biso	1.000000	Si
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Si	1.0	0.271492	0.079310	0.851378	Biso	1.000000	Si
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model 7

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# CRYSTAL DATA

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\_symmetry\_space\_group\_name\_H-M 'P 1'  
\_symmetry\_Int\_Tables\_number 1

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'x, y, z'

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\_atom\_site\_occupancy  
\_atom\_site\_fract\_x  
\_atom\_site\_fract\_y  
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\_atom\_site\_B\_iso\_or\_equiv  
\_atom\_site\_type\_symbol  
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O	1.0	0.437342	0.420097	0.233466	Biso	1.000000	O
O	1.0	0.437331	0.420409	0.567243	Biso	1.000000	O
O	1.0	0.436922	0.420107	0.900463	Biso	1.000000	O
O	1.0	0.437473	0.919680	0.233555	Biso	1.000000	O
O	1.0	0.437236	0.920219	0.567117	Biso	1.000000	O
O	1.0	0.437273	0.920131	0.900400	Biso	1.000000	O
O	1.0	0.563005	0.079746	0.099571	Biso	1.000000	O
O	1.0	0.562985	0.079816	0.433072	Biso	1.000000	O
O	1.0	0.562815	0.079772	0.766501	Biso	1.000000	O
O	1.0	0.562705	0.579472	0.099663	Biso	1.000000	O
O	1.0	0.563224	0.580238	0.432986	Biso	1.000000	O
O	1.0	0.562727	0.579843	0.766350	Biso	1.000000	O
O	1.0	0.062769	0.079262	0.066685	Biso	1.000000	O
O	1.0	0.062032	0.077053	0.397479	Biso	1.000000	O
O	1.0	0.062883	0.079968	0.733848	Biso	1.000000	O
O	1.0	0.062583	0.579685	0.067292	Biso	1.000000	O
O	1.0	0.062833	0.580573	0.401107	Biso	1.000000	O
O	1.0	0.062746	0.580317	0.733590	Biso	1.000000	O
O	1.0	0.938124	0.419706	0.267241	Biso	1.000000	O
O	1.0	0.936981	0.421059	0.600145	Biso	1.000000	O
O	1.0	0.936675	0.420471	0.931793	Biso	1.000000	O
O	1.0	0.937360	0.920842	0.266266	Biso	1.000000	O
O	1.0	0.936999	0.920287	0.599839	Biso	1.000000	O
O	1.0	0.937302	0.920475	0.933238	Biso	1.000000	O
O	1.0	0.311329	0.250810	0.015874	Biso	1.000000	O
O	1.0	0.310882	0.249295	0.347363	Biso	1.000000	O
O	1.0	0.311556	0.250940	0.681415	Biso	1.000000	O
O	1.0	0.311194	0.750551	0.014885	Biso	1.000000	O
O	1.0	0.311359	0.751282	0.348068	Biso	1.000000	O
O	1.0	0.311259	0.751190	0.681671	Biso	1.000000	O
O	1.0	0.688795	0.249070	0.318386	Biso	1.000000	O
O	1.0	0.688698	0.249101	0.651893	Biso	1.000000	O
O	1.0	0.688464	0.249180	0.985057	Biso	1.000000	O
O	1.0	0.688650	0.748947	0.318450	Biso	1.000000	O
O	1.0	0.688600	0.749106	0.652039	Biso	1.000000	O



O	1.0	0.688664	0.749044	0.985214	Biso	1.000000	O
O	1.0	0.190679	0.247530	0.190382	Biso	1.000000	O
O	1.0	0.188904	0.249748	0.512419	Biso	1.000000	O
O	1.0	0.188524	0.248428	0.848097	Biso	1.000000	O
O	1.0	0.188203	0.749206	0.181403	Biso	1.000000	O
O	1.0	0.187859	0.750500	0.514199	Biso	1.000000	O
O	1.0	0.188383	0.749334	0.848517	Biso	1.000000	O
O	1.0	0.811843	0.250872	0.152074	Biso	1.000000	O
O	1.0	0.812190	0.250642	0.484804	Biso	1.000000	O
O	1.0	0.811623	0.250881	0.817995	Biso	1.000000	O
O	1.0	0.811383	0.750899	0.151490	Biso	1.000000	O
O	1.0	0.811463	0.751053	0.484973	Biso	1.000000	O
O	1.0	0.811471	0.751044	0.818593	Biso	1.000000	O
O	1.0	0.688622	0.000822	0.151852	Biso	1.000000	O
O	1.0	0.688506	0.000790	0.485136	Biso	1.000000	O
O	1.0	0.688631	0.000943	0.818636	Biso	1.000000	O
O	1.0	0.688764	0.500779	0.151764	Biso	1.000000	O
O	1.0	0.688286	0.500815	0.485093	Biso	1.000000	O
O	1.0	0.688484	0.500898	0.818405	Biso	1.000000	O
O	1.0	0.310995	0.498646	0.181928	Biso	1.000000	O
O	1.0	0.311683	0.499680	0.515075	Biso	1.000000	O
O	1.0	0.311244	0.498861	0.848079	Biso	1.000000	O
O	1.0	0.311816	0.997587	0.180853	Biso	1.000000	O
O	1.0	0.311436	0.998714	0.515218	Biso	1.000000	O
O	1.0	0.311408	0.999490	0.848521	Biso	1.000000	O
O	1.0	0.812052	0.499070	0.318512	Biso	1.000000	O
O	1.0	0.811250	0.499316	0.651951	Biso	1.000000	O
O	1.0	0.811369	0.499040	0.984865	Biso	1.000000	O
O	1.0	0.810824	0.998573	0.318335	Biso	1.000000	O
O	1.0	0.811399	0.998959	0.651807	Biso	1.000000	O
O	1.0	0.811746	0.999368	0.985294	Biso	1.000000	O
O	1.0	0.189019	0.001512	0.015432	Biso	1.000000	O
O	1.0	0.186929	0.001116	0.345852	Biso	1.000000	O
O	1.0	0.188445	0.001513	0.681474	Biso	1.000000	O
O	1.0	0.187422	0.499005	0.017465	Biso	1.000000	O
O	1.0	0.191073	0.505365	0.351835	Biso	1.000000	O
O	1.0	0.188573	0.500953	0.681302	Biso	1.000000	O
O	1.0	0.432340	0.241029	0.229791	Biso	1.000000	O
O	1.0	0.432478	0.241179	0.563026	Biso	1.000000	O
O	1.0	0.432095	0.241046	0.896450	Biso	1.000000	O
O	1.0	0.432592	0.741022	0.229373	Biso	1.000000	O
O	1.0	0.432152	0.741472	0.562986	Biso	1.000000	O
O	1.0	0.432281	0.741130	0.896339	Biso	1.000000	O
O	1.0	0.567362	0.258684	0.103838	Biso	1.000000	O
O	1.0	0.567796	0.258585	0.437085	Biso	1.000000	O
O	1.0	0.567443	0.258719	0.770464	Biso	1.000000	O
O	1.0	0.567656	0.758489	0.103750	Biso	1.000000	O
O	1.0	0.567435	0.758627	0.437156	Biso	1.000000	O
O	1.0	0.567422	0.758745	0.770577	Biso	1.000000	O
O	1.0	0.067780	0.259642	0.063332	Biso	1.000000	O
O	1.0	0.056586	0.250850	0.404509	Biso	1.000000	O
O	1.0	0.067605	0.259299	0.728373	Biso	1.000000	O
O	1.0	0.067806	0.759222	0.063116	Biso	1.000000	O
O	1.0	0.067603	0.759007	0.396300	Biso	1.000000	O
O	1.0	0.067734	0.759115	0.729926	Biso	1.000000	O
O	1.0	0.933812	0.240278	0.269595	Biso	1.000000	O
O	1.0	0.932769	0.240622	0.602959	Biso	1.000000	O
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
O	1.0	0.932271	0.509823	0.437497	Biso	1.000000	O
O	1.0	0.932136	0.509337	0.770209	Biso	1.000000	O

O	1.0	0.067895	0.492384	0.233505	Biso	1.000000	O
O	1.0	0.067239	0.492189	0.563312	Biso	1.000000	O
O	1.0	0.067279	0.491551	0.895138	Biso	1.000000	O
O	1.0	0.068871	0.991395	0.230915	Biso	1.000000	O
O	1.0	0.067324	0.991486	0.563195	Biso	1.000000	O
O	1.0	0.067914	0.991505	0.896588	Biso	1.000000	O
O	1.0	0.305892	0.108011	0.278863	Biso	1.000000	O
O	1.0	0.302807	0.110116	0.612504	Biso	1.000000	O
O	1.0	0.302197	0.110760	0.945748	Biso	1.000000	O
O	1.0	0.303204	0.610817	0.278428	Biso	1.000000	O
O	1.0	0.303131	0.610803	0.612080	Biso	1.000000	O
O	1.0	0.302766	0.609832	0.945481	Biso	1.000000	O
O	1.0	0.697034	0.389675	0.054586	Biso	1.000000	O
O	1.0	0.697303	0.389543	0.387724	Biso	1.000000	O
O	1.0	0.696853	0.389695	0.721036	Biso	1.000000	O
O	1.0	0.697029	0.889600	0.054703	Biso	1.000000	O
O	1.0	0.696895	0.889384	0.388138	Biso	1.000000	O
O	1.0	0.696924	0.889685	0.721494	Biso	1.000000	O
O	1.0	0.195448	0.382335	0.108551	Biso	1.000000	O
O	1.0	0.198232	0.391695	0.445205	Biso	1.000000	O
O	1.0	0.196804	0.388935	0.777379	Biso	1.000000	O
O	1.0	0.196932	0.889792	0.111832	Biso	1.000000	O
O	1.0	0.196732	0.891590	0.445128	Biso	1.000000	O
O	1.0	0.196805	0.889884	0.778600	Biso	1.000000	O
O	1.0	0.802878	0.109914	0.221062	Biso	1.000000	O
O	1.0	0.803093	0.110084	0.554493	Biso	1.000000	O
O	1.0	0.803183	0.110409	0.887857	Biso	1.000000	O
O	1.0	0.803371	0.610542	0.221350	Biso	1.000000	O
O	1.0	0.803075	0.610568	0.554700	Biso	1.000000	O
O	1.0	0.803038	0.610431	0.887917	Biso	1.000000	O
O	1.0	0.697173	0.360242	0.221216	Biso	1.000000	O
O	1.0	0.696919	0.360169	0.554383	Biso	1.000000	O
O	1.0	0.696737	0.360346	0.887759	Biso	1.000000	O
O	1.0	0.696986	0.860286	0.221399	Biso	1.000000	O
O	1.0	0.696772	0.860307	0.554863	Biso	1.000000	O
O	1.0	0.696984	0.860387	0.888108	Biso	1.000000	O
O	1.0	0.302381	0.139331	0.112767	Biso	1.000000	O
O	1.0	0.304472	0.138818	0.446303	Biso	1.000000	O
O	1.0	0.302801	0.139878	0.778754	Biso	1.000000	O
O	1.0	0.302904	0.639179	0.112040	Biso	1.000000	O
O	1.0	0.302962	0.640172	0.445458	Biso	1.000000	O
O	1.0	0.302835	0.639715	0.778825	Biso	1.000000	O
O	1.0	0.803153	0.139803	0.054577	Biso	1.000000	O
O	1.0	0.803203	0.139081	0.387861	Biso	1.000000	O
O	1.0	0.803169	0.139506	0.721172	Biso	1.000000	O
O	1.0	0.803154	0.639602	0.054520	Biso	1.000000	O
O	1.0	0.803223	0.639705	0.387958	Biso	1.000000	O
O	1.0	0.803065	0.639883	0.721329	Biso	1.000000	O
O	1.0	0.199080	0.370770	0.275664	Biso	1.000000	O
O	1.0	0.197212	0.360404	0.610901	Biso	1.000000	O
O	1.0	0.196343	0.360408	0.943330	Biso	1.000000	O
O	1.0	0.196729	0.860629	0.278222	Biso	1.000000	O
O	1.0	0.196681	0.861294	0.611800	Biso	1.000000	O
O	1.0	0.196906	0.860931	0.945324	Biso	1.000000	O
O	1.0	0.448250	0.097084	0.201232	Biso	1.000000	O
O	1.0	0.448149	0.097218	0.534717	Biso	1.000000	O
O	1.0	0.447873	0.097213	0.868091	Biso	1.000000	O
O	1.0	0.447959	0.597095	0.201313	Biso	1.000000	O
O	1.0	0.448225	0.597676	0.534531	Biso	1.000000	O
O	1.0	0.447895	0.597359	0.867896	Biso	1.000000	O
O	1.0	0.552104	0.402644	0.132096	Biso	1.000000	O
O	1.0	0.551968	0.402481	0.465550	Biso	1.000000	O
O	1.0	0.551819	0.402655	0.798946	Biso	1.000000	O
O	1.0	0.552090	0.902382	0.132095	Biso	1.000000	O
O	1.0	0.551960	0.902553	0.465593	Biso	1.000000	O
O	1.0	0.552045	0.902658	0.798874	Biso	1.000000	O
O	1.0	0.051569	0.402892	0.032066	Biso	1.000000	O
O	1.0	0.052750	0.400208	0.368937	Biso	1.000000	O
O	1.0	0.051759	0.403840	0.701635	Biso	1.000000	O
O	1.0	0.052083	0.903460	0.034991	Biso	1.000000	O
O	1.0	0.052270	0.902657	0.368114	Biso	1.000000	O
O	1.0	0.051875	0.902943	0.701363	Biso	1.000000	O
O	1.0	0.945302	0.096077	0.299326	Biso	1.000000	O
O	1.0	0.947991	0.096964	0.632498	Biso	1.000000	O
O	1.0	0.948135	0.097210	0.965315	Biso	1.000000	O
O	1.0	0.947985	0.598100	0.299120	Biso	1.000000	O
O	1.0	0.947903	0.598083	0.632175	Biso	1.000000	O
O	1.0	0.947943	0.597589	0.965540	Biso	1.000000	O
O	1.0	0.552060	0.347228	0.298807	Biso	1.000000	O

O	1.0	0.552063	0.347437	0.632286	Biso	1.000000	O
O	1.0	0.551830	0.347315	0.965497	Biso	1.000000	O
O	1.0	0.552142	0.847142	0.298950	Biso	1.000000	O
O	1.0	0.551984	0.847341	0.632284	Biso	1.000000	O
O	1.0	0.552080	0.847204	0.965452	Biso	1.000000	O
O	1.0	0.447857	0.152577	0.034725	Biso	1.000000	O
O	1.0	0.448115	0.152411	0.367834	Biso	1.000000	O
O	1.0	0.448043	0.152612	0.701314	Biso	1.000000	O
O	1.0	0.447909	0.652646	0.034704	Biso	1.000000	O
O	1.0	0.448098	0.652823	0.367858	Biso	1.000000	O
O	1.0	0.447887	0.652848	0.701287	Biso	1.000000	O
O	1.0	0.947910	0.152823	0.131705	Biso	1.000000	O
O	1.0	0.946761	0.149012	0.466763	Biso	1.000000	O
O	1.0	0.948160	0.152630	0.798823	Biso	1.000000	O
O	1.0	0.948039	0.652950	0.132095	Biso	1.000000	O
O	1.0	0.948055	0.653767	0.465356	Biso	1.000000	O
O	1.0	0.948084	0.653147	0.798826	Biso	1.000000	O
O	1.0	0.051849	0.352458	0.196104	Biso	1.000000	O
O	1.0	0.051824	0.347812	0.535869	Biso	1.000000	O
O	1.0	0.051731	0.347284	0.867005	Biso	1.000000	O
O	1.0	0.052256	0.848675	0.200809	Biso	1.000000	O
O	1.0	0.051920	0.847731	0.534600	Biso	1.000000	O
O	1.0	0.051952	0.847642	0.868108	Biso	1.000000	O
Si	1.0	0.271210	0.170955	0.018068	Biso	1.000000	Si
Si	1.0	0.273615	0.167997	0.351434	Biso	1.000000	Si
Si	1.0	0.271302	0.171132	0.684178	Biso	1.000000	Si
Si	1.0	0.271450	0.670365	0.017619	Biso	1.000000	Si
Si	1.0	0.271645	0.670996	0.350794	Biso	1.000000	Si
Si	1.0	0.271540	0.671006	0.684263	Biso	1.000000	Si
Si	1.0	0.729031	0.329004	0.315649	Biso	1.000000	Si
Si	1.0	0.728470	0.329227	0.648931	Biso	1.000000	Si
Si	1.0	0.728307	0.329279	0.982280	Biso	1.000000	Si
Si	1.0	0.728369	0.829059	0.315919	Biso	1.000000	Si
Si	1.0	0.728342	0.829207	0.649358	Biso	1.000000	Si
Si	1.0	0.728460	0.829132	0.982527	Biso	1.000000	Si
Si	1.0	0.228529	0.333164	0.188354	Biso	1.000000	Si
Si	1.0	0.228527	0.329915	0.516028	Biso	1.000000	Si
Si	1.0	0.228183	0.328696	0.849523	Biso	1.000000	Si
Si	1.0	0.228384	0.828975	0.183646	Biso	1.000000	Si
Si	1.0	0.228053	0.830215	0.517464	Biso	1.000000	Si
Si	1.0	0.228190	0.829438	0.850832	Biso	1.000000	Si
Si	1.0	0.771860	0.170954	0.149226	Biso	1.000000	Si
Si	1.0	0.772165	0.170762	0.482114	Biso	1.000000	Si
Si	1.0	0.771787	0.170846	0.815567	Biso	1.000000	Si
Si	1.0	0.771799	0.670618	0.149128	Biso	1.000000	Si
Si	1.0	0.771750	0.670888	0.482406	Biso	1.000000	Si
Si	1.0	0.771632	0.670948	0.815832	Biso	1.000000	Si
Si	1.0	0.728760	0.420726	0.149167	Biso	1.000000	Si
Si	1.0	0.728392	0.420850	0.482310	Biso	1.000000	Si
Si	1.0	0.728252	0.420765	0.815564	Biso	1.000000	Si
Si	1.0	0.728384	0.920721	0.149239	Biso	1.000000	Si
Si	1.0	0.728219	0.920671	0.482649	Biso	1.000000	Si
Si	1.0	0.728414	0.920847	0.815949	Biso	1.000000	Si
Si	1.0	0.273374	0.077910	0.184538	Biso	1.000000	Si
Si	1.0	0.271571	0.078768	0.518248	Biso	1.000000	Si
Si	1.0	0.271398	0.079523	0.850901	Biso	1.000000	Si
Si	1.0	0.271280	0.578896	0.184442	Biso	1.000000	Si
Si	1.0	0.271408	0.579527	0.517586	Biso	1.000000	Si
Si	1.0	0.271446	0.578963	0.850701	Biso	1.000000	Si
Si	1.0	0.771532	0.079019	0.315809	Biso	1.000000	Si
Si	1.0	0.771714	0.079133	0.649004	Biso	1.000000	Si
Si	1.0	0.771793	0.079408	0.982429	Biso	1.000000	Si
Si	1.0	0.772112	0.579031	0.315698	Biso	1.000000	Si
Si	1.0	0.771618	0.579413	0.649174	Biso	1.000000	Si
Si	1.0	0.771655	0.579144	0.982414	Biso	1.000000	Si
Si	1.0	0.227520	0.419005	0.017170	Biso	1.000000	Si
Si	1.0	0.230024	0.424761	0.351784	Biso	1.000000	Si
Si	1.0	0.228256	0.420713	0.683247	Biso	1.000000	Si
Si	1.0	0.228693	0.921134	0.017382	Biso	1.000000	Si
Si	1.0	0.228292	0.920580	0.350029	Biso	1.000000	Si
Si	1.0	0.228264	0.921436	0.684283	Biso	1.000000	Si
Si	1.0	0.474115	0.168632	0.265977	Biso	1.000000	Si
Si	1.0	0.474025	0.168721	0.599306	Biso	1.000000	Si
Si	1.0	0.473833	0.168674	0.932662	Biso	1.000000	Si
Si	1.0	0.474045	0.668533	0.265883	Biso	1.000000	Si
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Si	1.0	0.473812	0.668600	0.932609	Biso	1.000000	Si
Si	1.0	0.526135	0.331338	0.067479	Biso	1.000000	Si
Si	1.0	0.526300	0.331092	0.400845	Biso	1.000000	Si

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Si	1.0	0.526289	0.831008	0.067384	Biso	1.000000	Si
Si	1.0	0.526091	0.831217	0.400929	Biso	1.000000	Si
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Si	1.0	0.025061	0.328670	0.433072	Biso	1.000000	Si
Si	1.0	0.026010	0.331638	0.764943	Biso	1.000000	Si
Si	1.0	0.026010	0.831572	0.099063	Biso	1.000000	Si
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Si	1.0	0.026073	0.831534	0.766082	Biso	1.000000	Si
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Si	1.0	0.473818	0.581400	0.765909	Biso	1.000000	Si
Si	1.0	0.973631	0.081386	0.067358	Biso	1.000000	Si
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Si	1.0	0.973636	0.581411	0.067482	Biso	1.000000	Si
Si	1.0	0.973968	0.581952	0.401039	Biso	1.000000	Si
Si	1.0	0.973809	0.581744	0.734015	Biso	1.000000	Si
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Si	1.0	0.025830	0.918930	0.599491	Biso	1.000000	Si
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model 8

#=====

# CRYSTAL DATA

#-----

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\_cell\_angle\_gamma 90  
\_symmetry\_space\_group\_name\_H-M 'P 1'  
\_symmetry\_Int\_Tables\_number 1

loop\_  
\_symmetry\_equiv\_pos\_as\_xyz  
'x, y, z'

loop\_  
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\_atom\_site\_occupancy  
\_atom\_site\_fract\_x  
\_atom\_site\_fract\_y  
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\_atom\_site\_B\_iso\_or\_equiv  
\_atom\_site\_type\_symbol  
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Mg 1.0 0.376086 0.326408 0.622090 Biso 1.000000 Mg  
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Fe 1.0 0.122903 0.179660 0.447501 Biso 1.000000 Fe  
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O	1.0	0.062812	0.670402	0.233809	Biso	1.000000	O
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O	1.0	0.437126	0.920150	0.900454	Biso	1.000000	O
O	1.0	0.562836	0.079679	0.099659	Biso	1.000000	O
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O	1.0	0.562806	0.079696	0.766436	Biso	1.000000	O
O	1.0	0.562733	0.579537	0.099678	Biso	1.000000	O
O	1.0	0.563319	0.580283	0.433048	Biso	1.000000	O
O	1.0	0.562659	0.579671	0.766372	Biso	1.000000	O
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
O	1.0	0.937184	0.919906	0.266260	Biso	1.000000	O
O	1.0	0.937430	0.920577	0.599663	Biso	1.000000	O
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
O	1.0	0.688404	0.249048	0.985113	Biso	1.000000	O
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
O	1.0	0.191323	0.247943	0.189976	Biso	1.000000	O
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
O	1.0	0.188479	0.749435	0.515215	Biso	1.000000	O
O	1.0	0.188463	0.749112	0.848410	Biso	1.000000	O
O	1.0	0.811333	0.250973	0.151874	Biso	1.000000	O
O	1.0	0.811546	0.250762	0.484868	Biso	1.000000	O
O	1.0	0.811454	0.250896	0.818118	Biso	1.000000	O
O	1.0	0.811442	0.750992	0.151557	Biso	1.000000	O
O	1.0	0.811614	0.750986	0.485122	Biso	1.000000	O
O	1.0	0.811601	0.750961	0.818470	Biso	1.000000	O
O	1.0	0.688558	0.000827	0.151831	Biso	1.000000	O
O	1.0	0.688670	0.000837	0.485169	Biso	1.000000	O
O	1.0	0.688663	0.000958	0.818549	Biso	1.000000	O
O	1.0	0.688785	0.500824	0.151737	Biso	1.000000	O
O	1.0	0.688500	0.500901	0.485231	Biso	1.000000	O
O	1.0	0.688465	0.500864	0.818487	Biso	1.000000	O
O	1.0	0.311067	0.498509	0.181974	Biso	1.000000	O
O	1.0	0.311309	0.499048	0.515088	Biso	1.000000	O
O	1.0	0.311137	0.498567	0.847871	Biso	1.000000	O
O	1.0	0.311726	0.998821	0.181406	Biso	1.000000	O
O	1.0	0.311075	0.998928	0.515329	Biso	1.000000	O
O	1.0	0.311354	0.999393	0.848535	Biso	1.000000	O
O	1.0	0.811891	0.499193	0.318407	Biso	1.000000	O
O	1.0	0.811276	0.499144	0.651704	Biso	1.000000	O
O	1.0	0.811441	0.499005	0.984987	Biso	1.000000	O
O	1.0	0.811402	0.998874	0.318539	Biso	1.000000	O
O	1.0	0.811808	0.999160	0.651686	Biso	1.000000	O
O	1.0	0.811454	0.999067	0.984949	Biso	1.000000	O
O	1.0	0.188497	0.001083	0.015060	Biso	1.000000	O
O	1.0	0.187613	0.000945	0.347588	Biso	1.000000	O
O	1.0	0.188709	0.001292	0.681525	Biso	1.000000	O
O	1.0	0.187537	0.499115	0.016985	Biso	1.000000	O
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
O	1.0	0.432519	0.241345	0.229924	Biso	1.000000	O
O	1.0	0.432914	0.241259	0.563191	Biso	1.000000	O
O	1.0	0.432326	0.241127	0.896441	Biso	1.000000	O
O	1.0	0.432476	0.741135	0.229471	Biso	1.000000	O
O	1.0	0.432371	0.741318	0.563035	Biso	1.000000	O
O	1.0	0.432286	0.741107	0.896338	Biso	1.000000	O
O	1.0	0.567390	0.258668	0.103832	Biso	1.000000	O
O	1.0	0.567799	0.258712	0.437130	Biso	1.000000	O
O	1.0	0.567496	0.258678	0.770450	Biso	1.000000	O
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
O	1.0	0.932380	0.241164	0.936715	Biso	1.000000	O
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
O	1.0	0.932229	0.508941	0.770117	Biso	1.000000	O



O	1.0	0.068064	0.492263	0.233617	Biso	1.000000	O
O	1.0	0.067312	0.491900	0.563208	Biso	1.000000	O
O	1.0	0.067316	0.491481	0.894994	Biso	1.000000	O
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
O	1.0	0.067672	0.991137	0.896310	Biso	1.000000	O
O	1.0	0.304169	0.109747	0.279075	Biso	1.000000	O
O	1.0	0.302961	0.110121	0.612863	Biso	1.000000	O
O	1.0	0.302294	0.110562	0.946036	Biso	1.000000	O
O	1.0	0.303142	0.610584	0.278462	Biso	1.000000	O
O	1.0	0.303199	0.610285	0.612224	Biso	1.000000	O
O	1.0	0.302827	0.609571	0.945466	Biso	1.000000	O
O	1.0	0.697061	0.389602	0.054606	Biso	1.000000	O
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
O	1.0	0.696970	0.889542	0.388036	Biso	1.000000	O
O	1.0	0.697085	0.889771	0.721386	Biso	1.000000	O
O	1.0	0.195660	0.382810	0.108287	Biso	1.000000	O
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
O	1.0	0.196884	0.889626	0.112142	Biso	1.000000	O
O	1.0	0.196790	0.889969	0.445404	Biso	1.000000	O
O	1.0	0.196836	0.889854	0.778805	Biso	1.000000	O
O	1.0	0.802754	0.110112	0.221135	Biso	1.000000	O
O	1.0	0.803218	0.110306	0.554544	Biso	1.000000	O
O	1.0	0.803076	0.110358	0.887841	Biso	1.000000	O
O	1.0	0.803342	0.610556	0.221266	Biso	1.000000	O
O	1.0	0.803150	0.610424	0.554652	Biso	1.000000	O
O	1.0	0.803101	0.610346	0.887926	Biso	1.000000	O
O	1.0	0.696976	0.360373	0.221211	Biso	1.000000	O
O	1.0	0.696918	0.360246	0.554526	Biso	1.000000	O
O	1.0	0.696774	0.360255	0.887926	Biso	1.000000	O
O	1.0	0.696988	0.860354	0.221346	Biso	1.000000	O
O	1.0	0.697035	0.860367	0.554725	Biso	1.000000	O
O	1.0	0.697089	0.860439	0.888011	Biso	1.000000	O
O	1.0	0.303436	0.140093	0.112888	Biso	1.000000	O
O	1.0	0.305287	0.139715	0.446945	Biso	1.000000	O
O	1.0	0.302698	0.139832	0.779185	Biso	1.000000	O
O	1.0	0.302952	0.638977	0.112000	Biso	1.000000	O
O	1.0	0.303040	0.639606	0.445385	Biso	1.000000	O
O	1.0	0.302977	0.639439	0.778855	Biso	1.000000	O
O	1.0	0.802763	0.139657	0.054475	Biso	1.000000	O
O	1.0	0.802928	0.139473	0.387803	Biso	1.000000	O
O	1.0	0.803250	0.139639	0.721147	Biso	1.000000	O
O	1.0	0.803168	0.639618	0.054534	Biso	1.000000	O
O	1.0	0.803284	0.639677	0.387994	Biso	1.000000	O
O	1.0	0.803151	0.639699	0.721330	Biso	1.000000	O
O	1.0	0.199048	0.371089	0.275134	Biso	1.000000	O
O	1.0	0.196786	0.358576	0.610356	Biso	1.000000	O
O	1.0	0.196486	0.360498	0.942967	Biso	1.000000	O
O	1.0	0.196851	0.860169	0.278705	Biso	1.000000	O
O	1.0	0.196872	0.860690	0.612154	Biso	1.000000	O
O	1.0	0.196786	0.860458	0.945490	Biso	1.000000	O
O	1.0	0.448156	0.097421	0.201311	Biso	1.000000	O
O	1.0	0.448069	0.097298	0.534777	Biso	1.000000	O
O	1.0	0.447866	0.097301	0.868036	Biso	1.000000	O
O	1.0	0.447997	0.597120	0.201377	Biso	1.000000	O
O	1.0	0.448263	0.597520	0.534552	Biso	1.000000	O
O	1.0	0.447849	0.597250	0.867893	Biso	1.000000	O
O	1.0	0.552138	0.402671	0.132075	Biso	1.000000	O
O	1.0	0.552204	0.402676	0.465687	Biso	1.000000	O
O	1.0	0.551831	0.402635	0.798937	Biso	1.000000	O
O	1.0	0.551924	0.902507	0.132163	Biso	1.000000	O
O	1.0	0.551989	0.902681	0.465540	Biso	1.000000	O
O	1.0	0.551944	0.902655	0.798886	Biso	1.000000	O
O	1.0	0.051551	0.402921	0.031977	Biso	1.000000	O
O	1.0	0.052957	0.398560	0.367731	Biso	1.000000	O
O	1.0	0.051828	0.402933	0.701175	Biso	1.000000	O
O	1.0	0.052031	0.902392	0.034643	Biso	1.000000	O
O	1.0	0.051877	0.902790	0.368058	Biso	1.000000	O
O	1.0	0.052109	0.902931	0.701245	Biso	1.000000	O
O	1.0	0.946215	0.097137	0.299310	Biso	1.000000	O
O	1.0	0.948757	0.097637	0.631973	Biso	1.000000	O
O	1.0	0.947726	0.097055	0.964801	Biso	1.000000	O
O	1.0	0.948060	0.597547	0.299110	Biso	1.000000	O
O	1.0	0.948016	0.597619	0.632166	Biso	1.000000	O
O	1.0	0.948032	0.597361	0.965565	Biso	1.000000	O
O	1.0	0.552249	0.347415	0.298850	Biso	1.000000	O

O	1.0	0.552084	0.347437	0.632306	Biso	1.000000	O
O	1.0	0.551835	0.347301	0.965517	Biso	1.000000	O
O	1.0	0.552055	0.847269	0.298904	Biso	1.000000	O
O	1.0	0.551967	0.847367	0.632237	Biso	1.000000	O
O	1.0	0.551958	0.847252	0.965502	Biso	1.000000	O
O	1.0	0.447967	0.152667	0.034702	Biso	1.000000	O
O	1.0	0.448145	0.152849	0.368131	Biso	1.000000	O
O	1.0	0.447993	0.152634	0.701435	Biso	1.000000	O
O	1.0	0.447962	0.652578	0.034619	Biso	1.000000	O
O	1.0	0.448205	0.652839	0.367882	Biso	1.000000	O
O	1.0	0.447940	0.652634	0.701248	Biso	1.000000	O
O	1.0	0.946390	0.153162	0.131006	Biso	1.000000	O
O	1.0	0.946328	0.151745	0.466054	Biso	1.000000	O
O	1.0	0.948316	0.152950	0.798430	Biso	1.000000	O
O	1.0	0.948045	0.652542	0.132247	Biso	1.000000	O
O	1.0	0.947948	0.652915	0.465582	Biso	1.000000	O
O	1.0	0.948154	0.652792	0.798858	Biso	1.000000	O
O	1.0	0.051863	0.352392	0.195591	Biso	1.000000	O
O	1.0	0.051871	0.347964	0.535322	Biso	1.000000	O
O	1.0	0.051736	0.347359	0.866805	Biso	1.000000	O
O	1.0	0.051819	0.846450	0.201506	Biso	1.000000	O
O	1.0	0.051992	0.847445	0.534673	Biso	1.000000	O
O	1.0	0.051986	0.847336	0.867917	Biso	1.000000	O
Si	1.0	0.271352	0.170962	0.018439	Biso	1.000000	Si
Si	1.0	0.273904	0.169449	0.352326	Biso	1.000000	Si
Si	1.0	0.271539	0.170860	0.684712	Biso	1.000000	Si
Si	1.0	0.271512	0.670210	0.017617	Biso	1.000000	Si
Si	1.0	0.271614	0.670855	0.350834	Biso	1.000000	Si
Si	1.0	0.271631	0.670720	0.684345	Biso	1.000000	Si
Si	1.0	0.728649	0.329196	0.315589	Biso	1.000000	Si
Si	1.0	0.728272	0.329186	0.649110	Biso	1.000000	Si
Si	1.0	0.728388	0.329062	0.982451	Biso	1.000000	Si
Si	1.0	0.728467	0.829168	0.315804	Biso	1.000000	Si
Si	1.0	0.728519	0.829291	0.649258	Biso	1.000000	Si
Si	1.0	0.728485	0.829209	0.982511	Biso	1.000000	Si
Si	1.0	0.228875	0.333453	0.187845	Biso	1.000000	Si
Si	1.0	0.228602	0.329943	0.515270	Biso	1.000000	Si
Si	1.0	0.228332	0.328226	0.849570	Biso	1.000000	Si
Si	1.0	0.228260	0.829043	0.184163	Biso	1.000000	Si
Si	1.0	0.228222	0.829545	0.517576	Biso	1.000000	Si
Si	1.0	0.228159	0.829285	0.851020	Biso	1.000000	Si
Si	1.0	0.771679	0.170854	0.149122	Biso	1.000000	Si
Si	1.0	0.771770	0.170687	0.482263	Biso	1.000000	Si
Si	1.0	0.771717	0.170780	0.815685	Biso	1.000000	Si
Si	1.0	0.771816	0.670790	0.149077	Biso	1.000000	Si
Si	1.0	0.771833	0.670895	0.482430	Biso	1.000000	Si
Si	1.0	0.771727	0.670887	0.815835	Biso	1.000000	Si
Si	1.0	0.728723	0.420748	0.149098	Biso	1.000000	Si
Si	1.0	0.728322	0.420821	0.482389	Biso	1.000000	Si
Si	1.0	0.728191	0.420714	0.815796	Biso	1.000000	Si
Si	1.0	0.728513	0.920812	0.149200	Biso	1.000000	Si
Si	1.0	0.728460	0.920742	0.482469	Biso	1.000000	Si
Si	1.0	0.728586	0.920922	0.815917	Biso	1.000000	Si
Si	1.0	0.272025	0.078856	0.184357	Biso	1.000000	Si
Si	1.0	0.272123	0.079334	0.518184	Biso	1.000000	Si
Si	1.0	0.271306	0.079342	0.851414	Biso	1.000000	Si
Si	1.0	0.271336	0.578779	0.184380	Biso	1.000000	Si
Si	1.0	0.271542	0.579295	0.517621	Biso	1.000000	Si
Si	1.0	0.271524	0.578774	0.850732	Biso	1.000000	Si
Si	1.0	0.771624	0.078989	0.315653	Biso	1.000000	Si
Si	1.0	0.771818	0.079149	0.649039	Biso	1.000000	Si
Si	1.0	0.771620	0.079153	0.982369	Biso	1.000000	Si
Si	1.0	0.772059	0.579246	0.315621	Biso	1.000000	Si
Si	1.0	0.771662	0.579317	0.649161	Biso	1.000000	Si
Si	1.0	0.771705	0.579123	0.982477	Biso	1.000000	Si
Si	1.0	0.227697	0.419170	0.016746	Biso	1.000000	Si
Si	1.0	0.230078	0.424797	0.351255	Biso	1.000000	Si
Si	1.0	0.228030	0.419638	0.682968	Biso	1.000000	Si
Si	1.0	0.228179	0.920891	0.017719	Biso	1.000000	Si
Si	1.0	0.227880	0.921071	0.350634	Biso	1.000000	Si
Si	1.0	0.228332	0.921027	0.684322	Biso	1.000000	Si
Si	1.0	0.474088	0.168759	0.265977	Biso	1.000000	Si
Si	1.0	0.474126	0.168562	0.599496	Biso	1.000000	Si
Si	1.0	0.473891	0.168640	0.932708	Biso	1.000000	Si
Si	1.0	0.474042	0.668720	0.265853	Biso	1.000000	Si
Si	1.0	0.473954	0.668850	0.599344	Biso	1.000000	Si
Si	1.0	0.473819	0.668586	0.932588	Biso	1.000000	Si
Si	1.0	0.526122	0.331293	0.067510	Biso	1.000000	Si
Si	1.0	0.526632	0.331398	0.400843	Biso	1.000000	Si

Si	1.0	0.526161	0.331300	0.734215	Biso	1.000000	Si
Si	1.0	0.526081	0.831139	0.067480	Biso	1.000000	Si
Si	1.0	0.526120	0.831291	0.400872	Biso	1.000000	Si
Si	1.0	0.526073	0.831309	0.734208	Biso	1.000000	Si
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Si	1.0	0.024378	0.330918	0.433964	Biso	1.000000	Si
Si	1.0	0.025720	0.331278	0.765292	Biso	1.000000	Si
Si	1.0	0.026150	0.830980	0.099286	Biso	1.000000	Si
Si	1.0	0.026083	0.831418	0.432700	Biso	1.000000	Si
Si	1.0	0.026193	0.831481	0.765948	Biso	1.000000	Si
Si	1.0	0.975018	0.168085	0.233656	Biso	1.000000	Si
Si	1.0	0.973667	0.168691	0.566682	Biso	1.000000	Si
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Si	1.0	0.525926	0.418673	0.900901	Biso	1.000000	Si
Si	1.0	0.526168	0.918542	0.234161	Biso	1.000000	Si
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model 9

#=====

# CRYSTAL DATA

#-----

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\_cell\_angle\_gamma 90  
\_symmetry\_space\_group\_name\_H-M 'P 1'  
\_symmetry\_Int\_Tables\_number 1

loop\_  
\_symmetry\_equiv\_pos\_as\_xyz  
'x, y, z'

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\_atom\_site\_occupancy  
\_atom\_site\_fract\_x  
\_atom\_site\_fract\_y  
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\_atom\_site\_B\_iso\_or\_equiv  
\_atom\_site\_type\_symbol  
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O	1.0	0.063012	0.670614	0.233921	Biso	1.000000	O
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O	1.0	0.437378	0.919928	0.567216	Biso	1.000000	O
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O	1.0	0.562648	0.079683	0.099605	Biso	1.000000	O
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
O	1.0	0.562632	0.579613	0.099557	Biso	1.000000	O
O	1.0	0.562821	0.579931	0.432953	Biso	1.000000	O
O	1.0	0.562781	0.579737	0.766287	Biso	1.000000	O
O	1.0	0.063876	0.084433	0.069877	Biso	1.000000	O
O	1.0	0.062379	0.079529	0.401021	Biso	1.000000	O
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O	1.0	0.062941	0.579431	0.733760	Biso	1.000000	O
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O	1.0	0.937100	0.419973	0.598703	Biso	1.000000	O
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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
O	1.0	0.311456	0.499359	0.515323	Biso	1.000000	O
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
O	1.0	0.311305	0.999549	0.848984	Biso	1.000000	O
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
O	1.0	0.811565	0.498991	0.984835	Biso	1.000000	O
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
O	1.0	0.567442	0.258749	0.436984	Biso	1.000000	O
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
O	1.0	0.303360	0.610894	0.278988	Biso	1.000000	O
O	1.0	0.303252	0.610627	0.612499	Biso	1.000000	O
O	1.0	0.302971	0.610191	0.945726	Biso	1.000000	O
O	1.0	0.696903	0.389681	0.054320	Biso	1.000000	O
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
O	1.0	0.697062	0.889637	0.387884	Biso	1.000000	O
O	1.0	0.697033	0.889572	0.721303	Biso	1.000000	O
O	1.0	0.195312	0.388163	0.110893	Biso	1.000000	O
O	1.0	0.196556	0.389888	0.444035	Biso	1.000000	O
O	1.0	0.196562	0.388630	0.777954	Biso	1.000000	O
O	1.0	0.196542	0.889944	0.112690	Biso	1.000000	O
O	1.0	0.196918	0.889658	0.445621	Biso	1.000000	O
O	1.0	0.196736	0.889612	0.779202	Biso	1.000000	O
O	1.0	0.803017	0.110417	0.221146	Biso	1.000000	O
O	1.0	0.803075	0.110393	0.554476	Biso	1.000000	O
O	1.0	0.803335	0.110314	0.887935	Biso	1.000000	O
O	1.0	0.803140	0.610505	0.221031	Biso	1.000000	O
O	1.0	0.803167	0.610256	0.554413	Biso	1.000000	O
O	1.0	0.803237	0.610220	0.887808	Biso	1.000000	O
O	1.0	0.696866	0.360321	0.220967	Biso	1.000000	O
O	1.0	0.696807	0.360307	0.554339	Biso	1.000000	O
O	1.0	0.696793	0.360202	0.887632	Biso	1.000000	O
O	1.0	0.697346	0.860594	0.221162	Biso	1.000000	O
O	1.0	0.697029	0.860288	0.554606	Biso	1.000000	O
O	1.0	0.697068	0.860314	0.888042	Biso	1.000000	O
O	1.0	0.305105	0.139616	0.111938	Biso	1.000000	O
O	1.0	0.304836	0.139588	0.446701	Biso	1.000000	O
O	1.0	0.303002	0.139649	0.779361	Biso	1.000000	O
O	1.0	0.303255	0.640111	0.112269	Biso	1.000000	O
O	1.0	0.303271	0.640017	0.445734	Biso	1.000000	O
O	1.0	0.302966	0.639820	0.779165	Biso	1.000000	O
O	1.0	0.802875	0.140098	0.054502	Biso	1.000000	O
O	1.0	0.802977	0.139682	0.387682	Biso	1.000000	O
O	1.0	0.803285	0.139522	0.721123	Biso	1.000000	O
O	1.0	0.803200	0.639591	0.054458	Biso	1.000000	O
O	1.0	0.803096	0.639532	0.387737	Biso	1.000000	O
O	1.0	0.803197	0.639500	0.721150	Biso	1.000000	O
O	1.0	0.197679	0.364248	0.274781	Biso	1.000000	O
O	1.0	0.196411	0.360466	0.610997	Biso	1.000000	O
O	1.0	0.196331	0.360004	0.944547	Biso	1.000000	O
O	1.0	0.196845	0.859287	0.279153	Biso	1.000000	O
O	1.0	0.196857	0.860482	0.612396	Biso	1.000000	O
O	1.0	0.196530	0.860862	0.945835	Biso	1.000000	O
O	1.0	0.447917	0.097473	0.201175	Biso	1.000000	O
O	1.0	0.448259	0.097013	0.534745	Biso	1.000000	O
O	1.0	0.447759	0.097323	0.867935	Biso	1.000000	O
O	1.0	0.447974	0.597514	0.201103	Biso	1.000000	O
O	1.0	0.448057	0.597470	0.534529	Biso	1.000000	O
O	1.0	0.447980	0.597524	0.867748	Biso	1.000000	O
O	1.0	0.551899	0.402614	0.132118	Biso	1.000000	O
O	1.0	0.551861	0.402572	0.465337	Biso	1.000000	O
O	1.0	0.551848	0.402661	0.798770	Biso	1.000000	O
O	1.0	0.551744	0.902798	0.132224	Biso	1.000000	O
O	1.0	0.552144	0.902656	0.465559	Biso	1.000000	O
O	1.0	0.552021	0.902645	0.798986	Biso	1.000000	O
O	1.0	0.052192	0.397546	0.029916	Biso	1.000000	O
O	1.0	0.051968	0.400803	0.365465	Biso	1.000000	O
O	1.0	0.051854	0.401266	0.699331	Biso	1.000000	O
O	1.0	0.051873	0.903189	0.034864	Biso	1.000000	O
O	1.0	0.052022	0.902921	0.368182	Biso	1.000000	O
O	1.0	0.051857	0.902709	0.701229	Biso	1.000000	O
O	1.0	0.948068	0.098400	0.298813	Biso	1.000000	O
O	1.0	0.948375	0.097757	0.632437	Biso	1.000000	O
O	1.0	0.949383	0.097706	0.966043	Biso	1.000000	O
O	1.0	0.948253	0.597513	0.299334	Biso	1.000000	O
O	1.0	0.948224	0.597153	0.632244	Biso	1.000000	O
O	1.0	0.948349	0.597014	0.965764	Biso	1.000000	O
O	1.0	0.551905	0.347290	0.298738	Biso	1.000000	O



O	1.0	0.552000	0.347283	0.632035	Biso	1.000000	O
O	1.0	0.551747	0.347345	0.965477	Biso	1.000000	O
O	1.0	0.551735	0.847565	0.298742	Biso	1.000000	O
O	1.0	0.552193	0.847241	0.632327	Biso	1.000000	O
O	1.0	0.551903	0.847421	0.965647	Biso	1.000000	O
O	1.0	0.448084	0.152454	0.034118	Biso	1.000000	O
O	1.0	0.448216	0.152565	0.367970	Biso	1.000000	O
O	1.0	0.447954	0.152575	0.701333	Biso	1.000000	O
O	1.0	0.447958	0.652601	0.034477	Biso	1.000000	O
O	1.0	0.448036	0.652811	0.367867	Biso	1.000000	O
O	1.0	0.448046	0.652714	0.701202	Biso	1.000000	O
O	1.0	0.946020	0.154097	0.131645	Biso	1.000000	O
O	1.0	0.947816	0.152825	0.465568	Biso	1.000000	O
O	1.0	0.948626	0.152489	0.799311	Biso	1.000000	O
O	1.0	0.948339	0.651682	0.132463	Biso	1.000000	O
O	1.0	0.948169	0.652232	0.465769	Biso	1.000000	O
O	1.0	0.948179	0.652173	0.799081	Biso	1.000000	O
O	1.0	0.051136	0.352187	0.196418	Biso	1.000000	O
O	1.0	0.051392	0.347361	0.531955	Biso	1.000000	O
O	1.0	0.051730	0.346499	0.865549	Biso	1.000000	O
O	1.0	0.052165	0.848018	0.201337	Biso	1.000000	O
O	1.0	0.051825	0.847181	0.534653	Biso	1.000000	O
O	1.0	0.051972	0.847996	0.867865	Biso	1.000000	O
Si	1.0	0.272019	0.171638	0.019193	Biso	1.000000	Si
Si	1.0	0.270490	0.170498	0.352161	Biso	1.000000	Si
Si	1.0	0.272044	0.170248	0.684478	Biso	1.000000	Si
Si	1.0	0.271543	0.670818	0.017739	Biso	1.000000	Si
Si	1.0	0.271789	0.671084	0.351195	Biso	1.000000	Si
Si	1.0	0.271645	0.670949	0.684604	Biso	1.000000	Si
Si	1.0	0.728238	0.329102	0.315378	Biso	1.000000	Si
Si	1.0	0.728066	0.329192	0.648863	Biso	1.000000	Si
Si	1.0	0.728132	0.329146	0.982194	Biso	1.000000	Si
Si	1.0	0.728553	0.829288	0.315649	Biso	1.000000	Si
Si	1.0	0.728447	0.829132	0.649100	Biso	1.000000	Si
Si	1.0	0.728552	0.829249	0.982597	Biso	1.000000	Si
Si	1.0	0.226158	0.327567	0.184662	Biso	1.000000	Si
Si	1.0	0.227861	0.329511	0.516000	Biso	1.000000	Si
Si	1.0	0.228415	0.328745	0.850474	Biso	1.000000	Si
Si	1.0	0.228179	0.828978	0.184314	Biso	1.000000	Si
Si	1.0	0.228348	0.829315	0.517862	Biso	1.000000	Si
Si	1.0	0.228202	0.829365	0.851517	Biso	1.000000	Si
Si	1.0	0.771372	0.171003	0.149269	Biso	1.000000	Si
Si	1.0	0.771407	0.170674	0.482294	Biso	1.000000	Si
Si	1.0	0.771740	0.170627	0.815647	Biso	1.000000	Si
Si	1.0	0.771686	0.670940	0.148864	Biso	1.000000	Si
Si	1.0	0.771732	0.670743	0.482243	Biso	1.000000	Si
Si	1.0	0.771768	0.670681	0.815670	Biso	1.000000	Si
Si	1.0	0.728402	0.420728	0.148855	Biso	1.000000	Si
Si	1.0	0.728132	0.420764	0.482133	Biso	1.000000	Si
Si	1.0	0.728213	0.420704	0.815520	Biso	1.000000	Si
Si	1.0	0.728718	0.921173	0.149120	Biso	1.000000	Si
Si	1.0	0.728417	0.920743	0.482411	Biso	1.000000	Si
Si	1.0	0.728387	0.920705	0.815794	Biso	1.000000	Si
Si	1.0	0.272580	0.081192	0.185090	Biso	1.000000	Si
Si	1.0	0.272671	0.078831	0.517775	Biso	1.000000	Si
Si	1.0	0.271251	0.079489	0.851430	Biso	1.000000	Si
Si	1.0	0.271969	0.579716	0.184617	Biso	1.000000	Si
Si	1.0	0.271988	0.579571	0.517926	Biso	1.000000	Si
Si	1.0	0.271604	0.579194	0.851162	Biso	1.000000	Si
Si	1.0	0.771527	0.079082	0.315557	Biso	1.000000	Si
Si	1.0	0.771669	0.079113	0.648944	Biso	1.000000	Si
Si	1.0	0.771743	0.079316	0.982508	Biso	1.000000	Si
Si	1.0	0.771470	0.579354	0.315408	Biso	1.000000	Si
Si	1.0	0.771699	0.579107	0.648941	Biso	1.000000	Si
Si	1.0	0.771717	0.579098	0.982355	Biso	1.000000	Si
Si	1.0	0.227614	0.419859	0.017745	Biso	1.000000	Si
Si	1.0	0.228184	0.420707	0.348589	Biso	1.000000	Si
Si	1.0	0.228069	0.420342	0.683612	Biso	1.000000	Si
Si	1.0	0.227798	0.921210	0.018180	Biso	1.000000	Si
Si	1.0	0.228154	0.920364	0.350758	Biso	1.000000	Si
Si	1.0	0.228339	0.920722	0.684689	Biso	1.000000	Si
Si	1.0	0.473561	0.168895	0.265942	Biso	1.000000	Si
Si	1.0	0.473776	0.168564	0.599229	Biso	1.000000	Si
Si	1.0	0.473949	0.168705	0.932494	Biso	1.000000	Si
Si	1.0	0.473793	0.668784	0.265807	Biso	1.000000	Si
Si	1.0	0.473939	0.668734	0.599244	Biso	1.000000	Si
Si	1.0	0.473859	0.668717	0.932571	Biso	1.000000	Si
Si	1.0	0.525764	0.331332	0.067506	Biso	1.000000	Si
Si	1.0	0.525715	0.331172	0.400652	Biso	1.000000	Si

Si	1.0	0.526038	0.331312	0.734005	Biso	1.000000	Si
Si	1.0	0.525864	0.831407	0.067596	Biso	1.000000	Si
Si	1.0	0.526140	0.831384	0.400794	Biso	1.000000	Si
Si	1.0	0.526169	0.831258	0.734280	Biso	1.000000	Si
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Si	1.0	0.023785	0.334432	0.431689	Biso	1.000000	Si
Si	1.0	0.025780	0.330199	0.764023	Biso	1.000000	Si
Si	1.0	0.026282	0.831638	0.099550	Biso	1.000000	Si
Si	1.0	0.026123	0.831367	0.432560	Biso	1.000000	Si
Si	1.0	0.026086	0.831428	0.766004	Biso	1.000000	Si
Si	1.0	0.974281	0.169179	0.233124	Biso	1.000000	Si
Si	1.0	0.974273	0.168797	0.567323	Biso	1.000000	Si
Si	1.0	0.974459	0.169040	0.900926	Biso	1.000000	Si
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Si	1.0	0.525742	0.418622	0.234087	Biso	1.000000	Si
Si	1.0	0.525974	0.418610	0.567281	Biso	1.000000	Si
Si	1.0	0.525929	0.418702	0.900780	Biso	1.000000	Si
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Si	1.0	0.526263	0.918545	0.567582	Biso	1.000000	Si
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Si	1.0	0.974340	0.580446	0.067639	Biso	1.000000	Si
Si	1.0	0.974366	0.580999	0.401014	Biso	1.000000	Si
Si	1.0	0.974025	0.580988	0.734192	Biso	1.000000	Si
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Si	1.0	0.025964	0.418621	0.598145	Biso	1.000000	Si
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model 10

#=====

# CRYSTAL DATA

#-----

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\_cell\_angle\_gamma 90  
\_symmetry\_space\_group\_name\_H-M 'P 1'  
\_symmetry\_Int\_Tables\_number 1

loop\_  
\_symmetry\_equiv\_pos\_as\_xyz  
'x, y, z'

loop\_  
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\_atom\_site\_occupancy  
\_atom\_site\_fract\_x  
\_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	0.562789	0.079831	0.766292	Biso	1.000000	O
O	1.0	0.562823	0.579652	0.099569	Biso	1.000000	O
O	1.0	0.563120	0.580111	0.433016	Biso	1.000000	O
O	1.0	0.562711	0.579742	0.766200	Biso	1.000000	O
O	1.0	0.062926	0.078656	0.067776	Biso	1.000000	O
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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
O	1.0	0.063285	0.580013	0.401090	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	0.187792	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
O	1.0	0.688654	0.000949	0.818556	Biso	1.000000	O
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
O	1.0	0.433015	0.008383	0.396435	Biso	1.000000	O
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
O	1.0	0.196867	0.889666	0.778914	Biso	1.000000	O
O	1.0	0.802763	0.109842	0.221232	Biso	1.000000	O
O	1.0	0.803121	0.110135	0.554485	Biso	1.000000	O
O	1.0	0.803087	0.110466	0.887842	Biso	1.000000	O
O	1.0	0.803355	0.610493	0.221071	Biso	1.000000	O
O	1.0	0.803244	0.610267	0.554417	Biso	1.000000	O
O	1.0	0.803197	0.610186	0.887738	Biso	1.000000	O
O	1.0	0.696969	0.360086	0.220705	Biso	1.000000	O
O	1.0	0.696951	0.360036	0.554069	Biso	1.000000	O
O	1.0	0.696626	0.360206	0.887414	Biso	1.000000	O
O	1.0	0.697024	0.860268	0.221382	Biso	1.000000	O
O	1.0	0.696855	0.860243	0.554865	Biso	1.000000	O
O	1.0	0.697067	0.860329	0.888128	Biso	1.000000	O
O	1.0	0.303074	0.135838	0.111123	Biso	1.000000	O
O	1.0	0.303203	0.139441	0.445861	Biso	1.000000	O
O	1.0	0.303033	0.139518	0.778999	Biso	1.000000	O
O	1.0	0.303123	0.640954	0.112402	Biso	1.000000	O
O	1.0	0.303228	0.640789	0.446020	Biso	1.000000	O
O	1.0	0.303054	0.640309	0.779242	Biso	1.000000	O
O	1.0	0.803072	0.139808	0.054580	Biso	1.000000	O
O	1.0	0.803017	0.139325	0.387731	Biso	1.000000	O
O	1.0	0.803161	0.139540	0.721087	Biso	1.000000	O
O	1.0	0.803223	0.639489	0.054358	Biso	1.000000	O
O	1.0	0.803316	0.639605	0.387784	Biso	1.000000	O
O	1.0	0.803202	0.639449	0.721128	Biso	1.000000	O
O	1.0	0.198514	0.366764	0.274718	Biso	1.000000	O
O	1.0	0.196339	0.360096	0.611040	Biso	1.000000	O
O	1.0	0.196435	0.360261	0.944960	Biso	1.000000	O
O	1.0	0.196633	0.860676	0.278586	Biso	1.000000	O
O	1.0	0.196705	0.861318	0.611963	Biso	1.000000	O
O	1.0	0.196830	0.861039	0.945620	Biso	1.000000	O
O	1.0	0.447988	0.096966	0.201414	Biso	1.000000	O
O	1.0	0.447920	0.096950	0.534754	Biso	1.000000	O
O	1.0	0.447907	0.097204	0.867766	Biso	1.000000	O
O	1.0	0.448255	0.597583	0.201160	Biso	1.000000	O
O	1.0	0.448181	0.597765	0.534540	Biso	1.000000	O
O	1.0	0.447972	0.597614	0.867759	Biso	1.000000	O
O	1.0	0.552094	0.402478	0.132060	Biso	1.000000	O
O	1.0	0.551581	0.402389	0.465298	Biso	1.000000	O
O	1.0	0.551743	0.402584	0.798704	Biso	1.000000	O
O	1.0	0.552224	0.902471	0.132251	Biso	1.000000	O
O	1.0	0.552194	0.902648	0.465590	Biso	1.000000	O
O	1.0	0.552120	0.902710	0.798953	Biso	1.000000	O
O	1.0	0.051353	0.402036	0.030863	Biso	1.000000	O
O	1.0	0.052046	0.400305	0.364982	Biso	1.000000	O
O	1.0	0.051878	0.401489	0.698931	Biso	1.000000	O
O	1.0	0.051961	0.903578	0.034634	Biso	1.000000	O
O	1.0	0.052171	0.903318	0.368902	Biso	1.000000	O
O	1.0	0.051803	0.902750	0.701303	Biso	1.000000	O
O	1.0	0.945184	0.095516	0.299439	Biso	1.000000	O
O	1.0	0.948538	0.097245	0.632360	Biso	1.000000	O
O	1.0	0.948168	0.097529	0.965949	Biso	1.000000	O
O	1.0	0.948221	0.598077	0.299411	Biso	1.000000	O
O	1.0	0.948324	0.597354	0.632159	Biso	1.000000	O
O	1.0	0.948357	0.597461	0.965872	Biso	1.000000	O
O	1.0	0.551858	0.347139	0.298734	Biso	1.000000	O

O	1.0	0.551792	0.347202	0.631980	Biso	1.000000	O
O	1.0	0.551782	0.347202	0.965452	Biso	1.000000	O
O	1.0	0.552263	0.847226	0.298979	Biso	1.000000	O
O	1.0	0.552163	0.847311	0.632321	Biso	1.000000	O
O	1.0	0.552090	0.847359	0.965557	Biso	1.000000	O
O	1.0	0.448153	0.151855	0.034045	Biso	1.000000	O
O	1.0	0.447690	0.152387	0.368068	Biso	1.000000	O
O	1.0	0.447799	0.152518	0.701144	Biso	1.000000	O
O	1.0	0.448069	0.652824	0.034626	Biso	1.000000	O
O	1.0	0.448223	0.652994	0.367919	Biso	1.000000	O
O	1.0	0.447975	0.652851	0.701249	Biso	1.000000	O
O	1.0	0.948327	0.152277	0.132689	Biso	1.000000	O
O	1.0	0.949054	0.151081	0.465281	Biso	1.000000	O
O	1.0	0.948182	0.152384	0.799036	Biso	1.000000	O
O	1.0	0.948378	0.652395	0.132414	Biso	1.000000	O
O	1.0	0.948203	0.652507	0.465730	Biso	1.000000	O
O	1.0	0.948243	0.652337	0.799055	Biso	1.000000	O
O	1.0	0.050508	0.352184	0.195487	Biso	1.000000	O
O	1.0	0.051552	0.347245	0.531645	Biso	1.000000	O
O	1.0	0.051587	0.348048	0.865290	Biso	1.000000	O
O	1.0	0.052513	0.851234	0.200597	Biso	1.000000	O
O	1.0	0.051842	0.847792	0.534655	Biso	1.000000	O
O	1.0	0.051929	0.847879	0.868011	Biso	1.000000	O
Si	1.0	0.270779	0.170247	0.018834	Biso	1.000000	Si
Si	1.0	0.270652	0.169264	0.350379	Biso	1.000000	Si
Si	1.0	0.271829	0.170474	0.684612	Biso	1.000000	Si
Si	1.0	0.271532	0.671264	0.017643	Biso	1.000000	Si
Si	1.0	0.271739	0.671684	0.351366	Biso	1.000000	Si
Si	1.0	0.271730	0.671295	0.684686	Biso	1.000000	Si
Si	1.0	0.728496	0.328964	0.315029	Biso	1.000000	Si
Si	1.0	0.728163	0.329013	0.648733	Biso	1.000000	Si
Si	1.0	0.728055	0.329179	0.981953	Biso	1.000000	Si
Si	1.0	0.728418	0.829112	0.315859	Biso	1.000000	Si
Si	1.0	0.728349	0.829075	0.649381	Biso	1.000000	Si
Si	1.0	0.728523	0.829111	0.982581	Biso	1.000000	Si
Si	1.0	0.228069	0.328311	0.185480	Biso	1.000000	Si
Si	1.0	0.227728	0.330024	0.515621	Biso	1.000000	Si
Si	1.0	0.227920	0.329047	0.850886	Biso	1.000000	Si
Si	1.0	0.228382	0.829086	0.183964	Biso	1.000000	Si
Si	1.0	0.228199	0.830490	0.517520	Biso	1.000000	Si
Si	1.0	0.228388	0.829466	0.851339	Biso	1.000000	Si
Si	1.0	0.771671	0.170759	0.149205	Biso	1.000000	Si
Si	1.0	0.771461	0.170489	0.482318	Biso	1.000000	Si
Si	1.0	0.771579	0.170847	0.815590	Biso	1.000000	Si
Si	1.0	0.771813	0.670722	0.148777	Biso	1.000000	Si
Si	1.0	0.771780	0.670726	0.482290	Biso	1.000000	Si
Si	1.0	0.771728	0.670653	0.815646	Biso	1.000000	Si
Si	1.0	0.728467	0.420664	0.148635	Biso	1.000000	Si
Si	1.0	0.728320	0.420556	0.481963	Biso	1.000000	Si
Si	1.0	0.728136	0.420621	0.815301	Biso	1.000000	Si
Si	1.0	0.728326	0.920773	0.149227	Biso	1.000000	Si
Si	1.0	0.728128	0.920644	0.482627	Biso	1.000000	Si
Si	1.0	0.728383	0.920817	0.815977	Biso	1.000000	Si
Si	1.0	0.272883	0.078239	0.185444	Biso	1.000000	Si
Si	1.0	0.272180	0.078874	0.517875	Biso	1.000000	Si
Si	1.0	0.271505	0.079318	0.851469	Biso	1.000000	Si
Si	1.0	0.271997	0.580362	0.184739	Biso	1.000000	Si
Si	1.0	0.272065	0.580046	0.518076	Biso	1.000000	Si
Si	1.0	0.271711	0.579548	0.851246	Biso	1.000000	Si
Si	1.0	0.771116	0.078865	0.315734	Biso	1.000000	Si
Si	1.0	0.771535	0.079092	0.649111	Biso	1.000000	Si
Si	1.0	0.771658	0.079364	0.982388	Biso	1.000000	Si
Si	1.0	0.771708	0.579376	0.315440	Biso	1.000000	Si
Si	1.0	0.771735	0.579026	0.648926	Biso	1.000000	Si
Si	1.0	0.771663	0.578995	0.982262	Biso	1.000000	Si
Si	1.0	0.227765	0.420141	0.018151	Biso	1.000000	Si
Si	1.0	0.228677	0.422165	0.348851	Biso	1.000000	Si
Si	1.0	0.227910	0.420322	0.683654	Biso	1.000000	Si
Si	1.0	0.228565	0.921158	0.017916	Biso	1.000000	Si
Si	1.0	0.228183	0.921087	0.349862	Biso	1.000000	Si
Si	1.0	0.228499	0.921095	0.684732	Biso	1.000000	Si
Si	1.0	0.473185	0.168836	0.265946	Biso	1.000000	Si
Si	1.0	0.473533	0.168655	0.599169	Biso	1.000000	Si
Si	1.0	0.473765	0.168575	0.932580	Biso	1.000000	Si
Si	1.0	0.474059	0.668800	0.265839	Biso	1.000000	Si
Si	1.0	0.473899	0.668972	0.599328	Biso	1.000000	Si
Si	1.0	0.473896	0.668744	0.932589	Biso	1.000000	Si
Si	1.0	0.525645	0.331126	0.067501	Biso	1.000000	Si
Si	1.0	0.525510	0.331019	0.400550	Biso	1.000000	Si



Si	1.0	0.525814	0.331259	0.734025	Biso	1.000000	Si
Si	1.0	0.526258	0.831164	0.067495	Biso	1.000000	Si
Si	1.0	0.526228	0.831322	0.400903	Biso	1.000000	Si
Si	1.0	0.526209	0.831330	0.734320	Biso	1.000000	Si
Si	1.0	0.025318	0.332158	0.096906	Biso	1.000000	Si
Si	1.0	0.023910	0.334291	0.431412	Biso	1.000000	Si
Si	1.0	0.025802	0.330737	0.764250	Biso	1.000000	Si
Si	1.0	0.026145	0.832369	0.099273	Biso	1.000000	Si
Si	1.0	0.025805	0.831349	0.433001	Biso	1.000000	Si
Si	1.0	0.026097	0.831441	0.766165	Biso	1.000000	Si
Si	1.0	0.974400	0.165803	0.234638	Biso	1.000000	Si
Si	1.0	0.974486	0.168090	0.567369	Biso	1.000000	Si
Si	1.0	0.974053	0.168803	0.901064	Biso	1.000000	Si
Si	1.0	0.974126	0.668936	0.234274	Biso	1.000000	Si
Si	1.0	0.974017	0.668748	0.567610	Biso	1.000000	Si
Si	1.0	0.974086	0.668592	0.901058	Biso	1.000000	Si
Si	1.0	0.526209	0.418744	0.234064	Biso	1.000000	Si
Si	1.0	0.525854	0.418554	0.567266	Biso	1.000000	Si
Si	1.0	0.525796	0.418537	0.900806	Biso	1.000000	Si
Si	1.0	0.526386	0.918443	0.234162	Biso	1.000000	Si
Si	1.0	0.526287	0.918596	0.567608	Biso	1.000000	Si
Si	1.0	0.526170	0.918773	0.900944	Biso	1.000000	Si
Si	1.0	0.473818	0.081246	0.099178	Biso	1.000000	Si
Si	1.0	0.473879	0.081303	0.432732	Biso	1.000000	Si
Si	1.0	0.473849	0.081308	0.765918	Biso	1.000000	Si
Si	1.0	0.473847	0.581210	0.099161	Biso	1.000000	Si
Si	1.0	0.474180	0.581670	0.432666	Biso	1.000000	Si
Si	1.0	0.473754	0.581392	0.765915	Biso	1.000000	Si
Si	1.0	0.974368	0.081061	0.067755	Biso	1.000000	Si
Si	1.0	0.972548	0.079769	0.400245	Biso	1.000000	Si
Si	1.0	0.974115	0.081154	0.734525	Biso	1.000000	Si
Si	1.0	0.974394	0.580915	0.067713	Biso	1.000000	Si
Si	1.0	0.974403	0.581237	0.400950	Biso	1.000000	Si
Si	1.0	0.974105	0.581129	0.734165	Biso	1.000000	Si
Si	1.0	0.026372	0.419159	0.262997	Biso	1.000000	Si
Si	1.0	0.026017	0.418639	0.597869	Biso	1.000000	Si
Si	1.0	0.025534	0.418948	0.930104	Biso	1.000000	Si
Si	1.0	0.026172	0.920058	0.267550	Biso	1.000000	Si
Si	1.0	0.025686	0.918812	0.599698	Biso	1.000000	Si
Si	1.0	0.026109	0.919359	0.932499	Biso	1.000000	Si

model 11

#=====

# CRYSTAL DATA

#-----

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\_cell\_length\_b 17.83444  
\_cell\_length\_c 15.70671  
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\_cell\_angle\_beta 90  
\_cell\_angle\_gamma 90  
\_symmetry\_space\_group\_name\_H-M 'P 1'  
\_symmetry\_Int\_Tables\_number 1

loop\_  
\_symmetry\_equiv\_pos\_as\_xyz  
'x, y, z'

loop\_  
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\_atom\_site\_occupancy  
\_atom\_site\_fract\_x  
\_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	0.937189	0.829997	0.766492	Biso	1.000000	O
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O	1.0	0.562737	0.579397	0.099614	Biso	1.000000	O
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O	1.0	0.688624	0.000846	0.151850	Biso	1.000000	O
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O	1.0	0.688630	0.000946	0.818622	Biso	1.000000	O
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O	1.0	0.688451	0.500844	0.818340	Biso	1.000000	O
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
O	1.0	0.697023	0.860395	0.888124	Biso	1.000000	O
O	1.0	0.301559	0.138760	0.113068	Biso	1.000000	O
O	1.0	0.303925	0.138729	0.446215	Biso	1.000000	O
O	1.0	0.302806	0.139868	0.778820	Biso	1.000000	O
O	1.0	0.302902	0.639206	0.112046	Biso	1.000000	O
O	1.0	0.303007	0.640156	0.445511	Biso	1.000000	O
O	1.0	0.302807	0.639738	0.778837	Biso	1.000000	O
O	1.0	0.803210	0.139802	0.054606	Biso	1.000000	O
O	1.0	0.803259	0.139065	0.387819	Biso	1.000000	O
O	1.0	0.803175	0.139504	0.721120	Biso	1.000000	O
O	1.0	0.803208	0.639649	0.054486	Biso	1.000000	O
O	1.0	0.803234	0.639706	0.387888	Biso	1.000000	O
O	1.0	0.803044	0.639895	0.721269	Biso	1.000000	O
O	1.0	0.198912	0.370837	0.275609	Biso	1.000000	O
O	1.0	0.197113	0.360222	0.610823	Biso	1.000000	O
O	1.0	0.196289	0.360395	0.943353	Biso	1.000000	O
O	1.0	0.196718	0.860772	0.278228	Biso	1.000000	O
O	1.0	0.196695	0.861456	0.611670	Biso	1.000000	O
O	1.0	0.196854	0.861155	0.945307	Biso	1.000000	O
O	1.0	0.448138	0.096966	0.201265	Biso	1.000000	O
O	1.0	0.448113	0.097081	0.534750	Biso	1.000000	O
O	1.0	0.447852	0.097180	0.868102	Biso	1.000000	O
O	1.0	0.447998	0.597081	0.201246	Biso	1.000000	O
O	1.0	0.448197	0.597650	0.534474	Biso	1.000000	O
O	1.0	0.447893	0.597340	0.867857	Biso	1.000000	O
O	1.0	0.551992	0.402543	0.132140	Biso	1.000000	O
O	1.0	0.551675	0.402270	0.465494	Biso	1.000000	O
O	1.0	0.551740	0.402594	0.798949	Biso	1.000000	O
O	1.0	0.552113	0.902373	0.132085	Biso	1.000000	O
O	1.0	0.552009	0.902518	0.465580	Biso	1.000000	O
O	1.0	0.552059	0.902643	0.798872	Biso	1.000000	O
O	1.0	0.051598	0.402849	0.032017	Biso	1.000000	O
O	1.0	0.052749	0.400470	0.368996	Biso	1.000000	O
O	1.0	0.051722	0.403903	0.701651	Biso	1.000000	O
O	1.0	0.052086	0.903954	0.034764	Biso	1.000000	O
O	1.0	0.052483	0.902936	0.368501	Biso	1.000000	O
O	1.0	0.051887	0.903047	0.701351	Biso	1.000000	O
O	1.0	0.945396	0.095801	0.299119	Biso	1.000000	O
O	1.0	0.948019	0.096888	0.632388	Biso	1.000000	O
O	1.0	0.948202	0.097285	0.965435	Biso	1.000000	O
O	1.0	0.948037	0.598396	0.299145	Biso	1.000000	O
O	1.0	0.947938	0.598185	0.632198	Biso	1.000000	O
O	1.0	0.947958	0.597685	0.965592	Biso	1.000000	O
O	1.0	0.551862	0.347103	0.298837	Biso	1.000000	O

O	1.0	0.551964	0.347350	0.632274	Biso	1.000000	O
O	1.0	0.551746	0.347265	0.965523	Biso	1.000000	O
O	1.0	0.552157	0.847121	0.298937	Biso	1.000000	O
O	1.0	0.552014	0.847325	0.632271	Biso	1.000000	O
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O	1.0	0.447726	0.152490	0.034781	Biso	1.000000	O
O	1.0	0.447959	0.152301	0.367908	Biso	1.000000	O
O	1.0	0.448011	0.152587	0.701308	Biso	1.000000	O
O	1.0	0.447938	0.652598	0.034666	Biso	1.000000	O
O	1.0	0.448105	0.652724	0.367783	Biso	1.000000	O
O	1.0	0.447876	0.652796	0.701236	Biso	1.000000	O
O	1.0	0.948550	0.152967	0.131870	Biso	1.000000	O
O	1.0	0.947456	0.148782	0.466410	Biso	1.000000	O
O	1.0	0.948146	0.152600	0.798816	Biso	1.000000	O
O	1.0	0.948111	0.653112	0.132115	Biso	1.000000	O
O	1.0	0.948080	0.653885	0.465379	Biso	1.000000	O
O	1.0	0.948104	0.653195	0.798868	Biso	1.000000	O
O	1.0	0.051911	0.352600	0.196115	Biso	1.000000	O
O	1.0	0.051817	0.347913	0.535904	Biso	1.000000	O
O	1.0	0.051716	0.347309	0.866940	Biso	1.000000	O
O	1.0	0.052625	0.850890	0.200344	Biso	1.000000	O
O	1.0	0.051960	0.847748	0.534690	Biso	1.000000	O
O	1.0	0.051938	0.847768	0.868064	Biso	1.000000	O
Si	1.0	0.270991	0.170647	0.018283	Biso	1.000000	Si
Si	1.0	0.272713	0.167313	0.351221	Biso	1.000000	Si
Si	1.0	0.271286	0.171114	0.684235	Biso	1.000000	Si
Si	1.0	0.271421	0.670416	0.017636	Biso	1.000000	Si
Si	1.0	0.271731	0.670962	0.350845	Biso	1.000000	Si
Si	1.0	0.271558	0.671022	0.684253	Biso	1.000000	Si
Si	1.0	0.729150	0.328824	0.315572	Biso	1.000000	Si
Si	1.0	0.728471	0.329174	0.648864	Biso	1.000000	Si
Si	1.0	0.728318	0.329239	0.982245	Biso	1.000000	Si
Si	1.0	0.728473	0.829118	0.315903	Biso	1.000000	Si
Si	1.0	0.728341	0.829226	0.649311	Biso	1.000000	Si
Si	1.0	0.728518	0.829145	0.982546	Biso	1.000000	Si
Si	1.0	0.228354	0.333122	0.188360	Biso	1.000000	Si
Si	1.0	0.228362	0.329731	0.515897	Biso	1.000000	Si
Si	1.0	0.228098	0.328643	0.849550	Biso	1.000000	Si
Si	1.0	0.228419	0.829050	0.183695	Biso	1.000000	Si
Si	1.0	0.228044	0.830590	0.517213	Biso	1.000000	Si
Si	1.0	0.228179	0.829534	0.850864	Biso	1.000000	Si
Si	1.0	0.771910	0.170932	0.149269	Biso	1.000000	Si
Si	1.0	0.772225	0.170793	0.482035	Biso	1.000000	Si
Si	1.0	0.771789	0.170851	0.815515	Biso	1.000000	Si
Si	1.0	0.771893	0.670657	0.149110	Biso	1.000000	Si
Si	1.0	0.771767	0.670906	0.482324	Biso	1.000000	Si
Si	1.0	0.771650	0.670929	0.815804	Biso	1.000000	Si
Si	1.0	0.728801	0.420631	0.149156	Biso	1.000000	Si
Si	1.0	0.728404	0.420761	0.482212	Biso	1.000000	Si
Si	1.0	0.728241	0.420722	0.815512	Biso	1.000000	Si
Si	1.0	0.728463	0.920785	0.149254	Biso	1.000000	Si
Si	1.0	0.728334	0.920761	0.482616	Biso	1.000000	Si
Si	1.0	0.728404	0.920845	0.815934	Biso	1.000000	Si
Si	1.0	0.273030	0.077437	0.185124	Biso	1.000000	Si
Si	1.0	0.271440	0.078671	0.518395	Biso	1.000000	Si
Si	1.0	0.271396	0.079486	0.850938	Biso	1.000000	Si
Si	1.0	0.271288	0.578925	0.184455	Biso	1.000000	Si
Si	1.0	0.271393	0.579507	0.517607	Biso	1.000000	Si
Si	1.0	0.271416	0.578984	0.850717	Biso	1.000000	Si
Si	1.0	0.771508	0.079000	0.315854	Biso	1.000000	Si
Si	1.0	0.771742	0.079143	0.648914	Biso	1.000000	Si
Si	1.0	0.771807	0.079455	0.982433	Biso	1.000000	Si
Si	1.0	0.772127	0.579007	0.315649	Biso	1.000000	Si
Si	1.0	0.771602	0.579420	0.649110	Biso	1.000000	Si
Si	1.0	0.771709	0.579156	0.982413	Biso	1.000000	Si
Si	1.0	0.227451	0.419006	0.017183	Biso	1.000000	Si
Si	1.0	0.229887	0.424706	0.351807	Biso	1.000000	Si
Si	1.0	0.228139	0.420565	0.683176	Biso	1.000000	Si
Si	1.0	0.228705	0.921231	0.017473	Biso	1.000000	Si
Si	1.0	0.228111	0.921178	0.349675	Biso	1.000000	Si
Si	1.0	0.228317	0.921492	0.684244	Biso	1.000000	Si
Si	1.0	0.473960	0.168516	0.266056	Biso	1.000000	Si
Si	1.0	0.473934	0.168677	0.599261	Biso	1.000000	Si
Si	1.0	0.473754	0.168631	0.932717	Biso	1.000000	Si
Si	1.0	0.474078	0.668495	0.265837	Biso	1.000000	Si
Si	1.0	0.473808	0.668964	0.599243	Biso	1.000000	Si
Si	1.0	0.473830	0.668569	0.932573	Biso	1.000000	Si
Si	1.0	0.526043	0.331269	0.067495	Biso	1.000000	Si
Si	1.0	0.526005	0.330840	0.400825	Biso	1.000000	Si

Si	1.0	0.526015	0.331276	0.734161	Biso	1.000000	Si
Si	1.0	0.526323	0.830987	0.067383	Biso	1.000000	Si
Si	1.0	0.526085	0.831204	0.400909	Biso	1.000000	Si
Si	1.0	0.526093	0.831298	0.734211	Biso	1.000000	Si
Si	1.0	0.025620	0.332822	0.098367	Biso	1.000000	Si
Si	1.0	0.025134	0.328828	0.433077	Biso	1.000000	Si
Si	1.0	0.026010	0.331642	0.764892	Biso	1.000000	Si
Si	1.0	0.026110	0.832319	0.099101	Biso	1.000000	Si
Si	1.0	0.025975	0.831293	0.432993	Biso	1.000000	Si
Si	1.0	0.026084	0.831606	0.766038	Biso	1.000000	Si
Si	1.0	0.975019	0.166403	0.234924	Biso	1.000000	Si
Si	1.0	0.974646	0.167841	0.566994	Biso	1.000000	Si
Si	1.0	0.973881	0.168777	0.900681	Biso	1.000000	Si
Si	1.0	0.973940	0.669255	0.234148	Biso	1.000000	Si
Si	1.0	0.973853	0.669430	0.567494	Biso	1.000000	Si
Si	1.0	0.973935	0.668915	0.900881	Biso	1.000000	Si
Si	1.0	0.526136	0.418489	0.234174	Biso	1.000000	Si
Si	1.0	0.526111	0.418612	0.567508	Biso	1.000000	Si
Si	1.0	0.525824	0.418656	0.900871	Biso	1.000000	Si
Si	1.0	0.526497	0.918313	0.234102	Biso	1.000000	Si
Si	1.0	0.526207	0.918658	0.567575	Biso	1.000000	Si
Si	1.0	0.526239	0.918619	0.900819	Biso	1.000000	Si
Si	1.0	0.474128	0.081125	0.099216	Biso	1.000000	Si
Si	1.0	0.474112	0.081176	0.432797	Biso	1.000000	Si
Si	1.0	0.473939	0.081285	0.766029	Biso	1.000000	Si
Si	1.0	0.473845	0.581041	0.099175	Biso	1.000000	Si
Si	1.0	0.474305	0.581560	0.432645	Biso	1.000000	Si
Si	1.0	0.473792	0.581349	0.765866	Biso	1.000000	Si
Si	1.0	0.973813	0.081470	0.067452	Biso	1.000000	Si
Si	1.0	0.972689	0.079610	0.399893	Biso	1.000000	Si
Si	1.0	0.973936	0.081231	0.734115	Biso	1.000000	Si
Si	1.0	0.973649	0.581517	0.067530	Biso	1.000000	Si
Si	1.0	0.973968	0.582089	0.401036	Biso	1.000000	Si
Si	1.0	0.973811	0.581800	0.734034	Biso	1.000000	Si
Si	1.0	0.027717	0.417468	0.267058	Biso	1.000000	Si
Si	1.0	0.025938	0.419335	0.599124	Biso	1.000000	Si
Si	1.0	0.025585	0.418973	0.930974	Biso	1.000000	Si
Si	1.0	0.026250	0.919602	0.267493	Biso	1.000000	Si
Si	1.0	0.025837	0.919009	0.599475	Biso	1.000000	Si
Si	1.0	0.026118	0.919289	0.932326	Biso	1.000000	Si



model 12

#=====

# CRYSTAL DATA

#-----

data\_VESTA\_phase\_1

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\_cell\_length\_b 17.83444  
\_cell\_length\_c 15.70671  
\_cell\_angle\_alpha 90  
\_cell\_angle\_beta 90  
\_cell\_angle\_gamma 90  
\_symmetry\_space\_group\_name\_H-M 'P 1'  
\_symmetry\_Int\_Tables\_number 1

loop\_  
\_symmetry\_equiv\_pos\_as\_xyz  
'x, y, z'

loop\_  
\_atom\_site\_label  
\_atom\_site\_occupancy  
\_atom\_site\_fract\_x  
\_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 0.375792 0.326294 0.621790 Biso 1.000000 Mg  
Mg 1.0 0.375775 0.326568 0.955395 Biso 1.000000 Mg  
Mg 1.0 0.375817 0.826602 0.288854 Biso 1.000000 Mg  
Mg 1.0 0.375785 0.826620 0.622253 Biso 1.000000 Mg  
Mg 1.0 0.375632 0.826490 0.955663 Biso 1.000000 Mg  
Mg 1.0 0.624156 0.173299 0.044535 Biso 1.000000 Mg  
Mg 1.0 0.624436 0.173364 0.377733 Biso 1.000000 Mg  
Mg 1.0 0.624197 0.173316 0.711190 Biso 1.000000 Mg  
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Mg 1.0 0.624128 0.673474 0.711155 Biso 1.000000 Mg  
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Cr 1.0 0.123399 0.174012 0.452902 Biso 1.000000 Cr  
Mg 1.0 0.123661 0.173332 0.788583 Biso 1.000000 Mg  
Mg 1.0 0.124035 0.672779 0.122434 Biso 1.000000 Mg  
Mg 1.0 0.124103 0.673577 0.455660 Biso 1.000000 Mg  
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Mg	1.0	0.376912	0.243705	0.119947	Biso	1.000000	Mg
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Mg	1.0	0.123320	0.256510	0.952999	Biso	1.000000	Mg
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Mg	1.0	0.876909	0.243130	0.047115	Biso	1.000000	Mg
Mg	1.0	0.877199	0.243931	0.379476	Biso	1.000000	Mg
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Mg	1.0	0.623584	0.493878	0.713261	Biso	1.000000	Mg
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O	1.0	0.816935	0.420182	0.488127	Biso	1.000000	O
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O	1.0	0.816808	0.920229	0.154967	Biso	1.000000	O

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O	1.0	0.937294	0.830011	0.766176	Biso	1.000000	O
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O	1.0	0.063604	0.169736	0.564194	Biso	1.000000	O
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O	1.0	0.062849	0.670314	0.233813	Biso	1.000000	O
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O	1.0	0.436905	0.920600	0.566928	Biso	1.000000	O
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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
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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
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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
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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
O	1.0	0.196698	0.860562	0.945522	Biso	1.000000	O
O	1.0	0.447968	0.097536	0.201418	Biso	1.000000	O
O	1.0	0.447876	0.097344	0.534836	Biso	1.000000	O
O	1.0	0.447791	0.097334	0.867999	Biso	1.000000	O
O	1.0	0.448049	0.597187	0.201297	Biso	1.000000	O
O	1.0	0.448317	0.597563	0.534452	Biso	1.000000	O
O	1.0	0.447838	0.597273	0.867803	Biso	1.000000	O
O	1.0	0.552186	0.402696	0.132028	Biso	1.000000	O
O	1.0	0.552216	0.402677	0.465594	Biso	1.000000	O
O	1.0	0.551845	0.402647	0.798838	Biso	1.000000	O
O	1.0	0.551828	0.902573	0.132198	Biso	1.000000	O
O	1.0	0.551814	0.902780	0.465548	Biso	1.000000	O
O	1.0	0.551804	0.902711	0.798883	Biso	1.000000	O
O	1.0	0.051563	0.402950	0.032013	Biso	1.000000	O
O	1.0	0.053648	0.396480	0.367976	Biso	1.000000	O
O	1.0	0.051837	0.402852	0.701334	Biso	1.000000	O
O	1.0	0.051981	0.902431	0.034563	Biso	1.000000	O
O	1.0	0.051969	0.903208	0.368397	Biso	1.000000	O
O	1.0	0.052191	0.902971	0.701262	Biso	1.000000	O
O	1.0	0.947168	0.097386	0.299673	Biso	1.000000	O
O	1.0	0.949244	0.097797	0.631911	Biso	1.000000	O
O	1.0	0.947701	0.097041	0.964817	Biso	1.000000	O
O	1.0	0.948137	0.597451	0.299033	Biso	1.000000	O
O	1.0	0.948032	0.597594	0.632106	Biso	1.000000	O
O	1.0	0.948079	0.597306	0.965575	Biso	1.000000	O
O	1.0	0.552267	0.347410	0.298778	Biso	1.000000	O

O	1.0	0.552115	0.347433	0.632187	Biso	1.000000	O
O	1.0	0.551870	0.347292	0.965452	Biso	1.000000	O
O	1.0	0.551930	0.847404	0.298937	Biso	1.000000	O
O	1.0	0.551691	0.847544	0.632189	Biso	1.000000	O
O	1.0	0.551868	0.847310	0.965528	Biso	1.000000	O
O	1.0	0.447905	0.152726	0.034691	Biso	1.000000	O
O	1.0	0.448073	0.152988	0.368161	Biso	1.000000	O
O	1.0	0.447906	0.152742	0.701415	Biso	1.000000	O
O	1.0	0.447975	0.652579	0.034550	Biso	1.000000	O
O	1.0	0.448273	0.652812	0.367823	Biso	1.000000	O
O	1.0	0.447942	0.652648	0.701159	Biso	1.000000	O
O	1.0	0.946329	0.153088	0.131091	Biso	1.000000	O
O	1.0	0.945425	0.151733	0.466486	Biso	1.000000	O
O	1.0	0.948288	0.152930	0.798475	Biso	1.000000	O
O	1.0	0.948107	0.652567	0.132191	Biso	1.000000	O
O	1.0	0.947994	0.652923	0.465458	Biso	1.000000	O
O	1.0	0.948236	0.652712	0.798809	Biso	1.000000	O
O	1.0	0.052039	0.351857	0.195488	Biso	1.000000	O
O	1.0	0.052412	0.346923	0.536324	Biso	1.000000	O
O	1.0	0.051725	0.347159	0.866926	Biso	1.000000	O
O	1.0	0.051969	0.847000	0.201491	Biso	1.000000	O
O	1.0	0.052062	0.847599	0.534625	Biso	1.000000	O
O	1.0	0.051965	0.847355	0.867873	Biso	1.000000	O
Si	1.0	0.271347	0.171121	0.018286	Biso	1.000000	Si
Si	1.0	0.272432	0.170615	0.352710	Biso	1.000000	Si
Si	1.0	0.271159	0.171122	0.684838	Biso	1.000000	Si
Si	1.0	0.271495	0.670194	0.017579	Biso	1.000000	Si
Si	1.0	0.271605	0.670840	0.350805	Biso	1.000000	Si
Si	1.0	0.271625	0.670640	0.684255	Biso	1.000000	Si
Si	1.0	0.728867	0.329164	0.315621	Biso	1.000000	Si
Si	1.0	0.728406	0.329165	0.649006	Biso	1.000000	Si
Si	1.0	0.728381	0.329095	0.982433	Biso	1.000000	Si
Si	1.0	0.728546	0.829222	0.315792	Biso	1.000000	Si
Si	1.0	0.728548	0.829371	0.649144	Biso	1.000000	Si
Si	1.0	0.728485	0.829186	0.982460	Biso	1.000000	Si
Si	1.0	0.228826	0.333504	0.187793	Biso	1.000000	Si
Si	1.0	0.227962	0.328667	0.514339	Biso	1.000000	Si
Si	1.0	0.228433	0.328155	0.849378	Biso	1.000000	Si
Si	1.0	0.228187	0.829167	0.184222	Biso	1.000000	Si
Si	1.0	0.228098	0.829538	0.517548	Biso	1.000000	Si
Si	1.0	0.228055	0.829364	0.851069	Biso	1.000000	Si
Si	1.0	0.771697	0.170867	0.149134	Biso	1.000000	Si
Si	1.0	0.771861	0.170845	0.482274	Biso	1.000000	Si
Si	1.0	0.771653	0.170773	0.815694	Biso	1.000000	Si
Si	1.0	0.771924	0.670687	0.149143	Biso	1.000000	Si
Si	1.0	0.771884	0.670908	0.482346	Biso	1.000000	Si
Si	1.0	0.771730	0.670866	0.815755	Biso	1.000000	Si
Si	1.0	0.728860	0.420768	0.149142	Biso	1.000000	Si
Si	1.0	0.728632	0.420754	0.482309	Biso	1.000000	Si
Si	1.0	0.728197	0.420707	0.815713	Biso	1.000000	Si
Si	1.0	0.728485	0.920804	0.149145	Biso	1.000000	Si
Si	1.0	0.728610	0.920932	0.482382	Biso	1.000000	Si
Si	1.0	0.728552	0.920934	0.815861	Biso	1.000000	Si
Si	1.0	0.271810	0.079506	0.184603	Biso	1.000000	Si
Si	1.0	0.272070	0.080338	0.517802	Biso	1.000000	Si
Si	1.0	0.271223	0.079345	0.851395	Biso	1.000000	Si
Si	1.0	0.271315	0.578748	0.184353	Biso	1.000000	Si
Si	1.0	0.271467	0.579195	0.517522	Biso	1.000000	Si
Si	1.0	0.271538	0.578720	0.850657	Biso	1.000000	Si
Si	1.0	0.771749	0.079120	0.315719	Biso	1.000000	Si
Si	1.0	0.771846	0.079172	0.648981	Biso	1.000000	Si
Si	1.0	0.771562	0.079135	0.982388	Biso	1.000000	Si
Si	1.0	0.772309	0.579033	0.315670	Biso	1.000000	Si
Si	1.0	0.771724	0.579289	0.649037	Biso	1.000000	Si
Si	1.0	0.771743	0.579133	0.982454	Biso	1.000000	Si
Si	1.0	0.227717	0.419154	0.016598	Biso	1.000000	Si
Si	1.0	0.230087	0.424804	0.351277	Biso	1.000000	Si
Si	1.0	0.227992	0.419015	0.682332	Biso	1.000000	Si
Si	1.0	0.228019	0.921016	0.017794	Biso	1.000000	Si
Si	1.0	0.227775	0.921287	0.350626	Biso	1.000000	Si
Si	1.0	0.228283	0.920974	0.684255	Biso	1.000000	Si
Si	1.0	0.474039	0.168913	0.266010	Biso	1.000000	Si
Si	1.0	0.474074	0.168664	0.599469	Biso	1.000000	Si
Si	1.0	0.473867	0.168656	0.932691	Biso	1.000000	Si
Si	1.0	0.474090	0.668750	0.265803	Biso	1.000000	Si
Si	1.0	0.473954	0.668872	0.599257	Biso	1.000000	Si
Si	1.0	0.473797	0.668604	0.932519	Biso	1.000000	Si
Si	1.0	0.526156	0.331319	0.067470	Biso	1.000000	Si
Si	1.0	0.526605	0.331406	0.400763	Biso	1.000000	Si

Si	1.0	0.526152	0.331323	0.734093	Biso	1.000000	Si
Si	1.0	0.526002	0.831180	0.067518	Biso	1.000000	Si
Si	1.0	0.526005	0.831366	0.400880	Biso	1.000000	Si
Si	1.0	0.525953	0.831373	0.734183	Biso	1.000000	Si
Si	1.0	0.025668	0.332276	0.097690	Biso	1.000000	Si
Si	1.0	0.026234	0.327550	0.434245	Biso	1.000000	Si
Si	1.0	0.025647	0.331225	0.765379	Biso	1.000000	Si
Si	1.0	0.026205	0.831133	0.099344	Biso	1.000000	Si
Si	1.0	0.026105	0.831480	0.432721	Biso	1.000000	Si
Si	1.0	0.026207	0.831455	0.765926	Biso	1.000000	Si
Si	1.0	0.975323	0.168405	0.233596	Biso	1.000000	Si
Si	1.0	0.973446	0.168935	0.566524	Biso	1.000000	Si
Si	1.0	0.973810	0.168649	0.900736	Biso	1.000000	Si
Si	1.0	0.973940	0.668648	0.234200	Biso	1.000000	Si
Si	1.0	0.973856	0.668923	0.567406	Biso	1.000000	Si
Si	1.0	0.974003	0.668589	0.900879	Biso	1.000000	Si
Si	1.0	0.526468	0.418764	0.234046	Biso	1.000000	Si
Si	1.0	0.526193	0.418710	0.567492	Biso	1.000000	Si
Si	1.0	0.525965	0.418674	0.900821	Biso	1.000000	Si
Si	1.0	0.526063	0.918661	0.234184	Biso	1.000000	Si
Si	1.0	0.525904	0.918894	0.567483	Biso	1.000000	Si
Si	1.0	0.525966	0.918672	0.900896	Biso	1.000000	Si
Si	1.0	0.473839	0.081343	0.099393	Biso	1.000000	Si
Si	1.0	0.473844	0.081404	0.432792	Biso	1.000000	Si
Si	1.0	0.473814	0.081266	0.766065	Biso	1.000000	Si
Si	1.0	0.473894	0.581185	0.099157	Biso	1.000000	Si
Si	1.0	0.474518	0.581684	0.432608	Biso	1.000000	Si
Si	1.0	0.473719	0.581216	0.765812	Biso	1.000000	Si
Si	1.0	0.973187	0.081664	0.067411	Biso	1.000000	Si
Si	1.0	0.972987	0.082365	0.400806	Biso	1.000000	Si
Si	1.0	0.974192	0.081578	0.734158	Biso	1.000000	Si
Si	1.0	0.973763	0.581127	0.067557	Biso	1.000000	Si
Si	1.0	0.974048	0.581402	0.400917	Biso	1.000000	Si
Si	1.0	0.973896	0.581369	0.734017	Biso	1.000000	Si
Si	1.0	0.027921	0.416213	0.266586	Biso	1.000000	Si
Si	1.0	0.025889	0.418861	0.599262	Biso	1.000000	Si
Si	1.0	0.025642	0.418894	0.930992	Biso	1.000000	Si
Si	1.0	0.026230	0.918595	0.265946	Biso	1.000000	Si
Si	1.0	0.026478	0.918988	0.599232	Biso	1.000000	Si
Si	1.0	0.026131	0.918650	0.932704	Biso	1.000000	Si

model 13

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# CRYSTAL DATA

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data\_VESTA\_phase\_1

\_pd\_phase\_name 'MgSiO3'  
\_cell\_length\_a 18.43007  
\_cell\_length\_b 17.83444  
\_cell\_length\_c 15.70671  
\_cell\_angle\_alpha 90  
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O	1.0	0.567459	0.258616	0.770565	Biso	1.000000	O
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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
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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
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O	1.0	0.697042	0.889684	0.387928	Biso	1.000000	O
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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
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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
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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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O	1.0	0.051874	0.902408	0.034140	Biso	1.000000	O
O	1.0	0.051983	0.902790	0.367799	Biso	1.000000	O
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O	1.0	0.947893	0.096854	0.631356	Biso	1.000000	O
O	1.0	0.947175	0.096848	0.965021	Biso	1.000000	O
O	1.0	0.948015	0.597475	0.298755	Biso	1.000000	O
O	1.0	0.947985	0.597383	0.632046	Biso	1.000000	O
O	1.0	0.947951	0.597411	0.965358	Biso	1.000000	O

O	1.0	0.551962	0.347565	0.299293	Biso	1.000000	O
O	1.0	0.551913	0.347407	0.632411	Biso	1.000000	O
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O	1.0	0.552061	0.847222	0.298653	Biso	1.000000	O
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O	1.0	0.551997	0.847252	0.965383	Biso	1.000000	O
O	1.0	0.447296	0.153391	0.034434	Biso	1.000000	O
O	1.0	0.448330	0.152479	0.368189	Biso	1.000000	O
O	1.0	0.448252	0.152574	0.701114	Biso	1.000000	O
O	1.0	0.448090	0.652428	0.034420	Biso	1.000000	O
O	1.0	0.447973	0.652578	0.367882	Biso	1.000000	O
O	1.0	0.448090	0.652618	0.701275	Biso	1.000000	O
O	1.0	0.947682	0.152513	0.131765	Biso	1.000000	O
O	1.0	0.948106	0.152937	0.465019	Biso	1.000000	O
O	1.0	0.946349	0.152380	0.797560	Biso	1.000000	O
O	1.0	0.947945	0.652929	0.132135	Biso	1.000000	O
O	1.0	0.948003	0.652832	0.465413	Biso	1.000000	O
O	1.0	0.947892	0.652794	0.798725	Biso	1.000000	O
O	1.0	0.051664	0.347861	0.201332	Biso	1.000000	O
O	1.0	0.051931	0.347400	0.534732	Biso	1.000000	O
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O	1.0	0.051949	0.847496	0.201121	Biso	1.000000	O
O	1.0	0.051914	0.847201	0.534420	Biso	1.000000	O
O	1.0	0.051815	0.847194	0.867777	Biso	1.000000	O
Al	1.0	0.269284	0.162225	0.017836	Biso	1.000000	Al
Si	1.0	0.271764	0.170906	0.352413	Biso	1.000000	Si
Si	1.0	0.271572	0.170283	0.684402	Biso	1.000000	Si
Si	1.0	0.271434	0.671056	0.017553	Biso	1.000000	Si
Si	1.0	0.271487	0.670789	0.350824	Biso	1.000000	Si
Si	1.0	0.271502	0.670642	0.684082	Biso	1.000000	Si
Si	1.0	0.728463	0.329193	0.316005	Biso	1.000000	Si
Si	1.0	0.728547	0.329127	0.649278	Biso	1.000000	Si
Si	1.0	0.728278	0.329279	0.982590	Biso	1.000000	Si
Si	1.0	0.728464	0.829270	0.315740	Biso	1.000000	Si
Si	1.0	0.728472	0.829206	0.649008	Biso	1.000000	Si
Si	1.0	0.728388	0.829227	0.982444	Biso	1.000000	Si
Si	1.0	0.227794	0.330597	0.185653	Biso	1.000000	Si
Si	1.0	0.228099	0.329455	0.518323	Biso	1.000000	Si
Si	1.0	0.228608	0.329215	0.851110	Biso	1.000000	Si
Si	1.0	0.228264	0.829387	0.184126	Biso	1.000000	Si
Si	1.0	0.228273	0.828910	0.517393	Biso	1.000000	Si
Si	1.0	0.228342	0.828968	0.850690	Biso	1.000000	Si
Si	1.0	0.771713	0.170650	0.148929	Biso	1.000000	Si
Si	1.0	0.771863	0.170804	0.482298	Biso	1.000000	Si
Si	1.0	0.771574	0.170742	0.815546	Biso	1.000000	Si
Si	1.0	0.771767	0.670966	0.149198	Biso	1.000000	Si
Si	1.0	0.771754	0.670885	0.482445	Biso	1.000000	Si
Si	1.0	0.771839	0.670914	0.815712	Biso	1.000000	Si
Si	1.0	0.728292	0.420831	0.149374	Biso	1.000000	Si
Si	1.0	0.728469	0.420815	0.482638	Biso	1.000000	Si
Si	1.0	0.728470	0.420829	0.815877	Biso	1.000000	Si
Si	1.0	0.728194	0.920794	0.149049	Biso	1.000000	Si
Si	1.0	0.728579	0.920849	0.482390	Biso	1.000000	Si
Si	1.0	0.728451	0.920708	0.815748	Biso	1.000000	Si
Si	1.0	0.273900	0.081067	0.186346	Biso	1.000000	Si
Si	1.0	0.271529	0.079252	0.517992	Biso	1.000000	Si
Si	1.0	0.272596	0.076261	0.849330	Biso	1.000000	Si
Si	1.0	0.271524	0.579236	0.184146	Biso	1.000000	Si
Si	1.0	0.271438	0.579112	0.517437	Biso	1.000000	Si
Si	1.0	0.271392	0.579280	0.850909	Biso	1.000000	Si
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Si	1.0	0.771756	0.079122	0.648859	Biso	1.000000	Si
Si	1.0	0.771463	0.079077	0.982221	Biso	1.000000	Si
Si	1.0	0.771693	0.579273	0.315829	Biso	1.000000	Si
Si	1.0	0.771825	0.579239	0.649079	Biso	1.000000	Si
Si	1.0	0.771943	0.579458	0.982456	Biso	1.000000	Si
Si	1.0	0.229097	0.423453	0.018285	Biso	1.000000	Si
Si	1.0	0.228337	0.421391	0.352016	Biso	1.000000	Si
Si	1.0	0.228169	0.421043	0.684887	Biso	1.000000	Si
Si	1.0	0.228257	0.920876	0.017340	Biso	1.000000	Si
Si	1.0	0.228249	0.920745	0.350972	Biso	1.000000	Si
Si	1.0	0.228405	0.920338	0.684052	Biso	1.000000	Si
Si	1.0	0.474343	0.168669	0.266372	Biso	1.000000	Si
Si	1.0	0.474035	0.168703	0.599153	Biso	1.000000	Si
Si	1.0	0.473844	0.168121	0.932349	Biso	1.000000	Si
Si	1.0	0.473888	0.668750	0.265906	Biso	1.000000	Si
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Si	1.0	0.474115	0.668747	0.932584	Biso	1.000000	Si
Si	1.0	0.526074	0.330962	0.068046	Biso	1.000000	Si

Si	1.0	0.526088	0.331310	0.401178	Biso	1.000000	Si
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Si	1.0	0.526054	0.831370	0.067388	Biso	1.000000	Si
Si	1.0	0.526172	0.831224	0.400660	Biso	1.000000	Si
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Si	1.0	0.026106	0.331499	0.432696	Biso	1.000000	Si
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Si	1.0	0.026070	0.831490	0.099112	Biso	1.000000	Si
Si	1.0	0.026114	0.831390	0.432380	Biso	1.000000	Si
Si	1.0	0.026075	0.831311	0.765761	Biso	1.000000	Si
Si	1.0	0.973846	0.168613	0.233625	Biso	1.000000	Si
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Si	1.0	0.474200	0.581370	0.099338	Biso	1.000000	Si
Si	1.0	0.473946	0.581256	0.432594	Biso	1.000000	Si
Si	1.0	0.474035	0.581300	0.765893	Biso	1.000000	Si
Si	1.0	0.973249	0.080771	0.067169	Biso	1.000000	Si
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Si	1.0	0.973555	0.080977	0.733512	Biso	1.000000	Si
Si	1.0	0.973632	0.581596	0.067440	Biso	1.000000	Si
Si	1.0	0.973784	0.581469	0.400759	Biso	1.000000	Si
Si	1.0	0.973733	0.581443	0.734054	Biso	1.000000	Si
Si	1.0	0.025946	0.419096	0.266205	Biso	1.000000	Si
Si	1.0	0.026134	0.418669	0.599563	Biso	1.000000	Si
Si	1.0	0.026055	0.418871	0.932881	Biso	1.000000	Si
Si	1.0	0.026361	0.919031	0.265699	Biso	1.000000	Si
Si	1.0	0.026087	0.918594	0.599074	Biso	1.000000	Si
Si	1.0	0.026042	0.918751	0.932404	Biso	1.000000	Si

model 14

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# CRYSTAL DATA

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\_cell\_length\_b 17.83444  
\_cell\_length\_c 15.70671  
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\_cell\_angle\_beta 90  
\_cell\_angle\_gamma 90  
\_symmetry\_space\_group\_name\_H-M 'P 1'  
\_symmetry\_Int\_Tables\_number 1

loop\_  
\_symmetry\_equiv\_pos\_as\_xyz  
'x, y, z'

loop\_  
\_atom\_site\_label  
\_atom\_site\_occupancy  
\_atom\_site\_fract\_x  
\_atom\_site\_fract\_y  
\_atom\_site\_fract\_z  
\_atom\_site\_adp\_type  
\_atom\_site\_B\_iso\_or\_equiv  
\_atom\_site\_type\_symbol  
H 1.0 0.518881 0.235491 0.139193 Biso 1.000000 H  
Mg 1.0 0.377394 0.327062 0.287277 Biso 1.000000 Mg  
Mg 1.0 0.375666 0.326706 0.621709 Biso 1.000000 Mg  
Mg 1.0 0.375186 0.326988 0.955181 Biso 1.000000 Mg  
Mg 1.0 0.375818 0.826339 0.288798 Biso 1.000000 Mg  
Mg 1.0 0.375786 0.826616 0.622095 Biso 1.000000 Mg  
Mg 1.0 0.375678 0.826315 0.955411 Biso 1.000000 Mg  
Mg 1.0 0.625780 0.169474 0.043652 Biso 1.000000 Mg  
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Mg 1.0 0.623870 0.174241 0.712053 Biso 1.000000 Mg  
Mg 1.0 0.624041 0.672918 0.044865 Biso 1.000000 Mg  
Mg 1.0 0.624074 0.673436 0.378330 Biso 1.000000 Mg  
Mg 1.0 0.623989 0.673042 0.711612 Biso 1.000000 Mg  
Mg 1.0 0.123566 0.173149 0.122116 Biso 1.000000 Mg  
Mg 1.0 0.124366 0.173338 0.455489 Biso 1.000000 Mg  
Mg 1.0 0.123986 0.173293 0.788904 Biso 1.000000 Mg  
Mg 1.0 0.124032 0.673162 0.122265 Biso 1.000000 Mg  
Mg 1.0 0.124054 0.673260 0.455616 Biso 1.000000 Mg  
Mg 1.0 0.123908 0.673202 0.788845 Biso 1.000000 Mg  
Mg 1.0 0.876447 0.326861 0.211660 Biso 1.000000 Mg  
Mg 1.0 0.876120 0.326782 0.544840 Biso 1.000000 Mg  
Mg 1.0 0.875582 0.326740 0.878140 Biso 1.000000 Mg  
Mg 1.0 0.875931 0.826453 0.211390 Biso 1.000000 Mg  
Mg 1.0 0.875958 0.826693 0.544817 Biso 1.000000 Mg  
Mg 1.0 0.875785 0.826538 0.877940 Biso 1.000000 Mg  
Mg 1.0 0.624466 0.075906 0.211724 Biso 1.000000 Mg  
Mg 1.0 0.624076 0.076841 0.545086 Biso 1.000000 Mg  
Mg 1.0 0.623809 0.076960 0.877690 Biso 1.000000 Mg  
Mg 1.0 0.623901 0.576756 0.212208 Biso 1.000000 Mg  
Mg 1.0 0.623954 0.576807 0.545260 Biso 1.000000 Mg  
Mg 1.0 0.624001 0.576007 0.878493 Biso 1.000000 Mg  
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Mg 1.0 0.375841 0.423570 0.454871 Biso 1.000000 Mg  
Mg 1.0 0.375795 0.423759 0.788049 Biso 1.000000 Mg  
Mg 1.0 0.375538 0.922469 0.122045 Biso 1.000000 Mg  
Mg 1.0 0.375708 0.923171 0.455484 Biso 1.000000 Mg  
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Mg 1.0 0.875795 0.423247 0.044880 Biso 1.000000 Mg  
Mg 1.0 0.876417 0.423634 0.378368 Biso 1.000000 Mg  
Mg 1.0 0.876035 0.423227 0.711386 Biso 1.000000 Mg  
Mg 1.0 0.875961 0.923049 0.044621 Biso 1.000000 Mg  
Mg 1.0 0.876055 0.923162 0.378211 Biso 1.000000 Mg  
Mg 1.0 0.875818 0.923245 0.711320 Biso 1.000000 Mg  
Mg 1.0 0.124101 0.076592 0.288843 Biso 1.000000 Mg  
Mg 1.0 0.124069 0.076757 0.622231 Biso 1.000000 Mg

Mg	1.0	0.123623	0.076382	0.955420	Biso	1.000000	Mg
Mg	1.0	0.124270	0.576662	0.288951	Biso	1.000000	Mg
Mg	1.0	0.124008	0.576717	0.622273	Biso	1.000000	Mg
Mg	1.0	0.123591	0.576813	0.955393	Biso	1.000000	Mg
Mg	1.0	0.372726	0.246268	0.117591	Biso	1.000000	Mg
Mg	1.0	0.376790	0.244218	0.452790	Biso	1.000000	Mg
Mg	1.0	0.376473	0.244254	0.786279	Biso	1.000000	Mg
Mg	1.0	0.376412	0.743158	0.119798	Biso	1.000000	Mg
Mg	1.0	0.376312	0.743584	0.453205	Biso	1.000000	Mg
Mg	1.0	0.376427	0.743447	0.786385	Biso	1.000000	Mg
Mg	1.0	0.627801	0.257598	0.217270	Biso	1.000000	Mg
Mg	1.0	0.622992	0.256822	0.547242	Biso	1.000000	Mg
Mg	1.0	0.619145	0.259672	0.882532	Biso	1.000000	Mg
Mg	1.0	0.623549	0.756060	0.213687	Biso	1.000000	Mg
Mg	1.0	0.623475	0.756222	0.547194	Biso	1.000000	Mg
Mg	1.0	0.623383	0.755861	0.880334	Biso	1.000000	Mg
Mg	1.0	0.123213	0.256251	0.286606	Biso	1.000000	Mg
Mg	1.0	0.123461	0.256343	0.619981	Biso	1.000000	Mg
Mg	1.0	0.123214	0.256236	0.953218	Biso	1.000000	Mg
Mg	1.0	0.123378	0.756081	0.286751	Biso	1.000000	Mg
Mg	1.0	0.123363	0.756242	0.620034	Biso	1.000000	Mg
Mg	1.0	0.123367	0.756127	0.953354	Biso	1.000000	Mg
Mg	1.0	0.876791	0.243806	0.047128	Biso	1.000000	Mg
Mg	1.0	0.877287	0.243563	0.380804	Biso	1.000000	Mg
Mg	1.0	0.876526	0.243549	0.713818	Biso	1.000000	Mg
Mg	1.0	0.876402	0.743516	0.046885	Biso	1.000000	Mg
Mg	1.0	0.876513	0.743558	0.380410	Biso	1.000000	Mg
Mg	1.0	0.876329	0.743491	0.713645	Biso	1.000000	Mg
Mg	1.0	0.621653	0.492674	0.049078	Biso	1.000000	Mg
Mg	1.0	0.623308	0.494267	0.381366	Biso	1.000000	Mg
Mg	1.0	0.622159	0.492808	0.714333	Biso	1.000000	Mg
Mg	1.0	0.623336	0.992129	0.046876	Biso	1.000000	Mg
Mg	1.0	0.623412	0.993242	0.380702	Biso	1.000000	Mg
Mg	1.0	0.623306	0.993865	0.713671	Biso	1.000000	Mg
Mg	1.0	0.376134	0.005715	0.286233	Biso	1.000000	Mg
Mg	1.0	0.376143	0.006136	0.619969	Biso	1.000000	Mg
Mg	1.0	0.375873	0.005650	0.952876	Biso	1.000000	Mg
Mg	1.0	0.377536	0.505771	0.285584	Biso	1.000000	Mg
Mg	1.0	0.376574	0.506434	0.619221	Biso	1.000000	Mg
Mg	1.0	0.377340	0.506003	0.952061	Biso	1.000000	Mg
Mg	1.0	0.876625	0.005972	0.213720	Biso	1.000000	Mg
Mg	1.0	0.876498	0.006479	0.547132	Biso	1.000000	Mg
Mg	1.0	0.876646	0.006132	0.880089	Biso	1.000000	Mg
Mg	1.0	0.876548	0.506411	0.213762	Biso	1.000000	Mg
Mg	1.0	0.876836	0.506593	0.547317	Biso	1.000000	Mg
Mg	1.0	0.876455	0.506310	0.880358	Biso	1.000000	Mg
Mg	1.0	0.123228	0.493928	0.119970	Biso	1.000000	Mg
Mg	1.0	0.123575	0.493758	0.453369	Biso	1.000000	Mg
Mg	1.0	0.123379	0.493632	0.786677	Biso	1.000000	Mg
Mg	1.0	0.123178	0.993516	0.119932	Biso	1.000000	Mg
Mg	1.0	0.123466	0.993713	0.453408	Biso	1.000000	Mg
Mg	1.0	0.123123	0.993551	0.786493	Biso	1.000000	Mg
O	1.0	0.182007	0.168954	0.011541	Biso	1.000000	O
O	1.0	0.183845	0.170658	0.344933	Biso	1.000000	O
O	1.0	0.183147	0.170132	0.678461	Biso	1.000000	O
O	1.0	0.183052	0.670148	0.011884	Biso	1.000000	O
O	1.0	0.183185	0.670084	0.345201	Biso	1.000000	O
O	1.0	0.183075	0.670182	0.678451	Biso	1.000000	O
O	1.0	0.817865	0.330247	0.322342	Biso	1.000000	O
O	1.0	0.817006	0.329589	0.655042	Biso	1.000000	O
O	1.0	0.816086	0.328776	0.988839	Biso	1.000000	O
O	1.0	0.816771	0.829818	0.321785	Biso	1.000000	O
O	1.0	0.816709	0.829855	0.655163	Biso	1.000000	O
O	1.0	0.816667	0.829786	0.988371	Biso	1.000000	O
O	1.0	0.315672	0.329565	0.179521	Biso	1.000000	O
O	1.0	0.316739	0.329718	0.511181	Biso	1.000000	O
O	1.0	0.316482	0.330188	0.844598	Biso	1.000000	O
O	1.0	0.316534	0.829630	0.178485	Biso	1.000000	O
O	1.0	0.316534	0.829892	0.511752	Biso	1.000000	O
O	1.0	0.316464	0.829605	0.845057	Biso	1.000000	O
O	1.0	0.683482	0.171072	0.155321	Biso	1.000000	O
O	1.0	0.683301	0.170114	0.488790	Biso	1.000000	O
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
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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
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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
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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
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O	1.0	0.311334	0.998938	0.180669	Biso	1.000000	O
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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
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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
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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
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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
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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
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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
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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
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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
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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
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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
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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
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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
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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
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Si	1.0	0.974021	0.581400	0.400949	Biso	1.000000	Si
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Si	1.0	0.025867	0.418620	0.932658	Biso	1.000000	Si
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Si	1.0	0.025952	0.918493	0.932657	Biso	1.000000	Si

model 15

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# CRYSTAL DATA

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\_cell\_length\_b 17.83444  
\_cell\_length\_c 15.70671  
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\_cell\_angle\_beta 90  
\_cell\_angle\_gamma 90  
\_symmetry\_space\_group\_name\_H-M 'P 1'  
\_symmetry\_Int\_Tables\_number 1

loop\_  
\_symmetry\_equiv\_pos\_as\_xyz  
'x, y, z'

loop\_  
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\_atom\_site\_occupancy  
\_atom\_site\_fract\_x  
\_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 0.123702 0.079208 0.288873 Biso 1.000000 Mg  
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Mg 1.0 0.375626 0.326555 0.622057 Biso 1.000000 Mg  
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Mg 1.0 0.375878 0.826662 0.622381 Biso 1.000000 Mg  
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Mg 1.0 0.876015 0.826765 0.211078 Biso 1.000000 Mg  
Mg 1.0 0.876022 0.826673 0.544531 Biso 1.000000 Mg  
Mg 1.0 0.876071 0.826725 0.877835 Biso 1.000000 Mg  
Mg 1.0 0.624066 0.076557 0.211135 Biso 1.000000 Mg  
Mg 1.0 0.624013 0.076430 0.544575 Biso 1.000000 Mg  
Mg 1.0 0.624089 0.076577 0.877862 Biso 1.000000 Mg  
Mg 1.0 0.624173 0.576736 0.210999 Biso 1.000000 Mg  
Mg 1.0 0.624247 0.576876 0.544603 Biso 1.000000 Mg  
Mg 1.0 0.624018 0.576603 0.877847 Biso 1.000000 Mg  
Mg 1.0 0.376007 0.423279 0.122311 Biso 1.000000 Mg  
Mg 1.0 0.376755 0.423968 0.456024 Biso 1.000000 Mg  
Mg 1.0 0.375799 0.423087 0.788742 Biso 1.000000 Mg  
Mg 1.0 0.375983 0.923078 0.122191 Biso 1.000000 Mg  
Mg 1.0 0.376021 0.923093 0.455475 Biso 1.000000 Mg  
Mg 1.0 0.375777 0.923375 0.789202 Biso 1.000000 Mg  
Mg 1.0 0.875874 0.422941 0.043746 Biso 1.000000 Mg  
Mg 1.0 0.874968 0.423998 0.376913 Biso 1.000000 Mg  
Mg 1.0 0.875892 0.423022 0.710695 Biso 1.000000 Mg  
Mg 1.0 0.875976 0.923353 0.044531 Biso 1.000000 Mg  
Mg 1.0 0.875885 0.923128 0.377792 Biso 1.000000 Mg  
Mg 1.0 0.876055 0.923339 0.711170 Biso 1.000000 Mg

Mg	1.0	0.124095	0.076332	0.621778	Biso	1.000000	Mg
Mg	1.0	0.123896	0.077083	0.956542	Biso	1.000000	Mg
Mg	1.0	0.124530	0.578014	0.289822	Biso	1.000000	Mg
Mg	1.0	0.124003	0.577040	0.622628	Biso	1.000000	Mg
Mg	1.0	0.124186	0.575725	0.956085	Biso	1.000000	Mg
Mg	1.0	0.376971	0.243727	0.120302	Biso	1.000000	Mg
Mg	1.0	0.376965	0.243991	0.453444	Biso	1.000000	Mg
Mg	1.0	0.376674	0.243516	0.786471	Biso	1.000000	Mg
Mg	1.0	0.376372	0.743581	0.119996	Biso	1.000000	Mg
Mg	1.0	0.376472	0.743854	0.453437	Biso	1.000000	Mg
Mg	1.0	0.376507	0.743913	0.786857	Biso	1.000000	Mg
Mg	1.0	0.623550	0.256061	0.213252	Biso	1.000000	Mg
Mg	1.0	0.623410	0.256014	0.546795	Biso	1.000000	Mg
Mg	1.0	0.623434	0.256137	0.879976	Biso	1.000000	Mg
Mg	1.0	0.623614	0.756265	0.213358	Biso	1.000000	Mg
Mg	1.0	0.623705	0.756347	0.546869	Biso	1.000000	Mg
Mg	1.0	0.623588	0.756249	0.880184	Biso	1.000000	Mg
Mg	1.0	0.124567	0.255125	0.619487	Biso	1.000000	Mg
Mg	1.0	0.123859	0.256094	0.953766	Biso	1.000000	Mg
Mg	1.0	0.123416	0.756966	0.286570	Biso	1.000000	Mg
Mg	1.0	0.123572	0.756389	0.620363	Biso	1.000000	Mg
Mg	1.0	0.123538	0.755947	0.953704	Biso	1.000000	Mg
Mg	1.0	0.876270	0.243368	0.046365	Biso	1.000000	Mg
Mg	1.0	0.874365	0.243200	0.378823	Biso	1.000000	Mg
Mg	1.0	0.876388	0.243345	0.712623	Biso	1.000000	Mg
Mg	1.0	0.876730	0.743823	0.046647	Biso	1.000000	Mg
Mg	1.0	0.876632	0.743744	0.379972	Biso	1.000000	Mg
Mg	1.0	0.876595	0.743813	0.713439	Biso	1.000000	Mg
Mg	1.0	0.623449	0.493657	0.046636	Biso	1.000000	Mg
Mg	1.0	0.623615	0.494162	0.380010	Biso	1.000000	Mg
Mg	1.0	0.623551	0.493860	0.713387	Biso	1.000000	Mg
Mg	1.0	0.623676	0.993636	0.046712	Biso	1.000000	Mg
Mg	1.0	0.623523	0.993590	0.380137	Biso	1.000000	Mg
Mg	1.0	0.623533	0.993588	0.713572	Biso	1.000000	Mg
Mg	1.0	0.376470	0.006101	0.286678	Biso	1.000000	Mg
Mg	1.0	0.376737	0.005817	0.620228	Biso	1.000000	Mg
Mg	1.0	0.376471	0.006053	0.953603	Biso	1.000000	Mg
Mg	1.0	0.377596	0.506824	0.286597	Biso	1.000000	Mg
Mg	1.0	0.376474	0.506343	0.620252	Biso	1.000000	Mg
Mg	1.0	0.375910	0.505735	0.953545	Biso	1.000000	Mg
Mg	1.0	0.876807	0.006389	0.213840	Biso	1.000000	Mg
Mg	1.0	0.876526	0.006072	0.546628	Biso	1.000000	Mg
Mg	1.0	0.876771	0.006353	0.880057	Biso	1.000000	Mg
Mg	1.0	0.876159	0.506207	0.212793	Biso	1.000000	Mg
Mg	1.0	0.876337	0.506354	0.546276	Biso	1.000000	Mg
Mg	1.0	0.875966	0.506168	0.879326	Biso	1.000000	Mg
Mg	1.0	0.122117	0.493842	0.121353	Biso	1.000000	Mg
Mg	1.0	0.125262	0.495520	0.454387	Biso	1.000000	Mg
Mg	1.0	0.123937	0.493833	0.786474	Biso	1.000000	Mg
Mg	1.0	0.123929	0.994828	0.120987	Biso	1.000000	Mg
Mg	1.0	0.122791	0.993449	0.452284	Biso	1.000000	Mg
Mg	1.0	0.123538	0.993848	0.787085	Biso	1.000000	Mg
O	1.0	0.182928	0.171436	0.015392	Biso	1.000000	O
O	1.0	0.185951	0.168133	0.343285	Biso	1.000000	O
O	1.0	0.183496	0.169762	0.678080	Biso	1.000000	O
O	1.0	0.183226	0.669452	0.012063	Biso	1.000000	O
O	1.0	0.183357	0.671226	0.345404	Biso	1.000000	O
O	1.0	0.183305	0.670177	0.679076	Biso	1.000000	O
O	1.0	0.816460	0.330073	0.320759	Biso	1.000000	O
O	1.0	0.816518	0.329729	0.654503	Biso	1.000000	O
O	1.0	0.816518	0.329630	0.987601	Biso	1.000000	O
O	1.0	0.816795	0.829814	0.321474	Biso	1.000000	O
O	1.0	0.816851	0.829889	0.654890	Biso	1.000000	O
O	1.0	0.816873	0.829847	0.988131	Biso	1.000000	O
O	1.0	0.317037	0.329960	0.179392	Biso	1.000000	O
O	1.0	0.316541	0.329832	0.511461	Biso	1.000000	O
O	1.0	0.316580	0.329397	0.844836	Biso	1.000000	O
O	1.0	0.316742	0.829696	0.178458	Biso	1.000000	O
O	1.0	0.316678	0.829898	0.512025	Biso	1.000000	O
O	1.0	0.316603	0.829986	0.845419	Biso	1.000000	O
O	1.0	0.683263	0.170124	0.154752	Biso	1.000000	O
O	1.0	0.682993	0.169768	0.488283	Biso	1.000000	O
O	1.0	0.683305	0.170054	0.821413	Biso	1.000000	O
O	1.0	0.683339	0.670144	0.154716	Biso	1.000000	O
O	1.0	0.683503	0.670300	0.488278	Biso	1.000000	O
O	1.0	0.683384	0.670120	0.821550	Biso	1.000000	O
O	1.0	0.816664	0.420039	0.154393	Biso	1.000000	O
O	1.0	0.816459	0.420285	0.487877	Biso	1.000000	O
O	1.0	0.816539	0.419931	0.820928	Biso	1.000000	O

O	1.0	0.816854	0.920169	0.154911	Biso	1.000000	O
O	1.0	0.816756	0.919977	0.488223	Biso	1.000000	O
O	1.0	0.816885	0.920205	0.821497	Biso	1.000000	O
O	1.0	0.183886	0.081028	0.179065	Biso	1.000000	O
O	1.0	0.183885	0.079665	0.511577	Biso	1.000000	O
O	1.0	0.183047	0.080047	0.845861	Biso	1.000000	O
O	1.0	0.183226	0.579820	0.178810	Biso	1.000000	O
O	1.0	0.183522	0.580999	0.513219	Biso	1.000000	O
O	1.0	0.183350	0.579475	0.845630	Biso	1.000000	O
O	1.0	0.683121	0.079710	0.321539	Biso	1.000000	O
O	1.0	0.683301	0.079694	0.654915	Biso	1.000000	O
O	1.0	0.683301	0.079764	0.988089	Biso	1.000000	O
O	1.0	0.683279	0.580253	0.321379	Biso	1.000000	O
O	1.0	0.683470	0.579861	0.654884	Biso	1.000000	O
O	1.0	0.683263	0.579827	0.988114	Biso	1.000000	O
O	1.0	0.316095	0.419398	0.012132	Biso	1.000000	O
O	1.0	0.318505	0.421913	0.346692	Biso	1.000000	O
O	1.0	0.316546	0.419879	0.678205	Biso	1.000000	O
O	1.0	0.316584	0.920059	0.011934	Biso	1.000000	O
O	1.0	0.316571	0.920195	0.345203	Biso	1.000000	O
O	1.0	0.316677	0.920096	0.678857	Biso	1.000000	O
O	1.0	0.563062	0.170088	0.266327	Biso	1.000000	O
O	1.0	0.562758	0.170093	0.599830	Biso	1.000000	O
O	1.0	0.562750	0.170141	0.932928	Biso	1.000000	O
O	1.0	0.562871	0.670249	0.266241	Biso	1.000000	O
O	1.0	0.562935	0.670413	0.599849	Biso	1.000000	O
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O	1.0	0.437181	0.329849	0.067094	Biso	1.000000	O
O	1.0	0.437677	0.329939	0.400733	Biso	1.000000	O
O	1.0	0.437097	0.329669	0.733574	Biso	1.000000	O
O	1.0	0.437165	0.829611	0.067009	Biso	1.000000	O
O	1.0	0.437281	0.829789	0.400415	Biso	1.000000	O
O	1.0	0.437234	0.829778	0.733836	Biso	1.000000	O
O	1.0	0.936397	0.329466	0.097806	Biso	1.000000	O
O	1.0	0.935140	0.330529	0.431713	Biso	1.000000	O
O	1.0	0.936971	0.329259	0.765245	Biso	1.000000	O
O	1.0	0.937301	0.829740	0.099676	Biso	1.000000	O
O	1.0	0.937143	0.829759	0.433029	Biso	1.000000	O
O	1.0	0.937243	0.829816	0.766334	Biso	1.000000	O
O	1.0	0.061015	0.167481	0.235357	Biso	1.000000	O
O	1.0	0.063322	0.170406	0.565245	Biso	1.000000	O
O	1.0	0.062964	0.170289	0.900618	Biso	1.000000	O
O	1.0	0.062880	0.670791	0.233867	Biso	1.000000	O
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O	1.0	0.062922	0.670055	0.900586	Biso	1.000000	O
O	1.0	0.437583	0.420356	0.233601	Biso	1.000000	O
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O	1.0	0.436919	0.420010	0.900464	Biso	1.000000	O
O	1.0	0.437214	0.920091	0.233728	Biso	1.000000	O
O	1.0	0.437302	0.919995	0.567145	Biso	1.000000	O
O	1.0	0.437183	0.920161	0.900484	Biso	1.000000	O
O	1.0	0.562945	0.079659	0.099523	Biso	1.000000	O
O	1.0	0.562871	0.079522	0.433131	Biso	1.000000	O
O	1.0	0.562764	0.079685	0.766440	Biso	1.000000	O
O	1.0	0.562652	0.579589	0.099644	Biso	1.000000	O
O	1.0	0.563272	0.580347	0.433122	Biso	1.000000	O
O	1.0	0.562791	0.579746	0.766368	Biso	1.000000	O
O	1.0	0.062389	0.080240	0.067495	Biso	1.000000	O
O	1.0	0.062282	0.080177	0.400335	Biso	1.000000	O
O	1.0	0.063049	0.079730	0.733549	Biso	1.000000	O
O	1.0	0.062721	0.579585	0.067148	Biso	1.000000	O
O	1.0	0.063048	0.580183	0.401192	Biso	1.000000	O
O	1.0	0.062926	0.579610	0.733654	Biso	1.000000	O
O	1.0	0.936926	0.420952	0.266303	Biso	1.000000	O
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O	1.0	0.937255	0.920290	0.599713	Biso	1.000000	O
O	1.0	0.937236	0.920292	0.932988	Biso	1.000000	O
O	1.0	0.311276	0.250996	0.015746	Biso	1.000000	O
O	1.0	0.312821	0.249901	0.347883	Biso	1.000000	O
O	1.0	0.311341	0.250516	0.681419	Biso	1.000000	O
O	1.0	0.311266	0.750517	0.014847	Biso	1.000000	O
O	1.0	0.311672	0.751094	0.348317	Biso	1.000000	O
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O	1.0	0.688514	0.248994	0.651733	Biso	1.000000	O
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O	1.0	0.688709	0.749061	0.318400	Biso	1.000000	O



O	1.0	0.688776	0.749062	0.652030	Biso	1.000000	O
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O	1.0	0.188556	0.248212	0.847938	Biso	1.000000	O
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O	1.0	0.311591	0.499590	0.515288	Biso	1.000000	O
O	1.0	0.311243	0.498734	0.848127	Biso	1.000000	O
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O	1.0	0.811111	0.998770	0.318480	Biso	1.000000	O
O	1.0	0.811597	0.999029	0.651648	Biso	1.000000	O
O	1.0	0.811555	0.999111	0.984938	Biso	1.000000	O
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O	1.0	0.187958	0.000747	0.347767	Biso	1.000000	O
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O	1.0	0.432491	0.741374	0.563110	Biso	1.000000	O
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O	1.0	0.567487	0.258677	0.103682	Biso	1.000000	O
O	1.0	0.567862	0.258788	0.437092	Biso	1.000000	O
O	1.0	0.567427	0.258663	0.770383	Biso	1.000000	O
O	1.0	0.567559	0.758642	0.103739	Biso	1.000000	O
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O	1.0	0.068191	0.259510	0.063481	Biso	1.000000	O
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O	1.0	0.067602	0.257960	0.728594	Biso	1.000000	O
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O	1.0	0.932576	0.241407	0.602634	Biso	1.000000	O
O	1.0	0.932400	0.241161	0.936666	Biso	1.000000	O
O	1.0	0.932308	0.741362	0.270219	Biso	1.000000	O
O	1.0	0.932391	0.741214	0.603842	Biso	1.000000	O
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O	1.0	0.567881	0.491292	0.270343	Biso	1.000000	O
O	1.0	0.567665	0.491374	0.603809	Biso	1.000000	O
O	1.0	0.567314	0.491204	0.937062	Biso	1.000000	O
O	1.0	0.567580	0.991119	0.270417	Biso	1.000000	O
O	1.0	0.567595	0.991102	0.603902	Biso	1.000000	O
O	1.0	0.567577	0.991166	0.937125	Biso	1.000000	O
O	1.0	0.432527	0.008665	0.063035	Biso	1.000000	O
O	1.0	0.432509	0.008605	0.396382	Biso	1.000000	O
O	1.0	0.432492	0.008576	0.729847	Biso	1.000000	O
O	1.0	0.432027	0.508757	0.063024	Biso	1.000000	O
O	1.0	0.433515	0.508957	0.396498	Biso	1.000000	O
O	1.0	0.432333	0.508759	0.729782	Biso	1.000000	O
O	1.0	0.932263	0.008680	0.103716	Biso	1.000000	O
O	1.0	0.932446	0.008212	0.437203	Biso	1.000000	O
O	1.0	0.932492	0.008923	0.770139	Biso	1.000000	O
O	1.0	0.932407	0.508423	0.103370	Biso	1.000000	O
O	1.0	0.932646	0.508541	0.436836	Biso	1.000000	O

O	1.0	0.932412	0.508424	0.769850	Biso	1.000000	O
O	1.0	0.067383	0.493971	0.231935	Biso	1.000000	O
O	1.0	0.067852	0.490952	0.562520	Biso	1.000000	O
O	1.0	0.067320	0.491600	0.895071	Biso	1.000000	O
O	1.0	0.067792	0.991400	0.229963	Biso	1.000000	O
O	1.0	0.067774	0.991132	0.562798	Biso	1.000000	O
O	1.0	0.067663	0.991440	0.896745	Biso	1.000000	O
O	1.0	0.305627	0.109097	0.279164	Biso	1.000000	O
O	1.0	0.303299	0.109516	0.612837	Biso	1.000000	O
O	1.0	0.302250	0.110605	0.946274	Biso	1.000000	O
O	1.0	0.303234	0.610761	0.278651	Biso	1.000000	O
O	1.0	0.303410	0.610710	0.612492	Biso	1.000000	O
O	1.0	0.302950	0.609645	0.945789	Biso	1.000000	O
O	1.0	0.696845	0.389648	0.054263	Biso	1.000000	O
O	1.0	0.696824	0.389812	0.387667	Biso	1.000000	O
O	1.0	0.696719	0.389672	0.721021	Biso	1.000000	O
O	1.0	0.697080	0.889618	0.054694	Biso	1.000000	O
O	1.0	0.696944	0.889486	0.388080	Biso	1.000000	O
O	1.0	0.697057	0.889659	0.721405	Biso	1.000000	O
O	1.0	0.195577	0.382245	0.108771	Biso	1.000000	O
O	1.0	0.197449	0.391802	0.444838	Biso	1.000000	O
O	1.0	0.196616	0.388723	0.777458	Biso	1.000000	O
O	1.0	0.196856	0.889703	0.112366	Biso	1.000000	O
O	1.0	0.196848	0.889716	0.445471	Biso	1.000000	O
O	1.0	0.196812	0.889686	0.779038	Biso	1.000000	O
O	1.0	0.802824	0.110206	0.221221	Biso	1.000000	O
O	1.0	0.803040	0.110320	0.554569	Biso	1.000000	O
O	1.0	0.803142	0.110396	0.887815	Biso	1.000000	O
O	1.0	0.803195	0.610603	0.221081	Biso	1.000000	O
O	1.0	0.803260	0.610310	0.554516	Biso	1.000000	O
O	1.0	0.803139	0.610246	0.887797	Biso	1.000000	O
O	1.0	0.696666	0.360361	0.220884	Biso	1.000000	O
O	1.0	0.696799	0.360300	0.554426	Biso	1.000000	O
O	1.0	0.696722	0.360166	0.887622	Biso	1.000000	O
O	1.0	0.697001	0.860377	0.221342	Biso	1.000000	O
O	1.0	0.696988	0.860256	0.554760	Biso	1.000000	O
O	1.0	0.697086	0.860350	0.888037	Biso	1.000000	O
O	1.0	0.303658	0.139948	0.113107	Biso	1.000000	O
O	1.0	0.304572	0.139438	0.446789	Biso	1.000000	O
O	1.0	0.302965	0.139658	0.779313	Biso	1.000000	O
O	1.0	0.303140	0.639268	0.112173	Biso	1.000000	O
O	1.0	0.303159	0.640026	0.445546	Biso	1.000000	O
O	1.0	0.303060	0.639639	0.779127	Biso	1.000000	O
O	1.0	0.802911	0.139682	0.054423	Biso	1.000000	O
O	1.0	0.802679	0.139600	0.387794	Biso	1.000000	O
O	1.0	0.803178	0.139531	0.721088	Biso	1.000000	O
O	1.0	0.803151	0.639537	0.054444	Biso	1.000000	O
O	1.0	0.803215	0.639692	0.387891	Biso	1.000000	O
O	1.0	0.803273	0.639561	0.721250	Biso	1.000000	O
O	1.0	0.198952	0.370763	0.275661	Biso	1.000000	O
O	1.0	0.196624	0.360292	0.610924	Biso	1.000000	O
O	1.0	0.196341	0.360135	0.943419	Biso	1.000000	O
O	1.0	0.196939	0.860100	0.278880	Biso	1.000000	O
O	1.0	0.196868	0.860569	0.612308	Biso	1.000000	O
O	1.0	0.196747	0.860557	0.945715	Biso	1.000000	O
O	1.0	0.448367	0.097368	0.201133	Biso	1.000000	O
O	1.0	0.448097	0.097205	0.534678	Biso	1.000000	O
O	1.0	0.447856	0.097231	0.868020	Biso	1.000000	O
O	1.0	0.447980	0.597167	0.201409	Biso	1.000000	O
O	1.0	0.448296	0.597569	0.534645	Biso	1.000000	O
O	1.0	0.447948	0.597345	0.867919	Biso	1.000000	O
O	1.0	0.552189	0.402657	0.132035	Biso	1.000000	O
O	1.0	0.552334	0.402737	0.465689	Biso	1.000000	O
O	1.0	0.551765	0.402594	0.798864	Biso	1.000000	O
O	1.0	0.551984	0.902522	0.132171	Biso	1.000000	O
O	1.0	0.552111	0.902621	0.465576	Biso	1.000000	O
O	1.0	0.552052	0.902642	0.798895	Biso	1.000000	O
O	1.0	0.051348	0.402538	0.031392	Biso	1.000000	O
O	1.0	0.051925	0.400855	0.365531	Biso	1.000000	O
O	1.0	0.051913	0.401455	0.699212	Biso	1.000000	O
O	1.0	0.051966	0.902617	0.034655	Biso	1.000000	O
O	1.0	0.051944	0.902905	0.368191	Biso	1.000000	O
O	1.0	0.051999	0.902712	0.701248	Biso	1.000000	O
O	1.0	0.945641	0.096707	0.299055	Biso	1.000000	O
O	1.0	0.948526	0.097699	0.631957	Biso	1.000000	O
O	1.0	0.948021	0.097156	0.965163	Biso	1.000000	O
O	1.0	0.948139	0.597730	0.299258	Biso	1.000000	O
O	1.0	0.948218	0.597209	0.632113	Biso	1.000000	O
O	1.0	0.948029	0.597326	0.965580	Biso	1.000000	O

O	1.0	0.552290	0.347422	0.298883	Biso	1.000000	O
O	1.0	0.552089	0.347374	0.632237	Biso	1.000000	O
O	1.0	0.551881	0.347277	0.965443	Biso	1.000000	O
O	1.0	0.552070	0.847249	0.298868	Biso	1.000000	O
O	1.0	0.552135	0.847228	0.632281	Biso	1.000000	O
O	1.0	0.552023	0.847252	0.965509	Biso	1.000000	O
O	1.0	0.448038	0.152592	0.034597	Biso	1.000000	O
O	1.0	0.448446	0.152583	0.367952	Biso	1.000000	O
O	1.0	0.447894	0.152543	0.701388	Biso	1.000000	O
O	1.0	0.447945	0.652611	0.034644	Biso	1.000000	O
O	1.0	0.448187	0.652859	0.367938	Biso	1.000000	O
O	1.0	0.448044	0.652692	0.701321	Biso	1.000000	O
O	1.0	0.946673	0.152808	0.131501	Biso	1.000000	O
O	1.0	0.947315	0.152286	0.465269	Biso	1.000000	O
O	1.0	0.948361	0.152720	0.798629	Biso	1.000000	O
O	1.0	0.948063	0.652399	0.132368	Biso	1.000000	O
O	1.0	0.947994	0.652537	0.465760	Biso	1.000000	O
O	1.0	0.948169	0.652342	0.798908	Biso	1.000000	O
O	1.0	0.051077	0.353106	0.195682	Biso	1.000000	O
O	1.0	0.051462	0.347367	0.531440	Biso	1.000000	O
O	1.0	0.051719	0.347620	0.865810	Biso	1.000000	O
O	1.0	0.052012	0.847333	0.201488	Biso	1.000000	O
O	1.0	0.051881	0.847277	0.534696	Biso	1.000000	O
O	1.0	0.052000	0.847538	0.867940	Biso	1.000000	O
Si	1.0	0.271395	0.170916	0.018870	Biso	1.000000	Si
Si	1.0	0.273498	0.169395	0.351687	Biso	1.000000	Si
Si	1.0	0.271846	0.170294	0.684572	Biso	1.000000	Si
Si	1.0	0.271584	0.670374	0.017781	Biso	1.000000	Si
Si	1.0	0.271707	0.671091	0.350926	Biso	1.000000	Si
Si	1.0	0.271663	0.670942	0.684639	Biso	1.000000	Si
Si	1.0	0.728101	0.329365	0.315367	Biso	1.000000	Si
Si	1.0	0.728134	0.329164	0.648972	Biso	1.000000	Si
Si	1.0	0.728223	0.329101	0.982153	Biso	1.000000	Si
Si	1.0	0.728453	0.829188	0.315806	Biso	1.000000	Si
Si	1.0	0.728499	0.829190	0.649279	Biso	1.000000	Si
Si	1.0	0.728516	0.829170	0.982536	Biso	1.000000	Si
Si	1.0	0.229116	0.333043	0.188472	Biso	1.000000	Si
Si	1.0	0.228091	0.330101	0.515861	Biso	1.000000	Si
Si	1.0	0.228181	0.328451	0.849665	Biso	1.000000	Si
Si	1.0	0.228370	0.829126	0.184301	Biso	1.000000	Si
Si	1.0	0.228300	0.829457	0.517750	Biso	1.000000	Si
Si	1.0	0.228224	0.829296	0.851299	Biso	1.000000	Si
Si	1.0	0.771634	0.170754	0.149049	Biso	1.000000	Si
Si	1.0	0.771291	0.170516	0.482449	Biso	1.000000	Si
Si	1.0	0.771675	0.170739	0.815593	Biso	1.000000	Si
Si	1.0	0.771707	0.670927	0.148833	Biso	1.000000	Si
Si	1.0	0.771843	0.670869	0.482431	Biso	1.000000	Si
Si	1.0	0.771751	0.670790	0.815715	Biso	1.000000	Si
Si	1.0	0.728338	0.420757	0.148762	Biso	1.000000	Si
Si	1.0	0.728101	0.420837	0.482291	Biso	1.000000	Si
Si	1.0	0.728204	0.420658	0.815572	Biso	1.000000	Si
Si	1.0	0.728520	0.920817	0.149208	Biso	1.000000	Si
Si	1.0	0.728418	0.920672	0.482537	Biso	1.000000	Si
Si	1.0	0.728528	0.920821	0.815904	Biso	1.000000	Si
Si	1.0	0.272238	0.078909	0.184860	Biso	1.000000	Si
Si	1.0	0.272268	0.078647	0.518054	Biso	1.000000	Si
Si	1.0	0.271389	0.079378	0.851609	Biso	1.000000	Si
Si	1.0	0.271549	0.579050	0.184536	Biso	1.000000	Si
Si	1.0	0.271906	0.579771	0.517945	Biso	1.000000	Si
Si	1.0	0.271712	0.578965	0.851010	Biso	1.000000	Si
Si	1.0	0.771454	0.078908	0.315639	Biso	1.000000	Si
Si	1.0	0.771649	0.079030	0.649049	Biso	1.000000	Si
Si	1.0	0.771661	0.079151	0.982285	Biso	1.000000	Si
Si	1.0	0.771604	0.579589	0.315515	Biso	1.000000	Si
Si	1.0	0.771832	0.579163	0.649052	Biso	1.000000	Si
Si	1.0	0.771646	0.579095	0.982322	Biso	1.000000	Si
Si	1.0	0.227656	0.418692	0.017229	Biso	1.000000	Si
Si	1.0	0.230097	0.424919	0.351443	Biso	1.000000	Si
Si	1.0	0.228136	0.420474	0.683383	Biso	1.000000	Si
Si	1.0	0.228187	0.920974	0.017956	Biso	1.000000	Si
Si	1.0	0.228147	0.920942	0.350844	Biso	1.000000	Si
Si	1.0	0.228303	0.920873	0.684552	Biso	1.000000	Si
Si	1.0	0.474144	0.168638	0.265936	Biso	1.000000	Si
Si	1.0	0.473854	0.168553	0.599371	Biso	1.000000	Si
Si	1.0	0.473845	0.168597	0.932630	Biso	1.000000	Si
Si	1.0	0.473974	0.668757	0.265905	Biso	1.000000	Si
Si	1.0	0.474011	0.668880	0.599407	Biso	1.000000	Si
Si	1.0	0.473847	0.668634	0.932641	Biso	1.000000	Si
Si	1.0	0.526127	0.331281	0.067453	Biso	1.000000	Si

Si	1.0	0.526549	0.331432	0.400915	Biso	1.000000	Si
Si	1.0	0.526026	0.331251	0.734120	Biso	1.000000	Si
Si	1.0	0.526095	0.831183	0.067481	Biso	1.000000	Si
Si	1.0	0.526197	0.831280	0.400871	Biso	1.000000	Si
Si	1.0	0.526151	0.831265	0.734249	Biso	1.000000	Si
Si	1.0	0.025439	0.332433	0.097414	Biso	1.000000	Si
Si	1.0	0.023114	0.334501	0.431457	Biso	1.000000	Si
Si	1.0	0.025888	0.330566	0.764398	Biso	1.000000	Si
Si	1.0	0.026241	0.831359	0.099429	Biso	1.000000	Si
Si	1.0	0.026038	0.831424	0.432684	Biso	1.000000	Si
Si	1.0	0.026163	0.831407	0.766042	Biso	1.000000	Si
Si	1.0	0.973258	0.167661	0.233816	Biso	1.000000	Si
Si	1.0	0.974307	0.168739	0.566682	Biso	1.000000	Si
Si	1.0	0.974004	0.168642	0.900698	Biso	1.000000	Si
Si	1.0	0.973990	0.668812	0.234301	Biso	1.000000	Si
Si	1.0	0.973945	0.668731	0.567604	Biso	1.000000	Si
Si	1.0	0.974012	0.668556	0.900880	Biso	1.000000	Si
Si	1.0	0.526485	0.418715	0.234085	Biso	1.000000	Si
Si	1.0	0.526288	0.418768	0.567599	Biso	1.000000	Si
Si	1.0	0.525875	0.418620	0.900828	Biso	1.000000	Si
Si	1.0	0.526132	0.918579	0.234163	Biso	1.000000	Si
Si	1.0	0.526206	0.918544	0.567569	Biso	1.000000	Si
Si	1.0	0.526109	0.918631	0.900874	Biso	1.000000	Si
Si	1.0	0.474039	0.081219	0.099224	Biso	1.000000	Si
Si	1.0	0.473968	0.081141	0.432639	Biso	1.000000	Si
Si	1.0	0.473853	0.081177	0.766075	Biso	1.000000	Si
Si	1.0	0.473740	0.581203	0.099258	Biso	1.000000	Si
Si	1.0	0.474384	0.581734	0.432759	Biso	1.000000	Si
Si	1.0	0.473862	0.581310	0.765991	Biso	1.000000	Si
Si	1.0	0.973427	0.081370	0.067438	Biso	1.000000	Si
Si	1.0	0.973244	0.080998	0.400474	Biso	1.000000	Si
Si	1.0	0.974111	0.081394	0.733922	Biso	1.000000	Si
Si	1.0	0.973791	0.581164	0.067482	Biso	1.000000	Si
Si	1.0	0.974140	0.581342	0.400970	Biso	1.000000	Si
Si	1.0	0.973990	0.581096	0.734097	Biso	1.000000	Si
Si	1.0	0.026095	0.419570	0.263652	Biso	1.000000	Si
Si	1.0	0.025927	0.418538	0.598057	Biso	1.000000	Si
Si	1.0	0.025532	0.418845	0.930333	Biso	1.000000	Si
Si	1.0	0.026257	0.918949	0.266000	Biso	1.000000	Si
Si	1.0	0.026170	0.918716	0.599262	Biso	1.000000	Si
Si	1.0	0.026175	0.918797	0.932792	Biso	1.000000	Si