

Appendix A: Atomic Co-ordinates

Atom	x	y	z	U _{iso}
V1	0.40401(5)	-0.14673(5)	0.07206(4)	0.00974(13)
V2	0.23861(5)	0.18024(5)	0.17905(4)	0.01192(14)
F1	0.25615(18)	-0.00255(17)	0.13748(16)	0.0161(3)
F2	0.21063(17)	-0.14142(17)	-0.02569(16)	0.0160(3)
F3	0.41064(17)	0.07681(16)	-0.11345(15)	0.0132(3)
F4	0.45396(18)	0.22681(17)	0.04617(15)	0.0153(3)
F5	0.40034(19)	0.06448(18)	0.33467(16)	0.0192(4)
F6	0.26291(18)	0.36633(17)	0.20086(16)	0.0176(3)
F7	0.12994(19)	0.31732(18)	-0.00665(16)	0.0188(3)
O1	0.3988(2)	-0.3051(2)	0.21856(19)	0.0186(4)
O2	0.0734(2)	0.1473(2)	0.2759(2)	0.0181(4)
O3	0.0297(3)	0.4858(2)	0.2997(2)	0.0218(5)
N1	0.9465(3)	-0.1711(3)	0.1729(2)	0.0186(5)
N2	0.5508(3)	-0.2253(2)	0.5086(2)	0.0140(5)
N3	0.2062(3)	-0.3871(3)	0.9044(3)	0.0207(5)
C1	0.9745(3)	-0.1980(3)	0.3249(3)	0.0179(6)
C2	0.8163(3)	-0.1553(3)	0.3954(3)	0.0193(6)
C3	0.7004(3)	-0.2726(3)	0.4369(3)	0.0150(6)
C4	0.4297(3)	-0.3342(3)	0.5480(3)	0.0188(6)
C5	0.2926(4)	-0.3076(4)	0.6458(3)	0.0233(6)
C6	0.3456(3)	-0.3724(4)	0.8019(3)	0.0256(7)

Table A.1 Atomic Co-ordinates for **V-1**.

Atom	x	y	z	U _{iso}
V1	0.1747(4)	0.34014(17)	0.24779(15)	0.0353(7)
F1	0.6609(13)	0.3684(6)	0.2279(6)	0.0537(17)
F2	0.0806(13)	0.4182(6)	0.3725(5)	0.0383(14)
F3	0.2241(12)	0.3035(5)	0.0948(4)	0.0356(14)
O1	0.1366(15)	0.1754(7)	0.3569(6)	0.0421(18)
O2	0.2029(16)	0.5737(7)	0.0924(7)	0.0421(18)
N1	0.3710(18)	0.7429(9)	0.4200(8)	0.042(2)
C1	0.481(3)	0.6896(12)	0.3360(11)	0.050(3)
C2	0.438(2)	0.8808(11)	0.3895(10)	0.044(3)
C3	0.683(2)	0.7732(11)	0.2148(10)	0.041(3)
C4	0.633(2)	0.9686(10)	0.2714(10)	0.038(2)
C5	0.753(2)	0.9185(10)	0.1772(10)	0.039(3)
C6	0.955(2)	1.0156(12)	0.0514(10)	0.048(3)

Table A.2 Atomic Co-ordinates for **V-2**.

Atom	x	y	z	U _{iso}
V1	0.08616(8)	0.70296(6)	0.62326(5)	0.0058(3)
F1	0.0706(3)	0.5570(2)	0.39585(19)	0.0085(4)
F2	0.4077(3)	0.6164(3)	0.6469(2)	0.0103(4)
F3	0.2398(3)	0.9144(3)	0.5620(2)	0.0119(4)
O1	0.0702(4)	0.7765(3)	0.7941(2)	0.0127(5)
O2	-0.2362(4)	0.7799(3)	0.5423(3)	0.0097(5)
N1	0.4696(5)	0.3368(4)	0.7782(3)	0.0116(6)
C1	0.6339(7)	0.2145(5)	0.7644(4)	0.0181(7)
C2	0.6502(7)	0.0805(5)	0.8514(4)	0.0161(7)
C3	0.4933(5)	0.0729(4)	0.9533(3)	0.0092(6)
C4	0.3237(8)	0.2025(7)	0.9637(5)	0.0369(13)
C5	0.3160(8)	0.3330(7)	0.8747(5)	0.0346(11)

Table A.3 Atomic Co-ordinates for **V-3**.

Atom	x	y	z	U _{iso}
V1	0.28604(9)	0.38973(7)	0.88277(5)	0.01283(18)
V2	-0.04172(9)	1.12951(7)	0.59015(5)	0.01494(18)
F1	0.3724(3)	0.1611(3)	0.89831(18)	0.0206(5)
F2	0.2065(3)	0.6143(3)	0.82400(16)	0.0184(5)
F3	0.5400(3)	0.4102(3)	0.87804(18)	0.0198(5)
F4	0.0466(3)	0.3696(3)	0.84011(16)	0.0188(5)
F5	0.0316(3)	0.9240(2)	0.69592(15)	0.0127(4)
F6	-0.1238(3)	1.2973(2)	0.46754(16)	0.0154(4)
F7	0.1752(3)	1.0169(2)	0.48935(15)	0.0124(4)
F8	-0.2789(3)	1.1849(3)	0.66317(18)	0.0211(5)
O1	0.2222(4)	0.3970(3)	1.0046(2)	0.0220(6)
O2	0.3668(4)	0.3792(3)	0.7062(2)	0.0157(5)
O3	0.1113(3)	1.2224(3)	0.63622(18)	0.0112(5)
N1	0.0571(4)	1.0009(4)	0.8882(2)	0.0131(6)
N2	0.1661(4)	1.3244(4)	0.2995(3)	0.0171(7)
N3	0.5730(4)	1.2500(4)	0.3630(2)	0.0177(7)
C1	-0.1561(5)	1.0663(5)	0.9233(3)	0.0160(8)
C2	0.1672(6)	0.8684(5)	0.9745(3)	0.0178(8)
C3	0.3346(5)	1.2274(5)	0.2398(3)	0.0175(8)
C4	0.5015(5)	1.1331(5)	0.3134(3)	0.0179(8)
C5	0.4061(6)	1.3410(5)	0.4264(3)	0.0220(9)
C6	0.2337(6)	1.4386(5)	0.3554(3)	0.0225(9)

Table A.4 Atomic Co-ordinates for **V-4**.

Atom	x	y	z	U _{iso}
V1	0.21138(8)	0.73048(8)	0.40630(6)	0.0069(3)
V2	-0.22237(8)	0.25260(8)	0.07133(6)	0.0075(3)
F1	0.4265(3)	0.8078(3)	0.4253(2)	0.0110(6)
F2	0.1390(3)	0.8517(3)	0.2906(2)	0.0111(6)
F3	-0.0007(3)	0.6144(3)	0.3560(2)	0.0123(6)
F4	0.2911(3)	0.5630(3)	0.4701(2)	0.0147(6)
F5	-0.1456(3)	0.1506(3)	0.2153(2)	0.0111(6)
F6	0.0050(3)	0.3309(3)	0.1264(2)	0.0116(6)
F7	-0.1816(3)	0.0662(3)	-0.0162(2)	0.0124(6)
F8	-0.4283(3)	0.1654(3)	0.0585(2)	0.0105(6)
O1	0.1934(3)	0.8431(4)	0.5243(3)	0.0146(7)
O2	0.2274(3)	0.5681(3)	0.2335(3)	0.0103(7)
O3	-0.2759(4)	0.3302(4)	-0.0441(3)	0.0142(7)
O4	-0.2441(3)	0.4330(4)	0.1980(3)	0.0120(7)
O5	-0.4555(3)	0.4741(4)	0.3119(3)	0.0184(8)
N1	-0.9125(4)	0.1748(4)	-0.0671(3)	0.0108(8)
N2	-0.6361(4)	0.0855(4)	-0.1670(3)	0.0076(7)
N3	-0.3780(4)	-0.0858(4)	-0.3458(3)	0.0078(8)
N4	-0.0676(4)	-0.3134(4)	-0.4217(3)	0.0094(8)
C1	-0.7720(5)	0.2759(5)	-0.0594(4)	0.0110(9)
C2	-0.7135(5)	0.2271(5)	-0.1665(4)	0.0122(9)
C3	-0.5520(5)	0.0656(5)	-0.2571(4)	0.0072(8)
C4	-0.4655(5)	-0.0751(5)	-0.2557(4)	0.0072(8)
C5	-0.2619(5)	-0.1976(5)	-0.3339(4)	0.0093(9)
C6	-0.1910(5)	-0.2104(5)	-0.4373(4)	0.0095(9)

Table A.5 Atomic Co-ordinates for **V-5**.

Atom	x	y	z	U _{iso}
V1	0.13502(8)	0.41665(6)	0.41046(8)	0.0071(3)
F1	-0.0499(3)	0.3973(2)	0.2317(3)	0.0111(6)
F2	-0.0229(3)	0.3995(2)	0.5691(3)	0.0103(6)
F3	0.2570(3)	0.4984(2)	0.2591(3)	0.0138(6)
F4	0.3127(3)	0.4723(2)	0.5713(3)	0.0099(6)
O1	0.1971(4)	0.2722(3)	0.4042(4)	0.0114(7)
N1	0.5691(4)	0.2960(3)	0.5617(4)	0.0091(7)
N2	0.7651(4)	0.0425(3)	0.4496(4)	0.0078(7)
C1	0.5908(6)	0.2434(4)	0.4019(5)	0.0116(9)
C2	0.7613(5)	0.1777(4)	0.3977(5)	0.0119(9)
C3	0.9304(5)	-0.0213(4)	0.4353(4)	0.0068(8)

Table A.6 Atomic Co-ordinates for **V-6**.

Atom	x	y	z	U _{iso}
V1	0.12375(3)	0.12295(5)	0.02491(3)	0.01324(13)
F1	0.12630(11)	0.39852(17)	0.02351(9)	0.0192(3)
F2	0.09324(12)	0.14924(17)	0.17092(9)	0.0191(3)
F3	0.09079(11)	0.14550(17)	-0.13416(9)	0.0180(3)
F4	0.06853(11)	-0.14183(16)	0.01453(10)	0.0160(3)
O1	0.26124(14)	0.0748(2)	0.05320(13)	0.0232(4)
N1	0.12047(16)	0.5952(3)	-0.15759(14)	0.0162(4)
N2	0.11729(15)	0.9110(3)	-0.29770(14)	0.0152(4)
C1	0.22949(19)	0.7107(3)	-0.14834(17)	0.0166(5)
C2	0.23049(19)	0.8072(3)	-0.25700(17)	0.0160(4)
C3	0.3349(2)	0.9427(3)	-0.24062(19)	0.0211(5)
C4	0.4496(2)	0.8307(4)	-0.2020(2)	0.0286(6)
C5	0.4482(2)	0.7169(4)	-0.0987(2)	0.0341(6)
C6	0.3393(2)	0.5893(4)	-0.1134(2)	0.0266(5)

Table A.7 Atomic Co-ordinates for **V-7**.

Atom	x	y	z	U _{iso}
V1	0.28950(5)	0.91765(3)	0.23869(4)	0.00990(16)
F1	0.45223(18)	0.81306(11)	0.29465(15)	0.0200(4)
F2	0.14222(17)	0.80183(11)	0.18911(15)	0.0174(4)
F3	0.45513(16)	1.02088(11)	0.23686(15)	0.0164(4)
F4	0.14705(16)	1.01360(11)	0.12729(15)	0.0165(4)
F5	0.35226(16)	0.88488(11)	0.04343(13)	0.0121(3)
O1	0.2500(2)	0.94338(14)	0.39028(18)	0.0172(4)
O2	0.0058(2)	0.69333(16)	-0.0345(2)	0.0204(5)
N1	0.1150(2)	0.88734(15)	-0.1703(2)	0.0117(5)
N2	0.3235(2)	1.08610(15)	-0.0849(2)	0.0097(5)
N3	0.4858(2)	1.31797(15)	-0.0855(2)	0.0119(5)
C1	0.1775(3)	0.9634(2)	-0.2641(3)	0.0175(6)
C2	0.1942(3)	1.07503(19)	-0.2065(3)	0.0152(6)
C3	0.3095(3)	1.18558(19)	-0.0031(3)	0.0143(6)
C4	0.3214(3)	1.28769(19)	-0.0808(3)	0.0135(6)

Table A.8 Atomic Co-ordinates for **V-8**.

Atom	x	y	z	U _{iso}
V1	0.15955(7)	0.12341(7)	0.41367(6)	0.0091(3)
F1	0.2083(3)	0.2556(3)	0.1940(2)	0.0127(5)
F2	0.3432(3)	-0.0878(3)	0.3235(2)	0.0131(5)
F3	-0.0669(3)	0.3283(3)	0.4685(2)	0.0114(5)
F4	0.0454(3)	-0.0197(3)	0.6290(2)	0.0105(5)
O1	0.2897(3)	0.1857(3)	0.4987(3)	0.0127(5)
O2	0.7083(4)	-0.1803(3)	0.1226(3)	0.0158(6)
N1	0.0457(4)	-0.3687(4)	1.2266(4)	0.0129(6)
N2	0.3758(4)	-0.2973(4)	0.6191(3)	0.0092(6)
C1	0.1861(5)	-0.2830(5)	1.0924(4)	0.0133(7)
C2	0.2068(5)	-0.3363(5)	0.9240(4)	0.0108(7)
C3	0.3506(5)	-0.2483(5)	0.7876(4)	0.0110(7)
C4	0.4863(5)	-0.4871(5)	0.5900(4)	0.0111(7)

Table A.9 Atomic Co-ordinates for **V-9**.

Atom	x	y	z	U _{iso}
V1	0.13437(5)	0.14422(5)	0.51673(3)	0.01005(15)
F1	0.30604(17)	0.11986(17)	0.61449(11)	0.0138(3)
F2	0.26248(16)	0.03929(17)	0.42035(10)	0.0127(3)
F3	0.00738(16)	0.21458(17)	0.62910(10)	0.0114(3)
F4	0.06315(16)	-0.09100(17)	0.56232(10)	0.0123(3)
O1	0.1717(2)	0.3174(2)	0.0127(4)	0.0127(4)
O2	0.0335(2)	0.5286(2)	0.66067(14)	0.0163(4)
N1	0.3947(2)	-0.2283(2)	0.42066(15)	0.0105(4)
N2	0.3476(2)	-0.3644(2)	0.69142(15)	0.0104(4)
C1	0.4111(3)	-0.4587(3)	0.30195(18)	0.0105(5)
C2	0.3530(3)	-0.2939(3)	0.31683(18)	0.0118(5)
C3	0.3408(3)	-0.3263(3)	0.50568(18)	0.0119(5)
C4	0.3995(3)	-0.2601(3)	0.60790(18)	0.0118(5)
C5	0.4057(3)	-0.5289(3)	0.68952(18)	0.0102(5)

Table A.10 Atomic Co-ordinates for **V-10**.

Atom	x	y	z	U _{iso}
V1	0.37817(9)	0.19666(9)	0.11454(9)	0.0076(3)
F1	0.3292(3)	0.2348(3)	0.3627(3)	0.0137(6)
F2	0.1676(3)	0.0824(3)	0.1659(3)	0.0120(6)
F3	0.6217(3)	0.2368(3)	0.0852(3)	0.0101(6)
F4	0.5258(3)	-0.0751(3)	0.1355(3)	0.0094(6)
O1	0.2760(4)	0.3856(4)	0.0577(4)	0.0112(7)
N1	0.2169(5)	-0.2749(5)	0.2573(5)	0.0079(8)
N2	0.1540(5)	0.0033(5)	0.7640(5)	0.0087(8)
C1	0.0211(6)	-0.2943(6)	0.3254(6)	0.0105(9)
C2	0.3378(6)	-0.3559(6)	0.3712(6)	0.0103(9)
C3	0.2656(6)	-0.2755(6)	0.5659(6)	0.0095(9)
C4	0.2550(6)	-0.0781(6)	0.5781(6)	0.0138(10)
C5	0.1056(6)	0.2043(6)	0.7826(6)	0.0105(9)

Table A.11 Atomic Co-ordinates for **V-11**.

Atom	x	y	z	U _{iso}
V1	0.36018(8)	0.49449(6)	0.47856(13)	0.0144(3)
F1	0.4991(2)	0.5753(2)	0.5389(4)	0.0131(8)
F2	0.3760(3)	0.4690(2)	0.7336(4)	0.0163(8)
F3	0.2708(3)	0.5841(3)	0.5068(5)	0.0325(10)
O1	0.2755(3)	0.4098(3)	0.4299(5)	0.0207(10)

Table A.12 Atomic Co-ordinates for **V-12**.

Atom	x	y	z	U _{iso}
V1	0.11950(7)	0.47767(6)	0.70694(5)	0.0061(3)
V2	0.53347(7)	0.92143(6)	0.76922(5)	0.0061(3)
F1	-0.0028(2)	0.4010(2)	0.81441(19)	0.0086(5)
F2	0.2814(3)	0.5599(3)	0.8220(2)	0.0145(5)
F3	0.0067(2)	0.6613(2)	0.7553(2)	0.0107(5)
F4	-0.0420(2)	0.3869(2)	0.57431(19)	0.0093(5)
F5	0.2073(2)	0.2775(2)	0.6479(2)	0.0099(5)
F6	0.6505(2)	0.9866(2)	0.6524(2)	0.0090(5)
F7	0.6802(3)	1.0177(2)	0.9008(2)	0.0136(5)
F8	0.6420(3)	0.7346(2)	0.7264(2)	0.0116(5)
F9	0.3832(2)	0.8177(2)	0.63244(19)	0.0107(5)
F10	0.4249(2)	1.1075(2)	0.8020(2)	0.0122(5)
O1	0.2322(3)	0.5483(3)	0.5808(3)	0.0097(6)
O2	0.3989(4)	0.8445(4)	0.8800(3)	0.0212(8)
N1	0.5020(3)	0.2149(3)	0.5949(3)	0.0079(6)
N2	0.7276(3)	0.5422(3)	0.8384(3)	0.0067(6)
N3	0.8605(3)	0.8315(3)	1.1449(3)	0.0059(6)
N4	1.0846(3)	1.1678(3)	1.3799(3)	0.0072(6)
C1	0.6083(4)	0.3552(4)	0.6520(3)	0.0090(7)
C2	0.6139(4)	0.4076(4)	0.7905(3)	0.0074(7)
C3	0.7294(4)	0.6238(4)	0.9721(3)	0.0092(7)
C4	0.8484(4)	0.7612(4)	1.0093(3)	0.0085(7)
C5	0.9660(4)	0.9730(4)	1.1926(3)	0.0080(7)
C6	0.9683(4)	1.0350(4)	1.3312(3)	0.0075(7)

Table A.13 Atomic Co-ordinates for **V-13**.

Atom	x	y	z	U _{iso}
V1	0.5000	1.0000	0.5000	0.01545(18)
F1	0.5000	0.82896(15)	0.5000	0.0207(4)
F2	0.0000	1.0000	0.5000	0.0258(6)
N1	0.5000	1.0000	0.68820(18)	0.0118(4)
C1	0.5000	1.0000	0.9346(2)	0.0126(5)
C2	0.3908(6)	0.8960(2)	0.8714(2)	0.0138(4)
C3	0.3917(6)	0.9002(2)	0.7497(2)	0.0143(4)

Table A.14 Atomic Co-ordinates for **V-14**.

Atom	x	y	z	U _{iso}
V1	0.33346(8)	0.85663(7)	0.27611(6)	0.0121(2)
V2	0.13619(7)	0.67317(7)	0.25789(6)	0.00873(19)
V3	-0.15626(7)	0.83045(7)	0.22600(6)	0.0112(2)
V4	-0.33238(7)	0.63033(7)	0.22959(6)	0.00765(19)
V5	-0.19895(8)	0.35192(7)	0.25412(6)	0.0128(2)
F1	0.4915(2)	0.7289(3)	0.2371(2)	0.0176(6)
F2	0.4191(3)	0.9597(3)	0.2748(3)	0.0284(8)
F3	0.3617(3)	0.8216(3)	0.4150(2)	0.0231(7)
F4	0.2501(3)	0.7439(2)	0.2830(2)	0.0166(6)
F5	0.3145(3)	0.8857(3)	0.1343(2)	0.0198(7)
F6	0.1807(3)	0.9735(3)	0.3079(2)	0.0211(7)
F7	0.1646(2)	0.6979(2)	0.1151(2)	0.0118(6)
F8	0.0771(3)	0.6887(2)	0.3963(2)	0.0121(6)
F9	-0.0018(2)	0.8518(2)	0.2458(2)	0.0098(6)
F10	-0.0214(2)	0.6620(2)	0.2333(2)	0.0090(5)
F11	-0.1069(3)	0.8211(2)	0.0861(2)	0.0155(6)
F12	-0.1821(2)	0.8115(2)	0.3694(2)	0.0129(6)
F13	-0.2797(3)	0.7650(2)	0.2025(2)	0.0144(6)
F14	-0.3320(3)	0.6503(3)	0.3675(2)	0.0156(6)
F15	-0.3425(3)	0.6222(2)	0.0885(2)	0.0145(6)
F16	-0.1665(2)	0.5183(2)	0.2275(2)	0.0120(6)
F17	-0.3646(2)	0.4847(2)	0.2466(2)	0.0117(6)
F18	-0.2057(3)	0.3928(2)	0.3916(2)	0.0146(6)
F19	-0.0275(3)	0.2773(3)	0.2509(3)	0.0274(8)
F20	-0.1861(3)	0.3575(2)	0.1092(2)	0.0158(6)
O1	0.5358(3)	0.5358(3)	0.2611(3)	0.0129(7)
O2	-0.2575(3)	0.9702(3)	0.2206(3)	0.0150(7)
O3	-0.2503(4)	0.2490(3)	0.2744(3)	0.0209(8)
N1	0.9107(4)	0.0704(4)	0.9329(3)	0.0139(9)
N2	0.9200(4)	0.5582(4)	0.4212(3)	0.0143(9)
N3	0.5987(4)	0.3870(4)	0.4991(3)	0.0190(10)
N4	0.0293(4)	0.5970(4)	0.0217(3)	0.0147(9)
N5	0.4212(4)	0.0751(4)	0.5768(3)	0.0200(10)
N6	0.3689(4)	0.5461(4)	0.0179(3)	0.0183(10)
N7	0.0134(5)	0.9106(4)	0.4348(3)	0.0203(10)
N8	0.4555(7)	0.0535(9)	-0.0891(5)	0.105(4)
C1	0.8882(5)	0.0885(4)	1.0446(4)	0.0149(10)
C2	0.9902(5)	-0.0522(4)	0.9084(4)	0.0152(10)
C3	1.0246(5)	0.4457(4)	0.4042(4)	0.0151(10)
C4	0.8721(5)	0.5694(5)	0.5294(4)	0.0150(10)
C5	0.5705(5)	0.4640(5)	0.5876(4)	0.0187(11)
C6	0.4858(5)	0.4111(5)	0.4450(4)	0.0210(12)
C7	0.0763(5)	0.4861(5)	0.0815(4)	0.0168(11)
C8	-0.0914(5)	0.6141(4)	-0.0183(4)	0.0158(10)
C9	0.4354(5)	0.1195(5)	0.4736(4)	0.0235(12)
C10	0.4393(5)	-0.0488(5)	0.5769(5)	0.0283(13)
C11	0.4482(5)	0.4625(5)	0.0911(4)	0.0205(11)
C12	0.4332(5)	0.6160(5)	-0.0366(5)	0.0229(12)
C13	-0.0989(5)	1.0186(5)	0.4358(4)	0.0223(12)
C14	-0.0669(5)	1.1175(4)	0.4661(4)	0.0218(12)
C15	0.4116(7)	0.1146(6)	0.0090(6)	0.058(3)
C16	0.5089(8)	0.0636(10)	0.0785(8)	0.080(4)

Table A.15 Atomic Co-ordinates for **V-15**.

Atom	x	y	z	U _{iso}
V1	0.13651(2)	0.73635(3)	0.08407(5)	0.00608(14)
Na1	-0.33078(6)	0.90272(8)	0.03384(12)	0.0094(2)
Na2	-0.10277(6)	0.89950(8)	-0.12619(12)	0.0090(2)
F1	0.15067(9)	0.80899(11)	0.35112(17)	0.0093(3)
F2	0.21245(9)	0.58305(11)	0.22727(17)	0.0081(2)
F3	0.09069(9)	0.90569(11)	-0.03905(17)	0.0084(2)
F4	0.31003(9)	0.80208(11)	0.15762(16)	0.0080(2)
O1	0.01662(11)	0.66880(14)	0.0119(2)	0.0100(3)

Table A.16 Atomic Co-ordinates for **V-16**.

Atom	x	y	z	U _{iso}
V1	0.18330(12)	0.2500	0.56602(8)	0.0143(3)
K1	0.67292(15)	0.2500	0.59072(10)	0.0136(3)
K2	-0.01450(16)	0.2500	0.27758(10)	0.0122(3)
F1	0.0000	0.0000	0.5000	0.0126(7)
F2	0.2786(4)	0.2500	0.4091(3)	0.0121(7)
F3	0.0264(4)	0.2500	0.6971(3)	0.0124(7)
F4	0.3181(3)	0.0105(4)	0.6137(2)	0.0120(6)
O1	0.3181(3)	0.0105(4)	0.6137(2)	0.0120(6)

Table A.17 Atomic Co-ordinates for **V-17**.

Atom	x	y	z	U _{iso}
V1	0.1921(3)	0.5173(2)	0.0000	0.0081(7)
Rb1	0.0076(2)	0.78010(15)	0.5000	0.0181(5)
F1	0.0317(11)	0.3962(8)	0.0000	0.021(2)
F2	0.1663(14)	0.5308(13)	-0.5000	0.043(4)
F3	0.2688(12)	0.6714(8)	0.0000	0.017(2)
O1	0.3455(14)	0.4404(10)	0.0000	0.026(3)

Table A.18 Atomic Co-ordinates for **V-18**.

Atom	x	y	z	U _{iso}
V1	0.17915(19)	0.96904(15)	0.0000	0.0041(4)
Cs1	-0.00408(6)	0.70451(6)	0.5000	0.0088(3)
F1	0.0439(6)	1.1008(5)	0.0000	0.0071(12)
F2	0.1557(7)	0.9561(5)	-0.5000	0.0133(14)
F3	0.2330(6)	0.8123(5)	0.0000	0.0091(13)
O1	0.3362(8)	1.0330(6)	0.0000	0.0109(15)

Table A.19 Atomic Co-ordinates for **V-19**.

Atom	x	y	z	U _{iso}
V1	0.71461(4)	0.06103(3)	0.26590(3)	0.01093(14)
F1	0.55832(13)	-0.02195(11)	0.13802(11)	0.0158(3)
F2	0.59733(15)	0.02967(13)	0.40125(12)	0.0210(3)
F3	0.82527(13)	-0.09808(11)	0.27672(11)	0.0156(3)
F4	0.83095(14)	0.10781(11)	0.12279(10)	0.0157(3)
F5	0.60315(14)	0.22063(11)	0.23361(11)	0.0185(3)
F6	0.88256(14)	0.13766(12)	0.38037(11)	0.0183(3)
N1	0.45680(19)	0.25203(16)	-0.00426(16)	0.0160(4)
N2	0.25930(19)	0.02949(15)	0.08243(15)	0.0114(3)
N3	0.12508(19)	-0.12847(16)	0.37034(15)	0.0130(3)
C1	0.2813(2)	0.25080(18)	-0.00407(19)	0.0144(4)
C2	0.2262(2)	0.16710(18)	0.09814(19)	0.0148(4)
C3	0.1681(2)	-0.05547(17)	0.16052(18)	0.0124(4)
C4	0.2076(2)	-0.03071(19)	0.30136(18)	0.0139(4)

Table A.20 Atomic Co-ordinates for **V-20**.

Atom	x	y	z	U _{iso}
V1	0.25148(3)	0.00057(4)	0.12542(6)	0.0010(2)
K1	0.02514(6)	0.2500	0.37369(11)	0.0062(2)
K2	0.01398(6)	0.2500	0.87455(11)	0.0054(2)
F1	0.10156(11)	0.0492(2)	0.11700(19)	0.0064(3)
F2	0.40172(11)	-0.0465(2)	0.13384(19)	0.0064(3)
F3	0.21704(17)	-0.2500	0.1654(3)	0.0058(5)
F4	0.28701(17)	0.2500	0.0858(3)	0.0067(5)
F5	0.25250(10)	-0.0441(2)	-0.12444(18)	0.0085(4)

Table A.21 Atomic Co-ordinates for **V-21**.

Atom	x	y	z	U _{iso}
V1	0.86376(5)	0.08179(10)	0.24673(4)	0.0052(2)
F1	0.7424(2)	0.3224(4)	0.22817(17)	0.0160(5)
F2	0.9758(2)	0.3106(4)	0.22289(17)	0.0141(5)
F3	0.8679(2)	0.1403(4)	0.38443(16)	0.0125(5)
F4	0.98831(19)	-0.1382(4)	0.26015(17)	0.0124(5)
F5	0.84607(19)	0.0158(4)	0.10961(15)	0.0109(5)
N1	0.9567(3)	-0.4375(6)	0.4050(2)	0.0139(7)
N2	0.9415(3)	-0.3848(6)	0.0776(2)	0.0114(7)
C1	0.8999(4)	-0.3505(7)	0.4941(3)	0.0147(9)
C2	1.0830(4)	-0.4820(8)	0.4223(3)	0.0175(9)
C3	1.0666(4)	-0.3373(7)	0.0581(3)	0.0144(9)
C4	0.8761(4)	-0.4577(7)	-0.0133(3)	0.0146(9)

Table A.22 Atomic Co-ordinates for **V-22**.

Atom	x	y	z	U _{iso}
V1	0.19975(10)	0.25615(13)	0.82733(10)	0.0057(6)
Na1	-0.1116(3)	0.7157(4)	0.6350(3)	0.0116(7)
F1	0.2925(4)	0.5558(6)	0.9642(4)	0.0099(10)
F2	-0.0522(4)	0.3637(6)	0.8267(3)	0.0098(10)
F3	0.1207(4)	-0.0210(6)	0.6874(4)	0.0113(10)
F4	0.1884(5)	0.4603(6)	0.6295(4)	0.0091(9)

Table A.23 Atomic Co-ordinates for **V-23**.

Atom	x	y	z	U _{iso}
V1	0.19279(8)	0.51623(7)	0.5000	0.0110(3)
F1	0.0299(4)	0.3977(2)	0.5000	0.0236(7)
F2	0.2753(4)	0.6665(3)	0.5000	0.0350(10)
F3A	0.1777(11)	0.5022(8)	0.0000	0.0253(19)
F3B	0.1623(9)	0.5560(7)	0.0000	0.0161(15)
O1	0.3439(5)	0.4355(4)	0.5000	0.0368(12)
N1	0.0082(7)	0.7791(4)	0.0000	0.0379(15)

Table A.24 Atomic Co-ordinates for **V-24**.

Atom	x	y	z	U _{iso}
V1	0.13818(18)	0.0000	0.0308(6)	0.0115(6)
F1	0.2225(6)	0.0871(6)	0.046(3)	0.069(3)
F2	0.0000	-0.0753(5)	0.0000	0.044(3)
F3	0.1214(9)	0.0288(6)	-0.471(3)	0.029(3)
O1	0.2225(6)	0.0871(6)	0.046(3)	0.069(3)
N1	0.0000	-0.2048(10)	-0.5000	0.047(4)
C1	-0.0874(10)	-0.2453(10)	-0.397(3)	0.051(3)
C2	-0.0893(12)	-0.3314(10)	-0.393(3)	0.058(4)
C3	0.0000	-0.3769(14)	-0.5000	0.068(5)
C4	-0.0432(19)	-0.4730(17)	-0.474(7)	0.060(7)

Table A.25 Atomic Co-ordinates for **V-25**.

Atom	x	y	z	U _{iso}
V1	0.45170(7)	0.23035(5)	0.75325(4)	0.00782(16)
F1	0.2806(3)	0.03663(18)	0.59744(15)	0.0145(3)
F2	0.3942(3)	0.38120(18)	0.62337(15)	0.0134(3)
F3	0.7134(3)	0.41656(17)	0.87188(15)	0.0130(3)
F4	0.6029(3)	0.08641(17)	0.85774(15)	0.0132(3)
O2	0.7675(4)	0.2145(2)	0.6333(2)	0.0147(4)
O1	0.2200(3)	0.2308(2)	0.8256(2)	0.0156(4)
N1	1.0405(4)	0.7215(2)	0.9114(2)	0.0090(4)
N2	0.9263(4)	0.7528(2)	0.6171(2)	0.0100(4)
C1	0.8946(5)	0.8384(3)	0.8626(3)	0.0111(5)
C2	0.7527(5)	0.7736(3)	0.7103(3)	0.0107(5)
C3	1.0702(5)	0.6342(3)	0.6648(3)	0.0119(5)
C4	1.2127(5)	0.6969(3)	0.8178(3)	0.0111(5)

Table A.26 Atomic Co-ordinates for **V-26**.

Atom	x	y	z	U _{iso}
V1	0.96085(9)	0.04176(5)	0.2500	0.0106(2)
F1	0.8945(2)	-0.08157(13)	0.36650(13)	0.0158(4)
O1	0.7812(4)	0.1469(2)	0.2500	0.0158(6)
N1	1.1215(3)	0.14267(19)	0.38146(18)	0.0120(5)
N2	1.2620(4)	-0.0613(3)	0.2500	0.0127(7)
C1	1.3359(4)	0.1121(2)	0.3897(2)	0.0166(6)
C2	1.3690(4)	-0.0297(2)	0.3568(2)	0.0160(6)

Table A.27 Atomic Co-ordinates for **V-27**.

Atom	x	y	z	U _{iso}
V1	0.12462(10)	0.12679(11)	0.15317(7)	0.0382(5)
V2	0.0000	0.0000	0.0000	0.0422(11)
F1	0.1582(4)	0.1582(4)	0.2500	0.0379(18)
F2	0.0900(3)	0.0003(3)	0.1723(2)	0.0362(12)
F3	0.2389(3)	0.1475(4)	0.1346(3)	0.0490(15)
F4	0.1525(4)	0.2411(4)	0.1350(3)	0.0539(15)
F5	0.0912(4)	0.0929(4)	0.0560(3)	0.0487(14)
N1	0.3443(12)	0.4309(12)	0.2738(9)	0.058(5)
N1A	0.2777(10)	0.3570(11)	0.2583(10)	0.046(4)
C1	0.3673(9)	0.3452(8)	0.1775(7)	0.073(4)
C2	0.3204(10)	0.3957(9)	0.2010(7)	0.076(4)

Table A.28 Atomic Co-ordinates for **V-28**.

Atom	x	y	z	U _{iso}
V1	0.0000	0.0000	0.5000	0.0076(3)
V2	1.0000	0.0000	0.5000	0.0099(3)
K1	0.5000	0.5000	0.5000	0.0182(4)
K2	1.21539(10)	0.28461(10)	0.2500	0.0154(3)
F1	0.4556(2)	0.1735(2)	0.38609(14)	0.0236(4)
F3	0.7531(3)	0.0724(3)	0.5000	0.0185(6)
F3	0.0000	0.0000	0.3356(3)	0.0159(7)

Table A.29 Atomic Co-ordinates for **V-29**.

Atom	x	y	z	U _{iso}
Mo1	0.423895(13)	0.12913(4)	0.312027(18)	0.00622(11)
F1	0.35938(10)	0.3977(2)	0.24566(14)	0.0110(4)
F2	0.31790(9)	0.0745(3)	0.33194(13)	0.0099(3)
F3	0.35425(10)	0.0267(3)	0.15830(13)	0.0114(4)
O1	0.45279(13)	-0.1284(3)	0.33577(17)	0.0122(5)
O2	0.46037(12)	0.2479(3)	0.43076(16)	0.0135(5)
O3	0.5000	0.2270(4)	0.2500	0.0114(6)
N1	0.29837(15)	0.6559(4)	0.3642(2)	0.0093(5)
N2	0.40003(15)	0.3551(4)	0.6088(2)	0.0098(5)
C1	0.35271(17)	0.6296(4)	0.4730(2)	0.0094(6)
C2	0.33360(17)	0.4218(5)	0.5173(2)	0.0098(6)

Table A.30 Atomic Co-ordinates for **Mo-1**.

Atom	x	y	z	U _{iso}
Mo1	0.38401(3)	0.21850(6)	0.52101(3)	0.0374(2)
Mo2	0.36706(3)	0.77225(6)	0.72579(3)	0.0412(2)
F1	0.37449(19)	0.0642(4)	0.5660(3)	0.0791(17)
F2	0.4544(2)	0.2296(5)	0.5809(3)	0.0733(15)
F3	0.3573(2)	0.2848(5)	0.5950(2)	0.0675(14)
F4	0.30094(17)	0.1994(4)	0.4771(2)	0.0469(11)
F5	0.3879(2)	0.7076(6)	0.6472(2)	0.102(2)
F6	0.44952(18)	0.7600(4)	0.7684(3)	0.0636(14)
F7	0.3740(2)	0.5962(4)	0.7465(3)	0.0916(19)
F8	0.2942(2)	0.7454(5)	0.6720(3)	0.0806(17)
F9	0.5000	1.0638(5)	0.7500	0.0378(14)
F10	0.0000	0.9008(5)	0.7500	0.0439(15)
O1	0.3965(3)	0.1376(6)	0.4618(3)	0.079(2)
O2	0.3774(2)	0.3683(5)	0.4869(3)	0.0589(16)
O3	0.3749(3)	0.9188(6)	0.6957(5)	0.124(3)
O4	0.3578(3)	0.8134(8)	0.7946(4)	0.112(3)
O5	0.3812(3)	0.5122(6)	0.8700(3)	0.0809(19)
N1	0.4471(3)	0.7476(4)	0.5402(3)	0.0324(15)
N2	0.4795(2)	0.5783(5)	0.6588(3)	0.0428(16)
N3	0.4649(2)	0.9322(5)	0.6411(3)	0.0338(14)
N4	0.3261(2)	0.7687(5)	0.5175(3)	0.0446(16)
N5	0.2025(2)	0.7477(4)	0.7949(3)	0.0279(14)
N6	0.2025(2)	0.9684(5)	0.8732(3)	0.0411(15)
N7	0.0796(2)	0.7343(5)	0.7735(3)	0.0418(16)
N8	0.2346(2)	0.6029(5)	0.9207(3)	0.0324(13)
C1	0.4929(3)	0.6553(6)	0.5589(4)	0.0421(19)
C2	0.4811(3)	0.5450(6)	0.5934(4)	0.045(2)
C3	0.4704(3)	0.8682(6)	0.5348(3)	0.0378(18)
C4	0.5014(3)	0.9266(7)	0.6016(3)	0.0398(19)
C5	0.4016(3)	0.7131(7)	0.4785(3)	0.047(2)
C6	0.3489(3)	0.7850(8)	0.4644(4)	0.051(2)
C7	0.2193(3)	0.8691(6)	0.7802(3)	0.0356(17)
C8	0.2443(3)	0.9452(6)	0.8421(4)	0.0393(18)
C9	0.1589(3)	0.6935(7)	0.7361(4)	0.0441(19)
C10	0.1026(3)	0.7507(7)	0.7200(4)	0.044(2)
C11	0.2520(3)	0.6685(6)	0.8201(3)	0.0329(16)
C12	0.2449(3)	0.5628(6)	0.8614(3)	0.0376(18)

Table A.31 Atomic Co-ordinates for **Mo-2**.

Atom	x	y	z	U _{iso}
Mo1	0.32228(7)	0.623954(18)	0.02656(6)	0.01910(17)
F1	0.2726(4)	0.62445(11)	-0.2816(4)	0.0177(6)
F2	0.1431(5)	0.68650(13)	0.0139(4)	0.0244(7)
F3	0.0863(5)	0.57764(13)	-0.0134(5)	0.0266(7)
F4	0.4603(5)	0.55831(13)	-0.0281(5)	0.0296(8)
O1	0.3420(6)	0.62063(15)	0.2661(5)	0.0247(8)
O2	0.5200(5)	0.66991(15)	-0.0195(5)	0.0193(7)
N1	0.2363(6)	0.51559(17)	-0.3860(7)	0.0214(9)
N2	0.2129(6)	0.22927(17)	-0.6070(6)	0.0175(9)
C1	0.2708(8)	0.4996(2)	-0.5618(8)	0.0220(11)
C2	0.1941(8)	0.4783(2)	-0.2507(8)	0.0217(11)
C3	0.2683(8)	0.4430(2)	-0.6102(7)	0.0196(10)
C4	0.1883(7)	0.4212(2)	-0.2924(7)	0.0187(10)
C5	0.2283(7)	0.4031(2)	-0.4723(7)	0.0153(10)
C6	0.2222(7)	0.34193(19)	-0.5170(7)	0.0156(9)
C7	0.1643(7)	0.3241(2)	-0.7010(7)	0.0178(10)
C8	0.2725(7)	0.3010(2)	-0.3817(7)	0.0181(10)
C9	0.1601(7)	0.2670(2)	-0.7411(7)	0.0173(10)
C10	0.2655(7)	0.2447(2)	-0.4289(7)	0.0186(10)

Table A.32 Atomic Co-ordinates for **Mo-3**.

Atom	x	y	z	U _{iso}
Mo1	0.19566(3)	0.93494(3)	0.25500(2)	0.01216(9)
F1	-0.00840(19)	0.85555(19)	0.08919(16)	0.0157(3)
F2	0.1834(2)	0.67705(19)	0.12883(17)	0.0173(3)
F3	0.0190(2)	0.82696(19)	0.33104(16)	0.0175(3)
F4	0.3282(2)	0.9682(2)	0.11317(17)	0.0189(4)
O1	0.3669(3)	0.9574(3)	0.3638(2)	0.0225(5)
O2	0.1713(3)	1.1343(2)	0.3275(2)	0.0203(4)
N1	0.0829(3)	0.7537(3)	-0.1577(2)	0.0140(5)
N2	0.6413(3)	0.4283(3)	-0.9355(2)	0.0134(5)
C1	0.0465(3)	0.5832(3)	-0.2312(3)	0.0142(6)
C2	0.1832(4)	0.8645(3)	-0.1999(3)	0.0167(6)
C3	0.1143(3)	0.5171(3)	-0.3532(3)	0.0125(5)
C4	0.2544(3)	0.8061(3)	-0.3198(3)	0.0144(6)
C5	0.2230(3)	0.6284(3)	-0.3991(3)	0.0121(5)
C6	0.2980(3)	0.5538(3)	-0.5260(3)	0.0131(5)
C7	0.4047(3)	0.6426(3)	-0.5819(3)	0.0148(6)
C8	0.4810(3)	0.5644(3)	-0.7074(3)	0.0129(5)
C9	0.4344(3)	0.3861(3)	-0.7925(3)	0.0126(5)
C10	0.6108(3)	0.6703(3)	-0.7443(3)	0.0139(6)
C11	0.5167(3)	0.3218(3)	-0.9046(3)	0.0145(6)
C12	0.6894(3)	0.5996(3)	-0.8586(3)	0.0138(6)

Table A.33 Atomic Co-ordinates for **Mo-4**.

Atom	x	y	z	U _{iso}
Mo1	0.0000	0.07041(6)	0.33897(4)	0.0069(2)
Mo2	0.0000	0.25787(6)	0.46168(4)	0.0064(2)
F1	0.2127(6)	-0.0608(3)	0.2784(2)	0.0148(7)
F2	-0.2232(5)	0.3404(3)	0.5464(2)	0.0125(7)
F3	0.0000	0.1083(4)	0.5720(3)	0.0108(9)
O1	0.0000	0.1784(5)	0.2490(3)	0.0104(11)
O2	0.0000	0.3998(6)	0.3949(4)	0.0152(12)
O3	0.2292(6)	0.1424(4)	0.4134(2)	0.0098(8)
N1	-0.5000	0.5624(7)	0.6053(5)	0.0200(17)
N2	0.0000	0.3367(7)	0.7148(4)	0.0128(14)
N3	0.5000	-0.1153(7)	0.4164(4)	0.0100(13)

Table A.34 Atomic Co-ordinates for **Mo-5**.

Atom	x	y	z	U _{iso}
Mo1	0.28726(5)	0.13314(14)	0.57073(7)	0.0257(3)
F1	0.2254(3)	-0.0391(9)	0.6273(5)	0.0257(13)
F2	0.3678(2)	0.2422(9)	0.5409(4)	0.0268(13)
O1	0.2472(3)	0.4165(9)	0.5890(5)	0.0164(14)
O2	0.4211(3)	0.5707(10)	0.4189(6)	0.0204(15)
N1	0.3381(4)	-0.1901(11)	0.5782(6)	0.0176(17)
N2	0.3343(3)	0.1263(12)	0.7515(6)	0.0172(16)
C1	0.3650(5)	-0.2430(16)	0.7001(8)	0.024(2)
C2	0.3880(4)	-0.0335(15)	0.7624(8)	0.021(2)
C3	0.4868(4)	0.5020(17)	0.4365(8)	0.025(2)

Table A.35 Atomic Co-ordinates for **Mo-6**.

Atom	x	y	z	U _{iso}
Mo1	0.0000	0.06939(7)	0.16627(5)	0.0066(2)
Mo2	0.0000	0.25852(7)	0.04026(4)	0.0064(2)
K1	0.0000	-0.0670(2)	0.39399(13)	0.0163(4)
K2	0.0000	-0.34067(19)	0.20564(13)	0.0123(4)
K3	-0.5000	-0.12457(19)	0.09012(12)	0.0099(4)
F1	0.2366(6)	0.3414(3)	-0.0447(2)	0.0101(7)
F2	0.2208(6)	-0.0632(3)	0.2258(2)	0.0109(7)
F3	0.0000	-0.1117(5)	0.0744(3)	0.0105(10)
O1	0.0000	0.4024(6)	0.1096(4)	0.0107(12)
O2	0.0000	0.1761(6)	0.2603(4)	0.0128(13)
O3	0.2381(7)	0.1410(4)	0.0897(3)	0.0103(9)

Table A.36 Atomic Co-ordinates for **Mo-7**.

Atom	x	y	z	U _{iso}
Mo1	-0.5000	0.0000	0.26730(12)	0.0162(6)
Mo2	0.0000	0.19884(18)	0.0000	0.0047(5)
K1	-0.5000	0.2671(4)	0.1614(2)	0.0142(8)
K2	0.0000	0.0000	0.1583(3)	0.0144(11)
K3	-0.5000	0.0000	0.0000	0.0115(14)
F1	-0.5000	0.0000	0.1616(8)	0.013(2)
F2	-0.7293(14)	0.1213(7)	0.2533(5)	0.0247(18)
F3	0.2232(12)	0.1672(6)	0.0705(4)	0.0142(14)
F4	0.0000	0.0000	0.0000	0.009(3)
O1	-0.5000	0.0000	0.3552(12)	0.069(9)
O2	0.0000	0.3454(17)	0.0000	0.025(5)
O3	-0.596(5)	0.5000	0.0898(14)	0.021(6)
C1	-0.5000	0.451(4)	0.032(2)	0.032(10)

Table A.37 Atomic Co-ordinates for **Mo-8**.

Atom	x	y	z	U _{iso}
Mo1	0.463286(15)	0.65002(2)	0.09855(2)	0.00900(8)
F1	0.32188(11)	0.59989(19)	-0.08942(17)	0.0140(3)
F2	0.52683(11)	0.60865(18)	-0.05777(17)	0.0118(3)
F3	0.39693(13)	0.6106(2)	0.2272(2)	0.0215(3)
O1	0.45832(16)	0.8486(2)	0.0646(3)	0.0167(4)
N1	0.24190(16)	0.7767(3)	-0.3561(2)	0.0130(4)
C1	0.1907(2)	0.6356(3)	-0.4627(3)	0.0143(5)
C2	0.33717(19)	0.8283(3)	-0.3651(3)	0.0136(4)

Table A.38 Atomic Co-ordinates for **Mo-9**.

Atom	x	y	z	U _{iso}
Ti1	0.0000	0.0000	0.0000	0.0129(3)
F1	0.1304(3)	-0.13525(16)	0.0000	0.0178(6)
F2	0.2252(3)	0.07834(17)	0.0000	0.0211(6)
F3	0.0000	0.0000	0.14343(17)	0.0180(6)
N1	0.0000	0.2087(3)	0.2500	0.0306(10)
C1	0.0642(4)	0.2623(2)	0.1684(3)	0.0269(8)
C2	0.0629(4)	0.3786(2)	0.1655(2)	0.0197(7)
C3	0.0000	0.4367(3)	0.2500	0.0123(9)

Table A.39 Atomic Co-ordinates for **Ti-1**.

Atom	x	y	z	U _{iso}
Ti1	0.7500	0.2500	0.2500	0.0295(6)
Ti2	0.2500	0.2500	0.24344(16)	0.0123(5)
O1	0.7500	0.2500	0.0000	0.0277(15)
O2	0.2500	0.2500	0.5194(7)	0.0215(14)
F1	0.60127(18)	0.24949(18)	0.2501(3)	0.0207(7)
F2A	0.3775(2)	0.1721(3)	0.2736(3)	0.0165(7)
F2B	0.3325(10)	0.1239(10)	0.2284(14)	0.018(2)
N1	0.4956(2)	0.1478(3)	-0.0084(4)	0.0175(8)
C1	0.5425(3)	0.0407(3)	-0.0044(5)	0.0152(9)

Table A.40 Atomic Co-ordinates for **Ti-2**.

Atom	x	y	z	U _{iso}
Ti1	1.0000	0.0000	1.0000	0.0061(6)
F1	0.7755(6)	0.1340(6)	0.8829(5)	0.0176(9)
F2	0.8904(6)	0.0405(5)	1.2637(5)	0.0152(9)
F3	1.2308(5)	0.2958(5)	1.0536(5)	0.0125(9)
N1	0.4658(8)	0.3549(8)	0.6679(7)	0.0091(11)
C1	0.5915(9)	0.2971(9)	0.4845(8)	0.0089(12)
C2	0.2834(9)	0.4818(9)	0.6068(8)	0.0103(12)

Table A.41 Atomic Co-ordinates for **Ti-3**.

Atom	x	y	z	U _{iso}
Ti1	0.0000	0.0000	0.0000	0.0132(2)
F1	0.2910(2)	-0.0156(2)	-0.0384(2)	0.0180(4)
F2	0.0321(3)	-0.1282(2)	0.2553(2)	0.0203(4)
F3	-0.0135(2)	-0.2389(2)	-0.0577(2)	0.0197(4)
N1	0.5019(4)	-0.3485(4)	0.1831(3)	0.0187(6)
C1	0.3497(5)	-0.4667(4)	0.1771(4)	0.0189(7)
C2	0.6783(5)	-0.4156(4)	0.2759(4)	0.0177(6)
C3	0.3691(5)	-0.6587(4)	0.2680(4)	0.0172(6)
C4	0.7059(4)	-0.6085(4)	0.3680(4)	0.0171(6)
C5	0.5500(4)	-0.7366(4)	0.3692(4)	0.0139(6)
C6	0.5769(4)	-0.9398(4)	0.4770(4)	0.0162(6)

Table A.42 Atomic Co-ordinates for **Ti-4**.

Atom	x	y	z	U _{iso}
Cs1	0.6667	0.3333	0.8040(3)	0.0062(11)
Ti1	1.0000	1.0000	0.5000	0.0056(17)
F1	0.8559(6)	0.7118(13)	0.2868(17)	0.0085(19)

Table A.43 Atomic Co-ordinates for **Ti-5**.

Atom	x	y	z	U _{iso}
Zr1	0.0000	0.5000	0.0000	0.0118(2)
F1	-0.0255(4)	0.4575(4)	0.2552(3)	0.0222(6)
F2	0.2668(5)	0.6759(5)	0.0676(4)	0.0353(8)
F3	0.1383(6)	0.2634(5)	-0.0511(4)	0.0383(9)
N1	0.6233(6)	0.2910(6)	0.3518(6)	0.0212(9)
C1	0.4666(7)	0.2105(7)	0.2334(6)	0.0205(10)
C2	0.6112(7)	0.3043(7)	0.5259(7)	0.0203(10)
C3	0.2832(7)	0.1337(7)	0.2936(6)	0.0207(10)
C4	0.4339(7)	0.2318(6)	0.5917(6)	0.0158(9)
C5	0.2652(6)	0.1424(7)	0.4740(6)	0.0145(8)
C6	0.0780(7)	0.0592(7)	0.5481(6)	0.0177(9)

Table A.44 Atomic Co-ordinates for **Zr-1**.

Atom	x	y	z	U _{iso}
Zr1	0.90856(4)	0.52680(3)	0.39743(2)	0.00751(9)
F1	0.8880(3)	0.4795(2)	0.54917(14)	0.0138(4)
F2	1.1185(2)	0.42339(19)	0.39216(17)	0.0157(4)
F3	0.7015(3)	0.6181(2)	0.42793(16)	0.0162(5)
F4	1.0605(3)	0.65237(19)	0.47438(14)	0.0128(5)
F5	0.7775(3)	0.3649(2)	0.39885(19)	0.0209(5)
F6	0.9401(3)	0.69030(19)	0.30941(15)	0.0141(5)
F7	0.8891(3)	0.4766(2)	0.25193(14)	0.0253(5)
N1	0.8937(4)	0.6606(3)	0.0987(2)	0.0120(6)
N2	1.2963(4)	0.3747(3)	0.1523(2)	0.0106(6)
N3	1.7420(4)	0.3058(3)	0.1395(2)	0.0134(7)
C1	1.0294(5)	0.6268(4)	0.0296(3)	0.0127(8)
C2	1.1021(5)	0.4980(3)	0.0505(2)	0.0135(8)
C3	1.2199(5)	0.5011(3)	0.1373(3)	0.0126(8)
C4	1.4174(5)	0.3762(3)	0.2345(2)	0.0120(7)
C5	1.5047(5)	0.2511(3)	0.2482(3)	0.0125(8)
C6	1.6132(5)	0.2109(3)	0.1627(3)	0.0114(7)

Table A.45 Atomic Co-ordinates for **Zr-2**.

Atom	x	y	z	U _{iso}
Zr1	0.26772(6)	0.25540(5)	0.24913(5)	0.01280(15)
Zr2	0.02905(6)	0.69181(5)	0.32067(5)	0.01272(15)
Zr3	-0.52826(6)	0.18611(5)	-0.19140(5)	0.01114(15)
F1	0.3347(4)	0.1348(3)	0.2758(3)	0.0221(8)
F2	0.4328(4)	0.3397(4)	0.4234(3)	0.0263(9)
F3	0.2583(4)	0.4100(4)	0.2625(3)	0.0284(9)
F4	0.4369(4)	0.3503(3)	0.2332(3)	0.0246(8)
F5	0.1723(4)	0.2204(3)	0.3465(4)	0.0303(9)
F6	0.1892(4)	0.2607(4)	0.0743(3)	0.0368(11)
F7	0.0859(4)	0.0964(3)	0.1487(4)	0.0300(9)
F8	-0.1807(4)	0.5822(3)	0.2082(3)	0.0251(9)
F9	0.0169(4)	0.5339(3)	0.2545(3)	0.0192(8)
F10	0.2256(4)	0.7248(3)	0.4511(3)	0.0222(8)
F11	-0.0376(4)	0.8013(3)	0.2323(3)	0.0244(8)
F12	0.1376(4)	0.7447(3)	0.2361(3)	0.0242(8)
F13	-0.0186(5)	0.5943(5)	0.4281(4)	0.0476(13)
F14	0.0809(6)	0.8235(5)	0.4487(4)	0.0642(17)
F15	-0.6154(4)	0.2911(3)	-0.2272(3)	0.0204(8)
F16	-0.3242(4)	0.2955(3)	-0.0672(3)	0.0229(8)
F17	-0.4473(4)	0.2837(3)	-0.2843(3)	0.0178(7)
F18	-0.5318(4)	0.2216(3)	-0.0347(3)	0.0167(7)
F19	-0.7287(3)	0.0594(3)	-0.2438(3)	0.0212(8)
F20	-0.5786(5)	0.0649(3)	-0.3324(4)	0.0320(10)
F21	-0.4888(4)	0.0592(3)	-0.1151(3)	0.0230(8)
F22	-0.8745(4)	-0.2193(3)	-0.2314(3)	0.0231(8)
N1	0.3441(5)	0.3550(5)	-0.0306(5)	0.0170(11)
N2	-0.2912(6)	0.0267(5)	0.0487(5)	0.0209(12)
N3	-0.0806(5)	0.1092(5)	-0.0953(5)	0.0188(11)
N4	0.1649(5)	0.5482(4)	0.1444(4)	0.0141(10)
N5	0.4826(5)	0.8458(5)	0.4868(4)	0.0174(11)
N6	-0.7194(5)	-0.1634(4)	-0.3301(4)	0.0169(11)
N7	-0.7359(5)	-0.3397(5)	-0.1702(5)	0.0198(12)
N8	0.4272(5)	0.4203(5)	0.6143(4)	0.0174(11)
N9	0.0996(6)	0.4179(5)	0.4142(5)	0.0233(12)
N10	-0.0001(5)	0.0081(5)	0.3580(5)	0.0194(11)
C1	0.4616(7)	0.4795(6)	0.0326(5)	0.0181(13)
C2	-0.2236(7)	0.0059(5)	-0.0101(5)	0.0166(13)
C3	-0.1780(8)	0.1093(6)	-0.0599(7)	0.0260(16)
C4	0.0340(6)	0.4662(5)	0.0355(5)	0.0187(14)
C5	0.5463(7)	0.9768(6)	0.5409(5)	0.0189(13)
C6	-0.6204(7)	-0.2059(6)	-0.2619(6)	0.0212(14)
C7	-0.6923(7)	-0.3325(6)	-0.2587(6)	0.0186(13)
C8	0.2864(6)	0.3994(6)	0.5737(6)	0.0184(13)
C9	0.2509(6)	0.4709(6)	0.4884(5)	0.0156(12)
C10	0.0490(6)	0.0464(6)	0.4854(6)	0.0197(14)

Table A.46 Atomic Co-ordinates for **Zr-3**.

Atom	x	y	z	U _{iso}
Hf1	0.17468(5)	0.05029(5)	0.098771(17)	0.00256(11)
Na1	-0.3269(5)	0.5016(6)	0.09185(18)	0.0062(6)
Na2	0.2442(5)	0.5358(5)	0.24745(18)	0.0077(6)
F1	0.4261(7)	0.2148(8)	0.1836(3)	0.0082(8)
F2	-0.0201(7)	0.2881(8)	0.1653(3)	0.0062(8)
F3	0.3966(7)	-0.2309(8)	0.1348(3)	0.0071(8)
F4	-0.0609(7)	-0.1822(8)	0.1489(3)	0.0072(8)
F5	0.3463(7)	0.2720(8)	0.0245(3)	0.0090(8)
F6	0.1295(7)	-0.1713(8)	-0.0116(2)	0.0060(8)

Table A.47 Atomic Co-ordinates for **Hf-1**.

Atom	x	y	z	U _{iso}
Hf1	0.77756(3)	0.45855(2)	0.23987(2)	0.01955(9)
F1	0.6283(4)	0.3392(3)	0.2144(4)	0.0445(11)
F2	0.6575(4)	0.5322(3)	0.0815(3)	0.0345(9)
F3	0.8710(4)	0.4105(3)	0.0665(3)	0.0348(10)
F4	0.9510(4)	0.3516(3)	0.2853(4)	0.0402(11)
F5	0.7882(5)	0.4389(4)	0.4341(4)	0.0675(17)
F6	0.6293(4)	0.5683(3)	0.3091(4)	0.0395(11)
F7	0.9318(4)	0.5788(3)	0.2409(4)	0.0339(10)
O1	0.4996(7)	0.6456(5)	0.5212(5)	0.0513(15)
N1	0.9967(5)	0.7905(4)	-0.0479(5)	0.0280(13)
N2	0.8024(5)	0.5774(4)	-0.1304(5)	0.0212(12)
N3	0.6071(5)	0.3587(4)	-0.1232(5)	0.0275(13)
C1	0.8457(7)	0.7570(5)	-0.0198(6)	0.0292(16)
C2	0.7611(7)	0.6956(5)	-0.1289(6)	0.0278(16)
C3	0.7202(8)	0.5147(5)	-0.2370(6)	0.0291(15)
C4	0.7172(7)	0.3930(5)	-0.2155(6)	0.0286(16)

Table A.48 Atomic Co-ordinates for **Hf-2**.

Atom	x	y	z	U _{iso}
Hf1	0.03266(3)	0.673236(19)	0.01111(2)	0.00839(8)
F1	0.0745(4)	0.8661(3)	0.0478(3)	0.0130(7)
F2	0.2950(4)	0.7129(3)	-0.0464(3)	0.0157(7)
F3	0.1030(4)	0.6463(3)	0.1842(3)	0.0153(7)
F4	-0.0631(4)	0.6814(3)	-0.1610(3)	0.0185(7)
F5	-0.2278(4)	0.7428(3)	0.0520(3)	0.0190(8)
F6	0.1658(4)	0.4902(2)	-0.0071(3)	0.0104(6)
N1	-0.0475(6)	1.1069(4)	-0.3058(4)	0.0142(10)
N2	0.2739(6)	1.0052(4)	-0.1038(4)	0.0082(9)
C1	0.0178(7)	0.9728(5)	-0.2745(5)	0.0133(11)
C2	0.2289(7)	0.9669(5)	-0.2316(5)	0.0105(10)
C3	0.4833(7)	0.9915(5)	-0.0668(5)	0.0101(11)

Table A.49 Atomic Co-ordinates for **Hf-3**.

Atom	x	y	z	U _{iso}
Hf1	0.5000	0.0000	0.5000	0.00583(8)
F1	0.1934(3)	-0.1279(3)	0.6010(3)	0.0133(4)
F2	0.4471(3)	-0.2664(3)	0.2576(3)	0.0134(4)
F3	0.3462(3)	0.1705(3)	0.3295(3)	0.0153(4)
N1	-0.0547(5)	-0.4069(5)	0.8251(4)	0.0071(5)
C1	-0.0801(6)	-0.2879(6)	1.0439(5)	0.0087(7)
C2	0.1307(6)	-0.5414(5)	0.8160(5)	0.0084(7)

Table A.50 Atomic Co-ordinates for **Hf-4**.

Atom	x	y	z	U _{iso}
Hf1	0.0000	0.0000	0.0000	0.01092(12)
F1	0.0000	0.0000	0.1460(3)	0.0306(10)
F2	0.2379(6)	0.0877(3)	0.0000	0.0321(11)
F3	0.1518(6)	-0.1384(3)	0.0000	0.0147(8)
N1	0.0000	-0.2128(6)	0.2500	0.093(5)
C1	-0.0524(8)	-0.2660(6)	0.1714(8)	0.070(3)
C2	-0.0528(7)	-0.3809(5)	0.1667(5)	0.0289(13)
C3	0.0000	-0.4386(4)	0.2500	0.0143(11)

Table A.51 Atomic Co-ordinates for **Hf-5**.

Atom	x	y	z	U _{iso}
Hf1	0.92688(4)	0.0000	0.25669(9)	0.0036(7)
Na1	0.7221(6)	-0.5000	0.1517(12)	0.0061(15)
Na2	1.0000	-0.5000	0.0000	0.013(2)
Na3	1.1647(6)	-0.5000	0.4281(11)	0.0061(15)
F1	1.0000	0.0000	0.5000	0.014(3)
F2	0.8198(6)	-0.2366(13)	0.3584(9)	0.0087(15)
F3	0.8673(6)	-0.2256(12)	0.0708(8)	0.0057(15)
F4	1.0611(7)	-0.2401(18)	0.2517(8)	0.006(2)

Table A.52 Atomic Co-ordinates for **Hf-6**.

Atom	x	y	z	U _{iso}
Nb1	0.0000	0.0000	0.5000	0.02091(16)
F1	0.2578(2)	0.1736(2)	0.57176(18)	0.0262(3)
F2	-0.1397(3)	0.2285(2)	0.54578(18)	0.0279(4)
F3	0.0297(2)	0.0395(2)	0.25953(17)	0.0215(3)
N1	0.3682(3)	0.2047(3)	0.1453(2)	0.0134(4)
C1	0.3807(3)	0.1924(3)	-0.0282(3)	0.0131(4)
C2	0.5290(3)	0.2846(3)	0.2617(3)	0.0147(5)
C3	0.5629(3)	0.2644(3)	-0.0926(3)	0.0123(4)
C4	0.7134(3)	0.3610(3)	0.2043(3)	0.0123(4)
C5	0.7329(3)	0.3538(3)	0.0239(3)	0.0104(4)
C6	0.9220(3)	0.4382(3)	-0.0478(3)	0.0113(4)

Table A.53 Atomic Co-ordinates for **Nb-1**.

Atom	x	y	z	U _{iso}
Nb1	0.29226(4)	0.78159(3)	0.77568(3)	0.01157(13)
F1	0.3629(3)	0.5370(2)	0.66859(19)	0.0145(3)
F2	0.0775(3)	0.6899(2)	0.9395(2)	0.0214(4)
F3	0.0663(3)	0.8527(2)	0.6596(2)	0.0221(4)
F4	0.5279(3)	0.8048(2)	0.5835(2)	0.0267(4)
F5	0.5371(3)	0.6490(2)	0.8642(2)	0.0213(4)
O1	0.2422(4)	0.9762(3)	0.8633(3)	0.0184(5)
N1	0.3840(4)	0.2683(3)	0.8657(3)	0.0160(5)
N2	0.8139(4)	0.3570(3)	0.6003(3)	0.0125(5)
C1	0.6186(5)	0.1572(4)	0.7798(4)	0.0174(6)
C2	0.8022(5)	0.2499(4)	0.7447(4)	0.0163(6)
C3	0.9855(5)	0.4534(4)	0.5784(3)	0.0142(6)

Table A.54 Atomic Co-ordinates for **Nb-2**.

Atom	x	y	z	U _{iso}
Nb1	0.21891(3)	0.72327(2)	0.05805(2)	0.00999(10)
F1	0.10133(18)	0.89715(13)	0.03819(13)	0.0109(3)
F2	0.3229(2)	0.78650(15)	-0.05644(16)	0.0211(4)
F3	0.0123(2)	0.69566(15)	-0.07357(15)	0.0204(4)
F4	0.0850(2)	0.70844(14)	0.16937(16)	0.0191(4)
F5	0.3965(2)	0.79985(14)	0.18590(15)	0.0187(4)
O1	0.3017(3)	0.58361(17)	0.07584(19)	0.0206(5)
O2	0.3749(3)	0.34967(18)	0.0576(2)	0.0222(5)
N1	0.2431(3)	1.1287(2)	0.0280(2)	0.0110(4)
N2	0.0350(3)	0.96797(19)	-0.1907(2)	0.0105(5)
C1	0.2963(3)	1.0778(2)	-0.0738(2)	0.0132(6)
C2	0.1490(3)	1.0704(2)	-0.1909(2)	0.0117(5)
C3	-0.1462(3)	0.9803(2)	-0.2723(2)	0.0132(6)
C4	-0.2659(3)	0.8871(2)	-0.2507(2)	0.0135(6)
C5	-0.3475(3)	0.9127(2)	-0.1519(2)	0.0122(5)

Table A.55 Atomic Co-ordinates for **Nb-3**.

Atom	x	y	z	U _{iso}
Nb1 Nb	0.19979(8)	0.26888(7)	0.34400(5)	0.0373(2)
F1 F	0.3375(8)	0.0690(5)	0.4383(3)	0.0591(12)
F2 F	0.4729(6)	0.2243(6)	0.2288(3)	0.0559(11)
F3 F	0.1237(10)	0.0837(9)	0.2608(5)	0.098(2)
F4 F	-0.0388(8)	0.2563(7)	0.4787(5)	0.0854(17)
F5 F	0.3137(8)	0.4080(5)	0.4437(4)	0.0617(12)
O1 O	0.0951(11)	0.4438(10)	0.2739(7)	0.096(3)
N1 N	-0.4568(9)	0.2764(7)	0.6064(6)	0.0511(15)
N2 N	-0.7590(16)	0.0447(12)	0.6882(8)	0.034(2)
N2A N	-0.881(2)	0.1759(16)	0.6683(10)	0.052(3)
C1 C	-0.6034(12)	0.3047(10)	0.7298(6)	0.0487(16)
C2 C	-0.7769(15)	0.1924(13)	0.7527(7)	0.079(3)
C3 C	-0.9184(15)	0.2132(15)	0.8790(7)	0.080(3)
C4 C	-0.8019(19)	0.1968(16)	0.9725(8)	0.091(3)
C5 C	-0.635(2)	0.3182(19)	0.9503(8)	0.102(4)
C6 C	-0.4833(17)	0.2799(16)	0.8213(9)	0.088(3)

Table A.56 Atomic Co-ordinates for **Nb-4**.

Atom	x	y	z	U _{iso}
Nb1	0.28989(4)	0.23163(4)	0.23838(3)	0.00347(16)
F1	0.2086(3)	-0.0017(3)	0.2462(3)	0.0136(5)
F2	0.0447(3)	0.3744(3)	0.1836(3)	0.0173(5)
F3	0.3962(3)	0.2322(3)	0.0007(3)	0.0162(5)
F4	0.5193(3)	0.0253(3)	0.2951(3)	0.0149(5)
F5	0.1682(4)	0.1817(4)	0.4801(3)	0.0184(5)
O1	0.3575(5)	0.4207(4)	0.2356(4)	0.0206(7)
N1	-0.0981(4)	0.0045(4)	0.1727(4)	0.0090(6)
N2	0.4484(4)	-0.3504(4)	0.3539(4)	0.0085(6)
C1	-0.0259(5)	-0.1767(5)	0.1169(5)	0.0106(7)
C2	-0.1477(6)	0.1746(5)	0.0282(5)	0.0113(7)
C3	0.6519(5)	-0.4437(5)	0.3658(5)	0.0105(7)
C4	0.3199(6)	-0.3540(5)	0.5258(5)	0.0116(7)

Table A.57 Atomic Co-ordinates for **Nb-5**.

Atom	x	y	z	U _{iso}
Ta1	0.63802(12)	0.22427(14)	0.08808(8)	0.0130(4)
F1	0.5964(18)	0.406(2)	0.1530(12)	0.022(3)
F2	0.7874(18)	0.381(2)	0.0995(12)	0.022(3)
F3	0.7552(17)	0.176(2)	0.2113(11)	0.022(3)
F4	0.4385(18)	0.228(2)	0.0474(12)	0.024(3)
F5	0.7571(19)	0.086(2)	0.0444(12)	0.026(4)
F6	0.5826(19)	0.011(2)	0.1113(13)	0.025(4)
F7	0.6040(19)	0.295(2)	-0.0260(13)	0.024(3)
F8	1.4635(17)	0.230(2)	0.2638(11)	0.018(4)
N1	1.149(2)	0.224(3)	0.1685(18)	0.024(5)
N2	1.352(2)	-0.026(3)	0.1544(15)	0.015(5)
N3	1.339(3)	0.485(3)	0.1660(18)	0.024(6)
N4	1.295(3)	0.207(4)	0.365(2)	0.030(6)
C1	1.121(3)	0.093(4)	0.104(2)	0.022(5)
C2	1.205(3)	-0.062(4)	0.138(2)	0.028(7)
C3	1.103(3)	0.380(4)	0.125(2)	0.022(6)
C4	1.213(3)	0.452(4)	0.0919(19)	0.017(5)
C5	1.081(4)	0.185(4)	0.241(2)	0.032(6)
C6	1.163(3)	0.274(3)	0.331(2)	0.020(5)

Table A.58 Atomic Co-ordinates for **Ta-1**.

Atom	x	y	z	U _{iso}
Ta1	0.95428(13)	0.02313(6)	0.06877(4)	0.0156(2)
Ta2	1.31437(14)	-0.32343(7)	0.27714(4)	0.0174(2)
Ta3	1.43804(14)	-0.74753(7)	0.38977(5)	0.0179(2)
F1	1.2102(19)	0.0371(10)	0.1403(6)	0.024(2)
F2	0.9928(18)	0.1702(10)	0.0366(6)	0.017(2)
F3	1.1652(19)	0.0241(11)	-0.0161(7)	0.025(2)
F4	1.040(2)	-0.1249(10)	0.0478(7)	0.024(3)
F5	0.796(2)	-0.0674(9)	0.1362(7)	0.029(3)
F6	0.775(2)	0.1149(10)	0.1335(7)	0.022(3)
F7	0.704(2)	0.0115(12)	-0.0070(7)	0.031(3)
F8	1.5290(19)	-0.3077(11)	0.3647(6)	0.028(3)
F9	1.469(2)	-0.2148(10)	0.2215(8)	0.033(3)
F10	1.564(2)	-0.3885(10)	0.2219(6)	0.025(3)
F11	1.3118(19)	-0.4745(11)	0.2973(8)	0.032(3)
F12	1.045(2)	-0.3491(12)	0.3382(7)	0.037(3)
F13	1.190(2)	-0.1869(11)	0.3060(8)	0.034(3)
F14	1.112(2)	-0.3469(12)	0.1886(7)	0.038(3)
F15	1.1814(19)	-0.6841(9)	0.3352(6)	0.020(2)
F16	1.545(2)	-0.7842(10)	0.2904(7)	0.030(3)
F17	1.679(2)	-0.6464(10)	0.3667(8)	0.033(3)
F18	1.434(2)	-0.6272(10)	0.4615(7)	0.026(3)
F19	1.226(2)	-0.7831(9)	0.4689(6)	0.019(2)
F20	1.3233(19)	-0.8896(9)	0.3679(6)	0.022(2)
F21	1.667(2)	-0.8168(11)	0.4535(7)	0.030(3)
N1	0.562(3)	0.0038(14)	0.2516(9)	0.020(4)
N2	0.875(3)	-0.1391(14)	0.4155(10)	0.021(4)
N3	1.221(3)	0.0379(13)	0.5540(9)	0.022(4)
N4	1.269(3)	0.2149(16)	-0.0907(9)	0.024(4)
N5	1.675(3)	0.3219(13)	0.0645(10)	0.021(4)
N6	1.873(3)	0.4442(15)	0.2510(9)	0.025(4)
C1	0.765(4)	-0.0221(17)	0.3040(11)	0.022(4)
C2	0.691(3)	-0.0756(17)	0.3784(11)	0.019(4)
C3	1.082(3)	-0.0809(17)	0.4508(10)	0.014(4)
C4	1.007(4)	-0.0182(18)	0.5201(12)	0.027(5)
C5	1.497(3)	0.2514(18)	-0.0514(10)	0.017(4)
C6	1.458(3)	0.2754(19)	0.0318(11)	0.023(5)
C7	1.658(3)	0.3594(18)	0.1442(12)	0.021(4)
C8	1.893(3)	0.3925(19)	0.1761(12)	0.026(5)

Table A.59 Atomic Co-ordinates for **Ta-2**.

Atom	x	y	z	U _{iso}
Ta1	0.0000	0.29516(3)	0.7500	0.00671(9)
F1	0.0000	0.5196(4)	0.7500	0.0145(7)
F2	0.0832(2)	0.2999(3)	0.9868(3)	0.0139(5)
F3	-0.07728(19)	0.1176(3)	0.7919(3)	0.0163(5)
F4	-0.14486(18)	0.3662(3)	0.7639(3)	0.0144(5)
N1	-0.2889(3)	0.1717(4)	0.8421(4)	0.0090(7)
C1	-0.3549(3)	0.3015(4)	0.8695(5)	0.0098(8)
C2	-0.2230(3)	0.0891(4)	1.0016(5)	0.0105(8)

Table A.60 Atomic Co-ordinates for **Ta-3**.