Acta Cryst. (1997). C**53**, IUC9700008 [**doi:10.1107/S0108270197099484**]

Bis[bis(triphenylphosphine)iminium] Di-μ-thio-bis[(pentasulfido)ferrate(III)]

J. W. van Hal and **K. H. Whitmire**

Abstract

Bis[bis(triphenylphosphine)iminium] di-μ-thio-bis[(pentasulfido)ferrate(III)] crystallizes in the monoclinic spacegroup $P2_1/c$. The S_5Fe units are in a chair conformation linked by a Fe_2S_2 core related by an inversion center. The iron iron distance is 2.7014 (12).

Comment

The structure of the title compound was undertaken to establish the chemical identity as one of several compounds obtained in a iron sulfur carbonyl cluster series. The compound had been previously obtained by different route and was structurally characterized as the tetraphenyl phosphonium salt (Coucouvanis, Swenson, Stremple, Baenziger, 1979; Rauchfuss, Dev, Wilson, 1992).

The title compound is build around a Fe_2S_2 core (Fe···Fe = 2.7014 (12)) where each of the irons is ligated with a S_5 ligand forming a chair conformation. Its bond metricals are very similar to those obtained from the Ph_4P structure.

Experimental

The title compound was obtained during attempts to synthesize a sulfur iron carbonyl cluster compound. A solution of 3.15 g. of KOH in 60 ml of MeOH was degassed by sparging with Ar for 30 minutes. To this solution was added 1.5 ml of $Fe(CO)_5$. After stirring for 30 more minutes, 3.45 g. of S was added in one portion. The solution was filtered and the crude product was precipitated by adding dropwise a solution of 9.45 g. of [PPN][Cl] in 60 ml of MeOH. The brown precipitate was filtered, washed with ether and dried *in vacuo*. Crystals of the title compound were obtained as black plates by dissolving the crude material in MeCN, filtering and allowing to let the solution stand at room temperature.

Computing details

Data collection: *TEXSAN* 5.0 (MSC, 1990); cell refinement: *TEXSAN* 5.0 (MSC, 1990); data reduction: *TEXSAN* 5.0 (MSC, 1990); program(s) used to solve structure: *SHELXS86* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL93* (Sheldrick, 1993); molecular graphics: *SHELXTL* PLUS (Siemens, 1992); software used to prepare material for publication: *SHELXL93* (Sheldrick, 1993).

Bis bistriphenylphosphineimine dodecasulfurdiirion

Crystal data

$(C_{36}H_{30}NP_2)_2[Fe_2S_{12}]$ $V = 3691.5\ (12)\ Å^3$

CIF access

M_r = 1573.52	Z = 2
Monoclinic, $P2_1/c$	Mo $K\alpha$
a = 11.379 (2) Å	μ = 0.86 mm^{-1}
b = 21.004 (4) Å	T = 296 (2) K
c = 15.488 (3) Å	0.50 × 0.30 × 0.30 mm
β = 94.26 (3)°	

Data collection

Rigaku AFC5S diffractometer	R_{int} = 0.030
Absorption correction: none	3 standard reflections
5192 measured reflections	every 150 reflections
4869 independent reflections	intensity decay: none
3680 reflections with $I > 2\sigma(I)$	

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.040	415 parameters
$wR(F^2)$ = 0.118	H-atom parameters constrained
S = 1.04	$\Delta\rho_{max}$ = 0.34 e Å^{-3}
4865 reflections	$\Delta\rho_{min}$ = −0.23 e Å^{-3}

Table 1
Selected geometric parameters (Å, °)

Fe1—S6^{i}	2.1816 (13)	S1—S2	2.049 (2)
Fe1—S6	2.2025 (12)	S2—S3	2.058 (2)
Fe1—S5	2.3178 (14)	S3—S4	2.051 (2)
Fe1—S1	2.3276 (14)	S4—S5	2.061 (2)
Fe1—Fe1^{i}	2.7014 (12)	S6—Fe1^{i}	2.1816 (13)
S6^{i}—Fe1—S6	103.93 (5)	S5—Fe1—Fe1^{i}	126.44 (5)
S6^{i}—Fe1—S5	109.76 (5)	S1—Fe1—Fe1^{i}	126.26 (5)
S6—Fe1—S5	113.18 (5)	S2—S1—Fe1	101.00 (6)
S6^{i}—Fe1—S1	107.94 (5)	S1—S2—S3	105.98 (8)
S6—Fe1—S1	114.85 (5)	S4—S3—S2	105.42 (8)
S5—Fe1—S1	107.00 (5)	S3—S4—S5	107.46 (8)
S6^{i}—Fe1—Fe1^{i}	52.31 (4)	S4—S5—Fe1	98.94 (7)
S6—Fe1—Fe1^{i}	51.61 (4)	Fe1^{i}—S6—Fe1	76.07 (5)

Symmetry codes: (i) −*x*+2, −*y*, −*z*+1.

Acknowledgements

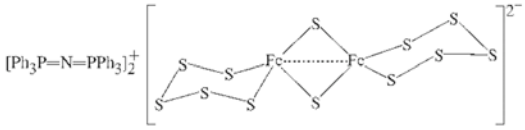
The Authors wish to thank the Robert A. Welch Foundation and the N·S·F. for their support for this research

References

Coucouvanis, P., Swenson, D., Stremple, P., Baenziger, N.C., J. Am. Chem. Soc., 101, 1979, 3392-3394.
Rauchfuss, T.B., Dev, S., Wilson, S.R., Inorg. Chem., 1992, 31, 154-156.
Sheldrick, G. M. (1986). *SHELXS86*. Program for structure solution of crystal structures. Univ. of Gőttingen, Germany.
Sheldrick, G. M. (1993). *SHELXL93*. In preparation for J. Appl. Cryst..
SHELXTL PLUS (1992). Siemens Xray Cooporation, Madison, Wisconson.
TEXSAN 5.0 (1990). The Molecular Structure Company, The Woodlands, Texas.

CIF access

Scheme 1



supplementary materials

Bis bistriphenylphosphineimine dodecasulfurdiirion

Crystal data

$(C_{36}H_{30}NP_2)_2[Fe_2S_{12}]$	F_{000} = 1620
M_r = 1573.52	D_x = 1.416 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 11.379 (2) Å	Cell parameters from 21 reflections
b = 21.004 (4) Å	θ = 3.5–7.5º
c = 15.488 (3) Å	μ = 0.86 mm^{-1}
β = 94.26 (3)º	T = 296 (2) K
V = 3691.5 (12) Å^3	Chunk, black
Z = 2	0.50 × 0.30 × 0.30 mm

Data collection

Rigaku AFC5S diffractometer	R_{int} = 0.030
Radiation source: normal-focus sealed tube	θ_{max} = 25.0º
Monochromator: graphite	θ_{min} = 2.0º
T = 296(2) K	h = 0→12
ω–scans	k = 0→22
Absorption correction: none	l = −18→18
5192 measured reflections	3 standard reflections
4869 independent reflections	every 150 reflections
3680 reflections with $I > 2\sigma(I)$	intensity decay: none

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.040	H-atom parameters constrained
$wR(F^2)$ = 0.118	Calculated $w = 1/[\sigma^2(F_o^2) + (0.0412P)^2 + 2.4083P]$ where $P = (F_o^2 + 2F_c^2)/3$?
S = 1.04	$\Delta\rho_{max}$ = 0.34 e Å^{-3}
4865 reflections	$\Delta\rho_{min}$ = −0.23 e Å^{-3}
415 parameters	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations

between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement on F^2 for ALL reflections except for 4 with very negative F^2 or flagged by the user for potential systematic errors. Weighted *R*-factors *wR* and all goodnesses of fit S are based on F^2, conventional *R*-factors *R* are based on F, with F set to zero for negative F^2. The observed criterion of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating R_factor_obs *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Fe1	0.94236 (5)	0.04986 (3)	0.53221 (4)	0.0424 (2)
S1	0.79242 (10)	0.04438 (5)	0.62630 (7)	0.0506 (3)
S2	0.65819 (11)	0.08933 (7)	0.55487 (8)	0.0689 (4)
S3	0.70687 (14)	0.18350 (7)	0.54878 (10)	0.0835 (5)
S4	0.82859 (14)	0.18720 (7)	0.45769 (9)	0.0818 (5)
S5	0.98725 (11)	0.15665 (6)	0.51621 (8)	0.0614 (3)
S6	0.90477 (10)	0.00034 (6)	0.40787 (7)	0.0487 (3)
N1	1.3528 (3)	0.3438 (2)	0.5410 (2)	0.0426 (8)
P1	1.33209 (9)	0.30615 (5)	0.45270 (6)	0.0351 (3)
C111	1.2017 (3)	0.3283 (2)	0.3878 (2)	0.0367 (9)
C112	1.1994 (4)	0.3858 (2)	0.3417 (3)	0.0539 (12)
H112	1.2670 (4)	0.4107 (2)	0.3417 (3)	0.065*
C113	1.0971 (5)	0.4056 (3)	0.2964 (3)	0.0683 (14)
H113	1.0955 (5)	0.4442 (3)	0.2669 (3)	0.082*
C114	0.9979 (5)	0.3686 (3)	0.2945 (3)	0.0740 (15)
H114	0.9299 (5)	0.3814 (3)	0.2621 (3)	0.089*
C115	0.9984 (4)	0.3130 (3)	0.3399 (3)	0.0651 (14)
H115	0.9299 (4)	0.2889 (3)	0.3402 (3)	0.078*
C116	1.0998 (4)	0.2924 (2)	0.3853 (3)	0.0490 (11)
H116	1.0997 (4)	0.2538 (2)	0.4147 (3)	0.059*
C121	1.4533 (3)	0.3182 (2)	0.3863 (2)	0.0374 (9)
C122	1.5640 (4)	0.3323 (2)	0.4244 (3)	0.0532 (12)
H122	1.5743 (4)	0.3378 (2)	0.4841 (3)	0.064*
C123	1.6591 (4)	0.3384 (3)	0.3750 (3)	0.0707 (15)
H123	1.7333 (4)	0.3476 (3)	0.4014 (3)	0.085*
C124	1.6440 (4)	0.3309 (2)	0.2868 (3)	0.0663 (14)
H124	1.7081 (4)	0.3357 (2)	0.2534 (3)	0.080*
C125	1.5364 (4)	0.3165 (2)	0.2480 (3)	0.0630 (13)
H125	1.5270 (4)	0.3113 (2)	0.1882 (3)	0.076*
C126	1.4410 (4)	0.3098 (2)	0.2972 (3)	0.0524 (12)
H126	1.3677 (4)	0.2994 (2)	0.2705 (3)	0.063*
C131	1.3272 (3)	0.2225 (2)	0.4762 (2)	0.0358 (9)
C132	1.3071 (4)	0.2014 (2)	0.5575 (3)	0.0530 (12)
H132	1.2953 (4)	0.2307 (2)	0.6011 (3)	0.064*
C133	1.3040 (4)	0.1369 (2)	0.5752 (3)	0.0620 (13)
H133	1.2868 (4)	0.1232 (2)	0.6299 (3)	0.074*

C134	1.3258 (4)	0.0937 (2)	0.5138 (3)	0.0560 (12)
H134	1.3247 (4)	0.0504 (2)	0.5263 (3)	0.067*
C135	1.3492 (5)	0.1140 (2)	0.4334 (3)	0.076 (2)
H135	1.3649 (5)	0.0844 (2)	0.3911 (3)	0.091*
C136	1.3498 (5)	0.1780 (2)	0.4143 (3)	0.071 (2)
H136	1.3657 (5)	0.1913 (2)	0.3591 (3)	0.085*
P2	1.30417 (9)	0.39674 (5)	0.59977 (6)	0.0381 (3)
C211	1.4208 (4)	0.4167 (2)	0.6799 (2)	0.0427 (10)
C212	1.4357 (4)	0.4782 (2)	0.7121 (3)	0.0611 (13)
H212	1.3850 (4)	0.5106 (2)	0.6920 (3)	0.073*
C213	1.5265 (5)	0.4912 (3)	0.7741 (3)	0.076 (2)
H213	1.5370 (5)	0.5324 (3)	0.7952 (3)	0.092*
C214	1.6006 (5)	0.4439 (3)	0.8045 (3)	0.082 (2)
H214	1.6616 (5)	0.4531 (3)	0.8460 (3)	0.098*
C215	1.5857 (5)	0.3825 (3)	0.7742 (3)	0.0695 (14)
H215	1.6356 (5)	0.3502 (3)	0.7957 (3)	0.083*
C216	1.4964 (4)	0.3693 (2)	0.7119 (3)	0.0549 (12)
H216	1.4867 (4)	0.3280 (2)	0.6910 (3)	0.066*
C221	1.1793 (4)	0.3721 (2)	0.6554 (2)	0.0419 (10)
C222	1.1031 (4)	0.3261 (2)	0.6219 (3)	0.0518 (11)
H222	1.1175 (4)	0.3064 (2)	0.5699 (3)	0.062*
C223	1.0060 (4)	0.3086 (2)	0.6641 (3)	0.0672 (14)
H223	0.9559 (4)	0.2769 (2)	0.6409 (3)	0.081*
C224	0.9831 (5)	0.3376 (3)	0.7395 (4)	0.0729 (15)
H224	0.9166 (5)	0.3262 (3)	0.7674 (4)	0.087*
C225	1.0572 (5)	0.3830 (3)	0.7743 (3)	0.082 (2)
H225	1.0414 (5)	0.4023 (3)	0.8263 (3)	0.098*
C226	1.1558 (5)	0.4008 (2)	0.7331 (3)	0.072 (2)
H226	1.2062 (5)	0.4319 (2)	0.7574 (3)	0.087*
C231	1.2624 (4)	0.4685 (2)	0.5415 (3)	0.0435 (10)
C232	1.1606 (4)	0.5014 (2)	0.5526 (3)	0.0614 (13)
H232	1.1110 (4)	0.4878 (2)	0.5940 (3)	0.074*
C233	1.1309 (5)	0.5547 (2)	0.5031 (4)	0.080 (2)
H233	1.0619 (5)	0.5768 (2)	0.5113 (4)	0.097*
C234	1.2044 (6)	0.5747 (3)	0.4416 (4)	0.080 (2)
H234	1.1840 (6)	0.6098 (3)	0.4073 (4)	0.097*
C235	1.3068 (5)	0.5429 (3)	0.4311 (3)	0.074 (2)
H235	1.3564 (5)	0.5569 (3)	0.3899 (3)	0.089*
C236	1.3374 (4)	0.4903 (2)	0.4807 (3)	0.0587 (12)
H236	1.4080 (4)	0.4693 (2)	0.4738 (3)	0.070*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Fe1	0.0463 (4)	0.0437 (4)	0.0378 (3)	−0.0027 (3)	0.0071 (3)	−0.0038 (3)
S1	0.0560 (7)	0.0552 (7)	0.0421 (6)	−0.0048 (6)	0.0129 (5)	0.0006 (5)
S2	0.0530 (8)	0.0925 (10)	0.0615 (8)	0.0052 (7)	0.0073 (6)	−0.0004 (7)
S3	0.0965 (11)	0.0735 (10)	0.0842 (10)	0.0305 (8)	0.0330 (9)	0.0134 (8)

S4	0.0896 (11)	0.0889 (11)	0.0693 (9)	0.0171 (9)	0.0211 (8)	0.0303 (8)
S5	0.0687 (8)	0.0483 (7)	0.0682 (8)	−0.0116 (6)	0.0116 (6)	0.0020 (6)
S6	0.0490 (7)	0.0578 (7)	0.0390 (6)	−0.0010 (6)	0.0008 (5)	−0.0059 (5)
N1	0.051 (2)	0.043 (2)	0.034 (2)	0.002 (2)	0.001 (2)	−0.006 (2)
P1	0.0396 (6)	0.0380 (6)	0.0281 (5)	−0.0027 (5)	0.0047 (4)	−0.0015 (4)
C111	0.041 (2)	0.043 (2)	0.027 (2)	−0.002 (2)	0.008 (2)	−0.001 (2)
C112	0.063 (3)	0.058 (3)	0.041 (2)	−0.012 (2)	0.001 (2)	0.014 (2)
C113	0.079 (4)	0.069 (3)	0.055 (3)	0.010 (3)	−0.007 (3)	0.025 (3)
C114	0.062 (3)	0.091 (4)	0.066 (3)	0.009 (3)	−0.017 (3)	0.012 (3)
C115	0.044 (3)	0.078 (4)	0.071 (3)	−0.006 (3)	−0.009 (2)	0.005 (3)
C116	0.048 (3)	0.056 (3)	0.043 (2)	0.000 (2)	0.002 (2)	0.005 (2)
C121	0.037 (2)	0.037 (2)	0.038 (2)	−0.005 (2)	0.006 (2)	0.002 (2)
C122	0.049 (3)	0.068 (3)	0.043 (3)	−0.007 (2)	0.007 (2)	−0.005 (2)
C123	0.043 (3)	0.096 (4)	0.074 (4)	−0.011 (3)	0.005 (3)	−0.006 (3)
C124	0.059 (3)	0.080 (4)	0.063 (3)	−0.007 (3)	0.026 (3)	−0.001 (3)
C125	0.059 (3)	0.089 (4)	0.043 (3)	−0.013 (3)	0.018 (2)	−0.001 (2)
C126	0.048 (3)	0.072 (3)	0.038 (2)	−0.016 (2)	0.008 (2)	−0.002 (2)
C131	0.037 (2)	0.037 (2)	0.033 (2)	−0.003 (2)	0.003 (2)	0.000 (2)
C132	0.072 (3)	0.047 (3)	0.039 (2)	0.006 (2)	0.000 (2)	0.003 (2)
C133	0.089 (4)	0.050 (3)	0.046 (3)	−0.006 (3)	0.003 (3)	0.016 (2)
C134	0.060 (3)	0.035 (3)	0.072 (3)	−0.003 (2)	0.003 (3)	0.006 (2)
C135	0.118 (5)	0.043 (3)	0.071 (4)	−0.003 (3)	0.032 (3)	−0.008 (3)
C136	0.122 (5)	0.045 (3)	0.050 (3)	−0.013 (3)	0.035 (3)	−0.003 (2)
P2	0.0457 (6)	0.0374 (6)	0.0313 (5)	−0.0015 (5)	0.0027 (5)	−0.0027 (5)
C211	0.049 (3)	0.044 (2)	0.035 (2)	−0.004 (2)	0.004 (2)	−0.001 (2)
C212	0.072 (3)	0.057 (3)	0.053 (3)	−0.005 (3)	−0.005 (3)	−0.014 (2)
C213	0.090 (4)	0.075 (4)	0.063 (3)	−0.021 (3)	−0.004 (3)	−0.023 (3)
C214	0.077 (4)	0.116 (5)	0.049 (3)	−0.028 (4)	−0.014 (3)	−0.002 (3)
C215	0.068 (3)	0.085 (4)	0.054 (3)	−0.001 (3)	−0.013 (3)	0.017 (3)
C216	0.067 (3)	0.056 (3)	0.041 (2)	−0.009 (3)	−0.005 (2)	0.008 (2)
C221	0.056 (3)	0.036 (2)	0.035 (2)	0.001 (2)	0.010 (2)	−0.003 (2)
C222	0.051 (3)	0.062 (3)	0.044 (2)	−0.005 (2)	0.012 (2)	−0.008 (2)
C223	0.060 (3)	0.072 (3)	0.071 (3)	−0.013 (3)	0.018 (3)	0.000 (3)
C224	0.069 (4)	0.078 (4)	0.076 (4)	0.005 (3)	0.036 (3)	0.015 (3)
C225	0.110 (5)	0.083 (4)	0.059 (3)	0.000 (4)	0.051 (3)	−0.008 (3)
C226	0.100 (4)	0.065 (3)	0.056 (3)	−0.013 (3)	0.030 (3)	−0.019 (3)
C231	0.048 (3)	0.038 (2)	0.044 (2)	−0.004 (2)	−0.002 (2)	0.005 (2)
C232	0.051 (3)	0.053 (3)	0.080 (3)	−0.001 (2)	0.004 (3)	0.010 (3)
C233	0.061 (3)	0.059 (3)	0.119 (5)	0.002 (3)	−0.013 (3)	0.022 (3)
C234	0.091 (4)	0.057 (3)	0.088 (4)	−0.011 (3)	−0.027 (4)	0.032 (3)
C235	0.092 (4)	0.065 (4)	0.065 (3)	−0.015 (3)	−0.002 (3)	0.023 (3)
C236	0.059 (3)	0.057 (3)	0.059 (3)	−0.008 (2)	0.000 (2)	0.007 (2)

Geometric parameters (Å, °)

Fe1—S6^{i}	2.1816 (13)	C131—C132	1.370 (5)
Fe1—S6	2.2025 (12)	C131—C136	1.376 (6)
Fe1—S5	2.3178 (14)	C132—C133	1.383 (6)
Fe1—S1	2.3276 (14)	C133—C134	1.351 (6)

Fe1—Fe1^{i}	2.7014 (12)	C134—C135	1.360 (6)
S1—S2	2.049 (2)	C135—C136	1.378 (6)
S2—S3	2.058 (2)	P2—C221	1.792 (4)
S3—S4	2.051 (2)	P2—C211	1.799 (4)
S4—S5	2.061 (2)	P2—C231	1.803 (4)
S6—Fe1^{i}	2.1816 (13)	C211—C216	1.384 (6)
N1—P2	1.563 (3)	C211—C212	1.390 (6)
N1—P1	1.583 (3)	C212—C213	1.384 (7)
P1—C111	1.790 (4)	C213—C214	1.364 (7)
P1—C131	1.796 (4)	C214—C215	1.378 (7)
P1—C121	1.799 (4)	C215—C216	1.377 (6)
C111—C116	1.383 (5)	C221—C222	1.374 (6)
C111—C112	1.403 (5)	C221—C226	1.390 (6)
C112—C113	1.378 (6)	C222—C223	1.375 (6)
C113—C114	1.369 (7)	C223—C224	1.360 (7)
C114—C115	1.364 (7)	C224—C225	1.357 (7)
C115—C116	1.376 (6)	C225—C226	1.383 (7)
C121—C122	1.383 (5)	C231—C232	1.371 (6)
C121—C126	1.387 (5)	C231—C236	1.393 (6)
C122—C123	1.377 (6)	C232—C233	1.384 (6)
C123—C124	1.373 (7)	C233—C234	1.378 (8)
C124—C125	1.358 (6)	C234—C235	1.363 (8)
C125—C126	1.380 (6)	C235—C236	1.376 (7)
S6^{i}—Fe1—S6	103.93 (5)	C132—C131—C136	118.2 (4)
S6^{i}—Fe1—S5	109.76 (5)	C132—C131—P1	120.8 (3)
S6—Fe1—S5	113.18 (5)	C136—C131—P1	120.8 (3)
S6^{i}—Fe1—S1	107.94 (5)	C131—C132—C133	120.4 (4)
S6—Fe1—S1	114.85 (5)	C134—C133—C132	120.7 (4)
S5—Fe1—S1	107.00 (5)	C133—C134—C135	119.5 (4)
S6^{i}—Fe1—Fe1^{i}	52.31 (4)	C134—C135—C136	120.5 (5)
S6—Fe1—Fe1^{i}	51.61 (4)	C131—C136—C135	120.6 (4)
S5—Fe1—Fe1^{i}	126.44 (5)	N1—P2—C221	113.7 (2)
S1—Fe1—Fe1^{i}	126.26 (5)	N1—P2—C211	107.0 (2)
S2—S1—Fe1	101.00 (6)	C221—P2—C211	107.8 (2)
S1—S2—S3	105.98 (8)	N1—P2—C231	113.2 (2)
S4—S3—S2	105.42 (8)	C221—P2—C231	107.1 (2)
S3—S4—S5	107.46 (8)	C211—P2—C231	107.7 (2)
S4—S5—Fe1	98.94 (7)	C216—C211—C212	119.0 (4)
Fe1^{i}—S6—Fe1	76.07 (5)	C216—C211—P2	119.1 (3)
P2—N1—P1	145.3 (2)	C212—C211—P2	121.9 (3)
N1—P1—C111	114.8 (2)	C213—C212—C211	119.7 (5)
N1—P1—C131	108.6 (2)	C214—C213—C212	120.5 (5)
C111—P1—C131	109.4 (2)	C213—C214—C215	120.4 (5)
N1—P1—C121	110.6 (2)	C216—C215—C214	119.5 (5)
C111—P1—C121	106.3 (2)	C215—C216—C211	120.8 (5)
C131—P1—C121	106.9 (2)	C222—C221—C226	118.4 (4)
C116—C111—C112	118.1 (4)	C222—C221—P2	121.5 (3)

C116—C111—P1	122.2 (3)	C226—C221—P2	120.1 (3)
C112—C111—P1	119.6 (3)	C221—C222—C223	121.1 (4)
C113—C112—C111	120.2 (4)	C224—C223—C222	120.0 (5)
C114—C113—C112	120.2 (5)	C225—C224—C223	120.2 (5)
C115—C114—C113	120.2 (5)	C224—C225—C226	120.5 (5)
C114—C115—C116	120.3 (5)	C225—C226—C221	119.8 (5)
C115—C116—C111	120.8 (4)	C232—C231—C236	119.0 (4)
C122—C121—C126	118.2 (4)	C232—C231—P2	123.5 (3)
C122—C121—P1	119.9 (3)	C236—C231—P2	117.5 (3)
C126—C121—P1	121.7 (3)	C231—C232—C233	120.8 (5)
C123—C122—C121	120.8 (4)	C234—C233—C232	119.6 (5)
C124—C123—C122	119.8 (5)	C235—C234—C233	120.1 (5)
C125—C124—C123	120.5 (4)	C234—C235—C236	120.6 (5)
C124—C125—C126	119.9 (4)	C235—C236—C231	119.9 (5)
C125—C126—C121	120.8 (4)		

Symmetry codes: (i) −*x*+2, −*y*, −*z*+1.