Crystal structure of $[Fe(C_6H_{16}P_2)_2(CO_3)]$.H₂CO₃ –nsw069

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Abstract

The crystal structure of $[Fe(C_6H_{16}P_2)_2(CO_3)]$. H₂CO₃ is reported.

Comment

The crystallographic asymmetric unit consists of one $[Fe(C_6H_{16}P_2)_2(CO_3)]$ molecule in close association with a H_2CO_3 molecule.

There is considerable disorder of the Me₂PCH₂CH₂PMe₂ ligands which has required the use of multiple sites for most atoms. Only Fe1, P1, P4 and the atoms of the carbonate and H_2CO_3 units have full occupancy. One major isomer is for P1 to link to P102 and P4 to link to P103, with the extra complication that the P1 to P102 connection can have either a λ or δ conformation. That is to say, there are dmpe ligand conformations described by sites P1, C101, C102, P102, C103, C104, C105, C106; P1, C201, C202, P102, C203, C204, C205, C206; and P103, C107, C108, P4, C109, C110, C111, C112. There is also a component in which P1 links to P302 (close to P103) and P4 to P303 (close to P102), consisting of sites . P1, C301, C302, P302, C303, C304, C305, C306; and P303, C307, C308, P4, C309, C310, C311, C312. As these various sites frequently overlap, restraints were imposed on P—C and C—C bonded distances and on C—P—C and P—C—C angles. Initial refinement was undertaken using isotropic displacement parameters for these sites, constraining the values for overlapping and near-overlapping sites to be equal. Later, anisotropic displacement parameters were used with the imposition of restraints that corresponding terms for overlapping sites should tend to be equal. H atoms of dmpe ligands were included at idealized positions, and ride on the atom to which they are attached. The relative occupancies of the various components of the disorder were refined.

Clearly O52 is hydrogen-bonded to O2 and O53 to O3 but the question arises as to the location of the H atoms and whether we have $[Fe(dmpe)_2(HCO_3)]^+(HCO_3)^-$ or $[Fe(dmpe)_2(CO_3)](H_2CO_3)$. A difference electron density map revealed peaks attributable to these H atoms close to O52 and O53. H atoms were added at these sites and refined positionally. Their final positions seem to favour $[Fe(dmpe)_2(CO_3)](H_2CO_3)$ but the reliability of this result is unknown. The biggest peaks in the final difference electron density map are located near the Fe atom and near the O atoms of the H_2CO_3 .

Experimental

The compound was prepared by OA and recrystallized from benzene. The sample identification code is Oa 2.47.

Crystal data	
$\mathrm{C}_{13}\mathrm{H}_{32}\mathrm{FeO}_{3}\mathrm{P}_{4}.\mathrm{CH}_{2}\mathrm{O}_{3}$	Cell parameters from 35060 reflections
$M_r = 478.17$	$\theta = 2.627.5^{\circ}$
Orthorhombic	$\mu = 0.996 \text{ mm}^{-1}$
Pbca	T = 200 K
a = 16.5175(3) Å	Plate
$b = 16.1088 (3) {\rm \AA}$	Orange
c = 16.6269 (3) Å	0.13 \times 0.13 \times 0.06 mm
$V = 4424.04(14){\rm \AA}^3$	Crystal source: from UNSW
Z = 8	
$D_x = 1.436 \text{ Mg m}^{-3}$	
D_m not measured	
Mo $K\alpha$ radiation	
$\lambda = 0.71073 \text{ \AA}$	
Data collection	
Nonius KappaCCD diffractometer	2956 reflections with
φ and ω scans with CCD	$I > 2.0\sigma(I)$
Absorption correction:	$R_{\rm int} = 0.099$
by integration via Gaussian method (Cop-	$\theta_{\rm max} = 27.493^{\circ}$
pens, 1970) implemented in maXus $\left(2000\right)$	$h = -21 \rightarrow 21$
$T_{\min} = 0.883, T_{\max} = 0.949$	$k = -20 \rightarrow 20$
57391 measured reflections	$l = -21 \rightarrow 21$
5060 independent reflections	

 $\begin{aligned} & Refinement \\ & Refinement & on \ F^2 \\ & R(F) &= 0.0384 \\ & wR(F^2) &= 0.1174 \\ & S &= 1.0039 \\ & 5050 \ \text{reflections} \\ & 409 \ \text{parameters} \\ & \text{H atoms treated by a mixture of independent} \\ & \text{ and constrained refinement} \end{aligned}$

Method, part 1, Chebychev polynomial, (Carruthers & Watkin, 1979, Prince, 1982) [weight] = $1.0/[A_0 * T_0(x) + A_1 * T_1(x) \dots + A_{n-1}] * T_{n-1}(x)$] where A_i are the Chebychev coefficients listed below and x= Fcalc/Fmax Method = Robust Weighting (Prince, 1982) W = [weight] * $[1-(deltaF/6^*sigmaF)^2]^2 A_i$ are: $40.2 \ 64.4 \ 37.5 \ 14.2 \ 2.56$ $(\Delta/\sigma)_{max} = 0.011699$ $\Delta\rho_{max} = 0.65 \text{ e } \text{Å}^{-3}$ $\Delta\rho_{min} = -0.60 \text{ e } \text{Å}^{-3}$ Extinction correction: none Scattering factors from International Tables Vol C 4.2.6.8 and 6.1.1.4

F 4 F 4	Table 1. Selected geome	tric parameters (Å, °)	
Fel—Pl	2.2400(10)	P102—C106	1.817 (17)
Fel—P4	2.2442 (10)	P102—C202	1.867 (13)
Fe1—P102	2.2195(15)	P102—C205	1.820 (17)
Fe1—P103	2.193(4)	P102—C206	1.804(13)
Fe1—P302	2.149(12)	P103—C107	1.845(7)
Fe1—P303	2.152(3)	P103—C109	1.815(7)
Fe1—O1	2.041(2)	P103—C110	1.826(9)
Fe1—O2	2.039(2)	P302—C302	1.794(13)
Fe1-C50	2.431(3)	P302—C305	1.810(19)
P1—C101	1.814(13)	P302—C306	1.831(13)
P1—C103	1.781(13)	P303—C307	1.817(11)
P1—C104	1.849(13)	P303—C309	1.807(18)
P1—C201	1.797(11)	P303—C310	1.824(19)
P1—C203	1.862(10)	O1—C50	1.281(4)
P1—C204	1.806(10)	O2—C50	1.313(4)
P1-C301	1.802(12)	O3—C50	1.262(4)
P1—C303	1.790(13)	O51—C51	1.213(4)
P1-C304	1.809(13)	O52—C51	1.311(5)
P4—C108	1.839(6)	O53—C51	1.275(5)
P4—C111	1.793~(6)	C101—C102	1.527(17)
P4—C112	1.837(8)	C101—C202	1.35(3)
P4—C308	1.713(15)	C107—C108	1.541 (9)
P4—C311	1.851(13)	C201 - C202	1.508(15)
P4—C312	1.834(13)	C301 - C302	1.530(17)
P102—C102	1.860(14)	C307—C308	1.478(16)
P102—C105	1.796(17)		
P1—Fe1—P4	177.33(4)	P4—Fe1—O1	88.68(7)
P1—Fe1—P102	83.33~(7)	P102—Fe1—O1	162.04 (8)
P4—Fe1—P102	98.91~(7)	P103—Fe1—O1	$97.35\ (14)$
P1—Fe1—P103	94.66(9)	P302—Fe1—O1	96.1(3)
P4—Fe1—P103	86.43~(9)	P1— $Fe1$ — $O2$	88.72(8)
P102—Fe1—P103	99.34(12)	P4—Fe1—O2	89.49(8)
P1—Fe1—P302	85.2(2)	P102—Fe1—O2	99.12(7)
P4—Fe1—P302	95.8(2)	P103—Fe1—O2	161.49(13)
P1—Fe1—P303	102.99(14)	P302—Fe1—O2	159.8(3)
P4—Fe1—P303	79.25(14)	P303—Fe1—O1	159.97(13)
P302—Fe1—P303	100.9(3)	P303—Fe1—O2	99.18 (10)
P1—Fe1—O1	88.76(7)	O1—Fe1—O2	64.48(9)

Fe1—P1—C101	113.8~(6)	Fe1 - P102 - C206	127.4(6)
Fe1—P1—C103	116.8(8)	C202—P102—C206	102.4(7)
C101—P1—C103	103.4(9)	Fe1—P102—C309	130.8(11)
Fe1—P1—C104	117.9(7)	C205—P102—C206	102.6(13)
C101—P1—C104	99.7(8)	Fe1—P103—C107	109.0(3)
C103—P1—C104	102.9(9)	Fe1—P103—C109	129.2(3)
Fe1—P1—C201	112.6(4)	C107—P103—C109	100.4(4)
Fe1—P1—C203	113.5(4)	Fe1—P103—C110	112.0(4)
C201—P1—C203	101.6(6)	C107—P103—C110	102.8~(6)
Fe1—P1—C204	122.5(4)	C109—P103—C110	100.1 (5)
C201—P1—C204	104.9(6)	Fe1—P302—C302	110.3~(6)
Fe1—P1—C301	112.1~(6)	Fe1 - P302 - C305	104.6(12)
Fe1—P1—C303	118.4(9)	C302—P302—C305	108.5(14)
Fe1—P1—C304	111.4(9)	Fe1—P302—C306	127.1(8)
C203—P1—C204	99.2(6)	C302—P302—C306	100.8 (9)
C301—P1—C303	103.8(9)	C305—P302—C306	104.6(12)
C301—P1—C304	104.0 (11)	Fe1—P303—C307	114.7(4)
C303—P1—C304	105.9(11)	Fe1—P303—C309	121.4(9)
Fe1—P4—C108	109.5(2)	Fe1—P303—C310	110.5(14)
Fe1—P4—C111	116.7(2)	C307—P303—C309	103.3(8)
C108—P4—C111	104.1 (3)	C307—P303—C310	102.8(12)
Fe1—P4—C112	119.3(3)	C309—P303—C310	102.0(14)
C108—P4—C112	102.8(4)	Fe1—O1—C50	91.12(18)
C111—P4—C112	102.7(4)	Fe1-O2-C50	90.29(19)
Fe1—P4—C308	118.0(6)	O2—C50—O1	114.1 (3)
Fe1—P4—C311	118.8(6)	O2—C50—O3	121.7(3)
C308—P4—C311	103.4(8)	O1—C50—O3	124.2(3)
Fe1—P4—C312	113.5(5)	O52—C51—O53	116.6(3)
C308—P4—C312	102.5(10)	O52— $C51$ — $O51$	120.2~(4)
C311—P4—C312	97.7(9)	O53—C51—O51	123.1(4)
Fe1—P102—C102	110.3(5)	P1—C101—C102	106.1 (10)
Fe1—P102—C105	120.8(10)	C101—C102—P102	110.6(10)
C102—P102—C105	100.4(8)	P103—C107—C108	109.2~(4)
Fe1—P102—C106	118.3(13)	C107—C108—P4	109.0(4)
C102—P102—C106	102.2(12)	P1-C301-C302	110.1 (10)
C105—P102—C106	102.0(13)	C301—C302—P302	114.1(10)
Fe1—P102—C202	109.4(5)	P303—C307—C308	114.8(9)
Fe1—P102—C205	113.1(14)	C307—C308—P4	106.4(10)
C202 - P102 - C205	97.8 (10)		

	Table 2. Hydr	rogen-bonding geom	$netry~(\AA,~^\circ)$	
D—H···A	D—H	$\mathrm{H}{\cdots}A$	$D \cdots A$	D—H···A
O52— $H2$ ··· $O2$	0.82(5)	1.77(5)	2.568(4)	163~(6)
O53—H3···O3	0.84(5)	1.63(5)	2.470(5)	175(5)

H atoms of dmpe ligands were included at idealized positions, and ride on the atom to which they are attached. H atoms of the H_2CO_3 were observed in a difference electron density map prior to their inclusion, and then were refined positionally.

Data collection: *COLLECT* (Nonius BV, 1997). Cell refinement: Denzo/Scalepack . Data reduction: Denzo/Scalepack (Otwinowski & Minor, 1997). Program(s) used to solve structure: *SIR*92 (Altomare *et al.* 1994). Program(s) used to refine structure: *CRYSTALS* (Watkin *et al.*2003). Molecular graphics: *ORTEP*–II (Johnson 1976) in teXsan (MSC, 1992–1997) . Software used to prepare material for publication: *CRYSTALS*.

References

- Mackay, S., Gilmore, C. J., Edwards, C., Stewart, N. & Shankland, K. (2000). maXus Computer Program for the Solution and Refinement of Crystal Structures. Nonius, The Netherlands, MacScience, Japan & The University of Glasgow.
- Coppens, P. (1970). The Evaluation of Absorption and Extinction in Single-Crystal Structure Analysis. Crystallographic Computing. F. R. Ahmed, S. R. Hall and C. P. Huber, Editors., Munksgaard. Copenhagen. pp 255–270.
- Altomare, A., Cascarano, G., Giacovazzo, C., Guagliardi, A., Burla, M. C., Polidori, G. & Camalli, M. (1994). SIR92 - a program for automatic solution of crystal structures by direct methods. J. Appl. Cryst. (27), 435–435
- Betteridge, P. W., Carruthers, J. R., Cooper, R. I., Prout, K., Watkin, D. J. (2003). J. Appl. Cryst. 36, 1487.
- Nonius BV, COLLECT Software, 1997-2001)
- Otwinowski, Z. & Minor, W. (1996). Processing of X-ray Diffraction Data Collected in Oscillation Mode. Methods Enzymol. 276, 1997, 307–326. Ed Carter, C. W. & Sweet, R. M., Academic Press.
- Molecular Structure Corporation. (1992–1997). teXsan. Single Crystal Structure Analysis Software. Version 1.8. MSC, 3200 Research Forest Drive, The Woodlands, TX 77381, USA.
- Johnson, C. K. (1976). ORTEP–II, A Fortran Thermal-Ellipsoid Plot Program, Report ORNL-5138, Oak Ridge National Laboratory, Oak Ridge, Tennessee, USA.
- Prince, E. Mathematical Techniques in Crystallography and Materials Science Springer-Verlag, New York, 1982.

Carruthers, J. R. & Watkin, D. J. (1979). Acta Cryst. A35, 698–699.

Supplementary data

		1	I	1 1	(
		$U_{\rm eq} = (1/3)\Sigma_i \Sigma_i$	$\Sigma_j U^{ij} a^i a^j \mathbf{a}_i . \mathbf{a}_j.$		
	Occupancy	x	11	7.	U_{aa}
Fe1	1.0000	0.54135(2)	0.24659(3)	0.61237(2)	0.0263
P1	1.0000	0.44830 (5)	0.34752(6)	0.61899(5)	0.0363
P4	1.0000	0.63205 (6)	0.14287(7)	0.61095(7)	0.0495
P102	0.705(4)	0.52864(12)	0.26550(13)	0.48076(8)	0.0370
P103	0.705(4)	0.64416(19)	0.3294 (3)	0.6355(3)	0.0381
P302	0.295(4)	0.6271(6)	0.3433(7)	0.6383(8)	0.0381
P303	0.295(4)	0.5592(2)	0.2314(3)	0.48503(17)	0.0290
O1	1.0000	0.51628(14)	0.21790(15)	0.72933(12)	0.0363
O2	1.0000	0.45118(14)	0.16193(16)	0.62926 (13)	0.0377
O3	1.0000	0.41618(16)	0.12747(18)	0.75564(16)	0.0522
O51	1.0000	0.21495 (18)	0.0186(2)	0.6048(2)	0.0654
O52	1.0000	0.3149(2)	0.1042(3)	0.5803(2)	0.0853
O53	1.0000	0.3039(2)	0.0448(3)	0.6989(2)	0.0924
C50	1.0000	0.4601(2)	0.1680(2)	0.70752(19)	0.0360
C51	1.0000	0.2761(2)	0.0528(2)	0.6278(2)	0.0482
C101	0.348(8)	0.4029(10)	0.3728(13)	0.5227(9)	0.0485
C102	0.348 (8)	0.4695(9)	0.3614(9)	0.4601(10)	0.0543
C103	0.348 (8)	0.3631(11)	0.3293(15)	0.6822(13)	0.0543
C104	0.348 (8)	0.4821(13)	0.4521(9)	0.6502(10)	0.0633
C105 C106	0.348(8)	0.6159(13) 0.4727(17)	0.2835(16)	0.4187(16)	0.0451
C106 C107	0.348(8)	0.4737(17)	0.1881(19)	0.423(2)	0.0442
C107	0.705(4) 0.705(4)	0.7389(3) 0.7222(2)	0.2743(5) 0.1824(5)	0.6110(4)	0.0679
C108	0.705(4)	0.7522(5) 0.6659(5)	0.1634(3) 0.4308(4)	0.0392(3) 0.5031(4)	0.0734
C110	0.705(4)	0.0059(3) 0.6558(8)	0.4503(4) 0.3521(10)	0.3331(4) 0.7424(6)	0.0713
C111	0.705(4)	0.0358(8) 0.6152(4)	0.0521(10) 0.0591(4)	0.7424(0) 0.6799(4)	0.0511
C112	0.705(4)	0.6102(4) 0.6528(6)	0.0885(6)	0.5160(5)	0.0895
C201	0.357(8)	0.4360(9)	0.4011(7)	0.5250(7)	0.0485
C202	0.357(8)	0.4407(9)	0.3353(9)	0.4607(9)	0.0528
C203	0.357(8)	0.3438(6)	0.3084(8)	0.6375(9)	0.0517
C204	0.357 (8)	0.4518 (8)	0.4286(8)	0.6939(7)	0.0587
C205	0.357 (8)	0.4909 (16)	0.1740 (17)	0.429(2)	0.0471
C206	0.357 (8)	0.6041 (9)	0.3046 (10)	0.4121 (11)	0.0297
C301	0.295(4)	0.4937(11)	0.4490 (9)	0.6255(15)	0.0774
C302	0.295(4)	0.5853(9)	0.4428(7)	0.6132(9)	0.0615
C303	0.295(4)	0.3776(12)	0.3461~(17)	0.7005(11)	0.0467
C304	0.295(4)	0.3881~(15)	0.3520(18)	0.5282(12)	0.0570
C305	0.295(4)	0.641(2)	0.338(2)	0.7462(14)	0.0547
C306	0.295(4)	0.7297(7)	0.3539(12)	0.5978~(9)	0.0655
C307	0.295(4)	0.6378 (9)	0.1577(11)	0.4578(7)	0.0752
C308	0.295(4)	0.6884(11)	0.1289(15)	0.5255 (10)	0.0903
C309	0.295(4)	0.5798(14)	0.3192(13)	0.4206(15)	0.0538
C310	0.295(4)	0.4690(17)	0.187(2)	0.438(2)	0.0487
C311	0.295(4)	0.7082(10)	0.1374(14)	0.6924(11)	0.0905
C312	0.295(4)	0.5868 (11)	0.0401 (8)	0.6260(12)	0.0757
H2	1.0000	0.361(3)	0.113(4)	0.597(3)	0.0850
H3	1.0000	0.342(3)	0.075(3)	0.716(3)	0.0920
H1011	0.3482	0.3832(10)	0.4315(13)	0.5227(9)	0.0583
П1012 Ц1091	0.3482	0.3000 (10)	0.3340 (13)	0.3112(9) 0.4617(10)	0.0383
111021 U1022	0.3482	0.3007 (9)	0.4104(9) 0.2572(0)	0.4017 (10) 0.4055 (10)	0.0052
H1022	0.3462	0.3261 (11)	0.3372 (9) 0.3784 (15)	0.4000 (10)	0.0052
H1032	0.3482	0.3201(11) 0.3810(11)	0.3704(15) 0.3204(15)	0.0002 (13) 0.7387 (13)	0.0052
H1032	0.3482	0.3335(11)	0.0204 (10) 0.02788 (15)	0.1301 (13) 0.6631 (13)	0.0052
H1041	0.3482	0.3333 (11) 0.4347 (13)	0.2100 (10)	0.0051(13) 0.6505(10)	0.0052
H1042	0.3482	0.5060(13)	0.4491(9)	0.7054(10)	0.0759
H1043	0.3482	0.5238(13)	0.4729(9)	0.6115(10)	0.0759
			(~)		

Table S1. Fractional atomic coordinates and equivalent isotropic displacement parameters (\mathring{A}^2)

H1051	0.3482	0.5984(13)	0.2906(16)	0.3615(16)	0.0541
H1052	0.3482	0.6443 (13)	0.3349(16)	0.4372(16)	0.0541
H1053	0.3482	0.6535(13)	0.2351(16)	0.4229(16)	0.0541
H1061	0.3482	0.4728(17)	0.2046 (19)	0.365(2)	0.0533
H1062	0.3482	0.5011(17)	0.1330(19)	0.429(2)	0.0533
H1063	0.3482	0.4170(17)	0.1840(19)	0.444(2)	0.0533
H1071 H1079	0.7054	0.7853(3) 0.7481(2)	0.3017(5) 0.2757(5)	0.6390(4) 0.5516(4)	0.0815
H1072	0.7054	0.7481(3) 0.7387(3)	0.2757(5) 0.1807(5)	0.5510(4) 0.6990(5)	0.0813
H1082	0.7054	0.7754(3)	0.1494(5)	0.6129(5)	0.0881
H1091	0.7054	0.7177 (5)	0.4524(4)	0.6161(4)	0.0856
H1092	0.7054	0.6208(5)	0.4699(4)	0.6066(4)	0.0856
H1093	0.7054	0.6710(5)	0.4261(4)	0.5334(4)	0.0856
H1101	0.7054	0.7032(8)	0.3899(10)	0.7504(6)	0.0613
H1102	0.7054	0.6651(8)	0.2993(10)	0.7726(6)	0.0613
H1103 H1111	0.7054	0.6007(8) 0.6592(4)	0.3797 (10) 0.0169 (4)	0.7629(6) 0.6738(4)	0.0013
H1112	0.7054	0.0332(4) 0.6153(4)	0.0109(4) 0.0810(4)	0.7362(4)	0.0748
H1113	0.7054	0.5617(4)	0.0327(4)	0.6683(4)	0.0748
H1121	0.7054	0.6943 (6)	0.0443 (6)	0.5254(5)	0.1074
H1122	0.7054	0.6737~(6)	0.1290(6)	0.4754(5)	0.1074
H1123	0.7054	0.6018(6)	0.0626~(6)	0.4956(5)	0.1074
H2011	0.3573	0.4801(9)	0.4429(7)	0.5176(7)	0.0582
H2012	0.3573	0.3823(9)	0.4297(7)	0.5232(7)	0.0582
H2021 H2022	0.3573	0.4470(9) 0.3806(0)	0.3623(9) 0.3010(0)	0.4070(9) 0.4609(9)	0.0634
H2031	0.3573	0.3890(9) 0.3054(6)	0.3019(9) 0.3564(8)	0.4009(9) 0.6398(9)	0.0034
H2032	0.3573	0.3423(6)	0.2777(8)	0.6897(9)	0.0621
H2033	0.3573	0.3276(6)	0.2703 (8)	0.5929(9)	0.0621
H2041	0.3573	0.4048(8)	0.4670(8)	0.6862(7)	0.0705
H2042	0.3573	0.5035(8)	0.4604 (8)	0.6883(7)	0.0705
H2043	0.3573	0.4489(8)	0.4033(8)	0.7488(7)	0.0705
H2051 H2052	0.3573	0.4865(16) 0.5201(16)	0.1863(17) 0.1267(17)	0.370(2) 0.427(2)	0.0566
H2053	0.3573	0.3291(10) 0.4364(16)	$0.1207 (17) \\ 0.1589 (17)$	0.457(2) 0.450(2)	0.0566
H2061	0.3573	0.5811(9)	0.3063(10)	0.3565(11)	0.0356
H2062	0.3573	0.6204 (9)	0.3618 (10)	0.4288 (11)	0.0356
H2063	0.3573	0.6525(9)	0.2673(10)	0.4130(11)	0.0356
H3011	0.2946	0.4824(11)	0.4733(9)	0.6797(15)	0.0928
H3012	0.2946	0.4701 (11)	0.4856(9)	0.5830(15)	0.0928
H3021	0.2946	0.6120(9) 0.5074(0)	0.4857(7) 0.4544(7)	0.6477(9)	0.0738
H3022	0.2940	0.3974(9) 0.3400(12)	0.4344(7) 0.3946(17)	0.5554(9) 0.6956(11)	0.0738
H3032	0.2946	0.4075(12)	0.3496(17)	0.7527(11)	0.0561
H3033	0.2946	0.3456(12)	0.2934(17)	0.6988 (11)	0.0561
H3041	0.2946	0.3473(15)	0.3975(18)	0.5330(12)	0.0684
H3042	0.2946	0.4242(15)	0.3631~(18)	0.4811(12)	0.0684
H3043	0.2946	0.3596(15)	0.2978(18)	0.5202(12)	0.0684
H3051	0.2946	0.681(2)	0.382(2)	0.7633(14)	0.0656
H3052 H2052	0.2946	0.662(2) 0.588(2)	0.282(2) 0.248(2)	0.7614(14) 0.7726(14)	0.0656
H3061	0.2946	0.7556(7)	0.348(2) 0.4049(12)	0.6205(9)	0.0030
H3062	0.2946	0.7624(7)	0.3040(12)	0.6129(9)	0.0787
H3063	0.2946	0.7270 (7)	0.3585(12)	0.5379(9)	0.0787
H3071	0.2946	0.6739(9)	0.1846(11)	0.4172(7)	0.0903
H3072	0.2946	0.6112(9)	0.1081~(11)	0.4331(7)	0.0903
H3081	0.2946	0.7394(11)	0.1623(15)	0.5285(10)	0.1083
H3082	0.2946	0.7023(11)	0.0689(15)	0.5187(10)	0.1083
H3091	0.2940	0.3802(14) 0.6308(14)	0.2997 (13) 0.3471 (13)	0.3038(15) 0.4385(15)	0.0646
H3093	0.2946	0.5338 (14)	0.3594 (13)	0.4237(15)	0.0646
H3101	0.2946	0.4783 (17)	0.181 (2)	0.379(2)	0.0586
H3102	0.2946	0.4574(17)	0.132(2)	0.463(2)	0.0586
H3103	0.2946	0.4219(17)	0.225(2)	0.448(2)	0.0586
H3111	0.2946	0.7441(10)	0.0882(14)	0.6836(11)	0.1086
H3112	0.2946	0.7416(10)	0.1892(14)	0.6923(11)	0.1086
H3113 H9191	0.2946	0.6801 (10)	$0.1318 (14) \\ 0.0021 (8)$	0.7454 (11) 0.6247 (12)	0.1086
H3122	0.2940	0.5588 (11)	0.0385 (8)	0.0247 (12) 0.6793 (12)	0.0908
H3123	0.2946	0.5468 (11)	0.0289 (8)	0.5823(12)	0.0908
		(-/	\ - /	/	

Table S2. Anisotropic displacement parameters (\AA^2)

	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Fe1	0.02097(19)	0.0335(2)	0.02428(19)	0.00051(17)	-0.00001(16)	-0.00009(18)
P1	0.0323(5)	0.0396(5)	0.0370(4)	0.0096(4)	0.0008(3)	0.0022(4)
P4	0.0366(5)	0.0480 (5)	0.0638 (6)	0.0147(4)	0.0050(5)	0.0013(5)
P102	0.0394(9)	0.0495 (10)	0.0221(6)	0.0017(8)	0.0004(6)	-0.0004(6)
P103	0.0321(16)	0.0491 (16)	0.0332(6)	-0.0127(10)	-0.0069(11)	0.0062(10)
P302	0.0321(16)	0.0491(16)	0.0332(6)	-0.0127(10)	-0.0069(11)	0.0062(10)
P303	0.0253(16)	0.0406 (19)	0.0212(13)	0.0082(14)	-0.0022(11)	0.0010(12)
O1	0.0340(12)	0.0485 (13)	0.0263(11)	-0.0063(10)	-0.0044(9)	0.0044(10)
O2	0.0328(13)	0.0516 (14)	0.0286(11)	-0.0091(11)	-0.0009(9)	0.0006(10)
O3	0.0483(15)	0.0704 (18)	0.0379(13)	-0.0193(13)	-0.0008(11)	0.0171(13)
O51	0.0474(16)	0.0657 (19)	0.083(2)	-0.0247(15)	-0.0080(15)	-0.0036(17)
O52	0.069(2)	0.130 (3)	0.0569(18)	-0.060(2)	-0.0214(17)	0.026(2)
O53	0.090(3)	0.103 (3)	0.084(2)	-0.062(2)	-0.030(2)	0.045(2)
C50	0.0324(16)	0.0445 (17)	0.0310 (16)	-0.0022(15)	-0.0015(13)	0.0068(14)
C51	0.043(2)	0.042(2)	0.060(2)	-0.0104(17)	-0.0007(17)	-0.0001(17)
C101	0.056(9)	0.041 (11)	0.048(5)	0.014(7)	-0.007(6)	-0.001(6)
C102	0.063(10)	0.066(10)	0.034(5)	0.013(7)	-0.002(7)	0.009(6)
C103	0.041 (7)	0.063(9)	0.059(8)	0.010(6)	0.021(7)	0.003 (8)
C104	0.091(8)	0.057(6)	0.041(9)	-0.011(5)	0.012(6)	-0.015(5)
C105	0.050(8)	0.054(11)	0.032(5)	0.000(7)	0.003(6)	0.007(6)
C106	0.039(9)	0.072(7)	0.021(8)	-0.008(7)	-0.003(7)	-0.010(7)
C107	0.032(3)	0.099(5)	0.073(4)	-0.008(3)	-0.001(3)	0.010(4)
C108	0.032(3)	0.100 (6)	0.089(5)	0.005(3)	-0.001(3)	0.027(4)
C109	0.096(5)	0.064(4)	0.054(4)	-0.035(4)	-0.006(4)	0.007(3)
C110	0.050(5)	0.068(6)	0.036(3)	-0.039(4)	-0.015(3)	0.005(3)
C111	0.058(4)	0.049(3)	0.080(5)	0.021(3)	0.003(3)	0.018(3)
C112	0.108 (8)	0.090(7)	0.071(4)	0.057(6)	0.003(5)	-0.008(5)
C201	0.062(9)	0.037(8)	0.047(5)	0.015(6)	0.003(6)	0.004(5)
C202	0.054(9)	0.074(10)	0.031(5)	0.013(7)	-0.006(6)	0.011(6)
C203	0.035~(6)	0.057(7)	0.062(8)	0.017(5)	0.016(6)	0.013(6)
C204	0.072(7)	0.057(6)	0.047(7)	0.013(6)	0.001(5)	-0.013(5)
C205	0.030(9)	0.073(9)	0.038(7)	-0.008(7)	-0.003(7)	-0.003(7)
C206	0.034(8)	0.040(10)	0.015(5)	-0.002(7)	0.001(5)	0.010(6)
C301	0.104(10)	0.063(7)	0.066(13)	-0.019(8)	0.017(9)	-0.006(8)
C302	0.091(8)	0.035(5)	0.058(7)	-0.018(6)	-0.012(7)	-0.003(6)
C303	0.034(7)	0.054(10)	0.052(9)	0.013(7)	0.009(7)	-0.004(7)
C304	0.060(9)	0.056(12)	0.055(7)	0.020(8)	-0.016(7)	0.001(7)
C305	0.054(10)	0.064(10)	0.047(7)	-0.041(9)	-0.012(6)	0.005~(6)
C306	0.034(6)	0.095(8)	0.067(7)	-0.032(6)	0.010(5)	0.003(7)
C307	0.070(10)	0.116(14)	0.040(7)	0.067(10)	0.023(7)	0.006(8)
C308	0.102(12)	0.101(12)	0.068(8)	0.050(9)	0.016(9)	-0.004(9)
C309	0.058(11)	0.066(11)	0.038(7)	-0.006(8)	0.005(8)	-0.001(7)
C310	0.048(9)	0.076(9)	0.022(10)	-0.007(8)	0.004(9)	-0.015(7)
C311	0.060(8)	0.114(10)	0.098(9)	0.024(8)	-0.021(7)	0.001(8)
C312	0.081(9)	0.045(7)	0.100(9)	0.022(7)	0.021(8)	0.009(7)

Table S3. Geometric parameters (Å, °)

Fe1—P1	2.2400 (10)	C107—H1072	1.000
Fe1—P4	2.2442 (10)	C108—H1081	1.000
Fe1—P102	2.2195 (15)	C108—H1082	1.000
Fe1—P103	2.193 (4)	C109—H1091	1.000
Fe1—P302	2.149 (12)	C109—H1092	1.000
Fe1—P303	2.152 (3)	C109—H1093	1.000
Fe1—O1	2.041 (2)	C110—H1101	1.000
Fe1—O2	2.039 (2)	C110—H1102	1.000
Fe1—C50	2.431 (3)	C110—H1103	1.000
P1-C101	1.814 (13)	C111—H1111	1.000
P1-C103	1.781 (13)	C111—H1112	1.000
P1-C104	1.849 (13)	C111—H1113	1.000
P1-C201	1.797 (11)	C112—H1121	1.000
P1-C203	1.862 (10)	C112—H1122	1.000
P1-C204	1.806 (10)	C112—H1123	1.000
P1-C301	1.802(12)	C201—C202	1.508(15)
P1-C303	1.790 (13)	C201—H2011	1.000
P1-C304	1.809 (13)	C201—H2012	1.000
P4-C108	1 839 (6)	C202—H2021	1 000
P4—C111	1 793 (6)	C202—H2022	1.000
P4—C112	1 837 (8)	C203—H2031	1.000
P4-C308	1.007(0) 1.713(15)	C203—H2032	1.000
P4_C311	1 851 (13)	C203 H2032	1.000
$P_4 = C_{212}$	1.001(10) 1.924(12)	C203—112033	1.000
P102 C102	1.634(13) 1.860(14)	$C_{204} = 112041$	1.000
P102—C102	1.800(14)	С204—Н2042	1.000
P102—C105	1.790(17)	С204—н2043	1.000
P102—C106	1.817(17)	C205—H2051	1.000
P102—C202	1.867 (13)	C205—H2052	1.000
P102—C205	1.820 (17)	C205—H2053	1.000
P102—C206	1.804 (13)	C206—H2061	1.000
P103—C107	1.845 (7)	C206—H2062	1.000
P103—C109	1.815 (7)	C206—H2063	1.000
P103-C110	1.826 (9)	C301—C302	1.530(17)
P302—C302	1.794 (13)	C301—H3011	1.000
P302—C305	1.810 (19)	C301—H3012	1.000
P302—C306	1.831 (13)	C302—H3021	1.000
P303—C307	1.817(11)	C302—H3022	1.000
P303—C309	1.807(18)	C303—H3031	1.000
P303—C310	1.824(19)	C303—H3032	1.000
O1-C50	1.281(4)	C303—H3033	1.000
O2—C50	1.313(4)	C304—H3041	1.000
O3-C50	1.262(4)	C304—H3042	1.000
O51—C51	1.213(4)	C304—H3043	1.000
O52—C51	1.311(5)	C305—H3051	1.000
O52—H2	0.83(5)	C305—H3052	1.000
O53—C51	1.275(5)	C305—H3053	1.000
O53—H3	0.84(6)	C306—H3061	1.000
C101—C102	1.527(17)	C306—H3062	1.000
C101— $C202$	1.35(3)	C306—H3063	1.000
C101—H1011	1.000	C307—C308	1.478(16)
C101—H1012	1.000	C307—H3071	1.000
C102—H1021	1.000	C307—H3072	1.000
C102—H1022	1.000	C308—H3081	1.000
C103—H1031	1.000	C308—H3082	1.000
C103—H1032	1.000	C309—H3091	1.000
C103—H1033	1.000	C309—H3092	1.000
C104—H1041	1.000	C309—H3093	1.000
C104—H1042	1.000	C310—H3101	1.000
C104—H1043	1.000	C310—H3102	1.000
C105—H1051	1.000	C310—H3103	1.000
C105—H1052	1.000	C311—H3111	1.000
C105—H1053	1.000	C311—H3112	1.000
C106—H1061	1.000	C311—H3113	1.000
C106—H1062	1.000	C312—H3121	1.000
C106—H1063	1.000	C312—H3122	1.000
C107—C108	1.541 (9)	C312—H3123	1.000
C107—H1071	1.000		
$P_1 = P_1 = P_4$	177.92(4)	$P_1 = F_{c1} = P_{102}$	09 99 (7)
r1—re1—r4	111.33 (4)	r1—re1—r102	83.33 (7)

P4—Fe1—P102
P1—Fe1—P103
P4—Fe1—P103
P102—Fe1—P103
P1—Fe1—P302
P4—Fe1—P302
P1—Fe1—P303 P4 Fe1 P202
P302_Fe1_P303
P1 = Fe1 = 01
P4—Fe1—O1
P102—Fe1—O1
P103—Fe1—O1
P302—Fe1—O1
P1—Fe1—O2
P4—Fe1—O2
P102—Fe1—O2
P103—Fe1—O2
P302—Fe1—O2
P303—Fe1—O1 P303—Fe1—O2
$01 - F_{e1} - 02$
Fe1-P1-C101
Fe1—P1—C103
C101-P1-C103
Fe1— $P1$ — $C104$
$\rm C101{}P1{}C104$
$\rm C103{}P1{}C104$
Fe1-P1-C201
Fe1—P1—C203
C201—P1—C203
Fel—Pl—C204
C201—P1—C204
Fe1—P1—C303
Fe1—P1—C304
C203—P1—C204
C301-P1-C303
C301—P1—C304
C303 - P1 - C304
Fe1-P4-C108
Fe1-P4-C111
C108—P4—C111
Fe1—P4—C112
C108—P4—C112
C111 - P4 - C112 E-1 D4 C208
Fe1 - P4 - C311
C308 - P4 - C311
Fe1—P4—C312
C308—P4—C312
C311—P4—C312
Fe1—P102—C102
$\rm Fe1{}P102{}C105$
C102 - P102 - C105
Fe1—P102—C106
C102—P102—C106
C105—P102—C106
Fe1—P102—C202
Fe1—P102—C205
Fe1—P102—C205 C202—P102—C205 Fe1—P102—C206
Fe1—P102—C205 C202—P102—C205 Fe1—P102—C206 C202—P102—C206
Fe1—P102—C205 C202—P102—C205 Fe1—P102—C206 C202—P102—C206 Fe1—P102—C206 Fe1—P102—C309
Fe1—P102—C205 C202—P102—C205 Fe1—P102—C206 C202—P102—C206 Fe1—P102—C206 Fe1—P102—C309 C205—P102—C206
$\begin{array}{c} \text{Fe1} P102-C205\\ \text{C202}-P102-C205\\ \text{Fe1}-P102-C206\\ \text{C202}-P102-C206\\ \text{Fe1}-P102-C206\\ \text{Fe1}-P102-C309\\ \text{C205}-P102-C206\\ \text{Fe1}-P103-C107\\ \end{array}$
$\begin{array}{c} \text{Fe1} P102-C205\\ \text{C202}-P102-C205\\ \text{Fe1}-P102-C206\\ \text{C202}-P102-C206\\ \text{Fe1}-P102-C206\\ \text{Fe1}-P102-C309\\ \text{C205}-P102-C206\\ \text{Fe1}-P103-C107\\ \text{Fe1}-P103-C109\\ \end{array}$
$\begin{array}{c} \text{Fe1-P102-C205} \\ \text{C202-P102-C205} \\ \text{Fe1-P102-C206} \\ \text{C202-P102-C206} \\ \text{Fe1-P102-C309} \\ \text{C205-P102-C206} \\ \text{Fe1-P103-C107} \\ \text{Fe1-P103-C107} \\ \text{Fe1-P103-C109} \\ \text{C107-P103-C109} \\ \end{array}$

98.91(7)
00.01 (1)
94.66(9)
86.43(9)
00.34 (12)
33.34 (12)
85.2(2)
95.8(2)
100.00 (14)
102.99(14)
79.25(14)
100.0 (2)
100.9(3)
88.76(7)
88 68 (7)
00.00 (1)
162.04(8)
97.35(14)
01.00 (11)
96.1(3)
88.72(8)
80 10 (8)
69.49 (6)
99.12(7)
161.49(13)
150.0 (0)
159.8(3)
159.97 (13)
00.18 (10)
<i>33.10</i> (10)
64.48(9)
113.8 (6)
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103.4(9)
117.0 (7)
117.9(7)
99.7(8)
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101.0 (0)
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102.2(12)
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112 1 (14)
113.1(14)
113.1 (14) 97.8 (10)
$\begin{array}{c} 113.1 \ (14) \\ 97.8 \ (10) \\ 127.4 \ (6) \end{array}$
$\begin{array}{c} 113.1 \ (14) \\ 97.8 \ (10) \\ 127.4 \ (6) \\ 122.4 \ (7) \end{array}$
$\begin{array}{c} 113.1 \ (14) \\ 97.8 \ (10) \\ 127.4 \ (6) \\ 102.4 \ (7) \end{array}$
$\begin{array}{c} 113.1 \ (14) \\ 97.8 \ (10) \\ 127.4 \ (6) \\ 102.4 \ (7) \\ 130.8 \ (11) \end{array}$
$\begin{array}{c} 113.1 \ (14) \\ 97.8 \ (10) \\ 127.4 \ (6) \\ 102.4 \ (7) \\ 130.8 \ (11) \\ 102.6 \ (12) \end{array}$
$\begin{array}{c} 113.1 \ (14) \\ 97.8 \ (10) \\ 127.4 \ (6) \\ 102.4 \ (7) \\ 130.8 \ (11) \\ 102.6 \ (13) \end{array}$
$\begin{array}{c} 113.1 \ (14) \\ 97.8 \ (10) \\ 127.4 \ (6) \\ 102.4 \ (7) \\ 130.8 \ (11) \\ 102.6 \ (13) \\ 109.0 \ (3) \end{array}$
$\begin{array}{c} 113.1 (14) \\ 97.8 (10) \\ 127.4 (6) \\ 102.4 (7) \\ 130.8 (11) \\ 102.6 (13) \\ 109.0 (3) \\ 129.2 (3) \end{array}$
$\begin{array}{c} 113.1 (14) \\ 97.8 (10) \\ 127.4 (6) \\ 102.4 (7) \\ 130.8 (11) \\ 102.6 (13) \\ 109.0 (3) \\ 129.2 (3) \\ 100.4 (1) \end{array}$

112.0 (4)

C107—P103—C110
C100 P102 C110
C109—F103—C110
Fe1—P302—C302
Fe1—P302—C305
C302—P302—C305
Fe1—P302—C306
C302—P302—C306
C305—P302—C306
E_{01} E
FeI—F303—C307
Fe1—P303—C309
Fe1—P303—C310
C307—P303—C309
C307—P303—C310
C309—P303—C310
Fe1 - O1 - C50
$F_{r}^{-1} = O_{r}^{-1} = O_{$
Fe1—02—050
C51—O52—H2
C51—O53—H3
O2-C50-O1
O2—C50—O3
O1-C50-O3
O52—C51—O53
052 - 051 - 051
053 - 051 - 051
055-051-051
P1-C101-C102
P1-C101-H1011
C102—C101—H1011
P1—C101—H1012
C102—C101—H1012
H1011—C101—H1012
C101-C102-P102
C101_C102_H1021
P102 C102 H1021
F 102-C102-II1021
C101—C102—H1022
P102—C102—H1022
H1021—C102—H1022
P1-C103-H1031
P1-C103-H1032
H1031—C103—H1032
P1-C103-H1033
H1021 C102 H1022
H1031 - C103 - H1033
H1032-C103-H1033
P1-C104-H1041
P1-C104-H1042
H1041—C104—H1042
P1—C104—H1043
H1041-C104-H1043
H1042-C104-H1043
P102-C105-H1051
$P_{102} = C_{105} = H_{1052}$
1102 - 0105 - 111052
H1051-C105-H1052
P102—C105—H1053
H1051—C105—H1053
H1052—C105—H1053
P102—C106—H1061
P102—C106—H1062
H1061—C106—H1062
P102—C106—H1063
$H_{1061} - C_{106} - H_{1063}$
H1001 - C100 - H1003
H1062—C106—H1063
P103—C107—C108
P103—C107—H1071
C108—C107—H1071
P103—C107—H1072
C108—C107—H1072
H1071—C107—H1072
C107—C108—P4
C107—C108—H1081
P4-C108-H1081

100.1 (5) 110.3(6)104.6 (12) 108.5 (14) 127.1 (8) 100.8 (9) 104.6(12)114.7 (4) 121.4 (9) 110.5 (14) 103.3 (8) 102.8 (12) 102.0 (14) 91.12 (18) 90.29 (19) 111 (4) 122 (4) 114.1(3)121.7 (3) 124.2 (3) 116.6 (3) 120.2(4)123.1 (4) 106.1 (10) 110.3 110.3 110.3110.3109.5110.6 (10) 109.2 109.2109.2109.2 109.5109.5109.5109.5109.5109.5109.5 109.5109.5109.5109.5109.5109.5109.5109.5109.5109.5109.5109.5109.5109.4109.5 109.4109.5109.5109.2(4)109.6 109.5109.5109.5109.5109.0 (4) 109.6

109.6

102.8(6)

C107—C108—H1082
D. C.C. W.C.C.
P4-C108-H1082
H1081 - C108 - H1082
P103—C109—H1091
P103_C109_H1092
H1001 G100 H1002
H1091—C109—H1092
P103—C109—H1093
H1091-C109-H1093
H1051 C105 H1055
H1092—C109—H1093
P103—C110—H1101
P103_C110_H1102
H1101 C110 H1102
H1101-C110-H1102
P103—C110—H1103
H1101-C110-H1103
H1100 G110 H1100
H1102—C110—H1103
P4—C111—H1111
P4—C111—H1112
H1111 C111 H1110
H1111-C111-H1112
P4—C111—H1113
H1111—C111—H1113
H1112_C111_H1112
п1112—С111—п1115
P4—C112—H1121
P4—C112—H1122
U1191 C119 U1199
IIII121—C112—III122
P4—C112—H1123
H1121-C112-H1123
H1122_C112_H1123
D1 C201 C202
P1—C201—C202
P1—C201—H2011
H1011—C201—H2011
$D_1 = C_{201} = U_{2012}$
P1=C201=H2012
C202—C201—H2012
H2011-C201-H2012
C201_C202_H2021
0201-0202-112021
C201—C202—H2022
P1—C203—H2031
P1_C203_H2032
P1—C203—H2032
P1—C203—H2032 H2031—C203—H2032
P1—C203—H2032 H2031—C203—H2032 P1—C203—H2033
P1—C203—H2032 H2031—C203—H2032 P1—C203—H2033 H2031—C203—H2033
P1—C203—H2032 H2031—C203—H2032 P1—C203—H2033 H2031—C203—H2033 H2031—C203—H2033
P1—C203—H2032 H2031—C203—H2032 P1—C203—H2033 H2031—C203—H2033 P1—C204—H2041
P1—C203—H2032 H2031—C203—H2032 P1—C203—H2033 H2031—C203—H2033 P1—C204—H2041 P1—C204—H2042
$\begin{array}{c} P1C203H2032 \\ H2031C203H2032 \\ P1C203H2033 \\ H2031C203H2033 \\ P1C204H2041 \\ P1C204H2042 \\ P1C204H2042 \\ P1C204H2043 \end{array}$
P1C203-H2032 H2031C203-H2032 P1C203-H2033 H2031C203-H2033 P1C204-H2041 P1C204-H2042 P1C204-H2042 P1C204-H2043 H2041-C204-H2043
P1—C203—H2032 H2031—C203—H2032 P1—C203—H2033 H2031—C203—H2033 P1—C204—H2041 P1—C204—H2042 P1—C204—H2043 H2041—C204—H2042
$\begin{array}{l} P1C203H2032\\ H2031C203H2032\\ P1C203H2033\\ H2031C203H2033\\ P1C204H2041\\ P1C204H2042\\ P1C204H2043\\ H2041C204H2042\\ H2041C204H2043\\ \end{array}$
$\begin{array}{l} P1-C203-H2032\\ H2031-C203-H2032\\ P1-C203-H2033\\ H2031-C203-H2033\\ P1-C204-H2043\\ P1-C204-H2042\\ P1-C204-H2042\\ H2041-C204-H2043\\ H2041-C204-H2043\\ H2042-C204-H2043\\ H2042-C204-H2043\\ \end{array}$
$\begin{array}{c} P1C203H2032\\ H2031C203H2032\\ P1C203H2033\\ H2031C203H2033\\ P1C204H2043\\ P1C204H2042\\ P1C204H2043\\ H2041C204H2042\\ H2041C204H2043\\ H2042C204H2043\\ H2042C205H2051\\ H2051\\ \end{array}$
$\begin{array}{c} P1C203H2032\\ H2031C203H2032\\ P1C203H2033\\ H2031C203H2033\\ P1C204H2041\\ P1C204H2042\\ P1C204H2043\\ H2041C204H2043\\ H2041C204H2043\\ H2042C204H2043\\ H2042C204H2043\\ P102C205H2051\\ P102C205H205H2051\\ P102C205H205H205\\ P102C205H205H205\\ P102C205H205H205\\ P102C205H205H205\\ P102C205H205H205\\ P102C205H205\\ P102C205H205H205\\ P102C205H205H205\\ P102C205H205P102\\ P102C205H205P102\\ P102C205H205P102\\ P102C205H205P102\\ P102P102P102P102\\ P102P102P102P102\\ P102P102P102P102\\ P102P102P102P102\\ P102P102P102P102P102P102\\ P102P1$
$\begin{array}{l} P1C203H2032\\ H2031C203H2032\\ P1C203H2033\\ H2031C203H2033\\ P1C204H2043\\ P1C204H2042\\ P1C204H2043\\ H2041C204H2043\\ H2041C204H2043\\ H2042C204H2043\\ H2042C204H2043\\ P102C205H2051\\ P102C205H2052\\ \end{array}$
$\begin{array}{l} P1C203H2032\\ H2031C203H2032\\ P1C203H2033\\ H2031C203H2033\\ P1C204H2043\\ P1C204H2042\\ P1C204H2043\\ H2041C204H2042\\ H2041C204H2043\\ H2042C204H2043\\ P102C205H2051\\ P102C205H2052\\ P102C205H2053\\ \end{array}$
$\begin{array}{l} P1C203H2032\\ H2031C203H2032\\ P1C203H2033\\ H2031C203H2033\\ P1C204H2043\\ P1C204H2042\\ P1C204H2043\\ H2041C204H2043\\ H2041C204H2043\\ H2042C204H2043\\ H2042C205H2053\\ P102C205H2052\\ P102C205H2053\\ H2051C205H2053\\ H2051C205H2052\\ H2052H2052\\ H2$
$\begin{array}{l} P1C203H2032\\ H2031C203H2032\\ P1C203H2033\\ H2031C203H2033\\ P1C204H2043\\ P1C204H2042\\ P1C204H2043\\ H2041C204H2043\\ H2041C204H2043\\ H2042C204H2043\\ H2042C205H2053\\ P102C205H2052\\ P102C205H2052\\ H2051C205H2052\\ H2051C205H205\\ H2051C205H205\\ H2051C205H$
$\begin{array}{l} P1C203H2032\\ H2031C203H2032\\ P1C203H2033\\ H2031C203H2033\\ P1C204H2043\\ P1C204H2042\\ P1C204H2042\\ H2041C204H2043\\ H2041C204H2043\\ H2042C204H2043\\ H2042C204H2043\\ P102C205H2051\\ P102C205H2052\\ H2051C205H2052\\ H2051C205H2053\\ \end{array}$
$\begin{array}{l} P1C203H2032\\ H2031C203H2032\\ P1C203H2033\\ H2031C203H2033\\ P1C204H2043\\ P1C204H2042\\ P1C204H2043\\ H2041C204H2043\\ H2041C204H2043\\ H2042C204H2043\\ H2042C205H2043\\ P102C205H2051\\ P102C205H2052\\ P102C205H2053\\ H2051C205H2053\\ H2051C205H2053\\ H2052C205H2053\\ H2052C205H2052\\ H2052C205H2052\\ H2052C205H2052\\ H2052C205H2052\\ H2052H2052\\ H2052H2052\\ H2052H2052\\ H2052H2052\\ H2052H2052\\ H2052H205\\ H2052H2052\\ H2052H205\\ H205H205\\ H2052H205\\ H205H205\\ H205H205\\ H205H20$
$\begin{array}{l} P1C203H2032\\ H2031C203H2032\\ P1C203H2033\\ H2031C203H2033\\ P1C204H2043\\ P1C204H2042\\ P1C204H2043\\ H2041C204H2043\\ H2041C204H2043\\ H2042C204H2043\\ H2042C205H2053\\ P102C205H2052\\ P102C205H2053\\ H2051C205H2053\\ H2051C205H2053\\ H2052C205H2053\\ H2051C205H2053\\ H2052C205H2053\\ H2051C205H2053\\ H2052C205H2053\\ H2051C205H2053\\ H2052C205H2053\\ H2051C205H2053\\ H2052C205H2053\\ H2051C205H2053\\ H2051H205H205\\ H2051$
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$\begin{array}{l} {\rm P1}{\rm C203}{\rm H2032}\\ {\rm H2031}{\rm C203}{\rm H2032}\\ {\rm P1}{\rm C203}{\rm H2033}\\ {\rm H2031}{\rm C203}{\rm H2033}\\ {\rm P1}{\rm C204}{\rm H2043}\\ {\rm P1}{\rm C204}{\rm H2042}\\ {\rm P1}{\rm C204}{\rm H2043}\\ {\rm H2041}{\rm C204}{\rm H2043}\\ {\rm H2041}{\rm C204}{\rm H2043}\\ {\rm H2042}{\rm C204}{\rm H2043}\\ {\rm H2042}{\rm C205}{\rm H2053}\\ {\rm P102}{\rm C205}{\rm H2052}\\ {\rm P102}{\rm C205}{\rm H2052}\\ {\rm H2051}{\rm C205}{\rm H2053}\\ {\rm H2051}{\rm C205}{\rm H2053}\\ {\rm H2052}{\rm C205}{\rm H2053}\\ {\rm P102}{\rm C206}{\rm H2061}\\ {\rm P102}{\rm C206}{\rm H2061}\\ {\rm P102}{\rm C206}{\rm H2062}\\ \end{array}$
$\begin{array}{l} {\rm P1}{\rm C203}{\rm H2032}\\ {\rm H2031}{\rm C203}{\rm H2032}\\ {\rm P1}{\rm C203}{\rm H2033}\\ {\rm H2031}{\rm C203}{\rm H2033}\\ {\rm P1}{\rm C204}{\rm H2043}\\ {\rm P1}{\rm C204}{\rm H2042}\\ {\rm P1}{\rm C204}{\rm H2043}\\ {\rm H2041}{\rm C204}{\rm H2043}\\ {\rm H2041}{\rm C204}{\rm H2043}\\ {\rm H2042}{\rm C204}{\rm H2043}\\ {\rm H2042}{\rm C205}{\rm H2053}\\ {\rm P102}{\rm C205}{\rm H2052}\\ {\rm P102}{\rm C205}{\rm H2053}\\ {\rm H2051}{\rm C205}{\rm H2053}\\ {\rm H2051}{\rm C205}{\rm H2053}\\ {\rm H2052}{\rm C205}{\rm H2053}\\ {\rm H2052}{\rm C205}{\rm H2053}\\ {\rm P102}{\rm C206}{\rm H2063}\\ {\rm P102}{\rm C206}{\rm H2063}\\ {\rm H2061}{\rm C206}{\rm H2062}\\ {\rm H2061}{\rm C206}{\rm H2062}\\ \end{array}$
$\begin{array}{l} P1C203H2032\\ H2031C203H2032\\ P1C203H2033\\ H2031C203H2033\\ P1C204H2033\\ P1C204H2042\\ P1C204H2042\\ H2041C204H2042\\ H2041C204H2043\\ H2042C204H2043\\ H2042C205H2043\\ P102C205H2052\\ P102C205H2052\\ P102C205H2053\\ H2051C205H2053\\ H2051C205H2053\\ H2051C205H2053\\ H2052C205H2053\\ P102C206H2063\\ P102C206H2062\\ H2061C206H2062\\ H2061L206H2062\\ H2061L206H2062\\ H2061L206H2062\\ H2061L206H206\\ H2061L206H206\\ H2061L206H206\\ H2061L206H206\\ H2061L206H206\\ H2061L206H206\\ H2061L206H206\\ H206L206H206\\ H206L206L206\\ H206$
$\begin{array}{c} P1C203H2032\\ H2031C203H2032\\ P1C203H2033\\ H2031C203H2033\\ P1C204H2033\\ P1C204H2042\\ P1C204H2042\\ H2041C204H2043\\ H2041C204H2043\\ H2041C204H2043\\ H2042C205H2053\\ P102C205H2053\\ H2051C205H2053\\ H2051C205H2053\\ H2051C205H2053\\ H2052C205H2053\\ H2052C205H2053\\ P102C206H2063\\ H2061C206H2062\\ H2061C206H2063\\ H2061$
$\begin{array}{l} P1C203H2032\\ H2031C203H2032\\ P1C203H2033\\ H2031C203H2033\\ P1C204H2033\\ P1C204H2041\\ P1C204H2042\\ P1C204H2043\\ H2041C204H2043\\ H2041C204H2043\\ H2042C204H2043\\ H2042C205H2052\\ P102C205H2052\\ P102C205H2053\\ H2051C205H2053\\ H2051C205H2053\\ H2051C205H2053\\ H2052C205H2053\\ H2052C205H2053\\ P102C206H2063\\ P102C206H2062\\ H2061C206H2063\\ P1C301C302\\ P102C301C302\\ P102C301C302\\ P102C301C302\\ P102C301C302\\ P102C301C302\\ P102C301C302\\ P102C301C302\\ P102C301C302\\ P102C301C302\\ P1C301C302\\ P1C301P1C302\\$
$\begin{array}{l} {\rm P1}{\rm C203}{\rm H2032}\\ {\rm H2031}{\rm C203}{\rm H2032}\\ {\rm P1}{\rm C203}{\rm H2033}\\ {\rm H2031}{\rm C203}{\rm H2033}\\ {\rm P1}{\rm C204}{\rm H2043}\\ {\rm P1}{\rm C204}{\rm H2042}\\ {\rm P1}{\rm C204}{\rm H2042}\\ {\rm H2041}{\rm C204}{\rm H2043}\\ {\rm H2041}{\rm C204}{\rm H2043}\\ {\rm H2042}{\rm C204}{\rm H2043}\\ {\rm H2042}{\rm C205}{\rm H2043}\\ {\rm P102}{\rm C205}{\rm H2053}\\ {\rm P102}{\rm C205}{\rm H2053}\\ {\rm H2051}{\rm C205}{\rm H2053}\\ {\rm H2051}{\rm C205}{\rm H2053}\\ {\rm H2051}{\rm C205}{\rm H2053}\\ {\rm H2052}{\rm C205}{\rm H2053}\\ {\rm H2051}{\rm C205}{\rm H2053}\\ {\rm H2051}{\rm C206}{\rm H2063}\\ {\rm P102}{\rm C206}{\rm H2063}\\ {\rm H2061}{\rm C206}{\rm H2062}\\ {\rm H2061}{\rm C206}{\rm H2063}\\ {\rm P10{\rm C301}{\rm C302}\\ {\rm P1{\rm C301}{\rm H3011}\\ \end{array}$
$\begin{array}{l} {\rm P1}{\rm C203}{\rm H2032}\\ {\rm H2031}{\rm C203}{\rm H2033}\\ {\rm H2031}{\rm C203}{\rm H2033}\\ {\rm P1}{\rm C204}{\rm H2043}\\ {\rm P1}{\rm C204}{\rm H2042}\\ {\rm P1}{\rm C204}{\rm H2043}\\ {\rm H2041}{\rm C204}{\rm H2043}\\ {\rm H2041}{\rm C204}{\rm H2043}\\ {\rm H2041}{\rm C204}{\rm H2043}\\ {\rm H2042}{\rm C204}{\rm H2043}\\ {\rm H2042}{\rm C205}{\rm H2053}\\ {\rm H2052}{\rm C205}{\rm H2053}\\ {\rm H2051}{\rm C205}{\rm H2053}\\ {\rm H2052}{\rm C205}{\rm H2053}\\ {\rm H2061}{\rm C206}{\rm H2062}\\ {\rm H2061}{\rm C206}{\rm H2062}\\ {\rm H2061}{\rm C206}{\rm H2063}\\ {\rm P1}{\rm C301}{\rm C302}\\ {\rm P1}-{\rm C301}{\rm H3011}\\ {\rm C302}{\rm C301}{\rm H3011}\\ \end{array}$
$\begin{array}{l} P1C203H2032\\ H2031C203H2032\\ P1C203H2033\\ H2031C203H2033\\ P1C204H2033\\ P1C204H2041\\ P1C204H2042\\ P1C204H2042\\ H2041C204H2043\\ H2041C204H2043\\ H2042C204H2043\\ H2042C205H2052\\ P102C205H2052\\ P102C205H2053\\ H2051C205H2053\\ H2051C205H2053\\ H2052C205H2053\\ H2052C205H2053\\ P102C206H2061\\ P102C206H2062\\ H2061C206H2062\\ H2061C206H2063\\ P1C301H3011\\ C302C301H3011\\ P1C301H3011\\ P1C301H3012\\ P1C301H302\\ P1C301H302$
$\begin{array}{l} {\rm P1}{\rm C203}{\rm H2032}\\ {\rm H2031}{\rm C203}{\rm H2032}\\ {\rm P1}{\rm C203}{\rm H2033}\\ {\rm H2031}{\rm C203}{\rm H2033}\\ {\rm P1}{\rm C204}{\rm H2043}\\ {\rm P1}{\rm C204}{\rm H2042}\\ {\rm P1}{\rm C204}{\rm H2042}\\ {\rm H2041}{\rm C204}{\rm H2043}\\ {\rm H2041}{\rm C204}{\rm H2043}\\ {\rm H2042}{\rm C204}{\rm H2043}\\ {\rm H2042}{\rm C205}{\rm H2043}\\ {\rm H2052}{\rm C205}{\rm H2052}\\ {\rm P102}{\rm C205}{\rm H2053}\\ {\rm H2051}{\rm C206}{\rm H2063}\\ {\rm H2061}{\rm C206}{\rm H2062}\\ {\rm H2061}{\rm C206}{\rm H2062}\\ {\rm H2061}{\rm C206}{\rm H2063}\\ {\rm P102}-{\rm C301}{\rm H3011}\\ {\rm C302}-{\rm C301}{\rm H3011}\\ {\rm P1}{\rm C301}{\rm H3012}\\ {\rm C205}{\rm H3012}\\ {\rm C205}{\rm H2052}\\ {\rm H2051}{\rm C205}{\rm H2053}\\ {\rm H2051}{\rm C301}-{\rm H3012}\\ {\rm C302}{\rm C301}-{\rm C302}\\ {\rm C302}-{\rm C301}-{\rm C302}\\ {\rm C302}{\rm C301}-{\rm C302}\\ {\rm C302}{\rm C301}-{\rm C302}\\ {\rm C302}{\rm C301}-{\rm C302}\\ {\rm C302}{\rm C301}-{\rm C30$
$\begin{array}{l} {\rm P1}{\rm C203}{\rm H2032}\\ {\rm H2031}{\rm C203}{\rm H2033}\\ {\rm H2031}{\rm C203}{\rm H2033}\\ {\rm P1}{\rm C204}{\rm H2043}\\ {\rm P1}{\rm C204}{\rm H2042}\\ {\rm P1}{\rm C204}{\rm H2043}\\ {\rm H2041}{\rm C204}{\rm H2043}\\ {\rm H2041}{\rm C204}{\rm H2043}\\ {\rm H2041}{\rm C204}{\rm H2043}\\ {\rm H2042}{\rm C204}{\rm H2043}\\ {\rm H2042}{\rm C205}{\rm H2053}\\ {\rm H2052}{\rm C205}{\rm H2053}\\ {\rm H2051}{\rm C205}{\rm H2053}\\ {\rm H2052}{\rm C205}{\rm H2053}\\ {\rm H2052}{\rm C205}{\rm H2053}\\ {\rm H2052}{\rm C205}{\rm H2062}\\ {\rm H2061}{\rm C206}{\rm H2063}\\ {\rm P1}{\rm C301}{\rm H3011}\\ {\rm C302}{\rm C301}-{\rm H3011}\\ {\rm C302}{\rm C301}{\rm H3012}\\ {\rm C302}{\rm C301}{\rm H3012}\\ \end{array}$
$\begin{array}{l} {\rm P1}{\rm C203}{\rm H2032}\\ {\rm H2031}{\rm C203}{\rm H2032}\\ {\rm P1}{\rm C203}{\rm H2033}\\ {\rm H2031}{\rm C203}{\rm H2033}\\ {\rm P1}{\rm C204}{\rm H2043}\\ {\rm P1}{\rm C204}{\rm H2042}\\ {\rm P1}{\rm C204}{\rm H2043}\\ {\rm H2041}{\rm C204}{\rm H2043}\\ {\rm H2041}{\rm C204}{\rm H2043}\\ {\rm H2042}{\rm C204}{\rm H2043}\\ {\rm H2042}{\rm C205}{\rm H2051}\\ {\rm P102}{\rm C205}{\rm H2052}\\ {\rm P102}{\rm C205}{\rm H2052}\\ {\rm H2051}{\rm C205}{\rm H2053}\\ {\rm H2051}{\rm C205}{\rm H2053}\\ {\rm H2052}{\rm C205}{\rm H2053}\\ {\rm H2052}{\rm C205}{\rm H2053}\\ {\rm H2052}{\rm C206}{\rm H2063}\\ {\rm P102}{\rm C206}{\rm H2062}\\ {\rm H2061}{\rm C206}{\rm H2062}\\ {\rm H2061}{\rm C206}{\rm H2062}\\ {\rm H2061}{\rm C206}{\rm H2063}\\ {\rm P1}{\rm C301}{\rm C302}\\ {\rm P1}{\rm C301}{\rm H3011}\\ {\rm C302}{\rm C301}{\rm H3011}\\ {\rm P1}{\rm C301}{\rm H3012}\\ {\rm H3011}{\rm C301}{\rm H3012}\\ {\rm H3011}{\rm C301}{\rm H3012}\\ \end{array}$
$\begin{array}{l} {\rm P1}{\rm C203}{\rm H2032}\\ {\rm H2031}{\rm C203}{\rm H2032}\\ {\rm P1}{\rm C203}{\rm H2033}\\ {\rm H2031}{\rm C203}{\rm H2033}\\ {\rm P1}{\rm C204}{\rm H2043}\\ {\rm P1}{\rm C204}{\rm H2042}\\ {\rm P1}{\rm C204}{\rm H2042}\\ {\rm H2041}{\rm C204}{\rm H2043}\\ {\rm H2041}{\rm C204}{\rm H2043}\\ {\rm H2042}{\rm C204}{\rm H2043}\\ {\rm H2042}{\rm C205}{\rm H2043}\\ {\rm H2042}{\rm C205}{\rm H2053}\\ {\rm H2051}{\rm C206}{\rm H2063}\\ {\rm H2061}{\rm C206}{\rm H2062}\\ {\rm H2061}{\rm C206}{\rm H2063}\\ {\rm H2061}{\rm C206}{\rm H2063}\\ {\rm H2061}{\rm C206}{\rm H2063}\\ {\rm P1}{\rm C301}{\rm H3011}\\ {\rm C302}{\rm C301}{\rm H3011}\\ {\rm P1}{\rm C301}{\rm H3012}\\ {\rm C302}{\rm C301}{\rm H3012}\\ {\rm H3011}{\rm C301}{\rm H3012}\\ {\rm H3011}{\rm C302}{\rm H3012}\\ {\rm C302}{\rm C302}{\rm H3012}\\ {\rm H3011}{\rm C302}{\rm H3012}\\ {\rm H3011}{\rm C302}{\rm H3012}\\ {\rm H3011}{\rm C302}{\rm H3012}\\ {\rm H3011}{\rm C302}{\rm H3012}\\ {\rm C302}{\rm C302}{\rm H3022}\\ {\rm H3011}{\rm C302}{\rm H3022}\\ {\rm H3011}{\rm C302}{\rm H3012}\\ {\rm H3011}{\rm C302}{\rm H3012}\\ {\rm C302}{\rm C302}{\rm H3022}\\ {\rm H3011}-{\rm C302}{\rm C302}\\ {\rm H3011}-{\rm C302}{\rm H3012}\\ {\rm H3011}-{\rm C302}{\rm H3012}\\ {\rm H3011}-{\rm C302}{\rm H3022}\\ {\rm H3011}-{\rm C302}-{\rm H3022}\\ {\rm H3011}-{\rm H3012}\\ {\rm H3011}-{\rm C302}-{\rm H3022}\\ {\rm H3011}-{\rm C302}-{\rm H3022}\\ {\rm H3011}-{\rm H3012}\\ {\rm H3011}-{\rm C302}-{\rm H3022}\\ {\rm H3011}-{\rm H3012}\\ {\rm H3011}-{\rm H3012}\\ {\rm H3011}-{\rm H3012}\\ {\rm H3011}-{\rm H3012}\\ {\rm H3011}\\ {\rm H3011}-{\rm H3012}\\ {\rm H3011}\\ {\rm H3$
$\begin{array}{l} {\rm P1}{\rm C203}{\rm H2032}\\ {\rm H2031}{\rm C203}{\rm H2033}\\ {\rm P1}{\rm C203}{\rm H2033}\\ {\rm P1}{\rm C204}{\rm H2043}\\ {\rm P1}{\rm C204}{\rm H2042}\\ {\rm P1}{\rm C204}{\rm H2043}\\ {\rm H2041}{\rm C204}{\rm H2043}\\ {\rm H2041}{\rm C204}{\rm H2043}\\ {\rm H2041}{\rm C204}{\rm H2043}\\ {\rm H2042}{\rm C204}{\rm H2043}\\ {\rm H2042}{\rm C205}{\rm H2053}\\ {\rm H2052}{\rm C205}{\rm H2053}\\ {\rm H2051}{\rm C205}{\rm H2053}\\ {\rm H2052}{\rm C205}{\rm H2053}\\ {\rm H2052}{\rm C205}{\rm H2053}\\ {\rm H2052}{\rm C205}{\rm H2062}\\ {\rm H2061}{\rm C206}{\rm H2062}\\ {\rm H2061}{\rm C206}{\rm H2062}\\ {\rm H2061}{\rm C206}{\rm H2062}\\ {\rm H2061}{\rm C206}{\rm H2063}\\ {\rm P1}{\rm C301}{\rm H3011}\\ {\rm C302}{\rm C301}{\rm H3011}\\ {\rm C302}{\rm C301}{\rm H3012}\\ {\rm C301}{\rm C301}{\rm H3012}\\ {\rm C301}{\rm C302}{\rm P302}\\ {\rm C301}{\rm C302}{\rm C302}\\ {\rm C301}{\rm C301}{\rm C302}\\ {\rm C301}{\rm C301}{\rm C302}\\ {\rm$
$\begin{array}{l} {\rm P1}{\rm C203}-+{\rm H2032}\\ {\rm H2031}{\rm C203}-+{\rm H2032}\\ {\rm P1}{\rm C203}-+{\rm H2033}\\ {\rm H2031}{\rm C203}-+{\rm H2033}\\ {\rm P1}{\rm C204}-+{\rm H2043}\\ {\rm P1}{\rm C204}-+{\rm H2042}\\ {\rm P1}{\rm C204}-+{\rm H2043}\\ {\rm H2041}{\rm C204}-+{\rm H2043}\\ {\rm H2041}{\rm C204}-+{\rm H2043}\\ {\rm H2042}{\rm C204}-+{\rm H2043}\\ {\rm H2042}{\rm C204}-+{\rm H2043}\\ {\rm H2042}{\rm C205}-+{\rm H2051}\\ {\rm P102}{\rm C205}-+{\rm H2052}\\ {\rm H2051}{\rm C205}-+{\rm H2053}\\ {\rm H2051}{\rm C205}-+{\rm H2053}\\ {\rm H2051}{\rm C205}-+{\rm H2053}\\ {\rm H2052}{\rm C205}-+{\rm H2053}\\ {\rm H2051}{\rm C206}-+{\rm H2062}\\ {\rm H2061}{\rm C206}-+{\rm H2062}\\ {\rm H2061}{\rm C206}-+{\rm H2062}\\ {\rm H2061}{\rm C206}-+{\rm H2063}\\ {\rm P1}{\rm C301}{\rm H3011}\\ {\rm C302}{\rm C301}-+{\rm H3011}\\ {\rm C302}{\rm C301}-+{\rm H3011}\\ {\rm P1}{\rm C301}-+{\rm H3012}\\ {\rm C301}{\rm H3012}\\ {\rm H3011}{\rm C301}-+{\rm H3012}\\ {\rm C301}{\rm C302}{\rm P302}\\ {\rm C301}{\rm C302}{\rm H3021}\\ \end{array}$
$\begin{array}{l} {\rm P1}{\rm C203}-+{\rm H2032}\\ {\rm H2031}{\rm C203}-+{\rm H2032}\\ {\rm P1}{\rm C203}-+{\rm H2033}\\ {\rm H2031}{\rm C203}-+{\rm H2033}\\ {\rm P1}{\rm C204}-+{\rm H2041}\\ {\rm P1}{\rm C204}-+{\rm H2042}\\ {\rm P1}{\rm C204}-+{\rm H2042}\\ {\rm H2041}{\rm C204}-+{\rm H2043}\\ {\rm H2041}{\rm C204}-+{\rm H2043}\\ {\rm H2042}{\rm C204}-+{\rm H2043}\\ {\rm H2042}{\rm C205}-+{\rm H2053}\\ {\rm H2051}{\rm C205}-+{\rm H2053}\\ {\rm H2061}{\rm C206}-+{\rm H2063}\\ {\rm H2061}{\rm C206}-+{\rm H2062}\\ {\rm H2061}{\rm C206}-+{\rm H2063}\\ {\rm H2061}{\rm C200}-+{\rm H2063}\\ {\rm H2061}{\rm C200}-{\rm H2063}\\ {\rm H2061}{\rm C200}-{\rm H2063}\\ {\rm H2061}{\rm C301}-{\rm H3011}\\ {\rm C302}{\rm C301}-{\rm H3011}\\ {\rm C302}{\rm C301}-{\rm H3012}\\ {\rm C301}{\rm C302}-{\rm P302}\\ {\rm C301}-{\rm C302}-{\rm P302}\\ {\rm C301}-{\rm C302}-{\rm H3021}\\ {\rm Fe1}-{\rm P1}-{\rm C101}-{\rm C102}\\ {\rm H2061}-{\rm C102}\\ {\rm H2061}-{\rm H2061}\\ {\rm H2061}\\ {\rm H2061}\\ {\rm H2061}-{\rm H2061}\\ {\rm H2061}\\ {\rm$
$\begin{array}{l} {\rm P1}{\rm C203}-+{\rm H2032}\\ {\rm H2031}{\rm C203}-+{\rm H2032}\\ {\rm P1}{\rm C203}-+{\rm H2033}\\ {\rm P1}{\rm C204}-+{\rm H2041}\\ {\rm P1}{\rm C204}-+{\rm H2042}\\ {\rm P1}{\rm C204}-+{\rm H2043}\\ {\rm H2041}{\rm C204}-+{\rm H2043}\\ {\rm H2042}{\rm C205}-+{\rm H2051}\\ {\rm P102}{\rm C205}-+{\rm H2052}\\ {\rm P102}{\rm C205}-+{\rm H2053}\\ {\rm H2051}{\rm C205}-+{\rm H2053}\\ {\rm H2052}{\rm C205}-+{\rm H2053}\\ {\rm H2052}{\rm C205}-+{\rm H2063}\\ {\rm P102}{\rm C206}-+{\rm H2062}\\ {\rm H2061}{\rm C206}-+{\rm H2062}\\ {\rm H2061}{\rm C206}-+{\rm H2062}\\ {\rm H2061}{\rm C206}-+{\rm H2063}\\ {\rm P1}{\rm C301}-+{\rm H3011}\\ {\rm C302}{\rm C301}-+{\rm H3011}\\ {\rm C302}{\rm C301}-+{\rm H3012}\\ {\rm C301}{\rm H3012}\\ {\rm C301}{\rm H3012}\\ {\rm C301}{\rm C302}-+{\rm H3021}\\ {\rm H3011}{\rm C302}-+{\rm H3021}\\ {\rm Fe1}{\rm P1}{\rm C101}{\rm C102}\\ {\rm Fe1}-{\rm P1}{\rm C101}{\rm C102}\\ {\rm Fe1}-{\rm P1}{\rm C201}-{\rm C202}\\ {\rm H2061}{\rm C202}-{\rm H2022}\\ {\rm H2061}{\rm C202}-{\rm H2062}\\ {\rm H2061}{\rm C206}-{\rm H2063}\\ {\rm H2061}-{\rm H2063}\\ {\rm H$
$\begin{array}{l} {\rm P1}{\rm C203}-+{\rm H2032}\\ {\rm H2031}{\rm C203}-+{\rm H2032}\\ {\rm P1}{\rm C203}-+{\rm H2033}\\ {\rm H2031}{\rm C203}-+{\rm H2033}\\ {\rm P1}{\rm C204}-+{\rm H2043}\\ {\rm P1}{\rm C204}-+{\rm H2042}\\ {\rm P1}{\rm C204}-+{\rm H2043}\\ {\rm H2041}{\rm C204}-+{\rm H2043}\\ {\rm H2041}{\rm C204}-+{\rm H2043}\\ {\rm H2042}{\rm C204}-+{\rm H2043}\\ {\rm H2042}{\rm C204}-+{\rm H2043}\\ {\rm H2042}{\rm C205}-+{\rm H2053}\\ {\rm H205}{\rm C205}-+{\rm H2052}\\ {\rm H2051}{\rm C205}-+{\rm H2053}\\ {\rm H2051}{\rm C205}-+{\rm H2053}\\ {\rm H2051}{\rm C205}-+{\rm H2053}\\ {\rm H2051}{\rm C205}-+{\rm H2053}\\ {\rm H2051}{\rm C206}-+{\rm H2062}\\ {\rm H2061}{\rm C206}-+{\rm H2062}\\ {\rm H2061}{\rm C206}-+{\rm H2062}\\ {\rm H2061}{\rm C206}-+{\rm H2063}\\ {\rm P1}{\rm C301}-+{\rm H3011}\\ {\rm C302}{\rm C301}-+{\rm H3011}\\ {\rm C302}{\rm C301}-+{\rm H3011}\\ {\rm C302}{\rm C301}-+{\rm H3012}\\ {\rm C301}{\rm H3012}\\ {\rm C301}{\rm H3012}\\ {\rm C301}{\rm C302}-+{\rm H3021}\\ {\rm Fe1}-{\rm P1}-{\rm C101}-{\rm C102}\\ {\rm Fe1}-{\rm P1}-{\rm C201}-{\rm C202}\\ \end{array}$
$\begin{array}{l} {\rm P1}{\rm C203}-+{\rm H2032}\\ {\rm H2031}{\rm C203}-+{\rm H2032}\\ {\rm P1}{\rm C203}-+{\rm H2033}\\ {\rm H2031}{\rm C203}-+{\rm H2033}\\ {\rm P1}{\rm C204}-+{\rm H2041}\\ {\rm P1}{\rm C204}-+{\rm H2042}\\ {\rm P1}{\rm C204}-+{\rm H2042}\\ {\rm H2041}{\rm C204}-+{\rm H2043}\\ {\rm H2041}{\rm C204}-+{\rm H2043}\\ {\rm H2042}{\rm C204}-+{\rm H2043}\\ {\rm H2042}{\rm C205}-+{\rm H2053}\\ {\rm H2051}{\rm C205}-+{\rm H2053}\\ {\rm H2061}{\rm C206}-+{\rm H2062}\\ {\rm H2061}{\rm C206}-+{\rm H2062}\\ {\rm H2061}{\rm C206}-+{\rm H2062}\\ {\rm H2061}{\rm C206}-+{\rm H2063}\\ {\rm P1}-{\rm C301}{\rm C302}\\ {\rm P1}{\rm C301}-+{\rm H3011}\\ {\rm C302}{\rm C301}-+{\rm H3011}\\ {\rm C302}{\rm C301}-+{\rm H3012}\\ {\rm C301}{\rm H3012}\\ {\rm C301}{\rm C302}{\rm P302}\\ {\rm C301}{\rm C302}{\rm H3021}\\ {\rm Fe1}{\rm P1}{\rm C101}{\rm C102}\\ {\rm Fe1}{\rm P1}{\rm C201}{\rm C202}\\ {\rm Fe1}{\rm P1}{\rm C301}{\rm C302}\\ \end{array}$

Fe1-P4-C308-C307

109.6
109.6
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109.5 105.0(8)
100.9 (8)
107.5
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109.5
110.1 (10)
109.3
109.3
109.3
109.3
109.5
114.1 (10)
108.3
-34(1)
40 (1)
8 (2)
-31.0(5)
-30(2)

P302-C302-H3021	108.3
C301-C302-H3022	108.3
P302_C302_H3022	108.3
1302 C302 113022 H2021 C202 H2022	100.5
D1 C202 H2021	109.5
P1-C303-H3031	109.5
P1—C303—H3032	109.5
P1—C303—H3033	109.5
H3031-C303-H3032	109.5
H3031-C303-H3033	109.5
H3032-C303-H3033	109.5
P1_C304_H3041	100.4
$P_1 = C_{204} = H_{2042}$	100.5
P1-C304-H3042	109.5
P1—C304—H3043	109.5
H3041 - C304 - H3042	109.5
H3041—C304—H3043	109.5
H3042-C304-H3043	109.5
P302-C305-H3051	109.5
P302—C305—H3052	109.4
$H_{3051} - C_{305} - H_{3052}$	100.5
D202 C205 H2052	109.5
P302—C305—H3053	109.5
H3051—C305—H3053	109.5
H3052—C305—H3053	109.5
P302-C306-H3061	109.5
P302-C306-H3062	109.5
H3061—C306—H3062	109.5
P302_C306_H3063	109.5
H3061C306H3063	100.5
113001—C306—113003	109.5
П3002—С300—П3003	109.0
P303-C307-C308	114.8 (9)
P303—C307—H3071	108.1
С308—С307—Н3071	108.1
P303—C307—H3072	108.1
C308—C307—H3072	108.1
H3071—C307—H3072	109.5
C307—C308—P4	106.4(10)
C307—C308—H3081	110.2
P4—C308—H3081	110.2
C307—C308—H3082	110.2
P4—C308—H3082	110.2
H3081-C308-H3082	109.5
P303-C309-H3091	109.5
P303-C309-H3092	109.5
P303-C309-H3093	109.5
H3001_C300_H3002	100.5
H2001 C200 H2002	109.5
Наова Сара Наова	109.5
H3092—C309—H3093	109.5
P303—C310—H3101	109.5
P303—C310—H3102	109.4
P303—C310—H3103	109.5
H3101—C310—H3102	109.5
H3101-C310-H3103	109.5
H3102-C310-H3103	109.5
P4-C311-H3111	109.5
P4-C311-H3112	109.5
H3111_C311_H3112	109.5
D4 C211 U2112	100.5
F 4-0311-113113	109.5
H3111-0311-H3113	109.5
Н3112—С311—Н3113	109.5
P4—C312—H3121	109.5
P4—C312—H3122	109.5
H3121—C312—H3122	109.5
P4—C312—H3123	109.5
H3121—C312—H3123	109.5
H3122—C312—H3123	109.5
Fe1-P102-C102-C101	-36(1)
Fe1—P102—C202—C201	37(1)
Fe1 = P103 = C107 = C108	_30 7 (5)
F_{e1} P303 C207 C208	-10(9)
$F_{01} = 0.007 = 0.007 = 0.000$	1 1 (9)
161-01-030-02	1.1 (3)

Eo1 01 CE0 02	-178.8(3)
T	11010 (0)
Fe1	-1.1(3)
Fe1-02-C50-O3	178.8(3)
D1 E-1 D100 C100	11.0 (5)
P1—Fe1—P102—C102	11.2(3)
P1—Fe1—P102—C105	128(1)
D1 E-1 D109 C106	106 (1)
F1—Fe1—F102—C100	-100(1)
P1—Fe1—P102—C202	-9.6(5)
D1 E-1 D109 C905	117 4 (0)
r 1—Fe1—F 102—C205	-117.4(9)
P1—Fe1—P102—C206	114.1(7)
D1 Eo1 D102 C107	166 2 (2)
11-101-0107	-100.3(3)
P1—Fe1—P103—C109	-44.6(4)
P1_Fe1_P103_C110	80.6 (5)
	00.0 (0)
P1—Fe1—P302—C302	-21.1(7)
P1—Fe1—P302—C305	96(1)
D1 E-1 D200 C20C	149 (1)
F1—Fe1—F302—C300	-143(1)
P1—Fe1—P303—C307	175.8(6)
P1—Fe1—P303—C309	50.7(9)
F1 F1 F00 C000	00.1 (0)
P1—Fe1—P303—C310	-69(1)
P1—Fe1—O1—C50	88.4(2)
$P1_{F_01_02_050}$	-885 (2)
	(2)
P1—C101—C102—P102	42(1)
P1-C201-C202-P102	-46(1)
D1 (2001 (2002 D200	
P1-C301-C302-P302	-25(2)
P4—Fe1—P102—C102	-170.2(5)
P4_Fo1_P102_C105	-54(1)
14-102-0105	-04 (1)
P4—Fe1—P102—C106	73(1)
P4—Fe1—P102—C202	168.9(5)
$D_{4} = 1$ $D_{100} = 0.05$	61 1 (0)
P4—Fe1—F102—C205	01.1(9)
P4—Fe1—P102—C206	-67.4(7)
P4—Fe1—P103—C107	16.1(3)
D4 D4 D400 C100	10.1 (0)
P4—Fe1—P103—C109	137.9(4)
P4—Fe1—P103—C110	-97.0(5)
D4 E ₂ 1 D202 C202	161 4 (7)
r 4—re1—r 302—0302	101.4 (7)
P4—Fe1—P302—C305	-82(1)
P4_Fo1_P302_C306	39(1)
	00 (1)
14-Fe1-1302-C300	
P4—Fe1—P303—C307	-5.6(6)
P4—Fe1—P303—C307 P4—Fe1—P303—C309	-5.6(6) -130.8(9)
P4 = Fe1 = P303 = C300 $P4 = Fe1 = P303 = C309$ $P4 = Fe1 = P303 = C309$	-5.6(6) -130.8(9) 110(1)
P4—Fe1—P303—C307 P4—Fe1—P303—C309 P4—Fe1—P303—C310	-5.6(6) -130.8(9) 110(1)
$\begin{array}{c} P4 - Fe1 - P303 - C307 \\ P4 - Fe1 - P303 - C309 \\ P4 - Fe1 - P303 - C310 \\ P4 - Fe1 - O1 - C50 \end{array}$	-5.6(6) -130.8(9) 110(1) -90.8(2)
P4-Fe1-P303-C307 P4-Fe1-P303-C309 P4-Fe1-P303-C310 P4-Fe1-O1-C50 P4-Fe1-O2-C50 P4-Fe1-O2-C50	-5.6(6) -130.8(9) 110(1) -90.8(2) 895(2)
P4-Fe1-P303-C307 P4-Fe1-P303-C309 P4-Fe1-P303-C310 P4-Fe1-O1-C50 P4-Fe1-O2-C50 P4-Fe1-O2-C50 P4-Fe1-O2-C50 P4-Fe1-O2-C50 P4-Fe1-O2-C50 P4-Fe1-P303-C310 P4-Fe1-P303-C310 P4-Fe1-P303-C310 P4-Fe1-P303-C309 P4-Fe1-P30-C309 P4-Fe1-P303-C309 P4-Fe1-P30-C309 P4-F61-P30-C309 P4-F61-P300-C309 P4-F61-P300	$\begin{array}{c} -5.6 \ (6) \\ -130.8 \ (9) \\ 110 \ (1) \\ -90.8 \ (2) \\ 89.5 \ (2) \end{array}$
$\begin{array}{c} P4 - Fe1 - P302 - C300 \\ P4 - Fe1 - P303 - C309 \\ P4 - Fe1 - P303 - C310 \\ P4 - Fe1 - P303 - C310 \\ P4 - Fe1 - O1 - C50 \\ P4 - Fe1 - O2 - C50 \\ P4 - C108 - C107 - P103 \end{array}$	$\begin{array}{c} -5.6 \ (6) \\ -130.8 \ (9) \\ 110 \ (1) \\ -90.8 \ (2) \\ 89.5 \ (2) \\ 44.0 \ (6) \end{array}$
$\begin{array}{c} P4 - Fe1 - P303 - C307 \\ P4 - Fe1 - P303 - C307 \\ P4 - Fe1 - P303 - C310 \\ P4 - Fe1 - O1 - C50 \\ P4 - Fe1 - O2 - C50 \\ P4 - C108 - C107 - P103 \\ P4 - C308 - C307 - P303 \end{array}$	$\begin{array}{c} -5.6 \ (6) \\ -130.8 \ (9) \\ 110 \ (1) \\ -90.8 \ (2) \\ 89.5 \ (2) \\ 44.0 \ (6) \\ 23 \ (2) \end{array}$
P4-Fe1-P303-C307 P4-Fe1-P303-C309 P4-Fe1-P303-C310 P4-Fe1-O1-C50 P4-Fe1-O2-C50 P4-Fe1-O2-C50 P4-C108-C107-P103 P4-C308-C307-P303 P102-Fe1-P1-C101 P102-Fe1-P1-C102 P102-Fe1-P1-C102 P102-Fe1-P1-C102 P102-Fe1-P1-C102 P102-Fe1-P1-C102 P102-Fe1-P1-C102 P102-Fe1-P1-C102 P102-Fe1-P1-C102 P102-Fe1-P1-C102 P102-Fe1-P103 P102-F61-F103 P102-F61-F103 P102-F61-F103 P102-F61-F103 P102-F61-F103 P102-F61-F103 P102-F61-F103 P102-F103 P102-F	$\begin{array}{c} -5.6 \ (6) \\ -130.8 \ (9) \\ 110 \ (1) \\ -90.8 \ (2) \\ 89.5 \ (2) \\ 44.0 \ (6) \\ 23 \ (2) \\ 100 \ 7 \ (6) \end{array}$
$\begin{array}{c} P4 - Fe1 - P302 - C300 \\ P4 - Fe1 - P303 - C309 \\ P4 - Fe1 - P303 - C310 \\ P4 - Fe1 - P303 - C310 \\ P4 - Fe1 - O1 - C50 \\ P4 - Fe1 - O2 - C50 \\ P4 - C108 - C107 - P103 \\ P4 - C308 - C307 - P303 \\ P102 - Fe1 - P1 - C101 \end{array}$	$\begin{array}{c} -5.6 \ (6) \\ -130.8 \ (9) \\ 110 \ (1) \\ -90.8 \ (2) \\ 89.5 \ (2) \\ 44.0 \ (6) \\ 23 \ (2) \\ 10.7 \ (6) \end{array}$
$P4-Fe1-P303-C307 \\ P4-Fe1-P303-C309 \\ P4-Fe1-P303-C310 \\ P4-Fe1-O1-C50 \\ P4-Fe1-O2-C50 \\ P4-Fe1-O2-C50 \\ P4-C108-C107-P103 \\ P4-C308-C307-P303 \\ P102-Fe1-P1-C101 \\ P102-Fe1-P1-C103 \\ P102-Fe1-P1-P1-C103 \\ P102-Fe1-P1-P1-P1-C103 \\ P102-Fe1-P1-P1-P1-P1-P1-P1-P1-P1-P1-P1-P1-P1-P1$	$\begin{array}{c} -5.6 \ (6) \\ -130.8 \ (9) \\ 110 \ (1) \\ -90.8 \ (2) \\ 89.5 \ (2) \\ 44.0 \ (6) \\ 23 \ (2) \\ 10.7 \ (6) \\ 131.1 \ (8) \end{array}$
$P4-Fe1-P303-C307 \\ P4-Fe1-P303-C309 \\ P4-Fe1-P303-C310 \\ P4-Fe1-O1-C50 \\ P4-Fe1-O2-C50 \\ P4-Fe1-O2-C50 \\ P4-C108-C107-P103 \\ P4-C308-C307-P303 \\ P102-Fe1-P1-C101 \\ P102-Fe1-P1-C103 \\ P102-Fe1-P1-C103 \\ P102-Fe1-P1-C104 \\ P102-Fe1-P1-F1-P1-F1-P1-F1-P1-F1-F1-F1-F1-F1-F1-F1-F1-F1-F1-F1-F1-F1$	$\begin{array}{r} -5.6 \ (6) \\ -130.8 \ (9) \\ 110 \ (1) \\ -90.8 \ (2) \\ 89.5 \ (2) \\ 44.0 \ (6) \\ 23 \ (2) \\ 10.7 \ (6) \\ 131.1 \ (8) \\ -105.5 \ (6) \end{array}$
$P4-Fe1-P303-C307 \\ P4-Fe1-P303-C307 \\ P4-Fe1-P303-C310 \\ P4-Fe1-O1-C50 \\ P4-Fe1-O2-C50 \\ P4-Fe1-O2-C50 \\ P4-C108-C107-P103 \\ P4-C308-C307-P303 \\ P102-Fe1-P1-C101 \\ P102-Fe1-P1-C103 \\ P102-Fe1-P1-C104 \\ P102-Fe1-P1-F10-F1-P1-C104 \\ P102-FE1-F10-F10-F10-F10-F10-F10 \\ P102-F10-F1$	$\begin{array}{c} -5.6 \ (6) \\ -130.8 \ (9) \\ 110 \ (1) \\ -90.8 \ (2) \\ 89.5 \ (2) \\ 44.0 \ (6) \\ 23 \ (2) \\ 10.7 \ (6) \\ 131.1 \ (8) \\ -105.5 \ (6) \\ 14.1 \ (7) \end{array}$
$\begin{array}{c} P4 - Fe1 - P302 - C300 \\ P4 - Fe1 - P303 - C307 \\ P4 - Fe1 - P303 - C309 \\ P4 - Fe1 - P303 - C310 \\ P4 - Fe1 - O1 - C50 \\ P4 - Fe1 - O2 - C50 \\ P4 - C108 - C107 - P103 \\ P4 - C308 - C307 - P303 \\ P102 - Fe1 - P1 - C101 \\ P102 - Fe1 - P1 - C103 \\ P102 - Fe1 - P1 - C104 \\ P102 - Fe1 - P1 - C201 \end{array}$	$\begin{array}{c} -5.6\ (6)\\ -130.8\ (9)\\ 110\ (1)\\ -90.8\ (2)\\ 89.5\ (2)\\ 44.0\ (6)\\ 23\ (2)\\ 10.7\ (6)\\ 131.1\ (8)\\ -105.5\ (6)\\ -14.1\ (5)\end{array}$
$P4-Fe1-P303-C307 \\ P4-Fe1-P303-C309 \\ P4-Fe1-P303-C310 \\ P4-Fe1-O1-C50 \\ P4-Fe1-O2-C50 \\ P4-Fe1-O2-C50 \\ P4-C108-C107-P103 \\ P4-C308-C307-P303 \\ P102-Fe1-P1-C101 \\ P102-Fe1-P1-C103 \\ P102-Fe1-P1-C104 \\ P102-Fe1-P1-C201 \\ P102-Fe1-P1-C201 \\ P102-Fe1-P1-C203 \\ P102-Fe1-P1-F1-P1-F1-P1-F1-P1-F1-F1-F1-F1-F1-F1-F1-F1-F1-F1-F1-F1-F1$	$\begin{array}{c} -5.6\ (6)\\ -130.8\ (9)\\ 110\ (1)\\ -90.8\ (2)\\ 89.5\ (2)\\ 44.0\ (6)\\ 23\ (2)\\ 10.7\ (6)\\ 131.1\ (8)\\ -105.5\ (6)\\ -14.1\ (5)\\ 100.6\ (5)\end{array}$
$P4-Fe1-P303-C307 \\ P4-Fe1-P303-C307 \\ P4-Fe1-P303-C309 \\ P4-Fe1-O1-C50 \\ P4-Fe1-O2-C50 \\ P4-Fe1-O2-C50 \\ P4-C108-C107-P103 \\ P4-C308-C307-P303 \\ P102-Fe1-P1-C101 \\ P102-Fe1-P1-C103 \\ P102-Fe1-P1-C104 \\ P102-Fe1-P1-C201 \\ P102-Fe1-P1-C203 \\ P102-Fe1-P1-C204 \\ P102-Fe1-P1-F1-C204 \\ P102-Fe1-F1-F1-F1-F1-F1-F1-F1-F1-F1-F1-F1-F1-F1$	$\begin{array}{c} -5.6 \ (6) \\ -130.8 \ (9) \\ 110 \ (1) \\ -90.8 \ (2) \\ 89.5 \ (2) \\ 44.0 \ (6) \\ 23 \ (2) \\ 10.7 \ (6) \\ 131.1 \ (8) \\ -105.5 \ (6) \\ -14.1 \ (5) \\ -140.6 \ (5) \\ -140.5 \ (5) \end{array}$
P4-Fe1-P303-C307 P4-Fe1-P303-C309 P4-Fe1-P303-C309 P4-Fe1-O1-C50 P4-Fe1-O2-C50 P4-C108-C107-P103 P4-C308-C307-P303 P102-Fe1-P1-C101 P102-Fe1-P1-C104 P102-Fe1-P1-C104 P102-Fe1-P1-C201 P102-Fe1-P1-C203 P102-Fe1-P1-C204 P102-FE1-P1-FE1	$\begin{array}{c} -5.6 \ (6) \\ -130.8 \ (9) \\ 110 \ (1) \\ -90.8 \ (2) \\ 89.5 \ (2) \\ 44.0 \ (6) \\ 23 \ (2) \\ 10.7 \ (6) \\ 131.1 \ (8) \\ -105.5 \ (6) \\ -14.1 \ (5) \\ 100.6 \ (5) \\ -140.5 \ (5) \end{array}$
$P4-Fe1-P303-C307 \\ P4-Fe1-P303-C309 \\ P4-Fe1-P303-C310 \\ P4-Fe1-O1-C50 \\ P4-Fe1-O2-C50 \\ P4-Fe1-O2-C50 \\ P4-C108-C107-P103 \\ P4-C308-C307-P303 \\ P102-Fe1-P1-C101 \\ P102-Fe1-P1-C101 \\ P102-Fe1-P1-C103 \\ P102-Fe1-P1-C201 \\ P102-Fe1-P1-C201 \\ P102-Fe1-P1-C203 \\ P102-Fe1-P1-C204 \\ P102-Fe1-P1-C301 \\ P102-Fe1-P1-C301 \\ P102-Fe1-P1-C301 \\ P102-Fe1-P1-C300 \\ P102-Fe1-P1-P1-C300 \\ P102-Fe1-P1-P1-P1-P1-P1-P1-P1-P1-P1-P1-P1-P1-P1$	$\begin{array}{c} -5.6\ (6)\\ -130.8\ (9)\\ 110\ (1)\\ -90.8\ (2)\\ 89.5\ (2)\\ 44.0\ (6)\\ 23\ (2)\\ 10.7\ (6)\\ 131.1\ (8)\\ -105.5\ (6)\\ -14.1\ (5)\\ 100.6\ (5)\\ -140.5\ (5)\\ -91.1\ (9)\end{array}$
$P4-Fe1-P303-C307 \\ P4-Fe1-P303-C307 \\ P4-Fe1-P303-C310 \\ P4-Fe1-O1-C50 \\ P4-Fe1-O2-C50 \\ P4-Fe1-O2-C50 \\ P4-C108-C107-P103 \\ P4-C308-C307-P303 \\ P102-Fe1-P1-C101 \\ P102-Fe1-P1-C103 \\ P102-Fe1-P1-C104 \\ P102-Fe1-P1-C201 \\ P102-Fe1-P1-C203 \\ P102-Fe1-P1-C203 \\ P102-Fe1-P1-C301 \\ P102-Fe1-P1-C301 \\ P102-Fe1-P1-C301 \\ P102-Fe1-P4-C108 \\ P102-Fe1-P1-C204 \\ P102-Fe1-P1-C204 \\ P102-Fe1-P1-C301 \\ P102-Fe1-P1-C301 \\ P102-Fe1-P1-C301 \\ P102-Fe1-P1-C108 \\ P102-Fe1-P1-C208 \\ P102-Fe1-P1-C301 \\ P102-Fe1-P1-F1-F1-F1-F1-F1-F1-F1-F1-F1-F1-F1-F1-F1$	$\begin{array}{c} -5.6 \ (6) \\ -130.8 \ (9) \\ 110 \ (1) \\ -90.8 \ (2) \\ 89.5 \ (2) \\ 44.0 \ (6) \\ 23 \ (2) \\ 10.7 \ (6) \\ 131.1 \ (8) \\ -105.5 \ (6) \\ -14.1 \ (5) \\ 100.6 \ (5) \\ -140.5 \ (5) \\ -91.1 \ (9) \\ 104.7 \ (3) \end{array}$
P4-Fe1-P303-C307 P4-Fe1-P303-C307 P4-Fe1-P303-C309 P4-Fe1-P303-C310 P4-Fe1-O1-C50 P4-Fe1-O2-C50 P4-C108-C107-P103 P4-C308-C307-P303 P102-Fe1-P1-C101 P102-Fe1-P1-C103 P102-Fe1-P1-C104 P102-Fe1-P1-C201 P102-Fe1-P1-C203 P102-Fe1-P1-C204 P102-Fe1-P1-C301 P102-Fe1-P1-C301 P102-Fe1-P4-C108 P102-Fe1-P4-C118 P102-Fe1-P1-C301 P102-FE1-P1-C30	$\begin{array}{c} -5.6 \ (6) \\ -130.8 \ (9) \\ 110 \ (1) \\ -90.8 \ (2) \\ 89.5 \ (2) \\ 44.0 \ (6) \\ 23 \ (2) \\ 10.7 \ (6) \\ 23 \ (2) \\ 10.7 \ (6) \\ 131.1 \ (8) \\ -105.5 \ (6) \\ -14.1 \ (5) \\ 100.6 \ (5) \\ -140.5 \ (5) \\ -91.1 \ (9) \\ 102.4 \ (2) \ (2) \ ($
$P4-Fe1-P303-C307 \\ P4-Fe1-P303-C309 \\ P4-Fe1-P303-C310 \\ P4-Fe1-O1-C50 \\ P4-Fe1-O2-C50 \\ P4-Fe1-O2-C50 \\ P4-C108-C107-P103 \\ P4-C308-C307-P303 \\ P102-Fe1-P1-C101 \\ P102-Fe1-P1-C103 \\ P102-Fe1-P1-C104 \\ P102-Fe1-P1-C201 \\ P102-Fe1-P1-C203 \\ P102-Fe1-P1-C204 \\ P102-Fe1-P1-C301 \\ P102-Fe1-P4-C108 \\ P102-Fe1-P4-C111 \\ P102-Fe1-P4-P4-C111 \\ P102-Fe1-P4-P4-P4-P4-P4-P4-P4-P4-P4-P4-P4-P4-P4-$	$\begin{array}{c} -5.6 \ (6) \\ -130.8 \ (9) \\ 110 \ (1) \\ -90.8 \ (2) \\ 89.5 \ (2) \\ 44.0 \ (6) \\ 23 \ (2) \\ 10.7 \ (6) \\ 131.1 \ (8) \\ -105.5 \ (6) \\ -14.1 \ (5) \\ 100.6 \ (5) \\ -91.1 \ (9) \\ 104.7 \ (3) \\ -137.4 \ (2) \end{array}$
$\begin{array}{l} P_{4} = Fe1 = P303 = C307 \\ P_{4} = Fe1 = P303 = C307 \\ P_{4} = Fe1 = P303 = C309 \\ P_{4} = Fe1 = P303 = C310 \\ P_{4} = Fe1 = O1 = C50 \\ P_{4} = Fe1 = O2 = C50 \\ P_{4} = C108 = C107 = P103 \\ P_{4} = C308 = C307 = P303 \\ P_{102} = Fe1 = P_{1} = C101 \\ P_{102} = Fe1 = P_{1} = C103 \\ P_{102} = Fe_{1} = P_{1} = C104 \\ P_{102} = Fe_{1} = P_{1} = C203 \\ P_{102} = Fe_{1} = P_{1} = C204 \\ P_{102} = Fe_{1} = P_{1} = C301 \\ P_{102} = Fe_{1} = P_{4} = C108 \\ P_{102} = Fe_{1} = P_{4} = C111 \\ P_{102} = Fe_{1} = P_{4} = C112 \\ \end{array}$	$\begin{array}{c} -5.6\ (6)\\ -130.8\ (9)\\ 110\ (1)\\ -90.8\ (2)\\ 89.5\ (2)\\ 44.0\ (6)\\ 23\ (2)\\ 10.7\ (6)\\ 131.1\ (8)\\ -105.5\ (6)\\ -14.1\ (5)\\ 100.6\ (5)\\ -140.5\ (5)\\ -91.1\ (9)\\ 104.7\ (3)\\ -137.4\ (2)\\ -13.1\ (4)\end{array}$
$P4-Fe1-P303-C307 \\ P4-Fe1-P303-C307 \\ P4-Fe1-P303-C309 \\ P4-Fe1-P303-C310 \\ P4-Fe1-O1-C50 \\ P4-Fe1-O2-C50 \\ P4-C108-C107-P103 \\ P4-C308-C307-P303 \\ P102-Fe1-P1-C101 \\ P102-Fe1-P1-C101 \\ P102-Fe1-P1-C103 \\ P102-Fe1-P1-C201 \\ P102-Fe1-P1-C201 \\ P102-Fe1-P1-C203 \\ P102-Fe1-P1-C301 \\ P102-Fe1-P1-C301 \\ P102-Fe1-P4-C108 \\ P102-Fe1-P4-C118 \\ P102-Fe1-P4-C112 \\ P102-Fe1-P4-C112 \\ P102-Fe1-P4-C107 \\ P102-Fe1-P103-C107 \\ P102-Fe1-P103-Fe1-P103-Fe10-Fe10-Fe10-Fe10-Fe10-Fe10-Fe10-Fe10$	$\begin{array}{c} -5.6 \ (6) \\ -130.8 \ (9) \\ 110 \ (1) \\ -90.8 \ (2) \\ 89.5 \ (2) \\ 44.0 \ (6) \\ 23 \ (2) \\ 10.7 \ (6) \\ 23 \ (2) \\ 10.7 \ (6) \\ 131.1 \ (8) \\ -105.5 \ (6) \\ -14.1 \ (5) \\ 100.6 \ (5) \\ -140.5 \ (5) \\ -91.1 \ (9) \\ 104.7 \ (3) \\ -137.4 \ (2) \\ -13.1 \ (4) \\ -82.3 \ (3) \end{array}$
$P4-Fe1-P303-C307 \\ P4-Fe1-P303-C309 \\ P4-Fe1-P303-C310 \\ P4-Fe1-O1-C50 \\ P4-Fe1-O2-C50 \\ P4-Fe1-O2-C50 \\ P4-C108-C107-P103 \\ P4-C308-C307-P303 \\ P102-Fe1-P1-C101 \\ P102-Fe1-P1-C101 \\ P102-Fe1-P1-C104 \\ P102-Fe1-P1-C201 \\ P102-Fe1-P1-C201 \\ P102-Fe1-P1-C203 \\ P102-Fe1-P1-C204 \\ P102-Fe1-P1-C301 \\ P102-Fe1-P4-C108 \\ P102-Fe1-P4-C111 \\ P102-Fe1-P4-C112 \\ P102-Fe1-P4-C112 \\ P102-Fe1-P103-C107 \\ P103-Fe1-P103-C107 \\ P103-Fe1-P103-Fe1-P103-C107 \\ P103-Fe1-P103-F$	$\begin{array}{c} -5.6 \ (6) \\ -130.8 \ (9) \\ 110 \ (1) \\ -90.8 \ (2) \\ 89.5 \ (2) \\ 44.0 \ (6) \\ 23 \ (2) \\ 10.7 \ (6) \\ 131.1 \ (8) \\ -105.5 \ (6) \\ -14.1 \ (5) \\ 100.6 \ (5) \\ -91.1 \ (9) \\ 104.7 \ (3) \\ -137.4 \ (2) \\ -13.1 \ (4) \\ -82.3 \ (3) \\ 20.4 \ (4) \end{array}$
$\begin{array}{l} P_{4} = Fe1 = P303 = C307 \\ P_{4} = Fe1 = P303 = C307 \\ P_{4} = Fe1 = P303 = C309 \\ P_{4} = Fe1 = O1 = C50 \\ P_{4} = Fe1 = O2 = C50 \\ P_{4} = C108 = C107 = P103 \\ P_{4} = C108 = C107 = P103 \\ P_{4} = C308 = C307 = P303 \\ P_{102} = Fe1 = P1 = C101 \\ P_{102} = Fe1 = P1 = C101 \\ P_{102} = Fe1 = P1 = C104 \\ P_{102} = Fe1 = P1 = C201 \\ P_{102} = Fe1 = P1 = C204 \\ P_{102} = Fe1 = P1 = C301 \\ P_{102} = Fe1 = P4 = C108 \\ P_{102} = Fe1 = P4 = C111 \\ P_{102} = Fe1 = P4 = C112 \\ P_{102} = Fe1 = P_{103} = C107 \\ P_{102} = Fe1 = P_{103} = C107 \\ P_{102} = Fe1 = P_{103} = C109 \\ \end{array}$	$\begin{array}{c} -5.6 \ (6) \\ -130.8 \ (9) \\ 110 \ (1) \\ -90.8 \ (2) \\ 89.5 \ (2) \\ 44.0 \ (6) \\ 23 \ (2) \\ 10.7 \ (6) \\ 131.1 \ (8) \\ -105.5 \ (6) \\ -14.1 \ (5) \\ 100.6 \ (5) \\ -140.5 \ (5) \\ -91.1 \ (9) \\ 104.7 \ (3) \\ -137.4 \ (2) \\ -13.1 \ (4) \\ -82.3 \ (3) \\ 39.4 \ (4) \end{array}$
$\begin{array}{l} P_{4} = Fe1 = P303 = C307 \\ P_{4} = Fe1 = P303 = C307 \\ P_{4} = Fe1 = P303 = C309 \\ P_{4} = Fe1 = P303 = C310 \\ P_{4} = Fe1 = O1 = C50 \\ P_{4} = Fe1 = O2 = C50 \\ P_{4} = C108 = C107 = P103 \\ P_{4} = C308 = C307 = P303 \\ P_{102} = Fe1 = P1 = C101 \\ P_{102} = Fe1 = P1 = C101 \\ P_{102} = Fe1 = P1 = C104 \\ P_{102} = Fe1 = P1 = C201 \\ P_{102} = Fe1 = P1 = C201 \\ P_{102} = Fe1 = P1 = C203 \\ P_{102} = Fe1 = P1 = C301 \\ P_{102} = Fe1 = P1 = C301 \\ P_{102} = Fe1 = P4 = C118 \\ P_{102} = Fe1 = P4 = C112 \\ P_{102} = Fe1 = P_{103} = C107 \\ P_{102} = Fe1 = P_{103} = C107 \\ P_{102} = Fe1 = P_{103} = C110 \\ P_{102} = Fe1 = P_{10$	$\begin{array}{c} -5.6 \ (6) \\ -130.8 \ (9) \\ 110 \ (1) \\ -90.8 \ (2) \\ 89.5 \ (2) \\ 44.0 \ (6) \\ 23 \ (2) \\ 10.7 \ (6) \\ 131.1 \ (8) \\ -105.5 \ (6) \\ -141. \ (5) \\ 100.6 \ (5) \\ -140.5 \ (5) \\ -91.1 \ (9) \\ 104.7 \ (3) \\ -137.4 \ (2) \\ -13.1 \ (4) \\ -82.3 \ (3) \\ 39.4 \ (4) \\ 164.6 \ (5) \end{array}$
$P4-Fe1-P303-C307 \\ P4-Fe1-P303-C309 \\ P4-Fe1-P303-C310 \\ P4-Fe1-O1-C50 \\ P4-Fe1-O2-C50 \\ P4-Fe1-O2-C50 \\ P4-C108-C107-P103 \\ P4-C308-C307-P303 \\ P102-Fe1-P1-C101 \\ P102-Fe1-P1-C103 \\ P102-Fe1-P1-C104 \\ P102-Fe1-P1-C201 \\ P102-Fe1-P1-C203 \\ P102-Fe1-P1-C204 \\ P102-Fe1-P1-C204 \\ P102-Fe1-P1-C301 \\ P102-Fe1-P4-C108 \\ P102-Fe1-P4-C111 \\ P102-Fe1-P4-C112 \\ P102-Fe1-P4-C112 \\ P102-Fe1-P4-C107 \\ P102-Fe1-P103-C107 \\ P102-Fe1-P103-C100 \\ P102-Fe1-P103-C110 \\ P102-Fe1-P103-C100 \\ P102-Fe1-P103-$	$\begin{array}{c} -5.6 \\ (6) \\ -130.8 \\ (9) \\ 110 \\ (1) \\ -90.8 \\ (2) \\ 89.5 \\ (2) \\ 44.0 \\ (23 \\ (2) \\ 10.7 \\ (6) \\ 131.1 \\ (8) \\ -105.5 \\ (6) \\ -14.1 \\ (5) \\ 100.6 \\ (5) \\ -140.5 \\ (5) \\ -140.5 \\ (5) \\ -140.5 \\ (5) \\ -1140.5 \\ (5) $
$P4-Fe1-P303-C307 \\ P4-Fe1-P303-C309 \\ P4-Fe1-P303-C309 \\ P4-Fe1-O1-C50 \\ P4-Fe1-O2-C50 \\ P4-Fe1-O2-C50 \\ P4-C108-C107-P103 \\ P4-C308-C307-P303 \\ P102-Fe1-P1-C101 \\ P102-Fe1-P1-C101 \\ P102-Fe1-P1-C103 \\ P102-Fe1-P1-C201 \\ P102-Fe1-P1-C203 \\ P102-Fe1-P1-C301 \\ P102-Fe1-P1-C301 \\ P102-Fe1-P1-C301 \\ P102-Fe1-P4-C108 \\ P102-Fe1-P4-C111 \\ P102-Fe1-P4-C112 \\ P102-Fe1-P4-C112 \\ P102-Fe1-P103-C107 \\ P102-Fe1-P103-C109 \\ P102-Fe1-P103-C302 \\ P102-Fe1-P103-C302 \\ P102-Fe1-P102-C302 \\ P102-Fe1-P103-C302 \\ P102-Fe1-P10$	$\begin{array}{c} -5.6 \ (6) \\ -130.8 \ (9) \\ 110 \ (1) \\ -90.8 \ (2) \\ 89.5 \ (2) \\ 44.0 \ (6) \\ 23 \ (2) \\ 10.7 \ (6) \\ 131.1 \ (8) \\ -105.5 \ (6) \\ -14.1 \ (5) \\ 100.6 \ (5) \\ -140.5 \ (5) \\ -140.5 \ (5) \\ 100.7 \ (3) \\ -137.4 \ (2) \\ -13.1 \ (4) \\ -82.3 \ (3) \\ 39.4 \ (4) \\ 164.6 \ (5) \\ 68.4 \ (4) \\ 166.4 \ (5) \\ \end{array}$
$\begin{array}{l} P_{4} = Fe1 = P303 = C307 \\ P_{4} = Fe1 = P303 = C307 \\ P_{4} = Fe1 = P303 = C309 \\ P_{4} = Fe1 = P303 = C310 \\ P_{4} = Fe1 = O1 = C50 \\ P_{4} = Fe1 = O2 = C50 \\ P_{4} = C108 = C107 = P103 \\ P_{4} = C308 = C307 = P303 \\ P_{102} = Fe1 = P1 = C101 \\ P_{102} = Fe1 = P1 = C101 \\ P_{102} = Fe1 = P1 = C104 \\ P_{102} = Fe1 = P1 = C201 \\ P_{102} = Fe1 = P1 = C201 \\ P_{102} = Fe1 = P1 = C203 \\ P_{102} = Fe1 = P1 = C204 \\ P_{102} = Fe1 = P1 = C301 \\ P_{102} = Fe1 = P4 = C108 \\ P_{102} = Fe1 = P4 = C112 \\ P_{102} = Fe1 = P_{103} = C107 \\ P_{102} = Fe1 = P_{103} = C107 \\ P_{102} = Fe1 = P_{103} = C109 \\ P_{102} = Fe1 = P_{103} = C302 \\ P_{102} = Fe1 = P_{103} = C302 \\ P_{102} = Fe1 = P_{103} = C305 \\ \end{array}$	$\begin{array}{c} -5.6\ (6)\\ -130.8\ (9)\\ 110\ (1)\\ -90.8\ (2)\\ 89.5\ (2)\\ 44.0\ (6)\\ 23\ (2)\\ 10.7\ (6)\\ 131.1\ (8)\\ -105.5\ (6)\\ -14.1\ (5)\\ 100.6\ (5)\\ -140.5\ (5)\\ -91.1\ (9)\\ 104.7\ (3)\\ -137.4\ (2)\\ -13.1\ (4)\\ -82.3\ (3)\\ 39.4\ (4)\\ 164.6\ (5)\\ 68.4\ (4)\\ 166\ (1)\\ \end{array}$
$\begin{array}{l} P_{4} = Fe1 = P303 = C307 \\ P_{4} = Fe1 = P303 = C307 \\ P_{4} = Fe1 = P303 = C309 \\ P_{4} = Fe1 = P303 = C310 \\ P_{4} = Fe1 = O1 = C50 \\ P_{4} = Fe1 = O2 = C50 \\ P_{4} = Fe1 = O2 = C50 \\ P_{4} = C108 = C107 = P103 \\ P_{4} = C308 = C307 = P303 \\ P_{4} = C308 = C307 \\ P_{4} = C308 \\ P_{4} = C$	$\begin{array}{c} -5.6\ (6)\\ -130.8\ (9)\\ 110\ (1)\\ -90.8\ (2)\\ 89.5\ (2)\\ 44.0\ (6)\\ 23\ (2)\\ 10.7\ (6)\\ 131.1\ (8)\\ -105.5\ (6)\\ -14.1\ (5)\\ 100.6\ (5)\\ -140.5\ (5)\\ 100.6\ (5)\\ -91.1\ (9)\\ 104.7\ (3)\\ -91.1\ (9)\\ 104.7\ (3)\\ -39.4\ (4)\\ 164.6\ (5)\\ 68.4\ (4)\\ 166\ (1)\\ -43\ (1)\\ \end{array}$
$P4-Fe1-P303-C307 \\ P4-Fe1-P303-C309 \\ P4-Fe1-P303-C310 \\ P4-Fe1-O1-C50 \\ P4-Fe1-O2-C50 \\ P4-Fe1-O2-C50 \\ P4-C108-C107-P103 \\ P4-C308-C307-P303 \\ P102-Fe1-P1-C101 \\ P102-Fe1-P1-C101 \\ P102-Fe1-P1-C104 \\ P102-Fe1-P1-C201 \\ P102-Fe1-P1-C204 \\ P102-Fe1-P1-C301 \\ P102-Fe1-P1-C301 \\ P102-Fe1-P4-C111 \\ P102-Fe1-P4-C111 \\ P102-Fe1-P4-C112 \\ P102-Fe1-P103-C107 \\ P102-Fe1-P103-C109 \\ P102-Fe1-P103-C302 \\ P102-Fe1-P103-C305 \\ P102-Fe1-P103-C306 \\ P102-Fe1-P01-C50 \\ P102-Fe1-O1-C50 \\ P102-Fe1-P01-C50 \\ P102-Fe1-P103-C50 \\$	$\begin{array}{c} -5.6\ (6)\\ -130.8\ (9)\\ 110\ (1)\\ -90.8\ (2)\\ 89.5\ (2)\\ 44.0\ (6)\\ 23\ (2)\\ 10.7\ (6)\\ 131.1\ (8)\\ -105.5\ (6)\\ -14.1\ (5)\\ 100.6\ (5)\\ -140.5\ (5)\\ -91.1\ (9)\\ 104.7\ (3)\\ 104.7\ (3)\\ 39.4\ (4)\\ 164.6\ (5)\\ 68.4\ (4)\\ 166\ (1)\\ -43\ (1)\\ -43\ (1)\\ 24\ 7\ (4)\end{array}$
P4-Fe1-P303-C307 $P4-Fe1-P303-C307$ $P4-Fe1-P303-C309$ $P4-Fe1-O1-C50$ $P4-Fe1-O2-C50$ $P4-Fe1-O2-C50$ $P4-C108-C107-P103$ $P4-C308-C307-P303$ $P102-Fe1-P1-C101$ $P102-Fe1-P1-C103$ $P102-Fe1-P1-C201$ $P102-Fe1-P1-C203$ $P102-Fe1-P1-C204$ $P102-Fe1-P1-C301$ $P102-Fe1-P4-C118$ $P102-Fe1-P4-C112$ $P102-Fe1-P4-C112$ $P102-Fe1-P103-C107$ $P102-Fe1-P103-C107$ $P102-Fe1-P103-C107$ $P102-Fe1-P103-C305$ $P102-Fe1-P103-C306$ $P102-Fe1-P103-C306$ $P102-Fe1-P1-C50$	$\begin{array}{c} -5.6\ (6)\\ -130.8\ (9)\\ 110\ (1)\\ -90.8\ (2)\\ 89.5\ (2)\\ 89.5\ (2)\\ 44.0\ (6)\\ 23\ (2)\\ 10.7\ (6)\\ 131.1\ (8)\\ -105.5\ (6)\\ -14.1\ (5)\\ 100.6\ (5)\\ -140.5\ (5)\\ -91.1\ (9)\\ 104.7\ (3)\\ -137.4\ (2)\\ -13.1\ (4)\\ -82.3\ (3)\\ 39.4\ (4)\\ 166.4\ (5)\\ 68.4\ (4)\\ 166\ (1)\\ -43\ (1)\\ 24.7\ (4)\\ 24.7\ (4)\\ 167.5\ (6)\\ -24.7\ (4)\\ 167.5\ (6)\\ -24.7\ (4)\\ 167.5\ (6)\\ -24.7\ (4)\\ -24.8\ (4)\\ -$
$\begin{array}{l} P_{4} = Fe1 = P303 = C307 \\ P_{4} = Fe1 = P303 = C307 \\ P_{4} = Fe1 = P303 = C309 \\ P_{4} = Fe1 = O1 = C50 \\ P_{4} = Fe1 = O2 = C50 \\ P_{4} = Fe1 = O2 = C50 \\ P_{4} = C108 = C107 = P103 \\ P_{4} = C308 = C307 = P303 \\ P_{102} = Fe1 = P_{1} = C101 \\ P_{102} = Fe_{1} = P_{1} = C103 \\ P_{102} = Fe_{1} = P_{1} = C201 \\ P_{102} = Fe_{1} = P_{1} = C204 \\ P_{102} = Fe_{1} = P_{1} = C301 \\ P_{102} = Fe_{1} = P_{4} = C108 \\ P_{102} = Fe_{1} = P_{4} = C108 \\ P_{102} = Fe_{1} = P_{4} = C108 \\ P_{102} = Fe_{1} = P_{4} = C111 \\ P_{102} = Fe_{1} = P_{4} = C112 \\ P_{102} = Fe_{1} = P_{103} = C107 \\ P_{102} = Fe_{1} = P_{103} = C107 \\ P_{102} = Fe_{1} = P_{103} = C109 \\ P_{102} = Fe_{1} = P_{103} = C302 \\ P_{102} = Fe_{1} = P_{103} = C305 \\ P_{102} = Fe_{1} = P_{103} = C306 \\ P_{102} = Fe_{1} = O_{1} = C50 \\ P_{102} = Fe_{1} = O_{2} = C50 \\ \end{array}$	$\begin{array}{c} -5.6\ (6)\\ -130.8\ (9)\\ 110\ (1)\\ -90.8\ (2)\\ 89.5\ (2)\\ 44.0\ (6)\\ 23\ (2)\\ 10.7\ (6)\\ 131.1\ (8)\\ -105.5\ (6)\\ -14.1\ (5)\\ 100.6\ (5)\\ -140.5\ (5)\\ -91.1\ (9)\\ 104.7\ (3)\\ -91.1\ (9)\\ 104.7\ (3)\\ 39.4\ (4)\\ 164.6\ (5)\\ 68.4\ (4)\\ 166\ (1)\\ -43\ (1)\\ 24.7\ (4)\\ -171.6\ (2)\\ \end{array}$
$\begin{array}{l} P_{4} = Fe1 = P303 = C300 \\ P_{4} = Fe1 = P303 = C307 \\ P_{4} = Fe1 = P303 = C309 \\ P_{4} = Fe1 = P303 = C310 \\ P_{4} = Fe1 = O1 = C50 \\ P_{4} = Fe1 = O2 = C50 \\ P_{4} = C108 = C107 = P103 \\ P_{4} = C308 = C307 = P303 \\ P_{4} = C308 = C307 = P303 \\ P_{102} = Fe1 = P_{1} = C101 \\ P_{102} = Fe1 = P_{1} = C101 \\ P_{102} = Fe_{1} = P_{1} = C201 \\ P_{102} = Fe_{1} = P_{1} = C201 \\ P_{102} = Fe_{1} = P_{1} = C201 \\ P_{102} = Fe_{1} = P_{1} = C203 \\ P_{102} = Fe_{1} = P_{1} = C301 \\ P_{102} = Fe_{1} = P_{1} = C108 \\ P_{102} = Fe_{1} = P_{1} = P_{1} = C107 \\ P_{102} = Fe_{1} = P_{1} = P_{1} = C107 \\ P_{102} = Fe_{1} = P_{1} = P_{1} = C302 \\ P_{102} = Fe_{1} = P_{1} = P_{1} = C305 \\ P_{102} = Fe_{1} = P_{1} = P_{1} = C306 \\ P_{102} = Fe_{1} = P_{1} = O_{1} = C50 \\ P_{102} = Fe_{1} = P_{1} = C101 \\ \end{array}$	$\begin{array}{c} -5.6\ (6)\\ -130.8\ (9)\\ 110\ (1)\\ -90.8\ (2)\\ 89.5\ (2)\\ 44.0\ (6)\\ 23\ (2)\\ 10.7\ (6)\\ 131.1\ (8)\\ -105.5\ (6)\\ -14.1\ (5)\\ 100.6\ (5)\\ -140.5\ (5)\\ -91.1\ (9)\\ 104.7\ (3)\\ -137.4\ (2)\\ -13.1\ (4)\\ -82.3\ (3)\\ 39.4\ (4)\\ 164.6\ (5)\\ 68.4\ (4)\\ 166\ (1)\\ -43\ (1)\\ 24.7\ (4)\\ -171.6\ (2)\\ 109.6\ (7)\\ \end{array}$
$P4-Fe1-P303-C307 \\ P4-Fe1-P303-C307 \\ P4-Fe1-P303-C309 \\ P4-Fe1-P303-C310 \\ P4-Fe1-O2-C50 \\ P4-Fe1-O2-C50 \\ P4-C108-C107-P103 \\ P4-C308-C307-P303 \\ P102-Fe1-P1-C101 \\ P102-Fe1-P1-C101 \\ P102-Fe1-P1-C103 \\ P102-Fe1-P1-C201 \\ P102-Fe1-P1-C201 \\ P102-Fe1-P1-C203 \\ P102-Fe1-P1-C301 \\ P102-Fe1-P1-C301 \\ P102-Fe1-P4-C118 \\ P102-Fe1-P4-C112 \\ P102-Fe1-P4-C112 \\ P102-Fe1-P103-C107 \\ P102-Fe1-P103-C107 \\ P102-Fe1-P103-C305 \\ P102-Fe1-P103-C306 \\ P102-Fe1-O1-C50 \\ P102-Fe1-O1-C50 \\ P102-Fe1-P1-C101 \\ P103-Fe1-P1-C101 \\ P103-Fe1-P1-C101 \\ P103-Fe1-P1-C103 \\ P103-Fe1-P1-C103 \\ P103-Fe1-P1-C101 \\ P103-Fe1-P1-C103 \\ P103-Fe1-P1-C101 \\ P103-Fe1-P1-C103 \\ P103-Fe1-P1-C101 \\ P103-Fe1-$	$\begin{array}{c} -5.6\ (6)\\ -130.8\ (9)\\ 110\ (1)\\ -90.8\ (2)\\ 89.5\ (2)\\ 44.0\ (6)\\ 23\ (2)\\ 10.7\ (6)\\ 131.1\ (8)\\ -105.5\ (6)\\ -14.1\ (5)\\ 100.6\ (5)\\ -140.5\ (5)\\ -140.5\ (5)\\ -91.1\ (9)\\ 104.7\ (3)\\ -137.4\ (2)\\ -13.1\ (4)\\ -82.3\ (3)\\ 39.4\ (4)\\ 164.6\ (5)\\ 68.4\ (4)\\ 166\ (1)\\ -43\ (1)\\ 24.7\ (4)\\ -171.6\ (2)\\ 109.6\ (7)\\ -120.0\ (6)\\ \end{array}$
$P4-Fe1-P303-C307 \\ P4-Fe1-P303-C309 \\ P4-Fe1-P303-C309 \\ P4-Fe1-P303-C310 \\ P4-Fe1-O1-C50 \\ P4-Fe1-O2-C50 \\ P4-C108-C107-P103 \\ P4-C308-C307-P303 \\ P102-Fe1-P1-C101 \\ P102-Fe1-P1-C103 \\ P102-Fe1-P1-C104 \\ P102-Fe1-P1-C201 \\ P102-Fe1-P1-C204 \\ P102-Fe1-P1-C301 \\ P102-Fe1-P1-C301 \\ P102-Fe1-P4-C108 \\ P102-Fe1-P4-C111 \\ P102-Fe1-P4-C112 \\ P102-Fe1-P4-C112 \\ P102-Fe1-P103-C107 \\ P102-Fe1-P103-C109 \\ P102-Fe1-P103-C305 \\ P102-Fe1-P103-C305 \\ P102-Fe1-P103-C306 \\ P102-Fe1-P103-C306 \\ P102-Fe1-P1-C301 \\ P102-Fe1-P103-C306 \\ P102-Fe1-P103-C50 \\ P102-Fe1-P1-C101 \\ P103-Fe1-P1-C101 \\ P103-Fe1-P1-C103 \\ P103-Fe1-P1-F103-P103 \\ P103-Fe1-P1-F103-P103 \\ P103-Fe1-P1-F103-P103 \\ P103-Fe1-P1-F103-P103 \\ P103-Fe1-P1-F103-P103 \\ P103-Fe1-P1-F103-P103 \\ P103-F1-$	$\begin{array}{c} -5.6 \ (6)\\ -130.8 \ (9)\\ 110 \ (1)\\ -90.8 \ (2)\\ 89.5 \ (2)\\ 44.0 \ (6)\\ 23 \ (2)\\ 10.7 \ (6)\\ 131.1 \ (8)\\ -105.5 \ (6)\\ -14.1 \ (5)\\ 100.6 \ (5)\\ -140.5 \ (5)\\ -91.1 \ (9)\\ 104.7 \ (3)\\ -91.1 \ (9)\\ 104.7 \ (3)\\ -39.4 \ (4)\\ 164.6 \ (5)\\ 68.4 \ (4)\\ 166. \ (1)\\ -43 \ (1)\\ 24.7 \ (4)\\ -171.6 \ (2)\\ 109.6 \ (7)\\ -130.0 \ (8)\\ \end{array}$
$P4-Fe1-P303-C307 \\ P4-Fe1-P303-C307 \\ P4-Fe1-P303-C309 \\ P4-Fe1-P303-C310 \\ P4-Fe1-O1-C50 \\ P4-Fe1-O2-C50 \\ P4-C108-C107-P103 \\ P4-C308-C307-P303 \\ P102-Fe1-P1-C101 \\ P102-Fe1-P1-C101 \\ P102-Fe1-P1-C104 \\ P102-Fe1-P1-C201 \\ P102-Fe1-P1-C201 \\ P102-Fe1-P1-C301 \\ P102-Fe1-P1-C301 \\ P102-Fe1-P4-C108 \\ P102-Fe1-P4-C112 \\ P102-Fe1-P4-C112 \\ P102-Fe1-P4-C112 \\ P102-Fe1-P103-C107 \\ P102-Fe1-P103-C107 \\ P102-Fe1-P103-C305 \\ P102-Fe1-P103-C306 \\ P102-Fe1-P1-C301 \\ P102-Fe1-P1-C301 \\ P102-Fe1-P1-C301 \\ P102-Fe1-P103-C306 \\ P102-Fe1-P103-C50 \\ P103-Fe1-P1-C101 \\ P103-Fe1-P1-C103 \\ P103-Fe1-P1-C103 \\ P103-Fe1-P1-C103 \\ P103-Fe1-P1-C104 \\ P103-Fe1-P1-F104 \\ P103-Fe1-P1-F104 \\ P103-Fe1-P1-F104 \\ P103-Fe1-P1-F104 \\ P103-Fe1-P1-F104 \\ P103-Fe1-P1-F104 \\ P103$	$\begin{array}{c} -5.6\ (6)\\ -130.8\ (9)\\ 110\ (1)\\ -90.8\ (2)\\ 89.5\ (2)\\ 44.0\ (6)\\ 23\ (2)\\ 10.7\ (6)\\ 131.1\ (8)\\ -105.5\ (6)\\ -14.1\ (5)\\ 100.6\ (5)\\ -140.5\ (5)\\ -91.1\ (9)\\ 104.7\ (3)\\ -137.4\ (2)\\ -13.1\ (4)\\ -82.3\ (3)\\ 39.4\ (4)\\ 164.6\ (5)\\ 68.4\ (4)\\ 166\ (1)\\ -43\ (1)\\ 24.7\ (4)\\ 109.6\ (7)\\ -130.0\ (8)\\ -6.6\ (6)\end{array}$
$\begin{array}{l} P_{4} = Fe1 = P303 = C307 \\ P_{4} = Fe1 = P303 = C307 \\ P_{4} = Fe1 = P303 = C309 \\ P_{4} = Fe1 = P303 = C310 \\ P_{4} = Fe1 = O1 = C50 \\ P_{4} = Fe1 = O2 = C50 \\ P_{4} = C108 = C107 = P103 \\ P_{4} = C308 = C307 = P303 \\ P_{4} = C308 = C307 \\ P_{4} = C308 = C308 \\ P_{4} = C308 \\ P_{4} = C308 = C308 \\ P_{4} = C308 = C308 \\ P_{4} = C308 \\ P_{4} = C308 = C308 \\ P_{4} = C308$	$\begin{array}{c} -5.6\ (6)\\ -130.8\ (9)\\ 110\ (1)\\ -90.8\ (2)\\ 89.5\ (2)\\ 44.0\ (6)\\ 23\ (2)\\ 10.7\ (6)\\ 131.1\ (8)\\ -105.5\ (6)\\ -14.1\ (5)\\ 100.6\ (5)\\ -140.5\ (5)\\ 0.140.5\ (5)\\ -91.1\ (9)\\ 0.140.5\ (5)\\ -91.1\ (9)\\ 0.137.4\ (2)\\ -137.4\ (2)\\ -137.4\ (2)\\ -131.1\ (4)\\ -82.3\ (3)\\ 39.4\ (4)\\ 166.6\ (1)\\ -43\ (1)\\ 24.7\ (4)\\ 166\ (1)\\ -43\ (1)\\ 24.7\ (4)\\ -171.6\ (2)\\ 109.6\ (7)\\ -130.0\ (8)\\ -6.6\ (6)\\ 84.8\ (5)\\ \end{array}$
$P4-Fe1-P303-C307 \\ P4-Fe1-P303-C307 \\ P4-Fe1-P303-C309 \\ P4-Fe1-O1-C50 \\ P4-Fe1-O2-C50 \\ P4-Fe1-O2-C50 \\ P4-C108-C107-P103 \\ P4-C308-C307-P303 \\ P102-Fe1-P1-C101 \\ P102-Fe1-P1-C101 \\ P102-Fe1-P1-C104 \\ P102-Fe1-P1-C201 \\ P102-Fe1-P1-C204 \\ P102-Fe1-P1-C301 \\ P102-Fe1-P1-C301 \\ P102-Fe1-P4-C108 \\ P102-Fe1-P4-C111 \\ P102-Fe1-P4-C112 \\ P102-Fe1-P4-C112 \\ P102-Fe1-P103-C107 \\ P102-Fe1-P103-C107 \\ P102-Fe1-P103-C305 \\ P102-Fe1-P103-C305 \\ P102-Fe1-P103-C305 \\ P102-Fe1-P1-C50 \\ P102-Fe1-P1-C101 \\ P103-Fe1-P1-C101 \\ P103-Fe1-P1-C103 \\ P103-Fe1-P1-C104 \\ P103-Fe1-P1-C104 \\ P103-Fe1-P1-C104 \\ P103-Fe1-P1-C201 \\ P102-Fe1-P1-C201 \\ P102-Fe1-$	$\begin{array}{c} -5.6\ (6)\\ -130.8\ (9)\\ 110\ (1)\\ -90.8\ (2)\\ 89.5\ (2)\\ 44.0\ (6)\\ 23\ (2)\\ 10.7\ (6)\\ 131.1\ (8)\\ -105.5\ (6)\\ -14.1\ (5)\\ 100.6\ (5)\\ -140.5\ (5)\\ -140.5\ (5)\\ -91.1\ (9)\\ 104.7\ (3)\\ -137.4\ (2)\\ -13.1\ (4)\\ -82.3\ (3)\\ 39.4\ (4)\\ 164.6\ (5)\\ 68.4\ (4)\\ 166.6\ (1)\\ -43\ (1)\\ 24.7\ (4)\\ -171.6\ (2)\\ 109.6\ (7)\\ -130.0\ (8)\\ -6.6\ (6)\\ 84.8\ (5)\\ 100.5\ (7)\\ -130.0\ (8)\\ -6.6\ (6)\\ 84.8\ (5)\\ 100.5\ (7)\\ -130.0\ (8)\\ -6.6\ (6)\\ 84.8\ (5)\\ 100.5\ (7)\\ -130.0\ (8)\\ -6.6\ (6)\\ 84.8\ (5)\\ 100.5\ (7)\\ -130.0\ (8)\\ -6.6\ (6)\\ 84.8\ (5)\\ 100.5\ (7)\\ -130.0\ (8)\\ -6.6\ (6)\\ 84.8\ (5)\\ 100.5\ (7)\\ -130.0\ (8)\\ -6.6\ (6)\\ 84.8\ (5)\\ 100.5\ (7)\\ -130.0\ (8)\\ -6.6\ (6)\\ 84.8\ (5)\\ 100.5\ (7)\\ -130.0\ (8)\\ -6.6\ (6)\\ 84.8\ (5)\\ 100.5\ (7)\\ -130.0\ (8)\\ -6.6\ (6)\\ 84.8\ (5)\\ 100.5\ (7)\\ -130.0\ (8)\\ -6.6\ (6)\ (6)\ (6)\ (6)\ (6)\ (6)\ (6)\ (6$
$\begin{array}{l} P_{4} = Fe1 = P303 = C307 \\ P_{4} = Fe1 = P303 = C307 \\ P_{4} = Fe1 = P303 = C309 \\ P_{4} = Fe1 = P303 = C310 \\ P_{4} = Fe1 = O1 = C50 \\ P_{4} = C108 = C107 = P103 \\ P_{4} = C108 = C107 = P103 \\ P_{4} = C308 = C307 = P303 \\ P_{102} = Fe1 = P1 = C101 \\ P_{102} = Fe1 = P1 = C104 \\ P_{102} = Fe1 = P1 = C201 \\ P_{102} = Fe1 = P1 = C204 \\ P_{102} = Fe1 = P1 = C204 \\ P_{102} = Fe1 = P1 = C301 \\ P_{102} = Fe1 = P1 = C301 \\ P_{102} = Fe1 = P4 = C112 \\ P_{102} = Fe1 = P4 = C112 \\ P_{102} = Fe1 = P_{103} = C107 \\ P_{102} = Fe1 = P_{103} = C107 \\ P_{102} = Fe1 = P_{103} = C107 \\ P_{102} = Fe1 = P_{103} = C302 \\ P_{102} = Fe1 = P_{103} = C302 \\ P_{102} = Fe1 = P_{103} = C306 \\ P_{103} = Fe1 = P_{1} = C103 \\ P_{103} = Fe_{1} = P_{1} = C103 \\ P_{103} = Fe_{1} = P_{1} = C201 \\ P_{103} = Fe_{1} = P_{1} = C201 \\ P_{103} = Fe_{1} = P_{1} = C203 \\ \end{array}$	$\begin{array}{c} -5.6 \ (6) \\ -130.8 \ (9) \\ 110 \ (1) \\ -90.8 \ (2) \\ 89.5 \ (2) \\ 44.0 \ (6) \\ 23 \ (2) \\ 10.7 \ (6) \\ 131.1 \ (8) \\ -105.5 \ (6) \\ -14.1 \ (5) \\ 100.6 \ (5) \\ -140.5 \ (5) \\ -91.1 \ (9) \\ 104.7 \ (3) \\ -137.4 \ (2) \\ -13.1 \ (4) \\ -82.3 \ (3) \\ 39.4 \ (4) \\ 164.6 \ (5) \\ 68.4 \ (4) \\ 166 \ (1) \\ -43 \ (1) \\ 24.7 \ (4) \\ -171.6 \ (2) \\ 109.6 \ (7) \\ -130.0 \ (8) \\ -6.6 \ (6) \\ 84.8 \ (5) \\ -160.5 \ (5) \end{array}$
$\begin{array}{l} P_{4} = Fe1 = P303 = C307 \\ P_{4} = Fe1 = P303 = C307 \\ P_{4} = Fe1 = P303 = C309 \\ P_{4} = Fe1 = O2 = C50 \\ P_{4} = Fe1 = O2 = C50 \\ P_{4} = C108 = C107 = P103 \\ P_{4} = C308 = C307 = P303 \\ P_{4} = C308 = C307 \\ P_{4} = C308 \\ P_{4} = C308 \\ P_{4} = C308 \\ P_$	$\begin{array}{c} -5.6\ (6)\\ -130.8\ (9)\\ 110\ (1)\\ -90.8\ (2)\\ 89.5\ (2)\\ 44.0\ (6)\\ 23\ (2)\\ 10.7\ (6)\\ 131.1\ (8)\\ -105.5\ (6)\\ -14.1\ (5)\\ 100.6\ (5)\\ -140.5\ (5)\\ 100.6\ (5)\\ -91.1\ (9)\\ 104.7\ (3)\\ -91.1\ (9)\\ 104.7\ (3)\\ -91.1\ (9)\\ -91.1\ (9)\\ 104.7\ (3)\\ -91.1\ (9)\ -91.1\ (9)\ -91.1\ (9)\ -91.1\ (9)\ -91.1\ (9)\ -91.1\ (9)\ -91.1\ (9)\ -91.1\ (9)\ -91.1\ (9)\ -91.1\ (9)\ -91.1\ (9)\ -91.1\ (9)\ -91.1\ (9)\ -91.1\ (9)\ -91.1\ (9)\ -91.1\ (9)\ -91.1\ (9)\ -91.1\ (9)\ -91.1\ (9)\ -91.1$
P4 - Fe1 - P303 - C307 $P4 - Fe1 - P303 - C307$ $P4 - Fe1 - P303 - C309$ $P4 - Fe1 - O1 - C50$ $P4 - Fe1 - O2 - C50$ $P4 - C108 - C107 - P103$ $P4 - C308 - C307 - P303$ $P102 - Fe1 - P1 - C101$ $P102 - Fe1 - P1 - C104$ $P102 - Fe1 - P1 - C201$ $P102 - Fe1 - P1 - C204$ $P102 - Fe1 - P1 - C301$ $P102 - Fe1 - P4 - C108$ $P102 - Fe1 - P4 - C111$ $P102 - Fe1 - P103 - C107$ $P102 - Fe1 - P103 - C302$ $P102 - Fe1 - P103 - C305$ $P102 - Fe1 - P103 - C306$ $P102 - Fe1 - P1 - C101$ $P103 - Fe1 - P1 - C101$ $P103 - Fe1 - P1 - C104$ $P103 - Fe1 - P1 - C104$ $P103 - Fe1 - P1 - C204$	$\begin{array}{c} -5.6\ (6)\\ -130.8\ (9)\\ 110\ (1)\\ -90.8\ (2)\\ 89.5\ (2)\\ 44.0\ (6)\\ 23\ (2)\\ 10.7\ (6)\\ 131.1\ (8)\\ -105.5\ (6)\\ -14.1\ (5)\\ 100.6\ (5)\\ -140.5\ (5)\\ -140.5\ (5)\\ 100.6\ (5)\\ -140.5\ (5)\\ 100.7\ (3)\\ 104.7\ (3)\\ 39.4\ (4)\\ 164.6\ (5)\\ 68.4\ (4)\\ 166.6\ (1)\\ -43\ (1)\\ 24.7\ (4)\\ -171.6\ (2)\\ 109.6\ (7)\\ -130.0\ (8)\\ -6.6\ (6)\\ 84.8\ (5)\\ -140.5\ (5)\\ -140.5\ (5)\\ -140.6\ (5)\\ 5.8\ (3)\\ \end{array}$
P4 - Fe1 - P303 - C307 $P4 - Fe1 - P303 - C307$ $P4 - Fe1 - P303 - C309$ $P4 - Fe1 - O1 - C50$ $P4 - Fe1 - O2 - C50$ $P4 - C108 - C107 - P103$ $P4 - C308 - C307 - P303$ $P102 - Fe1 - P1 - C101$ $P102 - Fe1 - P1 - C103$ $P102 - Fe1 - P1 - C201$ $P102 - Fe1 - P1 - C201$ $P102 - Fe1 - P1 - C204$ $P102 - Fe1 - P1 - C301$ $P102 - Fe1 - P4 - C118$ $P102 - Fe1 - P4 - C112$ $P102 - Fe1 - P103 - C107$ $P102 - Fe1 - P103 - C305$ $P102 - Fe1 - P103 - C306$ $P102 - Fe1 - P103 - C306$ $P102 - Fe1 - P1 - C101$ $P103 - Fe1 - P1 - C101$ $P103 - Fe1 - P1 - C103$ $P103 - Fe1 - P1 - C104$ $P103 - Fe1 - P1 - C104$ $P103 - Fe1 - P1 - C204$	$\begin{array}{c} -5.6\ (6)\\ -130.8\ (9)\\ 110\ (1)\\ -90.8\ (2)\\ 89.5\ (2)\\ 44.0\ (6)\\ 23\ (2)\\ 10.7\ (6)\\ 131.1\ (8)\\ -105.5\ (6)\\ -14.1\ (5)\\ 100.6\ (5)\\ -140.5\ (5)\\ -91.1\ (9)\\ 104.7\ (3)\\ -137.4\ (2)\\ -13.1\ (4)\\ -82.3\ (3)\\ 39.4\ (4)\\ 164.6\ (5)\\ 68.4\ (4)\\ 166\ (1)\\ -43\ (1)\\ 24.7\ (4)\\ -171.6\ (2)\\ 109.6\ (7)\\ -130.0\ (8)\\ -6.6\ (6)\\ 84.8\ (5)\\ -160.5\ (5)\\ -41.6\ (5)\\ 5.8\ (3)\\ 102.7\ (7)\\ -130.0\ (7)\\ -130.0\ (7)\\ -160.5\ (5)\\ -41.6\ (5)\\ 5.8\ (3)\\ 102.7\ (7)\\ -130.0\ (7)\\ -160.5\ (5)\\ -41.6\ (5)\\ 5.8\ (3)\\ 102.7\ (7)\\ -130.0\ (7)\\ -130.0\ (7)\\ -160.5\ (5)\\ -41.6\ (5)\\ 5.8\ (3)\\ 102.7\ (7)\\ -130.0\ (7)\\ -130.0\ (7)\\ -140.0\ (7)\\ -140.0\ (7)\\ -130.0\ (7)\\ -130.0\ (7)\\ -130.0\ (7)\\ -140.0\ (7)\ (7)\ (7)\ (7)\ (7)\ (7)\ (7)\ (7)$
$\begin{array}{l} P_{4} = Fe1 = P303 = C307 \\ P_{4} = Fe1 = P303 = C307 \\ P_{4} = Fe1 = P303 = C309 \\ P_{4} = Fe1 = P303 = C310 \\ P_{4} = Fe1 = O2 = C50 \\ P_{4} = C108 = C107 = P103 \\ P_{4} = C108 = C107 = P103 \\ P_{4} = C308 = C307 = P303 \\ P_{102} = Fe1 = P_{1} = C101 \\ P_{102} = Fe_{1} = P_{1} = C103 \\ P_{102} = Fe_{1} = P_{1} = C201 \\ P_{102} = Fe_{1} = P_{1} = C204 \\ P_{102} = Fe_{1} = P_{1} = C301 \\ P_{102} = Fe_{1} = P_{4} = C108 \\ P_{102} = Fe_{1} = P_{4} = C108 \\ P_{102} = Fe_{1} = P_{4} = C111 \\ P_{102} = Fe_{1} = P_{4} = C112 \\ P_{102} = Fe_{1} = P_{4} = C112 \\ P_{102} = Fe_{1} = P_{103} = C107 \\ P_{102} = Fe_{1} = P_{103} = C107 \\ P_{102} = Fe_{1} = P_{103} = C107 \\ P_{102} = Fe_{1} = P_{103} = C302 \\ P_{102} = Fe_{1} = P_{103} = C306 \\ P_{103} = Fe_{1} = P_{1} = C101 \\ P_{103} = Fe_{1} = P_{1} = C103 \\ P_{103} = Fe_{1} = P_{1} = C103 \\ P_{103} = Fe_{1} = P_{1} = C103 \\ P_{103} = Fe_{1} = P_{1} = C204 \\ P_{103} = Fe_{1} = P_{1} = C108 \\ P_{103} = Fe_{1} = P_{1} = C108 \\ P_{103} = Fe_{1} = P_{1} = C108 \\ P_{103} = Fe_{1} = P_{1} = C204 \\ P_{103} = Fe_{1} = P_{1} = C20$	$\begin{array}{c} -5.6\ (6)\\ -130.8\ (9)\\ 110\ (1)\\ -90.8\ (2)\\ 89.5\ (2)\\ 44.0\ (6)\\ 23\ (2)\\ 10.7\ (6)\\ 131.1\ (8)\\ -105.5\ (6)\\ -14.1\ (5)\\ 100.6\ (5)\\ -140.5\ (5)\\ -91.1\ (9)\\ 104.7\ (3)\\ -39.4\ (4)\\ 164.6\ (5)\\ 68.4\ (4)\\ 166\ (1)\\ -43\ (1)\\ 24.7\ (4)\\ -171.6\ (2)\\ 109.6\ (7)\\ -130.0\ (8)\\ -6.6\ (6)\\ 84.8\ (5)\\ -140.5\ (5)\\ -140.5\ (5)\\ -41.6\ (5)\\ 5.8\ (3)\\ 123.7\ (3)\\ \end{array}$
$P4-Fe1-P303-C307 \\ P4-Fe1-P303-C307 \\ P4-Fe1-P303-C309 \\ P4-Fe1-O1-C50 \\ P4-Fe1-O2-C50 \\ P4-Fe1-O2-C50 \\ P4-C108-C107-P103 \\ P4-C308-C307-P303 \\ P102-Fe1-P1-C101 \\ P102-Fe1-P1-C101 \\ P102-Fe1-P1-C104 \\ P102-Fe1-P1-C201 \\ P102-Fe1-P1-C203 \\ P102-Fe1-P1-C301 \\ P102-Fe1-P1-C301 \\ P102-Fe1-P4-C108 \\ P102-Fe1-P4-C112 \\ P102-Fe1-P4-C112 \\ P102-Fe1-P4-C112 \\ P102-Fe1-P103-C107 \\ P102-Fe1-P103-C107 \\ P102-Fe1-P103-C305 \\ P102-Fe1-P103-C306 \\ P102-Fe1-P1-C101 \\ P102-Fe1-P1-C101 \\ P103-Fe1-P1-C101 \\ P103-Fe1-P1-C101 \\ P103-Fe1-P1-C101 \\ P103-Fe1-P1-C103 \\ P103-Fe1-P1-C203 \\ P103-Fe1-P1-C203 \\ P103-Fe1-P1-C204 \\ P103-Fe1-P1-C204 \\ P103-Fe1-P1-C204 \\ P103-Fe1-P1-C204 \\ P103-Fe1-P4-C111 \\ P103-Fe1-P4-C112 \\ P103-Fe1-P$	$\begin{array}{c} -5.6\ (6)\\ -130.8\ (9)\\ 110\ (1)\\ -90.8\ (2)\\ 89.5\ (2)\\ 44.0\ (6)\\ 23\ (2)\\ 10.7\ (6)\\ 131.1\ (8)\\ -105.5\ (6)\\ -14.1\ (5)\\ 100.6\ (5)\\ -140.5\ (5)\\ -91.1\ (9)\\ 104.7\ (3)\\ 39.4\ (4)\\ 164.6\ (5)\\ 68.4\ (4)\\ 166\ (1)\\ -43\ (1)\\ 24.7\ (4)\\ 109.6\ (7)\\ -130.0\ (8)\\ -6.6\ (6)\\ 84.8\ (5)\\ -140.5\ (5)\\ -140.5\ (5)\\ -160.5\ (5)\\ -140.5\ (5)\\ 5.8\ (3)\\ 123.7\ (3)\\ -112.0\ (4)\\ \end{array}$

P103—Fe1—P102—C102	-824(5)
1100 Tel 1102 C102	02.1(0)
P103—Fe1—P102—C105	34(1)
P103—Fe1—P102—C106	161(1)
D100 D1 D100 C000	100 (1)
P103—Fe1—P102—C202	-103.3(5)
P103—Fe1—P102—C205	148.9(9)
D100 D1 D100 G000	
P103—Fe1—P102—C206	20.4(7)
P103—Fe1—O1—C50	-1770(2)
F100 FC1 O1 C00	111.0 (2)
P103—Fe1—O2—C50	12.3(5)
P302—Fe1—P1—C301	88(9)
1502 101 11 0501	0.0 (0)
P302—Fe1—P1—C303	-111.9(9)
$P_{302} = F_{01} = P_{1} = C_{304}$	125 (1)
1 302-141-1 1-0304	120 (1)
P302—Fe1—P4—C308	-80.6(9)
$P_{302} = F_{01} = P_{4} = C_{311}$	15 7 (8)
1 302-141-1 4-0311	40.7 (0)
P302—Fe1—P4—C312	159.6(8)
D202 Eo1 D202 C207	00 2 (7)
1 302-re1-1 303-0307	00.0 (1)
P302—Fe1—P303—C309	-36.8(9)
D202 Eo1 D202 C210	156 (1)
r 302—rei—r 303—0310	-130(1)
P302—Fe1—O1—C50	173.5(3)
D202 E-1 02 CE0	16 2 (0)
P 302—Pe1—O2—C30	-10.2(9)
P303—Fe1—P1—C301	-91.3(9)
D202 Eo1 D1 C202	1470 (9)
r 303—rei—r i—0303	141.9 (8)
P303—Fe1—P1—C304	24.8(9)
D202 Eo1 D4 C200	10 = (0)
P303—Fe1—P4—C308	19.5 (8)
P303—Fe1—P4—C311	145.7(7)
D202 E-1 D4 (2210	100.9 (7)
P303—Fe1—P4—C312	-100.3(7)
P303—Fe1—P302—C302	81.2(8)
Daoa E 1 Daoa Gaor	1 (0 (1)
P303—Fe1—P302—C305	-162(1)
P303—Fe1—P302—C306	-41(1)
D202 E-1 O1 CF0	20.0 (4)
P 305—Pe1—01—030	-36.2(4)
P303—Fe1—O2—C50	168.5(2)
O1 E-1 D1 C101	1529 (6)
01—Fe1—P1—C101	-153.2(0)
O1—Fe1—P1—C103	-32.8(8)
O1 = 1 = 1 = 01 = 0104	00 7 (6)
01—Fe1—F1—C104	90.7 (0)
O1—Fe1—P1—C201	-177.9(5)
O1 - Fe1 - P1 - C201	-177.9(5)
O1—Fe1—P1—C201 O1—Fe1—P1—C203	-177.9(5) -63.2(5)
O1-Fe1-P1-C201 O1-Fe1-P1-C203 O1-Fe1-P1-C204	-177.9(5) -63.2(5) 55.7(5)
$\begin{array}{c} O1 - Fe1 - P1 - C201 \\ O1 - Fe1 - P1 - C203 \\ O1 - Fe1 - P1 - C204 \\ O1 - Fe1 - P1 - C204 \end{array}$	-177.9 (5) -63.2 (5) 55.7 (5) 105.1 (0)
O1—Fe1—P1—C201 O1—Fe1—P1—C203 O1—Fe1—P1—C204 O1—Fe1—P1—C301	$\begin{array}{r} -177.9 (5) \\ -63.2 (5) \\ 55.7 (5) \\ 105.1 (9) \end{array}$
$\begin{array}{c} O1-Fe1-P1-C201\\ O1-Fe1-P1-C203\\ O1-Fe1-P1-C204\\ O1-Fe1-P1-C301\\ O1-Fe1-P1-C303\\ \end{array}$	-177.9 (5) -63.2 (5) 55.7 (5) 105.1 (9) -15.7 (8)
$\begin{array}{c} O1-Fe1-P1-C201\\ O1-Fe1-P1-C203\\ O1-Fe1-P1-C204\\ O1-Fe1-P1-C301\\ O1-Fe1-P1-C303\\ O1-Fe1-P1-C30\\ O1-Fe1-FF1-C30\\ O1-FF1-FF1-FF1-C30\\ O1-FF1-FF1-FF1-FF1-FF1-FF1-FF1-FF1-FF1-F$	$\begin{array}{c} -177.9 (5) \\ -63.2 (5) \\ 55.7 (5) \\ 105.1 (9) \\ -15.7 (8) \\ 122.8 (9) \end{array}$
O1—Fe1—P1—C201 O1—Fe1—P1—C203 O1—Fe1—P1—C204 O1—Fe1—P1—C301 O1—Fe1—P1—C303 O1—Fe1—P1—C304	$\begin{array}{r} -177.9 (5) \\ -63.2 (5) \\ 55.7 (5) \\ 105.1 (9) \\ -15.7 (8) \\ -138.8 (9) \end{array}$
$\begin{array}{c} O1-Fe1-P1-C201\\ O1-Fe1-P1-C203\\ O1-Fe1-P1-C204\\ O1-Fe1-P1-C301\\ O1-Fe1-P1-C303\\ O1-Fe1-P1-C304\\ O1-Fe1-P4-C108\\ \end{array}$	$\begin{array}{r} -177.9 (5) \\ -63.2 (5) \\ 55.7 (5) \\ 105.1 (9) \\ -15.7 (8) \\ -138.8 (9) \\ -91.7 (3) \end{array}$
$\begin{array}{c} O1-Fe1-P1-C201\\ O1-Fe1-P1-C203\\ O1-Fe1-P1-C204\\ O1-Fe1-P1-C301\\ O1-Fe1-P1-C303\\ O1-Fe1-P1-C304\\ O1-Fe1-P4-C108\\ O1-Fe1-P4-C108\\ O1-Fe1-P4-C111\\ \end{array}$	$\begin{array}{c} -177.9 (5) \\ -63.2 (5) \\ 55.7 (5) \\ 105.1 (9) \\ -15.7 (8) \\ -138.8 (9) \\ -91.7 (3) \\ 202 (2) \end{array}$
$\begin{array}{c} O1-Fe1-P1-C201\\ O1-Fe1-P1-C203\\ O1-Fe1-P1-C204\\ O1-Fe1-P1-C301\\ O1-Fe1-P1-C303\\ O1-Fe1-P1-C304\\ O1-Fe1-P1-C304\\ O1-Fe1-P4-C108\\ O1-Fe1-P4-C111\\ \end{array}$	$\begin{array}{c} -177.9 (5) \\ -63.2 (5) \\ 55.7 (5) \\ 105.1 (9) \\ -15.7 (8) \\ -138.8 (9) \\ -91.7 (3) \\ 26.2 (3) \end{array}$
$\begin{array}{c} O1-Fe1-P1-C201\\ O1-Fe1-P1-C203\\ O1-Fe1-P1-C204\\ O1-Fe1-P1-C301\\ O1-Fe1-P1-C303\\ O1-Fe1-P1-C304\\ O1-Fe1-P4-C108\\ O1-Fe1-P4-C111\\ O1-Fe1-P4-C112\\ \end{array}$	$\begin{array}{c} -177.9 (5) \\ -63.2 (5) \\ 55.7 (5) \\ 105.1 (9) \\ -15.7 (8) \\ -138.8 (9) \\ -91.7 (3) \\ 26.2 (3) \\ 150.5 (4) \end{array}$
$\begin{array}{c} O1-Fe1-P1-C201\\ O1-Fe1-P1-C203\\ O1-Fe1-P1-C204\\ O1-Fe1-P1-C301\\ O1-Fe1-P1-C303\\ O1-Fe1-P1-C303\\ O1-Fe1-P1-C304\\ O1-Fe1-P4-C108\\ O1-Fe1-P4-C111\\ O1-Fe1-P4-C112\\ O1-Fe1-P4-C122\\ O1-Fe1-F4-C12\\ O1-Fe1-F4-F4-C122\\ O1-F4-F4-F4-F4-F4-F4-F4-F4-F4-F4-F4-F4-F4-$	$\begin{array}{c} -177.9 (5) \\ -63.2 (5) \\ 55.7 (5) \\ 105.1 (9) \\ -15.7 (8) \\ -138.8 (9) \\ -91.7 (3) \\ 26.2 (3) \\ 150.5 (4) \end{array}$
$\begin{array}{c} \text{O1Fe1P1C201} \\ \text{O1Fe1P1C203} \\ \text{O1Fe1P1C304} \\ \text{O1Fe1P1C303} \\ \text{O1Fe1P1C304} \\ \text{O1Fe1P4C108} \\ \text{O1Fe1P4C111} \\ \text{O1Fe1P4C112} \\ \text{O1Fe1P4C112} \\ \text{O1Fe1P4C308} \end{array}$	$\begin{array}{c} -177.9 \ (5) \\ -63.2 \ (5) \\ 55.7 \ (5) \\ 105.1 \ (9) \\ -15.7 \ (8) \\ -138.8 \ (9) \\ -91.7 \ (3) \\ 26.2 \ (3) \\ 150.5 \ (4) \\ -176.6 \ (8) \end{array}$
$\begin{array}{c} O1-Fe1-P1-C201\\ O1-Fe1-P1-C203\\ O1-Fe1-P1-C204\\ O1-Fe1-P1-C301\\ O1-Fe1-P1-C303\\ O1-Fe1-P1-C304\\ O1-Fe1-P4-C108\\ O1-Fe1-P4-C111\\ O1-Fe1-P4-C112\\ O1-Fe1-P4-C112\\ O1-Fe1-P4-C308\\ O1-Fe1-P4-C311\\ \end{array}$	$\begin{array}{c} -177.9 \text{ (s)} \\ -63.2 \text{ (s)} \\ 55.7 \text{ (s)} \\ 105.1 \text{ (g)} \\ -15.7 \text{ (g)} \\ -138.8 \text{ (g)} \\ -91.7 \text{ (3)} \\ 26.2 \text{ (3)} \\ 150.5 \text{ (3)} \\ 150.6 \text{ (s)} \\ -176.6 \text{ (s)} \\ -50.4 \text{ (7)} \end{array}$
$\begin{array}{c} O1-Fe1-P1-C201\\ O1-Fe1-P1-C203\\ O1-Fe1-P1-C204\\ O1-Fe1-P1-C301\\ O1-Fe1-P1-C303\\ O1-Fe1-P1-C304\\ O1-Fe1-P4-C108\\ O1-Fe1-P4-C111\\ O1-Fe1-P4-C112\\ O1-Fe1-P4-C308\\ O1-Fe1-P4-C311\\ O1-Fe1-P4-C311\\ O1-Fe1-P4-C312\\ O1-Fe1-F4-C312\\ O1-Fe1-F4-C312\\ O1-Fe1-F4-C312\\ O1-F61-F4-C312\\ O1-F61-F4-C312\\ O1-F61-F4-F4-C312\\ O1-F61-F4-F4-F4-F4-F4-F4-F4\\ O1-F61-F4-F4-F4-F4-F4-F4-F4-F4-F4-F4-F4-F4-F4-$	-177.9 (5) -63.2 (5) 55.7 (5) 105.1 (9) -15.7 (8) -138.8 (9) -91.7 (3) 26.2 (3) 150.5 (4) -176.6 (8) -50.4 (7) e_2 (6)
$\begin{array}{c} \text{O1}-\text{Fe1}-\text{P1}-\text{C201} \\ \text{O1}-\text{Fe1}-\text{P1}-\text{C203} \\ \text{O1}-\text{Fe1}-\text{P1}-\text{C204} \\ \text{O1}-\text{Fe1}-\text{P1}-\text{C301} \\ \text{O1}-\text{Fe1}-\text{P1}-\text{C303} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C108} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C108} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C111} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C112} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C308} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C308} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C311} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C312} \end{array}$	$\begin{array}{c} -177.9 \text{ (s)} \\ -63.2 \text{ (s)} \\ 55.7 \text{ (s)} \\ 105.1 \text{ (g)} \\ -15.7 \text{ (s)} \\ -91.7 \text{ (3)} \\ 26.2 \text{ (3)} \\ 150.5 \text{ (4)} \\ -176.6 \text{ (8)} \\ -50.4 \text{ (7)} \\ 63.6 \text{ (7)} \end{array}$
$\begin{array}{c} \text{O1}-\text{Fe1}-\text{P1}-\text{C201} \\ \text{O1}-\text{Fe1}-\text{P1}-\text{C203} \\ \text{O1}-\text{Fe1}-\text{P1}-\text{C204} \\ \text{O1}-\text{Fe1}-\text{P1}-\text{C301} \\ \text{O1}-\text{Fe1}-\text{P1}-\text{C303} \\ \text{O1}-\text{Fe1}-\text{P1}-\text{C304} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C108} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C111} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C112} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C308} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C308} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C311} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C312} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C312} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C102} \end{array}$	$\begin{array}{c} -177.9 \text{ (s)} \\ -63.2 \text{ (s)} \\ 55.7 \text{ (s)} \\ 105.1 \text{ (g)} \\ -15.7 \text{ (g)} \\ -15.7 \text{ (g)} \\ -15.7 \text{ (g)} \\ -138.8 \text{ (g)} \\ -91.7 \text{ (g)} \\ 26.2 \text{ (g)} \\ 150.5 \text{ (4)} \\ -176.6 \text{ (g)} \\ -50.4 \text{ (f)} \\ 63.6 \text{ (f)} \\ 75.7 \text{ (g)} \end{array}$
$\begin{array}{c} O1-Fe1-P1-C201\\ O1-Fe1-P1-C203\\ O1-Fe1-P1-C204\\ O1-Fe1-P1-C301\\ O1-Fe1-P1-C303\\ O1-Fe1-P1-C304\\ O1-Fe1-P4-C108\\ O1-Fe1-P4-C112\\ O1-Fe1-P4-C112\\ O1-Fe1-P4-C308\\ O1-Fe1-P4-C311\\ O1-Fe1-P4-C312\\ O1-Fe1-P102-C102\\ O1-Fe1-P102-C105\\ \end{array}$	$\begin{array}{c} -177.9 \text{ (s)} \\ -63.2 \text{ (s)} \\ 55.7 \text{ (s)} \\ 105.1 \text{ (g)} \\ -15.7 \text{ (s)} \\ 105.1 \text{ (g)} \\ -15.8 \text{ (g)} \\ -91.7 \text{ (3)} \\ 26.2 \text{ (3)} \\ 150.5 \text{ (4)} \\ -91.7 \text{ (3)} \\ 26.2 \text{ (3)} \\ 150.5 \text{ (4)} \\ -176.6 \text{ (8)} \\ -50.4 \text{ (7)} \\ 75.7 \text{ (6)} \\ -168 \text{ (1)} \end{array}$
$\begin{array}{l} \text{O1Fe1P1C201} \\ \text{O1Fe1P1C203} \\ \text{O1Fe1P1C204} \\ \text{O1Fe1P1C301} \\ \text{O1Fe1P1C303} \\ \text{O1Fe1P4C108} \\ \text{O1Fe1P4C111} \\ \text{O1Fe1P4C112} \\ \text{O1Fe1P4C112} \\ \text{O1Fe1P4C311} \\ \text{O1Fe1P4C312} \\ \text{O1Fe1P4C312} \\ \text{O1Fe1P102C102} \\ \text{O1Fe1P102C102} \\ \text{O1Fe1P102C105} \end{array}$	$\begin{array}{c} -177.9~(5)\\ -63.2~(5)\\ 55.7~(5)\\ 105.1~(9)\\ -15.7~(8)\\ -138.8~(9)\\ -91.7~(3)\\ 26.2~(3)\\ 150.5~(4)\\ -176.6~(8)\\ -50.4~(7)\\ 63.6~(7)\\ 75.7~(6)\\ -168~(1) \end{array}$
$\begin{array}{c} \text{O1}-\text{Fe1}-\text{P1}-\text{C201} \\ \text{O1}-\text{Fe1}-\text{P1}-\text{C203} \\ \text{O1}-\text{Fe1}-\text{P1}-\text{C204} \\ \text{O1}-\text{Fe1}-\text{P1}-\text{C301} \\ \text{O1}-\text{Fe1}-\text{P1}-\text{C303} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C304} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C111} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C112} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C318} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C311} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C312} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C312} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C102} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C105} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C106} \\ \end{array}$	$\begin{array}{c} -177.9 \text{ (s)} \\ -63.2 \text{ (s)} \\ 55.7 \text{ (s)} \\ 105.1 \text{ (g)} \\ -15.7 \text{ (g)} \\ -15.7 \text{ (g)} \\ -138.8 \text{ (g)} \\ -91.7 \text{ (g)} \\ 26.2 \text{ (g)} \\ 150.5 \text{ (g)} \\ -91.7 \text{ (g)} \\ 150.5 \text{ (g)} \\ -176.6 \text{ (g)} \\ -176.6 \text{ (g)} \\ -57.6 \text{ (g)} \\ -168 \text{ (g)} \\ -168 \text{ (g)} \\ -41 \text{ (g)} \end{array}$
$\begin{array}{c} \text{O1-Fe1-P1-C201} \\ \text{O1-Fe1-P1-C203} \\ \text{O1-Fe1-P1-C301} \\ \text{O1-Fe1-P1-C301} \\ \text{O1-Fe1-P1-C303} \\ \text{O1-Fe1-P4-C108} \\ \text{O1-Fe1-P4-C112} \\ \text{O1-Fe1-P4-C112} \\ \text{O1-Fe1-P4-C112} \\ \text{O1-Fe1-P4-C308} \\ \text{O1-Fe1-P4-C311} \\ \text{O1-Fe1-P4-C312} \\ \text{O1-Fe1-P4-C312} \\ \text{O1-Fe1-P102-C102} \\ \text{O1-Fe1-P102-C105} \\ \text{O1-Fe1-P102-C106} \\ \text{O1-Fe1-P102-C302} \\ \text{O1-Fe1-P102-C302}$	-177.9 (s) -63.2 (s) 55.7 (s) 105.1 (9) -15.7 (8) -91.7 (3) 26.2 (3) 150.5 (4) -176.6 (8) -50.4 (7) 63.6 (7) 75.7 (6) -168 (1) -41 (1) 54.9 (6)
$\begin{array}{c} \text{O1}-\text{Fe1}-\text{P1}-\text{C201} \\ \text{O1}-\text{Fe1}-\text{P1}-\text{C203} \\ \text{O1}-\text{Fe1}-\text{P1}-\text{C204} \\ \text{O1}-\text{Fe1}-\text{P1}-\text{C301} \\ \text{O1}-\text{Fe1}-\text{P1}-\text{C303} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C108} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C111} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C112} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C308} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C311} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C312} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C312} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C312} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C102} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C102} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C105} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C106} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C202} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C106} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C106} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C106} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C106} \\ \text{O1}-\text{Fe1}-\text{P10}-\text{C1}-\text{C10}-\text{C10}-\text{C10}-\text{C10}-\text{C1}-C$	$\begin{array}{c} -177.9 \text{ (s)} \\ -63.2 \text{ (s)} \\ 55.7 \text{ (s)} \\ 105.1 \text{ (g)} \\ -15.7 \text{ (k)} \\ -138.8 \text{ (g)} \\ -91.7 \text{ (3)} \\ 26.2 \text{ (3)} \\ 150.5 \text{ (4)} \\ -176.6 \text{ (8)} \\ -50.4 \text{ (7)} \\ 63.6 \text{ (7)} \\ 75.7 \text{ (6)} \\ -168 \text{ (1)} \\ -41 \text{ (1)} \\ 54.9 \text{ (6)} \\ -50.4 \text{ (7)} \end{array}$
$\begin{array}{c} \text{O1}-\text{Fe1}-\text{P1}-\text{C201} \\ \text{O1}-\text{Fe1}-\text{P1}-\text{C203} \\ \text{O1}-\text{Fe1}-\text{P1}-\text{C204} \\ \text{O1}-\text{Fe1}-\text{P1}-\text{C301} \\ \text{O1}-\text{Fe1}-\text{P1}-\text{C303} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C108} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C112} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C112} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C308} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C311} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C312} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C312} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C102} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C105} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C106} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C202} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C205} \\ \end{array}$	$\begin{array}{c} -177.9 \text{ (s)} \\ -63.2 \text{ (s)} \\ 55.7 \text{ (s)} \\ 105.1 \text{ (g)} \\ -15.7 \text{ (s)} \\ -15.7 \text{ (s)} \\ -138.8 \text{ (g)} \\ -91.7 \text{ (s)} \\ 26.2 \text{ (s)} \\ 150.5 \text{ (4)} \\ -176.6 \text{ (s)} \\ -50.4 \text{ (7)} \\ 75.7 \text{ (6)} \\ -168 \text{ (1)} \\ -41 \text{ (1)} \\ 54.9 \text{ (6)} \\ -53 \text{ (1)} \end{array}$
$\begin{array}{l} \text{O1}-\text{Fe1}-\text{P1}-\text{C201} \\ \text{O1}-\text{Fe1}-\text{P1}-\text{C203} \\ \text{O1}-\text{Fe1}-\text{P1}-\text{C204} \\ \text{O1}-\text{Fe1}-\text{P1}-\text{C301} \\ \text{O1}-\text{Fe1}-\text{P1}-\text{C303} \\ \text{O1}-\text{Fe1}-\text{P1}-\text{C304} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C108} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C112} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C112} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C308} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C311} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C312} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C312} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C102} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C105} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C106} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C202} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C205} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C205} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C206} \\ \end{array}$	$\begin{array}{c} -177.9 \text{ (s)} \\ -63.2 \text{ (s)} \\ 55.7 \text{ (s)} \\ 105.1 \text{ (g)} \\ -15.7 \text{ (k)} \\ -138.8 \text{ (g)} \\ -91.7 \text{ (3)} \\ 26.2 \text{ (3)} \\ 150.5 \text{ (4)} \\ -176.6 \text{ (8)} \\ -50.4 \text{ (7)} \\ 63.6 \text{ (7)} \\ 75.7 \text{ (6)} \\ -168 \text{ (1)} \\ -41 \text{ (1)} \\ 54.9 \text{ (6)} \\ -53 \text{ (1)} \\ 178.5 \text{ (7)} \end{array}$
$\begin{array}{c} \text{O1}-\text{Fe1}-\text{P1}-\text{C201} \\ \text{O1}-\text{Fe1}-\text{P1}-\text{C203} \\ \text{O1}-\text{Fe1}-\text{P1}-\text{C204} \\ \text{O1}-\text{Fe1}-\text{P1}-\text{C301} \\ \text{O1}-\text{Fe1}-\text{P1}-\text{C303} \\ \text{O1}-\text{Fe1}-\text{P1}-\text{C304} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C108} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C111} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C112} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C308} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C312} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C312} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C102} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C102} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C105} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C205} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C205} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C206} \\ \end{array}$	$\begin{array}{c} -177.9~(5)\\ -63.2~(5)\\ 55.7~(5)\\ 105.1~(9)\\ -15.7~(8)\\ -138.8~(9)\\ -91.7~(3)\\ 26.2~(3)\\ 150.5~(4)\\ -176.6~(8)\\ -50.4~(7)\\ 63.6~(7)\\ 75.7~(6)\\ -168~(1)\\ -41~(1)\\ 54.9~(6)\\ -53~(1)\\ 178.5~(7)\\ (2)~(2)~(2)\\ -53~(2)~(2)\\ -53~(2)~(2)~(2)\\ -53~(2)~(2)~(2)\\ -53~(2)~(2)~(2)~(2)\\ -53~(2)~(2)~(2)~(2)~(2)\\ -53~(2)~(2)~(2)~(2)~(2)\\ -53~(2)~(2)~(2)~(2)~(2)\\ -53~(2)~(2)~(2)~(2)~(2)~(2)\\ -53~(2)~(2)~(2)~(2)~(2)~(2)~(2)~(2)\\ -53~(2)~(2)~(2)~(2)~(2)~(2)~(2)~(2)~(2)~(2)$
$\begin{array}{c} \text{O1}-\text{Fe1}-\text{P1}-\text{C201} \\ \text{O1}-\text{Fe1}-\text{P1}-\text{C203} \\ \text{O1}-\text{Fe1}-\text{P1}-\text{C301} \\ \text{O1}-\text{Fe1}-\text{P1}-\text{C303} \\ \text{O1}-\text{Fe1}-\text{P1}-\text{C304} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C108} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C112} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C112} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C308} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C311} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C312} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C312} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C102} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C105} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C106} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C202} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C202} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C206} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C206} \\ \text{O1}-\text{Fe1}-\text{P103}-\text{C107} \\ \end{array}$	$\begin{array}{c} -177.9~(5)\\ -63.2~(5)\\ 55.7~(5)\\ 105.1~(9)\\ -15.7~(8)\\ -138.8~(9)\\ -91.7~(3)\\ 26.2~(3)\\ 150.5~(4)\\ -176.6~(8)\\ -50.4~(7)\\ 75.7~(6)\\ -168~(1)\\ -41~(1)\\ 54.9~(6)\\ -53~(1)\\ 178.5~(7)\\ 104.3~(3)\\ \end{array}$
$\begin{array}{c} \text{O1}-\text{Fe1}-\text{P1}-\text{C201} \\ \text{O1}-\text{Fe1}-\text{P1}-\text{C203} \\ \text{O1}-\text{Fe1}-\text{P1}-\text{C301} \\ \text{O1}-\text{Fe1}-\text{P1}-\text{C303} \\ \text{O1}-\text{Fe1}-\text{P1}-\text{C304} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C108} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C111} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C112} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C308} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C312} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C312} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C102} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C102} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C105} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C106} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C202} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C205} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C206} \\ \text{O1}-\text{Fe1}-\text{P103}-\text{C107} \\ \text{O1}-\text{Fe1}-\text{P103}-\text{C109} \\ \end{array}$	$\begin{array}{c} -177.9 \text{ (s)} \\ -177.9 \text{ (s)} \\ -63.2 \text{ (s)} \\ 55.7 \text{ (s)} \\ 105.1 \text{ (g)} \\ -15.7 \text{ (g)} \\ -15.7 \text{ (g)} \\ -138.8 \text{ (g)} \\ -91.7 \text{ (g)} \\ 26.2 \text{ (g)} \\ 150.5 \text{ (4)} \\ -176.6 \text{ (g)} \\ -50.4 \text{ (f)} \\ 63.6 \text{ (f)} \\ 75.7 \text{ (f)} \\ -41 \text{ (1)} \\ 54.9 \text{ (f)} \\ -43 \text{ (g)} \\ -53 \text{ (1)} \\ 178.5 \text{ (f)} \\ 104.3 \text{ (g)} \\ -133 \text{ (g)} \text{ (4)} \end{array}$
$\begin{array}{c} \text{O1}-\text{Fe1}-\text{P1}-\text{C201} \\ \text{O1}-\text{Fe1}-\text{P1}-\text{C203} \\ \text{O1}-\text{Fe1}-\text{P1}-\text{C204} \\ \text{O1}-\text{Fe1}-\text{P1}-\text{C303} \\ \text{O1}-\text{Fe1}-\text{P1}-\text{C304} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C108} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C112} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C112} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C308} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C311} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C312} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C102} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C105} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C105} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C205} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C205} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C206} \\ \text{O1}-\text{Fe1}-\text{P103}-\text{C107} \\ \text{O1}-\text{Fe1}-\text{P103}-\text{C109} \\ \end{array}$	$\begin{array}{c} -177.9~(5)\\ -63.2~(5)\\ 55.7~(5)\\ 105.1~(9)\\ -15.7~(8)\\ -138.8~(9)\\ -91.7~(3)\\ 26.2~(3)\\ 150.5~(4)\\ -176.6~(8)\\ -50.4~(7)\\ 63.6~(7)\\ 75.7~(6)\\ -168~(1)\\ -41~(1)\\ 54.9~(6)\\ -53~(1)\\ 178.5~(7)\\ 104.3~(3)\\ -133.9~(4)\\ \end{array}$
$\begin{array}{c} \text{O1}-\text{Fe1}-\text{P1}-\text{C201} \\ \text{O1}-\text{Fe1}-\text{P1}-\text{C203} \\ \text{O1}-\text{Fe1}-\text{P1}-\text{C301} \\ \text{O1}-\text{Fe1}-\text{P1}-\text{C303} \\ \text{O1}-\text{Fe1}-\text{P1}-\text{C304} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C108} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C111} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C112} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C308} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C311} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C312} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C312} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C102} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C105} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C106} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C205} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C206} \\ \text{O1}-\text{Fe1}-\text{P103}-\text{C107} \\ \text{O1}-\text{Fe1}-\text{P103}-\text{C107} \\ \text{O1}-\text{Fe1}-\text{P103}-\text{C109} \\ \text{O1}-\text{Fe1}-\text{P103}-\text{C110} \end{array}$	$\begin{array}{c} -177.9 \text{ (s)} \\ -63.2 \text{ (s)} \\ 55.7 \text{ (s)} \\ 105.1 \text{ (g)} \\ -15.7 \text{ (k)} \\ 105.1 \text{ (g)} \\ -138.8 \text{ (g)} \\ -91.7 \text{ (a)} \\ 26.2 \text{ (a)} \\ 150.5 \text{ (4)} \\ -176.6 \text{ (k)} \\ -50.4 \text{ (7)} \\ 75.7 \text{ (6)} \\ -168 \text{ (1)} \\ -41 \text{ (1)} \\ 54.9 \text{ (6)} \\ -53 \text{ (1)} \\ 178.5 \text{ (7)} \\ 104.3 \text{ (a)} \\ -8.8 \text{ (6)} \end{array}$
$\begin{array}{c} \text{O1}-\text{Fe1}-\text{P1}-\text{C201} \\ \text{O1}-\text{Fe1}-\text{P1}-\text{C203} \\ \text{O1}-\text{Fe1}-\text{P1}-\text{C301} \\ \text{O1}-\text{Fe1}-\text{P1}-\text{C303} \\ \text{O1}-\text{Fe1}-\text{P1}-\text{C304} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C108} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C111} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C112} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C308} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C312} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C312} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C102} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C102} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C105} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C205} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C205} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C206} \\ \text{O1}-\text{Fe1}-\text{P103}-\text{C107} \\ \text{O1}-\text{Fe1}-\text{P103}-\text{C107} \\ \text{O1}-\text{Fe1}-\text{P103}-\text{C110} \\ \text{O1}-\text{Fe1}-\text{P103}-\text{C110} \\ \text{O1}-\text{Fe1}-\text{P103}-\text{C110} \\ \text{O1}-\text{Fe1}-\text{P103}-\text{C110} \\ \text{O1}-\text{Fe1}-\text{P103}-\text{C110} \\ \text{O1}-\text{Fe1}-\text{P103}-\text{C107} \\ \end{array}$	$\begin{array}{c} -177.9 \text{ (s)} \\ -63.2 \text{ (s)} \\ 55.7 \text{ (s)} \\ 105.1 \text{ (g)} \\ -15.7 \text{ (8)} \\ -138.8 \text{ (g)} \\ -91.7 \text{ (3)} \\ 26.2 \text{ (3)} \\ 150.5 \text{ (4)} \\ -176.6 \text{ (8)} \\ -50.4 \text{ (7)} \\ 63.6 \text{ (7)} \\ 75.7 \text{ (6)} \\ -168 \text{ (1)} \\ -53 \text{ (1)} \\ 178.5 \text{ (7)} \\ 104.3 \text{ (3)} \\ -133.9 \text{ (4)} \\ -8.8 \text{ (6)} \\ -109.3 \text{ (8)} \end{array}$
$\begin{array}{l} \text{O1}-\text{Fe1}-\text{P1}-\text{C201} \\ \text{O1}-\text{Fe1}-\text{P1}-\text{C203} \\ \text{O1}-\text{Fe1}-\text{P1}-\text{C204} \\ \text{O1}-\text{Fe1}-\text{P1}-\text{C301} \\ \text{O1}-\text{Fe1}-\text{P1}-\text{C303} \\ \text{O1}-\text{Fe1}-\text{P1}-\text{C304} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C108} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C112} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C112} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C313} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C312} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C312} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C102} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C105} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C106} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C202} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C205} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C205} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C206} \\ \text{O1}-\text{Fe1}-\text{P103}-\text{C107} \\ \text{O1}-\text{Fe1}-\text{P103}-\text{C109} \\ \text{O1}-\text{Fe1}-\text{P103}-\text{C109} \\ \text{O1}-\text{Fe1}-\text{P103}-\text{C110} \\ \text{O1}-\text{Fe1}-\text{P103}-\text{C110} \\ \text{O1}-\text{Fe1}-\text{P103}-\text{C302} \\ \text{O1}-\text{Fe1}-\text{P103}-\text{C302} \\ \text{O1}-\text{Fe1}-\text{P103}-\text{C302} \\ \text{O1}-\text{Fe1}-\text{P103}-\text{C109} \\ \text{O1}-\text{Fe1}-\text{P103}-\text{C106} \\ \text{O1}-\text{Fe1}-\text{P103}-\text{C107} \\ \text{O1}-\text{Fe1}-\text{P103}-\text{C107} \\ \text{O1}-\text{Fe1}-\text{P103}-\text{C108} \\ \text{O1}-$	$\begin{array}{c} -177.9 \text{ (s)} \\ -63.2 \text{ (s)} \\ 55.7 \text{ (s)} \\ 105.1 \text{ (g)} \\ -15.7 \text{ (g)} \\ -15.7 \text{ (g)} \\ -138.8 \text{ (g)} \\ -91.7 \text{ (3)} \\ 26.2 \text{ (3)} \\ 150.5 \text{ (4)} \\ -176.6 \text{ (g)} \\ -50.4 \text{ (7)} \\ 75.7 \text{ (6)} \\ -168 \text{ (1)} \\ -41 \text{ (1)} \\ 54.9 \text{ (6)} \\ -53 \text{ (1)} \\ 178.5 \text{ (7)} \\ 104.3 \text{ (3)} \\ -133.9 \text{ (4)} \\ -8.8 \text{ (6)} \\ -109.3 \text{ (g)} \\ -109.3 \text{ (g)} \\ -54.2 \text{ (g)} \\ -54.2 \text{ (g)} \\ -109.3 \text{ (g)} \\ -54.2 ($
$\begin{array}{c} \text{O1}-\text{Fe1}-\text{P1}-\text{C201} \\ \text{O1}-\text{Fe1}-\text{P1}-\text{C203} \\ \text{O1}-\text{Fe1}-\text{P1}-\text{C301} \\ \text{O1}-\text{Fe1}-\text{P1}-\text{C303} \\ \text{O1}-\text{Fe1}-\text{P1}-\text{C304} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C108} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C111} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C112} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C308} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C308} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C312} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C312} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C102} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C102} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C106} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C202} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C205} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C206} \\ \text{O1}-\text{Fe1}-\text{P103}-\text{C107} \\ \text{O1}-\text{Fe1}-\text{P103}-\text{C109} \\ \text{O1}-\text{Fe1}-\text{P103}-\text{C109} \\ \text{O1}-\text{Fe1}-\text{P103}-\text{C110} \\ \text{O1}-\text{Fe1}-\text{P302}-\text{C302} \\ \text{O1}-\text{Fe1}-\text{P302}-\text{C302} \\ \text{O1}-\text{Fe1}-\text{P302}-\text{C305} \\ \end{array}$	$\begin{array}{c} -177.9~(5)\\ -63.2~(5)\\ 55.7~(5)\\ 105.1~(9)\\ -15.7~(8)\\ -138.8~(9)\\ -91.7~(3)\\ 26.2~(3)\\ 150.5~(4)\\ -176.6~(8)\\ -50.4~(7)\\ 63.6~(7)\\ 75.7~(6)\\ -168~(1)\\ -41~(1)\\ 54.9~(6)\\ -53~(1)\\ 178.5~(7)\\ 104.3~(3)\\ -133.9~(4)\\ -8.8~(6)\\ -109.3~(8)\\ 7~(1) \end{array}$
$\begin{array}{c} \text{O1}-\text{Fe1}-\text{P1}-\text{C201} \\ \text{O1}-\text{Fe1}-\text{P1}-\text{C203} \\ \text{O1}-\text{Fe1}-\text{P1}-\text{C303} \\ \text{O1}-\text{Fe1}-\text{P1}-\text{C303} \\ \text{O1}-\text{Fe1}-\text{P1}-\text{C304} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C108} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C112} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C112} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C308} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C311} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C312} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C102} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C105} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C105} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C205} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C206} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C206} \\ \text{O1}-\text{Fe1}-\text{P103}-\text{C107} \\ \text{O1}-\text{Fe1}-\text{P103}-\text{C107} \\ \text{O1}-\text{Fe1}-\text{P103}-\text{C109} \\ \text{O1}-\text{Fe1}-\text{P103}-\text{C109} \\ \text{O1}-\text{Fe1}-\text{P302}-\text{C302} \\ \text{O1}-\text{Fe1}-\text{P302}-\text{C305} \\ \text{O1}-\text{Fe1}-\text{P302}-\text{C305} \\ \text{O1}-\text{Fe1}-\text{P302}-\text{C306} \\ \end{array}$	$\begin{array}{c} -177.9~(5)\\ -63.2~(5)\\ 55.7~(5)\\ 105.1~(9)\\ -15.7~(8)\\ -138.8~(9)\\ -91.7~(3)\\ 26.2~(3)\\ 150.5~(4)\\ -176.6~(8)\\ -50.4~(7)\\ 63.6~(7)\\ 75.7~(6)\\ -168~(1)\\ -41~(1)\\ 54.9~(6)\\ -53~(1)\\ 178.5~(7)\\ 104.3~(3)\\ -133.9~(4)\\ -8.8~(6)\\ -109.3~(8)\\ 7~(1)\\ 129~(1)\\ \end{array}$
$\begin{array}{c} \text{O1}-\text{Fe1}-\text{P1}-\text{C201} \\ \text{O1}-\text{Fe1}-\text{P1}-\text{C203} \\ \text{O1}-\text{Fe1}-\text{P1}-\text{C301} \\ \text{O1}-\text{Fe1}-\text{P1}-\text{C303} \\ \text{O1}-\text{Fe1}-\text{P1}-\text{C304} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C108} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C111} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C112} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C308} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C311} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C312} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C312} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C102} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C105} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C106} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C202} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C205} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C206} \\ \text{O1}-\text{Fe1}-\text{P103}-\text{C107} \\ \text{O1}-\text{Fe1}-\text{P103}-\text{C107} \\ \text{O1}-\text{Fe1}-\text{P103}-\text{C109} \\ \text{O1}-\text{Fe1}-\text{P103}-\text{C110} \\ \text{O1}-\text{Fe1}-\text{P302}-\text{C302} \\ \text{O1}-\text{Fe1}-\text{P302}-\text{C305} \\ \text{O1}-\text{Fe1}-\text{P302}-\text{C306} \\ \text{O1}-\text{Fe1}-\text{P103}-\text{C170} \\ \text{O1}-\text{Fe1}-\text{P103}-\text{C106} \\ \text{O1}-\text{Fe1}-\text{P103}-\text{C305} \\ \text{O1}-\text{Fe1}-\text{P103}-\text{C305} \\ \text{O1}-\text{Fe1}-\text{P103}-\text{C306} \\ \text{O1}-\text{Fe1}-\text{C306} \\ \text{O1}-\text{Fe1}-\text{C306} \\ \text{O1}-\text{C306} \\ O1$	$\begin{array}{c} -177.9~(5)\\ -63.2~(5)\\ 55.7~(5)\\ 105.1~(9)\\ -138.8~(9)\\ -91.7~(3)\\ 26.2~(3)\\ 150.5~(4)\\ -176.6~(8)\\ -50.4~(7)\\ 63.6~(7)\\ 75.7~(6)\\ -168~(1)\\ -41~(1)\\ 54.9~(6)\\ -53~(1)\\ 178.5~(7)\\ 104.3~(3)\\ -133.9~(4)\\ -8.8~(6)\\ -109.3~(8)\\ 7~(1)\\ 129~(1)\\ 129~(1)\\ 129~(1)\\ 129~(1)\\ 129~(1)\\ 129~(1)\\ 129~(1)\\ 129~(1)\\ 129~(1)\\ 129~(1)\\ 129~(1)\\ 129~(1)\\ 120~(1)$
$\begin{array}{l} {\rm O1-Fe1-P1-C201} \\ {\rm O1-Fe1-P1-C203} \\ {\rm O1-Fe1-P1-C301} \\ {\rm O1-Fe1-P1-C303} \\ {\rm O1-Fe1-P1-C304} \\ {\rm O1-Fe1-P4-C108} \\ {\rm O1-Fe1-P4-C112} \\ {\rm O1-Fe1-P4-C112} \\ {\rm O1-Fe1-P4-C312} \\ {\rm O1-Fe1-P4-C312} \\ {\rm O1-Fe1-P4-C312} \\ {\rm O1-Fe1-P102-C102} \\ {\rm O1-Fe1-P102-C102} \\ {\rm O1-Fe1-P102-C105} \\ {\rm O1-Fe1-P102-C202} \\ {\rm O1-Fe1-P102-C205} \\ {\rm O1-Fe1-P102-C206} \\ {\rm O1-Fe1-P103-C109} \\ {\rm O1-Fe1-P103-C109} \\ {\rm O1-Fe1-P103-C109} \\ {\rm O1-Fe1-P302-C305} \\ {\rm O1-Fe1-P302-C305} \\ {\rm O1-Fe1-P302-C306} \\ {\rm O1-Fe1-P303-C307} \\ \end{array}$	$\begin{array}{c} -177.9~(5)\\ -63.2~(5)\\ 55.7~(5)\\ 105.1~(9)\\ -15.7~(8)\\ -138.8~(9)\\ -91.7~(3)\\ 26.2~(3)\\ 150.5~(4)\\ -176.6~(8)\\ -50.4~(7)\\ 63.6~(7)\\ 63.6~(7)\\ 75.7~(6)\\ -168~(1)\\ -41~(1)\\ 54.9~(6)\\ -53~(1)\\ 178.5~(7)\\ 104.3~(3)\\ -139.9~(4)\\ -8.8~(6)\\ -109.3~(8)\\ 7~(1)\\ 129~(1)\\ -59.5~(7)\end{array}$
$\begin{array}{l} \text{O1}-\text{Fe1}-\text{P1}-\text{C201} \\ \text{O1}-\text{Fe1}-\text{P1}-\text{C203} \\ \text{O1}-\text{Fe1}-\text{P1}-\text{C204} \\ \text{O1}-\text{Fe1}-\text{P1}-\text{C301} \\ \text{O1}-\text{Fe1}-\text{P1}-\text{C303} \\ \text{O1}-\text{Fe1}-\text{P1}-\text{C304} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C108} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C112} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C112} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C311} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C312} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C312} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C312} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C102} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C105} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C202} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C205} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C205} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C206} \\ \text{O1}-\text{Fe1}-\text{P103}-\text{C107} \\ \text{O1}-\text{Fe1}-\text{P103}-\text{C109} \\ \text{O1}-\text{Fe1}-\text{P303}-\text{C302} \\ \text{O1}-\text{Fe1}-\text{P303}-\text{C306} \\ \text{O1}-\text{Fe1}-\text{P303}-\text{C307} \\ \text{O1}-\text{Fe1}-\text{P303}-\text{C309} \\ \end{array}$	$\begin{array}{c} -177.9~(5)\\ -63.2~(5)\\ 55.7~(5)\\ 105.1~(9)\\ -15.7~(8)\\ -138.8~(9)\\ -91.7~(3)\\ 26.2~(3)\\ 150.5~(4)\\ -176.6~(8)\\ -50.4~(7)\\ 63.6~(7)\\ 75.7~(6)\\ -168~(1)\\ -41~(1)\\ 54.9~(6)\\ -53~(1)\\ 178.5~(7)\\ 104.3~(3)\\ -133.9~(4)\\ -8.8~(6)\\ -109.3~(8)\\ 7~(1)\\ 129~(1)\\ -59.5~(7)\\ 175.3~(9)\\ \end{array}$
$\begin{array}{c} \text{O1}-\text{Fe1}-\text{P1}-\text{C201} \\ \text{O1}-\text{Fe1}-\text{P1}-\text{C203} \\ \text{O1}-\text{Fe1}-\text{P1}-\text{C301} \\ \text{O1}-\text{Fe1}-\text{P1}-\text{C303} \\ \text{O1}-\text{Fe1}-\text{P1}-\text{C304} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C108} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C111} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C112} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C308} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C308} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C312} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C312} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C102} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C105} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C106} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C202} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C206} \\ \text{O1}-\text{Fe1}-\text{P103}-\text{C107} \\ \text{O1}-\text{Fe1}-\text{P103}-\text{C109} \\ \text{O1}-\text{Fe1}-\text{P103}-\text{C109} \\ \text{O1}-\text{Fe1}-\text{P302}-\text{C305} \\ \text{O1}-\text{Fe1}-\text{P302}-\text{C305} \\ \text{O1}-\text{Fe1}-\text{P303}-\text{C307} \\ \text{O1}-\text{Fe1}-\text{P303}-\text{C307} \\ \text{O1}-\text{Fe1}-\text{P303}-\text{C309} \\ \text{O1}-\text{Fe1}-\text{C100}-\text{C100} \\ \text{O1}-\text{C100}-\text{C100}-\text{C100} \\ \text{O1}-\text{C100}-C10$	$\begin{array}{c} -177.9 \text{ (s)} \\ -63.2 \text{ (s)} \\ 55.7 \text{ (s)} \\ 105.1 \text{ (g)} \\ -15.7 \text{ (g)} \\ -15.7 \text{ (g)} \\ -15.7 \text{ (g)} \\ -138.8 \text{ (g)} \\ -91.7 \text{ (g)} \\ 26.2 \text{ (g)} \\ 150.5 \text{ (4)} \\ -176.6 \text{ (g)} \\ -50.4 \text{ (f)} \\ 63.6 \text{ (f)} \\ 75.7 \text{ (g)} \\ -53 \text{ (1)} \\ 178.5 \text{ (f)} \\ 104.3 \text{ (g)} \\ -8.8 \text{ (g)} \\ -109.3 \text{ (g)} \\ 7 \text{ (1)} \\ 129 \text{ (1)} \\ -59.5 \text{ (f)} \\ 129.5 \text{ (f)} \\ 129.5 \text{ (g)} \\ -53.4 \text{ (g)} \\ -59.5 \text{ (f)} \\ -53.4 \text{ (g)} \\ -59.5 \text{ (f)} \\ 129.5 \text{ (g)} \\ -59.5 \text{ (f)} \\ $
$\begin{array}{l} {\rm O1-Fe1-P1-C201} \\ {\rm O1-Fe1-P1-C203} \\ {\rm O1-Fe1-P1-C303} \\ {\rm O1-Fe1-P1-C303} \\ {\rm O1-Fe1-P1-C304} \\ {\rm O1-Fe1-P4-C108} \\ {\rm O1-Fe1-P4-C112} \\ {\rm O1-Fe1-P4-C112} \\ {\rm O1-Fe1-P4-C311} \\ {\rm O1-Fe1-P4-C312} \\ {\rm O1-Fe1-P4-C312} \\ {\rm O1-Fe1-P4-C312} \\ {\rm O1-Fe1-P102-C102} \\ {\rm O1-Fe1-P102-C105} \\ {\rm O1-Fe1-P102-C105} \\ {\rm O1-Fe1-P102-C205} \\ {\rm O1-Fe1-P102-C205} \\ {\rm O1-Fe1-P102-C205} \\ {\rm O1-Fe1-P102-C206} \\ {\rm O1-Fe1-P102-C206} \\ {\rm O1-Fe1-P103-C107} \\ {\rm O1-Fe1-P103-C107} \\ {\rm O1-Fe1-P103-C109} \\ {\rm O1-Fe1-P302-C302} \\ {\rm O1-Fe1-P302-C305} \\ {\rm O1-Fe1-P302-C305} \\ {\rm O1-Fe1-P303-C307} \\ {\rm O1-Fe1-P303-C309} \\ {\rm O1-Fe1-P303-C310} \\ \end{array}$	$\begin{array}{c} -177.9~(5)\\ -63.2~(5)\\ 55.7~(5)\\ 105.1~(9)\\ -15.7~(8)\\ -138.8~(9)\\ -91.7~(3)\\ 26.2~(3)\\ 150.5~(4)\\ -176.6~(8)\\ -50.4~(7)\\ 75.7~(6)\\ -168~(1)\\ -41~(1)\\ 54.9~(6)\\ -53~(1)\\ 178.5~(7)\\ 104.3~(3)\\ -133.9~(4)\\ -8.8~(6)\\ -109.3~(8)\\ 7~(1)\\ 129~(1)\\ -59.5~(7)\\ 175.3~(9)\\ 56~(1)\\ \end{array}$
$\begin{array}{c} \text{O1}-\text{Fe1}-\text{P1}-\text{C201} \\ \text{O1}-\text{Fe1}-\text{P1}-\text{C203} \\ \text{O1}-\text{Fe1}-\text{P1}-\text{C303} \\ \text{O1}-\text{Fe1}-\text{P1}-\text{C303} \\ \text{O1}-\text{Fe1}-\text{P1}-\text{C304} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C108} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C111} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C112} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C308} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C311} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C312} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C312} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C102} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C105} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C106} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C202} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C206} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C206} \\ \text{O1}-\text{Fe1}-\text{P103}-\text{C107} \\ \text{O1}-\text{Fe1}-\text{P103}-\text{C107} \\ \text{O1}-\text{Fe1}-\text{P103}-\text{C109} \\ \text{O1}-\text{Fe1}-\text{P302}-\text{C302} \\ \text{O1}-\text{Fe1}-\text{P303}-\text{C307} \\ \text{O1}-\text{Fe1}-\text{P303}-\text{C307} \\ \text{O1}-\text{Fe1}-\text{P303}-\text{C310} \\ \text{O1}-\text{Fe1}-\text{C20}-\text{C50} \\ \end{array} \\$	$\begin{array}{c} -177.9~(5)\\ -63.2~(5)\\ 55.7~(5)\\ 105.1~(9)\\ -15.7~(8)\\ -138.8~(9)\\ -91.7~(3)\\ 26.2~(3)\\ 150.5~(4)\\ -176.6~(8)\\ -50.4~(7)\\ 63.6~(7)\\ 75.7~(6)\\ -168~(1)\\ -41~(1)\\ 54.9~(6)\\ -53~(1)\\ 178.5~(7)\\ 104.3~(3)\\ -133.9~(4)\\ -8.8~(6)\\ -109.3~(8)\\ 7~(1)\\ 129~(1)\\ -59.5~(7)\\ 175.3~(9)\\ 56~(1)\\ 0.7~(2)\\ \end{array}$
$\begin{array}{c} \text{O1}-\text{Fe1}-\text{P1}-\text{C201} \\ \text{O1}-\text{Fe1}-\text{P1}-\text{C203} \\ \text{O1}-\text{Fe1}-\text{P1}-\text{C204} \\ \text{O1}-\text{Fe1}-\text{P1}-\text{C303} \\ \text{O1}-\text{Fe1}-\text{P1}-\text{C304} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C108} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C111} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C112} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C308} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C308} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C312} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C102} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C102} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C105} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C205} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C206} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C206} \\ \text{O1}-\text{Fe1}-\text{P103}-\text{C109} \\ \text{O1}-\text{Fe1}-\text{P103}-\text{C109} \\ \text{O1}-\text{Fe1}-\text{P103}-\text{C109} \\ \text{O1}-\text{Fe1}-\text{P302}-\text{C306} \\ \text{O1}-\text{Fe1}-\text{P303}-\text{C307} \\ \text{O1}-\text{Fe1}-\text{P303}-\text{C307} \\ \text{O1}-\text{Fe1}-\text{P303}-\text{C309} \\ \text{O1}-\text{Fe1}-\text{P303}-\text{C310} \\ \text{O1}-\text{Fe1}-\text{P303}-\text{C310} \\ \text{O1}-\text{Fe1}-\text{O2}-\text{C50} \\ \text{O2}-\text{Fe1}-\text{P1}-\text{O2}-\text{C50} \\ \end{array}$	$\begin{array}{c} -177.9~(5)\\ -63.2~(5)\\ 55.7~(5)\\ 105.1~(9)\\ -15.7~(8)\\ -138.8~(9)\\ -91.7~(3)\\ 26.2~(3)\\ 150.5~(4)\\ -176.6~(8)\\ -50.4~(7)\\ 63.6~(7)\\ 75.7~(6)\\ -168~(1)\\ -41~(1)\\ 54.9~(6)\\ -53~(1)\\ 178.5~(7)\\ 104.3~(3)\\ -139.9~(4)\\ -8.8~(6)\\ -109.3~(8)\\ 7~(1)\\ 129~(1)\\ -59.5~(7)\\ 175.3~(9)\\ 56~(1)\\ 0.7~(2)\\ 9.8~7~(6)\\ -8.8~(7)\\ 10.5~(7)\\ 129.5~(7)\\ 175.3~(9)\\ 56~(1)\\ 0.7~(2)\\ 9.8~7~(6)\\ -8.8~(7)\\ 10.5~(7)\\ 175.3~(9)\\ 56~(1)\\ 0.7~(2)\\ -8.8~(7)\\ 10.5~(7)\\$
$\begin{array}{c} \text{O1}-\text{Fe1}-\text{P1}-\text{C201} \\ \text{O1}-\text{Fe1}-\text{P1}-\text{C203} \\ \text{O1}-\text{Fe1}-\text{P1}-\text{C204} \\ \text{O1}-\text{Fe1}-\text{P1}-\text{C303} \\ \text{O1}-\text{Fe1}-\text{P1}-\text{C303} \\ \text{O1}-\text{Fe1}-\text{P1}-\text{C304} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C108} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C111} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C112} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C312} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C312} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C312} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C102} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C105} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C106} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C202} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C205} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C206} \\ \text{O1}-\text{Fe1}-\text{P103}-\text{C107} \\ \text{O1}-\text{Fe1}-\text{P103}-\text{C109} \\ \text{O1}-\text{Fe1}-\text{P303}-\text{C305} \\ \text{O1}-\text{Fe1}-\text{P303}-\text{C305} \\ \text{O1}-\text{Fe1}-\text{P303}-\text{C306} \\ \text{O1}-\text{Fe1}-\text{P303}-\text{C307} \\ \text{O1}-\text{Fe1}-\text{P303}-\text{C310} \\ \text{O1}-\text{Fe1}-\text{P103}-\text{C110} \\ \text{O1}-\text{Fe1}-\text{P103}-\text{C110} \\ \text{O1}-\text{Fe1}-\text{P303}-\text{C310} \\ \text{O1}-\text{Fe1}-\text{P303}-\text{C310} \\ \text{O1}-\text{Fe1}-\text{P303}-\text{C310} \\ \text{O1}-\text{Fe1}-\text{P103}-\text{C110} \\ \text{O1}-\text{Fe1}-\text{P103}-\text{C110} \\ \text{O1}-\text{Fe1}-\text{P103}-\text{C110} \\ \text{O1}-\text{Fe1}-\text{P103}-\text{C110} \\ \text{O1}-\text{Fe1}-\text{P103}-\text{C110} \\ \text{O1}-\text{Fe1}-\text{P103}-\text{C101} \\ \text{O1}-\text{Fe1}-\text{P103}-\text{C101} \\ \text{O1}-\text{Fe1}-\text{P103}-\text{C101} \\ \text{O1}-\text{Fe1}-\text{P103}-\text{C101} \\ \text{O1}-\text{Fe1}-\text{P103}-\text{C101} \\ \text{O1}-\text{Fe1}-\text{O2}-\text{C50} \\ \text{O2}-\text{Fe1}-\text{P1}-\text{C101} \\ \text{O1}-\text{Fe1}-\text{O2}-\text{C50} \\ \text{O2}-\text{Fe1}-\text{P1}-\text{C101} \\ \text{O1}-$	$\begin{array}{c} -177.9~(5)\\ -63.2~(5)\\ 55.7~(5)\\ 105.1~(9)\\ -15.7~(8)\\ -138.8~(9)\\ -91.7~(3)\\ 26.2~(3)\\ 150.5~(4)\\ -176.6~(8)\\ -50.4~(7)\\ 63.6~(7)\\ 75.7~(6)\\ -168~(1)\\ -41~(1)\\ 54.9~(6)\\ -53.~(1)\\ 178.5~(7)\\ 104.3~(3)\\ -133.9~(4)\\ -8.8~(6)\\ -109.3~(8)\\ 7~(1)\\ 129~(1)\\ -59.5~(7)\\ 175.3~(9)\\ 56~(1)\\ 0.7~(2)\\ -88.7~(6)\\ \end{array}$
$\begin{array}{c} \text{O1}-\text{Fe1}-\text{P1}-\text{C201} \\ \text{O1}-\text{Fe1}-\text{P1}-\text{C203} \\ \text{O1}-\text{Fe1}-\text{P1}-\text{C301} \\ \text{O1}-\text{Fe1}-\text{P1}-\text{C303} \\ \text{O1}-\text{Fe1}-\text{P1}-\text{C304} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C108} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C111} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C112} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C308} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C308} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C312} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C312} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C102} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C102} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C106} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C202} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C206} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C206} \\ \text{O1}-\text{Fe1}-\text{P103}-\text{C107} \\ \text{O1}-\text{Fe1}-\text{P103}-\text{C109} \\ \text{O1}-\text{Fe1}-\text{P103}-\text{C109} \\ \text{O1}-\text{Fe1}-\text{P302}-\text{C302} \\ \text{O1}-\text{Fe1}-\text{P303}-\text{C307} \\ \text{O1}-\text{Fe1}-\text{P303}-\text{C307} \\ \text{O1}-\text{Fe1}-\text{P303}-\text{C307} \\ \text{O1}-\text{Fe1}-\text{P303}-\text{C310} \\ \text{O1}-\text{Fe1}-\text{P103}-\text{C110} \\ \text{O2}-\text{Fe1}-\text{P1}-\text{C101} \\ \text{O2}-\text{Fe1}-\text{P1}-\text{C103} \\ \end{array}$	$\begin{array}{c} -177.9~(5)\\ -63.2~(5)\\ 55.7~(5)\\ 105.1~(9)\\ -15.7~(8)\\ -138.8~(9)\\ -91.7~(3)\\ 26.2~(3)\\ 150.5~(4)\\ -176.6~(8)\\ -50.4~(7)\\ 63.6~(7)\\ 75.7~(6)\\ -168~(1)\\ -41~(1)\\ 54.9~(6)\\ -53~(1)\\ 178.5~(7)\\ 104.3~(3)\\ -133.9~(4)\\ -8.8~(6)\\ -109.3~(8)\\ 7~(1)\\ 129~(1)\\ -59.5~(7)\\ 175.3~(9)\\ 56~(1)\\ 0.7~(2)\\ -88.7~(6)\\ 31.7~(8)\\ \end{array}$
$\begin{array}{l} \text{Ol}-\text{Fel}-\text{Pl}-\text{C201} \\ \text{Ol}-\text{Fel}-\text{Pl}-\text{C203} \\ \text{Ol}-\text{Fel}-\text{Pl}-\text{C204} \\ \text{Ol}-\text{Fel}-\text{Pl}-\text{C303} \\ \text{Ol}-\text{Fel}-\text{Pl}-\text{C303} \\ \text{Ol}-\text{Fel}-\text{Pl}-\text{C304} \\ \text{Ol}-\text{Fel}-\text{Pl}-\text{C108} \\ \text{Ol}-\text{Fel}-\text{P4}-\text{C112} \\ \text{Ol}-\text{Fel}-\text{P4}-\text{C112} \\ \text{Ol}-\text{Fel}-\text{P4}-\text{C308} \\ \text{Ol}-\text{Fel}-\text{P4}-\text{C312} \\ \text{Ol}-\text{Fel}-\text{P4}-\text{C312} \\ \text{Ol}-\text{Fel}-\text{P4}-\text{C312} \\ \text{Ol}-\text{Fel}-\text{P102}-\text{C102} \\ \text{Ol}-\text{Fel}-\text{P102}-\text{C105} \\ \text{Ol}-\text{Fel}-\text{P102}-\text{C106} \\ \text{Ol}-\text{Fel}-\text{P102}-\text{C205} \\ \text{Ol}-\text{Fel}-\text{P102}-\text{C205} \\ \text{Ol}-\text{Fel}-\text{P102}-\text{C206} \\ \text{Ol}-\text{Fel}-\text{P103}-\text{C107} \\ \text{Ol}-\text{Fel}-\text{P103}-\text{C107} \\ \text{Ol}-\text{Fel}-\text{P303}-\text{C302} \\ \text{Ol}-\text{Fel}-\text{P303}-\text{C306} \\ \text{Ol}-\text{Fel}-\text{P303}-\text{C306} \\ \text{Ol}-\text{Fel}-\text{P303}-\text{C306} \\ \text{Ol}-\text{Fel}-\text{P303}-\text{C307} \\ \text{Ol}-\text{Fel}-\text{P303}-\text{C310} \\ \text{Ol}-\text{Fel}-\text{P303}-\text{C310} \\ \text{Ol}-\text{Fel}-\text{P103}-\text{C110} \\ \text{Ol}-\text{Fel}-\text{P303}-\text{C310} \\ \text{Ol}-\text{Fel}-\text{P103}-\text{C104} \\ \text{Ol}-\text{Fel}-\text{P103}-\text{C104} \\ \text{Ol}-\text{Fel}-\text{P103}-\text{C104} \\ \text{Ol}-\text{Fel}-\text{P103}-\text{C100} \\ \text{Ol}-\text{Fel}-\text{P103}-\text{C306} \\ \text{Ol}-\text{Fel}-\text{P103}-\text{C306} \\ \text{Ol}-\text{Fel}-\text{P103}-\text{C307} \\ \text{Ol}-\text{Fel}-\text{P103}-\text{C306} \\ \text{Ol}-\text{Fel}-\text{P103}-\text{C306} \\ \text{Ol}-\text{Fel}-\text{P103}-\text{C307} \\ \text{Ol}-\text{Fel}-\text{P103}-\text{C306} \\ \text{Ol}-\text{Fel}-\text{P103}-\text{C306} \\ \text{Ol}-\text{Fel}-\text{P103}-\text{C307} \\ \text{Ol}-\text{Fel}-\text{P103}-\text{C307} \\ \text{Ol}-\text{Fel}-\text{P103}-\text{C306} \\ \text{Ol}-\text{Fel}-\text{P103}-\text{C306} \\ \text{Ol}-\text{Fel}-\text{P103}-\text{C306} \\ \text{Ol}-\text{Fel}-\text{P103}-\text{C306} \\ \text{Ol}-\text{Fel}-\text{P103}-\text{C306} \\ \text{Ol}-\text{Fel}-\text{P103}-\text{C306} \\ \text{Ol}-\text{Fel}-\text{P103}-\text{C101} \\ \text{Ol}-\text{Fel}-\text{P103}-\text{C101} \\ \text{Ol}-\text{Fel}-\text{P103}-\text{C104} \\ \end{array} \end{array}$	$\begin{array}{c} -177.9\ (s)\\ -177.9\ (s)\\ -63.2\ (s)\\ 55.7\ (s)\\ 105.1\ (9)\\ -15.7\ (8)\\ -138.8\ (9)\\ -91.7\ (3)\\ 26.2\ (3)\\ 150.5\ (4)\\ -176.6\ (8)\\ -50.4\ (7)\\ 75.7\ (6)\\ -168\ (1)\\ -41\ (1)\\ 54.9\ (6)\\ -53\ (1)\\ 178.5\ (7)\\ 104.3\ (3)\\ -133.9\ (4)\\ -8.8\ (6)\\ -109.3\ (8)\\ 7\ (1)\\ 129\ (1)\\ -59.5\ (7)\\ 175.3\ (9)\\ 56\ (1)\\ 0.7\ (2)\\ -88.7\ (6)\\ 31.7\ (8)\\ 155\ (2\ (6))\\ \end{array}$
$\begin{array}{l} {\rm O1-Fe1-P1-C201} \\ {\rm O1-Fe1-P1-C203} \\ {\rm O1-Fe1-P1-C303} \\ {\rm O1-Fe1-P1-C303} \\ {\rm O1-Fe1-P1-C304} \\ {\rm O1-Fe1-P4-C108} \\ {\rm O1-Fe1-P4-C112} \\ {\rm O1-Fe1-P4-C112} \\ {\rm O1-Fe1-P4-C311} \\ {\rm O1-Fe1-P4-C312} \\ {\rm O1-Fe1-P4-C312} \\ {\rm O1-Fe1-P4-C312} \\ {\rm O1-Fe1-P4-C312} \\ {\rm O1-Fe1-P102-C102} \\ {\rm O1-Fe1-P102-C105} \\ {\rm O1-Fe1-P102-C106} \\ {\rm O1-Fe1-P102-C202} \\ {\rm O1-Fe1-P102-C205} \\ {\rm O1-Fe1-P102-C206} \\ {\rm O1-Fe1-P103-C107} \\ {\rm O1-Fe1-P103-C107} \\ {\rm O1-Fe1-P103-C109} \\ {\rm O1-Fe1-P302-C302} \\ {\rm O1-Fe1-P302-C305} \\ {\rm O1-Fe1-P303-C307} \\ {\rm O1-Fe1-P303-C309} \\ {\rm O1-Fe1-P303-C309} \\ {\rm O1-Fe1-P303-C310} \\ {\rm O1-Fe1-P303-C310} \\ {\rm O2-Fe1-P1-C101} \\ {\rm O2-Fe1-P1-C104} \\ \end{array}$	$\begin{array}{c} -177.9~(s)\\ -63.2~(s)\\ 55.7~(s)\\ 105.1~(9)\\ -15.7~(8)\\ -138.8~(9)\\ -91.7~(3)\\ 26.2~(3)\\ 150.5~(4)\\ -176.6~(8)\\ -50.4~(7)\\ 75.7~(6)\\ -168~(1)\\ -41~(1)\\ 54.9~(6)\\ -53~(1)\\ 178.5~(7)\\ 104.3~(3)\\ -133.9~(4)\\ -8.8~(6)\\ -109.3~(8)\\ 7~(1)\\ 129~(1)\\ -59.5~(7)\\ 175.3~(9)\\ 56~(1)\\ 0.7~(2)\\ -88.7~(6)\\ 31.7~(8)\\ 155.2~(6)\\ \end{array}$
$\begin{array}{l} {\rm O1-Fe1-P1-C201} \\ {\rm O1-Fe1-P1-C203} \\ {\rm O1-Fe1-P1-C301} \\ {\rm O1-Fe1-P1-C303} \\ {\rm O1-Fe1-P1-C304} \\ {\rm O1-Fe1-P4-C108} \\ {\rm O1-Fe1-P4-C112} \\ {\rm O1-Fe1-P4-C112} \\ {\rm O1-Fe1-P4-C312} \\ {\rm O1-Fe1-P4-C312} \\ {\rm O1-Fe1-P4-C312} \\ {\rm O1-Fe1-P4-C312} \\ {\rm O1-Fe1-P102-C102} \\ {\rm O1-Fe1-P102-C102} \\ {\rm O1-Fe1-P102-C105} \\ {\rm O1-Fe1-P102-C205} \\ {\rm O1-Fe1-P102-C205} \\ {\rm O1-Fe1-P102-C206} \\ {\rm O1-Fe1-P102-C206} \\ {\rm O1-Fe1-P103-C109} \\ {\rm O1-Fe1-P103-C109} \\ {\rm O1-Fe1-P103-C109} \\ {\rm O1-Fe1-P302-C305} \\ {\rm O1-Fe1-P302-C305} \\ {\rm O1-Fe1-P302-C306} \\ {\rm O1-Fe1-P303-C307} \\ {\rm O1-Fe1-P303-C309} \\ {\rm O1-Fe1-P303-C310} \\ {\rm O1-Fe1-P303-C310} \\ {\rm O1-Fe1-P1-C101} \\ {\rm O2-Fe1-P1-C104} \\ {\rm O2-Fe1-P1-C104} \\ {\rm O2-Fe1-P1-C201} \\ \end{array}$	$\begin{array}{c} -177.9~(5)\\ -177.9~(5)\\ -63.2~(5)\\ 55.7~(5)\\ 105.1~(9)\\ -15.7~(8)\\ -138.8~(9)\\ -91.7~(3)\\ 26.2~(3)\\ 150.5~(4)\\ -176.6~(8)\\ -50.4~(7)\\ -63.6~(7)\\ 75.7~(6)\\ -168~(1)\\ -41~(1)\\ 54.9~(6)\\ -53~(1)\\ 178.5~(7)\\ 104.3~(3)\\ -133.9~(4)\\ -8.8~(6)\\ -109.3~(8)\\ 7~(1)\\ 129~(1)\\ -59.5~(7)\\ 175.3~(9)\\ 56~(1)\\ 0.7~(2)\\ -88.7~(6)\\ 31.7~(8)\\ 155.2~(6)\\ -113.4~(5)\\ \end{array}$
$\begin{array}{l} \text{O1}-\text{Fe1}-\text{P1}-\text{C201} \\ \text{O1}-\text{Fe1}-\text{P1}-\text{C203} \\ \text{O1}-\text{Fe1}-\text{P1}-\text{C303} \\ \text{O1}-\text{Fe1}-\text{P1}-\text{C303} \\ \text{O1}-\text{Fe1}-\text{P1}-\text{C304} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C108} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C111} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C112} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C308} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C311} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C312} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C312} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C102} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C102} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C105} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C202} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C206} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C206} \\ \text{O1}-\text{Fe1}-\text{P103}-\text{C107} \\ \text{O1}-\text{Fe1}-\text{P103}-\text{C107} \\ \text{O1}-\text{Fe1}-\text{P103}-\text{C107} \\ \text{O1}-\text{Fe1}-\text{P302}-\text{C305} \\ \text{O1}-\text{Fe1}-\text{P303}-\text{C307} \\ \text{O1}-\text{Fe1}-\text{P303}-\text{C307} \\ \text{O1}-\text{Fe1}-\text{P303}-\text{C307} \\ \text{O1}-\text{Fe1}-\text{P303}-\text{C307} \\ \text{O1}-\text{Fe1}-\text{P303}-\text{C310} \\ \text{O1}-\text{Fe1}-\text{P303}-\text{C310} \\ \text{O1}-\text{Fe1}-\text{P303}-\text{C310} \\ \text{O1}-\text{Fe1}-\text{P103}-\text{C110} \\ \text{O2}-\text{Fe1}-\text{P1}-\text{C101} \\ \text{O2}-\text{Fe1}-\text{P1}-\text{C101} \\ \text{O2}-\text{Fe1}-\text{P1}-\text{C104} \\ \text{O2}-\text{Fe1}-\text{P1}-\text{C203} \\ \end{array}$	$\begin{array}{c} -177.9 \text{ (s)} \\ -63.2 \text{ (s)} \\ 55.7 \text{ (s)} \\ 105.1 \text{ (g)} \\ -15.7 \text{ (s)} \\ 105.1 \text{ (g)} \\ -15.7 \text{ (s)} \\ 138.8 \text{ (g)} \\ -91.7 \text{ (a)} \\ 26.2 \text{ (a)} \\ 150.5 \text{ (4)} \\ -176.6 \text{ (s)} \\ -50.4 \text{ (7)} \\ 75.7 \text{ (6)} \\ -168 \text{ (1)} \\ -41 \text{ (1)} \\ 54.9 \text{ (6)} \\ -53 \text{ (1)} \\ 178.5 \text{ (7)} \\ 104.3 \text{ (a)} \\ -133.9 \text{ (4)} \\ -8.8 \text{ (6)} \\ -109.3 \text{ (s)} \\ 7 \text{ (1)} \\ 129 \text{ (1)} \\ -59.5 \text{ (7)} \\ 175.3 \text{ (g)} \\ 56 \text{ (1)} \\ 0.7 \text{ (2)} \\ -88.7 \text{ (6)} \\ 31.7 \text{ (8)} \\ 155.2 \text{ (6)} \\ -113.4 \text{ (5)} \\ 1.3 \text{ (s)} \end{array}$
$\begin{array}{l} \text{O1}-\text{Fe1}-\text{P1}-\text{C201} \\ \text{O1}-\text{Fe1}-\text{P1}-\text{C203} \\ \text{O1}-\text{Fe1}-\text{P1}-\text{C301} \\ \text{O1}-\text{Fe1}-\text{P1}-\text{C303} \\ \text{O1}-\text{Fe1}-\text{P1}-\text{C304} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C108} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C111} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C112} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C308} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C312} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C312} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C102} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C102} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C106} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C202} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C206} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C206} \\ \text{O1}-\text{Fe1}-\text{P103}-\text{C109} \\ \text{O1}-\text{Fe1}-\text{P103}-\text{C109} \\ \text{O1}-\text{Fe1}-\text{P103}-\text{C109} \\ \text{O1}-\text{Fe1}-\text{P302}-\text{C302} \\ \text{O1}-\text{Fe1}-\text{P303}-\text{C307} \\ \text{O1}-\text{Fe1}-\text{P303}-\text{C307} \\ \text{O1}-\text{Fe1}-\text{P303}-\text{C307} \\ \text{O1}-\text{Fe1}-\text{P303}-\text{C309} \\ \text{O1}-\text{Fe1}-\text{P303}-\text{C310} \\ \text{O2}-\text{Fe1}-\text{P1}-\text{C101} \\ \text{O2}-\text{Fe1}-\text{P1}-\text{C103} \\ \text{O2}-\text{Fe1}-\text{P1}-\text{C104} \\ \text{O2}-\text{Fe1}-\text{P1}-\text{C203} \\ \text{O2}-\text{Fe1}-\text{O1}-\text{C203} \\ \text{O2}-\text{O1}-$	$\begin{array}{c} -177.9~(s)\\ -177.9~(s)\\ -63.2~(s)\\ 55.7~(s)\\ 105.1~(9)\\ -15.7~(8)\\ -138.8~(9)\\ -91.7~(3)\\ 26.2~(3)\\ 150.5~(4)\\ -176.6~(8)\\ -50.4~(7)\\ 63.6~(7)\\ 75.7~(6)\\ -168~(1)\\ -41~(1)\\ 54.9~(6)\\ -53~(1)\\ 178.5~(7)\\ 104.3~(3)\\ -133.9~(4)\\ -8.8~(6)\\ -109.3~(8)\\ 7~(1)\\ 129~(1)\\ -59.5~(7)\\ 175.3~(9)\\ 56~(1)\\ 0.7~(2)\\ -88.7~(6)\\ 31.7~(8)\\ 155.2~(6)\\ -113.4~(5)\\ 1.3~(5)\\ $
$\begin{array}{l} {\rm O1-Fe1-P1-C201} \\ {\rm O1-Fe1-P1-C203} \\ {\rm O1-Fe1-P1-C303} \\ {\rm O1-Fe1-P1-C304} \\ {\rm O1-Fe1-P1-C304} \\ {\rm O1-Fe1-P4-C108} \\ {\rm O1-Fe1-P4-C112} \\ {\rm O1-Fe1-P4-C112} \\ {\rm O1-Fe1-P4-C312} \\ {\rm O1-Fe1-P102-C102} \\ {\rm O1-Fe1-P102-C105} \\ {\rm O1-Fe1-P102-C105} \\ {\rm O1-Fe1-P102-C205} \\ {\rm O1-Fe1-P102-C205} \\ {\rm O1-Fe1-P102-C205} \\ {\rm O1-Fe1-P102-C205} \\ {\rm O1-Fe1-P102-C206} \\ {\rm O1-Fe1-P103-C107} \\ {\rm O1-Fe1-P103-C109} \\ {\rm O1-Fe1-P302-C302} \\ {\rm O1-Fe1-P302-C302} \\ {\rm O1-Fe1-P302-C306} \\ {\rm O1-Fe1-P303-C306} \\ {\rm O1-Fe1-P303-C307} \\ {\rm O1-Fe1-P303-C310} \\ {\rm O1-Fe1-P303-C310} \\ {\rm O1-Fe1-P1-O2-C50} \\ {\rm O2-Fe1-P1-C101} \\ {\rm O2-Fe1-P1-C104} \\ {\rm O2-Fe1-P1-C203} \\ {\rm O2-Fe1-P1-C203} \\ {\rm O2-Fe1-P1-C204} \\ \end{array}$	$\begin{array}{c} -177.9~(\text{s})\\ -63.2~(\text{s})\\ 55.7~(\text{s})\\ 105.1~(\text{9})\\ -15.7~(\text{8})\\ -138.8~(\text{9})\\ -91.7~(\text{3})\\ 26.2~(\text{3})\\ 150.5~(\text{4})\\ -176.6~(\text{8})\\ -50.4~(7)\\ 63.6~(7)\\ 75.7~(\text{6})\\ -168~(1)\\ -41~(1)\\ 54.9~(\text{6})\\ -168~(1)\\ -41~(1)\\ 178.5~(7)\\ 104.3~(3)\\ -133.9~(4)\\ -8.8~(\text{6})\\ -109.3~(\text{8})\\ 7~(1)\\ 129~(1)\\ -59.5~(7)\\ 175.3~(9)\\ 56~(1)\\ 0.7~(2)\\ -88.7~(\text{6})\\ 31.7~(\text{8})\\ 155.2~(\text{6})\\ -1113.4~(\text{5})\\ 120.2~(\text{5})\\ 120.2~(\text{5})\\ \end{array}$
$\begin{array}{l} {\rm O1-Fe1-P1-C201} \\ {\rm O1-Fe1-P1-C203} \\ {\rm O1-Fe1-P1-C303} \\ {\rm O1-Fe1-P1-C303} \\ {\rm O1-Fe1-P1-C304} \\ {\rm O1-Fe1-P4-C108} \\ {\rm O1-Fe1-P4-C112} \\ {\rm O1-Fe1-P4-C112} \\ {\rm O1-Fe1-P4-C312} \\ {\rm O1-Fe1-P102-C102} \\ {\rm O1-Fe1-P102-C102} \\ {\rm O1-Fe1-P102-C106} \\ {\rm O1-Fe1-P102-C202} \\ {\rm O1-Fe1-P102-C205} \\ {\rm O1-Fe1-P102-C205} \\ {\rm O1-Fe1-P103-C107} \\ {\rm O1-Fe1-P103-C107} \\ {\rm O1-Fe1-P103-C109} \\ {\rm O1-Fe1-P302-C302} \\ {\rm O1-Fe1-P302-C305} \\ {\rm O1-Fe1-P302-C306} \\ {\rm O1-Fe1-P303-C307} \\ {\rm O1-Fe1-P303-C309} \\ {\rm O1-Fe1-P303-C309} \\ {\rm O1-Fe1-P303-C309} \\ {\rm O1-Fe1-P103-C101} \\ {\rm O2-Fe1-P1-C101} \\ {\rm O2-Fe1-P1-C104} \\ {\rm O2-Fe1-P1-C203} \\ {\rm O2-Fe1-P1-C204} \\ {\rm O2-Fe1-$	$\begin{array}{c} -177.9~(5)\\ -63.2~(5)\\ 55.7~(5)\\ 105.1~(9)\\ -15.7~(8)\\ -138.8~(9)\\ -91.7~(3)\\ 26.2~(3)\\ 150.5~(4)\\ -176.6~(8)\\ -50.4~(7)\\ 75.7~(6)\\ -168~(1)\\ -41~(1)\\ 54.9~(6)\\ -53~(1)\\ 178.5~(7)\\ 104.3~(3)\\ -133.9~(4)\\ -8.8~(6)\\ -109.3~(8)\\ 7~(1)\\ 129~(1)\\ -59.5~(7)\\ 175.3~(9)\\ 56~(1)\\ 0.7~(2)\\ -88.7~(6)\\ 31.7~(8)\\ 155.2~(6)\\ -113.4~(5)\\ 1.3~(5)\\ 120.2~(5)\\ 120.2~(6)\\ -120.2~(6)\\ -120.2~(6)\\ -120.2~(6)\\ -113.4~(5)\\ 1.20.2~(6)\\ -120.2~(6)\\ -120.2~(6)\\ -120.2~(6)\\ -113.4~(6)\\ -120.2~(6)\\ -12$
$\begin{array}{l} \text{O1}-\text{Fe1}-\text{P1}-\text{C201} \\ \text{O1}-\text{Fe1}-\text{P1}-\text{C203} \\ \text{O1}-\text{Fe1}-\text{P1}-\text{C301} \\ \text{O1}-\text{Fe1}-\text{P1}-\text{C303} \\ \text{O1}-\text{Fe1}-\text{P1}-\text{C304} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C108} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C111} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C112} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C308} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C312} \\ \text{O1}-\text{Fe1}-\text{P4}-\text{C312} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C102} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C102} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C105} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C205} \\ \text{O1}-\text{Fe1}-\text{P102}-\text{C206} \\ \text{O1}-\text{Fe1}-\text{P103}-\text{C109} \\ \text{O1}-\text{Fe1}-\text{P103}-\text{C109} \\ \text{O1}-\text{Fe1}-\text{P103}-\text{C109} \\ \text{O1}-\text{Fe1}-\text{P103}-\text{C302} \\ \text{O2}-\text{Fe1}-\text{P103}-\text{C306} \\ \text{O1}-\text{Fe1}-\text{P302}-\text{C306} \\ \text{O1}-\text{Fe1}-\text{P303}-\text{C307} \\ \text{O1}-\text{Fe1}-\text{P303}-\text{C309} \\ \text{O1}-\text{Fe1}-\text{P303}-\text{C309} \\ \text{O1}-\text{Fe1}-\text{P103}-\text{C101} \\ \text{O2}-\text{Fe1}-\text{P1}-\text{C101} \\ \text{O2}-\text{Fe1}-\text{P1}-\text{C104} \\ \text{O2}-\text{Fe1}-\text{P1}-\text{C104} \\ \text{O2}-\text{Fe1}-\text{P1}-\text{C203} \\ \text{O2}-\text{Fe1}-\text{P1}-\text{C204} \\ \text{O2}-\text{Fe1}-\text{P1}-\text{C204} \\ \text{O2}-\text{Fe1}-\text{P1}-\text{C301} \\ \text{O2}-\text{O1}-\text{O1}-\text{O1}-\text{O1}-\text{O1} \\$	$\begin{array}{c} -177.9~(5)\\ -63.2~(5)\\ 55.7~(5)\\ 105.1~(9)\\ -15.7~(8)\\ -138.8~(9)\\ -91.7~(3)\\ 26.2~(3)\\ 150.5~(4)\\ -50.4~(7)\\ 63.6~(7)\\ 75.7~(6)\\ -168~(1)\\ -41~(1)\\ 54.9~(6)\\ -53~(1)\\ 178.5~(7)\\ 104.3~(3)\\ -133.9~(4)\\ -8.8~(6)\\ -109.3~(8)\\ 7~(1)\\ 129~(1)\\ -59.5~(7)\\ 175.3~(9)\\ 56~(1)\\ 0.7~(2)\\ -88.7~(6)\\ 31.7~(8)\\ 155.2~(6)\\ -113.4~(5)\\ 120.2~(5)\\ $

O2—Fe1—P1—C304	-74.3(9)	O2—Fe1—O1—C50	-0.7(2)		
O2—Fe1—P4—C108	-156.1 (3)	C101-C102-P102-C105	-165(1)		
O2—Fe1—P4—C111	-38.3(2)	C101-C102-P102-C106	91(2)		
O2—Fe1—P4—C112	86.1(4)	C102-C101-P1-C103	-162(1)		
O2—Fe1—P4—C308	118.9 (8)	C102—C101—P1—C104	92(1)		
O2—Fe1—P4—C311	-114.8(7)	C107—C108—P4—C111	-156.6(5)		
O2—Fe1—P4—C312	-0.9(7)	C107-C108-P4-C112	96.6(6)		
O2-Fe1-P102-C102	98.9 (5)	C108—C107—P103—C109	-177.7(5)		
O2—Fe1—P102—C105	-145(1)	C108—C107—P103—C110	79.3(7)		
O2—Fe1—P102—C106	-18(1)	C201-C202-P102-C205	155 (1)		
O2—Fe1—P102—C202	78.0 (5)	C201-C202-P102-C206	-100(1)		
O2—Fe1—P102—C205	-29.8(9)	C202-C201-P1-C203	-82(1)		
O2—Fe1—P102—C206	-158.3(7)	C202-C201-P1-C204	174.9 (9)		
02—FeI—P103—C107	93.8 (5)	C301—C302—P302—C305	-81(2)		
02—Fe1—P103—C109	-144.5(4)	C301 - C302 - P302 - C306	169(1)		
O_2 —Fe1—P103—C110	-19.3(8)	C_{302} C_{301} P_1 C_{303} C_{302} C_{301} P_1 C_{304}	137(2)		
O_2 —FeI—P302—C302	-94(1)	$C_{302} = C_{301} = P_1 = C_{304}$	-113(2)		
O_2 —FeI—P302—C305 O_2 FeI—P302—C306	23(2)	$C_{307} = C_{308} = P_4 = C_{311}$	-103(1)		
O_2 Fe1 P302 C300	144.0(8)	$C_{208} = C_{207} = P_{203} = C_{200}$	90(2)		
O_2 Fe1 P303 C307	-93.4(0)	$C_{208} = C_{207} = P_{203} = C_{209}$	124(2) 120(2)		
O_2 —Fe1—F 303—C 309 O_2 —Fe1—P 303—C 310	141.3(9)	C308—C307—F305—C310	-130(2)		
	Table S4. Cont	$act \ distances \ (\AA)$			
$O1 \cdot \cdot \cdot C206^{i}$	3.39(2)	$O51 \cdots C103^{iii}$	3.55(2)		
$O1 \cdot \cdot \cdot C309^{i}$	3.40(2)	$O51 \cdot \cdot \cdot C203^{iii}$	3.56(1)		
$01 \cdots C105^{i}$	3.55 (3)	$O51 \cdot \cdot \cdot C308^V$	3.59(2)		
$O2 \cdot \cdot \cdot O52$	2.568(4)	$O52 \cdot \cdot \cdot C306^{iv}$	3.35(1)		
$O2 \cdot \cdot \cdot O53$	3.289 (5)	$O52 \cdot \cdot \cdot C50$	3.359(5)		
$O2 \cdot \cdot \cdot C51$	3.384 (4)	$O52 \cdot \cdot \cdot C203$	3.46 (1)		
O3· · · O53	2.470 (5)	$O52 \cdot \cdot \cdot C112^V$	3.53(1)		
$O3 \cdot \cdot \cdot C51$	3.364 (4)	$O53 \cdot \cdot \cdot C311^{ii}$	2.83(2)		
$O3 \cdot \cdot \cdot O52$	3.382 (4)	$O53 \cdot \cdot \cdot C50$	3.258(5)		
$O3 \cdot \cdot \cdot C202^{i}$	3.49(2)	$053 \cdots C110^{vi}$	3.32(2)		
$O3 \cdots C102^{i}$	3.52(2)	$053 \cdots C305^{vi}$	3.52(2)		
$O_3 \dots C_{311}^{ii}$	355(2)	$C_{53} = C_{503}$	3.07(3)		
	2.24(2)	C_{51} C_{112}^{V}	3.47(2)		
	3.34(2)		3.30(1)		
051···C206**	3.40(2)	$C102 \cdots C301$	3.42(2)		
$O51 \cdot \cdot \cdot C201$	3.40(1)	$C102 \cdots C302^{V11}$	3.50(2)		
$O51 \cdot \cdot \cdot C304^{111}$	3.42(3)	$C105 \cdots C305^{V111}$	3.50(4)		
$O51 \cdot \cdot \cdot C112^{v}$	3.43(1)	$C110 \cdot \cdot \cdot C307^{i}$	3.60(2)		
$O51 \cdot \cdot \cdot C204^{111}$	3.45(1)	$C111 \cdots C204^{vi}$	3.17(1)		
$O51 \cdot \cdot \cdot C309^{iv}$	3.46(2)	$C201 \cdots C302^{vii}$	3.42(2)		
$O51 \cdot \cdot \cdot C109^{iv}$	3.485 (7)	$C204 \cdots C312^{ix}$	355(2)		
$051\cdots C104^{iii}$	3.51(2)	C_{204} C_{200}^{iv}	2.00(2)		
OF1 C202 ⁱⁱⁱ	2 55 (2)		3.43(3)		
0.010009	ə.əə (2)	C305···C307 [*]	3.52 (3)		
Symmetry codes: (i) $x, \frac{1}{2} - y, \frac{1}{2} + z$; (ii) $x - \frac{1}{2}, y, \frac{3}{2} - z$; (iii) $\frac{1}{2} - x, y - \frac{1}{2}, z$; (iv) $x - \frac{1}{2}, \frac{1}{2} - y, 1 - z$; (v)					
$1-x, -y, 1-z; \text{(vi)} \ 1-x, y-\frac{1}{2}, \frac{3}{2}-z; \text{(vii)} \ 1-x, 1-y, 1-z; \text{(viii)} \ x, \frac{1}{2}-y, z-\frac{1}{2}; \text{(ix)} \ 1-x, \frac{1}{2}+y, \frac{3}{2}-z.$					
	2 2	2 2	4 4		