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Crystal structure of $[Fe(C_6H_{16}P_2)_2(CO_3)].H_2CO_3$ –nsw069

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Abstract

The crystal structure of $[Fe(C_6H_{16}P_2)_2(CO_3)].H_2CO_3$ 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 $Me_2PCH_2CH_2PMe_2$ 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 occcupancy. One major isomer is for P1 to link to P102 and P4 to link to P103, with the extra complication that the 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 displacemnt 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

$C_{13}H_{32}FeO_3P_4.CH_2O_3$
$M_r = 478.17$
Orthorhombic
Pbca
$a = 16.5175\,(3)$ Å
$b = 16.1088\,(3)$ Å
$c = 16.6269\,(3)$ Å
$V = 4424.04\,(14)$ Å^3
$Z = 8$
$D_x = 1.436$ Mg m^{-3}
D_m not measured
Mo $K\alpha$ radiation
$\lambda = 0.71073$ Å

Cell parameters from 35060 reflections
$\theta = 2.6$–$27.5°$
$\mu = 0.996$ mm^{-1}
$T = 200$ K
Plate
Orange
0.13 × 0.13 × 0.06 mm
Crystal source: from UNSW

Data collection

Nonius KappaCCD diffractometer
φ and ω scans with CCD
Absorption correction:
by integration *via* Gaussian method (Coppens, 1970) implemented in maXus (2000)
$T_{\min} = 0.883$, $T_{\max} = 0.949$
57391 measured reflections
5060 independent reflections

2956 reflections with
$I > 2.0\sigma(I)$
$R_{\rm int} = 0.099$
$\theta_{\max} = 27.493°$
$h = -21 \rightarrow 21$
$k = -20 \rightarrow 20$
$l = -21 \rightarrow 21$

Refinement
Refinement on F^2
$R(F) = 0.0384$
$wR(F^2) = 0.1174$
$S = 1.0039$
5050 reflections
409 parameters
H atoms treated by a mixture of independent and constrained refinement

Method, part 1, Chebychev polynomial, (Carruthers & Watkin, 1979, Prince, 1982) [weight] = $1.0/[A_0{*}T_0(x) + A_1{*}T_1(x) ... +A_{n-1}]{*}T_{n-1}(x)]$ 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
$(\Delta/\sigma)_{\max} = 0.011699$
$\Delta\rho_{\max} = 0.65$ e Å^{-3}
$\Delta\rho_{\min} = -0.60$ e Å^{-3}
Extinction correction: none
Scattering factors from International Tables Vol C 4.2.6.8 and 6.1.1.4

Table 1. *Selected geometric parameters (Å, °)*

Fe1—P1	2.2400 (10)	P102—C106	1.817 (17)
Fe1—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. *Hydrogen-bonding geometry (Å, °)*

D—H···*A*	*D*—H	H···*A*	*D*···*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* .

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Supplementary data

Table *S*1. *Fractional atomic coordinates and equivalent isotropic displacement parameters (Å²)*

$$U_{\mathrm{eq}} = (1/3)\Sigma_i\Sigma_j U^{ij} a^i a^j \mathbf{a}_i.\mathbf{a}_j.$$

	Occupancy	x	y	z	U_{eq}
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	0.348 (8)	0.6159 (13)	0.2835 (16)	0.4187 (16)	0.0451
C106	0.348 (8)	0.4737 (17)	0.1881 (19)	0.423 (2)	0.0442
C107	0.705 (4)	0.7389 (3)	0.2743 (5)	0.6110 (4)	0.0679
C108	0.705 (4)	0.7322 (3)	0.1834 (5)	0.6392 (5)	0.0734
C109	0.705 (4)	0.6659 (5)	0.4308 (4)	0.5931 (4)	0.0713
C110	0.705 (4)	0.6558 (8)	0.3521 (10)	0.7424 (6)	0.0511
C111	0.705 (4)	0.6152 (4)	0.0591 (4)	0.6799 (4)	0.0623
C112	0.705 (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
H1012	0.3482	0.3566 (10)	0.3346 (13)	0.5112 (9)	0.0583
H1021	0.3482	0.5067 (9)	0.4104 (9)	0.4617 (10)	0.0652
H1022	0.3482	0.4445 (9)	0.3572 (9)	0.4055 (10)	0.0652
H1031	0.3482	0.3261 (11)	0.3784 (15)	0.6802 (13)	0.0652
H1032	0.3482	0.3819 (11)	0.3204 (15)	0.7387 (13)	0.0652
H1033	0.3482	0.3335 (11)	0.2788 (15)	0.6631 (13)	0.0652
H1041	0.3482	0.4347 (13)	0.4908 (9)	0.6505 (10)	0.0759
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

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	0.7054	0.7853 (3)	0.3017 (5)	0.6390 (4)	0.0815
H1072	0.7054	0.7481 (3)	0.2757 (5)	0.5516 (4)	0.0815
H1081	0.7054	0.7387 (3)	0.1807 (5)	0.6990 (5)	0.0881
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	0.7054	0.6057 (8)	0.3797 (10)	0.7629 (6)	0.0613
H1111	0.7054	0.6592 (4)	0.0169 (4)	0.6738 (4)	0.0748
H1112	0.7054	0.6153 (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	0.3573	0.4476 (9)	0.3623 (9)	0.4070 (9)	0.0634
H2022	0.3573	0.3896 (9)	0.3019 (9)	0.4609 (9)	0.0634
H2031	0.3573	0.3054 (6)	0.3564 (8)	0.6398 (9)	0.0621
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	0.3573	0.4865 (16)	0.1863 (17)	0.370 (2)	0.0566
H2052	0.3573	0.5291 (16)	0.1267 (17)	0.437 (2)	0.0566
H2053	0.3573	0.4364 (16)	0.1589 (17)	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)	0.4857 (7)	0.6477 (9)	0.0738
H3022	0.2946	0.5974 (9)	0.4544 (7)	0.5554 (9)	0.0738
H3031	0.2946	0.3400 (12)	0.3946 (17)	0.6956 (11)	0.0561
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	0.2946	0.662 (2)	0.282 (2)	0.7614 (14)	0.0656
H3053	0.2946	0.588 (2)	0.348 (2)	0.7736 (14)	0.0656
H3061	0.2946	0.7556 (7)	0.4049 (12)	0.6205 (9)	0.0787
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	0.2946	0.5862 (14)	0.2997 (13)	0.3638 (15)	0.0646
H3092	0.2946	0.6308 (14)	0.3471 (13)	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	0.2946	0.6801 (10)	0.1318 (14)	0.7454 (11)	0.1086
H3121	0.2946	0.6303 (11)	−0.0031 (8)	0.6247 (12)	0.0908
H3122	0.2946	0.5588 (11)	0.0385 (8)	0.6793 (12)	0.0908
H3123	0.2946	0.5468 (11)	0.0289 (8)	0.5823 (12)	0.0908

Table *S*2. *Anisotropic displacement parameters* (Å^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 *S*3. *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	1.713 (15)	C203—H2032	1.000
P4—C311	1.851 (13)	C203—H2033	1.000
P4—C312	1.834 (13)	C204—H2041	1.000
P102—C102	1.860 (14)	C204—H2042	1.000
P102—C105	1.796 (17)	C204—H2043	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		
P1—Fe1—P4	177.33 (4)	P1—Fe1—P102	83.33 (7)

P4—Fe1—P102	98.91 (7)	C107—P103—C110	102.8 (6)
P1—Fe1—P103	94.66 (9)	C109—P103—C110	100.1 (5)
P4—Fe1—P103	86.43 (9)	Fe1—P302—C302	110.3 (6)
P102—Fe1—P103	99.34 (12)	Fe1—P302—C305	104.6 (12)
P1—Fe1—P302	85.2 (2)	C302—P302—C305	108.5 (14)
P4—Fe1—P302	95.8 (2)	Fe1—P302—C306	127.1 (8)
P1—Fe1—P303	102.99 (14)	C302—P302—C306	100.8 (9)
P4—Fe1—P303	79.25 (14)	C305—P302—C306	104.6 (12)
P302—Fe1—P303	100.9 (3)	Fe1—P303—C307	114.7 (4)
P1—Fe1—O1	88.76 (7)	Fe1—P303—C309	121.4 (9)
P4—Fe1—O1	88.68 (7)	Fe1—P303—C310	110.5 (14)
P102—Fe1—O1	162.04 (8)	C307—P303—C309	103.3 (8)
P103—Fe1—O1	97.35 (14)	C307—P303—C310	102.8 (12)
P302—Fe1—O1	96.1 (3)	C309—P303—C310	102.0 (14)
P1—Fe1—O2	88.72 (8)	Fe1—O1—C50	91.12 (18)
P4—Fe1—O2	89.49 (8)	Fe1—O2—C50	90.29 (19)
P102—Fe1—O2	99.12 (7)	C51—O52—H2	111 (4)
P103—Fe1—O2	161.49 (13)	C51—O53—H3	122 (4)
P302—Fe1—O2	159.8 (3)	O2—C50—O1	114.1 (3)
P303—Fe1—O1	159.97 (13)	O2—C50—O3	121.7 (3)
P303—Fe1—O2	99.18 (10)	O1—C50—O3	124.2 (3)
O1—Fe1—O2	64.48 (9)	O52—C51—O53	116.6 (3)
Fe1—P1—C101	113.8 (6)	O52—C51—O51	120.2 (4)
Fe1—P1—C103	116.8 (8)	O53—C51—O51	123.1 (4)
C101—P1—C103	103.4 (9)	P1—C101—C102	106.1 (10)
Fe1—P1—C104	117.9 (7)	P1—C101—H1011	110.3
C101—P1—C104	99.7 (8)	C102—C101—H1011	110.3
C103—P1—C104	102.9 (9)	P1—C101—H1012	110.3
Fe1—P1—C201	112.6 (4)	C102—C101—H1012	110.3
Fe1—P1—C203	113.5 (4)	H1011—C101—H1012	109.5
C201—P1—C203	101.6 (6)	C101—C102—P102	110.6 (10)
Fe1—P1—C204	122.5 (4)	C101—C102—H1021	109.2
C201—P1—C204	104.9 (6)	P102—C102—H1021	109.2
Fe1—P1—C301	112.1 (6)	C101—C102—H1022	109.2
Fe1—P1—C303	118.4 (9)	P102—C102—H1022	109.2
Fe1—P1—C304	111.4 (9)	H1021—C102—H1022	109.5
C203—P1—C204	99.2 (6)	P1—C103—H1031	109.5
C301—P1—C303	103.8 (9)	P1—C103—H1032	109.5
C301—P1—C304	104.0 (11)	H1031—C103—H1032	109.5
C303—P1—C304	105.9 (11)	P1—C103—H1033	109.5
Fe1—P4—C108	109.5 (2)	H1031—C103—H1033	109.5
Fe1—P4—C111	116.7 (2)	H1032—C103—H1033	109.5
C108—P4—C111	104.1 (3)	P1—C104—H1041	109.5
Fe1—P4—C112	119.3 (3)	P1—C104—H1042	109.5
C108—P4—C112	102.8 (4)	H1041—C104—H1042	109.5
C111—P4—C112	102.7 (4)	P1—C104—H1043	109.5
Fe1—P4—C308	118.0 (6)	H1041—C104—H1043	109.5
Fe1—P4—C311	118.8 (6)	H1042—C104—H1043	109.5
C308—P4—C311	103.4 (8)	P102—C105—H1051	109.5
Fe1—P4—C312	113.5 (5)	P102—C105—H1052	109.5
C308—P4—C312	102.5 (10)	H1051—C105—H1052	109.5
C311—P4—C312	97.7 (9)	P102—C105—H1053	109.5
Fe1—P102—C102	110.3 (5)	H1051—C105—H1053	109.5
Fe1—P102—C105	120.8 (10)	H1052—C105—H1053	109.5
C102—P102—C105	100.4 (8)	P102—C106—H1061	109.5
Fe1—P102—C106	118.3 (13)	P102—C106—H1062	109.4
C102—P102—C106	102.2 (12)	H1061—C106—H1062	109.5
C105—P102—C106	102.0 (13)	P102—C106—H1063	109.4
Fe1—P102—C202	109.4 (5)	H1061—C106—H1063	109.5
Fe1—P102—C205	113.1 (14)	H1062—C106—H1063	109.5
C202—P102—C205	97.8 (10)	P103—C107—C108	109.2 (4)
Fe1—P102—C206	127.4 (6)	P103—C107—H1071	109.6
C202—P102—C206	102.4 (7)	C108—C107—H1071	109.5
Fe1—P102—C309	130.8 (11)	P103—C107—H1072	109.5
C205—P102—C206	102.6 (13)	C108—C107—H1072	109.5
Fe1—P103—C107	109.0 (3)	H1071—C107—H1072	109.5
Fe1—P103—C109	129.2 (3)	C107—C108—P4	109.0 (4)
C107—P103—C109	100.4 (4)	C107—C108—H1081	109.6
Fe1—P103—C110	112.0 (4)	P4—C108—H1081	109.6

C107—C108—H1082	109.6	P302—C302—H3021	108.3
P4—C108—H1082	109.6	C301—C302—H3022	108.3
H1081—C108—H1082	109.5	P302—C302—H3022	108.3
P103—C109—H1091	109.5	H3021—C302—H3022	109.5
P103—C109—H1092	109.5	P1—C303—H3031	109.5
H1091—C109—H1092	109.5	P1—C303—H3032	109.5
P103—C109—H1093	109.5	P1—C303—H3033	109.5
H1091—C109—H1093	109.5	H3031—C303—H3032	109.5
H1092—C109—H1093	109.5	H3031—C303—H3033	109.5
P103—C110—H1101	109.5	H3032—C303—H3033	109.5
P103—C110—H1102	109.5	P1—C304—H3041	109.4
H1101—C110—H1102	109.5	P1—C304—H3042	109.5
P103—C110—H1103	109.5	P1—C304—H3043	109.5
H1101—C110—H1103	109.5	H3041—C304—H3042	109.5
H1102—C110—H1103	109.5	H3041—C304—H3043	109.5
P4—C111—H1111	109.5	H3042—C304—H3043	109.5
P4—C111—H1112	109.5	P302—C305—H3051	109.5
H1111—C111—H1112	109.5	P302—C305—H3052	109.4
P4—C111—H1113	109.5	H3051—C305—H3052	109.5
H1111—C111—H1113	109.5	P302—C305—H3053	109.5
H1112—C111—H1113	109.5	H3051—C305—H3053	109.5
P4—C112—H1121	109.5	H3052—C305—H3053	109.5
P4—C112—H1122	109.5	P302—C306—H3061	109.5
H1121—C112—H1122	109.5	P302—C306—H3062	109.5
P4—C112—H1123	109.5	H3061—C306—H3062	109.5
H1121—C112—H1123	109.5	P302—C306—H3063	109.5
H1122—C112—H1123	109.5	H3061—C306—H3063	109.5
P1—C201—C202	105.9 (8)	H3062—C306—H3063	109.5
P1—C201—H2011	110.4	P303—C307—C308	114.8 (9)
H1011—C201—H2011	107.5	P303—C307—H3071	108.1
P1—C201—H2012	110.4	C308—C307—H3071	108.1
C202—C201—H2012	110.4	P303—C307—H3072	108.1
H2011—C201—H2012	109.5	C308—C307—H3072	108.1
C201—C202—H2021	109.4	H3071—C307—H3072	109.5
C201—C202—H2022	109.4	C307—C308—P4	106.4 (10)
P1—C203—H2031	109.5	C307—C308—H3081	110.2
P1—C203—H2032	109.5	P4—C308—H3081	110.2
H2031—C203—H2032	109.5	C307—C308—H3082	110.2
P1—C203—H2033	109.5	P4—C308—H3082	110.2
H2031—C203—H2033	109.5	H3081—C308—H3082	109.5
P1—C204—H2041	109.5	P303—C309—H3091	109.5
P1—C204—H2042	109.5	P303—C309—H3092	109.5
P1—C204—H2043	109.5	P303—C309—H3093	109.5
H2041—C204—H2042	109.5	H3091—C309—H3092	109.5
H2041—C204—H2043	109.5	H3091—C309—H3093	109.5
H2042—C204—H2043	109.5	H3092—C309—H3093	109.5
P102—C205—H2051	109.4	P303—C310—H3101	109.5
P102—C205—H2052	109.5	P303—C310—H3102	109.4
P102—C205—H2053	109.5	P303—C310—H3103	109.5
H2051—C205—H2052	109.5	H3101—C310—H3102	109.5
H2051—C205—H2053	109.5	H3101—C310—H3103	109.5
H2052—C205—H2053	109.5	H3102—C310—H3103	109.5
P102—C206—H2061	109.5	P4—C311—H3111	109.5
P102—C206—H2062	109.5	P4—C311—H3112	109.5
H2061—C206—H2062	109.5	H3111—C311—H3112	109.5
H2061—C206—H2063	109.5	P4—C311—H3113	109.5
P1—C301—C302	110.1 (10)	H3111—C311—H3113	109.5
P1—C301—H3011	109.3	H3112—C311—H3113	109.5
C302—C301—H3011	109.3	P4—C312—H3121	109.5
P1—C301—H3012	109.3	P4—C312—H3122	109.5
C302—C301—H3012	109.3	H3121—C312—H3122	109.5
H3011—C301—H3012	109.5	P4—C312—H3123	109.5
C301—C302—P302	114.1 (10)	H3121—C312—H3123	109.5
C301—C302—H3021	108.3	H3122—C312—H3123	109.5
Fe1—P1—C101—C102	−34 (1)	Fe1—P102—C102—C101	−36 (1)
Fe1—P1—C201—C202	40 (1)	Fe1—P102—C202—C201	37 (1)
Fe1—P1—C301—C302	8 (2)	Fe1—P103—C107—C108	−39.7 (5)
Fe1—P4—C108—C107	−31.0 (5)	Fe1—P303—C307—C308	−10 (2)
Fe1—P4—C308—C307	−30 (2)	Fe1—O1—C50—O2	1.1 (3)

Fe1—O1—C50—O3	−178.8 (3)
Fe1—O2—C50—O1	−1.1 (3)
Fe1—O2—C50—O3	178.8 (3)
P1—Fe1—P102—C102	11.2 (5)
P1—Fe1—P102—C105	128 (1)
P1—Fe1—P102—C106	−106 (1)
P1—Fe1—P102—C202	−9.6 (5)
P1—Fe1—P102—C205	−117.4 (9)
P1—Fe1—P102—C206	114.1 (7)
P1—Fe1—P103—C107	−166.3 (3)
P1—Fe1—P103—C109	−44.6 (4)
P1—Fe1—P103—C110	80.6 (5)
P1—Fe1—P302—C302	−21.1 (7)
P1—Fe1—P302—C305	96 (1)
P1—Fe1—P302—C306	−143 (1)
P1—Fe1—P303—C307	175.8 (6)
P1—Fe1—P303—C309	50.7 (9)
P1—Fe1—P303—C310	−69 (1)
P1—Fe1—O1—C50	88.4 (2)
P1—Fe1—O2—C50	−88.5 (2)
P1—C101—C102—P102	42 (1)
P1—C201—C202—P102	−46 (1)
P1—C301—C302—P302	−25 (2)
P4—Fe1—P102—C102	−170.2 (5)
P4—Fe1—P102—C105	−54 (1)
P4—Fe1—P102—C106	73 (1)
P4—Fe1—P102—C202	168.9 (5)
P4—Fe1—P102—C205	61.1 (9)
P4—Fe1—P102—C206	−67.4 (7)
P4—Fe1—P103—C107	16.1 (3)
P4—Fe1—P103—C109	137.9 (4)
P4—Fe1—P103—C110	−97.0 (5)
P4—Fe1—P302—C302	161.4 (7)
P4—Fe1—P302—C305	−82 (1)
P4—Fe1—P302—C306	39 (1)
P4—Fe1—P303—C307	−5.6 (6)
P4—Fe1—P303—C309	−130.8 (9)
P4—Fe1—P303—C310	110 (1)
P4—Fe1—O1—C50	−90.8 (2)
P4—Fe1—O2—C50	89.5 (2)
P4—C108—C107—P103	44.0 (6)
P4—C308—C307—P303	23 (2)
P102—Fe1—P1—C101	10.7 (6)
P102—Fe1—P1—C103	131.1 (8)
P102—Fe1—P1—C104	−105.5 (6)
P102—Fe1—P1—C201	−14.1 (5)
P102—Fe1—P1—C203	100.6 (5)
P102—Fe1—P1—C204	−140.5 (5)
P102—Fe1—P1—C301	−91.1 (9)
P102—Fe1—P4—C108	104.7 (3)
P102—Fe1—P4—C111	−137.4 (2)
P102—Fe1—P4—C112	−13.1 (4)
P102—Fe1—P103—C107	−82.3 (3)
P102—Fe1—P103—C109	39.4 (4)
P102—Fe1—P103—C110	164.6 (5)
P102—Fe1—P103—C302	68.4 (4)
P102—Fe1—P103—C305	166 (1)
P102—Fe1—P103—C306	−43 (1)
P102—Fe1—O1—C50	24.7 (4)
P102—Fe1—O2—C50	−171.6 (2)
P103—Fe1—P1—C101	109.6 (7)
P103—Fe1—P1—C103	−130.0 (8)
P103—Fe1—P1—C104	−6.6 (6)
P103—Fe1—P1—C201	84.8 (5)
P103—Fe1—P1—C203	−160.5 (5)
P103—Fe1—P1—C204	−41.6 (5)
P103—Fe1—P4—C108	5.8 (3)
P103—Fe1—P4—C111	123.7 (3)
P103—Fe1—P4—C112	−112.0 (4)
P103—Fe1—P102—C102	−82.4 (5)
P103—Fe1—P102—C105	34 (1)
P103—Fe1—P102—C106	161 (1)
P103—Fe1—P102—C202	−103.3 (5)
P103—Fe1—P102—C205	148.9 (9)
P103—Fe1—P102—C206	20.4 (7)
P103—Fe1—O1—C50	−177.0 (2)
P103—Fe1—O2—C50	12.3 (5)
P302—Fe1—P1—C301	8.8 (9)
P302—Fe1—P1—C303	−111.9 (9)
P302—Fe1—P1—C304	125 (1)
P302—Fe1—P4—C308	−80.6 (9)
P302—Fe1—P4—C311	45.7 (8)
P302—Fe1—P4—C312	159.6 (8)
P302—Fe1—P303—C307	88.3 (7)
P302—Fe1—P303—C309	−36.8 (9)
P302—Fe1—P303—C310	−156 (1)
P302—Fe1—O1—C50	173.5 (3)
P302—Fe1—O2—C50	−16.2 (9)
P303—Fe1—P1—C301	−91.3 (9)
P303—Fe1—P1—C303	147.9 (8)
P303—Fe1—P1—C304	24.8 (9)
P303—Fe1—P4—C308	19.5 (8)
P303—Fe1—P4—C311	145.7 (7)
P303—Fe1—P4—C312	−100.3 (7)
P303—Fe1—P302—C302	81.2 (8)
P303—Fe1—P302—C305	−162 (1)
P303—Fe1—P302—C306	−41 (1)
P303—Fe1—O1—C50	−38.2 (4)
P303—Fe1—O2—C50	168.5 (2)
O1—Fe1—P1—C101	−153.2 (6)
O1—Fe1—P1—C103	−32.8 (8)
O1—Fe1—P1—C104	90.7 (6)
O1—Fe1—P1—C201	−177.9 (5)
O1—Fe1—P1—C203	−63.2 (5)
O1—Fe1—P1—C204	55.7 (5)
O1—Fe1—P1—C301	105.1 (9)
O1—Fe1—P1—C303	−15.7 (8)
O1—Fe1—P1—C304	−138.8 (9)
O1—Fe1—P4—C108	−91.7 (3)
O1—Fe1—P4—C111	26.2 (3)
O1—Fe1—P4—C112	150.5 (4)
O1—Fe1—P4—C308	−176.6 (8)
O1—Fe1—P4—C311	−50.4 (7)
O1—Fe1—P4—C312	63.6 (7)
O1—Fe1—P102—C102	75.7 (6)
O1—Fe1—P102—C105	−168 (1)
O1—Fe1—P102—C106	−41 (1)
O1—Fe1—P102—C202	54.9 (6)
O1—Fe1—P102—C205	−53 (1)
O1—Fe1—P102—C206	178.5 (7)
O1—Fe1—P103—C107	104.3 (3)
O1—Fe1—P103—C109	−133.9 (4)
O1—Fe1—P103—C110	−8.8 (6)
O1—Fe1—P302—C302	−109.3 (8)
O1—Fe1—P302—C305	7 (1)
O1—Fe1—P302—C306	129 (1)
O1—Fe1—P303—C307	−59.5 (7)
O1—Fe1—P303—C309	175.3 (9)
O1—Fe1—P303—C310	56 (1)
O1—Fe1—O2—C50	0.7 (2)
O2—Fe1—P1—C101	−88.7 (6)
O2—Fe1—P1—C103	31.7 (8)
O2—Fe1—P1—C104	155.2 (6)
O2—Fe1—P1—C201	−113.4 (5)
O2—Fe1—P1—C203	1.3 (5)
O2—Fe1—P1—C204	120.2 (5)
O2—Fe1—P1—C301	169.6 (9)
O2—Fe1—P1—C303	48.8 (8)

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)
O2—Fe1—P103—C107	93.8 (5)	C301—C302—P302—C305	−81 (2)
O2—Fe1—P103—C109	−144.5 (4)	C301—C302—P302—C306	169 (1)
O2—Fe1—P103—C110	−19.3 (8)	C302—C301—P1—C303	137 (2)
O2—Fe1—P302—C302	−94 (1)	C302—C301—P1—C304	−113 (2)
O2—Fe1—P302—C305	23 (2)	C307—C308—P4—C311	−163 (1)
O2—Fe1—P302—C306	144.0 (8)	C307—C308—P4—C312	96 (2)
O2—Fe1—P303—C307	−93.4 (6)	C308—C307—P303—C309	124 (2)
O2—Fe1—P303—C309	141.5 (9)	C308—C307—P303—C310	−130 (2)
O2—Fe1—P303—C310	22 (1)		

Table *S*4. *Contact distances (Å)*

O1···C206^{i}	3.39 (2)	O51···C103^{iii}	3.55 (2)
O1···C309^{i}	3.40 (2)	O51···C203^{iii}	3.56 (1)
O1···C105^{i}	3.55 (3)	O51···C308^{v}	3.59 (2)
O2···O52	2.568 (4)	O52···C306^{iv}	3.35 (1)
O2···O53	3.289 (5)	O52···C50	3.359 (5)
O2···C51	3.384 (4)	O52···C203	3.46 (1)
O3···O53	2.470 (5)	O52···C112^{v}	3.53 (1)
O3···C51	3.364 (4)	O53···C311^{ii}	2.83 (2)
O3···O52	3.382 (4)	O53···C50	3.258 (5)
O3···C202^{i}	3.49 (2)	O53···C110^{vi}	3.32 (2)
O3···C102^{i}	3.52 (2)	O53···C305^{vi}	3.57 (3)
O3···C311^{ii}	3.55 (2)	C51···C311^{ii}	3.47 (2)
O51···C101^{iii}	3.34 (2)	C51···C112^{v}	3.50 (1)
O51···C206^{iv}	3.40 (2)	C102···C301^{vii}	3.42 (2)
O51···C201^{iii}	3.40 (1)	C102···C302^{vii}	3.50 (2)
O51···C304^{iii}	3.42 (3)	C105···C305^{viii}	3.50 (4)
O51···C112^{v}	3.43 (1)	C110···C307^{i}	3.60 (2)
O51···C204^{iii}	3.45 (1)	C111···C204^{vi}	3.17 (1)
O51···C309^{iv}	3.46 (2)	C201···C302^{vii}	3.42 (2)
O51···C109^{iv}	3.485 (7)	C204···C312^{ix}	3.55 (2)
O51···C104^{iii}	3.51 (2)	C304···C308^{iv}	3.43 (3)
O51···C303^{iii}	3.55 (2)	C305···C307^{i}	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) $1-x, -y, 1-z$; (vi) $1-x, y-\frac{1}{2}, \frac{3}{2}-z$; (vii) $1-x, 1-y, 1-z$; (viii) $x, \frac{1}{2}-y, z-\frac{1}{2}$; (ix) $1-x, \frac{1}{2}+y, \frac{3}{2}-z$.