

Table of Positional Parameters and Their E.S.D.

Atom	x	y	z	Ueqv
Fe1	0.27056(2)	-0.09751(2)	0.28351(2)	0.0274(1)
Ni1	0.23062(2)	-0.08192(2)	0.16077(1)	0.0319(1)
C1	0.3610(2)	-0.0941(1)	0.2461(1)	0.035(1)
O1	0.4235(1)	-0.09066(9)	0.2242(1)	0.047(1)
C2	0.1547(2)	-0.0881(1)	0.2587(1)	0.038(1)
O2	0.0781(1)	-0.0820(1)	0.2434(1)	0.050(1)
C3	0.2973(2)	-0.1338(1)	0.3609(1)	0.041(1)
O3	0.3149(2)	-0.1586(1)	0.4112(1)	0.068(1)
P1	0.28803(4)	0.00936(3)	0.31004(3)	0.0263(2)
C4	0.2073(1)	0.0414(1)	0.3536(1)	0.029(1)
C5	0.2179(2)	0.0247(1)	0.4185(1)	0.039(1)
C6	0.1554(2)	0.0439(2)	0.4533(1)	0.046(1)
C7	0.0822(2)	0.0802(1)	0.4229(1)	0.046(1)
C8	0.0709(2)	0.0964(1)	0.3588(1)	0.047(1)
C9	0.1324(2)	0.0768(1)	0.3239(1)	0.039(1)
C10	0.3932(1)	0.0399(1)	0.3597(1)	0.030(1)
C11	0.4548(2)	-0.0042(1)	0.3943(1)	0.037(1)
C12	0.5351(2)	0.0199(1)	0.4301(1)	0.041(1)
C13	0.5546(2)	0.0866(1)	0.4315(1)	0.041(1)
C14	0.4941(2)	0.1309(1)	0.3970(2)	0.046(1)
C15	0.4139(2)	0.1078(1)	0.3615(1)	0.040(1)
C16	0.2809(2)	0.0636(1)	0.2384(1)	0.031(1)
P2	0.23408(4)	0.02323(3)	0.16017(3)	0.0284(3)
C17	0.3069(2)	0.0568(1)	0.1103(1)	0.031(1)
C18	0.3983(2)	0.0477(1)	0.1314(1)	0.038(1)
C19	0.4558(2)	0.0685(1)	0.0939(1)	0.048(1)
C20	0.4233(2)	0.0986(1)	0.0349(1)	0.053(1)

Table of Positional Parameters and Their E.S.D. (cont.)

Atom	x	y	z	Ueqv
C21	0.3335(2)	0.1083(1)	0.0136(1)	0.045(1)
C22	0.2747(2)	0.0872(1)	0.0506(1)	0.037(1)
C23	0.1285(2)	0.0653(1)	0.1321(1)	0.037(1)
C24	0.0512(2)	0.0282(2)	0.1133(2)	0.055(2)
C25	-0.0298(2)	0.0617(2)	0.0927(2)	0.070(2)
C26	-0.0322(2)	0.1309(2)	0.0910(2)	0.078(2)
C27	0.0433(2)	0.1669(2)	0.1094(2)	0.075(2)
C28	0.1242(2)	0.1352(2)	0.1305(1)	0.053(2)
C29	0.1956(2)	-0.0771(1)	0.0666(1)	0.043(1)
O4	0.2295(1)	-0.18092(8)	0.15975(8)	0.0403(9)
C30	0.2101(2)	-0.2292(1)	0.1082(2)	0.055(2)
Si1	0.24620(5)	-0.20018(3)	0.23895(4)	0.0359(3)
O5	0.3204(1)	-0.25958(9)	0.25078(9)	0.048(1)
C31	0.4053(2)	-0.2559(2)	0.2371(2)	0.056(2)
O6	0.1573(1)	-0.2427(1)	0.2430(1)	0.067(1)
C32	0.1198(2)	-0.2490(2)	0.2968(2)	0.084(2)
Fe2	0.74454(2)	0.14259(2)	0.27772(1)	0.0252(1)
Ni2	0.71058(2)	0.15725(1)	0.15442(1)	0.0266(1)
C33	0.8385(2)	0.1502(1)	0.2437(1)	0.031(1)
O7	0.9033(1)	0.15495(9)	0.22468(9)	0.0418(9)
C34	0.6275(2)	0.1458(1)	0.2512(1)	0.036(1)
O8	0.5515(1)	0.1475(1)	0.2353(1)	0.052(1)
C35	0.7730(2)	0.1051(1)	0.3550(1)	0.036(1)
O9	0.7921(2)	0.0787(1)	0.4043(1)	0.056(1)
P3	0.75021(4)	0.24971(3)	0.30381(3)	0.0261(3)
C36	0.6800(2)	0.2780(1)	0.3581(1)	0.030(1)
C37	0.6093(3)	0.3184(2)	0.3405(2)	0.116(2)

Table of Positional Parameters and Their E.S.D. (cont.)

Atom	x	y	z	Ueqv
C38	0.5572(3)	0.3360(2)	0.3841(2)	0.148(3)
C39	0.5767(2)	0.3138(2)	0.4449(2)	0.067(2)
C40	0.6454(2)	0.2723(2)	0.4635(1)	0.051(2)
C41	0.6970(2)	0.2544(2)	0.4201(1)	0.048(1)
C42	0.8576(2)	0.2844(1)	0.3436(1)	0.031(1)
C43	0.9222(2)	0.2423(1)	0.3790(1)	0.035(1)
C44	1.0039(2)	0.2672(1)	0.4095(1)	0.040(1)
C45	1.0224(2)	0.3348(1)	0.4041(1)	0.044(1)
C46	0.9590(2)	0.3766(1)	0.3700(1)	0.044(1)
C47	0.8767(2)	0.3520(1)	0.3402(1)	0.039(1)
C48	0.7120(2)	0.3034(1)	0.2323(1)	0.040(1)
P4	0.70105(4)	0.26213(3)	0.15326(3)	0.0266(3)
C49	0.5967(2)	0.3000(1)	0.1109(1)	0.036(1)
C50	0.5889(2)	0.3696(1)	0.1061(1)	0.046(1)
C51	0.5078(2)	0.3978(2)	0.0785(2)	0.058(2)
C52	0.4355(2)	0.3583(2)	0.0554(2)	0.056(2)
C53	0.4428(2)	0.2899(2)	0.0598(2)	0.055(2)
C54	0.5230(2)	0.2601(1)	0.0878(1)	0.043(1)
C55	0.7853(2)	0.3000(1)	0.1169(1)	0.031(1)
C56	0.7663(2)	0.3189(1)	0.0517(1)	0.039(1)
C57	0.8340(2)	0.3400(1)	0.0228(1)	0.053(1)
C58	0.9203(2)	0.3437(1)	0.0589(2)	0.058(2)
C59	0.9381(2)	0.3269(1)	0.1234(2)	0.056(2)
C60	0.8720(2)	0.3049(1)	0.1526(2)	0.042(1)
C61	0.6848(2)	0.1610(1)	0.0601(1)	0.032(1)
O10	0.7229(1)	0.05850(8)	0.15432(8)	0.0333(8)
C62	0.7150(2)	0.0100(1)	0.1034(1)	0.039(1)

Table of Positional Parameters and Their E.S.D. (cont.)

Atom	X	Y	Z	Ueqv
Si2	0.72929(4)	0.04035(3)	0.23290(3)	0.0278(3)
O11	0.8040(1)	-0.01915(8)	0.25218(9)	0.0365(8)
C63	0.8962(2)	-0.0097(1)	0.2618(2)	0.055(2)
O12	0.6374(1)	-0.00129(8)	0.23036(9)	0.0390(8)
C64	0.6116(2)	-0.0193(2)	0.2890(2)	0.057(2)

Anisotropically refined atoms are given in the form
of the isotropic equivalent displacement parameter
defined as one third of the trace of the orthogonalized
Uij tensor.

Table of Positional Parameters for the Hydrogen Atoms

Atom	x	y	z	Ueqv	
H1	0.2684	-0.0001	0.4394	0.0520	*
H2	0.1631	0.0322	0.4975	0.0617	*
H3	0.0396	0.0939	0.4465	0.0574	*
H4	0.0204	0.1214	0.3381	0.0595	*
H5	0.1232	0.0877	0.2793	0.0509	*
H6	0.4424	-0.0508	0.3937	0.0489	*
H7	0.5769	-0.0106	0.4539	0.0561	*
H8	0.6096	0.1024	0.4561	0.0555	*
H9	0.5075	0.1773	0.3975	0.0622	*
H10	0.3724	0.1387	0.3381	0.0555	*
H11	0.3389	0.0785	0.2376	0.0405	*
H12	0.2448	0.1010	0.2428	0.0405	*
H13	0.4210	0.0271	0.1720	0.0495	*
H14	0.5177	0.0620	0.1087	0.0610	*
H15	0.4628	0.1126	0.0089	0.0656	*
H16	0.3115	0.1296	-0.0268	0.0623	*
H17	0.2128	0.0934	0.0353	0.0493	*
H18	0.0531	-0.0193	0.1143	0.0803	*
H19	-0.0830	0.0368	0.0799	0.1150	*
H20	-0.0871	0.1533	0.0769	0.1191	*
H21	0.0407	0.2144	0.1079	0.1056	*
H22	0.1766	0.1610	0.1438	0.0709	*
H23	0.1910	-0.0316	0.0535	0.0636	*
H24	0.2387	-0.0989	0.0483	0.0636	*
H25	0.1399	-0.0985	0.0524	0.0636	*
H26	0.2034	-0.2069	0.0678	0.0758	*
H27	0.2574	-0.2604	0.1129	0.0758	*

Table of Positional Parameters for the Hydrogen Atoms (cont.)

Atom	x	y	z	Ueqv	
H28	0.1569	-0.2521	0.1098	0.0758	*
H29	0.4355	-0.2970	0.2483	0.0753	*
H30	0.3999	-0.2475	0.1923	0.0753	*
H31	0.4377	-0.2205	0.2614	0.0753	*
H32	0.0685	-0.2764	0.2861	0.1035	*
H33	0.1614	-0.2690	0.3312	0.1035	*
H34	0.1039	-0.2060	0.3097	0.1035	*
H35	0.5945	0.3354	0.2976	0.1489	*
H36	0.5073	0.3641	0.3702	0.1860	*
H37	0.5423	0.3273	0.4746	0.0828	*
H38	0.6588	0.2551	0.5063	0.0683	*
H39	0.7456	0.2250	0.4341	0.0651	*
H40	0.9100	0.1960	0.3822	0.0463	*
H41	1.0473	0.2383	0.4341	0.0536	*
H42	1.0790	0.3519	0.4241	0.0565	*
H43	0.9717	0.4228	0.3668	0.0560	*
H44	0.8329	0.3816	0.3173	0.0509	*
H45	0.7530	0.3391	0.2344	0.0679	*
H46	0.6557	0.3209	0.2345	0.0679	*
H47	0.6389	0.3974	0.1216	0.0604	*
H48	0.5022	0.4451	0.0754	0.0761	*
H49	0.3802	0.3782	0.0364	0.0771	*
H50	0.3925	0.2627	0.0436	0.0752	*
H51	0.5276	0.2127	0.0912	0.0570	*
H52	0.7071	0.3173	0.0272	0.0515	*
H53	0.8213	0.3519	-0.0217	0.0680	*
H54	0.9667	0.3578	0.0392	0.0760	*

Table of Positional Parameters for the Hydrogen Atoms (cont.)

Atom	x	y	z	Ueqv	
H55	0.9969	0.3304	0.1482	0.0794	*
H56	0.8855	0.2932	0.1971	0.0589	*
H57	0.6755	0.2062	0.0464	0.0424	*
H58	0.7333	0.1431	0.0449	0.0424	*
H59	0.6331	0.1356	0.0432	0.0424	*
H60	0.7125	0.0323	0.0635	0.0517	*
H61	0.7647	-0.0191	0.1121	0.0517	*
H62	0.6624	-0.0154	0.1009	0.0517	*
H63	0.9255	-0.0513	0.2724	0.0752	*
H64	0.9100	0.0073	0.2233	0.0752	*
H65	0.9154	0.0212	0.2960	0.0752	*
H66	0.5572	-0.0431	0.2790	0.0720	*
H67	0.6559	-0.0468	0.3144	0.0720	*
H68	0.6045	0.0201	0.3125	0.0720	*

Table of General Displacement Parameter Expressions - U's

Name	U(1,1)	U(2,2)	U(3,3)	U(1,2)	U(1,3)	U(2,3)
Fe1	.0283(1)	.0282(1)	.0257(1)	-.0020(1)	.0075(1)	-.0020(1)
Ni1	.0395(1)	.0333(1)	.0246(1)	-.0068(1)	.0066(1)	-.0051(1)
C1	.036(1)	.029(1)	.039(1)	-.002(1)	.0108(9)	-.001(1)
O1	.0369(8)	.049(1)	.059(1)	-.0028(8)	.0215(7)	-.0015(9)
C2	.037(1)	.039(1)	.039(1)	-.003(1)	.0119(9)	-.010(1)
O2	.0287(8)	.062(1)	.072(1)	.0009(9)	.0098(8)	-.012(1)
C3	.048(1)	.039(1)	.037(1)	-.008(1)	.004(1)	.005(1)
O3	.106(2)	.073(1)	.041(1)	-.021(1)	-.001(1)	.022(1)
P1	.0292(2)	.0284(3)	.0219(2)	-.0003(2)	.0056(2)	-.0023(2)
C4	.032(1)	.030(1)	.026(1)	-.0011(9)	.0079(8)	-.0025(9)
C5	.040(1)	.053(1)	.028(1)	.001(1)	.0093(9)	-.000(1)
C6	.049(1)	.066(2)	.030(1)	-.004(1)	.015(1)	-.005(1)
C7	.045(1)	.045(1)	.048(1)	-.004(1)	.023(1)	-.013(1)
C8	.044(1)	.043(1)	.054(1)	.010(1)	.019(1)	-.001(1)
C9	.043(1)	.042(1)	.034(1)	.012(1)	.011(1)	.003(1)
C10	.028(1)	.037(1)	.025(1)	-.003(1)	.0046(8)	-.0031(9)
C11	.038(1)	.037(1)	.036(1)	-.005(1)	.005(1)	.001(1)
C12	.036(1)	.051(1)	.038(1)	.001(1)	-.002(1)	.003(1)
C13	.036(1)	.052(1)	.038(1)	-.008(1)	.002(1)	-.007(1)
C14	.048(1)	.038(1)	.053(2)	-.012(1)	.000(1)	-.010(1)
C15	.045(1)	.035(1)	.042(1)	.002(1)	-.004(1)	-.004(1)
C16	.038(1)	.031(1)	.025(1)	-.005(1)	.0080(9)	-.0023(9)
P2	.0304(3)	.0342(3)	.0221(2)	-.0008(2)	.0062(2)	-.0014(2)
C17	.038(1)	.030(1)	.026(1)	.002(1)	.0113(8)	-.0004(9)
C18	.037(1)	.042(1)	.036(1)	-.002(1)	.010(1)	.006(1)
C19	.042(1)	.050(1)	.053(1)	-.002(1)	.020(1)	-.001(1)
C20	.062(1)	.053(2)	.045(1)	-.014(1)	.029(1)	-.002(1)

Table of General Displacement Parameter Expressions (Continued)

Name	U(1,1)	U(2,2)	U(3,3)	U(1,2)	U(1,3)	U(2,3)
C21	.075(2)	.046(1)	.026(1)	-.007(1)	.018(1)	.002(1)
C22	.048(1)	.039(1)	.026(1)	-.002(1)	.007(1)	-.001(1)
C23	.033(1)	.062(2)	.025(1)	.008(1)	.0047(9)	-.001(1)
C24	.037(1)	.101(3)	.044(2)	-.008(2)	.003(1)	.013(2)
C25	.034(1)	.170(4)	.058(2)	-.005(2)	.002(1)	.027(2)
C26	.058(2)	.169(4)	.050(2)	.053(2)	.014(1)	.022(2)
C27	.073(2)	.115(2)	.050(2)	.058(2)	.001(2)	-.009(2)
C28	.051(1)	.068(2)	.042(1)	.027(1)	.004(1)	-.012(1)
C29	.069(2)	.048(1)	.024(1)	-.011(1)	-.001(1)	-.007(1)
O4	.059(1)	.0321(8)	.0344(9)	-.0074(8)	.0069(8)	-.0099(7)
C30	.081(2)	.043(1)	.048(2)	-.015(2)	.010(2)	-.017(1)
Si1	.0399(3)	.0291(3)	.0400(3)	-.0059(3)	.0179(2)	-.0049(3)
O5	.059(1)	.0364(9)	.052(1)	.0069(9)	.0229(8)	.0007(8)
C31	.049(1)	.046(2)	.080(2)	.006(1)	.016(1)	-.006(2)
O6	.066(1)	.054(1)	.083(1)	-.0314(9)	.0437(8)	-.025(1)
C32	.076(2)	.073(2)	.104(2)	-.028(2)	.053(1)	-.006(2)
Fe2	.0324(1)	.0209(1)	.0236(1)	.0008(1)	.0064(1)	-.0009(1)
Ni2	.0352(1)	.0237(1)	.0226(1)	.0011(1)	.0070(1)	-.0025(1)
C33	.039(1)	.023(1)	.032(1)	-.000(1)	.0058(9)	-.0014(9)
O7	.0352(8)	.045(1)	.047(1)	-.0032(8)	.0140(7)	.0017(8)
C34	.035(1)	.032(1)	.041(1)	.004(1)	.007(1)	-.004(1)
O8	.0352(9)	.058(1)	.067(1)	.0100(9)	.0081(9)	-.006(1)
C35	.048(1)	.028(1)	.033(1)	-.005(1)	.005(1)	.002(1)
O9	.088(2)	.054(1)	.036(1)	-.007(1)	-.002(1)	.0143(9)
P3	.0398(3)	.0218(2)	.0206(2)	.0021(2)	.0058(2)	-.0002(2)
C36	.036(1)	.025(1)	.030(1)	.0006(9)	.0068(9)	-.0038(9)
C37	.136(2)	.144(2)	.080(2)	.108(2)	.060(2)	.063(2)

Table of General Displacement Parameter Expressions (Continued)

Name	U(1,1)	U(2,2)	U(3,3)	U(1,2)	U(1,3)	U(2,3)
C38	.155(2)	.184(3)	.115(3)	.137(2)	.083(2)	.070(3)
C39	.065(2)	.068(2)	.068(2)	.010(2)	.034(1)	-.007(2)
C40	.058(1)	.069(2)	.034(1)	-.002(2)	.017(1)	-.007(1)
C41	.054(1)	.067(2)	.031(1)	.022(1)	.012(1)	.001(1)
C42	.036(1)	.029(1)	.030(1)	-.0031(9)	.0125(8)	-.0035(9)
C43	.042(1)	.031(1)	.034(1)	-.004(1)	.008(1)	-.002(1)
C44	.041(1)	.046(1)	.035(1)	.000(1)	.004(1)	-.004(1)
C45	.044(1)	.050(1)	.040(1)	-.015(1)	.016(1)	-.014(1)
C46	.050(1)	.034(1)	.050(1)	-.008(1)	.022(1)	-.010(1)
C47	.046(1)	.028(1)	.046(1)	-.002(1)	.017(1)	-.004(1)
C48	.101(2)	.031(1)	.021(1)	.016(1)	.006(1)	-.001(1)
P4	.0362(3)	.0249(3)	.0209(2)	.0039(2)	.0063(2)	-.0004(2)
C49	.037(1)	.042(1)	.029(1)	.010(1)	.0081(9)	.002(1)
C50	.051(1)	.039(1)	.049(2)	.012(1)	.010(1)	.004(1)
C51	.065(2)	.056(2)	.052(2)	.031(1)	.010(1)	.010(1)
C52	.046(1)	.086(2)	.044(2)	.029(1)	.008(1)	.004(2)
C53	.041(1)	.082(2)	.050(2)	.010(1)	.007(1)	-.005(2)
C54	.038(1)	.055(2)	.039(1)	.006(1)	.009(1)	-.003(1)
C55	.040(1)	.023(1)	.034(1)	.002(1)	.0087(9)	.0014(9)
C56	.049(1)	.040(1)	.031(1)	-.005(1)	.012(1)	-.001(1)
C57	.078(2)	.039(1)	.049(1)	-.009(1)	.032(1)	-.004(1)
C58	.063(2)	.035(1)	.088(2)	-.011(1)	.040(1)	-.009(1)
C59	.045(1)	.041(1)	.096(2)	-.004(1)	.012(2)	.011(2)
C60	.039(1)	.033(1)	.059(2)	-.002(1)	-.000(1)	.010(1)
C61	.039(1)	.033(1)	.026(1)	-.000(1)	.0086(9)	-.0062(9)
O10	.0508(9)	.0239(7)	.0305(8)	-.0017(7)	.0118(7)	-.0061(6)
C62	.055(1)	.030(1)	.036(1)	-.002(1)	.014(1)	-.011(1)

Table of General Displacement Parameter Expressions (Continued)

Name	U(1,1)	U(2,2)	U(3,3)	U(1,2)	U(1,3)	U(2,3)
Si2	.0315(3)	.0217(3)	.0316(3)	-.0012(2)	.0098(2)	-.0021(2)
O11	.0383(8)	.0248(7)	.051(1)	.0038(7)	.0134(7)	.0005(7)
C63	.041(1)	.045(1)	.090(2)	.010(1)	.019(1)	.017(2)
O12	.0391(8)	.0353(8)	.0430(9)	-.0110(7)	.0134(7)	-.0077(7)
C64	.052(1)	.058(2)	.060(2)	-.023(1)	.021(1)	.004(1)

Table of Bond Distances in Angstroms

Atom 1	Atom 2	Distance	Atom 1	Atom 2	Distance
=====	=====	=====	=====	=====	=====
FE1	NI1	2.5597(5)	C3	O3	1.153(4)
FE1	C1	1.756(3)	P1	C4	1.825(2)
FE1	C2	1.767(3)	P1	C10	1.839(2)
FE1	C3	1.759(3)	P1	C16	1.850(2)
FE1	P1	2.2098(7)	C4	C5	1.392(4)
FE1	SI1	2.2558(8)	C4	C9	1.386(3)
NI1	C1	2.411(3)	C5	C6	1.393(4)
NI1	P2	2.1020(7)	C6	C7	1.380(4)
NI1	C29	1.953(3)	C7	C8	1.372(4)
NI1	O4	1.978(2)	C8	C9	1.385(4)
FE2	NI2	2.5688(4)	C10	C11	1.386(4)
FE2	C33	1.766(3)	C10	C15	1.393(4)
FE2	C34	1.777(3)	C11	C12	1.392(4)
FE2	C35	1.767(3)	C12	C13	1.367(4)
FE2	P3	2.2077(7)	C13	C14	1.377(4)
FE2	SI2	2.2438(7)	C14	C15	1.383(4)
NI2	C33	2.427(3)	C16	P2	1.844(2)
NI2	P4	2.1005(7)	P2	C17	1.833(2)
NI2	C61	1.954(3)	P2	C23	1.818(3)
NI2	O10	1.982(2)	C17	C18	1.400(4)
FE1	C1	1.756(3)	C17	C22	1.394(4)
FE1	C2	1.767(3)	C18	C19	1.381(4)
FE1	C3	1.759(3)	C19	C20	1.381(5)
NI1	C29	1.953(3)	C20	C21	1.379(5)
NI1	O4	1.978(2)	C21	C22	1.392(4)
C1	O1	1.163(3)	C23	C24	1.390(4)
C2	O2	1.165(3)	C23	C28	1.399(4)

Bond Distances (cont.)

Atom 1	Atom 2	Distance	Atom 1	Atom 2	Distance
=====	=====	=====	=====	=====	=====
C24	C25	1.404(5)	C42	C43	1.394(4)
C25	C26	1.382(7)	C42	C47	1.389(3)
C26	C27	1.355(7)	C43	C44	1.382(4)
C27	C28	1.388(4)	C44	C45	1.389(4)
O4	C30	1.440(3)	C45	C46	1.369(4)
O4	SI1	1.687(2)	C46	C47	1.383(4)
SI1	O5	1.633(2)	C48	P4	1.843(3)
SI1	O6	1.636(2)	P4	C49	1.832(3)
O5	C31	1.409(4)	P4	C55	1.819(3)
O6	C32	1.394(4)	C49	C50	1.398(4)
FE2	C33	1.766(3)	C49	C54	1.391(4)
FE2	C34	1.777(3)	C50	C51	1.385(4)
FE2	C35	1.767(3)	C51	C52	1.370(5)
NI2	C61	1.954(3)	C52	C53	1.373(5)
NI2	O10	1.982(2)	C53	C54	1.389(4)
C33	O7	1.164(3)	C55	C56	1.401(4)
C34	O8	1.152(3)	C55	C60	1.394(4)
C35	O9	1.151(3)	C56	C57	1.391(4)
P3	C36	1.836(2)	C57	C58	1.389(5)
P3	C42	1.829(3)	C58	C59	1.377(6)
P3	C48	1.846(3)	C59	C60	1.379(4)
C36	C37	1.346(4)	O10	C62	1.437(3)
C36	C41	1.368(4)	O10	SI2	1.687(2)
C37	C38	1.398(6)	SI2	O11	1.647(2)
C38	C39	1.334(6)	SI2	O12	1.638(2)
C39	C40	1.338(5)	O11	C63	1.410(3)
C40	C41	1.391(4)	O12	C64	1.433(4)

Table of Bond Angles in Degrees

At 1	At 2	At 3	Angle	At 1	At 2	At 3	Angle
====	====	====	=====	====	====	====	=====
N11	FE1	C1	64.83(9)	N12	FE2	C35	161.12(9)
N11	FE1	C2	71.35(9)	N12	FE2	P3	97.62(2)
N11	FE1	C3	162.6(1)	N12	FE2	SI2	72.15(2)
N11	FE1	P1	97.48(2)	C33	FE2	C34	137.9(1)
N11	FE1	SI1	72.75(2)	C33	FE2	C35	110.8(1)
C1	FE1	C2	136.1(1)	C33	FE2	P3	91.58(8)
C1	FE1	C3	113.0(1)	C33	FE2	SI2	85.73(8)
C1	FE1	P1	90.69(8)	C34	FE2	C35	109.8(1)
C1	FE1	SI1	85.58(9)	C34	FE2	P3	91.51(8)
C2	FE1	C3	109.8(1)	C34	FE2	SI2	83.86(9)
C2	FE1	P1	91.87(9)	C35	FE2	P3	100.94(9)
C2	FE1	SI1	84.62(9)	C35	FE2	SI2	89.38(9)
C3	FE1	P1	99.8(1)	P3	FE2	SI2	169.62(3)
C3	FE1	SI1	90.0(1)	FE2	N12	C33	41.28(6)
P1	FE1	SI1	170.22(3)	FE2	N12	P4	97.12(2)
FE1	N11	C1	41.25(6)	FE2	N12	C61	175.65(7)
FE1	N11	P2	97.29(2)	FE2	N12	O10	83.64(5)
FE1	N11	C29	175.38(9)	C33	NI2	P4	96.33(6)
FE1	N11	O4	83.63(6)	C33	NI2	C61	138.6(1)
C1	N11	P2	94.99(6)	C33	NI2	O10	83.16(8)
C1	N11	C29	140.5(1)	P4	NI2	C61	87.23(7)
C1	N11	O4	84.92(8)	P4	NI2	O10	178.20(6)
P2	N11	C29	86.92(9)	C61	NI2	O10	92.02(9)
P2	N11	O4	178.50(6)	C1	FE1	C2	136.1(1)
C29	N11	O4	92.2(1)	C1	FE1	C3	113.0(1)
N12	FE2	C33	65.06(8)	C2	FE1	C3	109.8(1)
N12	FE2	C34	72.90(9)	C29	N11	O4	92.2(1)

Bond Angles (cont.)

At 1	At 2	At 3	Angle	At 1	At 2	At 3	Angle
=====	=====	=====	=====	=====	=====	=====	=====
FE1	C1	O1	176.6(3)	P2	C17	C22	122.7(2)
FE1	C2	O2	178.9(3)	C18	C17	C22	118.9(2)
FE1	C3	O3	178.9(3)	C17	C18	C19	120.8(3)
C4	P1	C10	102.3(1)	C18	C19	C20	120.0(3)
C4	P1	C16	106.6(1)	C19	C20	C21	120.0(3)
C10	P1	C16	99.4(1)	C20	C21	C22	120.7(3)
P1	C4	C5	118.0(2)	C17	C22	C21	119.7(3)
P1	C4	C9	123.2(2)	P2	C23	C24	120.3(3)
C5	C4	C9	118.6(2)	P2	C23	C28	120.3(2)
C4	C5	C6	120.8(3)	C24	C23	C28	119.5(3)
C5	C6	C7	119.6(3)	C23	C24	C25	119.3(4)
C6	C7	C8	120.0(3)	C24	C25	C26	120.1(4)
C7	C8	C9	120.7(3)	C25	C26	C27	120.5(4)
C4	C9	C8	120.4(3)	C26	C27	C28	120.8(4)
P1	C10	C11	120.9(2)	C23	C28	C27	119.9(4)
P1	C10	C15	120.6(2)	NI1	O4	C30	132.7(2)
C11	C10	C15	118.4(2)	NI1	O4	SI1	102.61(9)
C10	C11	C12	119.9(2)	C30	O4	SI1	124.4(2)
C11	C12	C13	121.1(3)	O4	SI1	O5	105.6(1)
C12	C13	C14	119.6(3)	O4	SI1	O6	102.9(1)
C13	C14	C15	120.0(3)	O5	SI1	O6	100.8(1)
C10	C15	C14	121.0(3)	SI1	O5	C31	126.0(2)
P1	C16	P2	115.1(1)	SI1	O6	C32	126.6(2)
C16	P2	C17	100.9(1)	C33	FE2	C34	137.9(1)
C16	P2	C23	103.9(1)	C33	FE2	C35	110.8(1)
C17	P2	C23	105.4(1)	C34	FE2	C35	109.8(1)
P2	C17	C18	118.4(2)	C61	NI2	O10	92.02(9)

Bond Angles (cont.)

At 1	At 2	At 3	Angle	At 1	At 2	At 3	Angle
=====	=====	=====	=====	=====	=====	=====	=====
FE2	C33	O7	176.3(2)	C49	P4	C55	104.9(1)
FE2	C34	O8	178.5(3)	P4	C49	C50	120.0(2)
FE2	C35	O9	177.6(3)	P4	C49	C54	120.2(2)
C36	P3	C42	101.4(1)	C50	C49	C54	119.6(3)
C36	P3	C48	102.0(1)	C49	C50	C51	119.4(3)
C42	P3	C48	104.8(1)	C50	C51	C52	120.8(3)
P3	C36	C37	124.6(3)	C51	C52	C53	120.0(3)
P3	C36	C41	118.8(2)	C52	C53	C54	120.6(3)
C37	C36	C41	116.5(3)	C49	C54	C53	119.5(3)
C36	C37	C38	121.3(4)	P4	C55	C56	121.0(2)
C37	C38	C39	120.9(4)	P4	C55	C60	119.6(2)
C38	C39	C40	119.3(3)	C56	C55	C60	119.2(3)
C39	C40	C41	119.9(3)	C55	C56	C57	120.1(3)
C36	C41	C40	122.0(3)	C56	C57	C58	120.0(3)
P3	C42	C43	119.6(2)	C57	C58	C59	119.6(3)
P3	C42	C47	121.8(2)	C58	C59	C60	121.1(3)
C43	C42	C47	118.6(2)	C55	C60	C59	120.0(3)
C42	C43	C44	120.7(2)	NI2	O10	C62	132.9(2)
C43	C44	C45	119.7(3)	NI2	O10	SI2	101.41(8)
C44	C45	C46	120.0(3)	C62	O10	SI2	125.1(2)
C45	C46	C47	120.5(3)	O10	SI2	O11	106.7(1)
C42	C47	C46	120.5(3)	O10	SI2	O12	102.3(1)
P3	C48	P4	115.8(1)	O11	SI2	O12	101.5(1)
C48	P4	C49	99.0(1)	SI2	O11	C63	125.0(2)
C48	P4	C55	105.5(1)	SI2	O12	C64	120.3(2)