Table 2. Refined Positional Parameters for Compound 762

Atom	x	y	z	U_{eq}, Å^2
C1	0.66825(13)	0.89282(7)	0.3327(3)	0.0289(4)
C2	0.6116(2)	0.91471(9)	0.1447(4)	0.0378(4)
C3	0.5764(2)	0.97124(9)	0.1491(4)	0.0477(5)
C4	0.5992(2)	1.00668(10)	0.3400(4)	0.0497(6)
C5	0.6564(2)	0.98548(9)	0.5267(4)	0.0470(5)
C6	0.6904(2)	0.92888(9)	0.5238(4)	0.0379(4)
C7	0.70570(14)	0.83190(8)	0.3243(3)	0.0302(4)
C8	0.63881(12)	0.77072(7)	0.6317(3)	0.0258(4)
C9	0.54635(12)	0.70611(8)	0.9088(3)	0.0267(4)
C10	0.56576(14)	0.64069(7)	0.9008(3)	0.0316(4)
C11	0.6793(2)	0.62846(9)	0.8817(5)	0.0465(5)
C12	0.7083(2)	0.56513(11)	0.9038(7)	0.0625(7)
C13	0.5041(2)	0.61040(10)	0.7105(5)	0.0514(6)
C14	0.43965(13)	0.72200(8)	0.9948(3)	0.0309(4)
C15	0.4236(2)	0.78693(8)	1.0115(3)	0.0345(4)
C17	0.3969(2)	0.90180(11)	0.5650(5)	0.0538(6)
C18	0.39325(13)	0.81494(8)	0.7830(3)	0.0332(4)
N1	0.56304(11)	0.73354(6)	0.6770(3)	0.0285(3)
O1	0.62842(9)	0.79192(5)	0.4089(2)	0.0315(3)
O2	0.70672(9)	0.78471(5)	0.7678(2)	0.0333(3)
O3	0.42783(11)	0.86912(6)	0.7717(3)	0.0441(4)
O4	0.34077(11)	0.79359(6)	0.6296(2)	0.0451(4)
O5	0.42635(11)	0.69634(6)	1.2244(2)	0.0408(3)
H1	0.519(2)	0.7246(9)	0.564(4)	0.045(6)
H2	0.597(2)	0.8899(9)	0.003(4)	0.043(6)
H3	0.535(2)	0.9869(10)	0.017(5)	0.055(7)
H4	0.573(2)	1.0484(11)	0.331(5)	0.070(8)
H5	0.673(2)	1.0092(11)	0.656(5)	0.060(7)
H5a	0.361(3)	0.7009(12)	1.276(6)	0.088(10)
H6	0.731(2)	0.9129(9)	0.657(4)	0.047(6)
H7a	0.722(2)	0.8181(8)	0.154(4)	0.032(5)
H7b	0.771(2)	0.8259(8)	0.430(4)	0.032(5)
H9	0.5955(14)	0.7230(8)	1.020(3)	0.023(4)
H10	0.5446(14)	0.6249(8)	1.062(4)	0.027(5)
H11a	0.702(2)	0.6443(11)	0.733(5)	0.068(8)
H11b	0.714(2)	0.6488(13)	1.028(6)	0.089(10)
H12b	0.683(2)	0.5419(13)	0.762(6)	0.086(10)
H12c	0.681(3)	0.5491(13)	1.052(6)	0.083(10)
H12a	0.786(3)	0.5581(13)	0.905(5)	0.085(9)
H13a	0.430(2)	0.6194(11)	0.712(5)	0.072(8)
H13b	0.515(2)	0.5692(12)	0.718(5)	0.070(8)
H13c	0.524(2)	0.6260(13)	0.539(6)	0.095(10)
H14	0.389(2)	0.7064(9)	0.882(4)	0.037(5)
H15a	0.368(2)	0.7926(10)	1.121(4)	0.052(6)
H15b	0.483(2)	0.8061(8)	1.069(4)	0.033(5)
H17a	0.430(2)	0.9372(13)	0.575(6)	0.079(9)
H17b	0.323(2)	0.9054(11)	0.566(5)	0.063(8)
H17c	0.417(2)	0.8816(12)	0.407(6)	0.077(9)

$$U_{eq}={}^{1}/_{3}[U_{11}(aa^*)^2+U_{22}(bb^*)^2+U_{33}(cc^*)^2+2U_{12}aa^*bb^*cos\gamma+2U_{13}aa^*cc^*cos\beta+2U_{23}bb^*cc^*cos\alpha]$$

Table 3. Refined Thermal Parameters (U's) for Compound 762

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C1	0.0281(9)	0.0320(9)	0.0266(9)	0.0027(7)	0.0020(7)	-0.0044(7)
C2	0.0409(11)	0.0394(10)	0.0333(10)	0.0047(9)	-0.0032(9)	-0.0027(8)
C3	0.0483(12)	0.0456(11)	0.0491(13)	0.0145(10)	-0.0006(11)	0.0056(10)
C4	0.0501(13)	0.0375(11)	0.0615(14)	0.0036(11)	0.0136(11)	0.0065(9)
C5	0.0540(13)	0.0374(11)	0.0497(12)	-0.0113(10)	0.0076(11)	-0.0038(10)
C6	0.0405(11)	0.0398(11)	0.0334(10)	-0.0017(9)	-0.0004(9)	-0.0051(8)
C7	0.0285(9)	0.0312(9)	0.0310(9)	0.0035(8)	0.0036(8)	-0.0053(7)
C8	0.0254(8)	0.0250(8)	0.0271(8)	-0.0010(7)	0.0008(7)	0.0012(6)
C9	0.0240(8)	0.0307(8)	0.0252(8)	0.0039(8)	-0.0004(7)	-0.0036(7)
C10	0.0330(9)	0.0303(9)	0.0316(9)	0.0028(8)	-0.0011(8)	-0.0021(8)
C11	0.0384(11)	0.0378(11)	0.063(2)	0.0050(11)	0.0094(11)	0.0048(9)
C12	0.060(2)	0.0421(13)	0.086(2)	0.008(2)	0.006(2)	0.0159(12)
C13	0.061(2)	0.0350(11)	0.058(2)	-0.0016(11)	-0.0158(12)	-0.0084(10)
C14	0.0266(9)	0.0388(10)	0.0273(8)	0.0055(8)	0.0001(7)	-0.0032(8)
C15	0.0328(10)	0.0379(10)	0.0328(9)	-0.0005(8)	-0.0023(8)	0.0037(9)
C17	0.066(2)	0.0462(13)	0.0493(14)	0.0155(12)	-0.0092(12)	-0.0061(12)
C18	0.0289(9)	0.0342(9)	0.0365(10)	-0.0016(8)	0.0009(8)	0.0032(7)
N1	0.0263(7)	0.0336(7)	0.0257(7)	0.0020(6)	-0.0028(6)	-0.0062(6)
O1	0.0327(7)	0.0343(6)	0.0275(6)	0.0061(6)	-0.0026(5)	-0.0071(5)
O2	0.0292(6)	0.0428(7)	0.0278(6)	-0.0003(6)	-0.0022(5)	-0.0084(5)
O3	0.0503(8)	0.0386(7)	0.0434(8)	0.0059(7)	-0.0113(7)	-0.0059(6)
O4	0.0500(8)	0.0435(7)	0.0417(8)	0.0040(7)	-0.0143(7)	-0.0040(7)
O5	0.0333(7)	0.0549(8)	0.0342(7)	0.0153(6)	0.0081(6)	0.0039(6)

The form of the anisotropic displacement parameter is:

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

Table 4. Bond Distances in Compound 762, Å

C1-C2	1.389(3)	C1-C6	1.393(3)	C1-C7	1.495(2)
C2-C3	1.389(3)	C2-H2	1.00(2)	C3-C4	1.385(3)
C3-H3	0.99(2)	C4-C5	1.382(3)	C4-H4	1.02(3)
C5-C6	1.386(3)	C5-H5	0.94(3)	C6-H6	0.99(2)
C7-O1	1.455(2)	C7-H7a	1.03(2)	C7-H7b	1.05(2)
C8-O2	1.220(2)	C8-N1	1.341(2)	C8-O1	1.353(2)
C9-N1	1.467(2)	C9-C14	1.528(2)	C9-C10	1.538(2)
C9-H9	0.98(2)	C10-C13	1.515(3)	C10-C11	1.522(3)
C10-H10	1.02(2)	C11-C12	1.521(3)	C11-H11a	0.96(3)
C11-H11b	1.05(3)	C12-H12b	1.02(3)	C12-H12c	0.98(3)
C12-H12a	1.03(3)	C13-H13a	0.99(3)	C13-H13b	0.97(3)
C13-H13c	1.06(3)	C14-O5	1.433(2)	C14-C15	1.522(3)
C14-H14	0.99(2)	C15-C18	1.495(3)	C15-H15a	0.97(2)
C15-H15b	0.95(2)	C17-O3	1.446(3)	C17-H17a	0.93(3)
C17-H17b	0.98(3)	C17-H17c	1.04(3)	C18-O4	1.210(2)
C18-O3	1.337(2)	N1-H1	0.88(2)	O5-H5a	0.91(3)

Table 5. Bond Angles in Compound 762, °

C2-C1-C6	118.7(2)	C2-C1-C7	119.8(2)	C6-C1-C7	121.4(2)
C3-C2-C1	120.6(2)	C3-C2-H2	119.4(12)	C1-C2-H2	120.0(13)
C4-C3-C2	120.0(2)	C4-C3-H3	119.0(14)	C2-C3-H3	121.0(14)
C5-C4-C3	119.8(2)	C5-C4-H4	124(2)	C3-C4-H4	117(2)
C4-C5-C6	120.2(2)	C4-C5-H5	121(2)	C6-C5-H5	119(2)
C5-C6-C1	120.6(2)	C5-C6-H6	121.3(12)	C1-C6-H6	118.1(12)
O1-C7-C1	111.17(14)	O1-C7-H7a	104.5(11)	C1-C7-H7a	112.9(11)
O1-C7-H7b	107.5(10)	C1-C7-H7b	112.0(10)	H7a-C7-H7b	108(2)
O2-C8-N1	126.5(2)	O2-C8-O1	124.0(2)	N1-C8-O1	109.54(14)
N1-C9-C14	108.31(14)	N1-C9-C10	112.1(2)	C14-C9-C10	113.51(14)
N1-C9-H9	107.2(10)	C14-C9-H9	107.9(10)	C10-C9-H9	107.6(10)
C13-C10-C11	112.8(2)	C13-C10-C9	112.9(2)	C11-C10-C9	110.4(2)
C13-C10-H10	108.6(11)	C11-C10-H10	105.3(11)	C9-C10-H10	106.4(10)
C12-C11-C10	114.8(2)	C12-C11-H11a	111(2)	C10-C11-H11a	107(2)
C12-C11-H11b	105(2)	C10-C11-H11b	106(2)	H11a-C11-H11b	112(2)
C11-C12-H12b	111(2)	C11-C12-H12c	110(2)	H12b-C12-H12c	110(2)
C11-C12-H12a	114(2)	H12b-C12-H12a	104(2)	H12C-C12-H12a	107(3)
C10-C13-H13a	115(2)	C10-C13-H13b	110(2)	H13a-C13-H13b	111(2)
C10-C13-H13c	110(2)	H13a-C13-H13c	100(2)	H13b-C13-H13c	110(2)
O5-C14-C15	109.7(2)	O5-C14-C9	107.30(14)	C15-C14-C9	112.6(2)
O5-C14-H14	110.4(12)	C15-C14-H14	108.0(12)	C9-C14-H14	108.8(12)
C18-C15-C14	114.4(2)	C18-C15-H15a	106.6(14)	C14-C15-H15a	106.2(14)
C18-C15-H15b	107.8(12)	C14-C15-H15b	111.7(11)	H15a-C15-H15b	110(2)
O3-C17-H17a	106(2)	O3-C17-H17b	109(2)	H17a-C17-H17b	113(2)
O3-C17-H17c	112(2)	H17a-C17-H17c	109(2)	H17b-C17-H17c	107(2)
O4-C18-O3	122.9(2)	O4-C18-C15	126.0(2)	O3-C18-C15	111.0(2)
C8-N1-C9	123.9(2)	C8-N1-H1	119.9(14)	C9-N1-H1	116.1(14)
C8-O1-C7	117.63(14)	C18-O3-C17	115.7(2)	C14-O5-H5a	111(2)