Table 1. Atomic coordinates, B_{iso}/B_{eq} and occupancy

atom	x	y	z	B_{eq}	occ
V(1)	0.22051(2)	0.87418(2)	0.64140(4)	1.40(1)	1.0000
V(2)	0.10948(2)	0.79940(2)	0.52794(4)	1.49(2)	1.0000
V(3)	0.36139(3)	0.82174(3)	0.50984(6)	2.89(2)	1.0000
Cl(1)	0.0415(3)	1.0171(3)	1.0299(4)	4.9(1)	0.2500
Cl(2)	0.0000	1.0000	1.0706(10)	6.2(3)	0.0833
F(1)	0.16417(8)	0.83427(8)	0.5871(1)	1.84(5)	1.0000
F(2)	-0.1241(4)	1.0290(4)	0.6370(6)	11.2219	0.6000
F(3)	-0.0784(3)	1.0088(4)	0.6705(7)	11.2219	0.6000
F(4)	-0.1449(3)	0.9734(3)	0.7091(7)	11.2219	0.6000
F(5)	-0.1012(4)	1.0383(4)	0.7499(5)	11.2219	0.6000
F(6)	-0.1395(6)	0.9683(5)	0.644(1)	12.1669	0.4000
F(7)	-0.0964(7)	1.0374(5)	0.6281(9)	12.1669	0.4000
F(8)	-0.0870(6)	1.0046(7)	0.721(1)	12.1669	0.4000
F(9)	-0.1425(6)	1.0144(7)	0.718(1)	12.1669	0.4000
O(1)	0.23205(10)	0.90970(10)	0.5627(2)	1.72(6)	1.0000
O(2)	0.1869(1)	0.8822(1)	0.7046(2)	2.05(6)	1.0000
O(3)	0.2656(1)	0.90099(10)	0.6797(2)	1.98(6)	1.0000
O(4)	0.1412(1)	0.7830(1)	0.4740(2)	2.05(6)	1.0000
O(5)	0.0896(1)	0.7659(1)	0.6089(2)	2.19(7)	1.0000
O(6)	0.0662(1)	0.7764(1)	0.4832(2)	2.16(7)	1.0000
O(7)	0.3567(1)	0.8525(1)	0.4281(3)	3.41(9)	1.0000
O(8)	0.3546(1)	0.8602(1)	0.5718(3)	3.60(10)	1.0000
O(9)	0.4079(1)	0.8297(2)	0.5252(3)	3.9(1)	1.0000
N(1)	0.2447(1)	0.8434(1)	0.5797(2)	1.63(7)	1.0000

Table 1. Atomic coordinates, B_{iso}/B_{eq} and occupancy

atom	x	y	z	B_{eq}	occ
N(2)	0.2020(1)	0.8173(1)	0.6971(2)	1.87(7)	1.0000
N(3)	0.1386(1)	0.8559(1)	0.4665(2)	1.78(7)	1.0000
N(4)	0.0900(1)	0.8376(1)	0.5770(2)	1.90(7)	1.0000
N(5)	0.3362(2)	0.7703(2)	0.4432(3)	4.1(1)	1.0000
N(6)	0.3221(2)	0.7747(2)	0.5797(3)	3.8(1)	1.0000
C(1)	0.2695(1)	0.9293(1)	0.5298(2)	1.67(8)	1.0000
C(2)	0.2869(2)	0.9717(2)	0.5075(3)	2.29(9)	1.0000
C(3)	0.3259(2)	0.9915(2)	0.4727(3)	2.50(10)	1.0000
C(4)	0.3472(2)	0.9699(2)	0.4562(3)	2.61(10)	1.0000
C(5)	0.3302(2)	0.9281(2)	0.4765(3)	2.32(10)	1.0000
C(6)	0.2917(1)	0.9073(2)	0.5146(3)	1.86(8)	1.0000
C(7)	0.2747(1)	0.8632(1)	0.5337(3)	1.83(9)	1.0000
C(8)	0.2307(2)	0.7994(1)	0.5983(3)	2.17(9)	1.0000
C(9)	0.2277(2)	0.7982(2)	0.6808(3)	2.4(1)	1.0000
C(10)	0.1688(2)	0.7980(1)	0.7369(3)	2.17(9)	1.0000
C(11)	0.1411(2)	0.8136(2)	0.7558(3)	2.12(9)	1.0000
C(12)	0.1043(2)	0.7873(2)	0.7948(3)	2.53(10)	1.0000
C(13)	0.0770(2)	0.8011(2)	0.8146(3)	2.7(1)	1.0000
C(14)	0.0864(2)	0.8420(2)	0.7973(3)	2.6(1)	1.0000
C(15)	0.1230(2)	0.8690(2)	0.7601(3)	2.5(1)	1.0000
C(16)	0.1505(1)	0.8549(2)	0.7386(3)	2.03(9)	1.0000
C(17)	0.1772(1)	0.8028(2)	0.4367(3)	1.96(9)	1.0000
C(18)	0.1978(2)	0.7809(2)	0.4171(3)	2.5(1)	1.0000
C(19)	0.2345(2)	0.8003(2)	0.3766(3)	2.9(1)	1.0000

Table 1. Atomic coordinates, B_{iso}/B_{eq} and occupancy

atom	x	y	z	B_{eq}	occ
C(20)	0.2511(2)	0.8425(2)	0.3531(3)	3.2(1)	1.0000
C(21)	0.2303(2)	0.8641(2)	0.3714(3)	2.6(1)	1.0000
C(22)	0.1936(1)	0.8454(2)	0.4133(2)	1.95(8)	1.0000
C(23)	0.1727(1)	0.8689(1)	0.4283(3)	1.93(8)	1.0000
C(24)	0.1208(2)	0.8835(2)	0.4775(3)	2.34(10)	1.0000
C(25)	0.1128(2)	0.8828(2)	0.5573(3)	2.42(10)	1.0000
C(26)	0.0571(2)	0.8228(2)	0.6172(3)	2.36(10)	1.0000
C(27)	0.0340(2)	0.7795(2)	0.6423(3)	2.60(10)	1.0000
C(28)	-0.0057(2)	0.7652(2)	0.6766(3)	3.0(1)	1.0000
C(29)	-0.0273(2)	0.7265(2)	0.7063(3)	3.8(1)	1.0000
C(30)	-0.0094(2)	0.6999(2)	0.7051(3)	3.6(1)	1.0000
C(31)	0.0301(2)	0.7130(2)	0.6731(3)	2.9(1)	1.0000
C(32)	0.0514(1)	0.7534(2)	0.6394(3)	2.32(9)	1.0000
C(33)	0.3507(2)	0.8440(2)	0.3613(5)	3.7(1)	1.0000
C(34)	0.3572(2)	0.8773(2)	0.3116(4)	4.0(2)	1.0000
C(35)	0.3492(2)	0.8687(3)	0.2380(5)	4.7(2)	1.0000
C(36)	0.3358(2)	0.8296(3)	0.2082(5)	4.9(2)	1.0000
C(37)	0.3308(3)	0.7957(3)	0.2567(5)	5.3(2)	1.0000
C(38)	0.3376(2)	0.8041(2)	0.3284(4)	4.3(2)	1.0000
C(39)	0.3299(3)	0.7682(2)	0.3753(4)	4.7(2)	1.0000
C(40)	0.3229(3)	0.7303(2)	0.4850(4)	4.7(2)	1.0000
C(41)	0.2982(2)	0.7314(2)	0.5489(4)	4.4(2)	1.0000
C(42)	0.3194(2)	0.7798(2)	0.6478(4)	3.6(1)	1.0000
C(43)	0.3368(2)	0.8202(2)	0.6830(4)	3.5(1)	1.0000

Table 1. Atomic coordinates, B_{iso}/B_{eq} and occupancy

atom	x	y	z	B_{eq}	occ
C(44)	0.3355(2)	0.8220(3)	0.7587(4)	4.1(1)	1.0000
C(45)	0.3476(2)	0.8579(3)	0.7944(4)	4.4(2)	1.0000
C(46)	0.3606(2)	0.8961(3)	0.7550(4)	4.2(2)	1.0000
C(47)	0.3619(2)	0.8954(2)	0.6815(4)	4.2(2)	1.0000
C(48)	0.3515(2)	0.8594(2)	0.6421(4)	3.5(1)	1.0000
C(49)	0.0000	1.0000	1.0000	3.7(3)	0.1667
B(1)	-0.1122(3)	1.0124(3)	0.6916(4)	11.2219	0.6000
B(2)	-0.1163(4)	1.0062(4)	0.6777(7)	12.1669	0.4000
H(2)	0.2722	0.9866	0.5161	2.7314	1.0000
H(3)	0.3383	1.0205	0.4600	2.9860	1.0000
H(4)	0.3733	0.9838	0.4309	3.1242	1.0000
H(5)	0.3447	0.9133	0.4647	2.7673	1.0000
H(7)	0.2864	0.8479	0.5111	2.1811	1.0000
H(8a)	0.2038	0.7808	0.5775	2.5974	1.0000
H(8b)	0.2507	0.7916	0.5825	2.5974	1.0000
H(9a)	0.2550	0.8141	0.7018	2.9279	1.0000
H(9b)	0.2145	0.7698	0.6979	2.9279	1.0000
H(10)	0.1622	0.7711	0.7553	2.5990	1.0000
H(12)	0.0982	0.7596	0.8079	3.0212	1.0000
H(13)	0.0517	0.7828	0.8399	3.2813	1.0000
H(14)	0.0675	0.8516	0.8113	3.1640	1.0000
H(15)	0.1293	0.8971	0.7493	3.0188	1.0000
H(18)	0.1866	0.7523	0.4319	2.9593	1.0000
H(19)	0.2486	0.7852	0.3645	3.5000	1.0000

Table 1. Atomic coordinates, B_{iso}/B_{eq} and occupancy

atom	x	y	z	B_{eq}	occ
H(20)	0.2762	0.8559	0.3249	3.7984	1.0000
H(21)	0.2413	0.8925	0.3552	3.1452	1.0000
H(23)	0.1849	0.8966	0.4084	2.3020	1.0000
H(24a)	0.1403	0.9116	0.4622	2.7991	1.0000
H(24b)	0.0951	0.8732	0.4516	2.7991	1.0000
H(25a)	0.0960	0.8954	0.5674	2.8884	1.0000
H(25b)	0.1388	0.8974	0.5828	2.8884	1.0000
H(26)	0.0473	0.8414	0.6315	2.8247	1.0000
H(28)	-0.0173	0.7835	0.6785	3.6367	1.0000
H(29)	-0.0543	0.7171	0.7277	4.5935	1.0000
H(30)	-0.0245	0.6726	0.7264	4.2740	1.0000
H(31)	0.0423	0.6953	0.6739	3.4640	1.0000
H(34)	0.3668	0.9052	0.3290	4.7321	1.0000
H(35)	0.3533	0.8912	0.2070	5.6669	1.0000
H(36)	0.3302	0.8245	0.1582	5.8570	1.0000
H(37)	0.3225	0.7693	0.2384	6.3565	1.0000
H(39)	0.3194	0.7413	0.3530	5.6624	1.0000
H(40a)	0.3057	0.7063	0.4560	5.6080	1.0000
H(40b)	0.3472	0.7292	0.5005	5.6080	1.0000
H(41a)	0.2955	0.7110	0.5836	5.2676	1.0000
H(41b)	0.2707	0.7255	0.5342	5.2676	1.0000
H(42)	0.3049	0.7551	0.6767	4.3490	1.0000
H(44)	0.3254	0.7965	0.7853	4.8690	1.0000
H(45)	0.3477	0.8582	0.8455	5.3150	1.0000

Table 1. Atomic coordinates, B_{iso}/B_{eq} and occupancy

atom	x	y	z	B_{eq}	occ
H(46)	0.3682	0.9218	0.7796	5.0461	1.0000
H(47)	0.3706	0.9211	0.6563	5.0404	1.0000

$$B_{eq} = \frac{8}{3}\pi^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}aa^*bb^*\cos\gamma + 2U_{13}aa^*cc^*\cos\beta + 2U_{23}bb^*cc^*\cos\alpha)$$

Table 2. Anisotropic Displacement Parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
V(1)	0.0146(4)	0.0132(4)	0.0211(4)	0.0038(3)	-0.0004(3)	-0.0011(3)
V(2)	0.0133(4)	0.0158(4)	0.0208(4)	0.0023(3)	0.0013(3)	-0.0026(3)
V(3)	0.0275(5)	0.0343(5)	0.0483(6)	0.0155(4)	-0.0044(4)	0.0021(4)
F(1)	0.015(1)	0.020(1)	0.026(1)	0.0023(10)	-0.0019(10)	-0.001(1)
O(1)	0.019(1)	0.017(1)	0.027(2)	0.007(1)	0.001(1)	0.002(1)
O(2)	0.024(2)	0.022(2)	0.028(2)	0.009(1)	0.007(1)	0.000(1)
O(3)	0.020(2)	0.021(2)	0.030(2)	0.007(1)	-0.002(1)	-0.004(1)
O(4)	0.023(2)	0.019(1)	0.029(2)	0.005(1)	0.006(1)	-0.004(1)
O(5)	0.020(2)	0.026(2)	0.028(2)	0.004(1)	0.003(1)	0.002(1)
O(6)	0.021(2)	0.026(2)	0.025(2)	0.005(1)	-0.004(1)	-0.006(1)
O(7)	0.035(2)	0.043(2)	0.053(3)	0.021(2)	0.007(2)	0.014(2)
O(8)	0.029(2)	0.041(2)	0.065(3)	0.016(2)	0.005(2)	0.014(2)
O(9)	0.036(2)	0.051(3)	0.061(3)	0.022(2)	0.002(2)	0.002(2)
N(1)	0.021(2)	0.018(2)	0.023(2)	0.010(1)	-0.004(1)	-0.004(1)
N(2)	0.023(2)	0.018(2)	0.026(2)	0.008(2)	-0.006(2)	0.002(1)
N(3)	0.020(2)	0.020(2)	0.023(2)	0.007(1)	-0.001(1)	0.000(1)
N(4)	0.018(2)	0.024(2)	0.025(2)	0.006(2)	-0.004(1)	-0.004(2)
N(5)	0.056(3)	0.038(3)	0.059(4)	0.023(3)	-0.019(3)	0.001(2)
N(6)	0.037(3)	0.037(3)	0.067(4)	0.016(2)	-0.004(2)	0.011(3)
C(1)	0.015(2)	0.020(2)	0.021(2)	0.004(2)	-0.003(2)	0.000(2)
C(2)	0.022(2)	0.023(2)	0.034(3)	0.006(2)	0.002(2)	0.005(2)
C(3)	0.025(2)	0.026(2)	0.031(3)	0.002(2)	0.000(2)	0.009(2)
C(4)	0.022(2)	0.040(3)	0.025(3)	0.007(2)	0.002(2)	0.007(2)
C(5)	0.024(2)	0.039(3)	0.024(2)	0.014(2)	0.001(2)	0.003(2)

Table 2. Anisotropic Displacement Parameters (continued)

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(6)	0.016(2)	0.027(2)	0.024(2)	0.009(2)	-0.003(2)	0.000(2)
C(7)	0.018(2)	0.026(2)	0.026(2)	0.011(2)	-0.004(2)	-0.006(2)
C(8)	0.029(2)	0.020(2)	0.032(3)	0.011(2)	-0.001(2)	-0.004(2)
C(9)	0.037(3)	0.024(2)	0.030(3)	0.015(2)	-0.003(2)	0.004(2)
C(10)	0.032(2)	0.020(2)	0.023(2)	0.007(2)	-0.005(2)	0.003(2)
C(11)	0.024(2)	0.026(2)	0.020(2)	0.005(2)	-0.002(2)	0.000(2)
C(12)	0.030(2)	0.030(2)	0.021(2)	0.003(2)	-0.002(2)	0.003(2)
C(13)	0.025(2)	0.043(3)	0.021(2)	0.005(2)	0.002(2)	-0.001(2)
C(14)	0.028(2)	0.048(3)	0.022(2)	0.017(2)	-0.002(2)	-0.005(2)
C(15)	0.032(3)	0.037(3)	0.023(2)	0.015(2)	0.003(2)	-0.003(2)
C(16)	0.021(2)	0.027(2)	0.021(2)	0.006(2)	-0.001(2)	0.000(2)
C(17)	0.022(2)	0.028(2)	0.020(2)	0.010(2)	0.001(2)	-0.006(2)
C(18)	0.031(3)	0.040(3)	0.027(3)	0.021(2)	-0.002(2)	-0.008(2)
C(19)	0.031(3)	0.050(3)	0.033(3)	0.022(3)	-0.001(2)	-0.012(2)
C(20)	0.017(2)	0.066(4)	0.033(3)	0.017(2)	0.003(2)	-0.006(3)
C(21)	0.024(2)	0.041(3)	0.025(3)	0.008(2)	0.002(2)	-0.002(2)
C(22)	0.017(2)	0.028(2)	0.018(2)	0.003(2)	-0.001(2)	-0.003(2)
C(23)	0.022(2)	0.020(2)	0.021(2)	0.003(2)	-0.003(2)	-0.002(2)
C(24)	0.030(2)	0.025(2)	0.036(3)	0.015(2)	0.000(2)	0.001(2)
C(25)	0.031(2)	0.024(2)	0.036(3)	0.012(2)	0.001(2)	-0.006(2)
C(26)	0.022(2)	0.040(3)	0.026(2)	0.015(2)	0.000(2)	-0.009(2)
C(27)	0.020(2)	0.040(3)	0.026(3)	0.006(2)	0.001(2)	-0.007(2)
C(28)	0.025(2)	0.055(4)	0.030(3)	0.016(2)	0.003(2)	-0.004(2)
C(29)	0.022(3)	0.067(4)	0.033(3)	0.004(3)	0.009(2)	0.004(3)

Table 2. Anisotropic Displacement Parameters (continued)

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(30)	0.033(3)	0.047(3)	0.026(3)	-0.003(3)	0.002(2)	0.011(2)
C(31)	0.029(3)	0.036(3)	0.027(3)	0.003(2)	-0.002(2)	0.007(2)
C(32)	0.018(2)	0.036(3)	0.020(2)	0.002(2)	0.001(2)	0.001(2)
C(33)	0.016(2)	0.037(3)	0.090(5)	0.016(2)	0.001(3)	0.011(3)
C(34)	0.037(3)	0.063(4)	0.058(4)	0.031(3)	0.022(3)	0.024(3)
C(35)	0.028(3)	0.064(5)	0.099(6)	0.031(3)	0.019(3)	0.029(4)
C(36)	0.039(3)	0.075(5)	0.066(5)	0.024(4)	-0.012(3)	0.010(4)
C(37)	0.065(5)	0.050(4)	0.082(6)	0.025(4)	-0.008(4)	0.005(4)
C(38)	0.042(3)	0.044(4)	0.071(5)	0.018(3)	-0.020(3)	0.002(3)
C(39)	0.067(5)	0.043(4)	0.062(5)	0.021(3)	-0.014(4)	-0.009(3)
C(40)	0.074(5)	0.032(3)	0.063(5)	0.021(3)	-0.016(4)	0.000(3)
C(41)	0.050(4)	0.040(3)	0.065(5)	0.013(3)	-0.012(3)	0.016(3)
C(42)	0.035(3)	0.051(4)	0.051(4)	0.020(3)	-0.005(3)	0.010(3)
C(43)	0.026(3)	0.046(3)	0.056(4)	0.014(2)	0.000(3)	0.006(3)
C(44)	0.034(3)	0.071(5)	0.045(4)	0.023(3)	-0.003(3)	0.016(3)
C(45)	0.032(3)	0.076(5)	0.052(4)	0.020(3)	0.000(3)	0.008(4)
C(46)	0.028(3)	0.067(4)	0.059(4)	0.018(3)	0.008(3)	0.001(3)
C(47)	0.034(3)	0.060(4)	0.073(5)	0.029(3)	0.014(3)	0.006(4)
C(48)	0.019(2)	0.057(4)	0.048(4)	0.013(2)	-0.001(2)	0.013(3)

The general temperature factor expression:

$$\exp(-2\pi^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl))$$

Table 3. Bond Lengths(Å)

atom	atom	distance	atom	atom	distance
V(1)	F(1)	2.088(2)	V(1)	O(1)	1.857(3)
V(1)	O(2)	1.823(4)	V(1)	O(3)	1.598(3)
V(1)	N(1)	2.082(5)	V(1)	N(2)	2.103(4)
V(2)	F(1)	2.064(2)	V(2)	O(4)	1.839(4)
V(2)	O(5)	1.844(4)	V(2)	O(6)	1.599(3)
V(2)	N(3)	2.117(4)	V(2)	N(4)	2.065(5)
V(3)	O(7)	1.945(5)	V(3)	O(8)	1.922(6)
V(3)	O(9)	1.596(5)	V(3)	N(5)	2.042(6)
V(3)	N(6)	2.055(5)	Cl(1)	Cl(1)	1.72(1)
Cl(1)	Cl(1)	2.28(2)	Cl(1)	Cl(1)	1.72(1)
Cl(1)	Cl(1)	2.28(2)	Cl(1)	Cl(2)	1.52(1)
Cl(1)	Cl(2)	2.29(2)	Cl(1)	C(49)	1.428(9)
Cl(2)	C(49)	1.31(2)	O(1)	C(1)	1.329(5)
O(2)	C(16)	1.352(5)	O(4)	C(17)	1.352(6)
O(5)	C(32)	1.352(8)	O(7)	C(33)	1.273(10)
O(8)	C(48)	1.311(8)	N(1)	C(7)	1.287(6)
N(1)	C(8)	1.462(7)	N(2)	C(9)	1.451(9)
N(2)	C(10)	1.284(6)	N(3)	C(23)	1.298(6)
N(3)	C(24)	1.458(9)	N(4)	C(25)	1.470(6)
N(4)	C(26)	1.280(6)	N(5)	C(39)	1.28(1)
N(5)	C(40)	1.501(10)	N(6)	C(41)	1.482(9)
N(6)	C(42)	1.292(10)	C(1)	C(2)	1.405(7)
C(1)	C(6)	1.427(9)	C(2)	C(3)	1.391(7)
C(3)	C(4)	1.38(1)	C(4)	C(5)	1.379(8)

Table 3. Bond Lengths(Å) (continued)

atom	atom	distance	atom	atom	distance
C(5)	C(6)	1.407(7)	C(6)	C(7)	1.447(7)
C(8)	C(9)	1.538(7)	C(10)	C(11)	1.427(9)
C(11)	C(12)	1.399(6)	C(11)	C(16)	1.404(8)
C(12)	C(13)	1.37(1)	C(13)	C(14)	1.390(10)
C(14)	C(15)	1.381(7)	C(15)	C(16)	1.397(10)
C(17)	C(18)	1.39(1)	C(17)	C(22)	1.423(7)
C(18)	C(19)	1.380(8)	C(19)	C(20)	1.411(10)
C(20)	C(21)	1.38(1)	C(21)	C(22)	1.395(7)
C(22)	C(23)	1.429(9)	C(24)	C(25)	1.510(8)
C(26)	C(27)	1.444(8)	C(27)	C(28)	1.422(8)
C(27)	C(32)	1.38(1)	C(28)	C(29)	1.344(9)
C(29)	C(30)	1.41(1)	C(30)	C(31)	1.404(9)
C(31)	C(32)	1.421(8)	C(33)	C(34)	1.45(1)
C(33)	C(38)	1.42(1)	C(34)	C(35)	1.40(1)
C(35)	C(36)	1.37(1)	C(36)	C(37)	1.44(1)
C(37)	C(38)	1.36(1)	C(38)	C(39)	1.48(1)
C(40)	C(41)	1.50(1)	C(42)	C(43)	1.437(10)
C(43)	C(44)	1.412(10)	C(43)	C(48)	1.46(1)
C(44)	C(45)	1.33(1)	C(45)	C(46)	1.43(1)
C(46)	C(47)	1.37(1)	C(47)	C(48)	1.38(1)
B(1)	F(2)	1.36(2)	B(1)	F(3)	1.36(2)
B(1)	F(4)	1.36(1)	B(1)	F(5)	1.36(1)
B(1)	B(2)	0.33(1)	B(1)	F(6)	1.66(2)
B(1)	F(7)	1.43(2)	B(1)	F(8)	1.22(3)

Table 3. Bond Lengths($\AA$) (continued)

atom	atom	distance	atom	atom	distance
B(1)	F(9)	1.24(3)	F(2)	B(2)	1.26(2)
F(2)	F(7)	0.91(3)	F(2)	F(9)	1.63(2)
F(3)	B(2)	1.34(2)	F(3)	F(7)	1.68(3)
F(3)	F(8)	0.97(2)	F(4)	B(2)	1.27(1)
F(4)	F(6)	1.26(2)	F(4)	F(9)	1.46(3)
F(5)	B(2)	1.68(2)	F(5)	F(8)	1.64(3)
F(5)	F(9)	1.43(2)	B(2)	F(6)	1.36(2)
B(2)	F(7)	1.36(2)	B(2)	F(8)	1.36(3)
B(2)	F(9)	1.36(3)			

Table 4. Bond Lengths(Å)

atom	atom	distance	atom	atom	distance
C(2)	H(2)	0.95	C(3)	H(3)	0.95
C(4)	H(4)	0.95	C(5)	H(5)	0.95
C(7)	H(7)	0.95	C(8)	H(8a)	0.95
C(8)	H(8b)	0.95	C(9)	H(9a)	0.95
C(9)	H(9b)	0.95	C(10)	H(10)	0.95
C(12)	H(12)	0.95	C(13)	H(13)	0.95
C(14)	H(14)	0.95	C(15)	H(15)	0.95
C(18)	H(18)	0.95	C(19)	H(19)	0.95
C(20)	H(20)	0.95	C(21)	H(21)	0.95
C(23)	H(23)	0.95	C(24)	H(24a)	0.95
C(24)	H(24b)	0.95	C(25)	H(25a)	0.95
C(25)	H(25b)	0.95	C(26)	H(26)	0.95
C(28)	H(28)	0.95	C(29)	H(29)	0.95
C(30)	H(30)	0.95	C(31)	H(31)	0.95
C(34)	H(34)	0.95	C(35)	H(35)	0.95
C(36)	H(36)	0.95	C(37)	H(37)	0.95
C(39)	H(39)	0.95	C(40)	H(40a)	0.95
C(40)	H(40b)	0.95	C(41)	H(41a)	0.95
C(41)	H(41b)	0.95	C(42)	H(42)	0.95
C(44)	H(44)	0.95	C(45)	H(45)	0.95
C(46)	H(46)	0.95	C(47)	H(47)	0.95

Table 5. Bond Angles(°)

atom	atom	atom	angle	atom	atom	atom	angle
F(1)	V(1)	O(1)	84.6(1)	F(1)	V(1)	O(2)	85.3(1)
F(1)	V(1)	O(3)	173.1(2)	F(1)	V(1)	N(1)	83.8(1)
F(1)	V(1)	N(2)	80.4(1)	O(1)	V(1)	O(2)	109.4(2)
O(1)	V(1)	O(3)	96.9(2)	O(1)	V(1)	N(1)	86.0(2)
O(1)	V(1)	N(2)	157.5(2)	O(2)	V(1)	O(3)	100.5(2)
O(2)	V(1)	N(1)	160.1(1)	O(2)	V(1)	N(2)	86.0(2)
O(3)	V(1)	N(1)	89.6(2)	O(3)	V(1)	N(2)	96.2(2)
N(1)	V(1)	N(2)	75.8(2)	F(1)	V(2)	O(4)	85.5(1)
F(1)	V(2)	O(5)	84.9(1)	F(1)	V(2)	O(6)	174.0(2)
F(1)	V(2)	N(3)	80.2(1)	F(1)	V(2)	N(4)	84.3(1)
O(4)	V(2)	O(5)	109.5(2)	O(4)	V(2)	O(6)	99.2(2)
O(4)	V(2)	N(3)	86.0(2)	O(4)	V(2)	N(4)	160.5(1)
O(5)	V(2)	O(6)	96.9(2)	O(5)	V(2)	N(3)	157.6(2)
O(5)	V(2)	N(4)	86.1(2)	O(5)	V(2)	N(3)	96.4(2)
O(6)	V(2)	N(4)	90.1(2)	N(3)	V(2)	N(4)	75.9(2)
O(7)	V(3)	O(8)	88.3(2)	O(7)	V(3)	O(9)	115.2(2)
O(7)	V(3)	N(5)	85.8(2)	O(7)	V(3)	N(6)	138.5(2)
O(8)	V(3)	O(9)	105.8(2)	O(8)	V(3)	N(5)	150.5(2)
O(8)	V(3)	N(6)	86.5(2)	O(9)	V(3)	N(5)	102.9(3)
O(9)	V(3)	N(6)	105.8(3)	N(5)	V(3)	N(6)	79.1(2)
Cl(1)	Cl(1)	Cl(1)	48.6(3)	Cl(1)	Cl(1)	Cl(1)	82.8(7)
Cl(1)	Cl(1)	Cl(1)	90.000(5)	Cl(1)	Cl(1)	Cl(2)	89.5(5)
Cl(1)	Cl(1)	Cl(2)	41.6(3)	Cl(1)	Cl(1)	C(49)	52.9(2)
Cl(1)	Cl(1)	Cl(1)	90.000(7)	Cl(1)	Cl(1)	Cl(1)	60.000(8)

Table 5. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
Cl(1)	Cl(1)	Cl(2)	41.4(4)	Cl(1)	Cl(1)	Cl(2)	60.1(3)
Cl(1)	Cl(1)	C(49)	37.1(2)	Cl(1)	Cl(1)	Cl(1)	48.6(3)
Cl(1)	Cl(1)	Cl(2)	89.5(5)	Cl(1)	Cl(1)	Cl(2)	41.6(3)
Cl(1)	Cl(1)	C(49)	52.9(2)	Cl(1)	Cl(1)	Cl(2)	41.4(4)
Cl(1)	Cl(1)	Cl(2)	60.1(3)	Cl(1)	Cl(1)	C(49)	37.1(2)
Cl(2)	Cl(1)	Cl(2)	84.8(9)	Cl(2)	Cl(1)	C(49)	52.9(7)
Cl(2)	Cl(1)	C(49)	31.9(3)	Cl(1)	Cl(2)	Cl(1)	48.9(5)
Cl(1)	Cl(2)	Cl(1)	97.3(9)	Cl(1)	Cl(2)	Cl(1)	95.2(9)
Cl(1)	Cl(2)	Cl(1)	48.9(5)	Cl(1)	Cl(2)	Cl(1)	97.3(9)
Cl(1)	Cl(2)	C(49)	60.1(7)	Cl(1)	Cl(2)	Cl(1)	48.9(5)
Cl(1)	Cl(2)	Cl(1)	59.8(5)	Cl(1)	Cl(2)	Cl(1)	59.8(5)
Cl(1)	Cl(2)	Cl(1)	95.2(9)	Cl(1)	Cl(2)	C(49)	35.1(3)
Cl(1)	Cl(2)	Cl(1)	48.9(5)	Cl(1)	Cl(2)	Cl(1)	95.2(9)
Cl(1)	Cl(2)	Cl(1)	97.3(9)	Cl(1)	Cl(2)	C(49)	60.1(7)
Cl(1)	Cl(2)	Cl(1)	59.8(5)	Cl(1)	Cl(2)	Cl(1)	48.9(5)
Cl(1)	Cl(2)	C(49)	35.1(3)	Cl(1)	Cl(2)	Cl(1)	48.9(5)
Cl(1)	Cl(2)	C(49)	35.1(3)	Cl(1)	Cl(2)	C(49)	60.1(7)
V(1)	F(1)	V(2)	174.9(2)	V(1)	O(1)	C(1)	123.5(4)
V(1)	O(2)	C(16)	132.4(4)	V(2)	O(4)	C(17)	135.8(3)
V(2)	O(5)	C(32)	124.2(4)	V(3)	O(7)	C(33)	132.6(5)
V(3)	O(8)	C(48)	128.6(5)	V(1)	N(1)	C(7)	122.4(4)
V(1)	N(1)	C(8)	116.8(3)	C(7)	N(1)	C(8)	120.2(5)
V(1)	N(2)	C(9)	113.8(3)	V(1)	N(2)	C(10)	125.0(5)
C(9)	N(2)	C(10)	120.9(5)	V(2)	N(3)	C(23)	125.0(4)

Table 5. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
V(2)	N(3)	C(24)	114.5(3)	C(23)	N(3)	C(24)	120.0(4)
V(2)	N(4)	C(25)	116.8(3)	V(2)	N(4)	C(26)	122.5(4)
C(25)	N(4)	C(26)	120.3(5)	V(3)	N(5)	C(39)	129.6(5)
V(3)	N(5)	C(40)	110.8(5)	C(39)	N(5)	C(40)	119.5(6)
V(3)	N(6)	C(41)	115.9(5)	V(3)	N(6)	C(42)	124.8(4)
C(41)	N(6)	C(42)	119.0(5)	O(1)	C(1)	C(2)	120.4(5)
O(1)	C(1)	C(6)	120.4(4)	C(2)	C(1)	C(6)	119.2(4)
C(1)	C(2)	C(3)	119.4(6)	C(2)	C(3)	C(4)	121.7(5)
C(3)	C(4)	C(5)	119.8(5)	C(4)	C(5)	C(6)	120.6(6)
C(1)	C(6)	C(5)	119.3(5)	C(1)	C(6)	C(7)	121.9(4)
C(5)	C(6)	C(7)	118.8(6)	N(1)	C(7)	C(6)	123.8(5)
N(1)	C(8)	C(9)	104.4(4)	N(2)	C(9)	C(8)	104.4(5)
N(2)	C(10)	C(11)	125.7(5)	C(10)	C(11)	C(12)	118.9(5)
C(10)	C(11)	C(16)	121.9(4)	C(12)	C(11)	C(16)	119.2(6)
C(11)	C(12)	C(13)	120.7(6)	C(12)	C(13)	C(14)	119.8(5)
C(13)	C(14)	C(15)	120.9(7)	C(14)	C(15)	C(16)	119.7(6)
O(2)	C(16)	C(11)	121.2(6)	O(2)	C(16)	C(15)	118.9(5)
C(11)	C(16)	C(15)	119.7(4)	O(4)	C(17)	C(18)	119.7(5)
O(4)	C(17)	C(22)	120.9(6)	C(18)	C(17)	C(22)	119.4(4)
C(17)	C(18)	C(19)	120.7(6)	C(18)	C(19)	C(20)	120.3(7)
C(19)	C(20)	C(21)	119.1(5)	C(20)	C(21)	C(22)	121.5(6)
C(17)	C(22)	C(21)	118.9(6)	C(17)	C(22)	C(23)	122.2(4)
C(21)	C(22)	C(23)	118.9(5)	N(3)	C(23)	C(22)	126.0(4)
N(3)	C(24)	C(25)	105.9(5)	N(4)	C(25)	C(24)	105.1(4)

Table 5. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
N(4)	C(26)	C(27)	124.1(6)	C(26)	C(27)	C(28)	118.4(7)
C(26)	C(27)	C(32)	121.5(5)	C(28)	C(27)	C(32)	119.9(5)
C(27)	C(28)	C(29)	121.6(8)	C(28)	C(29)	C(30)	119.0(6)
C(29)	C(30)	C(31)	121.4(6)	C(30)	C(31)	C(32)	118.3(7)
O(5)	C(32)	C(27)	122.2(5)	O(5)	C(32)	C(31)	118.0(6)
C(27)	C(32)	C(31)	119.7(5)	O(7)	C(33)	C(34)	119.0(6)
O(7)	C(33)	C(38)	126.6(7)	C(34)	C(33)	C(38)	114.4(7)
C(33)	C(34)	C(35)	120.5(7)	C(34)	C(35)	C(36)	123.6(9)
C(35)	C(36)	C(37)	116.3(8)	C(36)	C(37)	C(38)	121.1(8)
C(33)	C(38)	C(37)	124.1(8)	C(33)	C(38)	C(39)	118.1(7)
C(37)	C(38)	C(39)	117.8(7)	N(5)	C(39)	C(38)	125.5(7)
N(5)	C(40)	C(41)	106.9(7)	N(6)	C(41)	C(40)	107.0(5)
N(6)	C(42)	C(43)	124.5(6)	C(42)	C(43)	C(44)	119.5(6)
C(42)	C(43)	C(48)	121.6(6)	C(44)	C(43)	C(48)	118.5(7)
C(43)	C(44)	C(45)	122.7(7)	C(44)	C(45)	C(46)	119.2(7)
C(45)	C(46)	C(47)	119.5(8)	C(46)	C(47)	C(48)	123.6(8)
O(8)	C(48)	C(43)	121.6(6)	O(8)	C(48)	C(47)	122.0(7)
C(43)	C(48)	C(47)	116.4(6)	Cl(1)	C(49)	Cl(1)	74.2(4)
Cl(1)	C(49)	Cl(1)	105.8(4)	Cl(1)	C(49)	Cl(1)	180.0
Cl(1)	C(49)	Cl(1)	74.2(4)	Cl(1)	C(49)	Cl(1)	105.8(4)
Cl(1)	C(49)	Cl(2)	67.1(3)	Cl(1)	C(49)	Cl(2)	112.9(3)
Cl(1)	C(49)	Cl(1)	74.2(4)	Cl(1)	C(49)	Cl(1)	105.8(4)
Cl(1)	C(49)	Cl(1)	105.8(4)	Cl(1)	C(49)	Cl(1)	180.0000(1)
Cl(1)	C(49)	Cl(2)	112.9(3)	Cl(1)	C(49)	Cl(2)	67.1(3)

Table 5. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
Cl(1)	C(49)	Cl(1)	74.2(4)	Cl(1)	C(49)	Cl(1)	180.0000(2)
Cl(1)	C(49)	Cl(1)	105.8(4)	Cl(1)	C(49)	Cl(2)	67.1(3)
Cl(1)	C(49)	Cl(2)	112.9(3)	Cl(1)	C(49)	Cl(1)	105.8(4)
Cl(1)	C(49)	Cl(1)	74.2(4)	Cl(1)	C(49)	Cl(2)	112.9(3)
Cl(1)	C(49)	Cl(2)	67.1(3)	Cl(1)	C(49)	Cl(1)	74.2(4)
Cl(1)	C(49)	Cl(2)	112.9(3)	Cl(1)	C(49)	Cl(2)	67.1(3)
Cl(1)	C(49)	Cl(2)	67.1(3)	Cl(1)	C(49)	Cl(2)	112.9(3)
Cl(2)	C(49)	Cl(2)	180.0	F(2)	B(1)	F(3)	109(1)
F(2)	B(1)	F(4)	109.5(9)	F(2)	B(1)	F(5)	109(1)
F(2)	B(1)	B(2)	65(3)	F(2)	B(1)	F(6)	81.9(10)
F(2)	B(1)	F(7)	38(1)	F(2)	B(1)	F(8)	152(1)
F(2)	B(1)	F(9)	77(1)	F(3)	B(1)	F(4)	109(1)
F(3)	B(1)	F(5)	109.4(10)	F(3)	B(1)	B(2)	80(3)
F(3)	B(1)	F(6)	83(1)	F(3)	B(1)	F(7)	74(1)
F(3)	B(1)	F(8)	44(1)	F(3)	B(1)	F(9)	173(1)
F(4)	B(1)	F(5)	109.4(9)	F(4)	B(1)	B(2)	66(2)
F(4)	B(1)	F(6)	48.1(9)	F(4)	B(1)	F(7)	136(1)
F(4)	B(1)	F(8)	91(1)	F(4)	B(1)	F(9)	67(1)
F(5)	B(1)	B(2)	170(3)	F(5)	B(1)	F(6)	157.5(9)
F(5)	B(1)	F(7)	109.4(10)	F(5)	B(1)	F(8)	79(1)
F(5)	B(1)	F(9)	66(1)	B(2)	B(1)	F(6)	20(2)
B(2)	B(1)	F(7)	71(2)	B(2)	B(1)	F(8)	109(4)
B(2)	B(1)	F(9)	103(3)	F(6)	B(1)	F(7)	91(1)
F(6)	B(1)	F(8)	99(1)	F(6)	B(1)	F(9)	98(1)

Table 5. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
F(7)	B(1)	F(8)	114(1)	F(7)	B(1)	F(9)	112(1)
F(8)	B(1)	F(9)	129(1)	B(1)	F(2)	B(2)	13.6(7)
B(1)	F(2)	F(7)	74(1)	B(1)	F(2)	F(9)	48(1)
B(2)	F(2)	F(7)	75(1)	B(2)	F(2)	F(9)	54(1)
F(7)	F(2)	F(9)	118(1)	B(1)	F(3)	B(2)	13.9(6)
B(1)	F(3)	F(7)	54.7(10)	B(1)	F(3)	F(8)	60(1)
B(2)	F(3)	F(7)	51(1)	B(2)	F(3)	F(8)	69(1)
F(7)	F(3)	F(8)	110(2)	B(1)	F(4)	B(2)	13.7(7)
B(1)	F(4)	F(6)	78.6(9)	B(1)	F(4)	F(9)	52.3(9)
B(2)	F(4)	F(6)	65(1)	B(2)	F(4)	F(9)	59(1)
F(6)	F(4)	F(9)	109(1)	B(1)	F(5)	B(2)	1.9(7)
B(1)	F(5)	F(8)	46.5(9)	B(1)	F(5)	F(9)	52(1)
B(2)	F(5)	F(8)	48.2(10)	B(2)	F(5)	F(9)	51(1)
F(8)	F(5)	F(9)	62(1)	B(1)	B(2)	F(2)	101(3)
B(1)	B(2)	F(3)	85(3)	B(1)	B(2)	F(4)	99(2)
B(1)	B(2)	F(5)	7(3)	B(1)	B(2)	F(6)	155(3)
B(1)	B(2)	F(7)	95(2)	B(1)	B(2)	F(8)	57(3)
B(1)	B(2)	F(9)	62(3)	F(2)	B(2)	F(3)	117(1)
F(2)	B(2)	F(4)	123(1)	F(2)	B(2)	F(5)	97(1)
F(2)	B(2)	F(6)	99(1)	F(2)	B(2)	F(7)	40(1)
F(2)	B(2)	F(8)	145(1)	F(2)	B(2)	F(9)	76(1)
F(3)	B(2)	F(4)	116(1)	F(3)	B(2)	F(5)	93(1)
F(3)	B(2)	F(6)	96(1)	F(3)	B(2)	F(7)	76(1)
F(3)	B(2)	F(8)	42(1)	F(3)	B(2)	F(9)	148(1)

Table 5. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
F(4)	B(2)	F(5)	96(1)	F(4)	B(2)	F(6)	57(1)
F(4)	B(2)	F(7)	160(1)	F(4)	B(2)	F(8)	89(1)
F(4)	B(2)	F(9)	67(1)	F(5)	B(2)	F(6)	153(1)
F(5)	B(2)	F(7)	96(1)	F(5)	B(2)	F(8)	64(1)
F(5)	B(2)	F(9)	54(1)	F(6)	B(2)	F(7)	109(1)
F(6)	B(2)	F(8)	109(1)	F(6)	B(2)	F(9)	109(1)
F(7)	B(2)	F(8)	109(1)	F(7)	B(2)	F(9)	109(1)
F(8)	B(2)	F(9)	109(1)	B(1)	F(6)	F(4)	53.3(8)
B(1)	F(6)	B(2)	4.7(6)	F(4)	F(6)	B(2)	57(1)
B(1)	F(7)	F(2)	66(1)	B(1)	F(7)	F(3)	51.1(9)
B(1)	F(7)	B(2)	13.2(6)	F(2)	F(7)	F(3)	114(1)
F(2)	F(7)	B(2)	63(1)	F(3)	F(7)	B(2)	51(1)
B(1)	F(8)	F(3)	75(1)	B(1)	F(8)	F(5)	54(1)
B(1)	F(8)	B(2)	13.1(8)	F(3)	F(8)	F(5)	113(2)
F(3)	F(8)	B(2)	68(1)	F(5)	F(8)	B(2)	67(1)
B(1)	F(9)	F(2)	54(1)	B(1)	F(9)	F(4)	59(1)
B(1)	F(9)	F(5)	60(1)	B(1)	F(9)	B(2)	13.5(7)
F(2)	F(9)	F(4)	91(1)	F(2)	F(9)	F(5)	92(1)
F(2)	F(9)	B(2)	48(1)	F(4)	F(9)	F(5)	100(1)
F(4)	F(9)	B(2)	53(1)	F(5)	F(9)	B(2)	74(1)

Table 6. Bond Angles(°)

atom	atom	atom	angle	atom	atom	atom	angle
C(1)	C(2)	H(2)	120.3	C(3)	C(2)	H(2)	120.3
C(2)	C(3)	H(3)	119.2	C(4)	C(3)	H(3)	119.2
C(3)	C(4)	H(4)	120.1	C(5)	C(4)	H(4)	120.1
C(4)	C(5)	H(5)	119.7	C(6)	C(5)	H(5)	119.7
N(1)	C(7)	H(7)	118.1	C(6)	C(7)	H(7)	118.1
N(1)	C(8)	H(8a)	110.7	N(1)	C(8)	H(8b)	110.7
C(9)	C(8)	H(8a)	110.7	C(9)	C(8)	H(8b)	110.7
H(8a)	C(8)	H(8b)	109.5	N(2)	C(9)	H(9a)	110.7
N(2)	C(9)	H(9b)	110.7	C(8)	C(9)	H(9a)	110.7
C(8)	C(9)	H(9b)	110.7	H(9a)	C(9)	H(9b)	109.5
N(2)	C(10)	H(10)	117.2	C(11)	C(10)	H(10)	117.2
C(11)	C(12)	H(12)	119.6	C(13)	C(12)	H(12)	119.7
C(12)	C(13)	H(13)	120.1	C(14)	C(13)	H(13)	120.1
C(13)	C(14)	H(14)	119.6	C(15)	C(14)	H(14)	119.6
C(14)	C(15)	H(15)	120.2	C(16)	C(15)	H(15)	120.2
C(17)	C(18)	H(18)	119.6	C(19)	C(18)	H(18)	119.6
C(18)	C(19)	H(19)	119.8	C(20)	C(19)	H(19)	119.8
C(19)	C(20)	H(20)	120.4	C(21)	C(20)	H(20)	120.4
C(20)	C(21)	H(21)	119.3	C(22)	C(21)	H(21)	119.2
N(3)	C(23)	H(23)	117.0	C(22)	C(23)	H(23)	117.0
N(3)	C(24)	H(24a)	110.4	N(3)	C(24)	H(24b)	110.4
C(25)	C(24)	H(24a)	110.4	C(25)	C(24)	H(24b)	110.4
H(24a)	C(24)	H(24b)	109.5	N(4)	C(25)	H(25a)	110.6
N(4)	C(25)	H(25b)	110.6	C(24)	C(25)	H(25a)	110.5

Table 6. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C(24)	C(25)	H(25b)	110.5	H(25a)	C(25)	H(25b)	109.5
N(4)	C(26)	H(26)	117.9	C(27)	C(26)	H(26)	117.9
C(27)	C(28)	H(28)	119.2	C(29)	C(28)	H(28)	119.2
C(28)	C(29)	H(29)	120.5	C(30)	C(29)	H(29)	120.5
C(29)	C(30)	H(30)	119.3	C(31)	C(30)	H(30)	119.3
C(30)	C(31)	H(31)	120.8	C(32)	C(31)	H(31)	120.8
C(33)	C(34)	H(34)	119.8	C(35)	C(34)	H(34)	119.8
C(34)	C(35)	H(35)	118.2	C(36)	C(35)	H(35)	118.2
C(35)	C(36)	H(36)	121.9	C(37)	C(36)	H(36)	121.8
C(36)	C(37)	H(37)	119.5	C(38)	C(37)	H(37)	119.4
N(5)	C(39)	H(39)	117.3	C(38)	C(39)	H(39)	117.2
N(5)	C(40)	H(40a)	110.1	N(5)	C(40)	H(40b)	110.1
C(41)	C(40)	H(40a)	110.2	C(41)	C(40)	H(40b)	110.1
H(40a)	C(40)	H(40b)	109.4	N(6)	C(41)	H(41a)	110.1
N(6)	C(41)	H(41b)	110.1	C(40)	C(41)	H(41a)	110.1
C(40)	C(41)	H(41b)	110.1	H(41a)	C(41)	H(41b)	109.4
N(6)	C(42)	H(42)	117.7	C(43)	C(42)	H(42)	117.7
C(43)	C(44)	H(44)	118.6	C(45)	C(44)	H(44)	118.7
C(44)	C(45)	H(45)	120.4	C(46)	C(45)	H(45)	120.4
C(45)	C(46)	H(46)	120.2	C(47)	C(46)	H(46)	120.2
C(46)	C(47)	H(47)	118.2	C(48)	C(47)	H(47)	118.2