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Supporting information for article:

The crystal structure of [Fe2(PIMIC6)(AnthCO2)(CH3CN)]·[Fe2(PIMIC6)(AnthCO2)(CH3CN)0.9(DCM)0.1]·[Fe2(PIMIC6)(AnthCO2) (OH2)]·0.75CH3CN: A Crystallographer's Nightmare or a Fascinating Case of Disorder?

Sabine Becker

Supporting Information

The crystal structure of $[Fe_2(PIMIC6)(AnthCO_2)(CH_3CN)]\cdot[Fe_2(PIMIC6)(AnthCO_2)(CH_3CN)_{0.9}(DCM)_{0.1}]\cdot[Fe_2(PIMIC6)(AnthCO_2)(OH_2)]\cdot 0.75CH_3CN$: A Crystallographer's Nightmare or a Fascinating Case of Disorder?

Sabine Becker

Contents

1. Nomenclature

All atoms were named according to Scheme S1. The nomenclature is identical throughout all residues, which enables a quick and efficient comparison of disordered atoms and restraints such as SADI, SAME, BIND, etc.

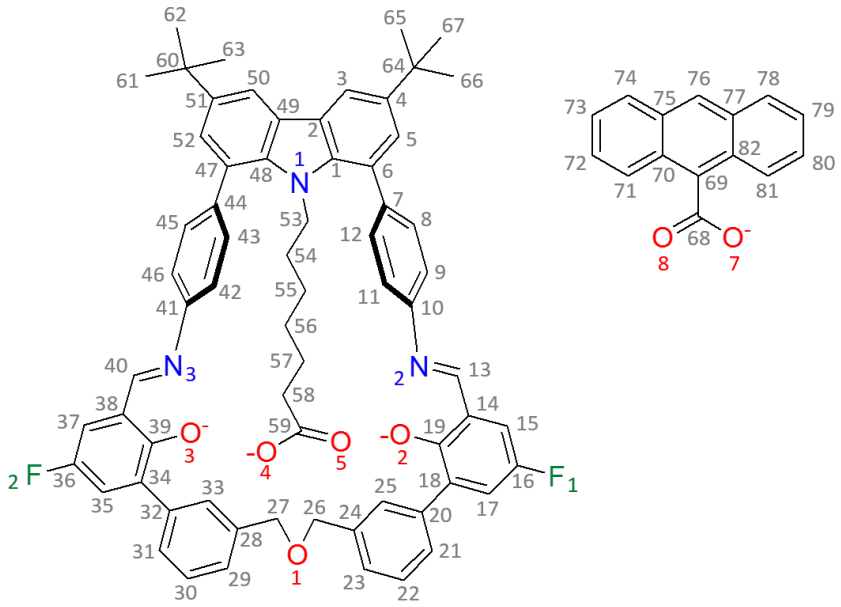
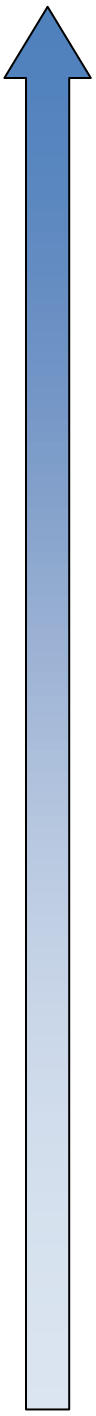


Figure S1. Nomenclature of the atoms of the organic ligands. Atoms were named identically throughout all residues.

The complexity of the disorder required a systematic approach in numbering all disordered atoms. This systematic numbering does not only facilitate the use of the SAME command, but furthermore, allows a quick and clear assignment of atoms that occur in restraints or in the CheckCif report. The nomenclature follows a simple system that is presented in Table S1. Atoms in non-disordered components as well as in the highest occupied disorder components were named according to Scheme S1 without the use of any suffices. Atoms of minor occupied disorder components were marked by adding letters in alphabetical order as suffices. The priority of the letters hereby corresponds to the occupancy, i.e. ***A*** marks the second highest occupied component, ***B*** the third highest occupied component, etc. The nomenclature of hydrogen atoms was carried out analogously. As it is good practice all hydrogen atoms were numbered the same way as the carbon atoms they are attached to. Hydrogen atoms attached to the same carbon atom were marked by adding suffices. Hereby, the suffices *A*, *B*, *C* were used for non-disordered as well as highest occupied components. Minor occupied disorder components were named by using the suffices *D-O* as listed in Table S1.

Please note that the nomenclature of atoms given in Table S4-S7 have additional numbers as suffices. These numbers are automatically added by *Ciftab* and correspond to the residue the atoms are a part of, i.e. Fe11 corresponds to Fe1 in residue 1, Fe12 to Fe1 in residue 2, etc.

Table S1. Overview of the nomenclature. Atoms in non-disordered components as well as in the highest occupied disorder component were named without any suffices. Minor occupied disorder components were marked with letters as suffices. The letters were added in alphabetical order with regard to the occupancy of the disorder component (second highest A, third highest B, etc.).



Occupancy

Disorder component	Atom numbering for carbon		Atom numbering for (methyl) hydrogens	
	general nomenclature	including residue number*	general nomenclature	including residue number*
1	C1	C11 *(residue 1)* C12 *(residue 2)* C13 *(residue 3)*	H1*A* H1*B* H1*C*	H1*A*1 *(residue 1)* H1*A*2 *(residue 2)* H1*A*3 *(residue 3)* H1*B*1 *(residue 1)* H1*B*2 *(residue 2)* H1*B*3 *(residue 3)* H1*C*1 *(residue 1)* H1*C*2 *(residue 2)* H1*C*3 *(residue 3)*
2	C1*A*	C1*A*1 *(residue 1)* C1*A*2 *(residue 2)* C1*A*3 *(residue 3)*	H1*D* H1*E* H1*F*	H1*D*1 *(residue 1)* H1*D*2 *(residue 2)* H1*D*3 *(residue 3)* H1*E*1 *(residue 1)* H1*E*2 *(residue 2)* H1*E*3 *(residue 3)* H1*F*1 *(residue 1)* H1*F*2 *(residue 2)* H1*F*3 *(residue 3)*
3	C1*B*	C1*B*1 *(residue 1)* C1*B*2 *(residue 2)* C1*B*3 *(residue 3)*	H1*G* H1*H* H1*I*	H1*G*1 *(residue 1)* H1*G*2 *(residue 2)* H1*G*3 *(residue 3)* H1*H*1 *(residue 1)* H1*H*2 *(residue 2)* H1*H*3 *(residue 3)* H1*I*1 *(residue 1)* H1*I*2 *(residue 2)* H1*I*3 *(residue 3)*
4	C1*C*	C1*C*1 *(residue 1)* C1*C*2 *(residue 2)* C1*C*3 *(residue 3)*	H1*J* H1*K* H1*L*	H1*J*1 *(residue 1)* H1*J*2 *(residue 2)* H1*J*3 *(residue 3)* H1*K*1 *(residue 1)* H1*K*2 *(residue 2)* H1*K*3 *(residue 3)* H1*L*1 *(residue 1)* H1*L*2 *(residue 2)* H1*L*3 *(residue 3)*
5	C1*D*	C1*D*1 *(residue 1)* C1*D*2 *(residue 2)* C1*D*3 *(residue 3)*	H1*M* H1*N* H1*O*	H1*M*1 *(residue 1)* H1*M*2 *(residue 2)* H1*M*3 *(residue 3)* H1*N*1 *(residue 1)* H1*N*2 *(residue 2)* H1*N*3 *(residue 3)* H1*O*1 *(residue 1)* H1*O*2 *(residue 2)* H1*O*3 *(residue 3)*

*The additional numbers are generated by Ciftab to differentiate between residues. This nomenclature is exclusively used in Tables S4-S7.

2. General Information

a. Intensity Statistics and Solvent Combinations Determined by SQUEEZE

Table S2. Intensity statistics of **1.**

Resolution	# Data	# Theory	% complete	redundancy	Mean I	Mean I/s	Rint	Rsigma
Inf – 2.05	3248	3253	99.8	12.47	97.6	50.01	0.0333	0.0143
2.05 – 1.60	3484	3486	99.9	12.85	34.5	37.06	0.0473	0.0179
1.60 – 1.40	3247	3248	100.0	11.73	19.9	26.54	0.0635	0.0255
1.40 – 1.25	3963	3963	100.0	10.12	13.7	19.05	0.0865	0.0377
1.25 – 1.15	3909	3910	100.0	9.05	10.2	13.80	0.1137	0.0540
1.15 – 1.05	5531	5531	100.0	8.22	7.6	10.15	0.1517	0.0777
1.05 – 1.00	3627	3627	100.0	7.63	5.9	7.75	0.2006	0.1072
1.00 – 0.95	4438	4438	100.0	7.24	4.3	5.70	0.2704	0.1515
0.95 – 0.90	5489	5490	100.0	6.81	3.3	4.25	0.3561	0.2134
0.90 – 0.85	6841	6841	100.0	6.39	2.4	2.95	0.5072	0.3182
0.85 – 0.80	8632	8632	100.0	5.94	1.6	1.89	0.7962	0.5101
0.80 – 0.75	11059	11091	99.7	5.41	1.1	1.20	1.2126	0.8269
0.75 – 0.75	397	601	66.1	1.27	0.8	0.55	1.3607	1.7490
0.85 – 0.75	**20088**	**20328**	**98.9**	**5.51**	**1.3**	**1.49**	**0.9847**	**0.6719**
Inf – 0.75	**63865**	**64111**	**99.6**	**7.76**	**11.6**	**10.80**	**0.0885**	**0.0648**

Table S3. Examples of possible solvent combinations and their total number of electrons. Combinations that match/are close to the electron equivalent of 691 and 692 found by SQUEEZE are highlighted in (dark) blue.

Entry	CH_2Cl_2		CH_3CN		ratio CH_3CN/CH_2Cl_2	# electrons (total)
	# molecules	# electrons	# molecules	# electrons		
1	0	0	31	682	----------	682
2	0	0	32	704	----------	704
3	1	42	30	660	30	702
4	2	84	28	616	14	700
5	3	126	26	572	8.7	698
6	4	168	24	528	6	696
7	5	210	22	484	4.4	694
8	6	252	20	440	3.3	692
9	7	294	18	396	2.6	690
10	8	336	16	352	2	688
11	9	378	14	308	1.6	686
12	10	420	12	264	1.2	684
13	11	462	10	220	0.91	682
14	12	504	8	176	0.67	680
15	13	546	6	132	0.46	678
16	14	588	4	88	0.29	676
17	15	630	2	44	0.13	674
18	16	672	0	0	----------	672

b. Structural Parameters

Table S4. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **1**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Fe11	1149(1)	7159(1)	2020(1)	41(1)
Fe21	1978(1)	6068(1)	2863(1)	54(1)
O41	1479(1)	6559(2)	1865(1)	55(1)
O51	1960(1)	5952(2)	2319(1)	58(1)
O61	975(1)	6893(2)	2448(1)	46(1)
O71	1431(1)	6198(2)	2870(1)	57(1)
C411	398(1)	6543(2)	1346(1)	33(1)
C421	323(1)	6128(2)	1601(1)	32(1)
C431	157(1)	5537(2)	1466(1)	32(1)
C441	66(1)	5338(2)	1073(1)	32(1)
C451	130(1)	5766(2)	817(1)	35(1)
C461	291(1)	6366(2)	949(1)	37(1)
C681	1115(2)	6552(2)	2756(1)	40(1)
C691	886(1)	6555(2)	3016(1)	37(1)
C701	995(1)	6986(2)	3333(1)	40(1)
C711	1329(2)	7429(2)	3426(2)	44(1)
C721	1437(2)	7820(3)	3747(2)	54(1)
C731	1223(2)	7803(3)	3994(2)	60(1)
C741	906(2)	7404(3)	3913(2)	54(1)
C751	775(2)	6972(2)	3578(1)	44(1)
C761	449(2)	6550(3)	3490(2)	48(1)
C771	335(2)	6119(2)	3175(2)	44(1)
C781	5(2)	5680(3)	3082(2)	53(1)
C791	-84(2)	5244(3)	2780(2)	55(1)
C801	149(2)	5227(3)	2557(2)	51(1)
C811	461(2)	5640(2)	2627(1)	45(1)
C821	564(1)	6111(2)	2934(1)	38(1)
C531	882(1)	4601(2)	1573(2)	41(1)
C541	1169(2)	4349(3)	1403(2)	47(2)
C551	1517(2)	4836(3)	1466(2)	52(2)
C561	1348(3)	5430(4)	1228(3)	54(2)
C571	1673(2)	5950(3)	1268(2)	68(2)
C581	1983(2)	6072(3)	1692(2)	58(1)
C591	1794(2)	6212(3)	1983(1)	45(1)
C54B1	948(7)	4555(10)	1167(6)	50(3)

C55B1	1297(6)	4936(9)	1178(7)	51(3)
C56B1	1253(7)	5645(10)	1179(10)	58(4)
C11	590(3)	3520(5)	1671(3)	37(2)
C21	271(3)	3135(4)	1409(3)	35(1)
C31	261(3)	2490(4)	1475(3)	35(1)
C41	573(3)	2219(4)	1813(3)	47(2)
C51	887(3)	2615(5)	2077(3)	47(2)
C61	913(4)	3262(5)	2019(4)	42(2)
C471	-53(4)	4673(4)	943(4)	31(1)
C481	159(5)	4160(5)	1180(6)	32(2)
C491	-14(4)	3546(5)	1095(5)	32(2)
C501	-382(4)	3435(5)	752(4)	31(1)
C511	-581(4)	3928(5)	488(4)	31(1)
C521	-416(5)	4539(6)	602(5)	31(1)
N11	539(10)	4150(6)	1530(11)	35(3)
C641	553(3)	1514(4)	1923(3)	59(2)
C651	994(4)	1214(8)	2084(5)	81(4)
C661	266(3)	1133(5)	1557(3)	70(3)
C671	385(4)	1500(6)	2246(4)	84(3)
C601	-950(4)	3797(5)	87(4)	33(2)
C611	-774(4)	3629(4)	-221(3)	36(1)
C621	-1210(4)	3236(6)	114(4)	36(1)
C631	-1239(5)	4368(6)	-73(6)	36(1)
C71	1233(4)	3685(5)	2324(4)	40(2)
C81	1651(4)	3667(7)	2403(4)	46(3)
C91	1929(4)	4118(7)	2649(4)	49(3)
C101	1788(4)	4606(7)	2812(5)	47(2)
C111	1376(4)	4621(9)	2753(6)	43(2)
C121	1105(4)	4156(7)	2518(5)	43(2)
C131	2422(4)	4863(6)	3341(4)	52(3)
C141	2769(3)	5229(5)	3611(3)	49(2)
C151	3097(4)	4881(5)	3908(3)	61(3)
C161	3437(4)	5204(5)	4169(3)	69(3)
C171	3465(3)	5856(5)	4169(3)	65(3)
C181	3149(3)	6209(4)	3881(3)	56(2)
C191	2791(4)	5893(5)	3590(4)	51(2)
O21	2503(4)	6237(5)	3310(4)	48(2)
F11	3755(4)	4873(4)	4460(3)	97(4)
N21	2083(5)	5079(6)	3052(5)	48(2)

C201	3206(3)	6907(4)	3875(3)	53(2)
C211	3592(3)	7163(5)	3938(3)	59(2)
C221	3638(3)	7810(5)	3934(3)	64(2)
C231	3308(3)	8214(5)	3879(4)	61(2)
C241	2924(3)	7960(4)	3806(3)	54(2)
C251	2875(3)	7312(4)	3803(4)	50(2)
C261	2560(3)	8405(5)	3728(3)	53(2)
O11	2405(3)	8623(4)	3321(3)	55(2)
C271	2055(3)	9024(5)	3226(3)	54(2)
C281	1931(3)	9276(4)	2803(3)	49(2)
C291	2188(3)	9710(5)	2738(3)	53(2)
C301	2084(3)	9943(5)	2358(3)	51(2)
C311	1722(3)	9739(6)	2039(3)	50(3)
C321	1458(4)	9307(7)	2099(3)	47(3)
C331	1564(3)	9083(6)	2488(3)	45(2)
C341	1050(5)	9104(8)	1761(6)	40(3)
C351	784(4)	9548(8)	1496(5)	38(4)
C361	415(4)	9357(7)	1179(5)	36(4)
C371	297(6)	8728(7)	1119(7)	38(4)
C381	563(9)	8273(7)	1381(11)	35(3)
C391	939(9)	8454(9)	1710(10)	37(3)
C401	433(11)	7634(6)	1286(12)	35(4)
O31	1196(10)	8032(10)	1959(11)	39(4)
F21	163(4)	9794(7)	920(4)	52(5)
N31	589(13)	7136(7)	1507(14)	34(3)
C1A1	690(5)	3559(9)	1649(6)	34(3)
C2A1	401(5)	3144(8)	1381(5)	35(1)
C3A1	468(6)	2491(9)	1424(6)	44(4)
C4A1	839(6)	2253(9)	1718(7)	51(4)
C5A1	1120(6)	2683(9)	1994(6)	46(4)
C6A1	1048(7)	3329(9)	1976(7)	41(4)
C47A1	-80(8)	4667(7)	981(9)	31(1)
C48A1	174(11)	4171(10)	1205(12)	32(4)
C49A1	63(8)	3532(9)	1105(10)	31(4)
C50A1	-312(9)	3393(12)	778(10)	34(4)
C51A1	-574(9)	3870(12)	549(8)	31(1)
C52A1	-453(8)	4507(12)	652(7)	31(1)
N1A1	565(16)	4194(10)	1540(20)	38(3)
C64A1	966(7)	1548(11)	1739(7)	69(4)

C65A1	1449(7)	1509(16)	1862(9)	84(7)
C66A1	861(11)	1160(20)	2025(10)	74(6)
C67A1	748(10)	1281(14)	1307(7)	93(8)
C60A1	-964(10)	3687(14)	151(8)	36(2)
C61A1	-861(8)	3455(17)	-193(8)	36(1)
C62A1	-1202(9)	3177(14)	264(8)	36(1)
C63A1	-1236(12)	4275(14)	-3(10)	36(1)
C7A1	1351(7)	3763(12)	2275(7)	43(4)
C8A1	1764(7)	3827(13)	2338(9)	46(4)
C9A1	2020(8)	4282(14)	2604(10)	49(4)
C10A1	1864(10)	4654(19)	2819(13)	49(3)
C11A1	1449(11)	4610(20)	2749(15)	44(4)
C12A1	1194(9)	4160(20)	2479(12)	44(4)
C13A1	2462(13)	4968(17)	3387(12)	48(4)
C14A1	2779(10)	5377(12)	3663(8)	51(4)
C15A1	3105(11)	5061(13)	3977(9)	55(4)
C16A1	3425(11)	5415(12)	4258(10)	58(4)
C17A1	3426(11)	6074(12)	4238(10)	59(4)
C18A1	3111(10)	6396(9)	3923(9)	53(4)
C19A1	2784(11)	6041(12)	3635(10)	49(4)
O2A1	2481(13)	6350(15)	3346(11)	54(5)
F1A1	3741(14)	5107(18)	4563(13)	97(4)
N2A1	2135(15)	5141(17)	3069(16)	50(3)
C20A1	3112(5)	7113(6)	3899(5)	52(3)
C21A1	3496(4)	7412(7)	4019(4)	55(3)
C22A1	3536(5)	8061(7)	4029(5)	60(3)
C23A1	3186(4)	8438(7)	3923(5)	60(3)
C24A1	2799(4)	8156(6)	3792(5)	55(3)
C25A1	2766(5)	7504(6)	3781(6)	53(3)
C26A1	2411(5)	8568(8)	3673(5)	63(3)
O1A1	2332(6)	8839(7)	3288(4)	61(3)
C27A1	2010(5)	9301(7)	3183(4)	57(3)
C28A1	1876(4)	9500(6)	2747(4)	51(3)
C29A1	2110(5)	9916(8)	2634(5)	57(3)
C30A1	1975(5)	10080(9)	2233(4)	52(3)
C31A1	1613(5)	9833(9)	1945(5)	41(3)
C32A1	1382(5)	9403(10)	2053(5)	42(3)
C33A1	1508(6)	9247(9)	2454(5)	49(4)
C34A1	970(4)	9161(7)	1744(5)	37(3)

C35A1	674(4)	9601(7)	1506(5)	43(3)
C36A1	296(4)	9398(6)	1211(5)	37(3)
C37A1	209(5)	8758(6)	1141(6)	37(3)
C38A1	501(6)	8302(6)	1380(8)	35(3)
C39A1	879(7)	8501(7)	1702(8)	38(3)
C40A1	386(10)	7648(5)	1294(12)	34(4)
O3A1	1163(8)	8084(8)	1937(9)	37(3)
F2A1	11(4)	9833(5)	989(5)	47(3)
N3A1	584(11)	7149(6)	1492(12)	34(3)
C1B1	626(8)	3550(14)	1678(9)	36(4)
C2B1	330(7)	3137(12)	1409(8)	35(1)
C3B1	371(7)	2484(12)	1476(9)	44(5)
C4B1	702(9)	2241(13)	1811(10)	54(4)
C5B1	994(10)	2668(15)	2073(11)	48(5)
C6B1	961(12)	3321(15)	2026(12)	41(4)
C47B1	-82(10)	4670(8)	954(13)	31(1)
C48B1	153(13)	4168(12)	1194(14)	32(4)
C49B1	26(12)	3533(12)	1102(13)	32(4)
C50B1	-341(12)	3389(15)	765(13)	33(4)
C51B1	-575(12)	3866(15)	509(13)	31(1)
C52B1	-427(13)	4491(15)	603(13)	31(1)
N1B1	530(30)	4183(17)	1550(30)	35(4)
C64B1	772(8)	1528(13)	1879(8)	65(4)
C65B1	1233(8)	1368(17)	1977(11)	79(6)
C66B1	494(10)	1134(15)	1524(9)	72(7)
C67B1	697(11)	1384(17)	2252(9)	82(6)
C60B1	-964(12)	3715(18)	119(11)	36(2)
C61B1	-759(9)	3424(18)	-137(9)	36(1)
C62B1	-1257(12)	3233(19)	178(12)	36(1)
C63B1	-1221(16)	4287(16)	-102(15)	36(1)
C7B1	1262(12)	3794(16)	2297(11)	43(4)
C8B1	1674(13)	3740(20)	2354(15)	45(4)
C9B1	1966(12)	4180(20)	2589(15)	47(4)
C10B1	1858(11)	4675(19)	2773(12)	49(4)
C11B1	1448(13)	4732(18)	2718(14)	45(4)
C12B1	1152(11)	4294(18)	2480(15)	45(4)
C13B1	2452(12)	5037(16)	3311(11)	48(4)
C14B1	2753(9)	5452(13)	3597(8)	51(4)
C15B1	3073(10)	5138(14)	3916(9)	57(4)

C16B1	3388(12)	5480(15)	4214(11)	60(4)
C17B1	3376(11)	6141(15)	4201(11)	59(4)
C18B1	3056(11)	6459(13)	3889(10)	53(4)
C19B1	2747(11)	6115(13)	3580(10)	50(4)
O2B1	2454(12)	6422(14)	3283(11)	56(5)
F1B1	3697(11)	5169(16)	4524(9)	64(6)
N2B1	2110(14)	5199(16)	3006(12)	50(3)
C13C1	2260(40)	5070(50)	3380(30)	51(4)
C14C1	2630(30)	5400(40)	3640(20)	52(4)
C15C1	2910(30)	5050(40)	3960(30)	57(5)
C16C1	3280(30)	5330(40)	4230(30)	61(5)
C17C1	3370(30)	5960(40)	4190(30)	58(5)
C18C1	3090(30)	6310(40)	3860(30)	55(4)
C19C1	2720(30)	6030(40)	3590(30)	52(4)
O2C1	2460(30)	6380(50)	3280(30)	55(5)
F1C1	3550(40)	4990(50)	4550(40)	70(11)
N2C1	2000(50)	5240(70)	3020(30)	49(4)
C20C1	3180(20)	6990(30)	3810(30)	54(4)
C21C1	3550(30)	7270(40)	4070(40)	57(5)
C22C1	3640(30)	7900(40)	4020(40)	59(5)
C23C1	3350(30)	8250(40)	3700(40)	58(6)
C24C1	2990(30)	7960(30)	3430(30)	56(6)
C25C1	2900(30)	7340(40)	3490(30)	54(6)
C26C1	2670(40)	8360(40)	3090(20)	56(6)
O1C1	2640(30)	8970(40)	3240(30)	56(6)
C27C1	2220(30)	9140(60)	3110(20)	54(4)
C28C1	2030(20)	9330(40)	2670(20)	51(4)
C29C1	2260(30)	9700(50)	2520(30)	52(4)
C30C1	2090(30)	9880(70)	2120(30)	50(5)
C31C1	1690(30)	9680(60)	1870(30)	47(4)
C32C1	1460(30)	9300(30)	2010(20)	44(4)
C33C1	1630(20)	9130(40)	2410(20)	47(4)
C34C1	1030(20)	9110(20)	1730(30)	41(4)
C35C1	740(30)	9570(20)	1510(40)	40(5)
C36C1	330(30)	9390(20)	1250(50)	39(5)
C37C1	220(30)	8750(20)	1210(40)	37(5)
C38C1	510(20)	8286(13)	1440(40)	36(4)
C39C1	910(20)	8460(20)	1700(40)	38(4)
C40C1	360(20)	7645(11)	1370(60)	34(4)

O3C1	1200(30)	8040(20)	1910(50)	41(4)
F2C1	50(40)	9830(40)	1040(70)	41(10)
N3C1	587(13)	7142(10)	1490(7)	36(4)
C34D1	1091(7)	9067(10)	1732(7)	42(4)
C35D1	873(6)	9499(9)	1433(6)	41(4)
C36D1	511(6)	9316(8)	1106(5)	40(4)
C37D1	366(7)	8696(8)	1062(7)	39(4)
C38D1	574(11)	8263(9)	1373(10)	35(4)
C39D1	948(11)	8436(11)	1702(11)	37(3)
C40D1	401(14)	7640(7)	1304(15)	33(4)
O3D1	1162(11)	8037(12)	1997(9)	40(4)
F2D1	283(6)	9757(10)	832(6)	53(5)
N3D1	582(15)	7138(7)	1510(16)	35(3)
N01A1	1934(2)	7170(3)	2681(2)	73(2)
C01A1	2114(2)	7569(3)	2608(2)	75(2)
C01B1	2237(3)	8101(4)	2428(3)	114(3)
C04A1	2182(5)	7250(30)	2437(9)	80(3)
Cl011	2666(4)	7473(10)	2823(5)	86(4)
Cl021	1766(4)	7378(9)	2568(6)	69(3)
F12	1562(1)	9098(1)	6303(1)	57(1)
O22	2371(1)	6865(2)	6907(1)	42(1)
N22	2981(1)	7595(2)	7509(1)	36(1)
Fe32	2891(1)	6650(1)	7344(1)	36(1)
N32	3818(1)	4291(2)	8034(1)	38(1)
Fe42	3323(1)	4811(1)	7571(1)	38(1)
O42	3680(1)	5480(2)	7492(1)	47(1)
O52	3372(1)	6403(2)	7247(1)	42(1)
C12	4787(1)	7447(2)	9025(1)	30(1)
C22	5170(1)	7500(2)	9367(1)	29(1)
C32	5319(1)	8094(2)	9524(1)	33(1)
C42	5097(1)	8644(2)	9344(1)	37(1)
C52	4714(1)	8572(2)	9006(1)	35(1)
C62	4548(1)	7983(2)	8843(1)	31(1)
C472	5101(1)	5794(2)	9214(1)	30(1)
C482	5042(1)	6453(2)	9192(1)	30(1)
C492	5334(1)	6862(2)	9470(1)	29(1)
C502	5707(1)	6618(2)	9766(1)	30(1)
C512	5790(1)	5973(2)	9781(1)	30(1)
C522	5480(1)	5575(2)	9511(1)	31(1)

N12	4706(1)	6806(2)	8908(1)	32(1)
C72	4129(1)	7932(2)	8502(1)	34(1)
C82	4030(1)	8261(2)	8145(1)	37(1)
C92	3648(1)	8167(2)	7816(1)	37(1)
C102	3363(1)	7746(2)	7846(1)	35(1)
C112	3449(1)	7440(2)	8208(1)	36(1)
C122	3828(1)	7536(2)	8531(1)	38(1)
C132	2740(1)	8057(2)	7310(1)	36(1)
C142	2350(1)	7997(2)	6961(1)	37(1)
C152	2141(2)	8573(2)	6801(1)	40(1)
C162	1769(2)	8549(2)	6464(1)	42(1)
C172	1592(2)	7982(3)	6282(1)	46(1)
C182	1789(1)	7413(2)	6429(1)	44(1)
C192	2180(1)	7406(2)	6781(1)	39(1)
C202	1616(5)	6829(5)	6198(4)	43(3)
C212	1500(4)	6813(6)	5787(4)	46(3)
C222	1350(3)	6263(5)	5569(3)	47(3)
C232	1309(3)	5715(5)	5760(3)	44(3)
C242	1427(4)	5725(5)	6174(3)	44(3)
C252	1582(7)	6282(6)	6393(3)	45(3)
C262	1410(4)	5115(5)	6378(3)	47(2)
O12	1704(4)	4697(5)	6342(4)	48(2)
C272	1634(4)	4059(5)	6444(4)	57(3)
C282	1964(4)	3633(6)	6431(4)	52(2)
C292	1891(5)	3308(7)	6076(4)	57(3)
C302	2175(5)	2868(7)	6072(4)	55(3)
C312	2525(5)	2737(8)	6414(4)	47(3)
C322	2610(4)	3074(7)	6767(4)	43(2)
C332	2331(5)	3526(8)	6767(4)	47(3)
C342	2984(4)	2924(6)	7141(4)	42(2)
C352	3090(4)	2294(6)	7242(4)	45(3)
C362	3438(4)	2135(6)	7587(4)	48(3)
C372	3688(5)	2591(6)	7846(5)	43(3)
C382	3588(6)	3233(7)	7751(5)	41(3)
C392	3240(5)	3417(6)	7399(5)	41(3)
O32	3147(7)	4008(6)	7293(7)	45(3)
F22	3532(5)	1510(6)	7681(5)	65(4)
C20A2	1597(8)	6783(8)	6262(7)	42(4)
C21A2	1441(7)	6731(10)	5846(7)	44(4)

C22A2	1267(7)	6161(10)	5654(6)	48(4)
C23A2	1244(7)	5643(9)	5880(5)	49(4)
C24A2	1400(8)	5680(8)	6296(5)	51(4)
C25A2	1579(12)	6255(10)	6483(7)	45(4)
C26A2	1391(6)	5111(8)	6544(6)	54(3)
O1A2	1714(4)	4665(6)	6598(4)	55(3)
C27A2	1614(6)	4224(10)	6279(5)	54(3)
C28A2	1924(8)	3701(11)	6357(7)	53(3)
C29A2	1855(9)	3285(13)	6041(7)	57(4)
C30A2	2121(10)	2784(14)	6091(8)	53(5)
C31A2	2466(10)	2704(16)	6451(8)	49(5)
C32A2	2537(8)	3116(14)	6772(7)	47(4)
C33A2	2258(9)	3596(14)	6725(7)	48(4)
C34A2	2895(7)	2974(11)	7158(7)	44(4)
C35A2	2974(6)	2339(10)	7270(7)	38(4)
C36A2	3318(6)	2165(10)	7615(7)	40(4)
C37A2	3595(9)	2617(12)	7866(9)	45(5)
C38A2	3529(11)	3257(12)	7752(10)	41(4)
C39A2	3174(10)	3440(12)	7406(10)	41(4)
O3A2	3095(15)	4038(12)	7304(14)	49(5)
F2A2	3401(8)	1540(11)	7711(10)	55(5)
C20B2	1646(10)	6837(12)	6165(11)	46(4)
C21B2	1583(10)	6859(14)	5763(11)	46(4)
C22B2	1456(10)	6323(14)	5521(9)	50(4)
C23B2	1388(11)	5755(13)	5676(8)	47(4)
C24B2	1449(13)	5714(11)	6076(8)	46(4)
C25B2	1576(16)	6261(15)	6314(9)	44(4)
C26B2	1384(12)	5096(13)	6249(10)	50(4)
O1B2	1687(15)	4632(15)	6281(15)	49(4)
C27B2	1696(11)	4096(14)	6526(11)	52(4)
C28B2	1975(8)	3561(12)	6525(7)	51(4)
C29B2	1876(8)	3162(12)	6196(7)	53(4)
C30B2	2134(9)	2662(13)	6210(7)	53(4)
C31B2	2496(9)	2553(13)	6551(7)	50(4)
C32B2	2597(8)	2948(12)	6882(6)	44(4)
C33B2	2341(10)	3449(15)	6865(8)	47(4)
C34B2	2976(7)	2813(10)	7248(6)	41(4)
C35B2	3089(9)	2185(10)	7363(7)	39(4)
C36B2	3448(9)	2050(11)	7707(7)	48(5)

C37B2	3687(11)	2538(12)	7950(9)	47(5)
C38B2	3577(10)	3169(12)	7834(9)	44(5)
C39B2	3218(10)	3317(10)	7485(8)	42(4)
O3B2	3105(11)	3907(11)	7378(10)	45(5)
F2B2	3544(13)	1432(11)	7815(9)	70(8)
C402	3852(2)	3685(2)	8046(2)	44(1)
C412	4150(1)	4628(2)	8350(1)	35(1)
C422	4052(1)	5051(2)	8591(1)	34(1)
C432	4367(1)	5399(2)	8881(1)	33(1)
C442	4777(1)	5354(2)	8938(1)	32(1)
C452	4872(1)	4907(2)	8706(1)	37(1)
C462	4559(2)	4552(2)	8417(1)	40(1)
C532	4550(1)	6646(2)	8476(1)	32(1)
C542	4842(3)	6920(11)	8311(2)	43(3)
C552	4700(4)	6708(11)	7870(2)	55(4)
C54A2	4845(4)	6695(14)	8289(3)	42(4)
C55A2	4647(6)	6530(13)	7844(3)	46(4)
C562	4302(2)	7017(3)	7591(1)	50(1)
C572	4096(2)	6797(2)	7160(1)	49(1)
C582	3935(2)	6116(2)	7110(2)	49(1)
C592	3640(2)	5994(2)	7297(1)	40(1)
C602	6197(1)	5674(2)	10085(1)	37(1)
C612	6389(2)	5253(2)	9870(2)	44(1)
C622	6106(2)	5260(2)	10384(1)	45(1)
C632	6518(1)	6176(2)	10323(1)	41(1)
C642	5269(2)	9297(2)	9511(2)	47(1)
C652	5688(2)	9398(2)	9499(2)	55(1)
C662	5318(2)	9339(2)	9949(2)	53(1)
C672	4977(2)	9837(2)	9273(2)	67(2)
C682	2898(1)	5646(2)	7965(1)	35(1)
C692	2697(2)	5643(5)	8250(2)	33(2)
C702	2908(3)	5880(4)	8644(2)	32(2)
C712	3323(3)	6125(5)	8794(2)	37(2)
C722	3521(3)	6328(5)	9184(2)	44(2)
C732	3318(4)	6314(4)	9438(2)	44(2)
C742	2913(4)	6105(4)	9297(2)	43(2)
C752	2701(3)	5882(4)	8896(2)	37(2)
C762	2292(3)	5658(4)	8748(3)	39(2)
C772	2086(3)	5413(4)	8360(3)	37(2)

C782	1675(3)	5167(5)	8212(3)	45(2)
C792	1479(2)	4914(5)	7835(3)	46(2)
C802	1689(3)	4896(6)	7585(3)	45(2)
C812	2081(3)	5140(6)	7712(3)	38(2)
C822	2294(3)	5399(6)	8105(3)	37(2)
O62	3052(4)	5122(5)	7919(3)	38(2)
O72	2890(4)	6158(5)	7792(3)	41(2)
C69A2	2618(8)	5630(20)	8183(8)	35(4)
C70A2	2790(9)	5871(19)	8579(7)	39(5)
C71A2	3204(9)	6090(20)	8769(8)	44(5)
C72A2	3368(11)	6320(20)	9163(8)	47(6)
C73A2	3132(12)	6296(17)	9385(7)	48(6)
C74A2	2725(11)	6061(16)	9205(7)	50(5)
C75A2	2555(9)	5842(17)	8806(7)	38(4)
C76A2	2146(9)	5613(14)	8624(8)	35(4)
C77A2	1987(8)	5323(18)	8246(8)	37(4)
C78A2	1584(8)	5055(15)	8078(10)	36(5)
C79A2	1427(8)	4753(17)	7704(9)	41(5)
C80A2	1667(9)	4760(20)	7483(10)	41(6)
C81A2	2068(10)	5020(20)	7649(10)	34(6)
C82A2	2229(9)	5320(20)	8026(9)	28(4)
O6A2	3103(15)	5240(20)	7947(15)	47(10)
O7A2	2949(16)	6210(20)	7859(14)	48(10)
Fe13	4174(1)	6693(1)	6158(1)	34(1)
N13	3336(1)	9544(2)	5628(1)	34(1)
C13	3592(1)	9984(2)	5910(1)	31(1)
Fe23	3212(1)	6512(1)	5182(1)	35(1)
N23	4599(1)	7355(2)	6568(1)	31(1)
C23	3442(1)	10603(2)	5797(1)	33(1)
N33	2718(1)	7009(2)	4712(1)	36(1)
C33	3636(1)	11119(2)	6047(1)	37(1)
O43	3659(1)	7082(2)	6142(1)	40(1)
C43	3987(1)	11026(2)	6406(1)	39(1)
O53	3064(1)	6812(2)	5623(1)	45(1)
C53	4146(1)	10409(2)	6496(1)	36(1)
O63	4289(1)	6927(1)	5678(1)	36(1)
C63	3964(1)	9879(2)	6258(1)	31(1)
O73	3694(1)	6910(2)	5114(1)	41(1)
C73	4159(1)	9245(2)	6357(1)	31(1)

C83	4294(1)	8973(2)	6740(1)	35(1)
C93	4452(1)	8363(2)	6817(1)	35(1)
C103	4476(1)	8004(2)	6511(1)	30(1)
C113	4355(1)	8276(2)	6132(1)	30(1)
C123	4206(1)	8887(2)	6061(1)	33(1)
C133	4937(1)	7208(2)	6882(1)	35(1)
C143	5086(6)	6576(5)	7020(5)	35(1)
C153	5460(5)	6546(6)	7374(5)	35(1)
C163	5571(4)	5989(6)	7585(4)	35(1)
C173	5326(4)	5448(6)	7464(4)	34(3)
C183	4954(4)	5461(6)	7113(4)	36(3)
C193	4841(5)	6019(6)	6876(5)	35(1)
O23	4510(6)	6015(10)	6531(6)	32(4)
F13	5939(6)	5944(12)	7922(6)	45(6)
C203	4658(4)	4908(6)	7002(4)	41(3)
C213	4553(5)	4627(7)	7291(4)	48(3)
C223	4277(5)	4128(7)	7195(4)	55(3)
C233	4104(5)	3888(7)	6810(4)	58(3)
C243	4188(4)	4172(6)	6510(3)	53(3)
C253	4463(4)	4679(6)	6611(4)	43(3)
C263	4011(4)	3881(6)	6092(3)	70(3)
O13	4066(3)	4289(6)	5807(3)	79(3)
C273	3932(4)	3939(7)	5429(4)	87(3)
C283	3454(4)	3901(5)	5229(3)	76(3)
C293	3245(4)	3381(6)	5282(5)	85(4)
C303	2813(4)	3374(6)	5119(5)	90(4)
C313	2591(4)	3875(6)	4882(5)	72(4)
C323	2794(4)	4397(6)	4815(4)	60(3)
C333	3226(3)	4411(6)	4990(4)	63(3)
C343	2539(4)	4905(6)	4528(5)	51(3)
C353	2177(4)	4750(7)	4189(4)	55(4)
C363	1927(4)	5209(7)	3939(4)	46(3)
C373	2017(5)	5845(7)	4010(5)	38(3)
C383	2381(5)	6020(6)	4354(5)	36(3)
C393	2651(4)	5554(6)	4611(4)	33(2)
C403	2439(5)	6696(7)	4411(6)	28(3)
O33	2983(5)	5707(9)	4941(6)	42(3)
F23	1577(4)	5034(8)	3606(4)	58(3)
C14A3	5057(7)	6558(7)	7032(7)	35(1)

C15A3	5430(7)	6458(9)	7383(7)	35(1)
C16A3	5522(6)	5863(8)	7559(6)	35(1)
C17A3	5245(8)	5363(10)	7424(8)	36(5)
C18A3	4884(7)	5440(9)	7073(7)	40(4)
C19A3	4796(9)	6022(10)	6867(9)	35(1)
O2A3	4452(10)	6057(18)	6529(10)	32(5)
F1A3	5881(10)	5804(15)	7904(10)	45(8)
C20A3	4609(6)	4867(9)	6914(6)	45(4)
C21A3	4416(6)	4613(8)	7139(5)	48(4)
C22A3	4173(7)	4069(9)	7013(6)	52(4)
C23A3	4117(7)	3800(10)	6648(6)	56(4)
C24A3	4308(7)	4052(9)	6422(5)	56(4)
C25A3	4564(7)	4583(9)	6560(6)	50(4)
C26A3	4293(5)	3697(9)	6056(4)	59(4)
O1A3	3992(4)	3964(9)	5700(5)	50(3)
C27A3	3579(4)	3853(10)	5659(5)	61(3)
C28A3	3274(4)	3875(7)	5214(4)	64(4)
C29A3	3247(7)	3354(8)	4979(5)	65(5)
C30A3	2981(5)	3370(7)	4575(5)	48(4)
C31A3	2725(5)	3892(7)	4421(5)	41(3)
C32A3	2759(7)	4429(8)	4648(5)	45(4)
C33A3	3020(7)	4400(8)	5056(5)	56(4)
C34A3	2490(6)	4990(7)	4448(5)	50(4)
C35A3	2105(7)	4859(10)	4132(5)	63(6)
C36A3	1828(7)	5340(9)	3931(5)	54(5)
C37A3	1926(7)	5965(9)	4018(7)	46(5)
C38A3	2309(7)	6112(8)	4342(7)	39(4)
C39A3	2587(7)	5635(8)	4569(7)	50(5)
C40A3	2369(8)	6776(8)	4441(8)	30(4)
O3A3	2953(9)	5760(12)	4877(8)	48(4)
F2A3	1451(7)	5179(10)	3633(6)	68(5)
C14B3	5101(10)	6615(7)	7047(8)	35(1)
C15B3	5470(9)	6613(9)	7399(8)	35(1)
C16B3	5650(6)	6016(9)	7525(6)	35(1)
C17B3	5428(7)	5475(9)	7338(6)	48(5)
C18B3	5077(6)	5500(7)	6967(6)	43(4)
C19B3	4914(6)	6095(7)	6806(5)	35(1)
O2B3	4572(7)	6112(13)	6465(6)	37(5)
F1B3	6006(11)	5977(19)	7875(11)	58(12)

C20B3	4870(7)	4898(9)	6747(6)	43(5)
C21B3	4871(9)	4361(11)	6965(7)	55(6)
C22B3	4671(12)	3816(12)	6770(8)	68(6)
C23B3	4466(13)	3786(13)	6355(8)	63(6)
C24B3	4459(11)	4314(11)	6126(6)	53(5)
C25B3	4660(9)	4857(11)	6332(6)	41(5)
C26B3	4225(11)	4323(12)	5669(6)	47(6)
O1B3	4165(8)	3701(10)	5496(6)	53(5)
C27B3	3888(8)	3722(15)	5083(7)	60(5)
C28B3	3428(7)	3825(12)	4979(6)	60(5)
C29B3	3201(10)	3395(15)	5088(11)	58(5)
C30B3	2779(10)	3486(18)	4973(14)	62(5)
C31B3	2579(9)	4022(19)	4763(13)	58(6)
C32B3	2802(10)	4469(17)	4660(12)	51(5)
C33B3	3224(9)	4375(14)	4781(11)	53(5)
C14C3	4995(10)	6555(9)	7032(10)	35(1)
C15C3	5365(10)	6515(15)	7386(11)	35(1)
C16C3	5480(10)	5954(17)	7604(10)	35(1)
C17C3	5221(13)	5425(17)	7484(12)	37(7)
C18C3	4875(13)	5432(14)	7111(12)	44(6)
C19C3	4744(12)	6006(14)	6900(11)	35(1)
O2C3	4403(14)	6000(30)	6559(13)	30(6)
F1C3	5842(13)	5920(30)	7947(15)	37(11)
C20C3	4580(12)	4876(15)	7022(11)	45(5)
C21C3	4537(17)	4600(20)	7345(11)	48(7)
C22C3	4256(19)	4110(30)	7289(11)	55(7)
C23C3	4004(15)	3910(20)	6903(11)	58(7)
C24C3	4077(11)	4140(20)	6586(9)	59(6)
C25C3	4351(13)	4640(20)	6639(11)	49(6)
C26C3	3773(9)	3950(20)	6161(11)	71(7)
O1C3	3362(10)	4103(17)	6113(10)	81(9)
C27C3	3065(10)	3683(19)	5836(8)	76(7)
C28C3	3004(7)	3746(14)	5404(8)	69(6)
C29C3	3142(11)	3270(15)	5230(11)	68(6)
C30C3	3088(14)	3321(18)	4836(12)	68(6)
C31C3	2892(12)	3847(19)	4607(10)	59(5)
C32C3	2758(10)	4331(17)	4778(10)	59(5)
C33C3	2816(9)	4276(14)	5173(9)	62(6)
C20D3	4919(10)	4932(16)	6893(11)	45(5)

C21D3	4844(14)	4519(19)	7145(11)	50(6)
C22D3	4677(17)	3925(19)	7006(12)	60(6)
C23D3	4581(18)	3745(18)	6615(12)	61(6)
C24D3	4669(15)	4156(18)	6368(9)	55(6)
C25D3	4818(15)	4761(16)	6500(11)	47(6)
C26D3	4556(12)	3960(20)	5937(9)	60(6)
O1D3	4111(12)	3960(40)	5727(12)	60(6)
C27D3	3991(12)	4290(30)	5352(13)	61(3)
C28D3	3536(11)	4113(19)	5092(10)	56(7)
C29D3	3417(14)	3480(18)	5048(15)	67(7)
C30D3	3006(15)	3310(20)	4810(20)	69(7)
C31D3	2712(13)	3780(30)	4630(18)	62(7)
C32D3	2829(12)	4420(20)	4673(14)	53(7)
C33D3	3244(13)	4581(19)	4900(15)	50(7)
C413	2695(1)	7684(2)	4736(1)	35(1)
C423	3032(1)	8052(2)	4771(1)	38(1)
C433	3023(1)	8703(2)	4816(1)	40(1)
C443	2686(1)	8999(2)	4846(1)	36(1)
C453	2344(1)	8627(2)	4794(1)	39(1)
C463	2346(1)	7979(2)	4743(1)	37(1)
C473	2715(1)	9682(2)	4955(1)	36(1)
C483	3030(1)	9905(2)	5320(1)	33(1)
C493	3081(1)	10549(2)	5413(1)	34(1)
C503	2814(1)	10997(2)	5147(1)	38(1)
C513	2491(1)	10793(2)	4787(1)	40(1)
C523	2450(1)	10140(2)	4704(1)	39(1)
C533	3215(1)	8957(2)	5771(1)	36(1)
C543	2852(2)	9071(2)	5885(1)	41(1)
C553	2765(2)	8494(2)	6085(2)	50(1)
C563	2570(2)	7937(2)	5814(2)	36(1)
C573	2602(2)	7312(3)	6030(2)	38(1)
C56A3	3170(7)	8206(8)	6388(7)	37(4)
C57A3	3113(10)	7556(9)	6528(7)	48(6)
C583	3042(2)	7069(2)	6241(1)	40(1)
C593	3273(1)	6986(2)	5984(1)	35(1)
C603	2199(2)	11263(2)	4473(2)	51(1)
C613	2269(2)	11941(2)	4629(2)	68(2)
C623	2282(2)	11223(3)	4098(2)	80(2)
C633	1748(2)	11091(3)	4362(2)	66(2)

C643	4178(2)	11583(2)	6698(1)	47(1)
C653	4582(4)	11393(12)	7059(5)	65(5)
C663	4260(6)	12157(10)	6493(8)	51(2)
C673	3848(5)	11750(13)	6848(5)	53(4)
C65A3	3939(6)	11724(15)	6946(6)	56(4)
C66A3	4174(7)	12179(12)	6453(9)	51(2)
C67A3	4639(4)	11460(15)	6987(6)	51(4)
C65B3	4210(20)	11420(30)	7118(10)	53(6)
C66B3	3905(16)	12187(19)	6557(19)	51(2)
C67B3	4615(9)	11760(30)	6742(19)	49(6)
C683	4080(1)	7001(2)	5307(1)	32(1)
C693	4316(1)	7213(2)	5074(1)	32(1)
C703	4522(1)	6762(2)	4946(1)	36(1)
C713	4493(2)	6101(2)	5005(2)	44(1)
C723	4682(2)	5674(3)	4861(2)	62(1)
C733	4921(2)	5884(3)	4660(2)	82(2)
C743	4960(2)	6507(3)	4603(2)	73(2)
C753	4752(2)	6971(2)	4732(2)	47(1)
C763	4778(2)	7610(2)	4661(2)	46(1)
C773	4573(1)	8061(2)	4784(1)	38(1)
C783	4584(2)	8722(2)	4700(1)	42(1)
C793	4369(2)	9151(2)	4803(1)	42(1)
C803	4125(1)	8955(2)	5003(1)	38(1)
C813	4108(1)	8335(2)	5096(1)	32(1)
C823	4332(1)	7867(2)	4992(1)	32(1)
O83	3718(1)	5941(2)	5731(1)	45(1)
N03A3	3292(2)	5213(3)	6105(2)	67(2)
C03A3	3155(3)	4764(4)	6189(3)	64(2)
C03B3	2984(3)	4203(4)	6310(3)	77(2)
N02A3	2798(1)	5240(2)	7028(1)	58(1)
C02A3	2626(2)	5388(3)	6700(2)	54(1)
C02B3	2411(2)	5635(3)	6298(2)	64(2)

Table S5. Bond lengths [Å] and angles [°] for **1**.

Fe11-O3D1	1.85(2)	C643-C663	1.515(11)	C302-C292-C282	119.8(9)
Fe11-O31	1.87(2)	C643-C65A3	1.525(12)	C302-C292-H292	120.1
Fe11-O3C1	1.92(7)	C643-C653	1.533(11)	C282-C292-H292	120.1
Fe11-O41	1.968(4)	C643-C67B3	1.536(16)	C312-C302-C292	120.4(10)
Fe11-O3A1	1.976(17)	C643-C673	1.539(11)	C312-C302-H302	119.8
Fe11-O61	2.007(3)	C643-C65B3	1.540(15)	C292-C302-H302	119.8
Fe11-N31	2.08(2)	C643-C66A3	1.541(12)	C302-C312-C322	120.3(9)
Fe11-N3D1	2.08(3)	C643-C67A3	1.542(11)	C302-C312-H312	119.9
Fe11-N3C1	2.11(3)	C643-C66B3	1.549(15)	C322-C312-H312	119.9
Fe11-N3A1	2.11(2)	C653-H65A3	0.9800	C332-C322-C312	119.0(8)
Fe11-Cl021	2.299(15)	C653-H65B3	0.9800	C332-C322-C342	120.4(8)
Fe21-N2C1	1.83(11)	C653-H65C3	0.9800	C312-C322-C342	120.5(9)
Fe21-O2C1	1.87(8)	C663-H66A3	0.9800	C322-C332-C282	121.2(9)
Fe21-O2B1	1.89(3)	C663-H66B3	0.9800	C322-C332-H332	119.4
Fe21-N2B1	1.91(3)	C663-H66C3	0.9800	C282-C332-H332	119.4
Fe21-O21	1.918(10)	C673-H67A3	0.9800	C352-C342-C392	119.4(8)
Fe21-O71	1.974(4)	C673-H67B3	0.9800	C352-C342-C322	119.1(8)
Fe21-O51	1.993(4)	C673-H67C3	0.9800	C392-C342-C322	121.5(8)
Fe21-O2A1	2.00(3)	C65A3-H65D3	0.9800	C362-C352-C342	120.9(8)
Fe21-N2A1	2.08(4)	C65A3-H65E3	0.9800	C362-C352-H352	119.6
Fe21-N21	2.176(14)	C65A3-H65F3	0.9800	C342-C352-H352	119.6
Fe21-N01A1	2.403(6)	C66A3-H66D3	0.9800	F22-C362-C372	118.8(10)
O41-C591	1.249(6)	C66A3-H66E3	0.9800	F22-C362-C352	119.5(9)
O51-C591	1.248(6)	C66A3-H66F3	0.9800	C372-C362-C352	121.7(8)
O61-C681	1.251(6)	C67A3-H67D3	0.9800	C362-C372-C382	118.7(9)
O71-C681	1.259(6)	C67A3-H67E3	0.9800	C362-C372-H372	120.7
C411-C421	1.389(6)	C67A3-H67F3	0.9800	C382-C372-H372	120.7
C411-C461	1.395(6)	C65B3-H65G3	0.9800	C372-C382-C392	121.5(9)
C411-N3C1	1.419(17)	C65B3-H65H3	0.9800	C372-C382-C402	115.6(10)
C411-N3D1	1.422(14)	C65B3-H65I3	0.9800	C392-C382-C402	122.8(10)
C411-N31	1.423(13)	C66B3-H66G3	0.9800	O32-C392-C382	123.3(10)
C411-N3A1	1.431(12)	C66B3-H66H3	0.9800	O32-C392-C342	118.9(10)
C421-C431	1.376(5)	C66B3-H66I3	0.9800	C382-C392-C342	117.8(8)
C421-H421	0.9500	C67B3-H67G3	0.9800	C392-O32-Fe42	133.6(14)
C431-C441	1.406(5)	C67B3-H67H3	0.9800	C21A2-C20A2-C25A2	118.9(12)
C431-H431	0.9500	C67B3-H67I3	0.9800	C21A2-C20A2-C182	114.7(16)
C441-C451	1.391(6)	C683-C693	1.503(6)	C25A2-C20A2-C182	126.4(16)

C441-C471	1.480(9)	C693-C703	1.401(6)	C22A2-C21A2-C20A2	120.3(13)
C441-C47A1	1.492(14)	C693-C823	1.416(6)	C22A2-C21A2-H21D2	119.8
C441-C47B1	1.499(15)	C703-C713	1.420(6)	C20A2-C21A2-H21D2	119.8
C451-C461	1.387(6)	C703-C753	1.428(7)	C21A2-C22A2-C23A2	119.8(14)
C451-H451	0.9500	C713-C723	1.358(7)	C21A2-C22A2-H22D2	120.1
C461-H461	0.9500	C713-H713	0.9500	C23A2-C22A2-H22D2	120.1
C681-C691	1.503(7)	C723-C733	1.418(9)	C24A2-C23A2-C22A2	121.1(13)
C691-C701	1.398(7)	C66B3-H66H3	0.9800	C24A2-C23A2-H23D2	119.4
C691-C821	1.407(7)	C66B3-H66I3	0.9800	C22A2-C23A2-H23D2	119.4
C701-C751	1.427(7)	C67B3-H67G3	0.9800	C23A2-C24A2-C25A2	118.1(13)
C701-C711	1.430(7)	C67B3-H67H3	0.9800	C23A2-C24A2-C26A2	121.4(13)
C711-C721	1.356(7)	C67B3-H67I3	0.9800	C25A2-C24A2-C26A2	120.5(13)
C711-H711	0.9500	C683-C693	1.503(6)	C20A2-C25A2-C24A2	121.7(13)
C721-C731	1.414(8)	C693-C703	1.401(6)	C20A2-C25A2-H25D2	119.2
C721-H721	0.9500	C693-C823	1.416(6)	C24A2-C25A2-H25D2	119.2
C731-C741	1.334(8)	C703-C713	1.420(6)	O1A2-C26A2-C24A2	112.4(15)
C731-H731	0.9500	C703-C753	1.428(7)	O1A2-C26A2-H26D2	109.1
C741-C751	1.442(7)	C713-C723	1.358(7)	C24A2-C26A2-H26D2	109.1
C741-H741	0.9500	C713-H713	0.9500	O1A2-C26A2-H26E2	109.1
C751-C761	1.382(7)	C723-C733	1.418(9)	C24A2-C26A2-H26E2	109.1
C761-C771	1.389(7)	C723-H723	0.9500	H26D2-C26A2-H26E2	107.9
C761-H761	0.9500	C733-C743	1.345(9)	C27A2-O1A2-C26A2	114.4(13)
C771-C781	1.414(7)	C733-H733	0.9500	O1A2-C27A2-C28A2	114.8(14)
C771-C821	1.440(7)	C743-C753	1.426(7)	O1A2-C27A2-H27D2	108.6
C781-C791	1.372(8)	C743-H743	0.9500	C28A2-C27A2-H27D2	108.6
C781-H781	0.9500	C753-C763	1.380(7)	O1A2-C27A2-H27E2	108.6
C791-C801	1.397(8)	C763-C773	1.387(7)	C28A2-C27A2-H27E2	108.6
C791-H791	0.9500	C763-H763	0.9500	H27D2-C27A2-H27E2	107.5
C801-C811	1.344(7)	C773-C783	1.431(7)	C33A2-C28A2-C29A2	119.3(14)
C801-H801	0.9500	C773-C823	1.433(6)	C33A2-C28A2-C27A2	123.8(14)
C811-C821	1.429(7)	C783-C793	1.342(7)	C29A2-C28A2-C27A2	116.9(14)
C811-H811	0.9500	C783-H783	0.9500	C30A2-C29A2-C28A2	120.4(15)
C531-N1A1	1.38(6)	C793-C803	1.418(7)	C30A2-C29A2-H29D2	119.8
C531-N1B1	1.49(10)	C793-H793	0.9500	C28A2-C29A2-H29D2	119.8
C531-N11	1.50(3)	C803-C813	1.359(6)	C29A2-C30A2-C31A2	120.1(16)
C531-C541	1.505(8)	C803-H803	0.9500	C29A2-C30A2-H30D2	119.9
C531-C54B1	1.614(17)	C813-C823	1.417(6)	C31A2-C30A2-H30D2	119.9
C531-H53A1	0.9900	C813-H813	0.9500	C30A2-C31A2-C32A2	119.9(15)

C531-H53B1	0.9900	O83-HO13	0.837(10)	C30A2-C31A2-H31D2	120.0
C531-H53D1	0.9900	O83-HO23	0.857(10)	C32A2-C31A2-H31D2	120.0
C531-H53E1	0.9900	N03A3-C03A3	1.167(9)	C33A2-C32A2-C31A2	119.6(14)
C541-C551	1.544(9)	C03A3-C03B3	1.484(10)	C33A2-C32A2-C34A2	123.0(14)
C541-H54A1	0.9900	C03B3-H3ZA3	0.9800	C31A2-C32A2-C34A2	117.2(14)
C541-H54B1	0.9900	C03B3-H3ZB3	0.9800	C32A2-C33A2-C28A2	120.5(14)
C551-C561	1.496(11)	C03B3-H3ZC3	0.9800	C32A2-C33A2-H33D2	119.7
C551-H55A1	0.9900	N02A3-C02A3	1.138(6)	C28A2-C33A2-H33D2	119.7
C551-H55B1	0.9900	C02A3-C02B3	1.443(7)	C35A2-C34A2-C39A2	118.7(13)
C561-C571	1.552(9)	C02B3-H2ZA3	0.9800	C35A2-C34A2-C32A2	117.4(14)
C561-H56A1	0.9900	C02B3-H2ZB3	0.9800	C39A2-C34A2-C32A2	123.8(14)
C561-H56B1	0.9900	C02B3-H2ZC3	0.9800	C36A2-C35A2-C34A2	120.8(13)
C571-C581	1.497(7)			C36A2-C35A2-H35D2	119.6
C571-C56B1	1.524(19)	O3D1-Fe11-O41	126.7(15)	C34A2-C35A2-H35D2	119.6
C571-H57A1	0.9900	O31-Fe11-O41	120.0(16)	F2A2-C36A2-C35A2	120.1(16)
C571-H57B1	0.9900	O3C1-Fe11-O41	116(6)	F2A2-C36A2-C37A2	118.2(16)
C571-H57D1	0.9900	O41-Fe11-O3A1	122.0(11)	C35A2-C36A2-C37A2	121.6(14)
C571-H57E1	0.9900	O3D1-Fe11-O61	109.6(15)	C36A2-C37A2-C38A2	118.5(14)
C581-C591	1.519(7)	O31-Fe11-O61	116.3(16)	C36A2-C37A2-H37D2	120.8
C581-H58A1	0.9900	O3C1-Fe11-O61	121(6)	C38A2-C37A2-H37D2	120.8
C581-H58B1	0.9900	O41-Fe11-O61	118.30(16)	C37A2-C38A2-C39A2	120.2(14)
C54B1-C55B1	1.462(19)	O3A1-Fe11-O61	115.6(12)	C37A2-C38A2-C402	112.6(17)
C54B1-H54D1	0.9900	O31-Fe11-N31	90.7(8)	C39A2-C38A2-C402	127.0(17)
C54B1-H54E1	0.9900	O41-Fe11-N31	100.3(16)	O3A2-C39A2-C38A2	121.3(18)
C55B1-C56B1	1.50(2)	O61-Fe11-N31	102.1(19)	O3A2-C39A2-C34A2	118.7(17)
C55B1-H55D1	0.9900	O3D1-Fe11-N3D1	90.7(9)	C38A2-C39A2-C34A2	120.0(13)
C55B1-H55E1	0.9900	O41-Fe11-N3D1	101.0(19)	C39A2-O3A2-Fe42	133(3)
C56B1-H56D1	0.9900	O61-Fe11-N3D1	101(2)	C25B2-C20B2-C21B2	118.1(15)
C56B1-H56E1	0.9900	O3C1-Fe11-N3C1	88(2)	C25B2-C20B2-C182	121(2)
C11-C21	1.390(9)	O41-Fe11-N3C1	99.5(9)	C21B2-C20B2-C182	121(3)
C11-N11	1.407(11)	O61-Fe11-N3C1	103.4(8)	C22B2-C21B2-C20B2	120.9(16)
C11-C61	1.412(9)	O41-Fe11-N3A1	100.1(14)	C22B2-C21B2-H21G2	119.5
C21-C31	1.384(9)	O3A1-Fe11-N3A1	86.8(7)	C20B2-C21B2-H21G2	119.5
C21-C491	1.450(9)	O61-Fe11-N3A1	103.1(16)	C21B2-C22B2-C23B2	120.1(16)
C31-C41	1.385(9)	O41-Fe11-Cl021	85.5(5)	C21B2-C22B2-H22G2	120.0
C31-H31	0.9500	O3A1-Fe11-Cl021	81.9(7)	C23B2-C22B2-H22G2	120.0
C41-C51	1.397(10)	O61-Fe11-Cl021	82.3(5)	C22B2-C23B2-C24B2	120.6(16)
C41-C641	1.550(13)	N3A1-Fe11-Cl021	168.8(6)	C22B2-C23B2-H23G2	119.7

C51-C61	1.388(10)	N2C1-Fe21-O2C1	100(3)	C24B2-C23B2-H23G2	119.7
C51-H51	0.9500	O2B1-Fe21-N2B1	97.1(11)	C23B2-C24B2-C25B2	118.4(15)
C61-C71	1.500(12)	N2C1-Fe21-O71	92(7)	C23B2-C24B2-C26B2	121.0(16)
C471-C521	1.388(9)	O2C1-Fe21-O71	120(5)	C25B2-C24B2-C26B2	120.6(17)
C471-C481	1.390(9)	O2B1-Fe21-O71	118.4(16)	C20B2-C25B2-C24B2	121.9(15)
C481-C491	1.408(9)	N2B1-Fe21-O71	104.9(18)	C20B2-C25B2-H25G2	119.0
C481-N11	1.412(8)	O21-Fe21-O71	124.3(5)	C24B2-C25B2-H25G2	119.0
C491-C501	1.394(9)	N2C1-Fe21-O51	100(6)	O1B2-C26B2-C24B2	112.3(19)
C501-C511	1.389(9)	O2C1-Fe21-O51	120(5)	O1B2-C26B2-H26G2	109.1
C501-H501	0.9500	O2B1-Fe21-O51	120.1(16)	C24B2-C26B2-H26G2	109.1
C511-C521	1.403(9)	N2B1-Fe21-O51	93.4(17)	O1B2-C26B2-H26H2	109.1
C511-C601	1.521(17)	O21-Fe21-O51	118.9(6)	C24B2-C26B2-H26H2	109.1
C521-H521	0.9500	O71-Fe21-O51	115.16(16)	H26G2-C26B2-H26H2	107.9
C641-C661	1.522(12)	O71-Fe21-O2A1	117.2(16)	C26B2-O1B2-C27B2	114(2)
C641-C671	1.544(14)	O51-Fe21-O2A1	124.1(17)	O1B2-C27B2-C28B2	115.2(19)
C641-C651	1.553(14)	O71-Fe21-N2A1	104(2)	O1B2-C27B2-H27G2	108.5
C651-H65A1	0.9800	O51-Fe21-N2A1	98(2)	C28B2-C27B2-H27G2	108.5
C651-H65B1	0.9800	O2A1-Fe21-N2A1	87.5(11)	O1B2-C27B2-H27H2	108.5
C651-H65C1	0.9800	O21-Fe21-N21	86.2(4)	C28B2-C27B2-H27H2	108.5
C661-H66A1	0.9800	O71-Fe21-N21	99.4(6)	H27G2-C27B2-H27H2	107.5
C661-H66B1	0.9800	O51-Fe21-N21	97.6(6)	C33B2-C28B2-C29B2	118.2(15)
C661-H66C1	0.9800	O21-Fe21-N01A1	88.9(4)	C33B2-C28B2-C27B2	119.5(17)
C671-H67A1	0.9800	O71-Fe21-N01A1	85.62(19)	C29B2-C28B2-C27B2	122.3(17)
C671-H67B1	0.9800	O51-Fe21-N01A1	82.4(2)	C30B2-C29B2-C28B2	120.8(16)
C671-H67C1	0.9800	N21-Fe21-N01A1	174.4(4)	C30B2-C29B2-H29G2	119.6
C601-C631	1.524(9)	C591-O41-Fe11	146.2(3)	C28B2-C29B2-H29G2	119.6
C601-C621	1.531(10)	C591-O51-Fe21	137.9(4)	C31B2-C30B2-C29B2	120.4(16)
C601-C611	1.554(10)	C681-O61-Fe11	137.3(3)	C31B2-C30B2-H30G2	119.8
C611-H61A1	0.9800	C681-O71-Fe21	145.0(3)	C29B2-C30B2-H30G2	119.8
C611-H61B1	0.9800	C421-C411-C461	119.8(4)	C30B2-C31B2-C32B2	119.2(16)
C611-H61C1	0.9800	C421-C411-N3C1	120.3(9)	C30B2-C31B2-H31G2	120.4
C621-H62A1	0.9800	C461-C411-N3C1	120.0(9)	C32B2-C31B2-H31G2	120.4
C621-H62B1	0.9800	C421-C411-N3D1	117(3)	C33B2-C32B2-C31B2	120.2(15)
C621-H62C1	0.9800	C461-C411-N3D1	123(3)	C33B2-C32B2-C34B2	121.2(14)
C631-H63A1	0.9800	C421-C411-N31	118(2)	C31B2-C32B2-C34B2	118.6(14)
C631-H63B1	0.9800	C461-C411-N31	122(2)	C32B2-C33B2-C28B2	121.3(16)
C631-H63C1	0.9800	C421-C411-N3A1	120(2)	C32B2-C33B2-H33G2	119.4
C71-C81	1.386(9)	C461-C411-N3A1	120(2)	C28B2-C33B2-H33G2	119.4

C71-C121	1.407(10)	C431-C421-C411	120.1(4)	C35B2-C34B2-C39B2	120.5(14)
C81-C91	1.391(10)	C431-C421-H421	120.0	C35B2-C34B2-C32B2	119.6(14)
C81-H81	0.9500	C411-C421-H421	120.0	C39B2-C34B2-C32B2	120.0(14)
C91-C101	1.389(10)	C421-C431-C441	121.1(4)	C36B2-C35B2-C34B2	120.2(15)
C91-H91	0.9500	C421-C431-H431	119.4	C36B2-C35B2-H35G2	119.9
C101-C111	1.383(9)	C441-C431-H431	119.4	C34B2-C35B2-H35G2	119.9
C101-N21	1.439(9)	C451-C441-C431	118.1(4)	F2B2-C36B2-C37B2	120.8(17)
C111-C121	1.385(10)	C451-C441-C471	120.1(7)	F2B2-C36B2-C35B2	118.7(17)
C111-H111	0.9500	C431-C441-C471	121.5(7)	C37B2-C36B2-C35B2	120.3(15)
C121-H121	0.9500	C451-C441-C47A1	127.0(14)	C36B2-C37B2-C38B2	119.6(16)
C131-N21	1.300(10)	C431-C441-C47A1	114.8(14)	C36B2-C37B2-H37G2	120.2
C131-C141	1.431(10)	C451-C441-C47B1	123(2)	C38B2-C37B2-H37G2	120.2
C131-H131	0.9500	C431-C441-C47B1	119(2)	C37B2-C38B2-C39B2	120.9(15)
C141-C191	1.404(10)	C461-C451-C441	121.1(4)	C37B2-C38B2-C402	120.9(18)
C141-C151	1.416(9)	C461-C451-H451	119.4	C39B2-C38B2-C402	117.8(17)
C151-C161	1.359(10)	C441-C451-H451	119.4	O3B2-C39B2-C38B2	121.7(17)
C151-H151	0.9500	C451-C461-C411	119.7(4)	O3B2-C39B2-C34B2	119.9(17)
C161-F11	1.366(9)	C451-C461-H461	120.1	C38B2-C39B2-C34B2	118.4(14)
C161-C171	1.377(10)	C411-C461-H461	120.1	C39B2-O3B2-Fe42	138(2)
C171-C181	1.384(10)	O61-C681-O71	126.4(5)	N32-C402-C38B2	134.3(12)
C171-H171	0.9500	O61-C681-C691	117.6(4)	N32-C402-C382	127.5(7)
C181-C191	1.427(9)	O71-C681-C691	116.1(4)	N32-C402-C38A2	123.0(12)
C181-C201	1.486(11)	C701-C691-C821	121.2(4)	N32-C402-H402	116.2
C191-O21	1.315(9)	C701-C691-C681	120.4(4)	C382-C402-H402	116.2
C201-C251	1.384(10)	C821-C691-C681	118.4(4)	C462-C412-C422	119.5(4)
C201-C211	1.396(10)	C691-C701-C751	119.0(4)	C462-C412-N32	121.4(4)
C211-C221	1.373(10)	C691-C701-C711	121.8(4)	C422-C412-N32	119.1(4)
C211-H211	0.9500	C751-C701-C711	119.2(4)	C432-C422-C412	119.1(4)
C221-C231	1.390(11)	C721-C711-C701	119.9(5)	C432-C422-H422	120.4
C221-H221	0.9500	C721-C711-H711	120.1	C412-C422-H422	120.4
C231-C241	1.383(10)	C701-C711-H711	120.1	C422-C432-C442	122.2(4)
C231-H231	0.9500	C711-C721-C731	121.3(5)	C422-C432-H432	118.9
C241-C251	1.374(10)	C711-C721-H721	119.4	C442-C432-H432	118.9
C241-C261	1.520(10)	C731-C721-H721	119.4	C432-C442-C452	117.8(4)
C251-H251	0.9500	C741-C731-C721	120.6(5)	C432-C442-C472	121.0(4)
C261-O11	1.431(9)	C741-C731-H731	119.7	C452-C442-C472	121.0(4)
C261-H26A1	0.9900	C721-C731-H731	119.7	C462-C452-C442	120.4(4)
C261-H26B1	0.9900	C731-C741-C751	121.3(5)	C462-C452-H452	119.8

O11-C271	1.419(10)	C731-C741-H741	119.3	C442-C452-H452	119.8
C271-C281	1.522(9)	C751-C741-H741	119.3	C412-C462-C452	120.8(4)
C271-H27A1	0.9900	C761-C751-C701	119.8(5)	C412-C462-H462	119.6
C271-H27B1	0.9900	C761-C751-C741	122.4(5)	C452-C462-H462	119.6
C281-C291	1.382(9)	C701-C751-C741	117.7(5)	N12-C532-C54A2	118.2(7)
C281-C331	1.385(9)	C751-C761-C771	122.1(5)	N12-C532-C542	109.9(6)
C291-C301	1.376(10)	C751-C761-H761	118.9	N12-C532-H53A2	109.7
C291-H291	0.9500	C771-C761-H761	118.9	C542-C532-H53A2	109.7
C301-C311	1.387(10)	C761-C771-C781	123.0(5)	N12-C532-H53B2	109.7
C301-H301	0.9500	C761-C771-C821	118.8(5)	C542-C532-H53B2	109.7
C311-C321	1.392(10)	C781-C771-C821	118.2(5)	H53A2-C532-H53B2	108.2
C311-H311	0.9500	C791-C781-C771	120.9(5)	N12-C532-H53E2	107.8
C321-C331	1.396(10)	C791-C781-H781	119.6	C54A2-C532-H53E2	107.8
C321-C341	1.513(13)	C771-C781-H781	119.6	N12-C532-H53F2	107.8
C331-H331	0.9500	C781-C791-C801	120.4(5)	C54A2-C532-H53F2	107.8
C341-C351	1.387(12)	C781-C791-H791	119.8	H53E2-C532-H53F2	107.1
C341-C391	1.414(12)	C801-C791-H791	119.8	C532-C542-C552	109.9(8)
C351-C361	1.389(11)	C811-C801-C791	121.3(5)	C532-C542-H54A2	109.7
C351-H351	0.9500	C811-C801-H801	119.3	C552-C542-H54A2	109.7
C361-F21	1.351(11)	C791-C801-H801	119.3	C532-C542-H54B2	109.7
C361-C371	1.379(12)	C801-C811-C821	120.7(5)	C552-C542-H54B2	109.7
C371-C381	1.401(12)	C801-C811-H811	119.7	H54A2-C542-H54B2	108.2
C371-H371	0.9500	C821-C811-H811	119.7	C562-C552-C542	112.5(8)
C381-C391	1.415(11)	C691-C821-C811	122.5(4)	C562-C552-H55A2	109.1
C381-C401	1.418(12)	C691-C821-C771	119.0(4)	C542-C552-H55A2	109.1
C391-O31	1.322(13)	C811-C821-C771	118.5(4)	C562-C552-H55B2	109.1
C401-N31	1.296(14)	N11-C531-C541	113(2)	C542-C552-H55B2	109.1
C401-H401	0.9500	N1A1-C531-C54B1	109(4)	H55A2-C552-H55B2	107.8
C1A1-C2A1	1.386(14)	N11-C531-H53A1	108.9	C532-C54A2-C55A2	113.2(11)
C1A1-C6A1	1.410(14)	C541-C531-H53A1	108.9	C532-C54A2-H54D2	108.9
C1A1-N1A1	1.411(15)	N11-C531-H53B1	108.9	C55A2-C54A2-H54D2	108.9
C2A1-C3A1	1.394(14)	C541-C531-H53B1	108.9	C532-C54A2-H54E2	108.9
C2A1-C49A1	1.447(13)	H53A1-C531-H53B1	107.7	C55A2-C54A2-H54E2	108.9
C3A1-C4A1	1.392(15)	N1A1-C531-H53D1	109.9	H54D2-C54A2-H54E2	107.8
C3A1-H3D1	0.9500	C54B1-C531-H53D1	109.9	C54A2-C55A2-C562	111.9(11)
C4A1-C5A1	1.405(15)	N1A1-C531-H53E1	109.9	C54A2-C55A2-H55D2	109.2
C4A1-C64A1	1.54(3)	C54B1-C531-H53E1	109.9	C562-C55A2-H55D2	109.2
C5A1-C6A1	1.381(15)	H53D1-C531-H53E1	108.3	C54A2-C55A2-H55E2	109.2

C5A1-H5D1	0.9500	C531-C541-C551	110.2(5)	C562-C55A2-H55E2	109.2
C6A1-C7A1	1.48(2)	C531-C541-H54A1	109.6	H55D2-C55A2-H55E2	107.9
C47A1-C48A1	1.396(13)	C551-C541-H54A1	109.6	C552-C562-C572	118.6(7)
C47A1-C52A1	1.399(14)	C531-C541-H54B1	109.6	C572-C562-C55A2	109.1(7)
C48A1-C49A1	1.406(14)	C551-C541-H54B1	109.6	C552-C562-H56A2	107.7
C48A1-N1A1	1.413(14)	H54A1-C541-H54B1	108.1	C572-C562-H56A2	107.7
C49A1-C50A1	1.391(14)	C561-C551-C541	111.9(6)	C552-C562-H56B2	107.7
C50A1-C51A1	1.383(14)	C561-C551-H55A1	109.2	C572-C562-H56B2	107.7
C50A1-H50D1	0.9500	C541-C551-H55A1	109.2	H56A2-C562-H56B2	107.1
C51A1-C52A1	1.410(14)	C561-C551-H55B1	109.2	C572-C562-H56D2	109.9
C51A1-C60A1	1.57(4)	C541-C551-H55B1	109.2	C55A2-C562-H56D2	109.9
C52A1-H52D1	0.9500	H55A1-C551-H55B1	107.9	C572-C562-H56E2	109.9
C64A1-C66A1	1.50(2)	C551-C561-C571	116.1(7)	C55A2-C562-H56E2	109.9
C64A1-C67A1	1.55(2)	C551-C561-H56A1	108.3	H56D2-C562-H56E2	108.3
C64A1-C65A1	1.58(2)	C571-C561-H56A1	108.3	C562-C572-C582	113.8(4)
C65A1-H65D1	0.9800	C551-C561-H56B1	108.3	C562-C572-H57A2	108.8
C65A1-H65E1	0.9800	C571-C561-H56B1	108.3	C582-C572-H57A2	108.8
C65A1-H65F1	0.9800	H56A1-C561-H56B1	107.4	C562-C572-H57B2	108.8
C66A1-H66D1	0.9800	C581-C571-C56B1	120.8(13)	C582-C572-H57B2	108.8
C66A1-H66E1	0.9800	C581-C571-C561	113.9(6)	H57A2-C572-H57B2	107.7
C66A1-H66F1	0.9800	C581-C571-H57A1	108.8	C592-C582-C572	113.8(4)
C67A1-H67D1	0.9800	C561-C571-H57A1	108.8	C592-C582-H58A2	108.8
C67A1-H67E1	0.9800	C581-C571-H57B1	108.8	C572-C582-H58A2	108.8
C67A1-H67F1	0.9800	C561-C571-H57B1	108.8	C592-C582-H58B2	108.8
C60A1-C63A1	1.522(16)	H57A1-C571-H57B1	107.7	C572-C582-H58B2	108.8
C60A1-C62A1	1.533(16)	C581-C571-H57D1	107.1	H58A2-C582-H58B2	107.7
C60A1-C61A1	1.543(16)	C56B1-C571-H57D1	107.1	O52-C592-O42	124.6(4)
C61A1-H61D1	0.9800	C581-C571-H57E1	107.1	O52-C592-C582	117.2(4)
C61A1-H61E1	0.9800	C56B1-C571-H57E1	107.1	O42-C592-C582	118.2(4)
C61A1-H61F1	0.9800	H57D1-C571-H57E1	106.8	C632-C602-C512	111.9(3)
C62A1-H62D1	0.9800	C571-C581-C591	114.7(5)	C632-C602-C612	108.0(4)
C62A1-H62E1	0.9800	C571-C581-H58A1	108.6	C512-C602-C612	110.4(4)
C62A1-H62F1	0.9800	C591-C581-H58A1	108.6	C632-C602-C622	108.4(4)
C63A1-H63D1	0.9800	C571-C581-H58B1	108.6	C512-C602-C622	109.5(4)
C63A1-H63E1	0.9800	C591-C581-H58B1	108.6	C612-C602-C622	108.6(4)
C63A1-H63F1	0.9800	H58A1-C581-H58B1	107.6	C602-C612-H61A2	109.5
C7A1-C8A1	1.390(13)	O51-C591-O41	125.1(5)	C602-C612-H61B2	109.5
C7A1-C12A1	1.393(13)	O51-C591-C581	116.8(5)	H61A2-C612-H61B2	109.5

C8A1-C9A1	1.391(14)	O41-C591-C581	118.0(5)	C602-C612-H61C2	109.5
C8A1-H8D1	0.9500	C55B1-C54B1-C531	113.7(14)	H61A2-C612-H61C2	109.5
C9A1-C10A1	1.389(14)	C55B1-C54B1-H54D1	108.8	H61B2-C612-H61C2	109.5
C9A1-H9D1	0.9500	C531-C54B1-H54D1	108.8	C602-C622-H62A2	109.5
C10A1-C11A1	1.387(13)	C55B1-C54B1-H54E1	108.8	C602-C622-H62B2	109.5
C10A1-N2A1	1.436(16)	C531-C54B1-H54E1	108.8	H62A2-C622-H62B2	109.5
C11A1-C12A1	1.393(14)	H54D1-C54B1-H54E1	107.7	C602-C622-H62C2	109.5
C11A1-H11D1	0.9500	C54B1-C55B1-C56B1	117.3(17)	H62A2-C622-H62C2	109.5
C12A1-H12D1	0.9500	C54B1-C55B1-H55D1	108.0	H62B2-C622-H62C2	109.5
C13A1-N2A1	1.298(16)	C56B1-C55B1-H55D1	108.0	C602-C632-H63A2	109.5
C13A1-C14A1	1.437(15)	C54B1-C55B1-H55E1	108.0	C602-C632-H63B2	109.5
C13A1-H13D1	0.9500	C56B1-C55B1-H55E1	108.0	H63A2-C632-H63B2	109.5
C14A1-C19A1	1.402(13)	H55D1-C55B1-H55E1	107.2	C602-C632-H63C2	109.5
C14A1-C15A1	1.404(13)	C55B1-C56B1-C571	109.1(17)	H63A2-C632-H63C2	109.5
C15A1-C16A1	1.381(13)	C55B1-C56B1-H56D1	109.9	H63B2-C632-H63C2	109.5
C15A1-H15D1	0.9500	C571-C56B1-H56D1	109.9	C42-C642-C652	109.8(4)
C16A1-F1A1	1.363(15)	C55B1-C56B1-H56E1	109.9	C42-C642-C672	112.5(4)
C16A1-C17A1	1.389(13)	C571-C56B1-H56E1	109.9	C652-C642-C672	107.9(5)
C17A1-C18A1	1.392(13)	H56D1-C56B1-H56E1	108.3	C42-C642-C662	108.7(4)
C17A1-H17D1	0.9500	C21-C11-N11	110.9(7)	C652-C642-C662	110.4(4)
C18A1-C19A1	1.407(13)	C21-C11-C61	120.6(7)	C672-C642-C662	107.6(4)
C18A1-C20A1	1.513(16)	N11-C11-C61	128.6(8)	C642-C652-H65A2	109.5
C19A1-O2A1	1.313(15)	C31-C21-C11	121.7(7)	C642-C652-H65B2	109.5
C20A1-C25A1	1.385(12)	C31-C21-C491	131.6(7)	H65A2-C652-H65B2	109.5
C20A1-C21A1	1.389(12)	C11-C21-C491	106.8(6)	C642-C652-H65C2	109.5
C21A1-C22A1	1.373(12)	C21-C31-C41	119.4(7)	H65A2-C652-H65C2	109.5
C21A1-H21D1	0.9500	C21-C31-H31	120.3	H65B2-C652-H65C2	109.5
C22A1-C23A1	1.383(12)	C41-C31-H31	120.3	C642-C662-H66A2	109.5
C22A1-H22D1	0.9500	C31-C41-C51	118.2(8)	C642-C662-H66B2	109.5
C23A1-C24A1	1.381(12)	C31-C41-C641	121.4(8)	H66A2-C662-H66B2	109.5
C23A1-H23D1	0.9500	C51-C41-C641	120.2(8)	C642-C662-H66C2	109.5
C24A1-C25A1	1.378(12)	C61-C51-C41	124.3(8)	H66A2-C662-H66C2	109.5
C24A1-C26A1	1.524(13)	C61-C51-H51	117.8	H66B2-C662-H66C2	109.5
C25A1-H25D1	0.9500	C41-C51-H51	117.8	C642-C672-H67A2	109.5
C26A1-O1A1	1.441(13)	C51-C61-C11	115.8(8)	C642-C672-H67B2	109.5
C26A1-H26D1	0.9900	C51-C61-C71	123.2(8)	H67A2-C672-H67B2	109.5
C26A1-H26E1	0.9900	C11-C61-C71	120.7(8)	C642-C672-H67C2	109.5
O1A1-C27A1	1.422(12)	C521-C471-C481	116.9(8)	H67A2-C672-H67C2	109.5

C27A1-C28A1	1.523(12)	C521-C471-C441	120.6(9)	H67B2-C672-H67C2	109.5
C27A1-H27D1	0.9900	C481-C471-C441	122.0(9)	O72-C682-O62	126.5(8)
C27A1-H27E1	0.9900	C471-C481-C491	120.5(8)	O6A2-C682-O7A2	120(3)
C28A1-C29A1	1.390(12)	C471-C481-N11	129.3(9)	O72-C682-C692	116.6(8)
C28A1-C33A1	1.395(12)	C491-C481-N11	110.1(7)	O62-C682-C692	116.8(7)
C29A1-C30A1	1.388(12)	C501-C491-C481	120.3(8)	O6A2-C682-C69A2	126(3)
C29A1-H29D1	0.9500	C501-C491-C21	133.3(8)	O7A2-C682-C69A2	113(3)
C30A1-C31A1	1.369(12)	C481-C491-C21	106.4(7)	C822-C692-C702	122.0(5)
C30A1-H30D1	0.9500	C511-C501-C491	120.5(9)	C822-C692-C682	116.9(5)
C31A1-C32A1	1.391(12)	C511-C501-H501	119.8	C702-C692-C682	121.0(5)
C31A1-H31D1	0.9500	C491-C501-H501	119.8	C692-C702-C752	118.8(5)
C32A1-C33A1	1.389(12)	C501-C511-C521	117.0(8)	C692-C702-C712	122.1(5)
C32A1-C34A1	1.505(12)	C501-C511-C601	120.8(9)	C752-C702-C712	119.1(5)
C33A1-H33D1	0.9500	C521-C511-C601	122.1(8)	C722-C712-C702	119.9(6)
C34A1-C35A1	1.394(11)	C471-C521-C511	124.3(8)	C722-C712-H712	120.1
C34A1-C39A1	1.419(11)	C471-C521-H521	117.8	C702-C712-H712	120.1
C35A1-C36A1	1.383(11)	C511-C521-H521	117.8	C712-C722-C732	121.0(6)
C35A1-H35D1	0.9500	C11-N11-C481	105.8(8)	C712-C722-H722	119.5
C36A1-F2A1	1.350(11)	C11-N11-C531	126(2)	C732-C722-H722	119.5
C36A1-C37A1	1.382(11)	C481-N11-C531	120(2)	C742-C732-C722	120.6(6)
C37A1-C38A1	1.411(11)	C661-C641-C671	109.8(9)	C742-C732-H732	119.7
C37A1-H37D1	0.9500	C661-C641-C41	111.3(8)	C722-C732-H732	119.7
C38A1-C39A1	1.422(11)	C671-C641-C41	107.2(8)	C732-C742-C752	119.9(6)
C38A1-C40A1	1.432(11)	C661-C641-C651	107.9(9)	C732-C742-H742	120.0
C39A1-O3A1	1.337(12)	C671-C641-C651	111.0(9)	C752-C742-H742	120.0
C40A1-N3A1	1.301(13)	C41-C641-C651	109.7(9)	C762-C752-C702	119.5(5)
C40A1-H40D1	0.9500	C641-C651-H65A1	109.5	C762-C752-C742	121.0(5)
C1B1-C2B1	1.396(14)	C641-C651-H65B1	109.5	C702-C752-C742	119.5(5)
C1B1-C6B1	1.407(14)	H65A1-C651-H65B1	109.5	C772-C762-C752	121.5(5)
C1B1-N1B1	1.409(15)	C641-C651-H65C1	109.5	C772-C762-H762	119.2
C2B1-C3B1	1.394(14)	H65A1-C651-H65C1	109.5	C752-C762-H762	119.2
C2B1-C49B1	1.446(13)	H65B1-C651-H65C1	109.5	C762-C772-C782	121.8(6)
C3B1-C4B1	1.387(15)	C641-C661-H66A1	109.5	C762-C772-C822	119.5(5)
C3B1-H3G1	0.9500	C641-C661-H66B1	109.5	C782-C772-C822	118.7(5)
C4B1-C5B1	1.400(16)	H66A1-C661-H66B1	109.5	C792-C782-C772	121.5(6)
C4B1-C64B1	1.52(4)	C641-C661-H66C1	109.5	C792-C782-H782	119.3
C5B1-C6B1	1.384(15)	H66A1-C661-H66C1	109.5	C772-C782-H782	119.3
C5B1-H5G1	0.9500	H66B1-C661-H66C1	109.5	C782-C792-C802	119.6(6)

C6B1-C7B1	1.49(3)	C641-C671-H67A1	109.5	C782-C792-H792	120.2
C47B1-C52B1	1.398(15)	C641-C671-H67B1	109.5	C802-C792-H792	120.2
C47B1-C48B1	1.401(14)	H67A1-C671-H67B1	109.5	C812-C802-C792	120.9(6)
C48B1-C49B1	1.405(14)	C641-C671-H67C1	109.5	C812-C802-H802	119.6
C48B1-N1B1	1.413(14)	H67A1-C671-H67C1	109.5	C792-C802-H802	119.6
C49B1-C50B1	1.394(14)	H67B1-C671-H67C1	109.5	C802-C812-C822	120.6(6)
C50B1-C51B1	1.386(15)	C511-C601-C631	112.9(11)	C802-C812-H812	119.7
C50B1-H50G1	0.9500	C511-C601-C621	111.5(9)	C822-C812-H812	119.7
C51B1-C52B1	1.404(15)	C631-C601-C621	107.9(8)	C692-C822-C812	122.7(6)
C51B1-C60B1	1.54(5)	C511-C601-C611	107.6(10)	C692-C822-C772	118.6(5)
C52B1-H52G1	0.9500	C631-C601-C611	108.3(8)	C812-C822-C772	118.7(5)
C64B1-C66B1	1.50(2)	C621-C601-C611	108.4(7)	C682-O62-Fe42	135.9(7)
C64B1-C67B1	1.54(2)	C601-C611-H61A1	109.5	C682-O72-Fe32	152.3(9)
C64B1-C65B1	1.56(2)	C601-C611-H61B1	109.5	C82A2-C69A2-C70A2	120.1(13)
C65B1-H65G1	0.9800	H61A1-C611-H61B1	109.5	C82A2-C69A2-C682	122.8(14)
C65B1-H65H1	0.9800	C601-C611-H61C1	109.5	C70A2-C69A2-C682	116.5(14)
C65B1-H65I1	0.9800	H61A1-C611-H61C1	109.5	C71A2-C70A2-C69A2	121.8(14)
C66B1-H66G1	0.9800	H61B1-C611-H61C1	109.5	C71A2-C70A2-C75A2	118.4(13)
C66B1-H66H1	0.9800	C601-C621-H62A1	109.5	C69A2-C70A2-C75A2	119.5(12)
C66B1-H66I1	0.9800	C601-C621-H62B1	109.5	C72A2-C71A2-C70A2	120.7(15)
C67B1-H67G1	0.9800	H62A1-C621-H62B1	109.5	C72A2-C71A2-H71D2	119.6
C67B1-H67H1	0.9800	C601-C621-H62C1	109.5	C70A2-C71A2-H71D2	119.6
C67B1-H67I1	0.9800	H62A1-C621-H62C1	109.5	C71A2-C72A2-C73A2	120.4(15)
C60B1-C63B1	1.520(17)	H62B1-C621-H62C1	109.5	C71A2-C72A2-H72D2	119.8
C60B1-C62B1	1.535(17)	C601-C631-H63A1	109.5	C73A2-C72A2-H72D2	119.8
C60B1-C61B1	1.546(17)	C601-C631-H63B1	109.5	C74A2-C73A2-C72A2	119.4(15)
C61B1-H61G1	0.9800	H63A1-C631-H63B1	109.5	C74A2-C73A2-H73D2	120.3
C61B1-H61H1	0.9800	C601-C631-H63C1	109.5	C72A2-C73A2-H73D2	120.3
C61B1-H61I1	0.9800	H63A1-C631-H63C1	109.5	C73A2-C74A2-C75A2	120.4(15)
C62B1-H62G1	0.9800	H63B1-C631-H63C1	109.5	C73A2-C74A2-H74D2	119.8
C62B1-H62H1	0.9800	C81-C71-C121	117.6(8)	C75A2-C74A2-H74D2	119.8
C62B1-H62I1	0.9800	C81-C71-C61	122.7(11)	C76A2-C75A2-C74A2	120.4(14)
C63B1-H63G1	0.9800	C121-C71-C61	119.5(11)	C76A2-C75A2-C70A2	119.1(13)
C63B1-H63H1	0.9800	C71-C81-C91	121.1(8)	C74A2-C75A2-C70A2	120.4(13)
C63B1-H63I1	0.9800	C71-C81-H81	119.5	C75A2-C76A2-C77A2	121.3(14)
C7B1-C8B1	1.390(14)	C91-C81-H81	119.5	C75A2-C76A2-H76D2	119.4
C7B1-C12B1	1.395(14)	C101-C91-C81	120.0(8)	C77A2-C76A2-H76D2	119.4
C8B1-C9B1	1.389(14)	C101-C91-H91	120.0	C76A2-C77A2-C78A2	120.7(13)

C8B1-H8G1	0.9500	C81-C91-H91	120.0	C76A2-C77A2-C82A2	119.2(13)
C9B1-C10B1	1.387(14)	C111-C101-C91	120.2(8)	C78A2-C77A2-C82A2	120.1(12)
C9B1-H9G1	0.9500	C111-C101-N21	121.5(11)	C79A2-C78A2-C77A2	120.9(14)
C10B1-C11B1	1.389(14)	C91-C101-N21	118.3(12)	C79A2-C78A2-H78D2	119.5
C10B1-N2B1	1.448(17)	C101-C111-C121	119.1(8)	C77A2-C78A2-H78D2	119.5
C11B1-C12B1	1.390(14)	C101-C111-H111	120.4	C78A2-C79A2-C80A2	118.8(15)
C11B1-H11G1	0.9500	C121-C111-H111	120.4	C78A2-C79A2-H79D2	120.6
C12B1-H12G1	0.9500	C111-C121-C71	121.8(8)	C80A2-C79A2-H79D2	120.6
C13B1-N2B1	1.296(17)	C111-C121-H121	119.1	C81A2-C80A2-C79A2	120.5(15)
C13B1-C14B1	1.433(16)	C71-C121-H121	119.1	C81A2-C80A2-H80D2	119.7
C13B1-H13G1	0.9500	N21-C131-C141	126.8(10)	C79A2-C80A2-H80D2	119.7
C14B1-C19B1	1.398(13)	N21-C131-H131	116.6	C80A2-C81A2-C82A2	121.0(15)
C14B1-C15B1	1.401(13)	C141-C131-H131	116.6	C80A2-C81A2-H81D2	119.5
C15B1-C16B1	1.386(14)	C191-C141-C151	120.8(7)	C82A2-C81A2-H81D2	119.5
C15B1-H15G1	0.9500	C191-C141-C131	123.4(8)	C69A2-C82A2-C81A2	121.8(14)
C16B1-F1B1	1.363(15)	C151-C141-C131	115.9(8)	C69A2-C82A2-C77A2	119.8(13)
C16B1-C17B1	1.391(14)	C161-C151-C141	118.3(8)	C81A2-C82A2-C77A2	118.4(13)
C17B1-C18B1	1.393(14)	C161-C151-H151	120.8	C682-O6A2-Fe42	143(4)
C17B1-H17G1	0.9500	C141-C151-H151	120.8	C682-O7A2-Fe32	137(3)
C18B1-C19B1	1.398(13)	C151-C161-F11	118.9(8)	O2B3-Fe13-O43	138.3(10)
C19B1-O2B1	1.310(15)	C151-C161-C171	122.8(8)	O2A3-Fe13-O43	120.6(15)
C13C1-N2C1	1.298(19)	F11-C161-C171	118.2(8)	O2C3-Fe13-O43	113.7(18)
C13C1-C14C1	1.436(18)	C161-C171-C181	120.1(8)	O43-Fe13-O23	126.2(9)
C13C1-H13J1	0.9500	C161-C171-H171	120.0	O2B3-Fe13-O63	107.8(10)
C14C1-C15C1	1.396(14)	C181-C171-H171	120.0	O2A3-Fe13-O63	124.6(16)
C14C1-C19C1	1.397(14)	C171-C181-C191	119.6(8)	O2C3-Fe13-O63	130.7(19)
C15C1-C16C1	1.393(14)	C171-C181-C201	118.1(8)	O43-Fe13-O63	113.71(13)
C15C1-H15J1	0.9500	C191-C181-C201	122.3(7)	O23-Fe13-O63	119.2(9)
C16C1-F1C1	1.359(17)	O21-C191-C141	123.2(8)	O2B3-Fe13-N23	82.8(8)
C16C1-C17C1	1.393(14)	O21-C191-C181	118.4(8)	O2A3-Fe13-N23	87.6(10)
C17C1-C18C1	1.394(14)	C141-C191-C181	118.4(7)	O2C3-Fe13-N23	90.7(13)
C17C1-H17J1	0.9500	C191-O21-Fe21	135.5(8)	O43-Fe13-N23	96.64(13)
C18C1-C19C1	1.397(14)	C131-N21-C101	115.8(10)	O23-Fe13-N23	87.0(6)
C18C1-C20C1	1.504(18)	C131-N21-Fe21	124.6(8)	O63-Fe13-N23	96.38(13)
C19C1-O2C1	1.315(17)	C101-N21-Fe21	119.1(9)	O2B3-Fe13-O83	95.2(7)
C20C1-C21C1	1.384(14)	C251-C201-C211	119.2(8)	O2A3-Fe13-O83	90.1(10)
C20C1-C25C1	1.386(14)	C251-C201-C181	120.1(8)	O2C3-Fe13-O83	87.0(13)
C21C1-C22C1	1.385(14)	C211-C201-C181	120.7(8)	O43-Fe13-O83	83.96(13)

C21C1-H21J1	0.9500	C221-C211-C201	119.6(8)	O23-Fe13-O83	90.8(6)
C22C1-C23C1	1.386(14)	C221-C211-H211	120.2	O63-Fe13-O83	85.41(12)
C22C1-H22J1	0.9500	C201-C211-H211	120.2	N23-Fe13-O83	177.68(13)
C23C1-C24C1	1.385(14)	C211-C221-C231	120.8(8)	C13-N13-C483	105.7(3)
C23C1-H23J1	0.9500	C211-C221-H221	119.6	C13-N13-C533	119.0(3)
C24C1-C25C1	1.384(14)	C231-C221-H221	119.6	C483-N13-C533	119.6(3)
C24C1-C26C1	1.525(15)	C241-C231-C221	119.5(8)	N13-C13-C23	110.7(4)
C25C1-H25J1	0.9500	C241-C231-H231	120.3	N13-C13-C63	128.9(4)
C26C1-O1C1	1.433(17)	C221-C231-H231	120.3	C23-C13-C63	120.3(4)
C26C1-H26J1	0.9900	C251-C241-C231	119.8(8)	O33-Fe23-O53	116.5(8)
C26C1-H26K1	0.9900	C251-C241-C261	121.1(7)	O3A3-Fe23-O53	120.3(12)
O1C1-C27C1	1.428(17)	C231-C241-C261	119.1(8)	O33-Fe23-O73	121.4(8)
C27C1-C28C1	1.526(15)	C241-C251-C201	121.0(8)	O3A3-Fe23-O73	119.1(12)
C27C1-H27J1	0.9900	C241-C251-H251	119.5	O53-Fe23-O73	119.93(14)
C27C1-H27K1	0.9900	C201-C251-H251	119.5	O33-Fe23-N33	91.2(5)
C28C1-C29C1	1.387(14)	O11-C261-C241	108.1(8)	O3A3-Fe23-N33	84.9(7)
C28C1-C33C1	1.387(14)	O11-C261-H26A1	110.1	O53-Fe23-N33	95.31(14)
C29C1-C30C1	1.385(14)	C241-C261-H26A1	110.1	O73-Fe23-N33	98.15(14)
C29C1-H29J1	0.9500	O11-C261-H26B1	110.1	O33-Fe23-O83	87.8(5)
C30C1-C31C1	1.385(14)	C241-C261-H26B1	110.1	O3A3-Fe23-O83	94.5(7)
C30C1-H30J1	0.9500	H26A1-C261-H26B1	108.4	O53-Fe23-O83	80.48(13)
C31C1-C32C1	1.386(14)	C271-O11-C261	110.6(7)	O73-Fe23-O83	86.76(12)
C31C1-H31J1	0.9500	O11-C271-C281	107.2(6)	N33-Fe23-O83	174.72(14)
C32C1-C33C1	1.385(14)	O11-C271-H27A1	110.3	C133-N23-C103	117.9(4)
C32C1-C34C1	1.504(18)	C281-C271-H27A1	110.3	C133-N23-Fe13	125.3(3)
C33C1-H33J1	0.9500	O11-C271-H27B1	110.3	C103-N23-Fe13	116.4(3)
C34C1-C35C1	1.398(14)	C281-C271-H27B1	110.3	C33-C23-C13	120.6(4)
C34C1-C39C1	1.401(14)	H27A1-C271-H27B1	108.5	C33-C23-C493	133.0(4)
C35C1-C36C1	1.396(14)	C291-C281-C331	120.1(7)	C13-C23-C493	106.4(4)
C35C1-H35J1	0.9500	C291-C281-C271	119.2(7)	C403-N33-C413	120.7(8)
C36C1-F2C1	1.346(17)	C331-C281-C271	120.7(7)	C40A3-N33-C413	110.9(9)
C36C1-C37C1	1.396(14)	C301-C291-C281	120.4(7)	C403-N33-Fe23	120.0(8)
C37C1-C38C1	1.400(14)	C301-C291-H291	119.8	C40A3-N33-Fe23	127.9(9)
C37C1-H37J1	0.9500	C281-C291-H291	119.8	C413-N33-Fe23	119.3(3)
C38C1-C39C1	1.403(13)	C291-C301-C311	119.8(8)	C43-C33-C23	120.3(4)
C38C1-C40C1	1.431(16)	C291-C301-H301	120.1	C43-C33-H33	119.9
C39C1-O3C1	1.333(17)	C311-C301-H301	120.1	C23-C33-H33	119.9
C40C1-N3C1	1.295(18)	C301-C311-C321	120.7(8)	C593-O43-Fe13	139.3(3)

C40C1-H40J1	0.9500	C301-C311-H311	119.6	C33-C43-C53	117.6(4)
C34D1-C35D1	1.383(13)	C321-C311-H311	119.6	C33-C43-C643	120.3(4)
C34D1-C39D1	1.410(13)	C311-C321-C331	118.7(8)	C53-C43-C643	122.1(4)
C35D1-C36D1	1.388(12)	C311-C321-C341	121.8(11)	C593-O53-Fe23	134.5(3)
C35D1-H35M1	0.9500	C331-C321-C341	119.4(11)	C63-C53-C43	124.2(4)
C36D1-F2D1	1.355(13)	C281-C331-C321	120.2(8)	C63-C53-H53	117.9
C36D1-C37D1	1.388(12)	C281-C331-H331	119.9	C43-C53-H53	117.9
C37D1-C38D1	1.400(13)	C321-C331-H331	119.9	C683-O63-Fe13	136.8(3)
C37D1-H37M1	0.9500	C351-C341-C391	119.5(11)	C53-C63-C13	116.6(4)
C38D1-C39D1	1.410(12)	C351-C341-C321	120.8(12)	C53-C63-C73	121.7(4)
C38D1-C40D1	1.424(14)	C391-C341-C321	119.7(13)	C13-C63-C73	121.7(4)
C39D1-O3D1	1.323(14)	C341-C351-C361	120.5(11)	C683-O73-Fe23	140.4(3)
C40D1-N3D1	1.300(15)	C341-C351-H351	119.8	C123-C73-C83	117.7(4)
C40D1-H40M1	0.9500	C361-C351-H351	119.8	C123-C73-C63	119.7(4)
N01A1-C01A1	1.1551(19)	F21-C361-C371	118.5(12)	C83-C73-C63	122.6(4)
C01A1-C01B1	1.462(2)	F21-C361-C351	119.7(12)	C93-C83-C73	121.3(4)
C01B1-H1ZA1	0.9800	C371-C361-C351	121.8(10)	C93-C83-H83	119.4
C01B1-H1ZB1	0.9800	C361-C371-C381	118.5(11)	C73-C83-H83	119.4
C01B1-H1ZC1	0.9800	C361-C371-H371	120.8	C83-C93-C103	119.9(4)
C04A1-Cl021	1.760(2)	C381-C371-H371	120.8	C83-C93-H93	120.0
C04A1-Cl011	1.760(2)	C371-C381-C391	121.0(10)	C103-C93-H93	120.0
C04A1-H4ZA1	0.9900	C371-C381-C401	115.2(12)	C93-C103-C113	119.4(4)
C04A1-H4ZB1	0.9900	C391-C381-C401	123.8(13)	C93-C103-N23	121.8(4)
F12-C162	1.363(5)	O31-C391-C341	119.3(14)	C113-C103-N23	118.8(4)
O22-C192	1.304(5)	O31-C391-C381	121.9(14)	C123-C113-C103	120.1(4)
O22-Fe32	1.910(3)	C341-C391-C381	118.7(10)	C123-C113-H113	120.0
N22-C132	1.294(6)	N31-C401-C381	127.2(18)	C103-C113-H113	120.0
N22-C102	1.426(5)	N31-C401-H401	116.4	C113-C123-C73	121.5(4)
N22-Fe32	2.065(4)	C381-C401-H401	116.4	C113-C123-H123	119.2
Fe32-O72	1.951(10)	C391-O31-Fe11	132.4(15)	C73-C123-H123	119.2
Fe32-O52	1.962(3)	C401-N31-C411	116.7(15)	N23-C133-C14B3	130.9(9)
Fe32-O7A2	2.04(5)	C401-N31-Fe11	122.5(14)	N23-C133-C143	126.6(7)
N32-C402	1.281(6)	C411-N31-Fe11	119.9(13)	N23-C133-C14C3	119.3(15)
N32-C412	1.437(5)	C2A1-C1A1-C6A1	120.9(14)	N23-C133-C14A3	124.6(10)
N32-Fe42	2.151(4)	C2A1-C1A1-N1A1	110.5(12)	N23-C133-H133	116.7
Fe42-O3A2	1.89(3)	C6A1-C1A1-N1A1	128.6(15)	C143-C133-H133	116.7
Fe42-O32	1.936(18)	C1A1-C2A1-C3A1	120.2(13)	C153-C143-C193	119.5(9)
Fe42-O42	2.001(3)	C1A1-C2A1-C49A1	106.4(11)	C153-C143-C133	115.2(10)

Fe42-O62	2.015(11)	C3A1-C2A1-C49A1	133.4(14)	C193-C143-C133	123.8(11)
Fe42-O3B2	2.06(3)	C4A1-C3A1-C2A1	120.2(15)	C163-C153-C143	119.4(10)
Fe42-O6A2	2.07(5)	C4A1-C3A1-H3D1	119.9	C163-C153-H153	120.3
Fe42-N02A3	2.259(4)	C2A1-C3A1-H3D1	119.9	C143-C153-H153	120.3
O42-C592	1.273(6)	C3A1-C4A1-C5A1	118.2(15)	F13-C163-C153	120.3(12)
O52-C592	1.238(6)	C3A1-C4A1-C64A1	122.8(16)	F13-C163-C173	117.4(11)
C12-C62	1.400(5)	C5A1-C4A1-C64A1	118.9(16)	C153-C163-C173	122.3(9)
C12-N12	1.407(5)	C6A1-C5A1-C4A1	122.8(15)	C163-C173-C183	119.6(9)
C12-C22	1.408(5)	C6A1-C5A1-H5D1	118.6	C163-C173-H173	120.2
C22-C32	1.383(5)	C4A1-C5A1-H5D1	118.6	C183-C173-H173	120.2
C22-C492	1.449(5)	C5A1-C6A1-C1A1	117.3(15)	C173-C183-C193	119.5(9)
C32-C42	1.398(6)	C5A1-C6A1-C7A1	120.9(17)	C173-C183-C203	120.7(8)
C32-H32	0.9500	C1A1-C6A1-C7A1	121.7(16)	C193-C183-C203	119.7(8)
C42-C52	1.403(6)	C48A1-C47A1-C52A1	117.7(14)	O23-C193-C183	119.4(10)
C42-C642	1.523(6)	C48A1-C47A1-C441	120.0(15)	O23-C193-C143	121.3(11)
C52-C62	1.393(6)	C52A1-C47A1-C441	122.1(16)	C183-C193-C143	119.3(8)
C52-H52	0.9500	C47A1-C48A1-C49A1	121.6(14)	C193-O23-Fe13	133.5(13)
C62-C72	1.483(6)	C47A1-C48A1-N1A1	129.6(16)	C253-C203-C213	117.6(9)
C472-C522	1.398(5)	C49A1-C48A1-N1A1	108.8(12)	C253-C203-C183	122.1(9)
C472-C482	1.400(5)	C50A1-C49A1-C48A1	119.0(14)	C213-C203-C183	120.3(9)
C472-C442	1.489(6)	C50A1-C49A1-C2A1	133.4(15)	C223-C213-C203	121.5(11)
C482-C492	1.397(5)	C48A1-C49A1-C2A1	107.6(12)	C223-C213-H213	119.3
C482-N12	1.415(5)	C51A1-C50A1-C49A1	121.3(16)	C203-C213-H213	119.3
C492-C502	1.403(5)	C51A1-C50A1-H50D1	119.4	C233-C223-C213	119.8(11)
C502-C512	1.386(6)	C49A1-C50A1-H50D1	119.4	C233-C223-H223	120.1
C502-H502	0.9500	C50A1-C51A1-C52A1	118.6(16)	C213-C223-H223	120.1
C512-C522	1.401(6)	C50A1-C51A1-C60A1	119(2)	C223-C233-C243	120.3(10)
C512-C602	1.533(6)	C52A1-C51A1-C60A1	121.9(19)	C223-C233-H233	119.8
C522-H522	0.9500	C47A1-C52A1-C51A1	121.8(16)	C243-C233-H233	119.8
N12-C532	1.482(5)	C47A1-C52A1-H52D1	119.1	C253-C243-C233	118.9(10)
C72-C82	1.390(6)	C51A1-C52A1-H52D1	119.1	C253-C243-C263	121.3(9)
C72-C122	1.400(6)	C531-N1A1-C1A1	115(4)	C233-C243-C263	119.4(9)
C82-C92	1.393(6)	C531-N1A1-C48A1	123(5)	C243-C253-C203	121.8(10)
C82-H82	0.9500	C1A1-N1A1-C48A1	106.6(13)	C243-C253-H253	119.1
C92-C102	1.389(6)	C66A1-C64A1-C4A1	113(2)	C203-C253-H253	119.1
C92-H92	0.9500	C66A1-C64A1-C67A1	111(2)	O13-C263-C243	111.9(9)
C102-C112	1.392(6)	C4A1-C64A1-C67A1	107.1(19)	O13-C263-H26A3	109.2
C112-C122	1.376(6)	C66A1-C64A1-C65A1	109.7(19)	C243-C263-H26A3	109.2

C112-H112	0.9500	C4A1-C64A1-C65A1	109(2)	O13-C263-H26B3	109.2
C122-H122	0.9500	C67A1-C64A1-C65A1	106.1(17)	C243-C263-H26B3	109.2
C132-C142	1.435(6)	C64A1-C65A1-H65D1	109.5	H26A3-C263-H26B3	107.9
C132-H132	0.9500	C64A1-C65A1-H65E1	109.5	C263-O13-C273	107.7(11)
C142-C152	1.412(6)	H65D1-C65A1-H65E1	109.5	O13-C273-C283	108.9(8)
C142-C192	1.417(6)	C64A1-C65A1-H65F1	109.5	O13-C273-H27A3	109.9
C152-C162	1.369(6)	H65D1-C65A1-H65F1	109.5	C283-C273-H27A3	109.9
C152-H152	0.9500	H65E1-C65A1-H65F1	109.5	O13-C273-H27B3	109.9
C162-C172	1.383(7)	C64A1-C66A1-H66D1	109.5	C283-C273-H27B3	109.9
C172-C182	1.374(7)	C64A1-C66A1-H66E1	109.5	H27A3-C273-H27B3	108.3
C172-H172	0.9500	H66D1-C66A1-H66E1	109.5	C293-C283-C333	119.7(10)
C182-C192	1.438(6)	C64A1-C66A1-H66F1	109.5	C293-C283-C273	121.5(10)
C182-C202	1.471(10)	H66D1-C66A1-H66F1	109.5	C333-C283-C273	118.8(10)
C182-C20A2	1.497(14)	H66E1-C66A1-H66F1	109.5	C283-C293-C303	120.5(11)
C182-C20B2	1.500(16)	C64A1-C67A1-H67D1	109.5	C283-C293-H293	119.8
C202-C252	1.390(10)	C64A1-C67A1-H67E1	109.5	C303-C293-H293	119.8
C202-C212	1.390(10)	H67D1-C67A1-H67E1	109.5	C313-C303-C293	119.5(12)
C212-C222	1.380(10)	C64A1-C67A1-H67F1	109.5	C313-C303-H303	120.3
C212-H212	0.9500	H67D1-C67A1-H67F1	109.5	C293-C303-H303	120.3
C222-C232	1.394(10)	H67E1-C67A1-H67F1	109.5	C303-C313-C323	120.9(11)
C222-H222	0.9500	C63A1-C60A1-C62A1	109.6(17)	C303-C313-H313	119.5
C232-C242	1.399(10)	C63A1-C60A1-C61A1	106.7(19)	C323-C313-H313	119.5
C232-H232	0.9500	C62A1-C60A1-C61A1	110.8(17)	C333-C323-C313	119.4(11)
C242-C252	1.394(10)	C63A1-C60A1-C51A1	108(2)	C333-C323-C343	121.6(10)
C242-C262	1.502(10)	C62A1-C60A1-C51A1	107(2)	C313-C323-C343	118.9(9)
C252-H252	0.9500	C61A1-C60A1-C51A1	115(2)	C323-C333-C283	120.0(11)
C262-O12	1.415(10)	C60A1-C61A1-H61D1	109.5	C323-C333-H333	120.0
C262-H26A2	0.9900	C60A1-C61A1-H61E1	109.5	C283-C333-H333	120.0
C262-H26B2	0.9900	H61D1-C61A1-H61E1	109.5	C353-C343-C393	118.9(8)
O12-C272	1.446(11)	C60A1-C61A1-H61F1	109.5	C353-C343-C323	120.7(8)
C272-C282	1.495(11)	H61D1-C61A1-H61F1	109.5	C393-C343-C323	120.4(8)
C272-H27A2	0.9900	H61E1-C61A1-H61F1	109.5	C363-C353-C343	121.5(9)
C272-H27B2	0.9900	C60A1-C62A1-H62D1	109.5	C363-C353-H353	119.2
C282-C332	1.378(10)	C60A1-C62A1-H62E1	109.5	C343-C353-H353	119.2
C282-C292	1.398(10)	H62D1-C62A1-H62E1	109.5	C353-C363-F23	119.5(9)
C292-C302	1.376(11)	C60A1-C62A1-H62F1	109.5	C353-C363-C373	121.8(8)
C292-H292	0.9500	H62D1-C62A1-H62F1	109.5	F23-C363-C373	118.7(9)
C302-C312	1.367(10)	H62E1-C62A1-H62F1	109.5	C363-C373-C383	118.2(8)

C302-H302	0.9500	C60A1-C63A1-H63D1	109.5	C363-C373-H373	120.9
C312-C322	1.397(10)	C60A1-C63A1-H63E1	109.5	C383-C373-H373	120.9
C312-H312	0.9500	H63D1-C63A1-H63E1	109.5	C393-C383-C373	120.9(8)
C322-C332	1.373(10)	C60A1-C63A1-H63F1	109.5	C393-C383-C403	125.2(9)
C322-C342	1.480(10)	H63D1-C63A1-H63F1	109.5	C373-C383-C403	113.9(9)
C332-H332	0.9500	H63E1-C63A1-H63F1	109.5	O33-C393-C383	121.9(9)
C342-C352	1.386(10)	C8A1-C7A1-C12A1	119.4(14)	O33-C393-C343	119.3(10)
C342-C392	1.437(9)	C8A1-C7A1-C6A1	124.2(19)	C383-C393-C343	118.6(7)
C352-C362	1.380(10)	C12A1-C7A1-C6A1	116(2)	N33-C403-C383	129.2(13)
C352-H352	0.9500	C7A1-C8A1-C9A1	120.5(15)	N33-C403-H403	115.4
C362-F22	1.364(9)	C7A1-C8A1-H8D1	119.8	C383-C403-H403	115.4
C362-C372	1.377(10)	C9A1-C8A1-H8D1	119.8	C393-O33-Fe23	132.3(11)
C372-C382	1.404(10)	C10A1-C9A1-C8A1	119.4(15)	C15A3-C14A3-C19A3	117.1(12)
C372-H372	0.9500	C10A1-C9A1-H9D1	120.3	C15A3-C14A3-C133	119.3(15)
C382-C392	1.408(10)	C8A1-C9A1-H9D1	120.3	C19A3-C14A3-C133	123.3(16)
C382-C402	1.445(13)	C11A1-C10A1-C9A1	120.7(15)	C16A3-C15A3-C14A3	120.3(13)
C392-O32	1.304(9)	C11A1-C10A1-N2A1	122(3)	C16A3-C15A3-H15D3	119.9
C20A2-C21A2	1.395(13)	C9A1-C10A1-N2A1	117(4)	C14A3-C15A3-H15D3	119.9
C20A2-C25A2	1.398(13)	C10A1-C11A1-C12A1	119.3(16)	F1A3-C16A3-C17A3	120.2(15)
C21A2-C22A2	1.394(13)	C10A1-C11A1-H11D1	120.3	F1A3-C16A3-C15A3	117.2(15)
C21A2-H21D2	0.9500	C12A1-C11A1-H11D1	120.3	C17A3-C16A3-C15A3	122.2(13)
C22A2-C23A2	1.395(13)	C7A1-C12A1-C11A1	120.4(16)	C16A3-C17A3-C18A3	118.5(13)
C22A2-H22D2	0.9500	C7A1-C12A1-H12D1	119.8	C16A3-C17A3-H17D3	120.7
C23A2-C24A2	1.392(13)	C11A1-C12A1-H12D1	119.8	C18A3-C17A3-H17D3	120.7
C23A2-H23D2	0.9500	N2A1-C13A1-C14A1	127(2)	C17A3-C18A3-C19A3	120.6(12)
C24A2-C25A2	1.402(13)	N2A1-C13A1-H13D1	116.7	C17A3-C18A3-C20A3	117.1(12)
C24A2-C26A2	1.514(14)	C14A1-C13A1-H13D1	116.7	C19A3-C18A3-C20A3	122.2(13)
C25A2-H25D2	0.9500	C19A1-C14A1-C15A1	120.1(14)	O2A3-C19A3-C18A3	117.4(16)
C26A2-O1A2	1.430(15)	C19A1-C14A1-C13A1	125.2(15)	O2A3-C19A3-C14A3	121.9(17)
C26A2-H26D2	0.9900	C15A1-C14A1-C13A1	114.7(16)	C18A3-C19A3-C14A3	120.6(12)
C26A2-H26E2	0.9900	C16A1-C15A1-C14A1	119.0(15)	C19A3-O2A3-Fe13	136(2)
O1A2-C27A2	1.418(15)	C16A1-C15A1-H15D1	120.5	C25A3-C20A3-C21A3	120.9(13)
C27A2-C28A2	1.497(14)	C14A1-C15A1-H15D1	120.5	C25A3-C20A3-C18A3	120.3(15)
C27A2-H27D2	0.9900	F1A1-C16A1-C15A1	118.9(17)	C21A3-C20A3-C18A3	118.8(14)
C27A2-H27E2	0.9900	F1A1-C16A1-C17A1	120.0(17)	C22A3-C21A3-C20A3	120.7(13)
C28A2-C33A2	1.383(13)	C15A1-C16A1-C17A1	121.2(14)	C22A3-C21A3-H21D3	119.6
C28A2-C29A2	1.393(13)	C16A1-C17A1-C18A1	120.8(15)	C20A3-C21A3-H21D3	119.6
C29A2-C30A2	1.374(13)	C16A1-C17A1-H17D1	119.6	C21A3-C22A3-C23A3	117.9(14)

C29A2-H29D2	0.9500	C18A1-C17A1-H17D1	119.6	C21A3-C22A3-H22D3	121.0
C30A2-C31A2	1.376(13)	C17A1-C18A1-C19A1	118.5(14)	C23A3-C22A3-H22D3	121.0
C30A2-H30D2	0.9500	C17A1-C18A1-C20A1	120.9(17)	C24A3-C23A3-C22A3	121.5(14)
C31A2-C32A2	1.400(13)	C19A1-C18A1-C20A1	120.5(17)	C24A3-C23A3-H23A3	119.2
C31A2-H31D2	0.9500	O2A1-C19A1-C14A1	121.5(16)	C22A3-C23A3-H23A3	119.2
C32A2-C33A2	1.375(13)	O2A1-C19A1-C18A1	118.2(17)	C23A3-C24A3-C25A3	120.0(13)
C32A2-C34A2	1.476(14)	C14A1-C19A1-C18A1	120.3(14)	C23A3-C24A3-C26A3	120.2(14)
C33A2-H33D2	0.9500	C19A1-O2A1-Fe21	133.0(19)	C25A3-C24A3-C26A3	119.1(14)
C34A2-C35A2	1.392(13)	C13A1-N2A1-C10A1	118(2)	C20A3-C25A3-C24A3	118.8(14)
C34A2-C39A2	1.414(12)	C13A1-N2A1-Fe21	126.1(17)	C20A3-C25A3-H25D3	120.6
C35A2-C36A2	1.381(13)	C10A1-N2A1-Fe21	116(2)	C24A3-C25A3-H25D3	120.6
C35A2-H35D2	0.9500	C25A1-C20A1-C21A1	116.7(11)	O1A3-C26A3-C24A3	110.8(14)
C36A2-F2A2	1.363(14)	C25A1-C20A1-C18A1	125.9(16)	O1A3-C26A3-H26D3	109.5
C36A2-C37A2	1.394(13)	C21A1-C20A1-C18A1	117.4(17)	C24A3-C26A3-H26D3	109.5
C37A2-C38A2	1.402(13)	C22A1-C21A1-C20A1	122.5(12)	O1A3-C26A3-H26E3	109.5
C37A2-H37D2	0.9500	C22A1-C21A1-H21D1	118.8	C24A3-C26A3-H26E3	109.5
C38A2-C39A2	1.410(13)	C20A1-C21A1-H21D1	118.8	H26D3-C26A3-H26E3	108.1
C38A2-C402	1.49(2)	C21A1-C22A1-C23A1	119.4(12)	C26A3-O1A3-C27A3	111.5(13)
C39A2-O3A2	1.307(14)	C21A1-C22A1-H22D1	120.3	O1A3-C27A3-C28A3	109.3(11)
C20B2-C25B2	1.399(14)	C23A1-C22A1-H22D1	120.3	O1A3-C27A3-H27D3	109.8
C20B2-C21B2	1.399(14)	C24A1-C23A1-C22A1	119.6(12)	C28A3-C27A3-H27D3	109.8
C21B2-C22B2	1.389(14)	C24A1-C23A1-H23D1	120.2	O1A3-C27A3-H27E3	109.8
C21B2-H21G2	0.9500	C22A1-C23A1-H23D1	120.2	C28A3-C27A3-H27E3	109.8
C22B2-C23B2	1.391(14)	C25A1-C24A1-C23A1	119.8(11)	H27D3-C27A3-H27E3	108.3
C22B2-H22G2	0.9500	C25A1-C24A1-C26A1	120.2(12)	C29A3-C28A3-C33A3	120.9(12)
C23B2-C24B2	1.396(13)	C23A1-C24A1-C26A1	119.9(12)	C29A3-C28A3-C27A3	118.6(14)
C23B2-H23G2	0.9500	C24A1-C25A1-C20A1	122.0(12)	C33A3-C28A3-C27A3	120.5(13)
C24B2-C25B2	1.401(14)	C24A1-C25A1-H25D1	119.0	C28A3-C29A3-C30A3	119.4(13)
C24B2-C26B2	1.512(15)	C20A1-C25A1-H25D1	119.0	C28A3-C29A3-H29D3	120.3
C25B2-H25G2	0.9500	O1A1-C26A1-C24A1	106.2(12)	C30A3-C29A3-H29D3	120.3
C26B2-O1B2	1.421(17)	O1A1-C26A1-H26D1	110.5	C29A3-C30A3-C31A3	119.2(13)
C26B2-H26G2	0.9900	C24A1-C26A1-H26D1	110.5	C29A3-C30A3-H30D3	120.4
C26B2-H26H2	0.9900	O1A1-C26A1-H26E1	110.5	C31A3-C30A3-H30D3	120.4
O1B2-C27B2	1.437(17)	C24A1-C26A1-H26E1	110.5	C32A3-C31A3-C30A3	122.1(13)
C27B2-C28B2	1.500(15)	H26D1-C26A1-H26E1	108.7	C32A3-C31A3-H31D3	118.9
C27B2-H27G2	0.9900	C27A1-O1A1-C26A1	109.6(11)	C30A3-C31A3-H31D3	118.9
C27B2-H27H2	0.9900	O1A1-C27A1-C28A1	109.0(9)	C31A3-C32A3-C33A3	117.7(13)
C28B2-C33B2	1.385(13)	O1A1-C27A1-H27D1	109.9	C31A3-C32A3-C34A3	118.5(14)

C28B2-C29B2	1.392(13)	C28A1-C27A1-H27D1	109.9	C33A3-C32A3-C34A3	123.7(14)
C29B2-C30B2	1.383(14)	O1A1-C27A1-H27E1	109.9	C32A3-C33A3-C28A3	120.1(13)
C29B2-H29G2	0.9500	C28A1-C27A1-H27E1	109.9	C32A3-C33A3-H33D3	120.0
C30B2-C31B2	1.379(14)	H27D1-C27A1-H27E1	108.3	C28A3-C33A3-H33D3	120.0
C30B2-H30G2	0.9500	C29A1-C28A1-C33A1	119.4(11)	C35A3-C34A3-C39A3	118.0(11)
C31B2-C32B2	1.391(13)	C29A1-C28A1-C27A1	122.3(11)	C35A3-C34A3-C32A3	116.4(13)
C31B2-H31G2	0.9500	C33A1-C28A1-C27A1	118.4(11)	C39A3-C34A3-C32A3	125.5(13)
C32B2-C33B2	1.375(13)	C30A1-C29A1-C28A1	119.9(11)	C36A3-C35A3-C34A3	121.3(12)
C32B2-C34B2	1.468(15)	C30A1-C29A1-H29D1	120.0	C36A3-C35A3-H35D3	119.4
C33B2-H33G2	0.9500	C28A1-C29A1-H29D1	120.0	C34A3-C35A3-H35D3	119.4
C34B2-C35B2	1.394(13)	C31A1-C30A1-C29A1	120.7(12)	F2A3-C36A3-C37A3	119.6(12)
C34B2-C39B2	1.409(13)	C31A1-C30A1-H30D1	119.7	F2A3-C36A3-C35A3	118.5(11)
C35B2-C36B2	1.388(13)	C29A1-C30A1-H30D1	119.7	C37A3-C36A3-C35A3	122.0(11)
C35B2-H35G2	0.9500	C30A1-C31A1-C32A1	120.1(11)	C36A3-C37A3-C38A3	117.9(12)
C36B2-F2B2	1.361(15)	C30A1-C31A1-H31D1	120.0	C36A3-C37A3-H37D3	121.1
C36B2-C37B2	1.387(13)	C32A1-C31A1-H31D1	120.0	C38A3-C37A3-H37D3	121.1
C37B2-C38B2	1.400(14)	C33A1-C32A1-C31A1	119.8(11)	C39A3-C38A3-C37A3	121.7(11)
C37B2-H37G2	0.9500	C33A1-C32A1-C34A1	119.3(12)	C39A3-C38A3-C40A3	123.7(12)
C38B2-C39B2	1.401(13)	C31A1-C32A1-C34A1	120.6(12)	C37A3-C38A3-C40A3	114.4(12)
C38B2-C402	1.44(2)	C32A1-C33A1-C28A1	120.1(12)	O3A3-C39A3-C38A3	122.9(13)
C39B2-O3B2	1.314(15)	C32A1-C33A1-H33D1	119.9	O3A3-C39A3-C34A3	118.1(14)
C402-H402	0.9500	C28A1-C33A1-H33D1	119.9	C38A3-C39A3-C34A3	118.8(11)
C412-C462	1.376(6)	C35A1-C34A1-C39A1	120.6(10)	N33-C40A3-C38A3	123.1(16)
C412-C422	1.404(6)	C35A1-C34A1-C32A1	118.4(12)	N33-C40A3-H40D3	118.4
C422-C432	1.379(6)	C39A1-C34A1-C32A1	121.0(12)	C38A3-C40A3-H40D3	118.4
C422-H422	0.9500	C36A1-C35A1-C34A1	120.3(11)	C39A3-O3A3-Fe23	134.8(17)
C432-C442	1.385(6)	C36A1-C35A1-H35D1	119.9	C19B3-C14B3-C15B3	126.4(13)
C432-H432	0.9500	C34A1-C35A1-H35D1	119.9	C19B3-C14B3-C133	115.4(13)
C442-C452	1.404(6)	F2A1-C36A1-C37A1	119.9(10)	C15B3-C14B3-C133	117.2(14)
C452-C462	1.385(6)	F2A1-C36A1-C35A1	119.3(10)	C14B3-C15B3-C16B3	115.2(13)
C452-H452	0.9500	C37A1-C36A1-C35A1	120.8(10)	C14B3-C15B3-H15G3	122.4
C462-H462	0.9500	C36A1-C37A1-C38A1	120.1(10)	C16B3-C15B3-H15G3	122.4
C532-C54A2	1.487(13)	C36A1-C37A1-H37D1	120.0	F1B3-C16B3-C17B3	121.0(18)
C532-C542	1.525(10)	C38A1-C37A1-H37D1	120.0	F1B3-C16B3-C15B3	118.4(19)
C532-H53A2	0.9900	C37A1-C38A1-C39A1	119.9(10)	C17B3-C16B3-C15B3	119.5(14)
C532-H53B2	0.9900	C37A1-C38A1-C40A1	116.9(11)	C16B3-C17B3-C18B3	122.1(14)
C532-H53E2	0.9900	C39A1-C38A1-C40A1	123.1(12)	C16B3-C17B3-H17G3	118.9
C532-H53F2	0.9900	O3A1-C39A1-C34A1	120.0(12)	C18B3-C17B3-H17G3	118.9

C542-C552	1.546(9)	O3A1-C39A1-C38A1	121.8(12)	C19B3-C18B3-C17B3	118.6(12)
C542-H54A2	0.9900	C34A1-C39A1-C38A1	117.9(10)	C19B3-C18B3-C20B3	120.2(13)
C542-H54B2	0.9900	N3A1-C40A1-C38A1	128.2(16)	C17B3-C18B3-C20B3	121.1(13)
C552-C562	1.495(9)	N3A1-C40A1-H40D1	115.9	O2B3-C19B3-C14B3	125.4(16)
C552-H55A2	0.9900	C38A1-C40A1-H40D1	115.9	O2B3-C19B3-C18B3	118.2(15)
C552-H55B2	0.9900	C39A1-O3A1-Fe11	133.3(13)	C14B3-C19B3-C18B3	115.9(11)
C54A2-C55A2	1.521(12)	C40A1-N3A1-C411	117.4(13)	C19B3-O2B3-Fe13	139(2)
C54A2-H54D2	0.9900	C40A1-N3A1-Fe11	125.4(11)	C21B3-C20B3-C25B3	117.2(14)
C54A2-H54E2	0.9900	C411-N3A1-Fe11	117.2(11)	C21B3-C20B3-C18B3	119.5(16)
C55A2-C562	1.563(12)	C2B1-C1B1-C6B1	121.1(15)	C25B3-C20B3-C18B3	123.3(15)
C55A2-H55D2	0.9900	C2B1-C1B1-N1B1	110.5(13)	C22B3-C21B3-C20B3	120.2(16)
C55A2-H55E2	0.9900	C6B1-C1B1-N1B1	128.4(17)	C22B3-C21B3-H21G3	119.9
C562-C572	1.509(6)	C3B1-C2B1-C1B1	120.1(15)	C20B3-C21B3-H21G3	119.9
C562-H56A2	0.9900	C3B1-C2B1-C49B1	133.8(16)	C21B3-C22B3-C23B3	121.4(17)
C562-H56B2	0.9900	C1B1-C2B1-C49B1	106.1(12)	C21B3-C22B3-H22G3	119.3
C562-H56D2	0.9900	C4B1-C3B1-C2B1	120.3(17)	C23B3-C22B3-H22G3	119.3
C562-H56E2	0.9900	C4B1-C3B1-H3G1	119.9	C22B3-C23B3-C24B3	119.9(16)
C572-C582	1.526(7)	C2B1-C3B1-H3G1	119.9	C22B3-C23B3-H23G3	120.1
C572-H57A2	0.9900	C3B1-C4B1-C5B1	118.1(17)	C24B3-C23B3-H23G3	120.1
C572-H57B2	0.9900	C3B1-C4B1-C64B1	122(2)	C23B3-C24B3-C25B3	117.2(15)
C582-C592	1.505(7)	C5B1-C4B1-C64B1	120(2)	C23B3-C24B3-C26B3	122.6(16)
C582-H58A2	0.9900	C6B1-C5B1-C4B1	123.7(18)	C25B3-C24B3-C26B3	120.1(16)
C582-H58B2	0.9900	C6B1-C5B1-H5G1	118.2	C20B3-C25B3-C24B3	124.1(15)
C602-C632	1.527(6)	C4B1-C5B1-H5G1	118.2	C20B3-C25B3-H25G3	118.0
C602-C612	1.533(6)	C5B1-C6B1-C1B1	116.6(17)	C24B3-C25B3-H25G3	118.0
C602-C622	1.543(7)	C5B1-C6B1-C7B1	126(2)	O1B3-C26B3-C24B3	112.8(17)
C612-H61A2	0.9800	C1B1-C6B1-C7B1	118(2)	O1B3-C26B3-H26G3	109.0
C612-H61B2	0.9800	C52B1-C47B1-C48B1	115.4(17)	C24B3-C26B3-H26G3	109.0
C612-H61C2	0.9800	C52B1-C47B1-C441	125(2)	O1B3-C26B3-H26H3	109.0
C622-H62A2	0.9800	C48B1-C47B1-C441	119.0(19)	C24B3-C26B3-H26H3	109.0
C622-H62B2	0.9800	C47B1-C48B1-C49B1	121.5(15)	H26G3-C26B3-H26H3	107.8
C622-H62C2	0.9800	C47B1-C48B1-N1B1	129.5(17)	C27B3-O1B3-C26B3	110.7(15)
C632-H63A2	0.9800	C49B1-C48B1-N1B1	108.9(13)	O1B3-C27B3-C28B3	116.8(18)
C632-H63B2	0.9800	C50B1-C49B1-C48B1	120.2(15)	O1B3-C27B3-H27G3	108.1
C632-H63C2	0.9800	C50B1-C49B1-C2B1	132.1(17)	C28B3-C27B3-H27G3	108.1
C642-C652	1.527(8)	C48B1-C49B1-C2B1	107.7(12)	O1B3-C27B3-H27H3	108.1
C642-C672	1.535(7)	C51B1-C50B1-C49B1	120.5(18)	C28B3-C27B3-H27H3	108.1
C642-C662	1.549(7)	C51B1-C50B1-H50G1	119.8	H27G3-C27B3-H27H3	107.3

C652-H65A2	0.9800	C49B1-C50B1-H50G1	119.8	C29B3-C28B3-C33B3	117.3(15)
C652-H65B2	0.9800	C50B1-C51B1-C52B1	117.3(18)	C29B3-C28B3-C27B3	122.0(18)
C652-H65C2	0.9800	C50B1-C51B1-C60B1	121(2)	C33B3-C28B3-C27B3	120.7(18)
C662-H66A2	0.9800	C52B1-C51B1-C60B1	121(2)	C28B3-C29B3-C30B3	120.8(17)
C662-H66B2	0.9800	C47B1-C52B1-C51B1	124.7(18)	C28B3-C29B3-H29G3	119.6
C662-H66C2	0.9800	C47B1-C52B1-H52G1	117.7	C30B3-C29B3-H29G3	119.6
C672-H67A2	0.9800	C51B1-C52B1-H52G1	117.7	C31B3-C30B3-C29B3	120.8(18)
C672-H67B2	0.9800	C1B1-N1B1-C48B1	106.6(14)	C31B3-C30B3-H30G3	119.6
C672-H67C2	0.9800	C1B1-N1B1-C531	118(7)	C29B3-C30B3-H30G3	119.6
C682-O6A2	1.15(5)	C48B1-N1B1-C531	121(7)	C30B3-C31B3-C32B3	119.5(17)
C682-O72	1.247(11)	C66B1-C64B1-C4B1	114(2)	C30B3-C31B3-H31G3	120.3
C682-O62	1.275(12)	C66B1-C64B1-C67B1	111(2)	C32B3-C31B3-H31G3	120.3
C682-O7A2	1.29(5)	C4B1-C64B1-C67B1	105(3)	C33B3-C32B3-C31B3	119.0(18)
C682-C692	1.502(7)	C66B1-C64B1-C65B1	108.3(19)	C32B3-C33B3-C28B3	122.3(17)
C682-C69A2	1.524(15)	C4B1-C64B1-C65B1	109(2)	C32B3-C33B3-H33G3	118.9
C692-C822	1.393(7)	C67B1-C64B1-C65B1	108.7(19)	C28B3-C33B3-H33G3	118.9
C692-C702	1.409(7)	C64B1-C65B1-H65G1	109.5	C15C3-C14C3-C19C3	118.2(16)
C702-C752	1.415(7)	C64B1-C65B1-H65H1	109.5	C15C3-C14C3-C133	109(2)
C702-C712	1.430(7)	H65G1-C65B1-H65H1	109.5	C19C3-C14C3-C133	132(2)
C712-C722	1.369(7)	C64B1-C65B1-H65I1	109.5	C16C3-C15C3-C14C3	121.1(17)
C712-H712	0.9500	H65G1-C65B1-H65I1	109.5	C16C3-C15C3-H15J3	119.5
C722-C732	1.404(8)	H65H1-C65B1-H65I1	109.5	C14C3-C15C3-H15J3	119.5
C722-H722	0.9500	C64B1-C66B1-H66G1	109.5	F1C3-C16C3-C15C3	121(2)
C732-C742	1.378(8)	C64B1-C66B1-H66H1	109.5	F1C3-C16C3-C17C3	119(2)
C732-H732	0.9500	H66G1-C66B1-H66H1	109.5	C15C3-C16C3-C17C3	120.5(16)
C742-C752	1.419(8)	C64B1-C66B1-H66I1	109.5	C16C3-C17C3-C18C3	119.2(17)
C742-H742	0.9500	H66G1-C66B1-H66I1	109.5	C16C3-C17C3-H17J3	120.4
C752-C762	1.397(8)	H66H1-C66B1-H66I1	109.5	C18C3-C17C3-H17J3	120.4
C762-C772	1.397(8)	C64B1-C67B1-H67G1	109.5	C17C3-C18C3-C19C3	119.8(16)
C762-H762	0.9500	C64B1-C67B1-H67H1	109.5	C17C3-C18C3-C20C3	116.1(18)
C772-C782	1.419(8)	H67G1-C67B1-H67H1	109.5	C19C3-C18C3-C20C3	121.0(18)
C772-C822	1.426(7)	C64B1-C67B1-H67I1	109.5	O2C3-C19C3-C18C3	118(2)
C782-C792	1.367(8)	H67G1-C67B1-H67I1	109.5	O2C3-C19C3-C14C3	121(2)
C782-H782	0.9500	H67H1-C67B1-H67I1	109.5	C18C3-C19C3-C14C3	120.3(15)
C792-C802	1.412(8)	C63B1-C60B1-C62B1	108(2)	C19C3-O2C3-Fe13	128(3)
C792-H792	0.9500	C63B1-C60B1-C51B1	115(3)	C25C3-C20C3-C21C3	119.4(16)
C802-C812	1.368(8)	C62B1-C60B1-C51B1	113(3)	C25C3-C20C3-C18C3	123.1(18)
C802-H802	0.9500	C63B1-C60B1-C61B1	109(2)	C21C3-C20C3-C18C3	117.4(18)

C812-C822	1.423(8)	C62B1-C60B1-C61B1	110(2)	C22C3-C21C3-C20C3	121.4(18)
C812-H812	0.9500	C51B1-C60B1-C61B1	101(3)	C22C3-C21C3-H21J3	119.3
C69A2-C82A2	1.406(12)	C60B1-C61B1-H61G1	109.5	C20C3-C21C3-H21J3	119.3
C69A2-C70A2	1.412(12)	C60B1-C61B1-H61H1	109.5	C23C3-C22C3-C21C3	119.1(18)
C70A2-C71A2	1.405(13)	H61G1-C61B1-H61H1	109.5	C23C3-C22C3-H22J3	120.5
C70A2-C75A2	1.417(13)	C60B1-C61B1-H61I1	109.5	C21C3-C22C3-H22J3	120.5
C71A2-C72A2	1.399(13)	H61G1-C61B1-H61I1	109.5	C22C3-C23C3-C24C3	119.2(17)
C71A2-H71D2	0.9500	H61H1-C61B1-H61I1	109.5	C22C3-C23C3-H23J3	120.4
C72A2-C73A2	1.404(13)	C60B1-C62B1-H62G1	109.5	C24C3-C23C3-H23J3	120.4
C72A2-H72D2	0.9500	C60B1-C62B1-H62H1	109.5	C25C3-C24C3-C23C3	121.4(17)
C73A2-C74A2	1.397(13)	H62G1-C62B1-H62H1	109.5	C25C3-C24C3-C26C3	120(2)
C73A2-H73D2	0.9500	C60B1-C62B1-H62I1	109.5	C23C3-C24C3-C26C3	117.5(19)
C74A2-C75A2	1.405(12)	H62G1-C62B1-H62I1	109.5	C20C3-C25C3-C24C3	118.9(17)
C74A2-H74D2	0.9500	H62H1-C62B1-H62I1	109.5	C20C3-C25C3-H25J3	120.6
C75A2-C76A2	1.399(12)	C60B1-C63B1-H63G1	109.5	C24C3-C25C3-H25J3	120.6
C76A2-C77A2	1.399(12)	C60B1-C63B1-H63H1	109.5	O1C3-C26C3-C24C3	108(2)
C76A2-H76D2	0.9500	H63G1-C63B1-H63H1	109.5	O1C3-C26C3-H26J3	110.2
C77A2-C78A2	1.409(13)	C60B1-C63B1-H63I1	109.5	C24C3-C26C3-H26J3	110.2
C77A2-C82A2	1.414(12)	H63G1-C63B1-H63I1	109.5	O1C3-C26C3-H26K3	110.2
C78A2-C79A2	1.399(13)	H63H1-C63B1-H63I1	109.5	C24C3-C26C3-H26K3	110.2
C78A2-H78D2	0.9500	C8B1-C7B1-C12B1	119.2(16)	H26J3-C26C3-H26K3	108.5
C79A2-C80A2	1.407(13)	C8B1-C7B1-C6B1	117(3)	C27C3-O1C3-C26C3	110.6(17)
C79A2-H79D2	0.9500	C12B1-C7B1-C6B1	124(3)	O1C3-C27C3-C28C3	115.2(19)
C80A2-C81A2	1.397(13)	C9B1-C8B1-C7B1	119.7(17)	O1C3-C27C3-H27J3	108.5
C80A2-H80D2	0.9500	C9B1-C8B1-H8G1	120.2	C28C3-C27C3-H27J3	108.5
C81A2-C82A2	1.410(12)	C7B1-C8B1-H8G1	120.2	O1C3-C27C3-H27K3	108.5
C81A2-H81D2	0.9500	C10B1-C9B1-C8B1	121.2(17)	C28C3-C27C3-H27K3	108.5
Fe13-O2B3	1.85(2)	C10B1-C9B1-H9G1	119.4	H27J3-C27C3-H27K3	107.5
Fe13-O2A3	1.87(3)	C8B1-C9B1-H9G1	119.4	C29C3-C28C3-C33C3	118.1(16)
Fe13-O2C3	1.98(4)	C9B1-C10B1-C11B1	119.3(16)	C29C3-C28C3-C27C3	120.1(19)
Fe13-O43	1.983(3)	C9B1-C10B1-N2B1	129(4)	C33C3-C28C3-C27C3	121.8(19)
Fe13-O23	1.987(15)	C11B1-C10B1-N2B1	111(3)	C30C3-C29C3-C28C3	120.8(18)
Fe13-O63	2.042(3)	C10B1-C11B1-C12B1	119.8(17)	C30C3-C29C3-H29J3	119.6
Fe13-N23	2.132(4)	C10B1-C11B1-H11G1	120.1	C28C3-C29C3-H29J3	119.6
Fe13-O83	2.328(3)	C12B1-C11B1-H11G1	120.1	C29C3-C30C3-C31C3	120.4(18)
N13-C13	1.397(5)	C11B1-C12B1-C7B1	120.9(17)	C29C3-C30C3-H30J3	119.8
N13-C483	1.410(5)	C11B1-C12B1-H12G1	119.6	C31C3-C30C3-H30J3	119.8
N13-C533	1.478(6)	C7B1-C12B1-H12G1	119.6	C32C3-C31C3-C30C3	119.4(18)

C13-C23	1.402(6)	N2B1-C13B1-C14B1	127(2)	C32C3-C31C3-H31J3	120.3
C13-C63	1.408(6)	N2B1-C13B1-H13G1	116.5	C30C3-C31C3-H31J3	120.3
Fe23-O33	1.924(16)	C14B1-C13B1-H13G1	116.5	C33C3-C32C3-C31C3	119.4(18)
Fe23-O3A3	1.93(2)	C19B1-C14B1-C15B1	120.1(14)	C32C3-C33C3-C28C3	121.8(17)
Fe23-O53	2.014(3)	C19B1-C14B1-C13B1	125.7(16)	C32C3-C33C3-H33J3	119.1
Fe23-O73	2.020(3)	C15B1-C14B1-C13B1	114.2(17)	C28C3-C33C3-H33J3	119.1
Fe23-N33	2.133(4)	C16B1-C15B1-C14B1	120.5(16)	C21D3-C20D3-C25D3	120.2(18)
Fe23-O83	2.377(4)	C16B1-C15B1-H15G1	119.8	C20D3-C21D3-C22D3	119.7(18)
N23-C133	1.297(5)	C14B1-C15B1-H15G1	119.8	C20D3-C21D3-H21M3	120.1
N23-C103	1.423(5)	F1B1-C16B1-C15B1	119.8(18)	C22D3-C21D3-H21M3	120.1
C23-C33	1.399(6)	F1B1-C16B1-C17B1	120.8(17)	C21D3-C22D3-C23D3	120.4(18)
C23-C493	1.449(6)	C15B1-C16B1-C17B1	119.3(15)	C21D3-C22D3-H22M3	119.8
N33-C403	1.306(14)	C16B1-C17B1-C18B1	120.8(16)	C23D3-C22D3-H22M3	119.8
N33-C40A3	1.31(2)	C16B1-C17B1-H17G1	119.6	C24D3-C23D3-C22D3	119.4(18)
N33-C413	1.429(6)	C18B1-C17B1-H17G1	119.6	C24D3-C23D3-H23M3	120.3
C33-C43	1.389(6)	C17B1-C18B1-C19B1	120.1(16)	C22D3-C23D3-H23M3	120.3
C33-H33	0.9500	O2B1-C19B1-C14B1	121.5(17)	C25D3-C24D3-C23D3	120.3(16)
O43-C593	1.254(5)	O2B1-C19B1-C18B1	119.3(17)	C25D3-C24D3-C26D3	121(2)
C43-C53	1.397(6)	C14B1-C19B1-C18B1	119.2(14)	C23D3-C24D3-C26D3	119(2)
C43-C643	1.539(6)	C19B1-O2B1-Fe21	126.8(18)	C20D3-C25D3-C24D3	119.7(17)
O53-C593	1.267(5)	C13B1-N2B1-C10B1	115(2)	C20D3-C25D3-H25M3	120.1
C53-C63	1.397(6)	C13B1-N2B1-Fe21	121.4(19)	C24D3-C25D3-H25M3	120.1
C53-H53	0.9500	C10B1-N2B1-Fe21	123(2)	O1D3-C26D3-C24D3	107(2)
O63-C683	1.251(5)	N2C1-C13C1-C14C1	126(3)	O1D3-C26D3-H26M3	110.3
C63-C73	1.476(6)	N2C1-C13C1-H13J1	116.9	C24D3-C26D3-H26M3	110.3
O73-C683	1.258(5)	C14C1-C13C1-H13J1	116.9	O1D3-C26D3-H26N3	110.3
C73-C123	1.395(6)	C15C1-C14C1-C19C1	119.8(17)	C24D3-C26D3-H26N3	110.3
C73-C83	1.402(6)	C15C1-C14C1-C13C1	115(2)	H26M3-C26D3-H26N3	108.5
C83-C93	1.382(6)	C19C1-C14C1-C13C1	125(2)	C26D3-O1D3-C27D3	108.6(18)
C83-H83	0.9500	C16C1-C15C1-C14C1	119.9(18)	O1D3-C27D3-C28D3	106.3(18)
C93-C103	1.389(6)	C16C1-C15C1-H15J1	120.0	O1D3-C27D3-H27M3	110.5
C93-H93	0.9500	C14C1-C15C1-H15J1	120.0	C28D3-C27D3-H27M3	110.5
C103-C113	1.398(6)	F1C1-C16C1-C17C1	121(2)	O1D3-C27D3-H27N3	110.5
C113-C123	1.374(6)	F1C1-C16C1-C15C1	119(2)	C28D3-C27D3-H27N3	110.5
C113-H113	0.9500	C17C1-C16C1-C15C1	120.4(17)	H27M3-C27D3-H27N3	108.7
C123-H123	0.9500	C16C1-C17C1-C18C1	119.7(18)	C33D3-C28D3-C29D3	120.1(16)
C133-C14B3	1.401(14)	C16C1-C17C1-H17J1	120.2	C33D3-C28D3-C27D3	121(2)
C133-C143	1.441(10)	C18C1-C17C1-H17J1	120.2	C29D3-C28D3-C27D3	119.3(19)

C133-C14C3	1.462(16)	C17C1-C18C1-C19C1	120.1(18)	C28D3-C29D3-C30D3	120.1(18)
C133-C14A3	1.468(13)	C17C1-C18C1-C20C1	120.1(14)	C28D3-C29D3-H29M3	119.9
C133-H133	0.9500	C19C1-C18C1-C20C1	119.8(14)	C30D3-C29D3-H29M3	119.9
C143-C153	1.406(10)	O2C1-C19C1-C14C1	121(2)	C29D3-C30D3-C31D3	119.7(18)
C143-C193	1.419(11)	O2C1-C19C1-C18C1	119(2)	C29D3-C30D3-H30M3	120.1
C153-C163	1.370(11)	C14C1-C19C1-C18C1	120.0(17)	C31D3-C30D3-H30M3	120.1
C153-H153	0.9500	C19C1-O2C1-Fe21	125(4)	C32D3-C31D3-C30D3	120.2(18)
C163-F13	1.366(10)	C13C1-N2C1-Fe21	120(5)	C32D3-C31D3-H31M3	119.9
C163-C173	1.385(11)	C21C1-C20C1-C25C1	119.9(19)	C30D3-C31D3-H31M3	119.9
C173-C183	1.397(10)	C21C1-C20C1-C18C1	120.2(14)	C31D3-C32D3-C33D3	119.8(18)
C173-H173	0.9500	C25C1-C20C1-C18C1	119.9(14)	C28D3-C33D3-C32D3	120.0(18)
C183-C193	1.417(10)	C20C1-C21C1-C22C1	120.1(19)	C28D3-C33D3-H33M3	120.0
C183-C203	1.502(11)	C20C1-C21C1-H21J1	119.9	C32D3-C33D3-H33M3	120.0
C193-O23	1.311(10)	C22C1-C21C1-H21J1	119.9	C423-C413-C463	119.2(4)
C203-C253	1.390(11)	C21C1-C22C1-C23C1	120.0(19)	C423-C413-N33	119.3(4)
C203-C213	1.401(11)	C21C1-C22C1-H22J1	120.0	C463-C413-N33	121.3(4)
C213-C223	1.378(11)	C23C1-C22C1-H22J1	120.0	C433-C423-C413	120.1(4)
C213-H213	0.9500	C24C1-C23C1-C22C1	119.8(18)	C433-C423-H423	120.0
C223-C233	1.378(12)	C24C1-C23C1-H23J1	120.1	C413-C423-H423	120.0
C223-H223	0.9500	C22C1-C23C1-H23J1	120.1	C423-C433-C443	121.2(4)
C233-C243	1.398(11)	C25C1-C24C1-C23C1	120.2(17)	C423-C433-H433	119.4
C233-H233	0.9500	C25C1-C24C1-C26C1	120(2)	C443-C433-H433	119.4
C243-C253	1.386(11)	C23C1-C24C1-C26C1	119(2)	C453-C443-C433	117.8(4)
C243-C263	1.520(12)	C24C1-C25C1-C20C1	119.9(18)	C453-C443-C473	122.6(4)
C253-H253	0.9500	C24C1-C25C1-H25J1	120.1	C433-C443-C473	119.5(4)
C263-O13	1.436(12)	C20C1-C25C1-H25J1	120.1	C463-C453-C443	121.5(5)
C263-H26A3	0.9900	O1C1-C26C1-C24C1	108(2)	C463-C453-H453	119.2
C263-H26B3	0.9900	O1C1-C26C1-H26J1	110.1	C443-C453-H453	119.2
O13-C273	1.464(12)	C24C1-C26C1-H26J1	110.1	C453-C463-C413	120.0(4)
C273-C283	1.536(13)	O1C1-C26C1-H26K1	110.1	C453-C463-H463	120.0
C273-H27A3	0.9900	C24C1-C26C1-H26K1	110.1	C413-C463-H463	120.0
C273-H27B3	0.9900	H26J1-C26C1-H26K1	108.4	C523-C473-C483	116.1(4)
C283-C293	1.383(12)	C27C1-O1C1-C26C1	109.7(18)	C523-C473-C443	123.0(4)
C283-C333	1.404(11)	O1C1-C27C1-C28C1	110(2)	C483-C473-C443	120.8(4)
C293-C303	1.388(12)	O1C1-C27C1-H27J1	109.6	C493-C483-N13	110.8(4)
C293-H293	0.9500	C28C1-C27C1-H27J1	109.6	C493-C483-C473	121.6(4)
C303-C313	1.381(12)	O1C1-C27C1-H27K1	109.6	N13-C483-C473	127.7(4)
C303-H303	0.9500	C28C1-C27C1-H27K1	109.6	C483-C493-C503	120.5(4)

C313-C323	1.393(12)	H27J1-C27C1-H27K1	108.1	C483-C493-C23	106.4(4)
C313-H313	0.9500	C29C1-C28C1-C33C1	119.9(17)	C503-C493-C23	133.0(4)
C323-C333	1.385(12)	C29C1-C28C1-C27C1	120(2)	C493-C503-C513	119.4(4)
C323-C343	1.504(14)	C33C1-C28C1-C27C1	120(2)	C493-C503-H503	120.3
C333-H333	0.9500	C30C1-C29C1-C28C1	120.2(18)	C513-C503-H503	120.3
C343-C353	1.392(10)	C30C1-C29C1-H29J1	119.9	C503-C513-C523	118.4(4)
C343-C393	1.420(9)	C28C1-C29C1-H29J1	119.9	C503-C513-C603	122.0(4)
C353-C363	1.367(10)	C31C1-C30C1-C29C1	119.9(19)	C523-C513-C603	119.5(4)
C353-H353	0.9500	C31C1-C30C1-H30J1	120.1	C473-C523-C513	123.9(4)
C363-F23	1.369(9)	C29C1-C30C1-H30J1	120.1	C473-C523-H523	118.1
C363-C373	1.376(10)	C30C1-C31C1-C32C1	120.0(19)	C513-C523-H523	118.1
C373-C383	1.419(9)	C30C1-C31C1-H31J1	120.0	N13-C533-C543	112.1(4)
C373-H373	0.9500	C32C1-C31C1-H31J1	120.0	N13-C533-H53A3	109.2
C383-C393	1.413(10)	C33C1-C32C1-C31C1	120.1(19)	C543-C533-H53A3	109.2
C383-C403	1.439(10)	C33C1-C32C1-C34C1	119.9(14)	N13-C533-H53B3	109.2
C393-O33	1.319(9)	C31C1-C32C1-C34C1	119.8(14)	C543-C533-H53B3	109.2
C403-H403	0.9500	C32C1-C33C1-C28C1	119.9(18)	H53A3-C533-H53B3	107.9
C14A3-C15A3	1.414(13)	C32C1-C33C1-H33J1	120.1	C553-C543-C533	112.2(4)
C14A3-C19A3	1.422(12)	C28C1-C33C1-H33J1	120.1	C553-C543-H54A3	109.2
C15A3-C16A3	1.385(12)	C35C1-C34C1-C39C1	120.3(18)	C533-C543-H54A3	109.2
C15A3-H15D3	0.9500	C35C1-C34C1-C32C1	119.8(14)	C553-C543-H54B3	109.2
C16A3-F1A3	1.367(13)	C39C1-C34C1-C32C1	119.9(13)	C533-C543-H54B3	109.2
C16A3-C17A3	1.379(13)	C36C1-C35C1-C34C1	119.8(18)	H54A3-C543-H54B3	107.9
C17A3-C18A3	1.386(12)	C36C1-C35C1-H35J1	120.1	C563-C553-C543	115.6(4)
C17A3-H17D3	0.9500	C34C1-C35C1-H35J1	120.1	C56A3-C553-C543	110.5(9)
C18A3-C19A3	1.403(12)	F2C1-C36C1-C37C1	120(2)	C563-C553-H55A3	108.4
C18A3-C20A3	1.506(13)	F2C1-C36C1-C35C1	120(2)	C543-C553-H55A3	108.4
C19A3-O2A3	1.318(13)	C37C1-C36C1-C35C1	120.4(17)	C563-C553-H55B3	108.4
C20A3-C25A3	1.383(13)	C36C1-C37C1-C38C1	119.9(18)	C543-C553-H55B3	108.4
C20A3-C21A3	1.392(13)	C36C1-C37C1-H37J1	120.1	H55A3-C553-H55B3	107.4
C21A3-C22A3	1.389(13)	C38C1-C37C1-H37J1	120.1	C56A3-C553-H55D3	109.6
C21A3-H21D3	0.9500	C37C1-C38C1-C39C1	120.1(16)	C543-C553-H55D3	109.6
C22A3-C23A3	1.392(13)	C37C1-C38C1-C40C1	115(2)	C56A3-C553-H55E3	109.6
C22A3-H22D3	0.9500	C39C1-C38C1-C40C1	124(2)	C543-C553-H55E3	109.6
C23A3-C24A3	1.386(13)	O3C1-C39C1-C34C1	118(2)	H55D3-C553-H55E3	108.1
C23A3-H23A3	0.9500	O3C1-C39C1-C38C1	122(2)	C553-C563-C573	114.8(4)
C24A3-C25A3	1.392(13)	C34C1-C39C1-C38C1	119.6(16)	C553-C563-H56A3	108.6
C24A3-C26A3	1.523(14)	N3C1-C40C1-C38C1	125(3)	C573-C563-H56A3	108.6

C25A3-H25D3	0.9500	N3C1-C40C1-H40J1	117.3	C553-C563-H56B3	108.6
C26A3-O1A3	1.405(14)	C38C1-C40C1-H40J1	117.3	C573-C563-H56B3	108.6
C26A3-H26D3	0.9900	C39C1-O3C1-Fe11	131(3)	H56A3-C563-H56B3	107.5
C26A3-H26E3	0.9900	C40C1-N3C1-C411	118(2)	C583-C573-C563	113.1(4)
O1A3-C27A3	1.428(14)	C40C1-N3C1-Fe11	120(5)	C583-C573-H57A3	109.0
C27A3-C28A3	1.528(14)	C411-N3C1-Fe11	117.9(18)	C563-C573-H57A3	109.0
C27A3-H27D3	0.9900	C35D1-C34D1-C39D1	119.9(14)	C583-C573-H57B3	109.0
C27A3-H27E3	0.9900	C34D1-C35D1-C36D1	120.1(14)	C563-C573-H57B3	109.0
C28A3-C29A3	1.376(13)	C34D1-C35D1-H35M1	119.9	H57A3-C573-H57B3	107.8
C28A3-C33A3	1.389(13)	C36D1-C35D1-H35M1	119.9	C57A3-C56A3-C553	113.0(18)
C29A3-C30A3	1.377(13)	F2D1-C36D1-C37D1	119.1(14)	C57A3-C56A3-H56D3	109.0
C29A3-H29D3	0.9500	F2D1-C36D1-C35D1	119.4(14)	C553-C56A3-H56D3	109.0
C30A3-C31A3	1.383(13)	C37D1-C36D1-C35D1	121.4(13)	C57A3-C56A3-H56E3	109.0
C30A3-H30D3	0.9500	C36D1-C37D1-C38D1	118.6(13)	C553-C56A3-H56E3	109.0
C31A3-C32A3	1.381(13)	C36D1-C37D1-H37M1	120.7	H56D3-C56A3-H56E3	107.8
C31A3-H31D3	0.9500	C38D1-C37D1-H37M1	120.7	C583-C57A3-C56A3	114.0(18)
C32A3-C33A3	1.387(13)	C37D1-C38D1-C39D1	120.5(13)	C583-C57A3-H57D3	108.7
C32A3-C34A3	1.499(15)	C37D1-C38D1-C40D1	114.6(15)	C56A3-C57A3-H57D3	108.7
C33A3-H33D3	0.9500	C39D1-C38D1-C40D1	124.6(15)	C583-C57A3-H57E3	108.7
C34A3-C35A3	1.393(12)	O3D1-C39D1-C38D1	122.6(16)	C56A3-C57A3-H57E3	108.7
C34A3-C39A3	1.423(11)	O3D1-C39D1-C34D1	118.3(16)	H57D3-C57A3-H57E3	107.6
C35A3-C36A3	1.384(12)	C38D1-C39D1-C34D1	119.0(13)	C57A3-C583-C593	125.7(13)
C35A3-H35D3	0.9500	N3D1-C40D1-C38D1	125(2)	C573-C583-C593	116.2(4)
C36A3-F2A3	1.361(12)	N3D1-C40D1-H40M1	117.4	C573-C583-H58A3	108.2
C36A3-C37A3	1.365(11)	C38D1-C40D1-H40M1	117.4	C593-C583-H58A3	108.2
C37A3-C38A3	1.405(12)	C39D1-O3D1-Fe11	130.8(18)	C573-C583-H58B3	108.2
C37A3-H37D3	0.9500	C40D1-N3D1-C411	116.6(16)	C593-C583-H58B3	108.2
C38A3-C39A3	1.405(11)	C40D1-N3D1-Fe11	123.7(15)	H58A3-C583-H58B3	107.4
C38A3-C40A3	1.439(12)	C411-N3D1-Fe11	119.4(15)	C57A3-C583-H58D3	105.9
C39A3-O3A3	1.334(13)	C01A1-N01A1-Fe21	142.3(6)	C593-C583-H58D3	105.9
C40A3-H40D3	0.9500	N01A1-C01A1-C01B1	165.2(8)	C57A3-C583-H58E3	105.9
C14B3-C19B3	1.387(13)	C01A1-C01B1-H1ZA1	109.5	C593-C583-H58E3	105.9
C14B3-C15B3	1.393(13)	C01A1-C01B1-H1ZB1	109.5	H58D3-C583-H58E3	106.2
C15B3-C16B3	1.395(13)	H1ZA1-C01B1-H1ZB1	109.5	O43-C593-O53	124.3(4)
C15B3-H15G3	0.9500	C01A1-C01B1-H1ZC1	109.5	O43-C593-C583	118.2(4)
C16B3-F1B3	1.366(14)	H1ZA1-C01B1-H1ZC1	109.5	O53-C593-C583	117.5(4)
C16B3-C17B3	1.388(13)	H1ZB1-C01B1-H1ZC1	109.5	C633-C603-C613	108.0(5)
C17B3-C18B3	1.401(13)	Cl021-C04A1-Cl011	112.5(3)	C633-C603-C623	109.6(5)

C17B3-H17G3	0.9500	Cl021-C04A1-H4ZA1	109.1	C613-C603-C623	109.2(5)
C18B3-C19B3	1.401(13)	Cl011-C04A1-H4ZA1	109.1	C633-C603-C513	110.0(4)
C18B3-C20B3	1.515(14)	Cl021-C04A1-H4ZB1	109.1	C613-C603-C513	111.7(4)
C19B3-O2B3	1.321(14)	Cl011-C04A1-H4ZB1	109.1	C623-C603-C513	108.3(5)
C20B3-C21B3	1.385(13)	H4ZA1-C04A1-H4ZB1	107.8	C603-C613-H61A3	109.5
C20B3-C25B3	1.386(13)	C04A1-Cl021-Fe11	109.0(9)	C603-C613-H61B3	109.5
C21B3-C22B3	1.380(14)	C192-O22-Fe32	132.3(3)	H61A3-C613-H61B3	109.5
C21B3-H21G3	0.9500	C132-N22-C102	118.5(4)	C603-C613-H61C3	109.5
C22B3-C23B3	1.387(14)	C132-N22-Fe32	125.0(3)	H61A3-C613-H61C3	109.5
C22B3-H22G3	0.9500	C102-N22-Fe32	116.1(3)	H61B3-C613-H61C3	109.5
C23B3-C24B3	1.387(14)	O22-Fe32-O72	119.0(4)	C603-C623-H62A3	109.5
C23B3-H23G3	0.9500	O22-Fe32-O52	120.87(14)	C603-C623-H62B3	109.5
C24B3-C25B3	1.387(13)	O72-Fe32-O52	109.4(4)	H62A3-C623-H62B3	109.5
C24B3-C26B3	1.527(15)	O22-Fe32-O7A2	124.4(14)	C603-C623-H62C3	109.5
C25B3-H25G3	0.9500	O52-Fe32-O7A2	107.5(15)	H62A3-C623-H62C3	109.5
C26B3-O1B3	1.431(15)	O22-Fe32-N22	89.53(14)	H62B3-C623-H62C3	109.5
C26B3-H26G3	0.9900	O72-Fe32-N22	108.6(4)	C603-C633-H63A3	109.5
C26B3-H26H3	0.9900	O52-Fe32-N22	105.78(14)	C603-C633-H63B3	109.5
O1B3-C27B3	1.414(15)	O7A2-Fe32-N22	102.9(14)	H63A3-C633-H63B3	109.5
C27B3-C28B3	1.526(15)	C402-N32-C412	115.6(4)	C603-C633-H63C3	109.5
C27B3-H27G3	0.9900	C402-N32-Fe42	124.5(3)	H63A3-C633-H63C3	109.5
C27B3-H27H3	0.9900	C412-N32-Fe42	119.8(3)	H63B3-C633-H63C3	109.5
C28B3-C29B3	1.384(14)	O3A2-Fe42-O42	133.3(18)	C663-C643-C653	109.6(9)
C28B3-C33B3	1.394(14)	O32-Fe42-O42	128.2(8)	C663-C643-C43	112.5(13)
C29B3-C30B3	1.386(14)	O32-Fe42-O62	119.2(9)	C65A3-C643-C43	112.1(12)
C29B3-H29G3	0.9500	O42-Fe42-O62	111.7(3)	C653-C643-C43	112.0(10)
C30B3-C31B3	1.381(14)	O42-Fe42-O3B2	140.2(11)	C67B3-C643-C43	113(2)
C30B3-H30G3	0.9500	O3A2-Fe42-O6A2	122(2)	C663-C643-C673	109.6(9)
C31B3-C32B3	1.385(14)	O42-Fe42-O6A2	103.7(12)	C653-C643-C673	108.6(8)
C31B3-H31G3	0.9500	O3A2-Fe42-N32	89.8(11)	C43-C643-C673	104.4(10)
C32B3-C33B3	1.383(14)	O32-Fe42-N32	86.8(6)	C67B3-C643-C65B3	107.9(14)
C33B3-H33G3	0.9500	O42-Fe42-N32	96.89(14)	C43-C643-C65B3	110(2)
C14C3-C15C3	1.401(14)	O62-Fe42-N32	96.5(3)	C65A3-C643-C66A3	109.0(10)
C14C3-C19C3	1.412(13)	O3B2-Fe42-N32	82.1(9)	C43-C643-C66A3	108.9(14)
C15C3-C16C3	1.388(14)	O6A2-Fe42-N32	96.1(14)	C65A3-C643-C67A3	108.6(9)
C15C3-H15J3	0.9500	O3A2-Fe42-N02A3	83.0(11)	C43-C643-C67A3	111.8(13)
C16C3-F1C3	1.363(15)	O32-Fe42-N02A3	85.6(6)	C66A3-C643-C67A3	106.3(9)
C16C3-C17C3	1.391(14)	O42-Fe42-N02A3	85.59(15)	C67B3-C643-C66B3	107.2(14)

C17C3-C18C3	1.397(14)	O62-Fe42-N02A3	89.7(3)	C43-C643-C66B3	112(2)
C17C3-H17J3	0.9500	O3B2-Fe42-N02A3	91.0(8)	C65B3-C643-C66B3	107.0(14)
C18C3-C19C3	1.403(13)	O6A2-Fe42-N02A3	90.7(14)	C643-C653-H65A3	109.5
C18C3-C20C3	1.510(15)	N32-Fe42-N02A3	171.90(16)	C643-C653-H65B3	109.5
C19C3-O2C3	1.321(15)	C592-O42-Fe42	139.2(3)	H65A3-C653-H65B3	109.5
C20C3-C25C3	1.385(14)	C592-O52-Fe32	146.4(3)	C643-C653-H65C3	109.5
C20C3-C21C3	1.390(14)	C62-C12-N12	128.7(4)	H65A3-C653-H65C3	109.5
C21C3-C22C3	1.383(14)	C62-C12-C22	121.2(4)	H65B3-C653-H65C3	109.5
C21C3-H21J3	0.9500	N12-C12-C22	110.1(3)	C643-C663-H66A3	109.5
C22C3-C23C3	1.382(14)	C32-C22-C12	119.7(4)	C643-C663-H66B3	109.5
C22C3-H22J3	0.9500	C32-C22-C492	133.7(4)	H66A3-C663-H66B3	109.5
C23C3-C24C3	1.388(14)	C12-C22-C492	106.6(3)	C643-C663-H66C3	109.5
C23C3-H23J3	0.9500	C22-C32-C42	120.9(4)	H66A3-C663-H66C3	109.5
C24C3-C25C3	1.386(14)	C22-C32-H32	119.5	H66B3-C663-H66C3	109.5
C24C3-C26C3	1.528(15)	C42-C32-H32	119.5	C643-C673-H67A3	109.5
C25C3-H25J3	0.9500	C32-C42-C52	117.8(4)	C643-C673-H67B3	109.5
C26C3-O1C3	1.431(16)	C32-C42-C642	120.6(4)	H67A3-C673-H67B3	109.5
C26C3-H26J3	0.9900	C52-C42-C642	121.6(4)	C643-C673-H67C3	109.5
C26C3-H26K3	0.9900	C62-C52-C42	123.3(4)	H67A3-C673-H67C3	109.5
O1C3-C27C3	1.418(15)	C62-C52-H52	118.4	H67B3-C673-H67C3	109.5
C27C3-C28C3	1.521(15)	C42-C52-H52	118.4	C643-C65A3-H65D3	109.5
C27C3-H27J3	0.9900	C52-C62-C12	117.0(4)	C643-C65A3-H65E3	109.5
C27C3-H27K3	0.9900	C52-C62-C72	121.1(4)	H65D3-C65A3-H65E3	109.5
C28C3-C29C3	1.387(14)	C12-C62-C72	121.9(4)	C643-C65A3-H65F3	109.5
C28C3-C33C3	1.387(14)	C522-C472-C482	116.2(4)	H65D3-C65A3-H65F3	109.5
C29C3-C30C3	1.386(14)	C522-C472-C442	122.1(4)	H65E3-C65A3-H65F3	109.5
C29C3-H29J3	0.9500	C482-C472-C442	121.7(4)	C643-C66A3-H66D3	109.5
C30C3-C31C3	1.387(14)	C492-C482-C472	121.5(4)	C643-C66A3-H66E3	109.5
C30C3-H30J3	0.9500	C492-C482-N12	110.1(3)	H66D3-C66A3-H66E3	109.5
C31C3-C32C3	1.387(14)	C472-C482-N12	128.4(4)	C643-C66A3-H66F3	109.5
C31C3-H31J3	0.9500	C482-C492-C502	120.0(4)	H66D3-C66A3-H66F3	109.5
C32C3-C33C3	1.387(14)	C482-C492-C22	107.0(3)	H66E3-C66A3-H66F3	109.5
C33C3-H33J3	0.9500	C502-C492-C22	133.0(4)	C643-C67A3-H67D3	109.5
C20D3-C21D3	1.381(14)	C512-C502-C492	120.2(4)	C643-C67A3-H67E3	109.5
C20D3-C25D3	1.383(14)	C512-C502-H502	119.9	H67D3-C67A3-H67E3	109.5
C21D3-C22D3	1.385(14)	C492-C502-H502	119.9	C643-C67A3-H67F3	109.5
C21D3-H21M3	0.9500	C502-C512-C522	118.0(4)	H67D3-C67A3-H67F3	109.5
C22D3-C23D3	1.387(14)	C502-C512-C602	123.3(4)	H67E3-C67A3-H67F3	109.5

C22D3-H22M3	0.9500	C522-C512-C602	118.7(4)	C643-C65B3-H65G3	109.5
C23D3-C24D3	1.384(14)	C472-C522-C512	123.8(4)	C643-C65B3-H65H3	109.5
C23D3-H23M3	0.9500	C472-C522-H522	118.1	H65G3-C65B3-H65H3	109.5
C24D3-C25D3	1.384(14)	C512-C522-H522	118.1	C643-C65B3-H65I3	109.5
C24D3-C26D3	1.521(15)	C12-N12-C482	106.3(3)	H65G3-C65B3-H65I3	109.5
C25D3-H25M3	0.9500	C12-N12-C532	118.6(3)	H65H3-C65B3-H65I3	109.5
C26D3-O1D3	1.430(16)	C482-N12-C532	118.7(3)	C643-C66B3-H66G3	109.5
C26D3-H26M3	0.9900	C82-C72-C122	118.7(4)	C643-C66B3-H66H3	109.5
C26D3-H26N3	0.9900	C82-C72-C62	121.3(4)	H66G3-C66B3-H66H3	109.5
O1D3-C27D3	1.441(17)	C122-C72-C62	120.0(4)	C643-C66B3-H66I3	109.5
C27D3-C28D3	1.530(15)	C72-C82-C92	120.6(4)	H66G3-C66B3-H66I3	109.5
C27D3-H27M3	0.9900	C72-C82-H82	119.7	H66H3-C66B3-H66I3	109.5
C27D3-H27N3	0.9900	C92-C82-H82	119.7	C643-C67B3-H67G3	109.5
C28D3-C33D3	1.384(14)	C102-C92-C82	119.5(4)	C643-C67B3-H67H3	109.5
C28D3-C29D3	1.386(14)	C102-C92-H92	120.3	H67G3-C67B3-H67H3	109.5
C29D3-C30D3	1.386(14)	C82-C92-H92	120.3	C643-C67B3-H67I3	109.5
C29D3-H29M3	0.9500	C92-C102-C112	120.5(4)	H67G3-C67B3-H67I3	109.5
C30D3-C31D3	1.388(14)	C92-C102-N22	121.7(4)	H67H3-C67B3-H67I3	109.5
C30D3-H30M3	0.9500	C112-C102-N22	117.8(4)	O63-C683-O73	126.1(4)
C31D3-C32D3	1.386(14)	C122-C112-C102	119.4(4)	O63-C683-C693	116.4(4)
C31D3-H31M3	0.9500	C122-C112-H112	120.3	O73-C683-C693	117.5(4)
C32D3-C33D3	1.388(14)	C102-C112-H112	120.3	C703-C693-C823	120.8(4)
C33D3-H33M3	0.9500	C112-C122-C72	121.1(4)	C703-C693-C683	119.5(4)
C413-C423	1.386(6)	C112-C122-H122	119.4	C823-C693-C683	119.7(4)
C413-C463	1.398(7)	C72-C122-H122	119.4	C693-C703-C713	122.1(4)
C423-C433	1.383(6)	N22-C132-C142	126.3(4)	C693-C703-C753	119.0(4)
C423-H423	0.9500	N22-C132-H132	116.8	C713-C703-C753	118.9(4)
C433-C443	1.397(7)	C142-C132-H132	116.8	C723-C713-C703	120.6(5)
C433-H433	0.9500	C152-C142-C192	121.1(4)	C723-C713-H713	119.7
C443-C453	1.389(6)	C152-C142-C132	115.6(4)	C703-C713-H713	119.7
C443-C473	1.485(6)	C192-C142-C132	123.2(4)	C713-C723-C733	120.4(5)
C453-C463	1.377(6)	C162-C152-C142	118.4(4)	C713-C723-H723	119.8
C453-H453	0.9500	C162-C152-H152	120.8	C733-C723-H723	119.8
C463-H463	0.9500	C142-C152-H152	120.8	C743-C733-C723	120.7(6)
C473-C523	1.386(6)	F12-C162-C152	119.6(4)	C743-C733-H733	119.6
C473-C483	1.412(6)	F12-C162-C172	118.3(4)	C723-C733-H733	119.6
C483-C493	1.393(6)	C152-C162-C172	122.1(4)	C733-C743-C753	120.9(6)
C493-C503	1.397(6)	C182-C172-C162	120.9(4)	C733-C743-H743	119.6

C503-C513	1.397(6)	C182-C172-H172	119.5	C753-C743-H743	119.6
C503-H503	0.9500	C162-C172-H172	119.5	C763-C753-C743	121.3(5)
C513-C523	1.402(7)	C172-C182-C192	119.6(5)	C763-C753-C703	120.3(4)
C513-C603	1.539(6)	C172-C182-C202	119.0(7)	C743-C753-C703	118.4(5)
C523-H523	0.9500	C192-C182-C202	121.1(7)	C753-C763-C773	121.2(5)
C533-C543	1.535(6)	C172-C182-C20A2	123.1(11)	C753-C763-H763	119.4
C533-H53A3	0.9900	C192-C182-C20A2	117.0(11)	C773-C763-H763	119.4
C533-H53B3	0.9900	C172-C182-C20B2	118.4(14)	C763-C773-C783	121.8(4)
C543-C553	1.521(6)	C192-C182-C20B2	120.2(14)	C763-C773-C823	120.0(4)
C543-H54A3	0.9900	O22-C192-C142	123.3(4)	C783-C773-C823	118.2(4)
C543-H54B3	0.9900	O22-C192-C182	118.9(4)	C793-C783-C773	121.4(5)
C553-C563	1.502(7)	C142-C192-C182	117.7(4)	C793-C783-H783	119.3
C553-C56A3	1.52(2)	C252-C202-C212	119.5(8)	C773-C783-H783	119.3
C553-H55A3	0.9900	C252-C202-C182	120.1(10)	C783-C793-C803	120.1(4)
C553-H55B3	0.9900	C212-C202-C182	120.3(10)	C783-C793-H793	119.9
C553-H55D3	0.9900	C222-C212-C202	120.9(8)	C803-C793-H793	119.9
C553-H55E3	0.9900	C222-C212-H212	119.5	C813-C803-C793	120.9(4)
C563-C573	1.518(7)	C202-C212-H212	119.5	C813-C803-H803	119.6
C563-H56A3	0.9900	C212-C222-C232	120.0(8)	C793-C803-H803	119.6
C563-H56B3	0.9900	C212-C222-H222	120.0	C803-C813-C823	120.7(4)
C573-C583	1.505(7)	C232-C222-H222	120.0	C803-C813-H813	119.7
C573-H57A3	0.9900	C222-C232-C242	119.5(8)	C823-C813-H813	119.7
C573-H57B3	0.9900	C222-C232-H232	120.3	C693-C823-C813	122.6(4)
C56A3-C57A3	1.51(2)	C242-C232-H232	120.3	C693-C823-C773	118.7(4)
C56A3-H56D3	0.9900	C252-C242-C232	120.1(8)	C813-C823-C773	118.7(4)
C56A3-H56E3	0.9900	C252-C242-C262	121.4(8)	Fe13-O83-Fe23	106.44(13)
C57A3-C583	1.42(2)	C232-C242-C262	118.3(8)	Fe13-O83-HO13	98(4)
C57A3-H57D3	0.9900	C202-C252-C242	120.0(8)	Fe23-O83-HO13	124(4)
C57A3-H57E3	0.9900	C202-C252-H252	120.0	Fe13-O83-HO23	119(4)
C583-C593	1.508(7)	C242-C252-H252	120.0	Fe23-O83-HO23	113(4)
C583-H58A3	0.9900	O12-C262-C242	107.1(9)	HO13-O83-HO23	96(5)
C583-H58B3	0.9900	O12-C262-H26A2	110.3	N03A3-C03A3-C03B3	178.1(10)
C583-H58D3	0.9900	C242-C262-H26A2	110.3	C03A3-C03B3-H3ZA3	109.5
C583-H58E3	0.9900	O12-C262-H26B2	110.3	C03A3-C03B3-H3ZB3	109.5
C603-C633	1.516(8)	C242-C262-H26B2	110.3	H3ZA3-C03B3-H3ZB3	109.5
C603-C613	1.520(8)	H26A2-C262-H26B2	108.6	C03A3-C03B3-H3ZC3	109.5
C603-C623	1.533(9)	C262-O12-C272	109.8(9)	H3ZA3-C03B3-H3ZC3	109.5
C613-H61A3	0.9800	O12-C272-C282	108.9(10)	H3ZB3-C03B3-H3ZC3	109.5

C613-H61B3	0.9800	O12-C272-H27A2	109.9	C02A3-N02A3-Fe42	155.9(5)
C613-H61C3	0.9800	C282-C272-H27A2	109.9	N02A3-C02A3-C02B3	174.8(6)
C623-H62A3	0.9800	O12-C272-H27B2	109.9	C02A3-C02B3-H2ZA3	109.5
C623-H62B3	0.9800	C282-C272-H27B2	109.9	C02A3-C02B3-H2ZB3	109.5
C623-H62C3	0.9800	H27A2-C272-H27B2	108.3	H2ZA3-C02B3-H2ZB3	109.5
C633-H63A3	0.9800	C332-C282-C292	119.0(9)	C02A3-C02B3-H2ZC3	109.5
C633-H63B3	0.9800	C332-C282-C272	121.4(9)	H2ZA3-C02B3-H2ZC3	109.5
C633-H63C3	0.9800	C292-C282-C272	119.4(9)	H2ZB3-C02B3-H2ZC3	109.5

Table S6. Anisotropic displacement parameters ($Å^2 \times 10^3$) for **1**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + \ldots + 2\,h\,k\,a^*b^*U^{12}]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Fe11	44(1)	40(1)	36(1)	2(1)	14(1)	-2(1)
Fe21	36(1)	83(1)	33(1)	-16(1)	6(1)	1(1)
O41	45(2)	68(2)	40(2)	-6(2)	7(2)	9(2)
O51	61(2)	70(2)	35(2)	-2(2)	12(2)	15(2)
O61	42(2)	60(2)	30(2)	1(1)	11(1)	-4(2)
O71	54(2)	61(2)	65(2)	13(2)	34(2)	14(2)
C411	31(2)	32(2)	33(2)	-2(1)	12(2)	-1(2)
C421	30(2)	32(2)	27(2)	-2(2)	8(2)	1(2)
C431	34(2)	28(2)	32(2)	0(2)	12(2)	3(2)
C441	30(2)	32(2)	32(2)	-3(1)	11(2)	0(2)
C451	40(2)	35(2)	31(2)	-4(2)	15(2)	0(2)
C461	44(3)	34(2)	34(2)	-2(2)	17(2)	-3(2)
C681	41(2)	42(2)	34(2)	-2(2)	14(2)	-2(2)
C691	37(2)	39(2)	31(2)	10(2)	11(2)	9(2)
C701	38(2)	41(2)	36(2)	6(2)	13(2)	10(2)
C711	44(3)	41(2)	43(2)	2(2)	15(2)	4(2)
C721	48(3)	51(3)	59(3)	-8(2)	21(2)	2(2)
C731	62(3)	67(3)	48(3)	-17(3)	21(2)	5(2)
C741	53(3)	70(3)	42(3)	-2(2)	24(2)	11(2)
C751	39(2)	53(3)	36(2)	6(2)	13(2)	13(2)
C761	43(2)	57(3)	45(3)	8(2)	22(2)	10(2)
C771	38(2)	50(3)	41(2)	12(2)	14(2)	9(2)
C781	44(3)	56(3)	57(3)	15(2)	22(2)	8(2)
C791	42(3)	49(3)	65(3)	10(2)	15(2)	-2(2)
C801	47(3)	48(3)	46(3)	3(2)	9(2)	1(2)
C811	44(2)	47(3)	36(2)	6(2)	10(2)	5(2)

C821	35(2)	39(2)	35(2)	10(2)	9(2)	9(2)
C531	38(2)	39(2)	44(3)	-10(2)	17(2)	-2(2)
C541	45(3)	50(3)	47(4)	-12(3)	20(3)	0(3)
C551	47(3)	66(4)	48(4)	-12(3)	24(3)	0(3)
C561	61(4)	63(4)	44(4)	-9(3)	29(3)	-6(3)
C571	68(3)	90(4)	53(3)	-19(3)	34(3)	-24(3)
C581	49(3)	70(4)	54(3)	-2(3)	23(2)	-1(3)
C591	34(2)	55(3)	40(2)	-2(2)	11(2)	-1(2)
C54B1	47(7)	58(7)	47(6)	-10(6)	23(6)	-1(6)
C55B1	53(7)	64(6)	42(7)	-12(6)	27(5)	-3(5)
C56B1	63(6)	64(7)	57(9)	-21(8)	35(6)	-13(6)
C11	40(4)	37(3)	36(3)	-3(2)	17(2)	5(2)
C21	34(2)	38(1)	38(2)	-1(1)	19(2)	2(2)
C31	34(2)	38(1)	38(2)	-1(1)	19(2)	2(2)
C41	42(4)	40(3)	52(3)	7(2)	14(3)	5(3)
C51	39(4)	46(3)	48(4)	6(3)	13(3)	6(3)
C61	40(4)	44(3)	40(3)	0(2)	16(3)	6(3)
C471	34(1)	35(1)	29(1)	-4(1)	18(1)	-2(1)
C481	34(3)	36(2)	28(3)	-5(2)	16(3)	0(2)
C491	35(4)	34(3)	32(3)	-4(2)	19(2)	2(2)
C501	34(1)	35(1)	29(1)	-4(1)	18(1)	-2(1)
C511	34(1)	35(1)	29(1)	-4(1)	18(1)	-2(1)
C521	34(1)	35(1)	29(1)	-4(1)	18(1)	-2(1)
N11	36(3)	35(3)	32(4)	-5(3)	12(3)	2(3)
C641	49(4)	45(3)	70(5)	19(3)	13(3)	3(3)
C651	54(5)	41(6)	119(9)	16(6)	9(5)	8(5)
C661	62(6)	39(5)	88(6)	13(4)	11(5)	-3(5)
C671	101(8)	65(7)	88(7)	23(5)	43(6)	-5(6)
C601	40(3)	32(4)	28(3)	-2(3)	16(2)	-7(2)
C611	41(2)	37(2)	28(2)	-3(2)	12(2)	-6(2)
C621	41(2)	37(2)	28(2)	-3(2)	12(2)	-6(2)
C631	41(2)	37(2)	28(2)	-3(2)	12(2)	-6(2)
C71	36(3)	42(4)	38(3)	6(3)	12(3)	11(3)
C81	39(4)	51(5)	44(5)	2(4)	16(3)	11(3)
C91	35(4)	61(5)	48(5)	-1(4)	16(3)	6(3)
C101	32(4)	65(4)	37(4)	-6(3)	8(3)	1(3)
C111	33(4)	56(5)	35(4)	-6(4)	10(3)	5(3)
C121	33(4)	51(5)	38(4)	-3(4)	9(3)	6(3)
C131	37(4)	72(5)	37(4)	-4(4)	7(3)	-3(3)

C141	37(3)	69(4)	32(4)	3(3)	6(3)	-3(3)
C151	48(4)	69(5)	42(4)	8(4)	-4(3)	-6(4)
C161	49(4)	71(4)	51(5)	16(4)	-12(4)	-9(4)
C171	48(4)	72(4)	44(4)	9(4)	-10(3)	-10(4)
C181	45(4)	68(4)	39(4)	9(3)	1(3)	-6(3)
C191	40(3)	70(4)	29(3)	5(3)	3(3)	-3(3)
O21	40(3)	68(4)	27(3)	1(3)	5(2)	-2(3)
F11	64(4)	82(6)	79(6)	28(5)	-31(4)	-11(4)
N21	34(4)	71(3)	34(4)	-6(3)	9(3)	-2(3)
C201	40(4)	69(4)	29(4)	5(3)	-4(3)	-5(3)
C211	43(4)	70(4)	45(5)	3(4)	2(4)	-6(3)
C221	45(4)	73(5)	53(5)	3(4)	2(4)	-10(3)
C231	50(4)	67(5)	50(5)	0(4)	7(4)	-9(3)
C241	48(4)	69(4)	30(4)	0(4)	4(3)	-7(3)
C251	41(4)	67(4)	25(4)	4(4)	-1(4)	-7(3)
C261	50(5)	69(5)	31(4)	-1(4)	8(4)	-6(4)
O11	55(4)	63(5)	32(3)	-3(3)	6(3)	-6(3)
C271	56(4)	65(6)	32(3)	-3(4)	9(3)	-5(4)
C281	51(4)	54(5)	31(3)	-3(3)	6(3)	-10(3)
C291	47(4)	59(5)	35(4)	-6(3)	1(3)	-15(4)
C301	47(5)	54(5)	42(5)	-3(4)	8(4)	-15(4)
C311	48(5)	51(5)	38(4)	3(4)	5(3)	-11(4)
C321	48(4)	42(5)	37(3)	-6(3)	5(3)	-13(4)
C331	42(4)	46(5)	35(3)	-4(3)	7(3)	-5(4)
C341	42(5)	38(3)	32(4)	-2(3)	10(4)	-8(3)
C351	41(6)	36(4)	36(5)	3(4)	16(4)	-10(4)
C361	39(6)	38(3)	32(5)	8(3)	16(4)	-4(4)
C371	39(6)	39(3)	30(5)	5(4)	11(5)	-7(4)
C381	40(5)	35(3)	26(4)	1(3)	10(4)	-6(3)
C391	40(5)	37(3)	27(4)	-1(3)	8(4)	-6(3)
C401	43(6)	35(3)	24(5)	-3(3)	12(5)	-4(3)
O31	39(5)	41(3)	27(6)	2(4)	4(4)	-6(3)
F21	48(8)	39(5)	54(9)	13(6)	7(6)	-5(6)
N31	39(4)	34(3)	28(4)	0(3)	14(4)	-4(3)
C1A1	33(5)	39(3)	34(5)	-2(3)	18(4)	3(3)
C2A1	34(2)	38(1)	38(2)	-1(1)	19(2)	2(2)
C3A1	41(6)	40(3)	44(6)	-1(4)	12(5)	2(4)
C4A1	45(5)	41(4)	54(6)	3(4)	10(5)	4(4)
C5A1	40(6)	45(4)	46(6)	0(4)	11(5)	6(4)

C6A1	40(5)	44(4)	38(5)	-1(4)	14(4)	5(4)
C47A1	34(1)	35(1)	29(1)	-4(1)	18(1)	-2(1)
C48A1	34(4)	35(3)	30(5)	-5(3)	17(4)	-1(3)
C49A1	32(4)	35(3)	31(5)	-4(3)	20(4)	0(3)
C50A1	36(5)	33(4)	35(5)	-6(4)	17(4)	-1(4)
C51A1	34(1)	35(1)	29(1)	-4(1)	18(1)	-2(1)
C52A1	34(1)	35(1)	29(1)	-4(1)	18(1)	-2(1)
N1A1	36(4)	38(4)	35(5)	-5(4)	11(3)	2(3)
C64A1	64(7)	42(5)	78(7)	3(5)	9(6)	8(5)
C65A1	73(9)	86(17)	85(16)	12(13)	27(9)	36(9)
C66A1	73(13)	38(10)	91(11)	7(9)	15(10)	4(12)
C67A1	114(16)	48(12)	82(9)	-5(8)	9(10)	18(14)
C60A1	41(4)	36(5)	30(4)	-4(4)	15(3)	-4(3)
C61A1	41(2)	37(2)	28(2)	-3(2)	12(2)	-6(2)
C62A1	41(2)	37(2)	28(2)	-3(2)	12(2)	-6(2)
C63A1	41(2)	37(2)	28(2)	-3(2)	12(2)	-6(2)
C7A1	37(5)	48(5)	39(5)	-4(5)	13(4)	6(4)
C8A1	36(5)	55(7)	44(6)	-1(5)	13(5)	8(5)
C9A1	35(6)	62(7)	44(6)	-6(5)	11(5)	8(5)
C10A1	32(5)	68(5)	38(5)	-7(4)	7(4)	7(4)
C11A1	33(5)	55(7)	35(6)	-8(5)	7(5)	8(5)
C12A1	32(6)	53(6)	37(6)	-6(5)	7(5)	9(5)
C13A1	33(5)	72(5)	35(5)	-7(5)	10(5)	-3(5)
C14A1	39(5)	69(4)	34(5)	-2(4)	5(4)	-5(4)
C15A1	43(5)	69(6)	37(6)	1(5)	2(4)	-5(5)
C16A1	46(5)	68(5)	37(6)	4(4)	-4(4)	-3(5)
C17A1	48(6)	68(5)	38(6)	3(5)	-2(5)	-6(5)
C18A1	45(5)	68(4)	32(5)	2(4)	4(4)	-6(4)
C19A1	40(5)	69(4)	30(5)	0(4)	6(4)	-4(4)
O2A1	44(5)	71(6)	31(5)	1(5)	3(5)	-4(5)
F1A1	64(4)	82(6)	79(6)	28(5)	-31(4)	-11(4)
N2A1	34(5)	76(4)	34(5)	-10(4)	9(4)	1(4)
C20A1	48(5)	68(4)	26(5)	0(4)	3(4)	-9(3)
C21A1	51(5)	73(5)	32(5)	4(5)	8(4)	-12(4)
C22A1	58(5)	72(5)	38(6)	8(5)	8(5)	-14(4)
C23A1	60(5)	71(6)	35(6)	4(5)	6(5)	-14(4)
C24A1	57(5)	65(5)	30(5)	-3(4)	7(5)	-10(4)
C25A1	48(5)	66(5)	29(5)	-4(5)	2(5)	-10(4)
C26A1	65(6)	70(7)	38(5)	-3(5)	8(5)	-2(5)

O1A1	58(6)	67(7)	39(4)	-2(4)	2(4)	-7(5)
C27A1	56(6)	63(7)	36(4)	-2(5)	5(4)	-11(5)
C28A1	50(5)	57(6)	36(4)	-4(4)	8(3)	-9(4)
C29A1	50(6)	61(7)	41(5)	-3(5)	3(4)	-19(5)
C30A1	45(6)	60(7)	41(5)	0(5)	7(4)	-15(5)
C31A1	39(6)	45(6)	34(5)	-7(4)	11(4)	-9(5)
C32A1	43(4)	42(5)	35(4)	-3(4)	10(3)	-9(4)
C33A1	51(5)	49(7)	36(4)	2(4)	10(3)	-14(5)
C34A1	40(4)	39(3)	31(4)	-4(3)	16(3)	-9(3)
C35A1	47(5)	38(4)	40(4)	0(4)	14(4)	-10(4)
C36A1	40(5)	36(3)	35(4)	8(3)	17(4)	-7(3)
C37A1	39(5)	37(3)	29(5)	4(3)	11(4)	-7(3)
C38A1	38(5)	35(3)	28(4)	2(3)	11(4)	-7(3)
C39A1	41(4)	40(3)	30(4)	-1(3)	10(4)	-9(3)
C40A1	41(5)	35(3)	25(5)	-1(3)	14(4)	-5(3)
O3A1	38(5)	41(3)	28(5)	-1(3)	10(4)	-10(3)
F2A1	55(6)	33(4)	53(6)	13(3)	23(4)	1(4)
N3A1	39(4)	34(3)	28(4)	0(3)	15(4)	-5(3)
C1B1	34(5)	39(4)	36(5)	-2(3)	18(4)	3(3)
C2B1	34(2)	38(1)	38(2)	-1(1)	19(2)	2(2)
C3B1	38(7)	40(3)	49(6)	4(4)	15(6)	2(4)
C4B1	49(6)	43(4)	57(6)	5(4)	8(5)	4(4)
C5B1	43(7)	45(4)	48(7)	4(4)	11(6)	6(5)
C6B1	38(5)	44(4)	40(5)	1(4)	16(5)	5(4)
C47B1	34(1)	35(1)	29(1)	-4(1)	18(1)	-2(1)
C48B1	35(4)	35(3)	29(5)	-5(3)	17(4)	-1(3)
C49B1	33(5)	35(3)	33(5)	-4(3)	19(4)	0(3)
C50B1	35(6)	33(4)	34(5)	-4(4)	18(4)	-2(4)
C51B1	34(1)	35(1)	29(1)	-4(1)	18(1)	-2(1)
C52B1	34(1)	35(1)	29(1)	-4(1)	18(1)	-2(1)
N1B1	36(4)	38(4)	32(6)	-4(4)	14(4)	2(4)
C64B1	57(7)	44(4)	74(7)	10(5)	10(6)	7(5)
C65B1	61(8)	58(12)	102(14)	18(12)	18(8)	13(8)
C66B1	72(12)	32(8)	85(10)	13(8)	9(10)	3(11)
C67B1	89(14)	58(12)	92(10)	19(9)	33(10)	4(12)
C60B1	41(4)	36(5)	30(4)	-3(4)	15(3)	-5(3)
C61B1	41(2)	37(2)	28(2)	-3(2)	12(2)	-6(2)
C62B1	41(2)	37(2)	28(2)	-3(2)	12(2)	-6(2)
C63B1	41(2)	37(2)	28(2)	-3(2)	12(2)	-6(2)

C7B1	35(5)	49(5)	40(6)	-2(5)	12(4)	6(4)
C8B1	36(5)	54(6)	41(7)	2(6)	14(5)	8(5)
C9B1	35(5)	62(6)	41(7)	-3(6)	14(5)	7(5)
C10B1	33(5)	69(5)	37(6)	-7(5)	7(4)	7(4)
C11B1	34(5)	57(6)	35(7)	-8(6)	9(5)	7(5)
C12B1	33(6)	52(6)	39(7)	-5(6)	7(5)	8(5)
C13B1	32(5)	75(5)	34(6)	-8(5)	11(5)	-2(5)
C14B1	39(5)	71(5)	32(5)	-2(4)	6(4)	-4(4)
C15B1	45(5)	69(5)	39(5)	0(5)	0(5)	-6(5)
C16B1	46(5)	68(5)	41(6)	2(5)	-5(5)	-4(5)
C17B1	48(6)	68(5)	38(6)	3(5)	-3(5)	-6(5)
C18B1	46(5)	68(5)	31(5)	2(4)	3(4)	-4(4)
C19B1	40(5)	71(5)	29(5)	-1(4)	6(4)	-3(4)
O2B1	47(5)	73(6)	32(5)	-2(5)	0(5)	-3(5)
F1B1	56(9)	65(9)	39(8)	-9(7)	-11(6)	2(8)
N2B1	34(5)	77(4)	33(5)	-12(4)	10(4)	2(4)
C13C1	35(6)	75(6)	36(5)	-10(5)	8(5)	-2(5)
C14C1	39(5)	70(5)	34(5)	-1(5)	4(5)	-4(4)
C15C1	44(6)	70(6)	39(6)	2(5)	1(5)	-5(5)
C16C1	47(6)	69(6)	42(6)	6(5)	-4(5)	-6(5)
C17C1	47(6)	69(5)	38(6)	5(5)	-2(5)	-6(5)
C18C1	45(5)	69(5)	34(5)	3(4)	1(5)	-5(4)
C19C1	42(5)	70(5)	32(5)	1(5)	4(4)	-4(4)
O2C1	46(6)	72(6)	31(6)	0(5)	1(5)	-3(6)
F1C1	55(13)	72(12)	50(12)	10(10)	-10(11)	-8(11)
N2C1	31(6)	77(4)	34(5)	-13(5)	10(5)	4(4)
C20C1	46(6)	69(5)	33(6)	3(5)	3(5)	-6(4)
C21C1	48(7)	71(6)	36(7)	4(6)	3(6)	-9(5)
C22C1	51(7)	71(6)	40(7)	4(6)	6(6)	-9(6)
C23C1	52(7)	69(7)	39(7)	3(6)	6(7)	-10(6)
C24C1	51(7)	67(6)	37(7)	1(6)	7(6)	-8(5)
C25C1	47(7)	67(6)	33(7)	2(6)	3(6)	-7(6)
C26C1	54(9)	64(8)	37(8)	0(7)	7(7)	-7(8)
O1C1	53(7)	64(8)	37(9)	-1(8)	6(7)	-9(8)
C27C1	53(7)	60(8)	35(5)	-2(6)	6(5)	-10(6)
C28C1	49(5)	55(7)	36(5)	-2(5)	7(4)	-12(6)
C29C1	48(7)	56(8)	38(6)	-2(6)	6(5)	-14(7)
C30C1	46(7)	53(8)	39(6)	-2(6)	7(6)	-14(7)
C31C1	45(6)	48(8)	37(6)	-2(6)	8(5)	-13(6)

C32C1	44(5)	44(6)	35(5)	-2(5)	8(4)	-10(5)
C33C1	47(6)	49(7)	35(5)	-1(6)	8(4)	-10(6)
C34C1	43(5)	39(4)	33(5)	-1(4)	10(5)	-8(4)
C35C1	43(5)	38(5)	35(6)	2(5)	13(5)	-8(4)
C36C1	42(6)	36(4)	34(6)	4(5)	13(5)	-6(4)
C37C1	40(6)	36(4)	30(6)	4(5)	12(6)	-6(4)
C38C1	40(5)	35(3)	27(5)	1(4)	10(5)	-6(3)
C39C1	41(5)	39(4)	29(5)	0(4)	9(5)	-7(3)
C40C1	40(5)	34(3)	28(6)	-1(4)	14(5)	-5(4)
O3C1	41(6)	42(4)	31(7)	1(5)	6(5)	-6(4)
F2C1	44(11)	37(9)	38(15)	7(10)	15(12)	-5(9)
N3C1	41(5)	35(3)	30(5)	-1(4)	14(5)	-4(3)
C34D1	43(5)	39(4)	34(5)	3(4)	7(4)	-8(4)
C35D1	46(6)	34(5)	36(5)	3(4)	10(5)	-7(4)
C36D1	44(6)	35(4)	33(5)	5(4)	10(4)	-2(4)
C37D1	44(6)	39(4)	29(5)	4(4)	9(5)	-6(4)
C38D1	40(5)	35(3)	26(4)	2(3)	10(4)	-5(3)
C39D1	40(5)	37(4)	28(4)	0(3)	9(4)	-5(4)
C40D1	41(6)	35(3)	25(5)	-2(4)	14(5)	-4(3)
O3D1	39(6)	40(3)	29(5)	2(4)	3(5)	-6(4)
F2D1	56(9)	45(6)	41(7)	13(5)	5(6)	2(6)
N3D1	40(5)	34(3)	29(4)	0(3)	13(5)	-4(3)
N01A1	65(4)	75(3)	79(4)	-14(3)	31(3)	-8(3)
C01A1	67(4)	80(4)	75(4)	-26(3)	27(3)	-25(3)
C01B1	122(7)	106(6)	139(8)	7(6)	80(6)	-12(5)
C04A1	68(5)	80(6)	83(6)	-9(6)	25(5)	-14(6)
Cl011	70(6)	105(10)	77(8)	-7(8)	28(6)	-20(8)
Cl021	61(4)	69(6)	62(5)	-2(4)	11(4)	-11(5)
F12	62(2)	56(2)	33(2)	5(1)	3(1)	26(1)
O22	38(2)	39(2)	35(2)	3(1)	4(1)	-4(1)
N22	34(2)	38(2)	25(2)	4(1)	4(1)	-3(1)
Fe32	32(1)	40(1)	30(1)	8(1)	7(1)	-1(1)
N32	45(2)	32(2)	35(2)	-9(1)	14(2)	-6(2)
Fe42	40(1)	33(1)	36(1)	-9(1)	11(1)	-7(1)
O42	38(2)	46(2)	51(2)	3(2)	14(2)	-3(1)
O52	42(2)	44(2)	41(2)	2(1)	19(2)	-4(1)
C12	33(2)	30(2)	23(2)	1(1)	7(2)	0(2)
C22	29(2)	31(2)	24(2)	0(1)	9(2)	2(2)
C32	35(2)	31(2)	24(2)	-2(2)	4(2)	3(2)

C42	41(2)	28(2)	30(2)	-2(2)	5(2)	5(2)
C52	39(2)	28(2)	30(2)	1(2)	7(2)	5(2)
C62	34(2)	30(2)	26(2)	2(2)	10(2)	3(2)
C472	33(2)	28(2)	25(2)	1(1)	9(2)	-1(2)
C482	32(2)	30(2)	24(2)	4(1)	9(2)	1(2)
C492	34(2)	29(2)	23(2)	0(1)	10(2)	1(2)
C502	33(2)	32(2)	22(2)	-1(2)	8(2)	0(2)
C512	33(2)	33(2)	23(2)	3(2)	11(2)	0(2)
C522	34(2)	27(2)	32(2)	3(2)	13(2)	3(2)
N12	35(2)	28(2)	24(2)	2(1)	4(1)	1(1)
C72	37(2)	26(2)	28(2)	-2(2)	4(2)	3(2)
C82	35(2)	33(2)	34(2)	4(2)	6(2)	-3(2)
C92	37(2)	35(2)	29(2)	6(2)	4(2)	-1(2)
C102	32(2)	32(2)	31(2)	4(2)	5(2)	3(2)
C112	37(2)	31(2)	32(2)	3(2)	7(2)	0(2)
C122	39(2)	33(2)	30(2)	6(2)	4(2)	2(2)
C132	38(2)	35(2)	27(2)	4(2)	7(2)	-2(2)
C142	34(2)	44(2)	27(2)	1(2)	8(2)	2(2)
C152	45(2)	42(2)	27(2)	3(2)	10(2)	7(2)
C162	44(2)	48(2)	28(2)	7(2)	9(2)	15(2)
C172	38(2)	60(2)	29(2)	5(2)	4(2)	4(2)
C182	35(2)	54(2)	32(2)	1(2)	4(2)	-3(2)
C192	36(2)	41(2)	30(2)	5(2)	6(2)	-2(2)
C202	28(4)	56(3)	34(4)	0(3)	3(3)	-3(3)
C212	34(6)	57(4)	35(4)	1(3)	3(4)	-13(4)
C222	34(6)	66(4)	33(4)	-3(3)	7(4)	-20(4)
C232	37(5)	57(4)	35(5)	-9(3)	13(4)	-18(4)
C242	37(4)	56(3)	35(5)	-5(3)	13(4)	-11(3)
C252	39(4)	54(3)	34(5)	-4(3)	7(5)	-7(3)
C262	46(4)	57(3)	37(6)	-4(4)	18(4)	-12(3)
O12	40(3)	53(3)	47(6)	-7(4)	17(4)	-13(3)
C272	56(5)	56(4)	55(6)	-5(4)	19(4)	-16(3)
C282	54(4)	51(4)	45(4)	-4(4)	15(4)	-18(3)
C292	58(5)	58(5)	43(4)	-8(4)	8(4)	-17(4)
C302	66(5)	48(5)	40(4)	-13(4)	12(3)	-22(4)
C312	58(5)	43(5)	39(4)	-11(3)	18(3)	-17(4)
C322	52(4)	37(4)	40(3)	-9(3)	20(3)	-20(3)
C332	55(4)	47(5)	38(4)	-9(4)	17(4)	-14(4)
C342	58(4)	33(3)	36(3)	-10(3)	21(3)	-15(3)

C352	68(5)	32(3)	39(4)	-9(3)	26(4)	-16(4)
C362	76(5)	29(3)	41(4)	-3(3)	27(4)	-8(4)
C372	65(6)	34(3)	35(4)	-3(3)	25(4)	-6(3)
C382	57(5)	31(3)	37(4)	-6(3)	22(4)	-12(3)
C392	57(5)	30(3)	37(4)	-7(3)	19(4)	-15(3)
O32	57(6)	30(3)	39(4)	-9(3)	13(4)	-17(3)
F22	107(9)	26(3)	48(6)	-5(3)	21(6)	-8(4)
C20A2	30(6)	56(4)	31(5)	0(4)	6(4)	-4(4)
C21A2	33(6)	57(5)	32(5)	-1(4)	6(5)	-8(5)
C22A2	37(7)	61(5)	34(5)	-3(4)	4(5)	-13(5)
C23A2	44(7)	59(5)	36(6)	-3(4)	9(5)	-12(5)
C24A2	47(6)	59(4)	36(6)	-4(4)	8(5)	-12(4)
C25A2	38(6)	55(4)	33(6)	-1(4)	8(6)	-7(4)
C26A2	52(6)	58(5)	42(7)	-3(5)	12(5)	-13(4)
O1A2	52(5)	59(5)	45(5)	-5(4)	11(5)	-12(4)
C27A2	55(6)	55(5)	43(6)	-3(5)	11(5)	-14(4)
C28A2	57(5)	51(5)	43(5)	-4(4)	14(4)	-16(4)
C29A2	61(6)	55(6)	43(5)	-9(5)	12(5)	-19(5)
C30A2	65(6)	50(7)	38(5)	-7(5)	18(5)	-21(6)
C31A2	61(7)	43(6)	40(5)	-8(5)	19(5)	-20(6)
C32A2	58(5)	40(5)	40(4)	-6(4)	18(4)	-18(4)
C33A2	56(6)	42(6)	40(5)	-4(5)	15(5)	-17(5)
C34A2	59(6)	33(4)	38(5)	-8(4)	20(4)	-15(4)
C35A2	60(6)	32(4)	33(5)	-9(4)	32(5)	-14(4)
C36A2	64(6)	31(4)	36(5)	-5(4)	32(5)	-8(4)
C37A2	63(7)	34(4)	41(6)	-7(4)	24(6)	-5(4)
C38A2	56(6)	31(4)	38(5)	-12(4)	22(5)	-7(4)
C39A2	55(6)	34(4)	36(5)	-11(4)	21(4)	-12(4)
O3A2	62(8)	35(4)	38(7)	-11(4)	11(6)	-14(4)
F2A2	85(11)	29(4)	55(9)	-4(5)	34(8)	-6(5)
C20B2	35(7)	57(4)	35(5)	0(4)	3(5)	-7(5)
C21B2	32(8)	60(6)	35(5)	-1(4)	3(5)	-12(6)
C22B2	39(8)	63(6)	36(6)	-3(4)	6(6)	-16(6)
C23B2	41(8)	60(6)	34(6)	-8(5)	10(6)	-15(6)
C24B2	40(6)	57(4)	36(6)	-5(4)	11(5)	-10(5)
C25B2	36(6)	56(4)	32(6)	-3(4)	7(6)	-7(5)
C26B2	49(6)	59(4)	39(7)	-5(5)	17(6)	-11(4)
O1B2	45(6)	55(5)	46(7)	-4(6)	19(6)	-15(5)
C27B2	49(6)	55(5)	47(7)	-4(5)	17(6)	-18(5)

C28B2	53(5)	54(5)	42(6)	-6(5)	17(5)	-18(5)
C29B2	57(6)	55(6)	41(6)	-6(5)	16(6)	-21(5)
C30B2	63(6)	51(7)	41(6)	-7(6)	18(5)	-22(6)
C31B2	62(6)	46(7)	40(5)	-9(5)	19(5)	-19(6)
C32B2	55(5)	40(5)	39(5)	-7(4)	22(4)	-21(4)
C33B2	52(6)	45(6)	41(6)	-7(5)	18(5)	-18(5)
C34B2	57(5)	34(4)	36(5)	-9(4)	23(5)	-16(4)
C35B2	60(6)	35(4)	33(6)	-9(5)	32(5)	-13(5)
C36B2	70(7)	35(5)	40(6)	-10(5)	24(6)	-9(5)
C37B2	65(7)	34(4)	40(7)	-10(4)	22(6)	-8(5)
C38B2	58(6)	34(4)	38(6)	-10(4)	20(5)	-10(4)
C39B2	55(6)	36(4)	37(6)	-12(4)	21(5)	-12(4)
O3B2	58(8)	36(4)	36(8)	-14(4)	16(6)	-12(4)
F2B2	95(14)	35(5)	48(13)	-13(6)	1(11)	-11(6)
C402	52(3)	33(2)	42(2)	-9(2)	17(2)	-5(2)
C412	40(2)	30(2)	32(2)	-6(2)	12(2)	-3(2)
C422	36(2)	28(2)	34(2)	-2(2)	12(2)	-2(2)
C432	40(2)	26(2)	28(2)	-3(2)	10(2)	0(2)
C442	37(2)	25(2)	28(2)	4(2)	9(2)	-1(2)
C452	36(2)	35(2)	36(2)	-3(2)	12(2)	0(2)
C462	45(2)	32(2)	42(2)	-12(2)	17(2)	-1(2)
C532	37(2)	25(2)	24(2)	0(2)	4(2)	1(2)
C542	32(4)	65(9)	27(3)	-7(4)	8(3)	1(4)
C552	42(5)	90(10)	30(3)	-11(4)	12(3)	1(6)
C54A2	39(6)	51(11)	31(4)	-9(5)	10(4)	-2(6)
C55A2	37(6)	68(10)	30(4)	-5(5)	11(4)	-13(6)
C562	48(3)	61(3)	31(2)	-1(2)	10(2)	-14(2)
C572	45(3)	66(3)	30(2)	0(2)	11(2)	-14(2)
C582	48(3)	60(3)	40(3)	-7(2)	21(2)	-7(2)
C592	41(2)	43(2)	34(2)	-4(2)	14(2)	-6(2)
C602	38(2)	31(2)	32(2)	3(2)	7(2)	7(2)
C612	39(3)	44(3)	40(3)	-2(2)	8(2)	9(2)
C622	47(3)	40(3)	35(2)	8(2)	6(2)	5(2)
C632	37(2)	37(2)	35(2)	2(2)	3(2)	5(2)
C642	49(2)	29(2)	41(2)	-3(2)	-1(2)	3(2)
C652	57(3)	36(3)	50(3)	-5(2)	4(2)	-5(2)
C662	55(3)	40(3)	46(2)	-14(2)	3(2)	11(2)
C672	71(3)	28(2)	57(3)	-5(2)	-14(3)	6(2)
C682	40(2)	32(2)	28(2)	3(2)	11(2)	-2(2)

C692	41(3)	26(3)	30(3)	11(3)	13(2)	7(3)
C702	41(4)	23(3)	32(3)	9(2)	15(3)	6(3)
C712	44(4)	29(3)	36(3)	7(2)	15(3)	3(3)
C722	55(5)	36(4)	36(3)	6(2)	15(3)	-3(4)
C732	58(5)	35(3)	33(3)	2(3)	15(3)	0(4)
C742	57(5)	40(4)	33(3)	3(3)	22(3)	1(4)
C752	49(4)	30(3)	33(3)	6(3)	17(3)	5(3)
C762	46(4)	40(4)	33(3)	11(3)	18(3)	7(3)
C772	43(3)	32(4)	35(4)	8(3)	16(3)	3(3)
C782	45(4)	54(5)	39(4)	7(3)	20(3)	2(3)
C792	38(3)	57(6)	41(5)	4(4)	15(3)	-6(3)
C802	47(3)	51(6)	36(4)	0(3)	16(3)	-5(3)
C812	43(3)	31(5)	40(4)	4(3)	19(3)	3(3)
C822	44(3)	28(4)	36(4)	6(3)	16(3)	3(3)
O62	45(4)	32(3)	35(3)	4(3)	17(3)	0(3)
O72	59(5)	33(3)	30(4)	3(3)	18(3)	-11(3)
C69A2	49(7)	24(10)	33(6)	6(7)	20(5)	7(7)
C70A2	50(8)	32(10)	36(6)	2(6)	19(6)	3(8)
C71A2	55(9)	46(12)	28(7)	12(7)	16(7)	-4(9)
C72A2	59(10)	41(11)	34(7)	5(7)	14(7)	-1(10)
C73A2	63(10)	46(12)	28(8)	2(7)	13(7)	-2(10)
C74A2	62(10)	50(11)	34(7)	-4(7)	16(7)	-1(10)
C75A2	52(8)	31(9)	31(6)	3(6)	17(6)	6(8)
C76A2	54(8)	35(9)	24(7)	3(7)	22(6)	2(8)
C77A2	51(7)	42(10)	26(7)	-1(7)	24(6)	3(7)
C78A2	48(7)	37(10)	34(10)	-4(9)	27(7)	5(7)
C79A2	46(9)	53(13)	40(9)	-12(8)	33(7)	-4(8)
C80A2	49(8)	50(14)	42(9)	-10(8)	36(7)	-7(7)
C81A2	49(8)	41(14)	28(7)	-2(7)	31(6)	-5(8)
C82A2	47(6)	21(10)	24(7)	8(6)	22(6)	10(6)
Fe13	42(1)	31(1)	26(1)	0(1)	12(1)	0(1)
N13	37(2)	32(2)	28(2)	-5(1)	10(1)	-2(1)
C13	32(2)	33(2)	29(2)	-7(2)	15(1)	-5(2)
Fe23	38(1)	31(1)	31(1)	-7(1)	9(1)	-6(1)
N23	36(2)	34(2)	26(2)	2(1)	15(1)	-2(1)
C23	33(2)	33(2)	33(2)	-4(2)	14(2)	-5(2)
N33	40(2)	36(2)	26(2)	-6(1)	10(1)	-6(1)
C33	38(2)	29(2)	42(2)	-7(2)	15(2)	-2(2)
O43	39(2)	37(2)	39(2)	-7(1)	11(1)	-3(1)

C43	41(2)	37(2)	38(2)	-14(2)	16(2)	-6(2)
O53	46(2)	52(2)	30(2)	-8(1)	10(1)	2(2)
C53	37(2)	39(2)	30(2)	-9(2)	13(2)	-3(2)
O63	41(2)	39(2)	25(1)	-2(1)	11(1)	-1(1)
C63	32(2)	36(2)	28(2)	-7(2)	14(2)	-4(2)
O73	38(2)	43(2)	34(2)	2(1)	10(1)	-4(1)
C73	29(2)	33(2)	29(2)	-4(1)	12(2)	-6(2)
C83	40(2)	38(2)	28(2)	-7(2)	14(2)	-8(2)
C93	40(2)	39(2)	24(2)	-1(2)	12(2)	-4(2)
C103	29(2)	33(2)	26(2)	-2(1)	10(2)	-7(2)
C113	31(2)	33(2)	26(2)	-3(2)	12(2)	1(2)
C123	35(2)	34(2)	26(2)	-1(2)	9(2)	-2(2)
C133	36(2)	43(1)	29(1)	4(1)	17(1)	6(1)
C143	36(2)	43(1)	29(1)	4(1)	17(1)	6(1)
C153	36(2)	43(1)	29(1)	4(1)	17(1)	6(1)
C163	36(2)	43(1)	29(1)	4(1)	17(1)	6(1)
C173	42(5)	40(4)	28(5)	8(4)	23(4)	8(3)
C183	40(5)	36(3)	34(4)	3(3)	18(3)	12(3)
C193	36(2)	43(1)	29(1)	4(1)	17(1)	6(1)
O23	46(6)	23(4)	30(4)	4(3)	18(4)	6(4)
F13	30(6)	73(10)	32(5)	21(6)	15(5)	7(5)
C203	46(5)	30(4)	46(5)	8(3)	17(4)	14(4)
C213	62(7)	28(5)	52(6)	11(5)	25(5)	11(4)
C223	71(7)	30(5)	69(6)	7(5)	35(6)	8(5)
C233	69(7)	31(6)	77(6)	0(5)	34(5)	1(5)
C243	52(6)	41(5)	65(4)	-4(4)	24(4)	4(4)
C253	44(6)	34(5)	47(4)	5(4)	17(4)	13(4)
C263	59(7)	66(7)	76(5)	-27(4)	21(5)	3(5)
O13	55(5)	112(8)	63(5)	-22(4)	19(4)	5(5)
C273	74(5)	98(9)	67(5)	-16(6)	11(5)	31(6)
C283	80(5)	51(5)	67(6)	-20(5)	4(5)	19(4)
C293	94(6)	43(5)	75(8)	-18(6)	-5(6)	12(5)
C303	96(6)	41(6)	81(9)	-3(5)	-10(6)	-1(5)
C313	73(6)	37(5)	70(8)	-5(5)	-3(6)	-7(4)
C323	65(4)	28(4)	63(7)	-20(4)	4(5)	-3(4)
C333	63(4)	47(5)	62(7)	-20(5)	13(5)	12(4)
C343	49(5)	36(4)	53(6)	-16(3)	9(4)	-6(3)
C353	56(5)	35(5)	56(6)	-15(4)	8(4)	-11(4)
C363	40(5)	48(5)	43(4)	-17(4)	10(3)	-10(4)

C373	35(5)	42(5)	31(4)	-8(4)	8(4)	-1(4)
C383	33(5)	36(4)	35(4)	-13(3)	11(3)	-1(3)
C393	29(4)	36(4)	32(4)	-10(3)	11(3)	-2(3)
C403	25(5)	38(4)	24(4)	-10(3)	11(3)	6(3)
O33	35(4)	34(4)	40(5)	-12(4)	1(3)	-3(3)
F23	50(5)	62(7)	46(3)	-20(4)	6(3)	-18(4)
C14A3	36(2)	43(1)	29(1)	4(1)	17(1)	6(1)
C15A3	36(2)	43(1)	29(1)	4(1)	17(1)	6(1)
C16A3	36(2)	43(1)	29(1)	4(1)	17(1)	6(1)
C17A3	41(6)	38(5)	32(6)	5(5)	19(5)	8(4)
C18A3	44(6)	39(4)	35(6)	3(4)	16(5)	8(4)
C19A3	36(2)	43(1)	29(1)	4(1)	17(1)	6(1)
O2A3	38(7)	33(5)	29(5)	1(4)	18(5)	5(5)
F1A3	50(9)	37(9)	35(7)	5(6)	7(7)	11(6)
C20A3	51(7)	32(5)	44(6)	8(4)	12(5)	10(5)
C21A3	61(8)	28(6)	48(7)	-1(6)	18(7)	1(6)
C22A3	67(9)	28(7)	51(7)	2(7)	14(7)	-2(6)
C23A3	72(8)	31(7)	54(7)	-2(6)	17(6)	-3(6)
C24A3	69(8)	33(6)	57(5)	1(5)	19(5)	3(6)
C25A3	62(8)	32(6)	45(6)	4(5)	15(6)	7(6)
C26A3	66(7)	42(7)	55(6)	-1(5)	13(5)	8(7)
O1A3	63(5)	21(6)	61(6)	8(5)	22(5)	8(6)
C27A3	63(5)	52(7)	58(5)	1(5)	18(4)	4(5)
C28A3	74(7)	39(6)	60(5)	-6(5)	11(5)	1(6)
C29A3	80(9)	36(6)	62(6)	-2(5)	13(6)	7(7)
C30A3	57(8)	26(6)	58(6)	-7(5)	23(6)	-5(5)
C31A3	53(7)	23(5)	46(6)	-8(5)	20(6)	-9(5)
C32A3	61(7)	25(5)	42(6)	-9(4)	14(5)	-8(5)
C33A3	72(8)	38(6)	44(5)	-8(5)	12(6)	2(6)
C34A3	65(6)	32(4)	34(6)	-11(4)	4(5)	-3(4)
C35A3	72(7)	39(7)	47(8)	-16(5)	-5(6)	-8(5)
C36A3	61(7)	47(6)	32(6)	-12(4)	-2(5)	-9(5)
C37A3	47(8)	43(6)	35(6)	-11(5)	7(6)	-4(5)
C38A3	43(7)	33(4)	35(6)	-10(4)	11(5)	-1(4)
C39A3	55(7)	32(4)	42(7)	-13(4)	0(5)	0(4)
C40A3	33(6)	30(4)	26(6)	-5(4)	12(5)	4(4)
O3A3	55(7)	31(5)	39(7)	-10(4)	3(4)	-4(4)
F2A3	71(8)	54(8)	43(6)	-15(5)	-10(6)	-19(6)
C14B3	36(2)	43(1)	29(1)	4(1)	17(1)	6(1)

C15B3	36(2)	43(1)	29(1)	4(1)	17(1)	6(1)
C16B3	36(2)	43(1)	29(1)	4(1)	17(1)	6(1)
C17B3	51(8)	41(5)	44(7)	9(5)	13(6)	7(5)
C18B3	44(7)	42(3)	41(6)	5(3)	16(5)	6(4)
C19B3	36(2)	43(1)	29(1)	4(1)	17(1)	6(1)
O2B3	40(6)	36(6)	35(5)	2(4)	16(5)	2(5)
F1B3	47(12)	85(14)	33(9)	12(9)	8(10)	13(8)
C20B3	41(9)	39(5)	48(6)	4(5)	18(6)	8(6)
C21B3	60(11)	45(6)	50(8)	7(6)	14(8)	-1(7)
C22B3	85(12)	48(7)	56(7)	5(7)	16(8)	-11(8)
C23B3	74(12)	50(8)	56(7)	3(7)	18(8)	-14(9)
C24B3	64(10)	44(7)	54(6)	-2(5)	27(6)	-4(7)
C25B3	38(11)	35(8)	48(6)	3(5)	17(6)	11(8)
C26B3	55(12)	44(9)	53(6)	-3(6)	36(7)	-8(9)
O1B3	64(9)	39(8)	54(7)	1(6)	25(7)	11(8)
C27B3	75(7)	40(12)	55(8)	-2(8)	20(7)	11(8)
C28B3	72(6)	41(8)	55(9)	-4(8)	16(7)	6(6)
C29B3	73(7)	35(8)	54(11)	-7(8)	16(8)	7(7)
C30B3	71(7)	34(8)	63(10)	-1(8)	13(8)	3(7)
C31B3	66(8)	33(9)	59(11)	-2(8)	13(8)	1(7)
C32B3	66(7)	29(8)	45(10)	-12(8)	12(7)	-2(6)
C33B3	68(7)	37(8)	46(10)	-9(8)	16(8)	4(7)
C14C3	36(2)	43(1)	29(1)	4(1)	17(1)	6(1)
C15C3	36(2)	43(1)	29(1)	4(1)	17(1)	6(1)
C16C3	36(2)	43(1)	29(1)	4(1)	17(1)	6(1)
C17C3	39(8)	42(6)	33(8)	6(6)	19(7)	7(6)
C18C3	47(7)	41(5)	37(7)	5(5)	13(6)	6(4)
C19C3	36(2)	43(1)	29(1)	4(1)	17(1)	6(1)
O2C3	35(7)	34(6)	30(5)	4(5)	21(5)	4(5)
F1C3	38(10)	45(18)	30(9)	12(11)	16(9)	4(10)
C20C3	48(9)	36(6)	45(7)	4(6)	16(6)	9(7)
C21C3	62(11)	31(10)	51(8)	6(7)	24(8)	10(9)
C22C3	70(12)	34(11)	60(8)	7(9)	26(9)	6(10)
C23C3	69(12)	35(12)	64(9)	4(8)	24(8)	5(10)
C24C3	66(9)	45(9)	56(8)	0(7)	17(7)	-2(8)
C25C3	55(9)	37(8)	47(7)	3(6)	14(7)	8(7)
C26C3	80(10)	48(13)	61(8)	-6(10)	9(8)	-2(10)
O1C3	76(10)	61(17)	75(12)	-17(14)	5(9)	-6(11)
C27C3	83(13)	48(16)	65(9)	-6(9)	3(9)	-4(13)

C28C3	76(11)	36(9)	68(8)	-6(7)	6(8)	0(8)
C29C3	74(12)	33(9)	68(8)	-5(8)	4(9)	1(9)
C30C3	74(11)	36(8)	68(8)	-6(7)	5(8)	4(8)
C31C3	66(9)	32(7)	62(8)	-9(7)	10(8)	0(7)
C32C3	63(10)	33(8)	61(8)	-12(7)	8(8)	-3(8)
C33C3	69(11)	36(9)	62(8)	-9(7)	10(8)	2(8)
C20D3	47(10)	35(8)	47(7)	7(6)	13(8)	10(8)
C21D3	59(10)	35(8)	49(8)	5(7)	17(8)	4(8)
C22D3	73(12)	38(8)	57(8)	2(8)	17(8)	-2(9)
C23D3	74(12)	40(9)	57(8)	0(7)	16(8)	-5(10)
C24D3	63(11)	37(8)	56(7)	2(6)	17(7)	5(9)
C25D3	52(13)	34(8)	48(8)	6(7)	15(8)	10(9)
C26D3	66(9)	46(12)	57(7)	-2(7)	17(6)	1(10)
O1D3	65(9)	47(12)	59(7)	0(8)	17(6)	2(10)
C27D3	63(5)	52(7)	58(5)	1(5)	18(4)	4(5)
C28D3	67(6)	36(7)	55(10)	-7(8)	18(7)	6(6)
C29D3	75(8)	36(7)	64(12)	-3(9)	6(9)	5(6)
C30D3	76(8)	36(7)	67(11)	-7(9)	5(9)	3(6)
C31D3	70(8)	33(7)	61(11)	-8(8)	6(9)	-1(6)
C32D3	66(7)	33(7)	49(11)	-11(8)	14(8)	-1(7)
C33D3	63(7)	31(8)	48(11)	-9(8)	17(8)	2(6)
C413	38(2)	36(2)	21(2)	-6(2)	3(2)	-4(2)
C423	39(2)	35(2)	32(2)	-4(2)	8(2)	-1(2)
C433	34(2)	39(2)	38(2)	-7(2)	8(2)	-6(2)
C443	35(2)	37(2)	25(2)	-3(2)	2(2)	-2(2)
C453	36(2)	39(2)	33(2)	-3(2)	8(2)	-2(2)
C463	36(2)	38(2)	27(2)	-3(2)	4(2)	-8(2)
C473	35(2)	37(2)	32(2)	-3(2)	11(2)	-6(2)
C483	29(2)	34(2)	34(2)	-4(2)	12(2)	-3(2)
C493	33(2)	35(2)	35(2)	-2(2)	15(2)	-2(2)
C503	40(2)	33(2)	39(2)	-1(2)	15(2)	-1(2)
C513	39(2)	38(2)	38(2)	6(2)	11(2)	1(2)
C523	36(2)	41(2)	33(2)	-1(2)	8(2)	-2(2)
C533	35(2)	31(2)	34(2)	-4(2)	8(2)	-4(2)
C543	49(3)	35(2)	40(3)	-3(2)	21(2)	-4(2)
C553	56(3)	42(2)	48(3)	0(2)	20(2)	-11(2)
C563	31(3)	38(3)	31(3)	2(2)	8(2)	-4(2)
C573	35(2)	39(3)	36(3)	4(2)	13(2)	-6(2)
C56A3	54(8)	42(6)	29(9)	-6(6)	31(7)	-2(7)

C57A3	59(17)	46(6)	49(8)	2(4)	32(10)	-3(7)
C583	45(2)	40(2)	36(2)	11(2)	17(2)	4(2)
C593	41(2)	30(2)	31(2)	1(2)	12(2)	0(2)
C603	49(3)	41(2)	47(3)	6(2)	5(2)	1(2)
C613	65(4)	36(2)	74(4)	11(2)	2(3)	2(2)
C623	99(5)	76(4)	54(3)	27(3)	23(3)	20(4)
C633	46(3)	44(3)	78(4)	8(3)	-2(3)	4(2)
C643	55(2)	39(2)	43(2)	-18(2)	16(2)	-8(2)
C653	67(6)	41(8)	60(8)	-25(5)	0(5)	-1(7)
C663	47(6)	42(2)	56(5)	-16(2)	15(5)	-11(3)
C673	70(7)	52(8)	36(8)	-30(7)	21(6)	-12(6)
C65A3	61(8)	59(9)	44(9)	-24(7)	19(8)	-8(7)
C66A3	47(6)	42(2)	56(5)	-16(2)	15(5)	-11(3)
C67A3	55(4)	55(9)	39(6)	-11(5)	18(4)	-15(5)
C65B3	66(15)	44(14)	42(6)	-21(6)	18(8)	-11(13)
C66B3	47(6)	42(2)	56(5)	-16(2)	15(5)	-11(3)
C67B3	52(6)	39(14)	45(15)	-19(13)	12(9)	-10(6)
C683	38(2)	26(2)	27(2)	-3(2)	10(1)	3(2)
C693	29(2)	36(2)	23(2)	-2(2)	5(2)	0(2)
C703	33(2)	37(2)	30(2)	-5(2)	6(2)	2(2)
C713	43(3)	37(2)	44(3)	-3(2)	11(2)	3(2)
C723	69(4)	39(3)	80(4)	-6(3)	35(3)	8(2)
C733	105(5)	52(3)	115(6)	-8(3)	73(5)	15(3)
C743	90(5)	55(3)	100(5)	-4(3)	67(4)	12(3)
C753	51(3)	49(2)	46(3)	-5(2)	25(2)	4(2)
C763	48(3)	53(2)	45(3)	3(2)	27(2)	3(2)
C773	35(2)	44(2)	31(2)	-1(2)	11(2)	-2(2)
C783	39(2)	47(2)	37(2)	4(2)	13(2)	-4(2)
C793	48(3)	36(2)	41(3)	5(2)	17(2)	-5(2)
C803	41(2)	33(2)	34(2)	-2(2)	12(2)	-1(2)
C813	35(2)	35(2)	25(2)	-1(2)	11(2)	-4(2)
C823	29(2)	36(2)	24(2)	-3(2)	5(2)	-4(2)
O83	52(2)	38(2)	46(2)	-6(1)	21(2)	-7(1)
N03A3	67(4)	66(4)	71(4)	15(3)	34(4)	-1(3)
C03A3	66(5)	62(4)	69(5)	13(4)	33(4)	2(4)
C03B3	76(6)	66(5)	91(7)	14(5)	38(5)	-7(4)
N02A3	51(2)	67(3)	42(2)	3(2)	7(2)	-14(2)
C02A3	54(3)	58(3)	42(2)	-6(2)	13(2)	-22(2)
C02B3	63(4)	76(4)	50(3)	9(3)	20(3)	-11(3)

Table S7. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for **1**.

	x	y	z	U(eq)
H421	387	6253	1869	38
H431	103	5259	1641	38
H451	62	5645	548	42
H461	329	6656	770	45
H711	1475	7449	3262	53
H721	1660	8112	3807	64
H731	1307	8079	4219	71
H741	763	7405	4080	65
H761	299	6555	3649	57
H781	-156	5687	3231	63
H791	-307	4951	2721	66
H801	86	4918	2352	61
H811	615	5619	2471	54
H53A1	1048	4697	1862	49
H53B1	757	5004	1436	49
H53D1	1143	4483	1808	49
H53E1	810	5042	1612	49
H54A1	1008	4264	1112	56
H54B1	1295	3944	1537	56
H55A1	1662	4944	1755	63
H55B1	1723	4642	1385	63
H56A1	1141	5615	1311	65
H56B1	1199	5313	941	65
H57A1	1825	5821	1109	81
H57B1	1524	6350	1152	81
H57D1	1812	5678	1143	81
H57E1	1616	6362	1126	81
H58A1	2160	6437	1694	69
H58B1	2167	5697	1791	69
H54D1	996	4106	1120	60
H54E1	690	4697	938	60
H55D1	1347	4818	942	61
H55E1	1549	4814	1421	61
H56D1	1160	5773	1386	70
H56E1	1042	5791	914	70
H31	41	2235	1291	42
H51	1097	2428	2311	56

H501	-498	3020	698	37
H521	-561	4885	435	37
H65A1	1185	1451	2320	98
H65B1	981	771	2160	98
H65C1	1094	1230	1875	98
H66A1	373	1143	1353	105
H66B1	253	692	1637	105
H66C1	-14	1318	1446	105
H67A1	571	1746	2480	126
H67B1	105	1686	2136	126
H67C1	373	1060	2326	126
H61A1	-1006	3542	-484	54
H61B1	-610	3986	-245	54
H61C1	-597	3251	-129	54
H62A1	-1444	3165	-148	54
H62B1	-1036	2854	196	54
H62C1	-1316	3330	314	54
H63A1	-1470	4258	-331	54
H63B1	-1349	4486	120	54
H63C1	-1083	4726	-110	54
H81	1749	3341	2287	55
H91	2216	4093	2705	58
H111	1281	4946	2871	52
H121	826	4155	2487	51
H131	2442	4416	3376	62
H151	3081	4432	3925	73
H171	3701	6064	4367	78
H211	3821	6891	3984	71
H221	3898	7983	3969	77
H231	3347	8661	3892	73
H251	2609	7140	3751	60
H26A1	2338	8179	3770	64
H26B1	2654	8770	3915	64
H27A1	2126	9380	3420	65
H27B1	1821	8783	3238	65
H291	2437	9847	2956	63
H301	2260	10244	2315	61
H311	1653	9896	1777	60
H331	1383	8798	2536	54

H351	854	9986	1533	45
H371	40	8605	904	45
H401	205	7562	1032	42
H3D1	261	2207	1251	53
H5D1	1369	2522	2202	55
H50D1	-389	2962	710	41
H52D1	-630	4837	494	37
H65D1	1516	1761	1674	126
H65E1	1602	1677	2135	126
H65F1	1529	1066	1854	126
H66D1	949	723	2025	112
H66E1	1007	1340	2297	112
H66F1	560	1178	1943	112
H67D1	823	1541	1127	140
H67E1	839	842	1304	140
H67F1	446	1289	1216	140
H61D1	-685	3076	-106	54
H61E1	-1120	3353	-428	54
H61F1	-713	3791	-263	54
H62D1	-1027	2799	363	54
H62E1	-1276	3340	474	54
H62F1	-1457	3064	27	54
H63D1	-1084	4601	-75	54
H63E1	-1491	4163	-241	54
H63F1	-1310	4439	207	54
H8D1	1872	3559	2199	56
H9D1	2298	4337	2637	59
H11D1	1340	4890	2884	53
H12D1	910	4126	2433	52
H13D1	2494	4526	3443	58
H15D1	3105	4611	3997	66
H17D1	3643	6307	4441	71
H21D1	3739	7158	4096	66
H22D1	3803	8250	4109	72
H23D1	3211	8887	3939	72
H25D1	2498	7316	3690	63
H26D1	2171	8307	3654	76
H26E1	2459	8907	3875	76
H27D1	2113	9676	3361	68

H27E1	1769	9121	3216	68
H29D1	2363	10087	2831	68
H30D1	2135	10366	2157	63
H31D1	1520	9956	1672	49
H33D1	1344	8968	2529	58
H35D1	732	10043	1546	52
H37D1	-48	8625	931	44
H40D1	133	7569	1063	40
H3G1	171	2203	1290	53
H5G1	1228	2501	2296	58
H50G1	-432	2960	711	40
H52G1	-570	4815	415	37
H65G1	1419	1621	2207	119
H65H1	1284	916	2041	119
H65I1	1286	1467	1743	119
H66G1	555	683	1588	107
H66H1	202	1219	1464	107
H66I1	544	1244	1291	107
H67G1	882	1648	2477	123
H67H1	406	1479	2193	123
H67I1	754	935	2323	123
H61G1	-592	3054	2	54
H61H1	-976	3292	-398	54
H61I1	-579	3741	-178	54
H62G1	-1096	2860	320	54
H62H1	-1388	3428	336	54
H62I1	-1472	3104	-85	54
H63G1	-1040	4602	-143	54
H63H1	-1437	4153	-363	54
H63I1	-1353	4477	57	54
H8G1	1754	3396	2234	54
H9G1	2246	4144	2623	56
H11G1	1369	5069	2843	53
H12G1	871	4336	2441	53
H13G1	2508	4595	3349	58
H15G1	3074	4687	3929	69
H17G1	3588	6377	4408	71
H13J1	2201	4682	3476	62
H15J1	2848	4626	4001	68

H17J1	3616	6155	4378	70
H21J1	3745	7030	4292	68
H22J1	3892	8083	4202	71
H23J1	3407	8681	3673	69
H25J1	2638	7161	3314	65
H26J1	2765	8403	2871	67
H26K1	2398	8145	2975	67
H27J1	2194	9498	3273	65
H27K1	2060	8775	3146	65
H29J1	2531	9834	2701	62
H30J1	2245	10133	2025	60
H31J1	1572	9810	1592	56
H33J1	1474	8880	2507	57
H35J1	815	10002	1531	48
H37J1	-60	8625	1032	44
H40J1	63	7585	1234	41
H35M1	972	9923	1451	50
H37M1	130	8567	827	47
H40M1	131	7588	1090	40
H1ZA1	2394	8411	2637	171
H1ZB1	1988	8304	2224	171
H1ZC1	2413	7946	2302	171
H4ZA1	2132	7497	2192	96
H4ZB1	2191	6795	2375	96
H32	5575	8128	9758	40
H52	4561	8943	8882	42
H502	5903	6896	9958	36
H522	5529	5130	9532	38
H82	4225	8552	8126	45
H92	3583	8391	7572	45
H112	3247	7168	8232	43
H122	3885	7329	8779	45
H132	2831	8475	7403	43
H152	2255	8968	6924	48
H172	1331	7985	6053	55
H212	1525	7187	5654	55
H222	1275	6258	5288	56
H232	1201	5337	5610	53
H252	1663	6288	6674	54

H26A2	1480	5193	6665	56
H26B2	1127	4930	6248	56
H27A2	1356	3908	6251	68
H27B2	1644	4053	6717	68
H292	1645	3391	5838	69
H302	2128	2654	5829	66
H312	2712	2415	6413	56
H332	2393	3769	7003	57
H352	2922	1968	7071	54
H372	3924	2473	8085	52
H21D2	1454	7085	5692	53
H22D2	1164	6126	5371	57
H23D2	1120	5259	5747	59
H25D2	1690	6286	6768	54
H26D2	1423	5259	6811	65
H26E2	1118	4897	6410	65
H27D2	1585	4458	6036	65
H27E2	1339	4033	6222	65
H29D2	1622	3347	5789	68
H30D2	2066	2493	5878	63
H31D2	2657	2369	6481	59
H33D2	2294	3857	6948	57
H35D2	2789	2020	7107	45
H37D2	3822	2493	8109	54
H21G2	1628	7245	5655	55
H22G2	1416	6344	5249	60
H23G2	1299	5390	5508	57
H25G2	1615	6241	6586	53
H26G2	1397	5176	6519	59
H26H2	1103	4929	6076	59
H27G2	1409	3930	6432	62
H27H2	1787	4243	6806	62
H29G2	1628	3234	5958	64
H30G2	2062	2393	5983	64
H31G2	2675	2212	6560	60
H33G2	2418	3724	7090	56
H35G2	2920	1848	7205	46
H37G2	3923	2444	8193	56
H402	4077	3512	8274	52

H422	3772	5097	8555	41
H432	4300	5678	9047	39
H452	5153	4849	8749	45
H462	4627	4252	8262	48
H53A2	4267	6821	8326	38
H53B2	4535	6179	8443	38
H53E2	4310	6925	8324	38
H53F2	4444	6204	8440	38
H54A2	5130	6772	8476	52
H54B2	4840	7390	8325	52
H55A2	4921	6812	7784	66
H55B2	4662	6241	7854	66
H54D2	5084	6407	8431	51
H54E2	4955	7134	8323	51
H55D2	4523	6100	7807	55
H55E2	4865	6522	7745	55
H56A2	4356	7478	7589	59
H56B2	4099	6963	7706	59
H56D2	4092	7051	7700	59
H56E2	4427	7442	7606	59
H57A2	4298	6832	7042	58
H57B2	3859	7084	7006	58
H58A2	3790	6016	6819	58
H58B2	4175	5824	7231	58
H61A2	6204	4892	9745	66
H61B2	6661	5096	10064	66
H61C2	6425	5502	9662	66
H62A2	5908	4924	10236	67
H62B2	5986	5524	10526	67
H62C2	6366	5068	10578	67
H63A2	6567	6460	10137	61
H63B2	6779	5968	10500	61
H63C2	6413	6424	10486	61
H65A2	5649	9407	9219	82
H65B2	5877	9049	9641	82
H65C2	5809	9801	9629	82
H66A2	5048	9268	9953	80
H66B2	5423	9761	10059	80
H66C2	5516	9015	10113	80

H67A2	4967	9856	9003	100
H67B2	5082	10241	9411	100
H67C2	4697	9758	9251	100
H712	3462	6146	8624	44
H722	3799	6480	9285	53
H732	3462	6451	9709	52
H742	2775	6110	9468	51
H762	2150	5673	8916	47
H782	1533	5179	8379	54
H792	1204	4752	7741	55
H802	1555	4711	7325	54
H812	2213	5137	7536	45
H71D2	3374	6074	8629	53
H72D2	3641	6494	9280	56
H73D2	3248	6438	9656	57
H74D2	2562	6049	9353	60
H76D2	1972	5656	8760	42
H78D2	1418	5080	8221	44
H79D2	1164	4549	7600	49
H80D2	1554	4586	7220	50
H81D2	2235	4984	7506	41
H33	3526	11534	5971	44
H53	4395	10347	6735	43
H83	4275	9212	6950	42
H93	4545	8189	7079	42
H113	4376	8038	5922	36
H123	4133	9071	5804	39
H133	5102	7550	7037	42
H153	5634	6910	7465	42
H173	5411	5070	7619	41
H213	4675	4784	7558	57
H223	4205	3949	7394	66
H233	3926	3527	6747	70
H253	4520	4874	6408	51
H26A3	4151	3470	6104	84
H26B3	3710	3796	6002	84
H27A3	4052	3506	5482	104
H27B3	4030	4158	5248	104
H293	3399	3025	5431	102

H303	2672	3028	5171	108
H313	2295	3864	4763	86
H333	3367	4765	4947	75
H353	2103	4316	4131	66
H373	1839	6158	3834	46
H403	2248	6949	4199	34
H15D3	5618	6800	7498	42
H17D3	5300	4975	7569	43
H21D3	4451	4813	7383	57
H22D3	4048	3885	7170	63
H23A3	3945	3436	6552	67
H25D3	4706	4748	6412	59
H26D3	4569	3715	6053	71
H26E3	4224	3245	6072	71
H27D3	3504	4182	5808	73
H27E3	3565	3433	5773	73
H29D3	3409	2986	5093	78
H30D3	2973	3027	4405	57
H31D3	2520	3882	4150	50
H33D3	3024	4740	5227	67
H35D3	2031	4431	4052	76
H37D3	1742	6291	3864	55
H40D3	2144	7059	4304	36
H15G3	5591	6991	7542	42
H17G3	5518	5076	7466	57
H21G3	5011	4369	7251	66
H22G3	4673	3453	6924	81
H23G3	4331	3405	6226	76
H25G3	4653	5224	6179	49
H26G3	3949	4525	5591	56
H26H3	4382	4585	5558	56
H27G3	3914	3317	4959	72
H27H3	3980	4066	4956	72
H29G3	3336	3034	5244	70
H30G3	2625	3175	5040	74
H31G3	2291	4084	4690	69
H33G3	3381	4697	4728	64
H15J3	5540	6877	7478	42
H17J3	5280	5063	7653	45

H21J3	4703	4750	7609	58
H22J3	4236	3919	7513	66
H23J3	3784	3621	6854	69
H25J3	4382	4817	6416	59
H26J3	3837	4179	5960	85
H26K3	3795	3487	6123	85
H27J3	2793	3755	5844	91
H27K3	3151	3242	5926	91
H29J3	3276	2906	5384	81
H30J3	3186	2992	4722	82
H31J3	2850	3876	4335	71
H33J3	2725	4610	5289	75
H21M3	4906	4642	7413	60
H22M3	4627	3639	7180	72
H23M3	4457	3344	6516	73
H25M3	4851	5057	6321	57
H26M3	4676	4259	5809	71
H26N3	4667	3528	5931	71
H27M3	4168	4153	5219	73
H27N3	4021	4751	5397	73
H29M3	3619	3160	5179	80
H30M3	2925	2880	4781	82
H31M3	2428	3672	4473	75
H33M3	3327	5013	4924	60
H423	3269	7856	4763	46
H433	3250	8953	4827	47
H453	2103	8824	4792	46
H463	2110	7733	4714	44
H503	2851	11437	5210	46
H523	2226	10003	4461	47
H53A3	3458	8794	6009	43
H53B3	3132	8630	5558	43
H54A3	2918	9439	6069	49
H54B3	2598	9177	5639	49
H55A3	3031	8353	6305	59
H55B3	2579	8626	6209	59
H55D3	2591	8622	6223	59
H55E3	2608	8174	5879	59
H56A3	2704	7888	5630	43

H56B3	2272	8032	5649	43
H57A3	2488	7367	6230	45
H57B3	2429	6990	5833	45
H56D3	3368	8175	6265	44
H56E3	3294	8491	6624	44
H57D3	3365	7448	6775	58
H57E3	2875	7569	6599	58
H58A3	3036	6654	6364	49
H58B3	3203	7366	6462	49
H58D3	2743	7098	6051	49
H58E3	3075	6663	6387	49
H61A3	2553	12073	4684	102
H61B3	2232	11963	4877	102
H61C3	2068	12223	4427	102
H62A3	2225	10790	3990	120
H62B3	2573	11331	4170	120
H62C3	2099	11522	3895	120
H63A3	1564	11377	4151	99
H63B3	1693	11132	4600	99
H63C3	1697	10652	4265	99
H65A3	4529	11022	7191	98
H65B3	4796	11288	6968	98
H65C3	4679	11747	7250	98
H66A3	4002	12278	6262	76
H66B3	4356	12511	6684	76
H66C3	4473	12052	6402	76
H67A3	3796	11379	6980	80
H67B3	3949	12102	7040	80
H67C3	3589	11875	6620	80
H65D3	4070	12081	7127	84
H65E3	3650	11834	6767	84
H65F3	3942	11349	7104	84
H66D3	4328	12092	6293	76
H66E3	3886	12292	6275	76
H66F3	4307	12533	6637	76
H67D3	4797	11368	6831	76
H67E3	4755	11837	7154	76
H67F3	4657	11096	7159	76
H65G3	3939	11301	7098	79

H65H3	4406	11058	7228	79
H65I3	4321	11785	7296	79
H66G3	3622	12091	6525	76
H66H3	4025	12524	6757	76
H66I3	3893	12329	6299	76
H67G3	4723	12118	6930	73
H67H3	4802	11396	6845	73
H67I3	4599	11885	6479	73
H713	4341	5955	5147	52
H723	4652	5232	4894	75
H733	5056	5581	4565	98
H743	5128	6639	4475	87
H763	4939	7743	4525	56
H783	4749	8860	4569	50
H793	4379	9588	4742	51
H803	3971	9262	5072	45
H813	3945	8213	5232	39
HO13	3895(14)	5700(20)	5712(18)	68
HO23	3610(17)	5660(20)	5828(17)	68
H3ZA3	2679	4210	6169	115
H3ZB3	3070	4214	6601	115
H3ZC3	3089	3814	6240	115
H2ZA3	2200	5330	6130	97
H2ZB3	2612	5705	6184	97
H2ZC3	2277	6039	6304	97

3. CSD statistics

a. Metal-dichloromethane distances

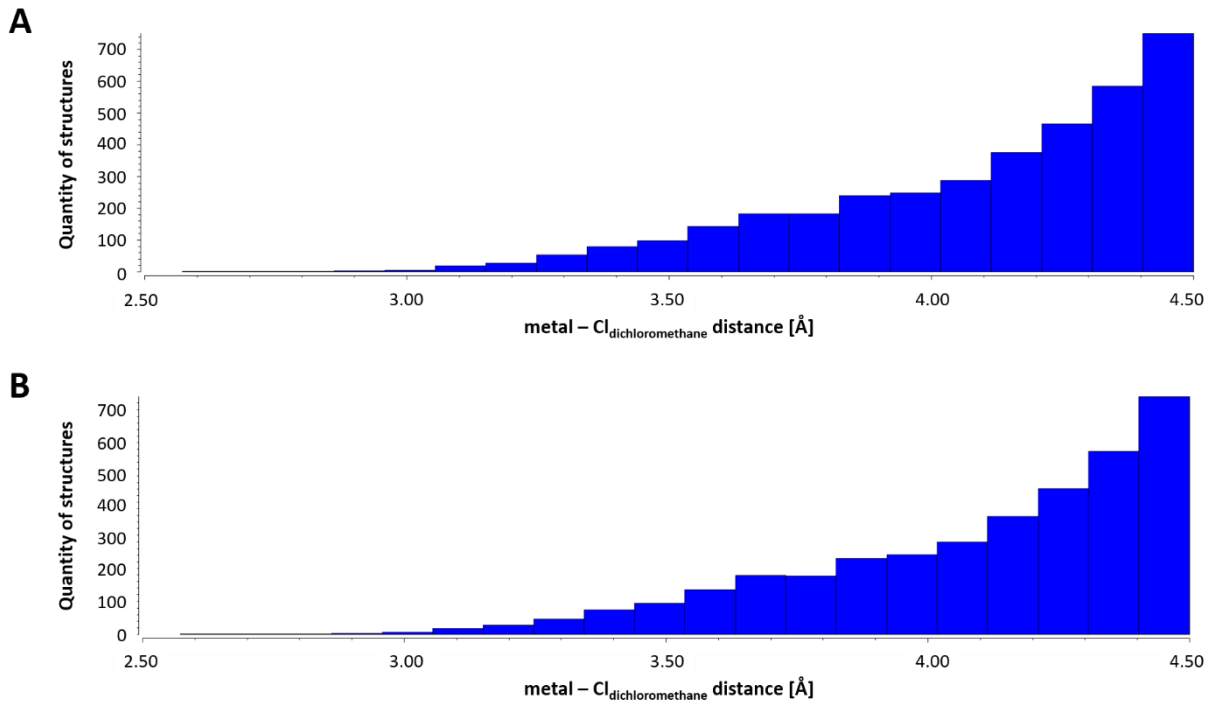


Figure S2. CSD statistics about metal – dichloromethane distances (search range: 1.0-4.5 Å, range shown 2.5-4.0 Å). **A**: All structures included. **B**: Only structures with R1≤ 0.10 included.

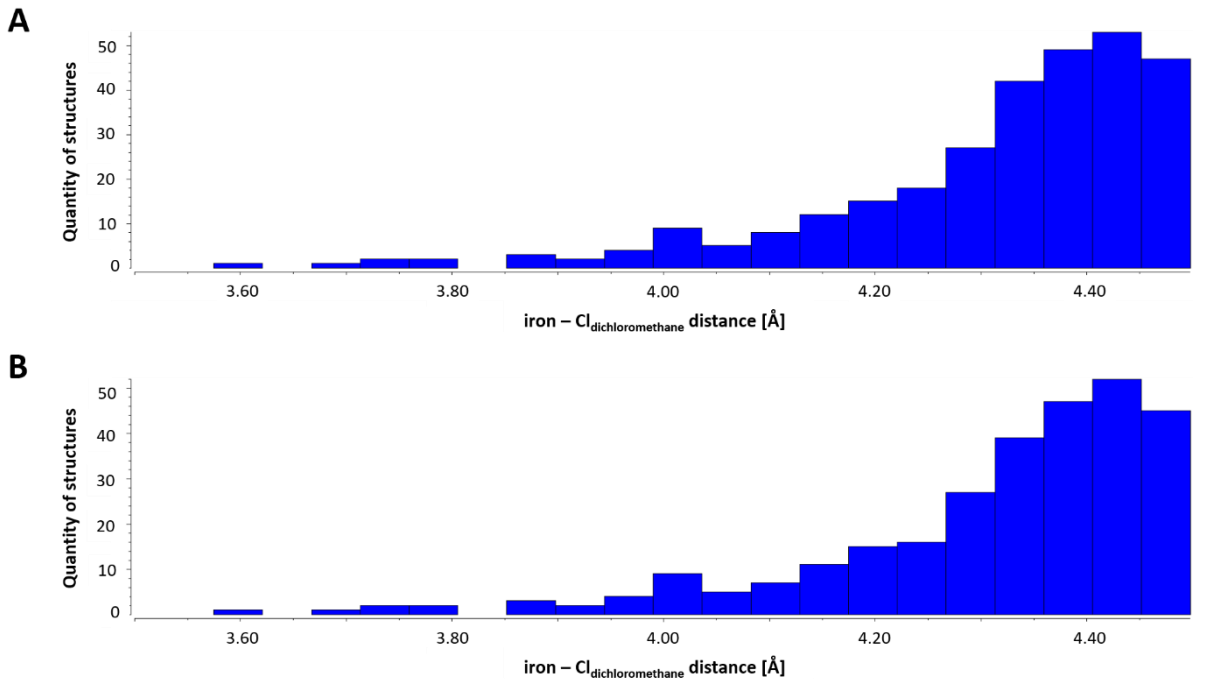


Figure S3. CSD statistics about iron – dichloromethane distances (search range: 1.0-4.5 Å, range shown 2.5-4.0 Å). **A**: All structures included. **B**: Only structures with R1≤ 0.10 included.

b. Quantity of refined parameters in complex structures

Table S8. Overview of structures in the CSD, which have the highest number of refined parameters.

Entry	CCDC number	Number of refined parameters	Entry	CCDC number	Number of refined parameters	Entry	CCDC number	Number of refined parameters
1	1400565	16805	**60**	900299	5623	**119**	221330	4879
2	263723	14394	**61**	784032	5620	**120**	790790	4873
3	911281	13399	**62**	1024739	5610	**121**	802905	4861
4	1001444	13276	**63**	1449018	5575	**122**	674852	4801
5	1450226	12854	**64**	1052767	5572	**123**	864176	4799
6	297539	12058	**65**	994963	5551	**124**	756308	4796
7	1032732	11257	**66**	1052769	5497	**125**	1444589	4784
8	166177	9913	**67**	1052764	5495	**126**	1022485	4782
9	1413935	8713	**68**	1052765	5425	**127**	1022486	4780
10	1004918	8702	**69**	279421	5423	**128**	183287	4774
11	221328	8535	**70**	728098	5381	**129**	1417966	4771
12	1465058	8418	**71**	755554	5372	**130**	1450317	4762
13	1430512	7885	**72**	624529	5369	**131**	1450318	4762
14	1430507	7885	**73**	1024740	5365	**132**	991298	4748
15	1421094	7718	**74**	1054511	5364	**133**	806042	4742
16	206636	7648	**75**	1054509	5333	**134**	1405497	4741
17	903567	7386	**76**	986850	5322	**135**	875312	4741
18	693249	7226	**77**	1052771	5298	**136**	1054510	4721
19	619904	7205	**78**	1001148	5290	**137**	655381	4714
20	1442991	6999	**79**	816801	5269	**138**	143710	4711
21	281545	6950	**80**	1473147	5258	**139**	1061926	4699
22	996385	6908	**81**	972369	5258	**140**	1061927	4699
23	1022488	6893	**82**	1052766	5254	**141**	1061928	4699
24	1022433	6891	**83**	972370	5246	**142**	1037545	4693
25	1442990	6872	**84**	825074	5240	**143**	689511	4672
26	159454	6859	**85**	278914	5233	**144**	1400134	4670
27	115146	6817	**86**	696017	5224	**145**	1432903	4651
28	648053	6774	**87**	1439853	5204	**146**	1012307	4650
29	869522	6746	**88**	902397	5186	**147**	958793	4643
30	750246	6724	**89**	1045907	5173	**148**	624579	4637
31	919657	6653	**90**	1052523	5163	**149**	702905	4631
32	1021784	6637	**91**	918145	5158	**150**	906753	4618
33	693248	6621	**92**	1013078	5155	**151**	191871	4593
34	660927	6538	**93**	1007472	5140	**152**	1023237	4592
35	1432685	6369	**94**	1052770	5125	**153**	945577	4592
36	990918	6364	**95**	1456932	5123	**154**	978061	4583
37	836226	6358	**96**	744112	5120	**155**	757946	4583
38	805517	6355	**97**	201753	5095	**156**	900297	4580
39	1007930	6312	**98**	278915	5093	**157**	631614	4577
40	980496	6265	**99**	789802	5093	**158**	1023236	4576
41	1434974	6226	**100**	657242	5055	**159**	754718	4569
42	609463	6203	**101**	673329	5049	**160**	619903	4564
43	1037547	6154	**102**	1439924	5041	**161**	745521	4558
44	740086	6154	**103**	900298	5038	**162**	806425	4544
45	120381	6004	**104**	660928	4995	**163**	985519	4543
46	900301	5886	**105**	186988	4995	**164**	978062	4543
47	1033040	5878	**106**	952425	4994	**165**	1448815	4529
48	866915	5865	**107**	146884	4989	**166**	877945	4441
49	1052773	5838	**108**	1416987	4968	**167**	868361	4441
50	1456933	5805	**109**	1418808	4956	**168**	294736	4441
51	1417965	5798	**110**	164710	4943	**169**	802297	4423
52	932596	5786	**111**	221238	4932	**170**	1421596	4417
53	1052774	5773	**112**	273452	4922	**171**	990110	4403
54	1448676	5769	**113**	947541	4901	**172**	829669	4395
55	1052772	5765	**114**	800136	4897	**173**	224752	4392
56	1011628	5723	**115**	898850	4891	**174**	1438968	4384
57	1052763	5718	**116**	1410005	4890	**175**	750248	4383

58	900300	5718	**117**	268805	4890
59	1052768	5654	**118**	1420853	4883

4. Refinement details

a. Crystal data and refinement details

Table S9. Crystal data and structure refinement for **1**.

CCDC entry	1586610
Empirical formula	$C_{251.40}H_{217.15}Cl_{0.20}F_6Fe_6N_{11.65}O_{22}$
Formula weight	4209.59
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	$P2_1/n$
Unit cell dimensions	a = 35.549(4) Å
	b = 21.056(2) Å β = 115.485(2)°
	c = 36.869(4) Å
Volume	24912(5) $Å^3$
Z	4
Density (calculated)	1.122 Mg/m^3
Absorption coefficient	0.407 mm^{-1}
F(000)	8786
Crystal size	0.40 x 0.35 x 0.35 mm^3
Theta range for data collection	1.144 to 26.373°
Index ranges	-44<=h<=44, -26<=k<=26, -46<=l<=45
Reflections collected	428848
Independent reflections	50900 [R(int) = 0.0779]
Completeness to theta = 25.242°	99.9 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	50900 / 32297 / 5311
Goodness-of-fit on F^2	1.058
Final R indices [I>2sigma(I)]	R1 = 0.0741, wR2 = 0.1815
R indices (all data)	R1 = 0.1298, wR2 = 0.2283
Largest diff. peak and hole	2.147 and -0.552 e.$Å^{-3}$

b. Overview of all free variables used

Table S10. Overview of all free variables used including occupancies and disorder components they were used for.

Free variable	occupancy [%]	residue	disorder component
2	75.2	*1*	1
3	59.2	*1*	1
4	34.4	*1*	1
5	21.5	*1*	2
6	38.7	*1*	2
7	19.2	*1*	3
8	17.2	*1*	3
9	2.0	*1*	4
10	24.8	*1*	5
11	60.9	*2*	1
12	54.5	*2*	1
13	78.2	*2*	1
14	27.5	*2*	2
15	18.1	*2*	3
16	84.2	*3*	1
17	49.0	*3*	1
18	43.5	*3*	1
19	58.0	*3*	1
20	44.6	*3*	1
21	25.8	*3*	2
22	6.3	*3*	2
23	20.3	*3*	3
24	12.5	*3*	3
25	10.4	*3*	4
26	7.7	*3*	5

c. BIND and SUMP commands

Table S11. Overview of all BIND commands used.

BIND command	Residue	Disorder components that are connected
BIND_1 C18B C20A	1	components 2 and 3 at phenolate imine moiety/dibenzyl ether
BIND_1 N2C C10B	1	components 3 and 4 at carbazole-benzyl/phenolate imine moiety
BIND_1 C32 C34D	1	components 1 and 5 at dibenzyl ether/phenolate imine moiety
BIND_3 C20D C18B	3	components 3 and 5, phenolate imine moiety/dibenzyl ether moiety
BIND_3 C34 C32C	3	components 4 and 1, dibenzyl ether/phenolate imine moiety
BIND_3 C34A C32B	3	components 3 and 2, dibenzyl ether/phenolate imine moiety
BIND_3 C34A C32D	3	components 5 and 2, dibenzyl ether/phenolate imine moiety
BIND_3 Fe1 O8	3	----------
BIND_3 Fe2 O8	3	----------

Table S12. Overview of all SUMP commands used.

SUMP command	Residue	Disordered moiety
SUMP 1.0 0 1 3 1 5 1 7	1	threefold disorder at carbazole and benzyl moiety
SUMP 1.0 0 1 3 1 5 1 8 1 9	1	fourfold disorder at phenolate imine moiety
SUMP 1.0 0 1 3 1 6 1 9	1	threefold disorder at dibenzyl ether moiety
SUMP 1.0 0 1 4 1 6 1 9 1 10	1	fourfold disorder at phenolate imine moiety
SUMP 1.0 0 1 12 1 14 1 15	2	threefold disorder at dibenzyl ether and phenolate imine moiety
SUMP 1.0 0 1 18 1 21 1 23 1 25	3	fourfold disorder at phenolate imine moiety

SUMP 1.0 0 1 18 1 21 1 24 1 25 1 26	3	fivefold disorder at dibenzyl ether moiety
SUMP 1.0 0 1 17 1 20 1 22	3	threefold disorder at tert-butyl moiety

d. SHELX restraints and constraints instructions used

Table S13. SHELX restraints and constraints instructions used*

Instruction	Strength	Description
RIGU	twice the default strength	Apply enhanced rigid bond *restraints* for 1,2- and 1,3-distances.[#]
SADI	default strength	The distances between specified atoms are *restrained* to be equal with an effective standard deviation.
FLAT	default strength	The named atoms are *restrained* to lie on a common plane.
SIMU	twice the default strength	Atoms are *restrained* with effective standard deviation to have the same Uij components.
ISOR	twice the default strength	The named atoms are *restrained* with effective standard deviation so that their U_{ij} components approximate to isotropic behavior; however the corresponding isotropic U is free to vary.
EADP	----------	The same isotropic or anisotropic displacement parameters are used for all the named atoms.
SUMP	----------	*Restrains* the sum of the occupancies of the specified free variables to unity. A standard deviation of 0 was applied.

*Descriptions taken and modified from http://shelx.uni-goettingen.de/shelxl_html.php#TheTop

[#] Thorn, Dittrich, Sheldrick, *Acta Cryst.* A**68** (2012) 448-451

Table S14. Additional SHELX instructions used*

Instruction	Description
RESI	Until the next RESI instruction, all atoms are considered to be in the specified 'residue', which may be defined by a class or number or both. The same atom names may be employed in different residues, enabling them to be referenced globally or selectively.
FREE	The specified 'bond' is deleted from the connectivity list (if present).
BIND	The specified 'bond' (which may be of any length) is added to the connectivity list if it is not there already.

*Descriptions taken and modified from http://shelx.uni-goettingen.de/shelxl_html.php#TheTop

e. ORTEP plots of minor occupied components

For obvious reasons it is not possible to show all of the possible combinations of disorder components. Thus, only a selection is shown below. The combination of disorder components was chosen in such a way that each disorder component is depicted at least in one ORTEP plot.

Residue 1

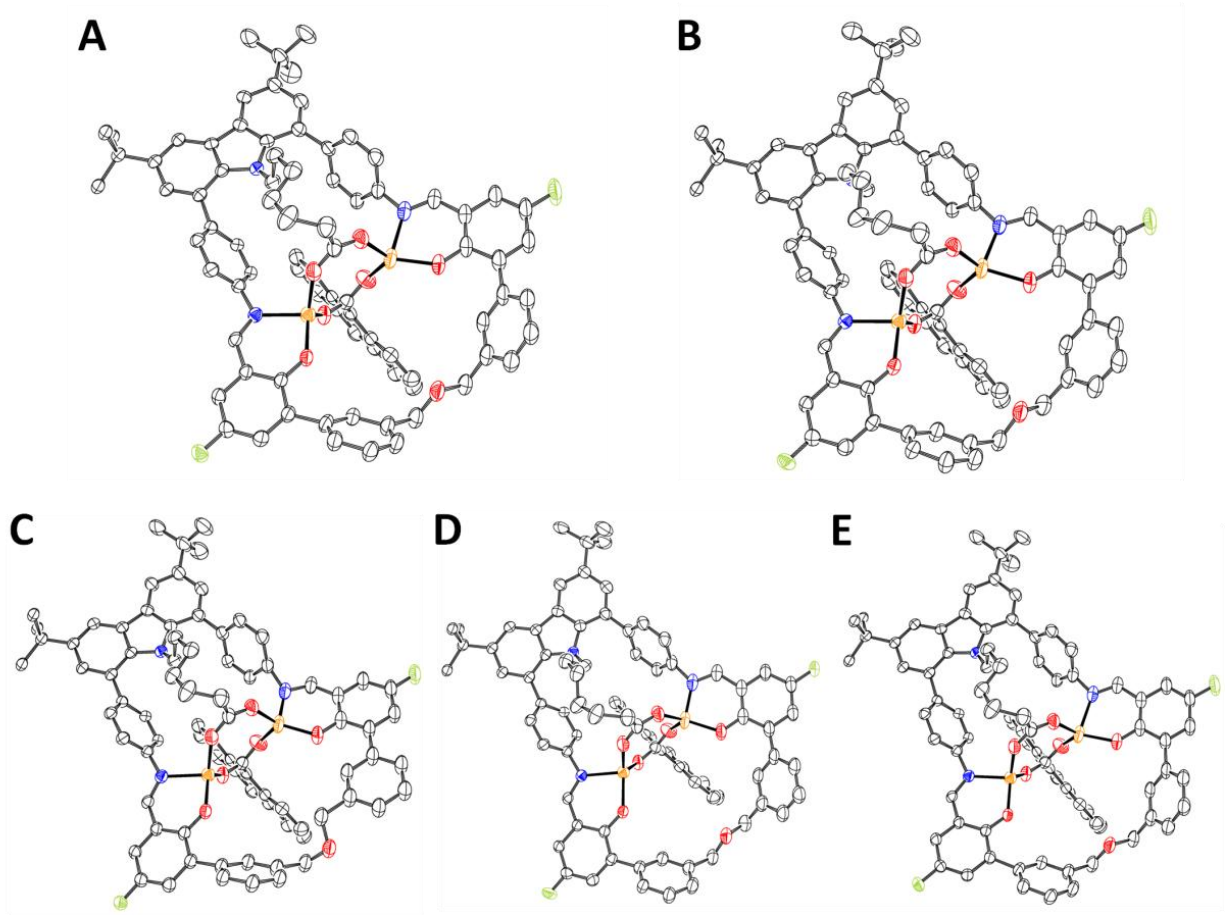


Figure S4. Thermal ellipsoid representation of selected disorder components of residue 1. Hydrogen atoms and coordinated solvent molecules are omitted for clarity. Thermal ellipsoids are set at 50%. Representations of the minor occupied species show component 1 of the internal carboxylate disorder. **A** & **B** main occupied species: component 1 (**A**) and 2 (**B**). **C-E** minor occupied species: component 3 and 4 (**C**); component 3 and 2 (**D**); component 1 and 5 (**E**).

Residue 2

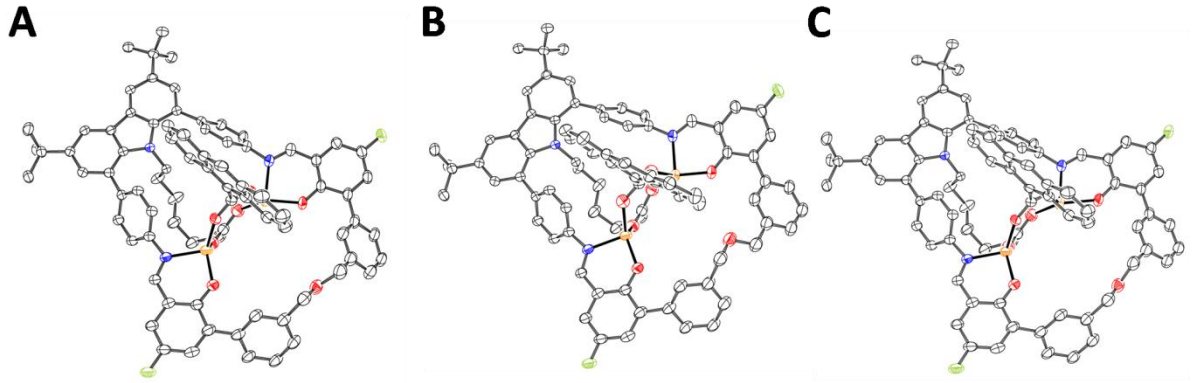


Figure S5. Thermal ellipsoid representation of selected disorder components of residue 2. Hydrogen atoms and coordinated solvent molecules are omitted for clarity. Thermal ellipsoids are set at 50%. **A** main occupied species: component 1. **B-C** minor occupied species: component 2 (**B**) and component 3 (**C**). Representation of component 3 shows component 1 of the carboxylate disorders.

Residue 3

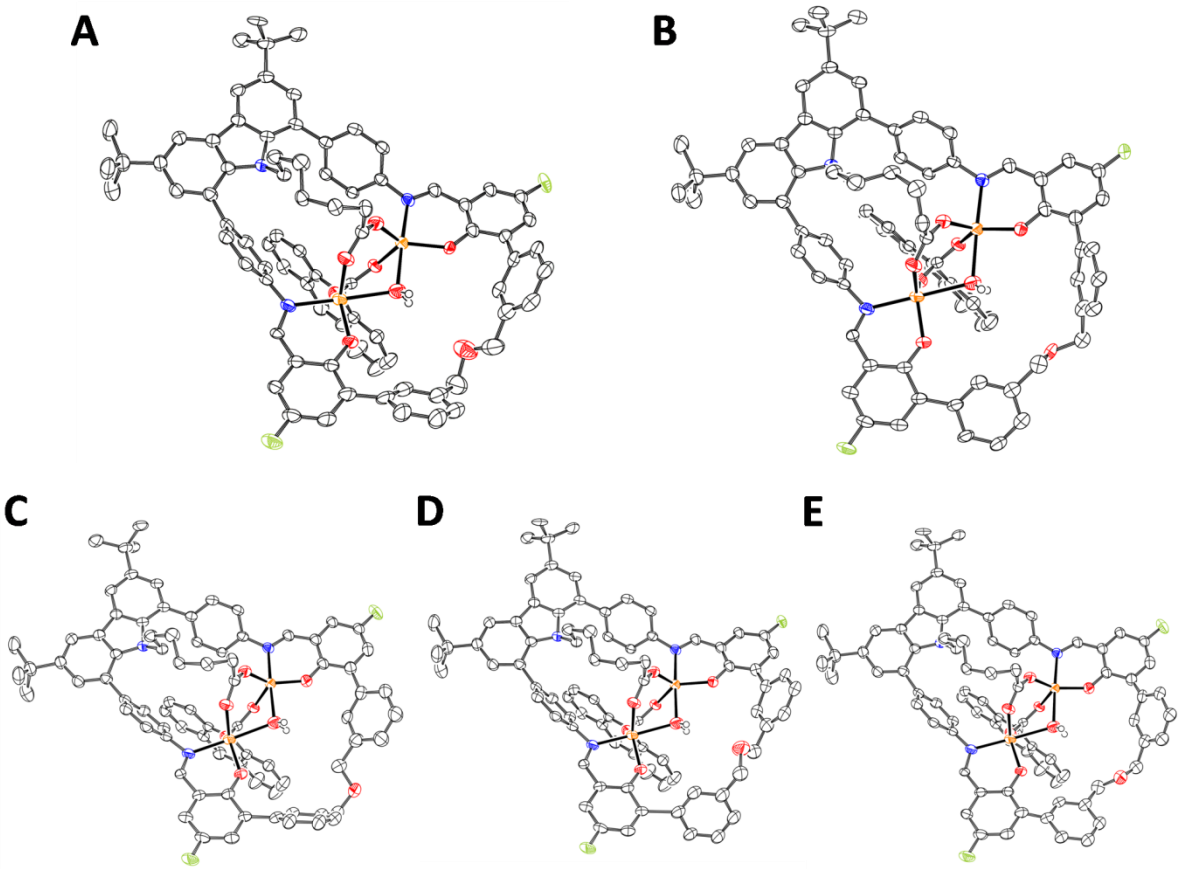


Figure S6. Thermal ellipsoid representation of selected disorder components of residue 3. Hydrogen atoms except O-hydrogens and coordinated solvent molecules are omitted for clarity. Thermal ellipsoids are set at 50%. Representations of the minor occupied species show component 1 of the internal carboxylate and *tert*-butyl disorder. **A** & **B** main occupied species: component 1 (**A**) and 2 (**B**). **C-E** minor occupied species: component 3 (**C**); component 4 (**D**); component 5 (**E**).