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Bromidocarbonyl{(1*S*,2*S*)-*N*-[2-(dicyclohexylphosphanyl)ethylidenyl]-*N*′-[2-(diphenylphosphanyl)ethyl]-1,2-diphenylethane-1,2-diamine}iron(II) tetraphenylborate

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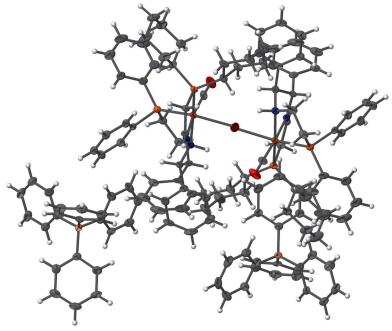
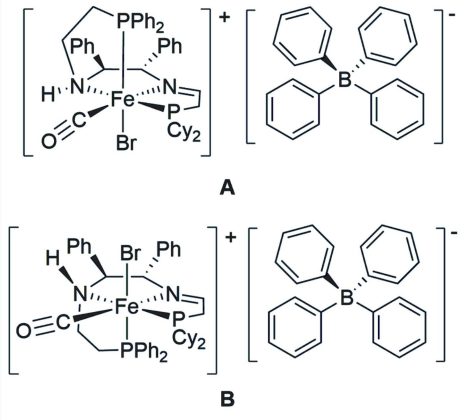
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, *trans*-(*S*,*S*)-[FeBr(CO)($PPh_2CH_2CH_2NHCHPhCHPhNCHCH_2PCy_2$)]$BPh_4$, the Fe^{II} ion is in a distorted octahedral complex geometry with a *cis*-β ligand geometry in which two diastereomers co-crystallized in the asymmetric unit. These diastereomers differ by the orientation of the N—H moieties on the ligand; one is in the *S* conformation (**A**), and the other *R* (**B**). Diastereomer **A** has a P—Fe—P angle of 104.36 (6)° and **B** has a P—Fe—P angle of 102.70 (6)°. During the refinement of the structure, electron density peaks were located that were believed to be highly disordered solvent molecules (possibly diethyl ether). Attempts made to model the solvent molecule were not successful. The SQUEEZE [Spek (2015). *Acta Cryst.* C**71**, 9–18] option in *PLATON* indicated there was a large solvent cavity of 363 Å^3. In the final cycles of refinement, this contribution of 117 electrons to the electron density was removed from the observed data. The density, the *F*(000) value, the molecular weight and the formula are given without taking into account the results obtained with SQUEEZE.

3D view



Chemical scheme



Structure description

This is the first time our group has observed that our P—N—NH—P ligands adopt a *cis*-β ligand geometry on the iron(II) center. The initial report of this complex (Smith & Morris, 2015) had assumed that there was a *mer*-geometry of the tetradentate ligand; however, it was not until after the article had been published that crystals were obtained for X-ray diffraction study. This complex has been applied in the catalytic asymmetric

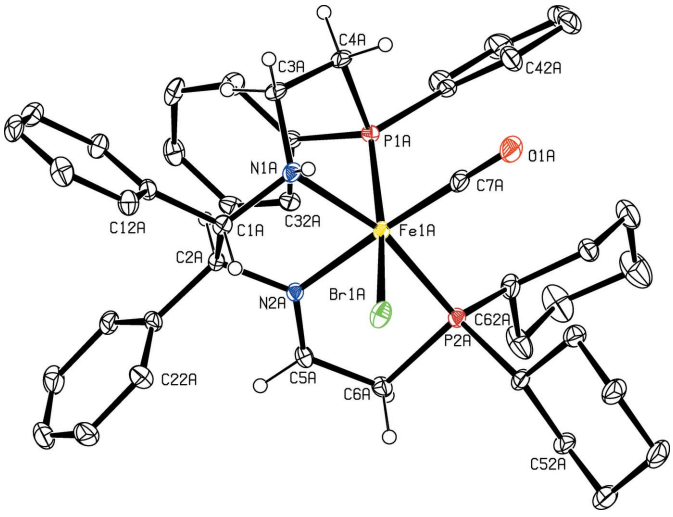


Figure 1
The molecular structure of one of the cations in the asymmetric unit, showing 30% displacement ellipsoids (phenyl-H atoms have been omitted for clarity).

transfer hydrogenation of ketones yielding high enantioselectivities for a variety of ketones.

The molecular structures of the two cations in the asymmetric unit are shown in Figs. 1 and 2. The Fe^{II} ions are in distorted octahedral coordination environments.

Synthesis and crystallization

A 100 mL Schlenk flask was charged with sodium methoxide (64 mg, 1.176 mmol) and dicyclohexylphosphonium bromide dimer (378 mg, 5.88×10^{-1} mmol) in 25 ml methanol and stirred for no more than two minutes. A solution of dissolved $[Fe(H_2O)_6][BF_4]_2$ (496 mg, 1.47 mmol) in 20 mL acetonitrile

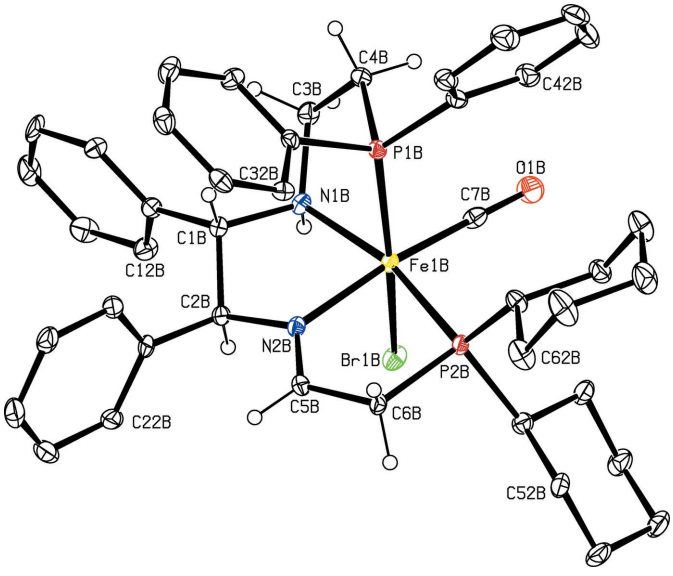


Figure 2
The molecular structure of the other cation in the asymmetric unit showing 30% displacement ellipsoids (phenyl H atoms have been omitted for clarity).

Table 1
Experimental details.

Crystal data	
Chemical formula	$[FeBr(C_{43}H_{52}N_2OP_2)](C_{24}H_{20}B)$
M_r	1129.77
Crystal system, space group	Triclinic, *P*1
Temperature (K)	147
a, *b*, *c* (Å)	12.8083 (8), 14.637 (1), 18.9082 (12)
α, β, γ (°)	106.916 (2), 98.406 (2), 110.635 (2)
V (Å^3)	3048.9 (3)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	1.00
Crystal size (mm)	0.27 × 0.24 × 0.08
Data collection	
Diffractometer	Bruker Kappa APEX DUO CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2014)
T_{min}, T_{max}	0.699, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	100485, 27968, 23633
R_{int}	0.040
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.651
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.040, 0.089, 1.04
No. of reflections	27968
No. of parameters	1351
No. of restraints	3
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.46, −0.72
Absolute structure	Flack *x* determined using 10019 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons et al., 2013)
Absolute structure parameter	0.031 (4)

Computer programs: *APEX2* and *SAINT* (Bruker, 2014), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2014* (Sheldrick, 2015*b*), *PLATON* (Spek, 2009) and *SHELXTL* (Sheldrick, 2008).

was added to the Schlenk flask, followed by a solution of (*S,S*)-$PPh_2CH_2CH_2NHCH(Ph)CH(Ph)NH_2$ (Zuo *et al.*, 2013; Zuo & Morris, 2015) in 10 mL methanol. This resulted in a purple solution, which was left to stir at room temperature for 16 h, after which a colour change from purple to pink was observed. The solvent was removed *in vacuo*. KBr (140 mg, 4.70 mmol) was added to the flask, which was sealed and removed from the glovebox. The atmosphere of the flask was replaced with CO using Schlenk techniques. 20 mL dry acetone was added to the flask and stirred for 1.5 h. The solvent was removed under vacuum to ensure maximum removal of acetonitrile and the residual orange solid was redissolved in 20 ml acetone while under CO atmosphere. This was stirred for 1 h, after which the solvent was removed and the flask brought into the glovebox, where the remaining steps occurred. The solid residue was dissolved in 20 ml dichloromethane and filtered through a pad of celite, then through a 25 mm Syringe Filter PTFE membrane (pore size 0.45 µm). The clear orange solution was dried *in vacuo*, then dissolved in minimal methanol. This solution was added to a vial charged with a stir bar and $NaBPh_4$ (402 mg, 1.294 mmol) dissolved in minimal methanol, from which a yellow solid precipitated. This solid was filtered off and washed with diethyl ether (3 × 15 ml) and dried overnight. Yield: 530 mg (40%). Suitable crystals for an X-ray

diffraction study were obtained by layering a concentrated solution of the title compound in dichloromethane with diethyl ether.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1. During the refinement of the structure, electron density peaks were located that were believed to be highly disordered solvent molecules (possibly diethyl ether). Attempts made to model the solvent molecule were not successful. The SQUEEZE (Spek, 2015) option in *PLATON* (Spek, 2009) indicated there was a large solvent cavity of 363 Å^3. In the final cycles of refinement, this contribution of 117 electrons to the electron density was removed from the observed data. The density, the *F*(000) value, the molecular weight and the formula are given without taking into account the results obtained with SQUEEZE.

Acknowledgements

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full crystallographic data

IUCrData (2017). **2**, x170452 [https://doi.org/10.1107/S2414314617004527]

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Crystal data

$[FeBr(C_{43}H_{52}N_2OP_2)](C_{24}H_{20}B)$
M_r = 1129.77
Triclinic, $P\overline{1}$
a = 12.8083 (8) Å
b = 14.637 (1) Å
c = 18.9082 (12) Å
α = 106.916 (2)°
β = 98.406 (2)°
γ = 110.635 (2)°
V = 3048.9 (3) Å^3
Z = 2
$F(000)$ = 1184
D_x = 1.231 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9764 reflections
θ = 2.3–26.9°
μ = 1.00 mm^{-1}
T = 147 K
Plate, brown
0.27 × 0.24 × 0.08 mm

Data collection

Bruker Kappa APEX DUO CCD diffractometer
Radiation source: sealed tube with Bruker Triumph monochormator
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2014)
T_{min} = 0.699, T_{max} = 0.746
100485 measured reflections
27968 independent reflections
23633 reflections with $I > 2\sigma(I)$
R_{int} = 0.040
θ_{max} = 27.6°, θ_{min} = 1.6°
h = −16→16
k = −19→19
l = −24→24

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.089
S = 1.04
27968 reflections
1351 parameters
3 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0286P)^2 + 2.0989P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.007
$\Delta\rho_{max}$ = 0.46 e Å^{-3}
$\Delta\rho_{min}$ = −0.72 e Å^{-3}
Absolute structure: Flack x determined using 10019 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons et al., 2013)
Absolute structure parameter: 0.031 (4)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Fe1A	0.47961 (6)	0.31754 (5)	0.58673 (4)	0.01673 (16)
Br1A	0.32265 (4)	0.24165 (4)	0.46381 (3)	0.02753 (13)
P1A	0.64697 (11)	0.37862 (10)	0.67748 (8)	0.0182 (3)
P2A	0.36422 (12)	0.37319 (10)	0.65025 (8)	0.0187 (3)
O1A	0.5753 (4)	0.5059 (4)	0.5521 (3)	0.0383 (11)
N1A	0.5539 (4)	0.2289 (3)	0.5222 (3)	0.0189 (9)
H1A	0.5428	0.2380	0.4717	0.023*
N2A	0.4039 (3)	0.1867 (3)	0.6051 (2)	0.0164 (9)
C1A	0.4789 (4)	0.1144 (3)	0.5042 (3)	0.0207 (9)
H1AA	0.4044	0.0967	0.4667	0.025*
C2A	0.4481 (4)	0.1047 (3)	0.5776 (2)	0.0179 (8)
H2AA	0.5217	0.1243	0.6167	0.021*
C3A	0.6810 (5)	0.2611 (4)	0.5508 (3)	0.0228 (11)
H3AA	0.7161	0.2604	0.5074	0.027*
H3AB	0.6940	0.2100	0.5715	0.027*
C4A	0.7396 (5)	0.3704 (4)	0.6132 (3)	0.0237 (12)
H4AA	0.7495	0.4243	0.5900	0.028*
H4AB	0.8172	0.3823	0.6421	0.028*
C5A	0.3177 (5)	0.1690 (4)	0.6339 (3)	0.0198 (11)
H5AA	0.2808	0.1023	0.6374	0.024*
C6A	0.2745 (5)	0.2502 (4)	0.6617 (3)	0.0216 (11)
H6AA	0.2774	0.2645	0.7166	0.026*
H6AB	0.1927	0.2244	0.6322	0.026*
C7A	0.5378 (5)	0.4313 (5)	0.5655 (3)	0.0245 (12)
C11A	0.5265 (5)	0.0373 (4)	0.4657 (3)	0.0213 (11)
C12A	0.4866 (5)	−0.0115 (4)	0.3862 (3)	0.0261 (12)
H12A	0.4309	0.0036	0.3584	0.031*
C13A	0.5266 (5)	−0.0816 (5)	0.3468 (3)	0.0327 (13)
H13A	0.4989	−0.1136	0.2923	0.039*
C14A	0.6050 (5)	−0.1051 (5)	0.3853 (4)	0.0311 (13)
H14A	0.6319	−0.1537	0.3580	0.037*
C15A	0.6462 (5)	−0.0576 (5)	0.4653 (4)	0.0302 (13)
H15A	0.7021	−0.0730	0.4926	0.036*
C16A	0.6055 (5)	0.0120 (4)	0.5048 (3)	0.0249 (12)
H16A	0.6321	0.0428	0.5594	0.030*
C21A	0.3644 (5)	−0.0046 (4)	0.5680 (3)	0.0214 (11)
C22A	0.2671 (5)	−0.0636 (4)	0.5058 (3)	0.0321 (12)
H22A	0.2541	−0.0379	0.4661	0.038*
C23A	0.1882 (5)	−0.1605 (4)	0.5010 (4)	0.0410 (14)

H23A	0.1215	−0.2011	0.4580	0.049*
C24A	0.2062 (6)	−0.1976 (5)	0.5581 (5)	0.0460 (19)
H24A	0.1508	−0.2632	0.5549	0.055*
C25A	0.3038 (6)	−0.1409 (5)	0.6205 (4)	0.0382 (15)
H25A	0.3168	−0.1679	0.6593	0.046*
C26A	0.3831 (5)	−0.0434 (4)	0.6254 (4)	0.0276 (12)
H26A	0.4502	−0.0034	0.6681	0.033*
C31A	0.6613 (4)	0.2952 (4)	0.7300 (3)	0.0178 (10)
C32A	0.5845 (5)	0.2698 (4)	0.7747 (3)	0.0229 (12)
H32A	0.5253	0.2946	0.7757	0.027*
C33A	0.5950 (5)	0.2092 (4)	0.8168 (3)	0.0254 (12)
H33A	0.5441	0.1939	0.8477	0.030*
C34A	0.6788 (5)	0.1708 (5)	0.8142 (3)	0.0298 (13)
H34A	0.6847	0.1281	0.8427	0.036*
C35A	0.7534 (6)	0.1938 (5)	0.7709 (4)	0.0312 (13)
H35A	0.8104	0.1663	0.7691	0.037*
C36A	0.7468 (5)	0.2570 (5)	0.7294 (3)	0.0270 (12)
H36A	0.8007	0.2741	0.7006	0.032*
C41A	0.7270 (5)	0.5109 (4)	0.7524 (3)	0.0245 (12)
C42A	0.7577 (6)	0.5977 (5)	0.7312 (4)	0.0380 (16)
H42A	0.7359	0.5887	0.6786	0.046*
C43A	0.8209 (6)	0.6990 (5)	0.7874 (5)	0.0462 (19)
H43A	0.8433	0.7586	0.7730	0.055*
C44A	0.8501 (6)	0.7112 (5)	0.8634 (5)	0.050 (2)
H44A	0.8915	0.7799	0.9015	0.060*
C45A	0.8208 (6)	0.6261 (5)	0.8853 (4)	0.0425 (17)
H45A	0.8426	0.6359	0.9381	0.051*
C46A	0.7588 (5)	0.5255 (5)	0.8297 (4)	0.0330 (14)
H46A	0.7381	0.4663	0.8447	0.040*
C51A	0.2532 (5)	0.4015 (5)	0.5971 (3)	0.0230 (12)
H51A	0.2029	0.3334	0.5536	0.028*
C52A	0.1692 (5)	0.4286 (5)	0.6408 (4)	0.0271 (13)
H52A	0.1357	0.3744	0.6625	0.033*
H52B	0.2126	0.4970	0.6842	0.033*
C53A	0.0720 (6)	0.4344 (6)	0.5886 (4)	0.0382 (16)
H53A	0.0227	0.3637	0.5490	0.046*
H53B	0.0228	0.4567	0.6192	0.046*
C54A	0.1186 (6)	0.5108 (6)	0.5495 (5)	0.0418 (17)
H54A	0.1605	0.5828	0.5887	0.050*
H54B	0.0531	0.5093	0.5135	0.050*
C55A	0.2007 (6)	0.4831 (6)	0.5054 (4)	0.0362 (16)
H55A	0.1570	0.4138	0.4630	0.043*
H55B	0.2325	0.5360	0.4824	0.043*
C56A	0.3001 (5)	0.4796 (5)	0.5579 (4)	0.0279 (13)
H56A	0.3482	0.5505	0.5975	0.033*
H56B	0.3499	0.4583	0.5274	0.033*
C61A	0.4324 (5)	0.4762 (5)	0.7484 (3)	0.0269 (13)
H61A	0.5040	0.4681	0.7686	0.032*

C62A	0.3672 (7)	0.4700 (5)	0.8077 (4)	0.0439 (18)
H62A	0.3439	0.3997	0.8111	0.053*
H62B	0.2959	0.4798	0.7923	0.053*
C63A	0.4431 (7)	0.5551 (6)	0.8871 (4)	0.0504 (19)
H63A	0.3977	0.5513	0.9251	0.061*
H63B	0.5114	0.5420	0.9043	0.061*
C64A	0.4838 (8)	0.6644 (6)	0.8834 (5)	0.057 (2)
H64A	0.4158	0.6802	0.8710	0.068*
H64B	0.5353	0.7173	0.9343	0.068*
C65A	0.5474 (6)	0.6714 (5)	0.8241 (4)	0.0393 (16)
H65A	0.6206	0.6646	0.8402	0.047*
H65B	0.5680	0.7414	0.8204	0.047*
C66A	0.4769 (5)	0.5870 (4)	0.7454 (3)	0.0251 (12)
H66A	0.5256	0.5908	0.7093	0.030*
H66B	0.4098	0.6002	0.7255	0.030*
Fe1B	0.52061 (5)	0.30550 (5)	0.25957 (4)	0.01600 (16)
Br1B	0.66082 (4)	0.37006 (4)	0.38985 (3)	0.02588 (13)
P1B	0.35682 (11)	0.25002 (10)	0.16651 (8)	0.0171 (3)
P2B	0.63287 (11)	0.24639 (10)	0.19442 (8)	0.0166 (3)
O1B	0.4105 (4)	0.1166 (4)	0.2908 (3)	0.0372 (11)
N1B	0.4429 (4)	0.3947 (3)	0.3173 (2)	0.0187 (9)
H1B	0.4770	0.4134	0.3733	0.022*
N2B	0.6168 (4)	0.4410 (3)	0.2523 (2)	0.0177 (9)
C1B	0.4795 (4)	0.4981 (3)	0.3045 (2)	0.0178 (8)
H1BA	0.4323	0.4842	0.2524	0.021*
C2B	0.6060 (4)	0.5344 (3)	0.3043 (3)	0.0185 (9)
H2BA	0.6525	0.5518	0.3575	0.022*
C3B	0.3130 (5)	0.3429 (4)	0.3028 (3)	0.0234 (12)
H3BA	0.2803	0.3948	0.3023	0.028*
H3BB	0.2952	0.3186	0.3452	0.028*
C4B	0.2560 (5)	0.2492 (4)	0.2261 (3)	0.0205 (11)
H4BA	0.1863	0.2518	0.1981	0.025*
H4BB	0.2310	0.1830	0.2360	0.025*
C5B	0.6992 (4)	0.4552 (4)	0.2212 (3)	0.0201 (11)
H5BA	0.7476	0.5243	0.2261	0.024*
C6B	0.7210 (5)	0.3644 (4)	0.1768 (3)	0.0188 (11)
H6BA	0.8045	0.3802	0.1933	0.023*
H6BB	0.6995	0.3514	0.1211	0.023*
C7B	0.4529 (5)	0.1906 (5)	0.2775 (3)	0.0231 (12)
C11B	0.4571 (4)	0.5798 (4)	0.3636 (3)	0.0202 (11)
C12B	0.5181 (5)	0.6212 (4)	0.4403 (3)	0.0263 (12)
H12B	0.5754	0.5990	0.4569	0.032*
C13B	0.4958 (5)	0.6950 (5)	0.4929 (3)	0.0314 (13)
H13B	0.5378	0.7233	0.5457	0.038*
C14B	0.4127 (6)	0.7275 (5)	0.4690 (4)	0.0370 (15)
H14B	0.3986	0.7788	0.5054	0.044*
C15B	0.3504 (6)	0.6863 (5)	0.3930 (4)	0.0318 (14)
H15B	0.2920	0.7076	0.3770	0.038*

C16B	0.3734 (5)	0.6132 (5)	0.3399 (4)	0.0243 (12)
H16B	0.3319	0.5857	0.2871	0.029*
C21B	0.6530 (5)	0.6309 (4)	0.2850 (3)	0.0223 (11)
C22B	0.7602 (4)	0.7130 (4)	0.3307 (3)	0.0290 (12)
H22B	0.7996	0.7100	0.3761	0.035*
C23B	0.8093 (5)	0.7993 (5)	0.3097 (5)	0.0428 (17)
H23B	0.8822	0.8545	0.3408	0.051*
C24B	0.7534 (5)	0.8050 (4)	0.2449 (4)	0.0449 (17)
H24B	0.7877	0.8637	0.2308	0.054*
C25B	0.6463 (5)	0.7248 (4)	0.1996 (4)	0.0349 (14)
H25B	0.6070	0.7292	0.1549	0.042*
C26B	0.5965 (5)	0.6383 (4)	0.2193 (3)	0.0249 (12)
H26B	0.5234	0.5836	0.1879	0.030*
C31B	0.7438 (5)	0.2208 (5)	0.2501 (3)	0.0219 (12)
H31A	0.7925	0.2898	0.2931	0.026*
C32B	0.4175 (5)	0.3573 (4)	0.0695 (3)	0.0210 (11)
H32B	0.4766	0.3323	0.0683	0.025*
C33B	0.4046 (5)	0.4152 (4)	0.0250 (3)	0.0240 (12)
H33B	0.4528	0.4273	−0.0080	0.029*
C34B	0.3215 (5)	0.4553 (5)	0.0286 (3)	0.0289 (13)
H34B	0.3131	0.4952	−0.0017	0.035*
C35B	0.2507 (6)	0.4370 (5)	0.0764 (4)	0.0313 (14)
H35B	0.1949	0.4659	0.0799	0.038*
C36B	0.2614 (5)	0.3764 (4)	0.1190 (3)	0.0232 (12)
H36B	0.2115	0.3624	0.1508	0.028*
C39B	0.3454 (4)	0.3358 (4)	0.1155 (3)	0.0188 (11)
C41B	0.2780 (5)	0.1189 (4)	0.0899 (3)	0.0225 (11)
C42B	0.2413 (5)	0.0301 (5)	0.1092 (4)	0.0285 (13)
H42B	0.2594	0.0372	0.1617	0.034*
C43B	0.1783 (5)	−0.0691 (5)	0.0519 (4)	0.0393 (16)
H43B	0.1555	−0.1295	0.0653	0.047*
C44B	0.1487 (5)	−0.0804 (5)	−0.0242 (4)	0.0393 (16)
H44B	0.1040	−0.1482	−0.0629	0.047*
C45B	0.1842 (5)	0.0073 (5)	−0.0442 (4)	0.0369 (15)
H45B	0.1645	−0.0003	−0.0967	0.044*
C46B	0.2490 (5)	0.1066 (5)	0.0129 (3)	0.0263 (12)
H46B	0.2736	0.1666	−0.0010	0.032*
C52B	0.8294 (5)	0.1960 (5)	0.2082 (4)	0.0270 (13)
H52C	0.8622	0.2500	0.1863	0.032*
H52D	0.7882	0.1270	0.1653	0.032*
C53B	0.9282 (5)	0.1938 (5)	0.2638 (4)	0.0333 (15)
H53C	0.9783	0.1708	0.2344	0.040*
H53D	0.9765	0.2658	0.3019	0.040*
C54B	0.8830 (6)	0.1204 (5)	0.3060 (4)	0.0339 (14)
H54C	0.8448	0.0469	0.2687	0.041*
H54D	0.9491	0.1266	0.3444	0.041*
C55B	0.7978 (6)	0.1456 (5)	0.3461 (4)	0.0319 (14)
H55C	0.8385	0.2157	0.3878	0.038*

H55D	0.7662	0.0933	0.3696	0.038*
C56B	0.6979 (5)	0.1448 (5)	0.2905 (4)	0.0264 (13)
H56C	0.6459	0.1653	0.3193	0.032*
H56D	0.6522	0.0729	0.2517	0.032*
C61B	0.5650 (5)	0.1411 (4)	0.0975 (3)	0.0213 (12)
H61B	0.4954	0.1501	0.0748	0.026*
C62B	0.6390 (6)	0.1465 (5)	0.0394 (4)	0.0338 (14)
H62C	0.6642	0.2163	0.0351	0.041*
H62D	0.7092	0.1368	0.0582	0.041*
C63B	0.5679 (7)	0.0609 (5)	−0.0396 (4)	0.0433 (17)
H63C	0.5025	0.0754	−0.0605	0.052*
H63D	0.6175	0.0627	−0.0752	0.052*
C64B	0.5211 (6)	−0.0463 (5)	−0.0357 (4)	0.0405 (16)
H64C	0.5866	−0.0638	−0.0201	0.049*
H64D	0.4728	−0.0986	−0.0875	0.049*
C65B	0.4491 (6)	−0.0529 (5)	0.0206 (4)	0.0369 (15)
H65C	0.4241	−0.1233	0.0239	0.044*
H65D	0.3786	−0.0436	0.0017	0.044*
C66B	0.5181 (5)	0.0317 (4)	0.1009 (4)	0.0266 (13)
H66C	0.4671	0.0285	0.1356	0.032*
H66D	0.5835	0.0176	0.1223	0.032*
C71A	0.9590 (5)	1.0170 (4)	0.6145 (3)	0.0211 (12)
C72A	0.9233 (5)	1.0988 (5)	0.6234 (3)	0.0259 (12)
H72A	0.8904	1.1166	0.6644	0.031*
C73A	0.9338 (5)	1.1550 (5)	0.5750 (4)	0.0323 (14)
H73A	0.9079	1.2096	0.5831	0.039*
C74A	0.9823 (5)	1.1313 (5)	0.5148 (4)	0.0345 (15)
H74A	0.9889	1.1687	0.4810	0.041*
C75A	1.0207 (6)	1.0526 (5)	0.5048 (3)	0.0354 (15)
H75A	1.0556	1.0368	0.4646	0.043*
C76A	1.0084 (5)	0.9964 (5)	0.5535 (4)	0.0289 (13)
H76A	1.0345	0.9419	0.5451	0.035*
C81A	0.8466 (5)	0.9485 (4)	0.7135 (3)	0.0207 (12)
C82A	0.8528 (5)	0.9599 (5)	0.7906 (3)	0.0280 (13)
H82A	0.9261	0.9803	0.8249	0.034*
C83A	0.7567 (6)	0.9426 (6)	0.8184 (4)	0.0375 (16)
H83A	0.7648	0.9505	0.8708	0.045*
C84A	0.6476 (6)	0.9136 (5)	0.7700 (4)	0.0341 (15)
H84A	0.5816	0.9037	0.7893	0.041*
C85A	0.6379 (5)	0.8997 (5)	0.6939 (4)	0.0318 (14)
H85A	0.5639	0.8771	0.6595	0.038*
C86A	0.7350 (5)	0.9185 (5)	0.6672 (4)	0.0300 (14)
H86A	0.7259	0.9108	0.6147	0.036*
C91A	1.0821 (5)	1.0341 (5)	0.7418 (3)	0.0227 (12)
C92A	1.0990 (5)	1.1283 (5)	0.7980 (3)	0.0274 (13)
H92A	1.0343	1.1453	0.8011	0.033*
C93A	1.2075 (5)	1.1990 (5)	0.8499 (3)	0.0307 (14)
H93A	1.2152	1.2623	0.8874	0.037*

C94A	1.3033 (5)	1.1768 (5)	0.8468 (4)	0.0331 (15)
H94A	1.3770	1.2238	0.8822	0.040*
C95A	1.2900 (5)	1.0853 (5)	0.7916 (4)	0.0339 (15)
H95A	1.3553	1.0692	0.7889	0.041*
C96A	1.1832 (5)	1.0164 (5)	0.7400 (3)	0.0265 (13)
H96A	1.1776	0.9546	0.7018	0.032*
C101	0.9399 (5)	0.8357 (4)	0.6352 (3)	0.0206 (11)
C102	0.9874 (5)	0.7845 (5)	0.6737 (4)	0.0270 (13)
H10A	1.0354	0.8229	0.7252	0.032*
C103	0.9670 (5)	0.6803 (5)	0.6395 (4)	0.0310 (14)
H10B	1.0016	0.6490	0.6675	0.037*
C104	0.8969 (5)	0.6209 (5)	0.5653 (4)	0.0293 (13)
H10C	0.8839	0.5495	0.5419	0.035*
C105	0.8459 (5)	0.6670 (5)	0.5257 (4)	0.0310 (13)
H10D	0.7963	0.6272	0.4748	0.037*
C106	0.8676 (5)	0.7722 (5)	0.5607 (3)	0.0277 (13)
H10E	0.8314	0.8024	0.5326	0.033*
B1A	0.9575 (5)	0.9583 (5)	0.6771 (4)	0.0201 (13)
C71B	0.0376 (4)	0.6074 (4)	0.2316 (3)	0.0186 (11)
C72B	−0.0066 (5)	0.6311 (4)	0.2948 (3)	0.0240 (12)
H72B	−0.0302	0.6871	0.3045	0.029*
C73B	−0.0172 (5)	0.5764 (5)	0.3437 (3)	0.0294 (13)
H73B	−0.0459	0.5962	0.3866	0.035*
C74B	0.0137 (5)	0.4933 (5)	0.3305 (4)	0.0320 (15)
H74B	0.0052	0.4548	0.3636	0.038*
C75B	0.0566 (5)	0.4667 (5)	0.2700 (4)	0.0308 (14)
H75B	0.0787	0.4097	0.2610	0.037*
C76B	0.0683 (5)	0.5218 (5)	0.2210 (4)	0.0262 (13)
H76B	0.0980	0.5012	0.1788	0.031*
C81B	0.0554 (4)	0.7861 (4)	0.2065 (3)	0.0202 (11)
C82B	0.1306 (5)	0.8528 (5)	0.2804 (4)	0.0300 (13)
H82B	0.1688	0.8249	0.3095	0.036*
C83B	0.1510 (6)	0.9577 (5)	0.3123 (4)	0.0328 (14)
H83B	0.2037	1.0000	0.3619	0.039*
C84B	0.0968 (5)	1.0012 (5)	0.2735 (4)	0.0321 (14)
H84B	0.1094	1.0726	0.2965	0.038*
C85B	0.0236 (6)	0.9401 (5)	0.2009 (4)	0.0329 (14)
H85B	−0.0147	0.9690	0.1727	0.039*
C86B	0.0057 (5)	0.8341 (5)	0.1682 (4)	0.0270 (13)
H86B	−0.0431	0.7938	0.1172	0.032*
C91B	−0.0856 (5)	0.5867 (4)	0.1026 (3)	0.0196 (11)
C92B	−0.1859 (5)	0.6011 (5)	0.1063 (3)	0.0252 (12)
H92B	−0.1808	0.6612	0.1461	0.030*
C93B	−0.2949 (5)	0.5316 (5)	0.0544 (4)	0.0315 (14)
H93B	−0.3614	0.5450	0.0588	0.038*
C94B	−0.3043 (5)	0.4424 (5)	−0.0038 (4)	0.0326 (14)
H94B	−0.3772	0.3947	−0.0400	0.039*
C95B	−0.2059 (5)	0.4245 (5)	−0.0080 (3)	0.0309 (13)

H95B	−0.2115	0.3631	−0.0466	0.037*
C96B	−0.1007 (5)	0.4944 (5)	0.0429 (3)	0.0288 (13)
H96B	−0.0346	0.4804	0.0379	0.035*
C111	0.1499 (5)	0.6735 (4)	0.1320 (3)	0.0205 (11)
C112	0.2595 (5)	0.6998 (4)	0.1787 (3)	0.0235 (12)
H11A	0.2675	0.7072	0.2311	0.028*
C113	0.3578 (5)	0.7156 (5)	0.1515 (4)	0.0298 (14)
H11B	0.4302	0.7311	0.1847	0.036*
C114	0.3494 (5)	0.7085 (5)	0.0763 (4)	0.0316 (14)
H11C	0.4163	0.7210	0.0579	0.038*
C115	0.2444 (6)	0.6834 (5)	0.0286 (4)	0.0318 (15)
H11D	0.2375	0.6763	−0.0237	0.038*
C116	0.1470 (5)	0.6681 (5)	0.0567 (4)	0.0266 (13)
H11E	0.0754	0.6533	0.0229	0.032*
B1B	0.0405 (5)	0.6641 (5)	0.1684 (3)	0.0200 (13)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Fe1A	0.0190 (4)	0.0166 (4)	0.0192 (4)	0.0096 (3)	0.0089 (3)	0.0085 (3)
Br1A	0.0350 (3)	0.0310 (3)	0.0214 (3)	0.0209 (2)	0.0059 (2)	0.0084 (2)
P1A	0.0167 (6)	0.0162 (6)	0.0225 (7)	0.0067 (5)	0.0082 (5)	0.0073 (5)
P2A	0.0210 (7)	0.0170 (7)	0.0217 (7)	0.0091 (6)	0.0098 (6)	0.0088 (6)
O1A	0.042 (3)	0.039 (3)	0.060 (3)	0.026 (2)	0.030 (2)	0.037 (2)
N1A	0.021 (2)	0.021 (2)	0.021 (2)	0.0121 (18)	0.0104 (18)	0.0087 (18)
N2A	0.018 (2)	0.0157 (19)	0.0168 (19)	0.0080 (16)	0.0068 (16)	0.0060 (16)
C1A	0.021 (2)	0.021 (2)	0.020 (2)	0.0103 (18)	0.0055 (18)	0.0068 (18)
C2A	0.019 (2)	0.016 (2)	0.022 (2)	0.0096 (18)	0.0076 (18)	0.0082 (17)
C3A	0.020 (3)	0.027 (3)	0.028 (3)	0.013 (2)	0.015 (2)	0.011 (2)
C4A	0.020 (3)	0.028 (3)	0.033 (3)	0.014 (2)	0.018 (2)	0.016 (2)
C5A	0.025 (3)	0.016 (2)	0.017 (2)	0.007 (2)	0.005 (2)	0.007 (2)
C6A	0.024 (3)	0.020 (3)	0.022 (3)	0.008 (2)	0.012 (2)	0.009 (2)
C7A	0.028 (3)	0.027 (3)	0.031 (3)	0.018 (2)	0.017 (3)	0.014 (3)
C11A	0.024 (3)	0.016 (2)	0.025 (3)	0.009 (2)	0.010 (2)	0.008 (2)
C12A	0.033 (3)	0.025 (3)	0.024 (3)	0.014 (2)	0.008 (2)	0.012 (2)
C13A	0.049 (4)	0.027 (3)	0.022 (3)	0.016 (3)	0.018 (2)	0.006 (2)
C14A	0.042 (3)	0.027 (3)	0.036 (3)	0.023 (3)	0.025 (3)	0.011 (3)
C15A	0.031 (3)	0.035 (3)	0.036 (3)	0.021 (3)	0.014 (3)	0.018 (3)
C16A	0.031 (3)	0.026 (3)	0.020 (3)	0.016 (2)	0.009 (2)	0.006 (2)
C21A	0.023 (3)	0.015 (2)	0.024 (3)	0.007 (2)	0.011 (2)	0.004 (2)
C22A	0.028 (3)	0.024 (3)	0.037 (3)	0.006 (2)	0.008 (2)	0.009 (2)
C23A	0.030 (3)	0.024 (3)	0.054 (4)	0.005 (2)	0.013 (3)	0.000 (3)
C24A	0.050 (4)	0.021 (3)	0.076 (5)	0.015 (3)	0.046 (4)	0.017 (3)
C25A	0.053 (4)	0.032 (3)	0.054 (4)	0.026 (3)	0.038 (4)	0.027 (3)
C26A	0.031 (3)	0.024 (3)	0.034 (3)	0.017 (2)	0.016 (2)	0.010 (2)
C31A	0.015 (2)	0.018 (2)	0.017 (2)	0.0055 (19)	0.0030 (19)	0.003 (2)
C32A	0.018 (3)	0.021 (3)	0.024 (3)	0.006 (2)	0.003 (2)	0.006 (2)
C33A	0.020 (3)	0.027 (3)	0.023 (3)	0.003 (2)	0.002 (2)	0.010 (2)

C34A	0.040 (3)	0.025 (3)	0.026 (3)	0.014 (3)	0.006 (3)	0.013 (3)
C35A	0.037 (3)	0.031 (3)	0.030 (3)	0.025 (3)	0.007 (3)	0.006 (3)
C36A	0.027 (3)	0.030 (3)	0.026 (3)	0.014 (2)	0.007 (2)	0.011 (2)
C41A	0.017 (3)	0.018 (3)	0.035 (3)	0.007 (2)	0.010 (2)	0.003 (2)
C42A	0.039 (4)	0.020 (3)	0.055 (4)	0.009 (3)	0.027 (3)	0.012 (3)
C43A	0.038 (4)	0.022 (3)	0.079 (5)	0.009 (3)	0.037 (4)	0.012 (3)
C44A	0.033 (4)	0.025 (3)	0.061 (5)	−0.001 (3)	0.014 (3)	−0.011 (3)
C45A	0.028 (3)	0.034 (4)	0.041 (4)	0.008 (3)	−0.002 (3)	−0.008 (3)
C46A	0.026 (3)	0.026 (3)	0.038 (3)	0.009 (2)	0.004 (3)	0.003 (3)
C51A	0.024 (3)	0.024 (3)	0.030 (3)	0.016 (2)	0.013 (3)	0.012 (3)
C52A	0.027 (3)	0.030 (3)	0.037 (3)	0.017 (3)	0.020 (3)	0.017 (3)
C53A	0.033 (3)	0.043 (4)	0.055 (4)	0.025 (3)	0.022 (3)	0.025 (3)
C54A	0.043 (4)	0.047 (4)	0.062 (5)	0.034 (3)	0.024 (4)	0.035 (4)
C55A	0.035 (3)	0.044 (4)	0.051 (4)	0.026 (3)	0.018 (3)	0.032 (3)
C56A	0.027 (3)	0.032 (3)	0.037 (3)	0.016 (3)	0.014 (3)	0.021 (3)
C61A	0.036 (3)	0.023 (3)	0.029 (3)	0.017 (3)	0.017 (3)	0.011 (3)
C62A	0.063 (5)	0.025 (3)	0.040 (4)	0.009 (3)	0.026 (3)	0.013 (3)
C63A	0.078 (5)	0.037 (4)	0.027 (3)	0.013 (3)	0.022 (3)	0.009 (3)
C64A	0.077 (6)	0.034 (4)	0.040 (4)	0.007 (4)	0.023 (4)	0.003 (3)
C65A	0.047 (4)	0.021 (3)	0.042 (4)	0.007 (3)	0.016 (3)	0.007 (3)
C66A	0.029 (3)	0.020 (3)	0.027 (3)	0.009 (2)	0.012 (3)	0.009 (2)
Fe1B	0.0180 (4)	0.0164 (4)	0.0174 (4)	0.0094 (3)	0.0073 (3)	0.0077 (3)
Br1B	0.0299 (3)	0.0314 (3)	0.0186 (3)	0.0178 (2)	0.0042 (2)	0.0075 (2)
P1B	0.0169 (6)	0.0157 (6)	0.0196 (6)	0.0066 (5)	0.0072 (5)	0.0071 (5)
P2B	0.0189 (7)	0.0153 (6)	0.0200 (7)	0.0096 (5)	0.0087 (6)	0.0080 (6)
O1B	0.034 (2)	0.040 (3)	0.051 (3)	0.015 (2)	0.017 (2)	0.033 (2)
N1B	0.021 (2)	0.021 (2)	0.018 (2)	0.0123 (18)	0.0069 (17)	0.0078 (18)
N2B	0.020 (2)	0.016 (2)	0.018 (2)	0.0096 (16)	0.0051 (17)	0.0049 (16)
C1B	0.020 (2)	0.017 (2)	0.019 (2)	0.0093 (17)	0.0058 (18)	0.0068 (17)
C2B	0.018 (2)	0.015 (2)	0.020 (2)	0.0075 (17)	0.0040 (17)	0.0014 (17)
C3B	0.027 (3)	0.025 (3)	0.025 (3)	0.014 (2)	0.015 (2)	0.011 (2)
C4B	0.018 (3)	0.020 (3)	0.025 (3)	0.007 (2)	0.010 (2)	0.011 (2)
C5B	0.020 (2)	0.014 (2)	0.023 (2)	0.0059 (19)	0.005 (2)	0.004 (2)
C6B	0.022 (3)	0.016 (2)	0.023 (3)	0.011 (2)	0.009 (2)	0.007 (2)
C7B	0.022 (3)	0.034 (3)	0.023 (3)	0.016 (2)	0.011 (2)	0.017 (3)
C11B	0.020 (2)	0.019 (2)	0.022 (2)	0.0086 (19)	0.010 (2)	0.0051 (19)
C12B	0.026 (3)	0.028 (3)	0.023 (3)	0.013 (2)	0.006 (2)	0.006 (2)
C13B	0.030 (3)	0.033 (3)	0.023 (3)	0.009 (2)	0.010 (2)	0.001 (2)
C14B	0.046 (4)	0.022 (3)	0.043 (4)	0.016 (3)	0.028 (3)	0.002 (3)
C15B	0.037 (3)	0.028 (3)	0.047 (4)	0.027 (3)	0.024 (3)	0.015 (3)
C16B	0.020 (3)	0.026 (3)	0.030 (3)	0.012 (2)	0.008 (2)	0.011 (2)
C21B	0.024 (3)	0.014 (2)	0.031 (3)	0.012 (2)	0.011 (2)	0.003 (2)
C22B	0.019 (3)	0.021 (3)	0.039 (3)	0.009 (2)	0.007 (2)	0.001 (2)
C23B	0.024 (3)	0.020 (3)	0.071 (5)	0.004 (2)	0.021 (3)	0.002 (3)
C24B	0.044 (4)	0.025 (3)	0.088 (5)	0.021 (3)	0.050 (4)	0.027 (3)
C25B	0.035 (3)	0.032 (3)	0.059 (4)	0.023 (3)	0.032 (3)	0.026 (3)
C26B	0.024 (3)	0.021 (3)	0.035 (3)	0.011 (2)	0.017 (2)	0.012 (2)
C31B	0.022 (3)	0.024 (3)	0.026 (3)	0.011 (2)	0.009 (2)	0.014 (3)

C32B	0.017 (3)	0.023 (3)	0.021 (3)	0.007 (2)	0.004 (2)	0.007 (2)
C33B	0.026 (3)	0.022 (3)	0.020 (3)	0.003 (2)	0.006 (2)	0.009 (2)
C34B	0.037 (3)	0.022 (3)	0.024 (3)	0.010 (3)	0.001 (3)	0.009 (2)
C35B	0.036 (3)	0.031 (3)	0.031 (3)	0.021 (3)	0.004 (3)	0.012 (3)
C36B	0.023 (3)	0.028 (3)	0.021 (3)	0.014 (2)	0.008 (2)	0.007 (2)
C39B	0.019 (2)	0.014 (2)	0.018 (2)	0.004 (2)	−0.001 (2)	0.004 (2)
C41B	0.016 (2)	0.019 (3)	0.028 (3)	0.005 (2)	0.007 (2)	0.005 (2)
C42B	0.025 (3)	0.026 (3)	0.034 (3)	0.009 (2)	0.013 (2)	0.010 (3)
C43B	0.035 (3)	0.020 (3)	0.057 (4)	0.005 (3)	0.022 (3)	0.010 (3)
C44B	0.020 (3)	0.024 (3)	0.053 (4)	0.001 (2)	0.010 (3)	−0.004 (3)
C45B	0.031 (3)	0.034 (3)	0.035 (3)	0.010 (3)	0.007 (3)	0.004 (3)
C46B	0.022 (3)	0.023 (3)	0.026 (3)	0.007 (2)	0.004 (2)	0.004 (2)
C52B	0.029 (3)	0.022 (3)	0.038 (3)	0.016 (2)	0.013 (3)	0.014 (3)
C53B	0.028 (3)	0.042 (4)	0.047 (4)	0.025 (3)	0.021 (3)	0.024 (3)
C54B	0.034 (3)	0.036 (3)	0.045 (4)	0.025 (3)	0.012 (3)	0.021 (3)
C55B	0.035 (3)	0.038 (3)	0.037 (3)	0.022 (3)	0.013 (3)	0.024 (3)
C56B	0.029 (3)	0.028 (3)	0.034 (3)	0.019 (3)	0.014 (3)	0.016 (3)
C61B	0.024 (3)	0.018 (3)	0.018 (3)	0.005 (2)	0.006 (2)	0.004 (2)
C62B	0.044 (4)	0.027 (3)	0.029 (3)	0.010 (3)	0.025 (3)	0.008 (3)
C63B	0.061 (4)	0.027 (3)	0.028 (3)	0.008 (3)	0.024 (3)	0.000 (3)
C64B	0.049 (4)	0.024 (3)	0.041 (4)	0.013 (3)	0.018 (3)	0.001 (3)
C65B	0.044 (4)	0.022 (3)	0.034 (3)	0.006 (3)	0.011 (3)	0.006 (3)
C66B	0.026 (3)	0.021 (3)	0.032 (3)	0.007 (2)	0.012 (3)	0.010 (3)
C71A	0.018 (3)	0.021 (3)	0.017 (3)	0.003 (2)	0.003 (2)	0.003 (2)
C72A	0.024 (3)	0.028 (3)	0.029 (3)	0.013 (2)	0.012 (3)	0.012 (3)
C73A	0.027 (3)	0.030 (3)	0.045 (4)	0.014 (3)	0.010 (3)	0.020 (3)
C74A	0.024 (3)	0.038 (4)	0.034 (3)	0.002 (3)	−0.003 (3)	0.021 (3)
C75A	0.035 (3)	0.040 (4)	0.017 (3)	0.003 (3)	0.009 (3)	0.008 (3)
C76A	0.030 (3)	0.027 (3)	0.028 (3)	0.011 (3)	0.010 (3)	0.007 (3)
C81A	0.026 (3)	0.012 (2)	0.022 (3)	0.008 (2)	0.008 (2)	0.002 (2)
C82A	0.035 (3)	0.028 (3)	0.023 (3)	0.013 (3)	0.008 (3)	0.011 (3)
C83A	0.046 (4)	0.041 (4)	0.029 (3)	0.018 (3)	0.017 (3)	0.014 (3)
C84A	0.038 (4)	0.023 (3)	0.049 (4)	0.014 (3)	0.028 (3)	0.014 (3)
C85A	0.025 (3)	0.028 (3)	0.038 (4)	0.009 (3)	0.007 (3)	0.008 (3)
C86A	0.032 (3)	0.031 (3)	0.027 (3)	0.011 (3)	0.010 (3)	0.011 (3)
C91A	0.024 (3)	0.025 (3)	0.018 (3)	0.008 (2)	0.005 (2)	0.008 (2)
C92A	0.028 (3)	0.025 (3)	0.024 (3)	0.012 (2)	−0.002 (2)	0.004 (2)
C93A	0.034 (3)	0.023 (3)	0.024 (3)	0.006 (3)	0.004 (3)	0.003 (2)
C94A	0.024 (3)	0.037 (4)	0.023 (3)	0.002 (3)	0.003 (3)	0.005 (3)
C95A	0.025 (3)	0.040 (4)	0.033 (3)	0.012 (3)	0.013 (3)	0.008 (3)
C96A	0.025 (3)	0.030 (3)	0.020 (3)	0.009 (2)	0.010 (2)	0.004 (3)
C101	0.017 (3)	0.021 (3)	0.024 (3)	0.008 (2)	0.009 (2)	0.007 (2)
C102	0.029 (3)	0.027 (3)	0.027 (3)	0.013 (3)	0.011 (3)	0.010 (3)
C103	0.031 (3)	0.031 (3)	0.046 (4)	0.020 (3)	0.017 (3)	0.022 (3)
C104	0.026 (3)	0.020 (3)	0.041 (3)	0.009 (2)	0.018 (3)	0.006 (3)
C105	0.023 (3)	0.029 (3)	0.030 (3)	0.007 (2)	0.002 (2)	0.003 (3)
C106	0.026 (3)	0.023 (3)	0.028 (3)	0.010 (2)	0.001 (2)	0.005 (2)
B1A	0.021 (3)	0.020 (3)	0.021 (3)	0.011 (2)	0.007 (3)	0.005 (3)

C71B	0.013 (2)	0.018 (3)	0.019 (3)	0.005 (2)	0.000 (2)	0.003 (2)
C72B	0.025 (3)	0.019 (3)	0.023 (3)	0.007 (2)	0.007 (2)	0.003 (2)
C73B	0.034 (3)	0.023 (3)	0.025 (3)	0.007 (2)	0.012 (3)	0.006 (2)
C74B	0.034 (3)	0.032 (3)	0.027 (3)	0.005 (3)	0.009 (3)	0.016 (3)
C75B	0.020 (3)	0.029 (3)	0.048 (4)	0.010 (2)	0.006 (3)	0.023 (3)
C76B	0.020 (3)	0.025 (3)	0.034 (3)	0.009 (2)	0.008 (2)	0.012 (3)
C81B	0.017 (3)	0.021 (3)	0.023 (3)	0.008 (2)	0.010 (2)	0.006 (2)
C82B	0.029 (3)	0.024 (3)	0.035 (3)	0.011 (3)	0.006 (3)	0.008 (3)
C83B	0.036 (3)	0.018 (3)	0.033 (3)	0.007 (2)	0.010 (3)	0.000 (2)
C84B	0.033 (3)	0.019 (3)	0.049 (4)	0.012 (2)	0.023 (3)	0.012 (3)
C85B	0.036 (3)	0.027 (3)	0.047 (4)	0.017 (3)	0.022 (3)	0.021 (3)
C86B	0.024 (3)	0.028 (3)	0.028 (3)	0.008 (2)	0.009 (2)	0.013 (3)
C91B	0.020 (3)	0.020 (3)	0.022 (3)	0.009 (2)	0.006 (2)	0.009 (2)
C92B	0.024 (3)	0.025 (3)	0.023 (3)	0.008 (2)	0.007 (2)	0.006 (2)
C93B	0.019 (3)	0.041 (4)	0.025 (3)	0.009 (3)	0.002 (2)	0.007 (3)
C94B	0.023 (3)	0.035 (3)	0.023 (3)	0.003 (3)	−0.002 (2)	0.002 (3)
C95B	0.030 (3)	0.028 (3)	0.024 (3)	0.010 (3)	0.002 (2)	0.000 (2)
C96B	0.027 (3)	0.026 (3)	0.028 (3)	0.011 (2)	0.006 (2)	0.004 (3)
C111	0.021 (3)	0.016 (3)	0.027 (3)	0.010 (2)	0.009 (2)	0.008 (2)
C112	0.023 (3)	0.024 (3)	0.023 (3)	0.011 (2)	0.007 (2)	0.005 (2)
C113	0.024 (3)	0.026 (3)	0.040 (4)	0.012 (3)	0.014 (3)	0.008 (3)
C114	0.028 (3)	0.028 (3)	0.044 (4)	0.012 (3)	0.021 (3)	0.014 (3)
C115	0.043 (4)	0.030 (3)	0.031 (3)	0.017 (3)	0.023 (3)	0.014 (3)
C116	0.025 (3)	0.028 (3)	0.029 (3)	0.013 (2)	0.010 (3)	0.011 (3)
B1B	0.019 (3)	0.020 (3)	0.017 (3)	0.007 (2)	0.003 (2)	0.005 (3)

Geometric parameters (Å, º)

Fe1A—C7A	1.758 (5)	C23B—H23B	0.9500
Fe1A—N2A	1.976 (4)	C24B—C25B	1.389 (9)
Fe1A—N1A	2.088 (4)	C24B—H24B	0.9500
Fe1A—P1A	2.2403 (16)	C25B—C26B	1.387 (7)
Fe1A—P2A	2.2557 (15)	C25B—H25B	0.9500
Fe1A—Br1A	2.4970 (9)	C26B—H26B	0.9500
P1A—C31A	1.823 (5)	C31B—C52B	1.526 (8)
P1A—C4A	1.827 (5)	C31B—C56B	1.528 (7)
P1A—C41A	1.840 (6)	C31B—H31A	1.0000
P2A—C51A	1.855 (6)	C32B—C39B	1.378 (7)
P2A—C6A	1.857 (5)	C32B—C33B	1.388 (7)
P2A—C61A	1.857 (6)	C32B—H32B	0.9500
O1A—C7A	1.146 (7)	C33B—C34B	1.385 (9)
N1A—C3A	1.489 (7)	C33B—H33B	0.9500
N1A—C1A	1.512 (6)	C34B—C35B	1.386 (8)
N1A—H1A	1.0000	C34B—H34B	0.9500
N2A—C5A	1.280 (6)	C35B—C36B	1.388 (8)
N2A—C2A	1.495 (6)	C35B—H35B	0.9500
C1A—C11A	1.521 (7)	C36B—C39B	1.401 (8)
C1A—C2A	1.530 (6)	C36B—H36B	0.9500

C1A—H1AA	1.0000	C41B—C46B	1.390 (8)
C2A—C21A	1.518 (6)	C41B—C42B	1.393 (8)
C2A—H2AA	1.0000	C42B—C43B	1.392 (9)
C3A—C4A	1.520 (8)	C42B—H42B	0.9500
C3A—H3AA	0.9900	C43B—C44B	1.378 (10)
C3A—H3AB	0.9900	C43B—H43B	0.9500
C4A—H4AA	0.9900	C44B—C45B	1.385 (9)
C4A—H4AB	0.9900	C44B—H44B	0.9500
C5A—C6A	1.477 (8)	C45B—C46B	1.394 (9)
C5A—H5AA	0.9500	C45B—H45B	0.9500
C6A—H6AA	0.9900	C46B—H46B	0.9500
C6A—H6AB	0.9900	C52B—C53B	1.539 (9)
C11A—C16A	1.382 (8)	C52B—H52C	0.9900
C11A—C12A	1.388 (7)	C52B—H52D	0.9900
C12A—C13A	1.381 (7)	C53B—C54B	1.525 (8)
C12A—H12A	0.9500	C53B—H53C	0.9900
C13A—C14A	1.354 (9)	C53B—H53D	0.9900
C13A—H13A	0.9500	C54B—C55B	1.504 (9)
C14A—C15A	1.395 (9)	C54B—H54C	0.9900
C14A—H14A	0.9500	C54B—H54D	0.9900
C15A—C16A	1.383 (8)	C55B—C56B	1.527 (8)
C15A—H15A	0.9500	C55B—H55C	0.9900
C16A—H16A	0.9500	C55B—H55D	0.9900
C21A—C22A	1.381 (8)	C56B—H56C	0.9900
C21A—C26A	1.391 (8)	C56B—H56D	0.9900
C22A—C23A	1.389 (7)	C61B—C66B	1.525 (7)
C22A—H22A	0.9500	C61B—C62B	1.552 (7)
C23A—C24A	1.368 (9)	C61B—H61B	1.0000
C23A—H23A	0.9500	C62B—C63B	1.529 (9)
C24A—C25A	1.382 (10)	C62B—H62C	0.9900
C24A—H24A	0.9500	C62B—H62D	0.9900
C25A—C26A	1.396 (8)	C63B—C64B	1.497 (9)
C25A—H25A	0.9500	C63B—H63C	0.9900
C26A—H26A	0.9500	C63B—H63D	0.9900
C31A—C36A	1.394 (8)	C64B—C65B	1.509 (9)
C31A—C32A	1.409 (7)	C64B—H64C	0.9900
C32A—C33A	1.379 (8)	C64B—H64D	0.9900
C32A—H32A	0.9500	C65B—C66B	1.538 (9)
C33A—C34A	1.378 (9)	C65B—H65C	0.9900
C33A—H33A	0.9500	C65B—H65D	0.9900
C34A—C35A	1.362 (8)	C66B—H66C	0.9900
C34A—H34A	0.9500	C66B—H66D	0.9900
C35A—C36A	1.392 (8)	C71A—C72A	1.399 (8)
C35A—H35A	0.9500	C71A—C76A	1.403 (8)
C36A—H36A	0.9500	C71A—B1A	1.650 (8)
C41A—C42A	1.385 (8)	C72A—C73A	1.390 (8)
C41A—C46A	1.391 (9)	C72A—H72A	0.9500
C42A—C43A	1.403 (9)	C73A—C74A	1.389 (9)

C42A—H42A	0.9500	C73A—H73A	0.9500
C43A—C44A	1.371 (11)	C74A—C75A	1.379 (10)
C43A—H43A	0.9500	C74A—H74A	0.9500
C44A—C45A	1.372 (10)	C75A—C76A	1.394 (8)
C44A—H44A	0.9500	C75A—H75A	0.9500
C45A—C46A	1.392 (9)	C76A—H76A	0.9500
C45A—H45A	0.9500	C81A—C82A	1.404 (8)
C46A—H46A	0.9500	C81A—C86A	1.404 (8)
C51A—C56A	1.535 (7)	C81A—B1A	1.647 (8)
C51A—C52A	1.540 (7)	C82A—C83A	1.380 (9)
C51A—H51A	1.0000	C82A—H82A	0.9500
C52A—C53A	1.516 (9)	C83A—C84A	1.397 (10)
C52A—H52A	0.9900	C83A—H83A	0.9500
C52A—H52B	0.9900	C84A—C85A	1.375 (9)
C53A—C54A	1.514 (9)	C84A—H84A	0.9500
C53A—H53A	0.9900	C85A—C86A	1.379 (8)
C53A—H53B	0.9900	C85A—H85A	0.9500
C54A—C55A	1.524 (9)	C86A—H86A	0.9500
C54A—H54A	0.9900	C91A—C92A	1.395 (8)
C54A—H54B	0.9900	C91A—C96A	1.411 (8)
C55A—C56A	1.521 (9)	C91A—B1A	1.634 (9)
C55A—H55A	0.9900	C92A—C93A	1.402 (8)
C55A—H55B	0.9900	C92A—H92A	0.9500
C56A—H56A	0.9900	C93A—C94A	1.380 (9)
C56A—H56B	0.9900	C93A—H93A	0.9500
C61A—C62A	1.498 (8)	C94A—C95A	1.373 (9)
C61A—C66A	1.540 (7)	C94A—H94A	0.9500
C61A—H61A	1.0000	C95A—C96A	1.380 (9)
C62A—C63A	1.543 (10)	C95A—H95A	0.9500
C62A—H62A	0.9900	C96A—H96A	0.9500
C62A—H62B	0.9900	C101—C106	1.399 (8)
C63A—C64A	1.524 (10)	C101—C102	1.404 (8)
C63A—H63A	0.9900	C101—B1A	1.654 (8)
C63A—H63B	0.9900	C102—C103	1.381 (9)
C64A—C65A	1.487 (9)	C102—H10A	0.9500
C64A—H64A	0.9900	C103—C104	1.379 (9)
C64A—H64B	0.9900	C103—H10B	0.9500
C65A—C66A	1.519 (9)	C104—C105	1.380 (9)
C65A—H65A	0.9900	C104—H10C	0.9500
C65A—H65B	0.9900	C105—C106	1.391 (9)
C66A—H66A	0.9900	C105—H10D	0.9500
C66A—H66B	0.9900	C106—H10E	0.9500
Fe1B—C7B	1.757 (5)	C71B—C72B	1.402 (8)
Fe1B—N2B	1.990 (4)	C71B—C76B	1.410 (8)
Fe1B—N1B	2.071 (4)	C71B—B1B	1.640 (8)
Fe1B—P1B	2.2462 (16)	C72B—C73B	1.379 (8)
Fe1B—P2B	2.2601 (15)	C72B—H72B	0.9500
Fe1B—Br1B	2.5183 (9)	C73B—C74B	1.375 (9)

P1B—C39B	1.822 (5)	C73B—H73B	0.9500
P1B—C4B	1.832 (5)	C74B—C75B	1.356 (9)
P1B—C41B	1.842 (6)	C74B—H74B	0.9500
P2B—C31B	1.853 (6)	C75B—C76B	1.386 (8)
P2B—C61B	1.854 (6)	C75B—H75B	0.9500
P2B—C6B	1.855 (5)	C76B—H76B	0.9500
O1B—C7B	1.146 (7)	C81B—C86B	1.379 (8)
N1B—C3B	1.508 (7)	C81B—C82B	1.408 (8)
N1B—C1B	1.521 (6)	C81B—B1B	1.648 (8)
N1B—H1B	1.0000	C82B—C83B	1.386 (9)
N2B—C5B	1.266 (6)	C82B—H82B	0.9500
N2B—C2B	1.498 (6)	C83B—C84B	1.364 (9)
C1B—C2B	1.518 (6)	C83B—H83B	0.9500
C1B—C11B	1.523 (7)	C84B—C85B	1.373 (10)
C1B—H1BA	1.0000	C84B—H84B	0.9500
C2B—C21B	1.502 (6)	C85B—C86B	1.411 (9)
C2B—H2BA	1.0000	C85B—H85B	0.9500
C3B—C4B	1.532 (8)	C86B—H86B	0.9500
C3B—H3BA	0.9900	C91B—C92B	1.381 (8)
C3B—H3BB	0.9900	C91B—C96B	1.416 (8)
C4B—H4BA	0.9900	C91B—B1B	1.656 (8)
C4B—H4BB	0.9900	C92B—C93B	1.402 (8)
C5B—C6B	1.494 (7)	C92B—H92B	0.9500
C5B—H5BA	0.9500	C93B—C94B	1.394 (9)
C6B—H6BA	0.9900	C93B—H93B	0.9500
C6B—H6BB	0.9900	C94B—C95B	1.384 (9)
C11B—C12B	1.380 (7)	C94B—H94B	0.9500
C11B—C16B	1.394 (8)	C95B—C96B	1.365 (8)
C12B—C13B	1.384 (7)	C95B—H95B	0.9500
C12B—H12B	0.9500	C96B—H96B	0.9500
C13B—C14B	1.380 (9)	C111—C116	1.398 (8)
C13B—H13B	0.9500	C111—C112	1.399 (8)
C14B—C15B	1.373 (10)	C111—B1B	1.630 (8)
C14B—H14B	0.9500	C112—C113	1.399 (8)
C15B—C16B	1.387 (8)	C112—H11A	0.9500
C15B—H15B	0.9500	C113—C114	1.380 (9)
C16B—H16B	0.9500	C113—H11B	0.9500
C21B—C26B	1.395 (8)	C114—C115	1.365 (10)
C21B—C22B	1.401 (7)	C114—H11C	0.9500
C22B—C23B	1.397 (8)	C115—C116	1.398 (8)
C22B—H22B	0.9500	C115—H11D	0.9500
C23B—C24B	1.366 (10)	C116—H11E	0.9500

C7A—Fe1A—N2A	176.0 (2)	C12B—C13B—H13B	119.9
C7A—Fe1A—N1A	98.6 (2)	C15B—C14B—C13B	120.6 (6)
N2A—Fe1A—N1A	82.10 (16)	C15B—C14B—H14B	119.7
C7A—Fe1A—P1A	88.3 (2)	C13B—C14B—H14B	119.7
N2A—Fe1A—P1A	95.73 (13)	C14B—C15B—C16B	119.4 (6)

N1A—Fe1A—P1A	82.94 (13)	C14B—C15B—H15B	120.3
C7A—Fe1A—P2A	94.01 (18)	C16B—C15B—H15B	120.3
N2A—Fe1A—P2A	84.82 (13)	C15B—C16B—C11B	120.4 (6)
N1A—Fe1A—P2A	165.62 (12)	C15B—C16B—H16B	119.8
P1A—Fe1A—P2A	104.36 (6)	C11B—C16B—H16B	119.8
C7A—Fe1A—Br1A	87.5 (2)	C26B—C21B—C22B	118.6 (5)
N2A—Fe1A—Br1A	88.58 (13)	C26B—C21B—C2B	121.6 (5)
N1A—Fe1A—Br1A	84.39 (13)	C22B—C21B—C2B	119.6 (5)
P1A—Fe1A—Br1A	165.92 (5)	C23B—C22B—C21B	120.1 (5)
P2A—Fe1A—Br1A	89.35 (5)	C23B—C22B—H22B	120.0
C31A—P1A—C4A	105.0 (3)	C21B—C22B—H22B	120.0
C31A—P1A—C41A	102.0 (3)	C24B—C23B—C22B	120.7 (6)
C4A—P1A—C41A	104.3 (3)	C24B—C23B—H23B	119.7
C31A—P1A—Fe1A	117.17 (17)	C22B—C23B—H23B	119.7
C4A—P1A—Fe1A	97.4 (2)	C23B—C24B—C25B	119.8 (5)
C41A—P1A—Fe1A	127.98 (19)	C23B—C24B—H24B	120.1
C51A—P2A—C6A	102.4 (3)	C25B—C24B—H24B	120.1
C51A—P2A—C61A	109.0 (3)	C26B—C25B—C24B	120.4 (6)
C6A—P2A—C61A	106.7 (2)	C26B—C25B—H25B	119.8
C51A—P2A—Fe1A	118.24 (18)	C24B—C25B—H25B	119.8
C6A—P2A—Fe1A	99.76 (18)	C25B—C26B—C21B	120.4 (5)
C61A—P2A—Fe1A	118.2 (2)	C25B—C26B—H26B	119.8
C3A—N1A—C1A	114.9 (4)	C21B—C26B—H26B	119.8
C3A—N1A—Fe1A	117.9 (3)	C52B—C31B—C56B	111.6 (5)
C1A—N1A—Fe1A	107.6 (3)	C52B—C31B—P2B	115.3 (4)
C3A—N1A—H1A	105.1	C56B—C31B—P2B	115.6 (4)
C1A—N1A—H1A	105.1	C52B—C31B—H31A	104.2
Fe1A—N1A—H1A	105.1	C56B—C31B—H31A	104.2
C5A—N2A—C2A	121.2 (4)	P2B—C31B—H31A	104.2
C5A—N2A—Fe1A	123.2 (4)	C39B—C32B—C33B	120.5 (5)
C2A—N2A—Fe1A	115.5 (3)	C39B—C32B—H32B	119.7
N1A—C1A—C11A	115.6 (4)	C33B—C32B—H32B	119.7
N1A—C1A—C2A	107.6 (3)	C34B—C33B—C32B	120.2 (5)
C11A—C1A—C2A	114.2 (4)	C34B—C33B—H33B	119.9
N1A—C1A—H1AA	106.2	C32B—C33B—H33B	119.9
C11A—C1A—H1AA	106.2	C33B—C34B—C35B	119.9 (5)
C2A—C1A—H1AA	106.2	C33B—C34B—H34B	120.0
N2A—C2A—C21A	113.4 (4)	C35B—C34B—H34B	120.0
N2A—C2A—C1A	105.1 (3)	C34B—C35B—C36B	119.7 (6)
C21A—C2A—C1A	114.6 (4)	C34B—C35B—H35B	120.1
N2A—C2A—H2AA	107.8	C36B—C35B—H35B	120.1
C21A—C2A—H2AA	107.8	C35B—C36B—C39B	120.4 (5)
C1A—C2A—H2AA	107.8	C35B—C36B—H36B	119.8
N1A—C3A—C4A	111.1 (4)	C39B—C36B—H36B	119.8
N1A—C3A—H3AA	109.4	C32B—C39B—C36B	119.1 (5)
C4A—C3A—H3AA	109.4	C32B—C39B—P1B	119.2 (4)
N1A—C3A—H3AB	109.4	C36B—C39B—P1B	121.6 (4)
C4A—C3A—H3AB	109.4	C46B—C41B—C42B	118.9 (5)

H3AA—C3A—H3AB	108.0	C46B—C41B—P1B	121.3 (4)
C3A—C4A—P1A	107.6 (3)	C42B—C41B—P1B	119.6 (4)
C3A—C4A—H4AA	110.2	C43B—C42B—C41B	120.0 (6)
P1A—C4A—H4AA	110.2	C43B—C42B—H42B	120.0
C3A—C4A—H4AB	110.2	C41B—C42B—H42B	120.0
P1A—C4A—H4AB	110.2	C44B—C43B—C42B	120.6 (6)
H4AA—C4A—H4AB	108.5	C44B—C43B—H43B	119.7
N2A—C5A—C6A	121.3 (4)	C42B—C43B—H43B	119.7
N2A—C5A—H5AA	119.4	C43B—C44B—C45B	119.9 (6)
C6A—C5A—H5AA	119.4	C43B—C44B—H44B	120.0
C5A—C6A—P2A	110.3 (3)	C45B—C44B—H44B	120.0
C5A—C6A—H6AA	109.6	C44B—C45B—C46B	119.7 (6)
P2A—C6A—H6AA	109.6	C44B—C45B—H45B	120.1
C5A—C6A—H6AB	109.6	C46B—C45B—H45B	120.1
P2A—C6A—H6AB	109.6	C41B—C46B—C45B	120.8 (5)
H6AA—C6A—H6AB	108.1	C41B—C46B—H46B	119.6
O1A—C7A—Fe1A	179.4 (6)	C45B—C46B—H46B	119.6
C16A—C11A—C12A	118.3 (5)	C31B—C52B—C53B	110.6 (5)
C16A—C11A—C1A	124.3 (5)	C31B—C52B—H52C	109.5
C12A—C11A—C1A	117.4 (5)	C53B—C52B—H52C	109.5
C13A—C12A—C11A	121.0 (5)	C31B—C52B—H52D	109.5
C13A—C12A—H12A	119.5	C53B—C52B—H52D	109.5
C11A—C12A—H12A	119.5	H52C—C52B—H52D	108.1
C14A—C13A—C12A	120.5 (6)	C54B—C53B—C52B	112.3 (5)
C14A—C13A—H13A	119.8	C54B—C53B—H53C	109.1
C12A—C13A—H13A	119.8	C52B—C53B—H53C	109.1
C13A—C14A—C15A	119.7 (6)	C54B—C53B—H53D	109.1
C13A—C14A—H14A	120.1	C52B—C53B—H53D	109.1
C15A—C14A—H14A	120.1	H53C—C53B—H53D	107.9
C16A—C15A—C14A	119.8 (6)	C55B—C54B—C53B	111.6 (5)
C16A—C15A—H15A	120.1	C55B—C54B—H54C	109.3
C14A—C15A—H15A	120.1	C53B—C54B—H54C	109.3
C11A—C16A—C15A	120.7 (5)	C55B—C54B—H54D	109.3
C11A—C16A—H16A	119.7	C53B—C54B—H54D	109.3
C15A—C16A—H16A	119.7	H54C—C54B—H54D	108.0
C22A—C21A—C26A	119.4 (5)	C54B—C55B—C56B	111.7 (5)
C22A—C21A—C2A	121.4 (5)	C54B—C55B—H55C	109.3
C26A—C21A—C2A	119.1 (5)	C56B—C55B—H55C	109.3
C21A—C22A—C23A	120.1 (5)	C54B—C55B—H55D	109.3
C21A—C22A—H22A	120.0	C56B—C55B—H55D	109.3
C23A—C22A—H22A	120.0	H55C—C55B—H55D	107.9
C24A—C23A—C22A	120.2 (6)	C55B—C56B—C31B	110.8 (5)
C24A—C23A—H23A	119.9	C55B—C56B—H56C	109.5
C22A—C23A—H23A	119.9	C31B—C56B—H56C	109.5
C23A—C24A—C25A	120.9 (5)	C55B—C56B—H56D	109.5
C23A—C24A—H24A	119.5	C31B—C56B—H56D	109.5
C25A—C24A—H24A	119.5	H56C—C56B—H56D	108.1
C24A—C25A—C26A	118.9 (6)	C66B—C61B—C62B	110.6 (5)

C24A—C25A—H25A	120.6	C66B—C61B—P2B	112.3 (4)
C26A—C25A—H25A	120.6	C62B—C61B—P2B	116.2 (4)
C21A—C26A—C25A	120.4 (6)	C66B—C61B—H61B	105.6
C21A—C26A—H26A	119.8	C62B—C61B—H61B	105.6
C25A—C26A—H26A	119.8	P2B—C61B—H61B	105.6
C36A—C31A—C32A	118.3 (5)	C63B—C62B—C61B	110.1 (5)
C36A—C31A—P1A	122.9 (4)	C63B—C62B—H62C	109.6
C32A—C31A—P1A	118.8 (4)	C61B—C62B—H62C	109.6
C33A—C32A—C31A	120.4 (5)	C63B—C62B—H62D	109.6
C33A—C32A—H32A	119.8	C61B—C62B—H62D	109.6
C31A—C32A—H32A	119.8	H62C—C62B—H62D	108.1
C34A—C33A—C32A	120.3 (5)	C64B—C63B—C62B	112.0 (6)
C34A—C33A—H33A	119.8	C64B—C63B—H63C	109.2
C32A—C33A—H33A	119.8	C62B—C63B—H63C	109.2
C35A—C34A—C33A	120.2 (5)	C64B—C63B—H63D	109.2
C35A—C34A—H34A	119.9	C62B—C63B—H63D	109.2
C33A—C34A—H34A	119.9	H63C—C63B—H63D	107.9
C34A—C35A—C36A	120.7 (6)	C63B—C64B—C65B	111.9 (6)
C34A—C35A—H35A	119.6	C63B—C64B—H64C	109.2
C36A—C35A—H35A	119.6	C65B—C64B—H64C	109.2
C35A—C36A—C31A	120.1 (5)	C63B—C64B—H64D	109.2
C35A—C36A—H36A	120.0	C65B—C64B—H64D	109.2
C31A—C36A—H36A	120.0	H64C—C64B—H64D	107.9
C42A—C41A—C46A	119.3 (6)	C64B—C65B—C66B	111.3 (5)
C42A—C41A—P1A	119.4 (5)	C64B—C65B—H65C	109.4
C46A—C41A—P1A	121.3 (4)	C66B—C65B—H65C	109.4
C41A—C42A—C43A	120.1 (7)	C64B—C65B—H65D	109.4
C41A—C42A—H42A	119.9	C66B—C65B—H65D	109.4
C43A—C42A—H42A	119.9	H65C—C65B—H65D	108.0
C44A—C43A—C42A	119.4 (6)	C61B—C66B—C65B	111.1 (5)
C44A—C43A—H43A	120.3	C61B—C66B—H66C	109.4
C42A—C43A—H43A	120.3	C65B—C66B—H66C	109.4
C43A—C44A—C45A	121.3 (7)	C61B—C66B—H66D	109.4
C43A—C44A—H44A	119.4	C65B—C66B—H66D	109.4
C45A—C44A—H44A	119.4	H66C—C66B—H66D	108.0
C44A—C45A—C46A	119.5 (7)	C72A—C71A—C76A	115.2 (5)
C44A—C45A—H45A	120.3	C72A—C71A—B1A	122.5 (5)
C46A—C45A—H45A	120.3	C76A—C71A—B1A	121.9 (5)
C41A—C46A—C45A	120.4 (6)	C73A—C72A—C71A	123.0 (5)
C41A—C46A—H46A	119.8	C73A—C72A—H72A	118.5
C45A—C46A—H46A	119.8	C71A—C72A—H72A	118.5
C56A—C51A—C52A	110.7 (5)	C74A—C73A—C72A	119.8 (6)
C56A—C51A—P2A	115.1 (4)	C74A—C73A—H73A	120.1
C52A—C51A—P2A	115.9 (4)	C72A—C73A—H73A	120.1
C56A—C51A—H51A	104.6	C75A—C74A—C73A	119.1 (5)
C52A—C51A—H51A	104.6	C75A—C74A—H74A	120.4
P2A—C51A—H51A	104.6	C73A—C74A—H74A	120.4
C53A—C52A—C51A	111.4 (5)	C74A—C75A—C76A	120.2 (6)

C53A—C52A—H52A	109.4	C74A—C75A—H75A	119.9
C51A—C52A—H52A	109.4	C76A—C75A—H75A	119.9
C53A—C52A—H52B	109.4	C75A—C76A—C71A	122.6 (6)
C51A—C52A—H52B	109.4	C75A—C76A—H76A	118.7
H52A—C52A—H52B	108.0	C71A—C76A—H76A	118.7
C54A—C53A—C52A	111.6 (5)	C82A—C81A—C86A	114.7 (5)
C54A—C53A—H53A	109.3	C82A—C81A—B1A	123.5 (5)
C52A—C53A—H53A	109.3	C86A—C81A—B1A	121.5 (5)
C54A—C53A—H53B	109.3	C83A—C82A—C81A	122.6 (6)
C52A—C53A—H53B	109.3	C83A—C82A—H82A	118.7
H53A—C53A—H53B	108.0	C81A—C82A—H82A	118.7
C53A—C54A—C55A	111.2 (5)	C82A—C83A—C84A	120.5 (6)
C53A—C54A—H54A	109.4	C82A—C83A—H83A	119.7
C55A—C54A—H54A	109.4	C84A—C83A—H83A	119.8
C53A—C54A—H54B	109.4	C85A—C84A—C83A	118.5 (6)
C55A—C54A—H54B	109.4	C85A—C84A—H84A	120.8
H54A—C54A—H54B	108.0	C83A—C84A—H84A	120.8
C56A—C55A—C54A	111.2 (6)	C84A—C85A—C86A	120.3 (6)
C56A—C55A—H55A	109.4	C84A—C85A—H85A	119.9
C54A—C55A—H55A	109.4	C86A—C85A—H85A	119.9
C56A—C55A—H55B	109.4	C85A—C86A—C81A	123.4 (6)
C54A—C55A—H55B	109.4	C85A—C86A—H86A	118.3
H55A—C55A—H55B	108.0	C81A—C86A—H86A	118.3
C55A—C56A—C51A	110.6 (5)	C92A—C91A—C96A	115.0 (5)
C55A—C56A—H56A	109.5	C92A—C91A—B1A	121.6 (5)
C51A—C56A—H56A	109.5	C96A—C91A—B1A	123.0 (5)
C55A—C56A—H56B	109.5	C91A—C92A—C93A	122.6 (6)
C51A—C56A—H56B	109.5	C91A—C92A—H92A	118.7
H56A—C56A—H56B	108.1	C93A—C92A—H92A	118.7
C62A—C61A—C66A	110.9 (5)	C94A—C93A—C92A	120.1 (6)
C62A—C61A—P2A	118.5 (5)	C94A—C93A—H93A	120.0
C66A—C61A—P2A	111.2 (4)	C92A—C93A—H93A	120.0
C62A—C61A—H61A	105.0	C95A—C94A—C93A	118.7 (6)
C66A—C61A—H61A	105.0	C95A—C94A—H94A	120.6
P2A—C61A—H61A	105.0	C93A—C94A—H94A	120.6
C61A—C62A—C63A	110.6 (6)	C94A—C95A—C96A	121.1 (6)
C61A—C62A—H62A	109.5	C94A—C95A—H95A	119.5
C63A—C62A—H62A	109.5	C96A—C95A—H95A	119.5
C61A—C62A—H62B	109.5	C95A—C96A—C91A	122.5 (6)
C63A—C62A—H62B	109.5	C95A—C96A—H96A	118.8
H62A—C62A—H62B	108.1	C91A—C96A—H96A	118.8
C64A—C63A—C62A	110.9 (6)	C106—C101—C102	114.8 (5)
C64A—C63A—H63A	109.4	C106—C101—B1A	122.1 (5)
C62A—C63A—H63A	109.4	C102—C101—B1A	122.9 (5)
C64A—C63A—H63B	109.4	C103—C102—C101	122.4 (6)
C62A—C63A—H63B	109.4	C103—C102—H10A	118.8
H63A—C63A—H63B	108.0	C101—C102—H10A	118.8
C65A—C64A—C63A	110.8 (6)	C104—C103—C102	121.0 (6)

C65A—C64A—H64A	109.5	C104—C103—H10B	119.5
C63A—C64A—H64A	109.5	C102—C103—H10B	119.5
C65A—C64A—H64B	109.5	C103—C104—C105	118.8 (6)
C63A—C64A—H64B	109.5	C103—C104—H10C	120.6
H64A—C64A—H64B	108.1	C105—C104—H10C	120.6
C64A—C65A—C66A	112.5 (6)	C104—C105—C106	119.6 (6)
C64A—C65A—H65A	109.1	C104—C105—H10D	120.2
C66A—C65A—H65A	109.1	C106—C105—H10D	120.2
C64A—C65A—H65B	109.1	C105—C106—C101	123.4 (6)
C66A—C65A—H65B	109.1	C105—C106—H10E	118.3
H65A—C65A—H65B	107.8	C101—C106—H10E	118.3
C65A—C66A—C61A	111.8 (5)	C91A—B1A—C81A	112.4 (4)
C65A—C66A—H66A	109.2	C91A—B1A—C71A	103.0 (4)
C61A—C66A—H66A	109.2	C81A—B1A—C71A	111.7 (5)
C65A—C66A—H66B	109.2	C91A—B1A—C101	114.0 (5)
C61A—C66A—H66B	109.2	C81A—B1A—C101	104.7 (4)
H66A—C66A—H66B	107.9	C71A—B1A—C101	111.2 (4)
C7B—Fe1B—N2B	171.5 (2)	C72B—C71B—C76B	114.6 (5)
C7B—Fe1B—N1B	98.9 (2)	C72B—C71B—B1B	123.7 (5)
N2B—Fe1B—N1B	82.35 (17)	C76B—C71B—B1B	121.4 (5)
C7B—Fe1B—P1B	87.17 (19)	C73B—C72B—C71B	122.8 (6)
N2B—Fe1B—P1B	101.30 (13)	C73B—C72B—H72B	118.6
N1B—Fe1B—P1B	80.18 (13)	C71B—C72B—H72B	118.6
C7B—Fe1B—P2B	95.29 (19)	C74B—C73B—C72B	120.2 (5)
N2B—Fe1B—P2B	83.33 (13)	C74B—C73B—H73B	119.9
N1B—Fe1B—P2B	165.68 (12)	C72B—C73B—H73B	119.9
P1B—Fe1B—P2B	102.70 (6)	C75B—C74B—C73B	119.5 (5)
C7B—Fe1B—Br1B	85.08 (19)	C75B—C74B—H74B	120.2
N2B—Fe1B—Br1B	86.68 (13)	C73B—C74B—H74B	120.2
N1B—Fe1B—Br1B	84.78 (13)	C74B—C75B—C76B	120.6 (6)
P1B—Fe1B—Br1B	161.80 (5)	C74B—C75B—H75B	119.7
P2B—Fe1B—Br1B	94.40 (4)	C76B—C75B—H75B	119.7
C39B—P1B—C4B	105.9 (3)	C75B—C76B—C71B	122.3 (6)
C39B—P1B—C41B	102.0 (2)	C75B—C76B—H76B	118.8
C4B—P1B—C41B	101.4 (2)	C71B—C76B—H76B	118.8
C39B—P1B—Fe1B	118.49 (17)	C86B—C81B—C82B	114.5 (5)
C4B—P1B—Fe1B	98.80 (19)	C86B—C81B—B1B	124.3 (5)
C41B—P1B—Fe1B	127.01 (19)	C82B—C81B—B1B	120.9 (5)
C31B—P2B—C61B	109.5 (3)	C83B—C82B—C81B	122.5 (6)
C31B—P2B—C6B	103.1 (2)	C83B—C82B—H82B	118.7
C61B—P2B—C6B	104.4 (2)	C81B—C82B—H82B	118.7
C31B—P2B—Fe1B	116.34 (18)	C84B—C83B—C82B	121.1 (6)
C61B—P2B—Fe1B	119.65 (19)	C84B—C83B—H83B	119.4
C6B—P2B—Fe1B	101.25 (17)	C82B—C83B—H83B	119.4
C3B—N1B—C1B	111.0 (4)	C83B—C84B—C85B	118.9 (6)
C3B—N1B—Fe1B	117.4 (3)	C83B—C84B—H84B	120.6
C1B—N1B—Fe1B	109.7 (3)	C85B—C84B—H84B	120.6
C3B—N1B—H1B	106.0	C84B—C85B—C86B	119.5 (6)

C1B—N1B—H1B	106.0	C84B—C85B—H85B	120.3
Fe1B—N1B—H1B	106.0	C86B—C85B—H85B	120.3
C5B—N2B—C2B	119.3 (4)	C81B—C86B—C85B	123.5 (6)
C5B—N2B—Fe1B	124.9 (4)	C81B—C86B—H86B	118.3
C2B—N2B—Fe1B	114.1 (3)	C85B—C86B—H86B	118.3
C2B—C1B—N1B	107.9 (3)	C92B—C91B—C96B	115.0 (5)
C2B—C1B—C11B	112.9 (4)	C92B—C91B—B1B	122.8 (5)
N1B—C1B—C11B	112.0 (4)	C96B—C91B—B1B	121.9 (5)
C2B—C1B—H1BA	108.0	C91B—C92B—C93B	123.3 (6)
N1B—C1B—H1BA	108.0	C91B—C92B—H92B	118.4
C11B—C1B—H1BA	108.0	C93B—C92B—H92B	118.4
N2B—C2B—C21B	114.0 (4)	C94B—C93B—C92B	119.2 (6)
N2B—C2B—C1B	106.3 (3)	C94B—C93B—H93B	120.4
C21B—C2B—C1B	114.8 (4)	C92B—C93B—H93B	120.4
N2B—C2B—H2BA	107.1	C95B—C94B—C93B	119.0 (6)
C21B—C2B—H2BA	107.1	C95B—C94B—H94B	120.5
C1B—C2B—H2BA	107.1	C93B—C94B—H94B	120.5
N1B—C3B—C4B	111.3 (4)	C96B—C95B—C94B	120.5 (6)
N1B—C3B—H3BA	109.4	C96B—C95B—H95B	119.8
C4B—C3B—H3BA	109.4	C94B—C95B—H95B	119.8
N1B—C3B—H3BB	109.4	C95B—C96B—C91B	123.1 (6)
C4B—C3B—H3BB	109.4	C95B—C96B—H96B	118.5
H3BA—C3B—H3BB	108.0	C91B—C96B—H96B	118.5
C3B—C4B—P1B	111.2 (3)	C116—C111—C112	114.8 (5)
C3B—C4B—H4BA	109.4	C116—C111—B1B	124.4 (5)
P1B—C4B—H4BA	109.4	C112—C111—B1B	120.5 (5)
C3B—C4B—H4BB	109.4	C113—C112—C111	122.7 (5)
P1B—C4B—H4BB	109.4	C113—C112—H11A	118.6
H4BA—C4B—H4BB	108.0	C111—C112—H11A	118.6
N2B—C5B—C6B	120.6 (5)	C114—C113—C112	119.8 (6)
N2B—C5B—H5BA	119.7	C114—C113—H11B	120.1
C6B—C5B—H5BA	119.7	C112—C113—H11B	120.1
C5B—C6B—P2B	108.9 (3)	C115—C114—C113	119.6 (5)
C5B—C6B—H6BA	109.9	C115—C114—H11C	120.2
P2B—C6B—H6BA	109.9	C113—C114—H11C	120.2
C5B—C6B—H6BB	109.9	C114—C115—C116	119.9 (6)
P2B—C6B—H6BB	109.9	C114—C115—H11D	120.1
H6BA—C6B—H6BB	108.3	C116—C115—H11D	120.1
O1B—C7B—Fe1B	178.5 (6)	C111—C116—C115	123.1 (6)
C12B—C11B—C16B	119.4 (5)	C111—C116—H11E	118.4
C12B—C11B—C1B	121.0 (5)	C115—C116—H11E	118.4
C16B—C11B—C1B	119.5 (5)	C111—B1B—C71B	112.9 (5)
C11B—C12B—C13B	120.0 (5)	C111—B1B—C81B	104.5 (4)
C11B—C12B—H12B	120.0	C71B—B1B—C81B	112.3 (4)
C13B—C12B—H12B	120.0	C111—B1B—C91B	112.0 (4)
C14B—C13B—C12B	120.2 (6)	C71B—B1B—C91B	102.8 (4)
C14B—C13B—H13B	119.9	C81B—B1B—C91B	112.6 (5)

C3A—N1A—C1A—C11A	−39.4 (6)
Fe1A—N1A—C1A—C11A	−172.8 (3)
C3A—N1A—C1A—C2A	89.7 (5)
Fe1A—N1A—C1A—C2A	−43.7 (4)
C5A—N2A—C2A—C21A	15.0 (6)
Fe1A—N2A—C2A—C21A	−160.7 (3)
C5A—N2A—C2A—C1A	140.9 (5)
Fe1A—N2A—C2A—C1A	−34.7 (4)
N1A—C1A—C2A—N2A	50.1 (4)
C11A—C1A—C2A—N2A	179.9 (4)
N1A—C1A—C2A—C21A	175.2 (4)
C11A—C1A—C2A—C21A	−55.0 (5)
C1A—N1A—C3A—C4A	−142.1 (4)
Fe1A—N1A—C3A—C4A	−13.6 (5)
N1A—C3A—C4A—P1A	43.0 (5)
C31A—P1A—C4A—C3A	71.2 (4)
C41A—P1A—C4A—C3A	178.1 (4)
Fe1A—P1A—C4A—C3A	−49.6 (4)
C2A—N2A—C5A—C6A	179.5 (5)
Fe1A—N2A—C5A—C6A	−5.2 (7)
N2A—C5A—C6A—P2A	−1.4 (7)
C51A—P2A—C6A—C5A	127.7 (4)
C61A—P2A—C6A—C5A	−117.8 (4)
Fe1A—P2A—C6A—C5A	5.7 (4)
N1A—C1A—C11A—C16A	84.0 (6)
C2A—C1A—C11A—C16A	−41.8 (7)
N1A—C1A—C11A—C12A	−96.8 (5)
C2A—C1A—C11A—C12A	137.5 (5)
C16A—C11A—C12A—C13A	−1.5 (8)
C1A—C11A—C12A—C13A	179.2 (5)
C11A—C12A—C13A—C14A	0.7 (8)
C12A—C13A—C14A—C15A	−0.4 (9)
C13A—C14A—C15A—C16A	0.9 (9)
C12A—C11A—C16A—C15A	2.0 (8)
C1A—C11A—C16A—C15A	−178.8 (5)
C14A—C15A—C16A—C11A	−1.7 (8)
N2A—C2A—C21A—C22A	76.5 (6)
C1A—C2A—C21A—C22A	−44.1 (7)
N2A—C2A—C21A—C26A	−100.0 (5)
C1A—C2A—C21A—C26A	139.3 (5)
C26A—C21A—C22A—C23A	0.6 (8)
C2A—C21A—C22A—C23A	−175.9 (5)
C21A—C22A—C23A—C24A	0.3 (9)
C22A—C23A—C24A—C25A	−1.4 (9)
C23A—C24A—C25A—C26A	1.5 (9)
C22A—C21A—C26A—C25A	−0.5 (8)
C2A—C21A—C26A—C25A	176.1 (5)
C24A—C25A—C26A—C21A	−0.6 (8)
C33B—C34B—C35B—C36B	−1.6 (9)
C34B—C35B—C36B—C39B	1.6 (9)
C33B—C32B—C39B—C36B	−2.4 (8)
C33B—C32B—C39B—P1B	174.7 (4)
C35B—C36B—C39B—C32B	0.4 (8)
C35B—C36B—C39B—P1B	−176.6 (5)
C4B—P1B—C39B—C32B	175.8 (4)
C41B—P1B—C39B—C32B	−78.5 (5)
Fe1B—P1B—C39B—C32B	66.2 (5)
C4B—P1B—C39B—C36B	−7.3 (5)
C41B—P1B—C39B—C36B	98.4 (5)
Fe1B—P1B—C39B—C36B	−116.9 (4)
C39B—P1B—C41B—C46B	13.1 (5)
C4B—P1B—C41B—C46B	122.3 (5)
Fe1B—P1B—C41B—C46B	−127.3 (4)
C39B—P1B—C41B—C42B	−163.7 (5)
C4B—P1B—C41B—C42B	−54.5 (5)
Fe1B—P1B—C41B—C42B	55.9 (5)
C46B—C41B—C42B—C43B	1.0 (9)
P1B—C41B—C42B—C43B	177.8 (5)
C41B—C42B—C43B—C44B	−1.8 (9)
C42B—C43B—C44B—C45B	1.6 (10)
C43B—C44B—C45B—C46B	−0.5 (10)
C42B—C41B—C46B—C45B	0.1 (8)
P1B—C41B—C46B—C45B	−176.8 (5)
C44B—C45B—C46B—C41B	−0.3 (9)
C56B—C31B—C52B—C53B	−54.6 (7)
P2B—C31B—C52B—C53B	170.9 (4)
C31B—C52B—C53B—C54B	53.3 (7)
C52B—C53B—C54B—C55B	−53.8 (8)
C53B—C54B—C55B—C56B	54.9 (8)
C54B—C55B—C56B—C31B	−56.2 (7)
C52B—C31B—C56B—C55B	56.3 (7)
P2B—C31B—C56B—C55B	−169.4 (4)
C31B—P2B—C61B—C66B	53.3 (5)
C6B—P2B—C61B—C66B	163.2 (4)
Fe1B—P2B—C61B—C66B	−84.6 (4)
C31B—P2B—C61B—C62B	−75.5 (5)
C6B—P2B—C61B—C62B	34.3 (5)
Fe1B—P2B—C61B—C62B	146.5 (4)
C66B—C61B—C62B—C63B	55.4 (7)
P2B—C61B—C62B—C63B	−175.0 (5)
C61B—C62B—C63B—C64B	−55.8 (8)
C62B—C63B—C64B—C65B	56.3 (9)
C63B—C64B—C65B—C66B	−55.4 (8)
C62B—C61B—C66B—C65B	−55.5 (7)
P2B—C61B—C66B—C65B	172.9 (4)
C64B—C65B—C66B—C61B	55.3 (7)

C4A—P1A—C31A—C36A	12.6 (5)
C41A—P1A—C31A—C36A	−96.0 (5)
Fe1A—P1A—C31A—C36A	119.3 (4)
C4A—P1A—C31A—C32A	−168.8 (4)
C41A—P1A—C31A—C32A	82.6 (5)
Fe1A—P1A—C31A—C32A	−62.2 (5)
C36A—C31A—C32A—C33A	0.4 (8)
P1A—C31A—C32A—C33A	−178.2 (4)
C31A—C32A—C33A—C34A	−1.5 (9)
C32A—C33A—C34A—C35A	1.0 (9)
C33A—C34A—C35A—C36A	0.6 (10)
C34A—C35A—C36A—C31A	−1.8 (9)
C32A—C31A—C36A—C35A	1.3 (8)
P1A—C31A—C36A—C35A	179.8 (5)
C31A—P1A—C41A—C42A	166.0 (5)
C4A—P1A—C41A—C42A	56.9 (5)
Fe1A—P1A—C41A—C42A	−54.7 (5)
C31A—P1A—C41A—C46A	−13.1 (5)
C4A—P1A—C41A—C46A	−122.2 (5)
Fe1A—P1A—C41A—C46A	126.2 (4)
C46A—C41A—C42A—C43A	0.5 (9)
P1A—C41A—C42A—C43A	−178.6 (5)
C41A—C42A—C43A—C44A	−1.2 (10)
C42A—C43A—C44A—C45A	1.4 (10)
C43A—C44A—C45A—C46A	−0.9 (11)
C42A—C41A—C46A—C45A	0.0 (9)
P1A—C41A—C46A—C45A	179.1 (5)
C44A—C45A—C46A—C41A	0.2 (10)
C6A—P2A—C51A—C56A	−162.8 (4)
C61A—P2A—C51A—C56A	84.5 (5)
Fe1A—P2A—C51A—C56A	−54.4 (5)
C6A—P2A—C51A—C52A	65.8 (5)
C61A—P2A—C51A—C52A	−46.9 (5)
Fe1A—P2A—C51A—C52A	174.2 (3)
C56A—C51A—C52A—C53A	55.0 (7)
P2A—C51A—C52A—C53A	−171.6 (4)
C51A—C52A—C53A—C54A	−55.1 (8)
C52A—C53A—C54A—C55A	55.6 (8)
C53A—C54A—C55A—C56A	−56.5 (8)
C54A—C55A—C56A—C51A	56.6 (7)
C52A—C51A—C56A—C55A	−55.6 (7)
P2A—C51A—C56A—C55A	170.5 (5)
C51A—P2A—C61A—C62A	78.0 (5)
C6A—P2A—C61A—C62A	−31.9 (6)
Fe1A—P2A—C61A—C62A	−143.1 (5)
C51A—P2A—C61A—C66A	−52.3 (5)
C6A—P2A—C61A—C66A	−162.2 (4)
Fe1A—P2A—C61A—C66A	86.6 (4)
C76A—C71A—C72A—C73A	1.0 (9)
B1A—C71A—C72A—C73A	174.1 (6)
C71A—C72A—C73A—C74A	−0.4 (9)
C72A—C73A—C74A—C75A	−0.8 (9)
C73A—C74A—C75A—C76A	1.4 (9)
C74A—C75A—C76A—C71A	−0.9 (10)
C72A—C71A—C76A—C75A	−0.3 (9)
B1A—C71A—C76A—C75A	−173.5 (5)
C86A—C81A—C82A—C83A	0.2 (9)
B1A—C81A—C82A—C83A	−174.3 (6)
C81A—C82A—C83A—C84A	−0.7 (10)
C82A—C83A—C84A—C85A	1.9 (10)
C83A—C84A—C85A—C86A	−2.7 (10)
C84A—C85A—C86A—C81A	2.3 (10)
C82A—C81A—C86A—C85A	−1.0 (9)
B1A—C81A—C86A—C85A	173.6 (6)
C96A—C91A—C92A—C93A	−1.6 (8)
B1A—C91A—C92A—C93A	−174.3 (5)
C91A—C92A—C93A—C94A	0.1 (9)
C92A—C93A—C94A—C95A	0.7 (9)
C93A—C94A—C95A—C96A	−0.1 (9)
C94A—C95A—C96A—C91A	−1.5 (9)
C92A—C91A—C96A—C95A	2.2 (8)
B1A—C91A—C96A—C95A	174.9 (5)
C106—C101—C102—C103	2.0 (8)
B1A—C101—C102—C103	176.4 (5)
C101—C102—C103—C104	−0.8 (9)
C102—C103—C104—C105	−0.8 (8)
C103—C104—C105—C106	1.0 (8)
C104—C105—C106—C101	0.3 (9)
C102—C101—C106—C105	−1.7 (8)
B1A—C101—C106—C105	−176.2 (5)
C92A—C91A—B1A—C81A	−41.7 (7)
C96A—C91A—B1A—C81A	146.1 (5)
C92A—C91A—B1A—C71A	78.7 (6)
C96A—C91A—B1A—C71A	−93.5 (6)
C92A—C91A—B1A—C101	−160.7 (5)
C96A—C91A—B1A—C101	27.1 (7)
C82A—C81A—B1A—C91A	−27.5 (7)
C86A—C81A—B1A—C91A	158.4 (5)
C82A—C81A—B1A—C71A	−142.7 (5)
C86A—C81A—B1A—C71A	43.2 (7)
C82A—C81A—B1A—C101	96.8 (6)
C86A—C81A—B1A—C101	−77.3 (6)
C72A—C71A—B1A—C91A	−85.5 (6)
C76A—C71A—B1A—C91A	87.2 (6)
C72A—C71A—B1A—C81A	35.3 (7)
C76A—C71A—B1A—C81A	−152.0 (5)

C66A—C61A—C62A—C63A	−55.5 (8)	C72A—C71A—B1A—C101	151.9 (5)
P2A—C61A—C62A—C63A	174.1 (5)	C76A—C71A—B1A—C101	−35.4 (7)
C61A—C62A—C63A—C64A	57.4 (9)	C106—C101—B1A—C91A	−153.0 (5)
C62A—C63A—C64A—C65A	−56.4 (10)	C102—C101—B1A—C91A	33.0 (7)
C63A—C64A—C65A—C66A	54.8 (9)	C106—C101—B1A—C81A	83.8 (6)
C64A—C65A—C66A—C61A	−53.6 (8)	C102—C101—B1A—C81A	−90.3 (6)
C62A—C61A—C66A—C65A	53.8 (7)	C106—C101—B1A—C71A	−37.0 (7)
P2A—C61A—C66A—C65A	−172.1 (4)	C102—C101—B1A—C71A	148.9 (5)
C3B—N1B—C1B—C2B	−168.9 (4)	C76B—C71B—C72B—C73B	1.1 (8)
Fe1B—N1B—C1B—C2B	−37.5 (4)	B1B—C71B—C72B—C73B	174.4 (5)
C3B—N1B—C1B—C11B	66.3 (5)	C71B—C72B—C73B—C74B	−1.4 (9)
Fe1B—N1B—C1B—C11B	−162.3 (3)	C72B—C73B—C74B—C75B	1.1 (9)
C5B—N2B—C2B—C21B	29.0 (6)	C73B—C74B—C75B—C76B	−0.6 (9)
Fe1B—N2B—C2B—C21B	−165.2 (3)	C74B—C75B—C76B—C71B	0.4 (9)
C5B—N2B—C2B—C1B	156.5 (4)	C72B—C71B—C76B—C75B	−0.6 (8)
Fe1B—N2B—C2B—C1B	−37.7 (4)	B1B—C71B—C76B—C75B	−174.1 (5)
N1B—C1B—C2B—N2B	47.6 (4)	C86B—C81B—C82B—C83B	1.1 (8)
C11B—C1B—C2B—N2B	171.9 (4)	B1B—C81B—C82B—C83B	175.8 (5)
N1B—C1B—C2B—C21B	174.6 (4)	C81B—C82B—C83B—C84B	1.2 (9)
C11B—C1B—C2B—C21B	−61.1 (5)	C82B—C83B—C84B—C85B	−2.0 (9)
C1B—N1B—C3B—C4B	105.2 (5)	C83B—C84B—C85B—C86B	0.4 (8)
Fe1B—N1B—C3B—C4B	−22.1 (5)	C82B—C81B—C86B—C85B	−2.8 (8)
N1B—C3B—C4B—P1B	−14.1 (5)	B1B—C81B—C86B—C85B	−177.2 (5)
C39B—P1B—C4B—C3B	−84.7 (4)	C84B—C85B—C86B—C81B	2.1 (9)
C41B—P1B—C4B—C3B	169.1 (4)	C96B—C91B—C92B—C93B	−1.2 (8)
Fe1B—P1B—C4B—C3B	38.4 (4)	B1B—C91B—C92B—C93B	−175.0 (5)
C2B—N2B—C5B—C6B	172.6 (4)	C91B—C92B—C93B—C94B	0.7 (9)
Fe1B—N2B—C5B—C6B	8.5 (7)	C92B—C93B—C94B—C95B	0.7 (9)
N2B—C5B—C6B—P2B	−11.4 (7)	C93B—C94B—C95B—C96B	−1.6 (9)
C31B—P2B—C6B—C5B	−112.0 (4)	C94B—C95B—C96B—C91B	1.0 (9)
C61B—P2B—C6B—C5B	133.6 (4)	C92B—C91B—C96B—C95B	0.4 (8)
Fe1B—P2B—C6B—C5B	8.7 (4)	B1B—C91B—C96B—C95B	174.2 (5)
C2B—C1B—C11B—C12B	−55.3 (6)	C116—C111—C112—C113	−2.3 (8)
N1B—C1B—C11B—C12B	66.8 (6)	B1B—C111—C112—C113	−175.7 (5)
C2B—C1B—C11B—C16B	125.0 (5)	C111—C112—C113—C114	2.0 (9)
N1B—C1B—C11B—C16B	−113.0 (5)	C112—C113—C114—C115	−1.7 (9)
C16B—C11B—C12B—C13B	0.1 (8)	C113—C114—C115—C116	1.9 (9)
C1B—C11B—C12B—C13B	−179.6 (5)	C112—C111—C116—C115	2.5 (9)
C11B—C12B—C13B—C14B	−0.1 (8)	B1B—C111—C116—C115	175.6 (6)
C12B—C13B—C14B—C15B	0.8 (9)	C114—C115—C116—C111	−2.3 (10)
C13B—C14B—C15B—C16B	−1.5 (9)	C116—C111—B1B—C71B	147.0 (5)
C14B—C15B—C16B—C11B	1.5 (8)	C112—C111—B1B—C71B	−40.2 (7)
C12B—C11B—C16B—C15B	−0.9 (8)	C116—C111—B1B—C81B	−90.7 (6)
C1B—C11B—C16B—C15B	178.9 (5)	C112—C111—B1B—C81B	82.1 (6)
N2B—C2B—C21B—C26B	71.2 (6)	C116—C111—B1B—C91B	31.5 (7)
C1B—C2B—C21B—C26B	−51.7 (6)	C112—C111—B1B—C91B	−155.7 (5)
N2B—C2B—C21B—C22B	−104.2 (5)	C72B—C71B—B1B—C111	148.8 (5)
C1B—C2B—C21B—C22B	132.8 (5)	C76B—C71B—B1B—C111	−38.3 (7)

C26B—C21B—C22B—C23B	−0.9 (8)	C72B—C71B—B1B—C81B	31.0 (7)
C2B—C21B—C22B—C23B	174.8 (5)	C76B—C71B—B1B—C81B	−156.2 (5)
C21B—C22B—C23B—C24B	0.3 (8)	C72B—C71B—B1B—C91B	−90.3 (6)
C22B—C23B—C24B—C25B	0.5 (9)	C76B—C71B—B1B—C91B	82.6 (6)
C23B—C24B—C25B—C26B	−0.8 (9)	C86B—C81B—B1B—C111	91.3 (6)
C24B—C25B—C26B—C21B	0.3 (8)	C82B—C81B—B1B—C111	−82.7 (6)
C22B—C21B—C26B—C25B	0.6 (8)	C86B—C81B—B1B—C71B	−145.9 (5)
C2B—C21B—C26B—C25B	−175.0 (5)	C82B—C81B—B1B—C71B	40.0 (7)
C61B—P2B—C31B—C52B	48.8 (5)	C86B—C81B—B1B—C91B	−30.5 (7)
C6B—P2B—C31B—C52B	−61.9 (5)	C82B—C81B—B1B—C91B	155.4 (5)
Fe1B—P2B—C31B—C52B	−171.7 (3)	C92B—C91B—B1B—C111	−149.2 (5)
C61B—P2B—C31B—C56B	−83.8 (5)	C96B—C91B—B1B—C111	37.5 (7)
C6B—P2B—C31B—C56B	165.5 (4)	C92B—C91B—B1B—C71B	89.3 (6)
Fe1B—P2B—C31B—C56B	55.7 (5)	C96B—C91B—B1B—C71B	−84.0 (6)
C39B—C32B—C33B—C34B	2.4 (8)	C92B—C91B—B1B—C81B	−31.8 (6)
C32B—C33B—C34B—C35B	−0.4 (9)	C96B—C91B—B1B—C81B	154.9 (5)