Table 2. Refined Positional Parameters for Compound 18

Atom	x	y	z	U_{eq}, Å^2
C1	0.0552(2)	0.09982(4)	0.7114(3)	0.0326(4)
C2	0.1942(2)	0.09641(4)	0.6707(3)	0.0334(4)
C3	0.2615(2)	0.10330(4)	0.5066(3)	0.0371(4)
C4	0.3920(2)	0.09586(4)	0.4962(3)	0.0409(4)
C5	0.4517(2)	0.08208(5)	0.6476(3)	0.0435(5)
C6	0.3850(2)	0.07581(4)	0.8126(3)	0.0407(4)
C7	0.2542(2)	0.08315(4)	0.8246(3)	0.0340(4)
C8	0.1614(2)	0.07965(4)	0.9869(3)	0.0363(4)
C9	0.0268(2)	0.08134(4)	0.8910(3)	0.0311(4)
C11	-0.2019(2)	0.07654(4)	0.9462(3)	0.0345(4)
C12	-0.1500(2)	0.04981(4)	0.8487(3)	0.0331(4)
C13	-0.0221(2)	0.05201(4)	0.8203(3)	0.0323(4)
C14	-0.2780(2)	0.07142(5)	1.1298(3)	0.0444(5)
C15	-0.2105(2)	0.09100(6)	1.2730(3)	0.0502(5)
C16	-0.0705(2)	0.09069(6)	1.2070(3)	0.0509(5)
C18	0.0603(2)	0.03072(4)	0.7170(3)	0.0347(4)
C21	0.1735(3)	-0.01346(6)	0.7421(4)	0.0601(7)
C22	-0.2277(2)	0.02518(4)	0.7791(3)	0.0368(4)
C25	-0.4391(2)	0.00767(6)	0.7276(5)	0.0557(6)
N10	-0.0826(2)	0.09284(3)	1.0002(2)	0.0348(3)
O17	-0.02577(13)	0.11355(3)	0.6238(2)	0.0420(3)
O19	0.10552(14)	0.01026(3)	0.8328(2)	0.0438(3)
O20	0.0844(2)	0.03226(3)	0.5517(2)	0.0494(4)
O23	-0.35476(12)	0.03039(3)	0.7950(2)	0.0411(3)
O24	-0.18337(14)	0.00330(3)	0.7122(3)	0.0553(4)
C1'	0.3691(2)	0.15089(4)	0.9910(3)	0.0337(4)
C2'	0.4684(2)	0.15249(4)	0.8424(3)	0.0344(4)
C3'	0.5939(2)	0.14139(4)	0.8412(3)	0.0407(4)
C4'	0.6693(2)	0.14533(5)	0.6825(4)	0.0499(5)
C5'	0.6188(2)	0.16018(5)	0.5272(3)	0.0506(5)
C6'	0.4944(2)	0.17136(4)	0.5281(3)	0.0463(5)
C7'	0.4187(2)	0.16745(4)	0.6881(3)	0.0359(4)
C8'	0.2795(2)	0.17646(4)	0.7209(3)	0.0395(4)
C9'	0.2596(2)	0.17241(4)	0.9351(3)	0.0326(4)
C11'	0.1071(2)	0.17612(4)	1.1871(3)	0.0389(4)
C12'	0.2003(2)	0.20159(4)	1.1919(3)	0.0327(4)
C13'	0.2851(2)	0.19993(4)	1.0507(2)	0.0315(4)
C14'	-0.0388(2)	0.18359(6)	1.1963(4)	0.0527(6)
C15'	-0.0922(2)	0.17173(5)	1.0103(4)	0.0558(6)
C16'	0.0218(2)	0.17408(5)	0.8789(4)	0.0473(5)
C18'	0.3961(2)	0.21950(4)	1.0075(3)	0.0332(4)
C21'	0.6158(2)	0.22924(6)	1.0784(4)	0.0566(6)
C22'	0.1953(2)	0.22416(4)	1.3394(3)	0.0347(4)
C25'	0.2929(3)	0.26760(5)	1.4493(4)	0.0541(6)
N10'	0.1303(2)	0.16286(3)	0.9965(3)	0.0383(4)
O17'	0.36975(14)	0.13628(3)	1.1331(2)	0.0433(3)
O19'	0.50005(12)	0.21204(3)	1.1073(2)	0.0389(3)
O20'	0.3930(2)	0.23883(3)	0.8934(2)	0.0499(4)
O23'	0.28647(14)	0.24452(3)	1.3113(2)	0.0452(3)

O24'	0.11926(14)	0.22445(3)	1.4688(2)	0.0470(3)
H3	0.216(2)	0.1124(4)	0.403(3)	0.037(5)
H4	0.444(2)	0.1002(4)	0.386(3)	0.036(5)
H5	0.543(2)	0.0762(5)	0.637(3)	0.051(6)
H6	0.431(2)	0.0667(5)	0.922(4)	0.056(7)
H8a	0.170(2)	0.0965(5)	1.070(3)	0.040(5)
H8b	0.177(2)	0.0617(5)	1.056(3)	0.046(6)
H11	-0.252(2)	0.0881(4)	0.850(3)	0.042(5)
H14a	-0.368(3)	0.0766(5)	1.119(4)	0.064(7)
H14b	-0.269(2)	0.0515(6)	1.176(3)	0.054(6)
H15a	-0.244(3)	0.1110(6)	1.265(4)	0.069(8)
H15b	-0.228(3)	0.0843(6)	1.410(4)	0.074(8)
H16a	-0.013(3)	0.1073(6)	1.265(4)	0.068(8)
H16b	-0.033(2)	0.0725(5)	1.243(3)	0.048(6)
H21a	0.208(3)	-0.0263(7)	0.843(5)	0.084(9)
H21b	0.250(4)	-0.0053(7)	0.666(5)	0.091(10)
H21c	0.114(3)	-0.0240(7)	0.663(5)	0.092(10)
H25a	-0.521(3)	0.0143(7)	0.754(5)	0.084(9)
H25b	-0.425(3)	-0.0101(8)	0.817(6)	0.110(12)
H25c	-0.430(3)	0.0050(6)	0.597(5)	0.074(9)
H3'	0.622(2)	0.1319(5)	0.952(4)	0.053(6)
H4'	0.761(2)	0.1375(5)	0.682(3)	0.053(6)
H5'	0.676(3)	0.1636(5)	0.410(4)	0.064(7)
H6'	0.461(2)	0.1830(5)	0.414(4)	0.055(7)
H8a'	0.224(3)	0.1629(6)	0.641(4)	0.068(8)
H8b'	0.260(3)	0.1977(6)	0.678(4)	0.064(7)
H11'	0.136(2)	0.1626(5)	1.291(4)	0.056(7)
H14a'	-0.074(3)	0.1744(7)	1.305(5)	0.082(9)
H14b'	-0.049(3)	0.2044(7)	1.207(5)	0.082(9)
H15a'	-0.111(3)	0.1515(7)	1.014(4)	0.083(9)
H15b'	-0.172(3)	0.1830(6)	0.961(4)	0.070(8)
H16a'	0.013(2)	0.1618(5)	0.773(3)	0.046(6)
H16b'	0.035(2)	0.1961(6)	0.838(4)	0.061(7)
H21a'	0.687(3)	0.2183(7)	1.133(5)	0.089(10)
H21b'	0.598(3)	0.2483(7)	1.110(5)	0.081(10)
H21c'	0.632(3)	0.2318(7)	0.940(5)	0.092(10)
H25a'	0.372(3)	0.2801(7)	1.400(5)	0.092(10)
H25b'	0.321(3)	0.2588(6)	1.573(4)	0.072(8)
H25c'	0.204(3)	0.2768(6)	1.470(4)	0.067(8)

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

Table 3. Refined Thermal Parameters (U's) for Compound 18

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C1	0.0353(9)	0.0295(8)	0.0331(9)	-0.0026(7)	-0.0043(8)	-0.0006(7)
C2	0.0354(9)	0.0311(8)	0.0336(9)	-0.0004(7)	-0.0040(8)	-0.0027(7)
C3	0.0415(10)	0.0362(9)	0.0336(10)	0.0006(8)	-0.0019(9)	-0.0006(8)
C4	0.0400(10)	0.0412(10)	0.0415(11)	0.0007(9)	0.0022(9)	-0.0027(9)
C5	0.0343(10)	0.0431(10)	0.0532(12)	0.0001(9)	-0.0010(9)	-0.0004(8)
C6	0.0354(10)	0.0418(10)	0.0447(11)	0.0044(9)	-0.0071(9)	0.0001(8)
C7	0.0340(9)	0.0316(8)	0.0364(10)	-0.0001(7)	-0.0052(8)	-0.0044(7)
C8	0.0352(10)	0.0387(10)	0.0348(10)	0.0023(8)	-0.0057(8)	-0.0029(8)
C9	0.0321(9)	0.0298(8)	0.0314(9)	-0.0018(7)	-0.0021(7)	-0.0012(7)
C11	0.0336(9)	0.0299(9)	0.0400(10)	-0.0043(7)	-0.0015(8)	0.0018(8)
C12	0.0334(9)	0.0283(8)	0.0375(10)	-0.0034(8)	-0.0032(8)	0.0013(7)
C13	0.0364(9)	0.0286(8)	0.0318(9)	-0.0022(7)	-0.0016(8)	0.0014(7)
C14	0.0436(12)	0.0426(11)	0.0469(12)	-0.0070(9)	0.0082(10)	-0.0013(9)
C15	0.0460(12)	0.0643(14)	0.0402(12)	-0.0107(10)	0.0063(10)	-0.0028(11)
C16	0.0448(12)	0.075(2)	0.0331(11)	-0.0077(11)	-0.0004(9)	-0.0021(12)
C18	0.0318(9)	0.0348(9)	0.0375(11)	-0.0052(8)	-0.0018(8)	-0.0011(7)
C21	0.063(2)	0.0501(13)	0.067(2)	-0.0140(12)	-0.0025(14)	0.0260(12)
C22	0.0347(9)	0.0340(9)	0.0417(10)	-0.0050(8)	0.0001(8)	-0.0001(8)
C25	0.0391(12)	0.0528(14)	0.075(2)	-0.0207(13)	0.0013(12)	-0.0147(10)
N10	0.0348(8)	0.0356(8)	0.0341(8)	-0.0067(7)	-0.0010(7)	-0.0027(6)
O17	0.0417(7)	0.0459(7)	0.0385(7)	0.0002(6)	-0.0068(6)	0.0088(6)
O19	0.0470(8)	0.0400(7)	0.0445(8)	-0.0036(6)	-0.0018(7)	0.0149(6)
O20	0.0566(9)	0.0503(8)	0.0412(9)	-0.0055(6)	0.0065(7)	0.0036(7)
O23	0.0322(7)	0.0388(7)	0.0524(8)	-0.0082(6)	-0.0043(6)	-0.0037(5)
O24	0.0417(8)	0.0405(8)	0.0836(11)	-0.0217(8)	0.0004(8)	-0.0004(6)
C1'	0.0357(9)	0.0302(8)	0.0350(10)	-0.0022(8)	-0.0030(8)	0.0021(7)
C2'	0.0359(9)	0.0301(8)	0.0371(10)	-0.0030(7)	-0.0020(8)	0.0007(7)
C3'	0.0378(10)	0.0366(10)	0.0478(12)	-0.0026(9)	-0.0003(9)	0.0018(8)
C4'	0.0402(11)	0.0467(11)	0.0628(14)	-0.0118(10)	0.0084(11)	-0.0049(9)
C5'	0.0548(13)	0.0476(11)	0.0495(12)	-0.0076(10)	0.0136(11)	-0.0107(10)
C6'	0.0596(13)	0.0418(11)	0.0375(11)	-0.0012(9)	0.0027(10)	-0.0045(10)
C7'	0.0441(10)	0.0310(9)	0.0327(10)	-0.0026(7)	-0.0006(8)	-0.0007(8)
C8'	0.0437(11)	0.0399(10)	0.0349(10)	-0.0034(8)	-0.0084(9)	0.0068(9)
C9'	0.0314(9)	0.0297(9)	0.0367(9)	-0.0022(7)	-0.0033(7)	0.0014(7)
C11'	0.0337(9)	0.0354(9)	0.0475(11)	-0.0010(8)	0.0040(9)	-0.0015(8)
C12'	0.0324(9)	0.0299(8)	0.0358(9)	0.0012(7)	-0.0026(8)	0.0003(7)
C13'	0.0317(9)	0.0285(8)	0.0343(9)	0.0020(7)	-0.0033(8)	0.0032(7)
C14'	0.0324(10)	0.0534(14)	0.072(2)	-0.0097(12)	0.0059(11)	-0.0044(10)
C15'	0.0331(10)	0.0436(12)	0.091(2)	-0.0144(12)	-0.0045(12)	0.0022(9)
C16'	0.0359(10)	0.0423(11)	0.0636(14)	-0.0144(11)	-0.0160(10)	0.0065(9)
C18'	0.0362(9)	0.0299(8)	0.0334(9)	-0.0009(7)	0.0004(8)	-0.0007(7)
C21'	0.0374(12)	0.059(2)	0.074(2)	0.0059(13)	-0.0021(12)	-0.0156(11)
C22'	0.0358(9)	0.0348(9)	0.0335(10)	0.0026(7)	-0.0033(8)	0.0049(8)
C25'	0.067(2)	0.0458(12)	0.0491(13)	-0.0177(10)	-0.0006(12)	-0.0024(12)
N10'	0.0295(8)	0.0352(8)	0.0502(9)	-0.0063(7)	-0.0039(7)	0.0012(6)
O17'	0.0469(8)	0.0429(7)	0.0401(7)	0.0093(6)	-0.0002(6)	0.0053(6)
O19'	0.0319(7)	0.0415(7)	0.0433(7)	0.0060(6)	-0.0017(6)	-0.0057(6)
O20'	0.0529(8)	0.0456(8)	0.0513(9)	0.0176(7)	-0.0027(7)	-0.0045(7)
O23'	0.0520(8)	0.0395(7)	0.0441(8)	-0.0108(6)	0.0049(7)	-0.0082(6)

O24'	0.0485(8)	0.0521(8)	0.0404(8)	-0.0019(6)	0.0070(7)	0.0060(7)

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 18, Å

C1-O17	1.217(2)	C1-C2	1.468(3)	C1-C9	1.559(2)
C2-C3	1.389(3)	C2-C7	1.394(3)	C3-C4	1.388(3)
C3-H3	0.97(2)	C4-C5	1.390(3)	C4-H4	0.97(2)
C5-C6	1.385(3)	C5-H5	0.98(2)	C6-C7	1.391(3)
C6-H6	1.00(3)	C7-C8	1.503(3)	C8-C9	1.545(2)
C8-H8a	0.98(2)	C8-H8b	0.98(2)	C9-N10	1.466(2)
C9-C13	1.528(2)	C11-N10	1.490(2)	C11-C12	1.511(2)
C11-C14	1.535(3)	C11-H11	1.01(2)	C12-C13	1.336(3)
C12-C22	1.474(3)	C13-C18	1.490(2)	C14-C15	1.526(3)
C14-H14a	0.96(3)	C14-H14b	0.98(2)	C15-C16	1.515(3)
C15-H15a	0.99(3)	C15-H15b	1.03(3)	C16-N10	1.473(3)
C16-H16a	1.05(3)	C16-H16b	0.96(2)	C18-O20	1.198(2)
C18-O19	1.335(2)	C21-O19	1.449(3)	C21-H21a	1.00(3)
C21-H21b	1.03(4)	C21-H21c	0.96(3)	C22-O24	1.205(2)
C22-O23	1.334(2)	C25-O23	1.442(3)	C25-H25a	0.92(3)
C25-H25b	1.05(4)	C25-H25c	0.94(3)	C1'-O17'	1.211(2)
C1'-C2'	1.469(3)	C1'-C9'	1.553(2)	C2'-C3'	1.389(3)
C2'-C7'	1.390(3)	C3'-C4'	1.378(3)	C3'-H3'	0.95(2)
C4'-C5'	1.396(3)	C4'-H4'	1.01(2)	C5'-C6'	1.381(3)
C5'-H5'	1.03(3)	C6'-C7'	1.387(3)	C6'-H6'	1.03(3)
C7'-C8'	1.510(3)	C8'-C9'	1.542(3)	C8'-H8a'	1.02(3)
C8'-H8b'	1.05(3)	C9'-N10'	1.467(2)	C9'-C13'	1.533(2)
C11'-N10'	1.501(3)	C11'-C12'	1.517(3)	C11'-C14'	1.542(3)
C11'-H11'	1.01(2)	C12'-C13'	1.329(3)	C12'-C22'	1.476(3)
C13'-C18'	1.488(3)	C14'-C15'	1.528(4)	C14'-H14a	0.95(3)
C14'-H14b	0.97(3)	C15'-C16'	1.501(4)	C15'-H15a	0.95(3)
C15'-H15b	1.03(3)	C16'-N10'	1.486(3)	C16'-H16a	0.95(2)
C16'-H16b	1.07(3)	C18'-O20'	1.204(2)	C18'-O19'	1.328(2)
C21'-O19'	1.446(3)	C21'-H21a'	0.97(3)	C21'-H21b'	0.93(3)
C21'-H21c'	1.00(4)	C22'-O24'	1.206(2)	C22'-O23'	1.342(2)
C25'-O23'	1.447(2)	C25'-H25a'	1.06(3)	C25'-H25b'	1.01(3)
C25'-H25c'	1.02(3)				

Table 5. Bond Angles in Compound 18, °

O17-C1-C2	128.6(2)	O17-C1-C9	124.9(2)	C2-C1-C9	106.5(2)
C3-C2-C7	122.2(2)	C3-C2-C1	128.7(2)	C7-C2-C1	109.0(2)
C4-C3-C2	118.1(2)	C4-C3-H3	122.6(12)	C2-C3-H3	119.3(12)
C5-C4-C3	120.0(2)	C5-C4-H4	118.1(12)	C3-C4-H4	121.9(12)
C6-C5-C4	121.8(2)	C6-C5-H5	118.7(14)	C4-C5-H5	119.5(14)
C5-C6-C7	118.7(2)	C5-C6-H6	120.3(14)	C7-C6-H6	120.9(14)
C6-C7-C2	119.2(2)	C6-C7-C8	129.5(2)	C2-C7-C8	111.3(2)
C7-C8-C9	103.2(2)	C7-C8-H8a	108.5(12)	C9-C8-H8a	107.9(13)
C7-C8-H8b	111.5(13)	C9-C8-H8b	114.4(13)	H8a-C8-H8b	111(2)
N10-C9-C13	103.90(14)	N10-C9-C8	118.4(2)	C13-C9-C8	113.2(2)
N10-C9-C1	112.12(14)	C13-C9-C1	106.22(14)	C8-C9-C1	102.57(14)
N10-C11-C12	103.76(14)	N10-C11-C14	106.3(2)	C12-C11-C14	116.2(2)
N10-C11-H11	109.0(12)	C12-C11-H11	107.7(12)	C14-C11-H11	113.3(12)
C13-C12-C22	122.9(2)	C13-C12-C11	110.8(2)	C22-C12-C11	126.2(2)
C12-C13-C18	125.8(2)	C12-C13-C9	110.0(2)	C18-C13-C9	123.9(2)
C15-C14-C11	103.9(2)	C15-C14-H14a	110(2)	C11-C14-H14a	113(2)
C15-C14-H14b	107.0(14)	C11-C14-H14b	112.0(14)	H14a-C14-H14b	111(2)
C16-C15-C14	102.9(2)	C16-C15-H15a	109(2)	C14-C15-H15a	111(2)
C16-C15-H15b	117(2)	C14-C15-H15b	112(2)	H15a-C15-H15b	106(2)
N10-C16-C15	103.0(2)	N10-C16-H16a	113(2)	C15-C16-H16a	114(2)
N10-C16-H16b	110.9(14)	C15-C16-H16b	108.2(14)	H16a-C16-H16b	108(2)
O20-C18-O19	124.8(2)	O20-C18-C13	124.0(2)	O19-C18-C13	111.3(2)
O19-C21-H21a	108(2)	O19-C21-H21b	109(2)	H21a-C21-H21b	109(3)
O19-C21-H21c	110(2)	H21a-C21-H21c	110(3)	H21b-C21-H21c	112(3)
O24-C22-O23	123.7(2)	O24-C22-C12	124.8(2)	O23-C22-C12	111.4(2)
O23-C25-H25a	104(2)	O23-C25-H25b	107(2)	H25a-C25-H25b	105(3)
O23-C25-H25c	111(2)	H25a-C25-H25c	110(3)	H25b-C25-H25c	119(3)
C9-N10-C16	115.8(2)	C9-N10-C11	108.38(13)	C16-N10-C11	106.9(2)
C18-O19-C21	115.5(2)	C22-O23-C25	115.5(2)	O17'-C1'-C2'	128.2(2)
O17'-C1'-C9'	124.8(2)	C2'-C1'-C9'	106.9(2)	C3'-C2'-C7'	121.4(2)
C3'-C2'-C1'	129.3(2)	C7'-C2'-C1'	109.4(2)	C4'-C3'-C2'	118.7(2)
C4'-C3'-H3'	124(2)	C2'-C3'-H3'	117(2)	C3'-C4'-C5'	119.8(2)
C3'-C4'-H4'	118.6(14)	C5'-C4'-H4'	121.6(14)	C6'-C5'-C4'	121.7(2)
C6'-C5'-H5'	118(2)	C4'-C5'-H5'	120(2)	C5'-C6'-C7'	118.4(2)
C5'-C6'-H6'	119.9(14)	C7'-C6'-H6'	121.6(14)	C6'-C7'-C2'	120.0(2)
C6'-C7'-C8'	128.5(2)	C2'-C7'-C8'	111.4(2)	C7'-C8'-C9'	104.1(2)
C7'-C8'-H8a'	106(2)	C9'-C8'-H8a'	114(2)	C7'-C8'-H8b'	113.3(14)
C9'-C8'-H8b'	112.0(14)	H8a'-C8'-H8b'	108(2)	N10'-C9'-C13'	104.22(14)
N10'-C9'-C8'	116.6(2)	C13'-C9'-C8'	113.7(2)	N10'-C9'-C1'	113.0(2)
C13'-C9'-C1'	105.63(14)	C8'-C9'-C1'	103.4(2)	N10'-C11'-C12'	103.6(2)
N10'-C11'-C14'	106.5(2)	C12'-C11'-C14'	116.2(2)	N10'-C11'-H11'	110.7(14)
C12'-C11'-H11'	105.9(14)	C14'-C11'-H11'	113.5(14)	C13'-C12'-C22'	126.6(2)
C13'-C12'-C11'	110.7(2)	C22'-C12'-C11'	122.7(2)	C12'-C13'-C18'	128.6(2)
C12'-C13'-C9'	109.7(2)	C18'-C13'-C9'	121.6(2)	C15'-C14'-C11'	103.5(2)
C15'-C14'-H14a'	114(2)	C11'-C14'-H14a'	108(2)	C15'-C14'-H14b'	112(2)
C11'-C14'-H14b'	110(2)	H14a'-C14'-H14b'	110(3)	C16'-C15'-C14'	103.1(2)
C16'-C15'-H15a'	104(2)	C14'-C15'-H15a'	114(2)	C16'-C15'-H15b'	112(2)
C14'-C15'-H15b'	113(2)	H15a'-C15'-H15b'	110(3)	N10'-C16'-C15'	102.4(2)
N10'-C16'-H16a'	107.9(14)	C15'-C16'-H16a'	111.9(14)	N10'-C16'-H16b'	112.6(14)
C15'-C16'-H16b'	109.8(14)	H16a'-C16'-H16b'	112(2)	O20'-C18'-O19'	124.8(2)
O20'-C18'-C13'	124.5(2)	O19'-C18'-C13'	110.63(14)	O19'-C21'-H21a'	106(2)

O19'-C21'-H21b'	109(2)	H21a'-C21'-H21b'	124(3)	O19'-C21'-H21c'	110(2)
H21a'-C21'-H21c'	109(3)	H21b'-C21'-H21c'	99(3)	O24'-C22'-O23'	124.0(2)
O24'-C22'-C12'	124.6(2)	O23'-C22'-C12'	111.4(2)	O23'-C25'-H25a'	102(2)
O23'-C25'-H25b	108(2)	H25a'-C25'-H25b'	107(2)	O23'-C25'-H25c'	111(2)
H25a'-C25'-H25c'	121(2)	H25b'-C25'-H25c'	107(2)	C9'-N10'-C16'	114.3(2)
C9'-N10'-C11'	106.76(14)	C16'-N10'-C11'	104.0(2)	C18'-O19'-C21'	116.5(2)
C22'-O23'-C25'	116.6(2)				

Table 1. Summary of Structure Determination of Compound 19

Formula:	$C_{23}H_{20}N_2O_3$
Formula weight:	372.41
Crystal class:	triclinic
Space group:	$P\bar{1}$ (#2)
Z	2
Cell constants:	
a	8.2314(2)Å
b	14.3827(4)Å
c	7.7342(2)Å
α	91.128(2)°
β	104.792(2)°
γ	86.249(2)°
V	883.40(4)Å^3
μ	0.94 cm^{-1}
crystal size, mm	0.25 x 0.20 x 0.08
D_{calc}	1.400 g/cm^3
F(000)	392
Radiation:	Mo -K_α (λ=0.71069Å)
2θ range	5.12 – 50.7 °
hkl collected:	$-9 \le h \le 9$; $-17 \le k \le 16$; $-9 \le l \le 9$
No. reflections measured:	7000
No. unique reflections:	2957 (R_{int}=0.0193)
No. observed reflections	2650 (F>4σ)
No. reflections used in refinement	2957
No. parameters	334
R indices (F>4σ)	R_1=0.0444
	wR_2=0.1016
R indices (all data)	R_1=0.0503
	wR_2=0.1057
GOF:	1.070
Final Difference Peaks, e/Å^3	+0.185, -0.179

Table 2. Refined Positional Parameters for Compound 19

Atom	x	y	z	U_{eq}, Å^2
C1	0.3562(2)	0.22781(12)	0.7232(2)	0.0307(4)
C2	0.2184(2)	0.18534(12)	0.7746(2)	0.0286(4)
C3	0.1792(2)	0.18789(14)	0.9403(3)	0.0352(4)
C4	0.0416(2)	0.1418(2)	0.9560(3)	0.0396(5)
C5	-0.0552(2)	0.0948(2)	0.8106(3)	0.0369(5)
C6	-0.0165(2)	0.09354(13)	0.6458(3)	0.0306(4)
C7	0.1224(2)	0.13885(12)	0.6289(2)	0.0278(4)
C8	0.1897(2)	0.14516(14)	0.4659(2)	0.0322(4)
C9	0.3430(2)	0.20572(12)	0.5218(2)	0.0288(4)
C11	0.4870(2)	0.33130(12)	0.4452(2)	0.0294(4)
C12	0.6171(2)	0.24652(13)	0.4843(2)	0.0308(4)
C13	0.5145(2)	0.16336(12)	0.5043(2)	0.0294(4)
C14	0.4854(2)	0.39354(14)	0.2882(3)	0.0348(4)
C15	0.3307(2)	0.45996(13)	0.2492(2)	0.0340(4)
C16	0.3241(3)	0.54005(14)	0.1469(3)	0.0411(5)
C17	0.1834(3)	0.6013(2)	0.1094(3)	0.0497(6)
C18	0.0461(3)	0.5835(2)	0.1732(3)	0.0513(6)
C19	0.0495(3)	0.5046(2)	0.2736(3)	0.0433(5)
C20	0.1910(2)	0.44257(13)	0.3131(2)	0.0339(4)
C21	0.1913(2)	0.35872(14)	0.4268(3)	0.0354(4)
C22	0.6923(2)	0.21985(13)	0.3303(3)	0.0335(4)
C24	0.5098(2)	0.10551(12)	0.3369(2)	0.0308(4)
C25	0.6529(3)	0.0989(2)	0.0882(3)	0.0431(5)
N10	0.3235(2)	0.28885(10)	0.4091(2)	0.0278(3)
N23	0.6164(2)	0.14162(11)	0.2478(2)	0.0329(4)
O26	0.4663(2)	0.27173(10)	0.8195(2)	0.0432(4)
O27	0.8007(2)	0.25736(10)	0.2815(2)	0.0440(4)
O28	0.4331(2)	0.03610(9)	0.2870(2)	0.0386(3)
H3	0.245(3)	0.223(2)	1.038(3)	0.051(6)
H4	0.008(3)	0.142(2)	1.071(3)	0.050(6)
H5	-0.155(3)	0.062(2)	0.821(3)	0.049(6)
H6	-0.089(3)	0.0615(14)	0.543(3)	0.036(5)
H8a	0.102(3)	0.176(2)	0.364(3)	0.048(6)
H8b	0.226(3)	0.083(2)	0.426(3)	0.044(6)
H11	0.502(2)	0.3715(13)	0.558(3)	0.031(5)
H12	0.710(3)	0.2586(13)	0.589(3)	0.035(5)
H13	0.569(2)	0.1213(13)	0.603(3)	0.030(5)
H14b	0.488(3)	0.355(2)	0.179(3)	0.040(6)
H14a	0.590(3)	0.430(2)	0.316(3)	0.048(6)
H16	0.429(3)	0.551(2)	0.097(3)	0.049(6)
H17	0.178(3)	0.658(2)	0.034(4)	0.071(8)
H18	-0.058(3)	0.626(2)	0.145(3)	0.070(8)
H19	-0.051(3)	0.488(2)	0.319(3)	0.057(7)
H21a	0.207(3)	0.382(2)	0.559(3)	0.047(6)
H21b	0.076(3)	0.332(2)	0.389(3)	0.048(6)

H25c	0.547(3)	0.078(2)	0.010(4)	0.065(8)
H25a	0.735(3)	0.045(2)	0.123(4)	0.070(8)
H25b	0.700(3)	0.151(2)	0.024(4)	0.075(8)

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

Table 3. Refined Thermal Parameters (U's) for Compound 19

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C1	0.0335(9)	0.0290(9)	0.0291(9)	0.0005(7)	0.0069(8)	-0.0043(8)
C2	0.0312(9)	0.0271(9)	0.0277(9)	0.0023(7)	0.0079(7)	-0.0012(8)
C3	0.0358(10)	0.0402(11)	0.0283(9)	0.0009(8)	0.0063(8)	0.0003(9)
C4	0.0365(10)	0.0554(13)	0.0296(10)	0.0046(9)	0.0133(8)	-0.0009(9)
C5	0.0312(10)	0.0454(11)	0.0360(10)	0.0050(9)	0.0118(8)	-0.0014(9)
C6	0.0274(9)	0.0316(9)	0.0337(10)	0.0015(8)	0.0092(8)	-0.0012(8)
C7	0.0272(9)	0.0267(9)	0.0293(9)	0.0020(7)	0.0081(7)	0.0025(7)
C8	0.0341(10)	0.0348(10)	0.0298(9)	-0.0036(8)	0.0111(8)	-0.0079(8)
C9	0.0304(9)	0.0281(9)	0.0288(9)	0.0005(7)	0.0082(7)	-0.0055(7)
C11	0.0274(9)	0.0278(9)	0.0326(9)	-0.0005(8)	0.0059(7)	-0.0061(7)
C12	0.0260(9)	0.0326(10)	0.0327(10)	0.0011(8)	0.0047(8)	-0.0041(8)
C13	0.0289(9)	0.0274(9)	0.0309(9)	0.0047(8)	0.0057(8)	-0.0012(7)
C14	0.0336(10)	0.0324(10)	0.0402(11)	0.0045(9)	0.0113(9)	-0.0065(8)
C15	0.0390(10)	0.0284(9)	0.0323(10)	-0.0018(8)	0.0047(8)	-0.0041(8)
C16	0.0534(13)	0.0294(10)	0.0374(11)	0.0024(8)	0.0050(10)	-0.0059(9)
C17	0.068(2)	0.0316(11)	0.0423(12)	0.0034(9)	0.0016(11)	0.0029(11)
C18	0.061(2)	0.0378(12)	0.0477(13)	-0.0005(10)	0.0039(11)	0.0140(11)
C19	0.0473(12)	0.0395(11)	0.0405(11)	-0.0002(9)	0.0093(10)	0.0089(10)
C20	0.0373(10)	0.0313(10)	0.0310(9)	-0.0031(8)	0.0058(8)	0.0007(8)
C21	0.0326(10)	0.0354(10)	0.0401(11)	0.0008(9)	0.0136(9)	0.0007(8)
C22	0.0242(9)	0.0345(10)	0.0411(11)	0.0066(8)	0.0070(8)	-0.0002(8)
C24	0.0280(9)	0.0286(9)	0.0354(10)	0.0055(8)	0.0080(8)	0.0019(8)
C25	0.0447(12)	0.0457(13)	0.0437(12)	-0.0030(10)	0.0215(10)	0.0022(11)
N10	0.0260(7)	0.0272(8)	0.0316(8)	0.0033(6)	0.0092(6)	-0.0025(6)
N23	0.0307(8)	0.0341(8)	0.0366(9)	0.0002(7)	0.0140(7)	-0.0006(7)
O26	0.0489(8)	0.0486(8)	0.0327(7)	-0.0037(6)	0.0070(6)	-0.0215(7)
O27	0.0300(7)	0.0501(9)	0.0560(9)	0.0054(7)	0.0171(7)	-0.0076(7)
O28	0.0437(8)	0.0305(7)	0.0445(8)	-0.0035(6)	0.0156(6)	-0.0067(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 19, Å

C1-O26	1.219(2)	C1-C2	1.466(3)	C1-C9	1.562(2)
C2-C7	1.388(2)	C2-C3	1.399(3)	C3-C4	1.381(3)
C3-H3	0.97(2)	C4-C5	1.393(3)	C4-H4	0.99(2)
C5-C6	1.389(3)	C5-H5	1.00(2)	C6-C7	1.388(3)
C6-H6	0.99(2)	C7-C8	1.507(2)	C8-C9	1.545(2)
C8-H8a	1.01(2)	C8-H8b	1.00(2)	C9-N10	1.469(2)
C9-C13	1.538(2)	C11-N10	1.473(2)	C11-C14	1.520(3)
C11-C12	1.550(2)	C11-H11	1.02(2)	C12-C22	1.508(3)
C12-C13	1.541(3)	C12-H12	0.98(2)	C13-C24	1.518(3)
C13-H13	0.98(2)	C14-C15	1.510(3)	C14-H14b	1.01(2)
C14-H14a	1.00(2)	C15-C16	1.400(3)	C15-C20	1.400(3)
C16-C17	1.381(3)	C16-H16	1.06(2)	C17-C18	1.383(4)
C17-H17	1.00(3)	C18-C19	1.382(3)	C18-H18	1.00(3)
C19-C20	1.393(3)	C19-H19	1.02(2)	C20-C21	1.506(3)
C21-N10	1.463(2)	C21-H21a	1.05(2)	C21-H21b	1.02(2)
C22-O27	1.214(2)	C22-N23	1.387(2)	C24-O28	1.219(2)
C24-N23	1.377(2)	C25-N23	1.458(2)	C25-H25c	0.99(3)
C25-H25a	0.99(3)	C25-H25b	1.05(3)		

Table 5. Bond Angles in Compound 19, °

O26-C1-C2	126.9(2)	O26-C1-C9	124.5(2)	C2-C1-C9	108.6(2)
C7-C2-C3	121.6(2)	C7-C2-C1	109.6(2)	C3-C2-C1	128.7(2)
C4-C3-C2	118.0(2)	C4-C3-H3	122.0(13)	C2-C3-H3	120.0(13)
C3-C4-C5	120.7(2)	C3-C4-H4	121.1(13)	C5-C4-H4	118.2(13)
C6-C5-C4	120.9(2)	C6-C5-H5	118.0(13)	C4-C5-H5	121.0(13)
C5-C6-C7	118.8(2)	C5-C6-H6	119.7(11)	C7-C6-H6	121.5(11)
C2-C7-C6	119.9(2)	C2-C7-C8	112.0(2)	C6-C7-C8	128.1(2)
C7-C8-C9	105.90(14)	C7-C8-H8a	110.8(13)	C9-C8-H8a	109.6(13)
C7-C8-H8b	111.6(12)	C9-C8-H8b	109.7(12)	H8a-C8-H8b	109(2)
N10-C9-C13	100.69(14)	N10-C9-C8	112.12(14)	C13-C9-C8	118.1(2)
N10-C9-C1	114.01(14)	C13-C9-C1	108.54(14)	C8-C9-C1	103.82(14)
N10-C11-C14	108.11(14)	N10-C11-C12	103.67(13)	C14-C11-C12	118.1(2)
N10-C11-H11	109.4(10)	C14-C11-H11	108.7(11)	C12-C11-H11	108.6(10)
C22-C12-C13	104.5(2)	C22-C12-C11	113.9(2)	C13-C12-C11	104.98(14)
C22-C12-H12	108.0(11)	C13-C12-H12	114.7(11)	C11-C12-H12	110.7(11)
C24-C13-C9	115.4(2)	C24-C13-C12	104.1(2)	C9-C13-C12	105.86(14)
C24-C13-H13	104.5(11)	C9-C13-H13	112.2(11)	C12-C13-H13	114.7(11)
C15-C14-C11	110.3(2)	C15-C14-H14b	109.7(12)	C11-C14-H14b	110.5(12)
C15-C14-H14a	110.0(12)	C11-C14-H14a	109.9(13)	H14b-C14-H14a	106(2)
C16-C15-C20	118.7(2)	C16-C15-C14	120.3(2)	C20-C15-C14	120.9(2)
C17-C16-C15	121.1(2)	C17-C16-H16	121.0(12)	C15-C16-H16	118.0(12)
C16-C17-C18	119.8(2)	C16-C17-H17	121(2)	C18-C17-H17	119(2)
C19-C18-C17	120.1(2)	C19-C18-H18	119(2)	C17-C18-H18	121(2)
C18-C19-C20	120.7(2)	C18-C19-H19	122.1(14)	C20-C19-H19	117.2(14)
C19-C20-C15	119.6(2)	C19-C20-C21	119.0(2)	C15-C20-C21	121.4(2)
N10-C21-C20	110.7(2)	N10-C21-H21a	111.8(12)	C20-C21-H21a	107.8(12)
N10-C21-H21b	110.4(12)	C20-C21-H21b	108.9(12)	H21a-C21-H21b	107(2)
O27-C22-N23	123.4(2)	O27-C22-C12	128.3(2)	N23-C22-C12	108.3(2)
O28-C24-N23	123.2(2)	O28-C24-C13	128.3(2)	N23-C24-C13	108.5(2)
N23-C25-H25c	108(2)	N23-C25-H25a	110(2)	H25c-C25-H25a	110(2)
N23-C25-H25b	107(2)	H25c-C25-H25b	110(2)	H25a-C25-H25b	112(2)
C21-N10-C9	115.90(14)	C21-N10-C11	110.20(14)	C9-N10-C11	108.42(13)
C24-N23-C22	113.2(2)	C24-N23-C25	123.4(2)	C22-N23-C25	123.3(2)

Table 1. Summary of Structure Determination of Compound 23

Formula:	$C_{33}H_{29}N_2O_6$
Formula weight:	549.58
Crystal class:	tetragonal
Space group:	$I4_1/a$ (#88)
Z	16
Cell constants:	
a	28.0824(5)Å
c	13.9256(4)Å
V	10982.0(4)Å^3
μ	0.92 cm^{-1}
crystal size, mm	0.40 x 0.25 x 0.18
D_{calc}	1.330 g/cm^3
F(000)	4624
Radiation:	Mo -K_α (λ=0.71069Å)
2θ range	5.24 – 50.7 °
hkl collected:	-31≤ h ≤33; -33≤ k ≤32; -16≤ l ≤16
No. reflections measured:	25651
No. unique reflections:	4987 (R_{int}=0.0346)
No. observed reflections	4494 (F>4σ)
No. reflections used in refinement	4987
No. parameters	373
R indices (F>4σ)	R_1=0.0867
	wR_2=0.1797
R indices (all data)	R_1=0.0970
	wR_2=0.1852
GOF:	1.203
Final Difference Peaks, e/Å^3	+0.448, -0.466

Table 2. Refined Positional Parameters for Compound 23

Atom	x	y	z	U_{eq}, Å^2
O1	0.81540(8)	0.36649(8)	0.6800(2)	0.0520(6)
O2	0.73224(9)	0.27309(10)	0.4537(2)	0.0676(7)
O3	0.82750(10)	0.27289(10)	0.3599(2)	0.0709(8)
O4	0.91333(8)	0.34269(8)	0.5968(2)	0.0552(6)
O5	0.90219(9)	0.38578(8)	1.0327(2)	0.0552(6)
O6	0.89982(9)	0.29966(8)	1.0899(2)	0.0578(6)
N1	0.78115(8)	0.27339(9)	0.6334(2)	0.0409(6)
N2	0.86446(9)	0.32100(9)	0.4717(2)	0.0449(6)
C1	0.82962(10)	0.33150(10)	0.7236(2)	0.0401(7)
C2	0.85079(11)	0.32886(10)	0.8186(2)	0.0397(7)
C3	0.86671(11)	0.36582(11)	0.8780(2)	0.0434(7)
H3	0.86544(11)	0.39731(11)	0.8575(2)	0.054
C4	0.88425(11)	0.35452(11)	0.9673(2)	0.0430(7)
C5	0.88420(11)	0.30622(11)	0.9987(2)	0.0445(7)
C6	0.86864(11)	0.27014(11)	0.9390(2)	0.0438(7)
H6	0.86908(11)	0.23862(11)	0.9595(2)	0.055
C7	0.85230(10)	0.28181(10)	0.8478(2)	0.0389(7)
C8	0.83236(11)	0.24858(10)	0.7729(2)	0.0411(7)
H8a	0.80198(11)	0.23559(10)	0.7932(2)	0.051
H8b	0.85418(11)	0.22256(10)	0.7601(2)	0.051
C9	0.82641(10)	0.28052(10)	0.6833(2)	0.0383(7)
C10	0.86630(10)	0.27020(10)	0.6058(2)	0.0393(7)
H10	0.89199(10)	0.25057(10)	0.6323(2)	0.049
C11	0.84032(10)	0.24463(11)	0.5234(2)	0.0415(7)
H11	0.85600(10)	0.21451(11)	0.5072(2)	0.052
C12	0.78872(10)	0.23601(11)	0.5625(2)	0.0412(7)
C13	0.78465(12)	0.18485(11)	0.6034(3)	0.0508(8)
H13a	0.81581(12)	0.17195(11)	0.6185(3)	0.063
H13b	0.76510(12)	0.18431(11)	0.6609(3)	0.063
C14	0.76153(12)	0.15748(13)	0.5233(3)	0.0565(9)
C15	0.7584(2)	0.1084(2)	0.5121(4)	0.0810(13)
H15	0.7725(2)	0.0879(2)	0.5563(4)	0.101
C16	0.7338(2)	0.0907(2)	0.4340(5)	0.101(2)
H16	0.7312(2)	0.0580(2)	0.4258(5)	0.126
C17	0.7132(2)	0.1208(2)	0.3681(4)	0.096(2)
H17	0.6969(2)	0.1079(2)	0.3161(4)	0.120
C18	0.71600(13)	0.1698(2)	0.3772(3)	0.0760(13)
H18	0.70192(13)	0.1901(2)	0.3327(3)	0.095
C19	0.74094(11)	0.18738(14)	0.4563(3)	0.0562(9)
C20	0.75056(11)	0.23710(13)	0.4834(2)	0.0497(8)
C21	0.84192(12)	0.27915(12)	0.4402(2)	0.0481(8)
C22	0.86849(12)	0.36374(12)	0.4162(2)	0.0487(8)
C23	0.88691(13)	0.36320(14)	0.3244(2)	0.0574(9)
H23	0.89702(13)	0.33477(14)	0.2968(2)	0.072
C24	0.89015(14)	0.4054(2)	0.2738(3)	0.0711(12)
H24	0.90228(14)	0.4054(2)	0.2117(3)	0.089
C25	0.8756(2)	0.4474(2)	0.3145(3)	0.0764(13)
H25	0.8782(2)	0.4756(2)	0.2802(3)	0.096
C26	0.8574(2)	0.4478(2)	0.4060(3)	0.0787(12)

H26	0.8476(2)	0.4763(2)	0.4334(3)	0.098
C27	0.8535(2)	0.40579(13)	0.4574(3)	0.0646(10)
H27	0.8408(2)	0.40593(13)	0.5191(3)	0.081
C28	0.88524(10)	0.31526(11)	0.5614(2)	0.0418(7)
C29	0.9053(2)	0.43441(12)	1.0039(3)	0.0688(11)
H29a	0.9206(9)	0.4525(2)	1.0536(9)	0.092
H29b	0.8739(2)	0.4467(3)	0.993(2)	0.092
H29c	0.9236(8)	0.4367(2)	0.9459(11)	0.092
C30	0.8969(2)	0.25223(14)	1.1281(3)	0.0836(14)
H30a	0.9056(11)	0.2526(2)	1.1947(6)	0.111
H30b	0.9182(8)	0.2318(3)	1.093(2)	0.111
H30c	0.8649(3)	0.2407(4)	1.122(2)	0.111
O7	0.5088(2)	0.20165(14)	0.6433(6)	0.163(2)
C32	0.5182(3)	0.2255(4)	0.7511(7)	0.195(5)
C33	0.5000	0.2500	0.696(2)	0.42(2)
C34	0.5000	0.2500	0.5703(10)	0.193(6)
H1	0.7716	0.2994	0.5977	0.050

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

Table 3. Refined Thermal Parameters (U's) for Compound 23

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O1	0.063(2)	0.0432(12)	0.0497(13)	0.0050(10)	-0.0057(11)	0.0079(11)
O2	0.066(2)	0.074(2)	0.063(2)	-0.0011(14)	-0.0153(13)	0.0144(14)
O3	0.091(2)	0.081(2)	0.0412(14)	-0.0065(13)	-0.0038(13)	-0.032(2)
O4	0.0485(13)	0.061(2)	0.0555(14)	0.0004(11)	-0.0068(11)	-0.0211(11)
O5	0.076(2)	0.0433(12)	0.0461(13)	0.0017(10)	-0.0125(12)	-0.0127(11)
O6	0.077(2)	0.0499(13)	0.0466(13)	0.0100(11)	-0.0190(12)	-0.0076(12)
N1	0.0360(13)	0.0456(14)	0.0411(14)	-0.0019(11)	-0.0014(11)	0.0005(10)
N2	0.048(2)	0.047(2)	0.039(2)	0.0024(11)	-0.0016(12)	-0.0099(12)
C1	0.039(2)	0.041(2)	0.040(2)	0.0018(13)	0.0029(13)	0.0013(12)
C2	0.042(2)	0.039(2)	0.038(2)	0.0012(13)	0.0002(13)	0.0001(13)
C3	0.050(2)	0.037(2)	0.043(2)	0.0044(13)	0.0007(14)	-0.0011(13)
C4	0.044(2)	0.044(2)	0.041(2)	0.0003(13)	-0.0012(13)	-0.0045(13)
C5	0.045(2)	0.046(2)	0.042(2)	0.0074(14)	-0.0024(14)	-0.0004(14)
C6	0.047(2)	0.037(2)	0.047(2)	0.0060(13)	0.0005(14)	-0.0019(13)
C7	0.036(2)	0.041(2)	0.039(2)	0.0019(13)	0.0008(12)	0.0011(12)
C8	0.042(2)	0.038(2)	0.043(2)	0.0023(13)	0.0023(13)	-0.0025(13)
C9	0.037(2)	0.039(2)	0.039(2)	0.0002(13)	-0.0002(12)	0.0002(12)
C10	0.035(2)	0.041(2)	0.042(2)	-0.0016(13)	0.0013(13)	-0.0004(12)
C11	0.038(2)	0.041(2)	0.046(2)	-0.0059(13)	0.0040(13)	-0.0022(12)
C12	0.038(2)	0.042(2)	0.044(2)	-0.0008(13)	0.0006(13)	-0.0036(12)
C13	0.043(2)	0.047(2)	0.063(2)	0.004(2)	0.001(2)	-0.0077(14)
C14	0.040(2)	0.054(2)	0.075(3)	-0.014(2)	0.006(2)	-0.014(2)
C15	0.068(3)	0.057(2)	0.118(4)	-0.017(2)	0.007(3)	-0.016(2)
C16	0.077(3)	0.078(3)	0.147(5)	-0.048(4)	0.008(3)	-0.026(3)
C17	0.054(3)	0.116(4)	0.118(4)	-0.067(4)	0.001(3)	-0.016(3)
C18	0.039(2)	0.108(4)	0.081(3)	-0.038(3)	-0.004(2)	0.000(2)
C19	0.034(2)	0.070(2)	0.065(2)	-0.021(2)	0.002(2)	-0.004(2)
C20	0.039(2)	0.062(2)	0.048(2)	-0.004(2)	0.0004(14)	-0.001(2)
C21	0.049(2)	0.052(2)	0.043(2)	-0.007(2)	0.005(2)	-0.011(2)
C22	0.049(2)	0.052(2)	0.045(2)	0.006(2)	-0.004(2)	-0.013(2)
C23	0.053(2)	0.073(2)	0.046(2)	0.009(2)	-0.001(2)	-0.011(2)
C24	0.059(2)	0.103(3)	0.051(2)	0.024(2)	-0.005(2)	-0.019(2)
C25	0.075(3)	0.076(3)	0.078(3)	0.035(2)	-0.019(2)	-0.025(2)
C26	0.097(3)	0.058(2)	0.081(3)	0.012(2)	-0.006(3)	-0.014(2)
C27	0.083(3)	0.056(2)	0.055(2)	0.007(2)	0.005(2)	-0.009(2)
C28	0.035(2)	0.047(2)	0.043(2)	-0.0027(14)	0.0025(13)	-0.0038(13)
C29	0.104(3)	0.044(2)	0.058(2)	-0.001(2)	-0.010(2)	-0.017(2)
C30	0.135(4)	0.058(2)	0.058(2)	0.019(2)	-0.031(3)	-0.004(2)
O7	0.155(4)	0.072(3)	0.262(7)	-0.012(3)	0.097(5)	-0.005(3)
C32	0.128(6)	0.222(10)	0.236(9)	0.171(8)	-0.118(6)	-0.097(6)
C33	0.75(7)	0.22(2)	0.30(3)	0.000	0.000	0.19(3)
C34	0.112(8)	0.32(2)	0.145(11)	0.000	0.000	0.035(11)

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 23, Å

O1-C1	1.222(3)	O2-C20	1.207(4)	O3-C21	1.202(4)
O4-C28	1.208(4)	O5-C4	1.361(4)	O5-C29	1.426(4)
O6-C5	1.356(4)	O6-C30	1.436(4)	N1-C12	1.457(4)
N1-C9	1.462(4)	N2-C28	1.388(4)	N2-C21	1.405(4)
N2-C22	1.432(4)	C1-C2	1.452(4)	C1-C9	1.540(4)
C2-C7	1.383(4)	C2-C3	1.401(4)	C3-C4	1.374(4)
C4-C5	1.425(4)	C5-C6	1.382(4)	C6-C7	1.391(4)
C7-C8	1.507(4)	C8-C9	1.545(4)	C9-C10	1.582(4)
C10-C28	1.506(4)	C10-C11	1.537(4)	C11-C21	1.512(5)
C11-C12	1.567(4)	C12-C20	1.537(4)	C12-C13	1.550(4)
C13-C14	1.503(5)	C14-C19	1.382(5)	C14-C15	1.390(5)
C15-C16	1.380(7)	C16-C17	1.376(8)	C17-C18	1.384(7)
C18-C19	1.395(5)	C19-C20	1.471(5)	C22-C23	1.380(5)
C22-C27	1.379(5)	C23-C24	1.382(5)	C24-C25	1.369(6)
C25-C26	1.373(6)	C26-C27	1.383(5)	O7-C32	1.665(12)
O7-C34	1.714(10)	O7-C33	1.56(2)	C32-C33	1.15(2)
C32-C32'	1.71(2)	C33-C32'	1.15(2)	C33-O7'	1.56(2)
C33-C34	1.75(3)	C34-O7'	1.714(10)		

Table 5. Bond Angles in Compound 23, °

C4-O5-C29	116.9(3)	C5-O6-C30	117.0(3)	C12-N1-C9	107.1(2)
C28-N2-C21	111.9(3)	C28-N2-C22	123.3(3)	C21-N2-C22	124.6(3)
O1-C1-C2	128.9(3)	O1-C1-C9	123.2(3)	C2-C1-C9	108.0(2)
C7-C2-C3	121.6(3)	C7-C2-C1	109.2(3)	C3-C2-C1	129.1(3)
C4-C3-C2	118.5(3)	O5-C4-C3	126.1(3)	O5-C4-C5	114.1(3)
C3-C4-C5	119.8(3)	O6-C5-C6	124.5(3)	O6-C5-C4	114.6(3)
C6-C5-C4	120.9(3)	C5-C6-C7	118.8(3)	C2-C7-C6	120.2(3)
C2-C7-C8	112.1(3)	C6-C7-C8	127.5(3)	C7-C8-C9	103.8(2)
N1-C9-C1	110.6(2)	N1-C9-C8	113.4(2)	C1-C9-C8	103.9(2)
N1-C9-C10	105.4(2)	C1-C9-C10	112.2(2)	C8-C9-C10	111.6(2)
C28-C10-C11	104.7(2)	C28-C10-C9	112.1(2)	C11-C10-C9	105.0(2)
C21-C11-C10	105.0(2)	C21-C11-C12	113.1(3)	C10-C11-C12	104.6(2)
N1-C12-C20	111.7(2)	N1-C12-C13	114.1(3)	C20-C12-C13	103.3(2)
N1-C12-C11	105.0(2)	C20-C12-C11	113.1(3)	C13-C12-C11	109.8(2)
C14-C13-C12	103.5(3)	C19-C14-C15	120.0(4)	C19-C14-C13	111.8(3)
C15-C14-C13	128.2(4)	C16-C15-C14	118.5(5)	C17-C16-C15	121.1(5)
C16-C17-C18	121.6(4)	C17-C18-C19	116.9(5)	C14-C19-C18	121.9(4)
C14-C19-C20	109.0(3)	C18-C19-C20	129.1(4)	O2-C20-C19	128.9(3)
O2-C20-C12	124.0(3)	C19-C20-C12	107.0(3)	O3-C21-N2	124.4(3)
O3-C21-C11	127.5(3)	N2-C21-C11	108.1(3)	C23-C22-C27	120.6(3)
C23-C22-N2	121.4(3)	C27-C22-N2	118.0(3)	C22-C23-C24	119.2(4)
C25-C24-C23	120.5(4)	C24-C25-C26	120.2(4)	C25-C26-C27	120.1(4)
C22-C27-C26	119.4(4)	O4-C28-N2	124.6(3)	O4-C28-C10	126.8(3)
N2-C28-C10	108.6(2)	C32-O7-C34	103.8(5)	C32-O7-C33	41.6(9)
C34-O7-C33	64.4(11)	C33-C32-O7	64.4(12)	C33-C32-C32'	42(2)
O7-C32-C32'	103.2(4)	C32'-C33-C32	96(3)	C32'-C33-O7'	74.0(7)
C32-C33-O7'	154.5(14)	C32'-C33-O7	154.5(14)	C32-C33-O7	74.0(7)
O7'-C33-O7	124(2)	C32'-C33-C34	132(2)	C32-C33-C34	132(2)
O7'-C33-C34	62.0(11)	O7-C33-C34	62.0(11)	O7'-C34-O7	107.2(9)
O7'-C34-C33	53.6(4)	O7-C34-C33	53.6(4)		

Table 1. Summary of Structure Determination of Compound 24

Formula:	$C_{28}H_{18}N_2O_5$
Formula weight:	462.44
Crystal class:	monoclinic
Space group:	$P2_1/c$ (#14)
Z	4
Cell constants:	
a	10.6739(5)Å
b	8.0149(3)Å
c	25.1159(8)Å
β	92.495(3)°
V	2146.6(2)Å^3
μ	1.00 cm^{-1}
crystal size, mm	0.50 x 0.15 x 0.12
D_{calc}	1.431 g/cm^3
F(000)	960
Radiation:	Mo -K_α (λ=0.71069Å)
2θ range	5.12 – 50.7 °
hkl collected:	-12≤ h ≤12; -9≤ k ≤9; -30≤ l ≤27
No. reflections measured:	16612
No. unique reflections:	3671 (R_{int}=0.0338)
No. observed reflections	3384 (F>4σ)
No. reflections used in refinement	3671
No. parameters	399
R indices (F>4σ)	R_1=0.0529
	wR_2=0.1059
R indices (all data)	R_1=0.0599
	wR_2=0.1089
GOF:	1.257
Final Difference Peaks, e/Å^3	+0.202, -0.199

Table 2. Refined Positional Parameters for Compound 24

Atom	x	y	z	U_{eq}, Å^2
C1	0.6683(2)	0.4957(3)	0.06324(8)	0.0313(5)
C2	0.7180(2)	0.3370(3)	0.04544(8)	0.0314(5)
C3	0.8356(2)	0.3040(3)	0.02611(9)	0.0377(5)
C4	0.8601(2)	0.1432(3)	0.01040(10)	0.0432(6)
C5	0.7702(2)	0.0185(3)	0.01431(10)	0.0445(6)
C6	0.6533(2)	0.0529(3)	0.03330(9)	0.0387(5)
C7	0.6262(2)	0.2149(3)	0.04848(8)	0.0309(5)
C8	0.5040(2)	0.2880(3)	0.06567(9)	0.0329(5)
C9	0.5416(2)	0.4606(2)	0.08841(8)	0.0287(5)
C10	0.5524(2)	0.4567(3)	0.15090(8)	0.0299(5)
C11	0.6687(2)	0.5431(3)	0.17401(8)	0.0309(5)
C12	0.5023(2)	0.6978(3)	0.20404(8)	0.0322(5)
C13	0.4423(2)	0.5610(3)	0.17012(8)	0.0301(5)
C14	0.3742(2)	0.6308(2)	0.11801(8)	0.0293(5)
C15	0.3461(2)	0.8187(3)	0.11965(9)	0.0320(5)
C16	0.2100(2)	0.8414(3)	0.12134(8)	0.0311(5)
C17	0.1429(2)	0.9896(3)	0.12513(9)	0.0372(5)
C18	0.0137(2)	0.9785(3)	0.12373(10)	0.0425(6)
C19	-0.0468(2)	0.8251(3)	0.11785(10)	0.0426(6)
C20	0.0196(2)	0.6781(3)	0.11317(9)	0.0382(5)
C21	0.1497(2)	0.6883(3)	0.11507(8)	0.0316(5)
C22	0.2430(2)	0.5530(3)	0.10959(9)	0.0337(5)
C23	0.7184(2)	0.8089(3)	0.22139(8)	0.0318(5)
C24	0.7077(2)	0.9711(3)	0.20282(10)	0.0375(5)
C25	0.7925(2)	1.0903(3)	0.22179(10)	0.0433(6)
C26	0.8867(2)	1.0460(3)	0.25862(10)	0.0449(6)
C27	0.8967(2)	0.8838(3)	0.27685(10)	0.0456(6)
C28	0.8120(2)	0.7638(3)	0.25841(9)	0.0389(5)
N1	0.4564(2)	0.5975(2)	0.07446(7)	0.0321(4)
N2	0.6321(2)	0.6862(2)	0.20037(7)	0.0310(4)
O1	0.7107(2)	0.6352(2)	0.05822(7)	0.0409(4)
O2	0.77594(14)	0.4979(2)	0.17025(6)	0.0393(4)
O3	0.45013(14)	0.8014(2)	0.22996(6)	0.0425(4)
O4	0.4262(2)	0.9250(2)	0.11723(7)	0.0441(4)
O5	0.2220(2)	0.4070(2)	0.10099(8)	0.0450(7)
H8a	0.463(3)	0.213(4)	0.0916(12)	0.042(7)
H8b	0.445(3)	0.306(4)	0.0312(12)	0.041(8)
O5'	0.401(2)	0.245(2)	0.0600(9)	0.054(6)
H1	0.506(2)	0.691(3)	0.0706(10)	0.042(7)
H3	0.896(2)	0.393(3)	0.0258(10)	0.047(7)
H4	0.942(3)	0.116(3)	-0.0019(11)	0.060(8)
H5	0.789(3)	-0.099(4)	0.0050(11)	0.060(8)
H6	0.591(2)	-0.033(3)	0.0358(9)	0.040(6)
H10	0.551(2)	0.343(3)	0.1654(9)	0.035(6)
H13	0.385(2)	0.501(3)	0.1915(9)	0.029(5)
H17	0.187(2)	1.096(3)	0.1280(9)	0.035(6)
H18	-0.039(2)	1.080(3)	0.1264(10)	0.045(7)
H19	-0.137(3)	0.824(3)	0.1157(10)	0.048(7)
H20	-0.024(3)	0.567(4)	0.1100(10)	0.054(7)

H24	0.646(2)	0.995(3)	0.1755(10)	0.048(7)
H25	0.785(2)	1.207(3)	0.2076(10)	0.053(7)
H26	0.945(3)	1.134(4)	0.2730(11)	0.060(8)
H27	0.961(3)	0.853(3)	0.3055(12)	0.063(8)
H28	0.814(2)	0.650(3)	0.2724(10)	0.047(7)
H22a	0.2342	0.5040	0.0743	0.042
H22b	0.2307	0.4674	0.1362	0.042

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

Table 3. Refined Thermal Parameters (U's) for Compound 24

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C1	0.0347(11)	0.0303(12)	0.0291(11)	0.0021(8)	0.0024(9)	-0.0004(9)
C2	0.0354(11)	0.0328(12)	0.0260(11)	0.0017(8)	0.0027(9)	0.0021(9)
C3	0.0379(12)	0.0419(13)	0.0338(13)	0.0005(10)	0.0066(10)	0.0018(11)
C4	0.0451(14)	0.0458(14)	0.0391(14)	0.0036(10)	0.0071(11)	0.0136(11)
C5	0.059(2)	0.0354(13)	0.0396(14)	0.0003(10)	0.0079(12)	0.0112(12)
C6	0.0506(14)	0.0301(12)	0.0356(13)	-0.0001(9)	0.0035(11)	0.0006(11)
C7	0.0394(12)	0.0301(11)	0.0231(11)	0.0022(8)	0.0014(9)	0.0009(9)
C8	0.0357(13)	0.0287(11)	0.0346(13)	-0.0009(9)	0.0031(10)	-0.0026(9)
C9	0.0310(11)	0.0264(10)	0.0288(11)	0.0021(8)	0.0030(9)	-0.0003(8)
C10	0.0365(11)	0.0261(11)	0.0273(11)	0.0024(8)	0.0038(9)	0.0009(9)
C11	0.0379(12)	0.0278(11)	0.0272(11)	0.0026(8)	0.0036(9)	0.0026(9)
C12	0.0344(11)	0.0340(12)	0.0287(12)	0.0009(9)	0.0071(9)	0.0003(9)
C13	0.0312(11)	0.0303(11)	0.0295(12)	0.0029(9)	0.0079(9)	-0.0026(9)
C14	0.0297(11)	0.0276(11)	0.0310(11)	0.0025(8)	0.0046(9)	-0.0002(8)
C15	0.0351(11)	0.0295(11)	0.0317(12)	0.0020(8)	0.0048(9)	-0.0015(9)
C16	0.0319(11)	0.0331(12)	0.0284(11)	0.0011(8)	0.0017(9)	0.0027(9)
C17	0.0422(13)	0.0360(13)	0.0335(13)	-0.0015(9)	0.0024(10)	0.0050(10)
C18	0.0406(13)	0.049(2)	0.0381(13)	-0.0012(11)	0.0035(11)	0.0125(12)
C19	0.0305(12)	0.059(2)	0.0382(14)	0.0040(11)	0.0031(10)	0.0056(11)
C20	0.0333(12)	0.0461(14)	0.0350(13)	0.0036(10)	0.0013(10)	-0.0020(10)
C21	0.0317(11)	0.0346(12)	0.0285(11)	0.0029(9)	0.0023(9)	-0.0011(9)
C22	0.0366(12)	0.0317(12)	0.0330(12)	0.0033(9)	0.0027(9)	-0.0021(9)
C23	0.0326(11)	0.0315(11)	0.0316(12)	-0.0051(9)	0.0049(9)	-0.0011(9)
C24	0.0383(13)	0.0359(13)	0.0385(13)	-0.0007(10)	0.0047(10)	0.0015(10)
C25	0.0483(14)	0.0336(13)	0.049(2)	-0.0038(11)	0.0154(12)	-0.0037(11)
C26	0.0432(14)	0.048(2)	0.0443(14)	-0.0136(11)	0.0104(11)	-0.0108(12)
C27	0.0420(14)	0.056(2)	0.0387(14)	-0.0093(11)	-0.0024(11)	-0.0015(12)
C28	0.0423(13)	0.0392(13)	0.0352(13)	-0.0023(10)	0.0005(11)	0.0012(10)
N1	0.0349(10)	0.0298(10)	0.0320(10)	0.0048(8)	0.0061(8)	0.0024(8)
N2	0.0314(9)	0.0294(9)	0.0323(10)	-0.0018(7)	0.0016(8)	0.0006(7)
O1	0.0443(9)	0.0309(9)	0.0482(10)	0.0012(7)	0.0114(8)	-0.0074(7)
O2	0.0349(9)	0.0396(9)	0.0433(9)	-0.0037(7)	0.0011(7)	0.0065(7)
O3	0.0398(9)	0.0451(10)	0.0434(10)	-0.0124(8)	0.0106(7)	0.0016(7)
O4	0.0386(9)	0.0301(8)	0.0641(12)	0.0062(7)	0.0075(8)	-0.0045(7)
O5	0.0448(11)	0.0281(11)	0.0624(14)	-0.0028(8)	0.0039(9)	-0.0068(8)
O5'	0.038(11)	0.050(11)	0.073(14)	-0.018(9)	0.000(9)	0.004(8)

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 24, Å

C1-O1	1.215(2)	C1-C2	1.456(3)	C1-C9	1.543(3)
C2-C7	1.390(3)	C2-C3	1.391(3)	C3-C4	1.376(3)
C3-H3	0.96(3)	C4-C5	1.392(4)	C4-H4	0.96(3)
C5-C6	1.383(3)	C5-H5	0.99(3)	C6-C7	1.387(3)
C6-H6	0.96(2)	C7-C8	1.510(3)	C8-O5'	1.15(2)
C8-C9	1.542(3)	C8-H8a	1.00(3)	C8-H8b	1.06(3)
C9-N1	1.458(3)	C9-C10	1.569(3)	C10-C11	1.515(3)
C10-C13	1.536(3)	C10-H10	0.98(2)	C11-O2	1.208(3)
C11-N2	1.389(3)	C12-O3	1.206(3)	C12-N2	1.395(3)
C12-C13	1.514(3)	C13-C14	1.572(3)	C13-H13	0.96(2)
C14-N1	1.457(3)	C14-C15	1.536(3)	C14-C22	1.539(3)
C15-O4	1.211(3)	C15-C16	1.467(3)	C16-C21	1.391(3)
C16-C17	1.392(3)	C17-C18	1.381(3)	C17-H17	0.97(2)
C18-C19	1.394(4)	C18-H18	0.99(3)	C19-C20	1.382(3)
C19-H19	0.96(3)	C20-C21	1.390(3)	C20-H20	1.01(3)
C21-C22	1.483(3)	C22-O5	1.209(3)	C22-H22a	0.970(2)
C22-H22b	0.971(2)	C23-C28	1.383(3)	C23-C24	1.384(3)
C23-N2	1.433(3)	C24-C25	1.386(3)	C24-H24	0.95(3)
C25-C26	1.383(4)	C25-H25	1.00(3)	C26-C27	1.381(4)
C26-H26	1.00(3)	C27-C28	1.386(3)	C27-H27	1.00(3)
C28-H28	0.98(3)	N1-H1	0.92(3)	O5-H22a	1.038(2)
O5-H22b	1.009(2)				

Table 5. Bond Angles in Compound 24, °

O1-C1-C2	129.0(2)	O1-C1-C9	123.2(2)	C2-C1-C9	107.7(2)
C7-C2-C3	122.3(2)	C7-C2-C1	109.3(2)	C3-C2-C1	128.3(2)
C4-C3-C2	117.7(2)	C4-C3-H3	124(2)	C2-C3-H3	119(2)
C3-C4-C5	120.8(2)	C3-C4-H4	119(2)	C5-C4-H4	120(2)
C6-C5-C4	121.1(2)	C6-C5-H5	117(2)	C4-C5-H5	121(2)
C5-C6-C7	118.9(2)	C5-C6-H6	121.0(14)	C7-C6-H6	120.1(14)
C6-C7-C2	119.2(2)	C6-C7-C8	129.5(2)	C2-C7-C8	111.2(2)
O5'-C8-C7	132.6(8)	O5'-C8-C9	123.0(8)	C7-C8-C9	103.9(2)
C7-C8-H8a	111(2)	C9-C8-H8a	114(2)	C7-C8-H8b	108(2)
C9-C8-H8b	109(2)	H8a-C8-H8b	111(2)	N1-C9-C8	115.9(2)
N1-C9-C1	108.2(2)	C8-C9-C1	103.3(2)	N1-C9-C10	105.8(2)
C8-C9-C10	111.1(2)	C1-C9-C10	112.7(2)	C11-C10-C13	104.8(2)
C11-C10-C9	113.4(2)	C13-C10-C9	106.3(2)	C11-C10-H10	107.7(13)
C13-C10-H10	111.6(13)	C9-C10-H10	112.8(13)	O2-C11-N2	124.8(2)
O2-C11-C10	126.7(2)	N2-C11-C10	108.5(2)	O3-C12-N2	124.4(2)
O3-C12-C13	127.5(2)	N2-C12-C13	108.1(2)	C12-C13-C10	105.1(2)
C12-C13-C14	112.3(2)	C10-C13-C14	105.3(2)	C12-C13-H13	108.1(13)
C10-C13-H13	114.7(12)	C14-C13-H13	111.3(12)	N1-C14-C15	109.0(2)
N1-C14-C22	113.4(2)	C15-C14-C22	102.9(2)	N1-C14-C13	106.7(2)
C15-C14-C13	114.2(2)	C22-C14-C13	110.8(2)	O4-C15-C16	128.1(2)
O4-C15-C14	123.3(2)	C16-C15-C14	108.5(2)	C21-C16-C17	121.6(2)
C21-C16-C15	109.9(2)	C17-C16-C15	128.4(2)	C18-C17-C16	117.3(2)
C18-C17-H17	122.4(13)	C16-C17-H17	120.3(13)	C17-C18-C19	121.1(2)
C17-C18-H18	121.0(14)	C19-C18-H18	117.9(14)	C20-C19-C18	121.6(2)
C20-C19-H19	120(2)	C18-C19-H19	118(2)	C19-C20-C21	117.5(2)
C19-C20-H20	122(2)	C21-C20-H20	121(2)	C20-C21-C16	120.8(2)
C20-C21-C22	128.9(2)	C16-C21-C22	110.3(2)	O5-C22-C21	127.1(2)
O5-C22-C14	125.3(2)	C21-C22-C14	107.5(2)	O5-C22-H22a	55.6(2)
C21-C22-H22a	110.0(2)	C14-C22-H22a	110.0(2)	O5-C22-H22b	53.81(14)
C21-C22-H22b	109.9(2)	C14-C22-H22b	110.0(2)	H22a-C22-H22b	109.4(2)
C28-C23-C24	121.3(2)	C28-C23-N2	120.1(2)	C24-C23-N2	118.6(2)
C23-C24-C25	119.2(2)	C23-C24-H24	118(2)	C25-C24-H24	122(2)
C26-C25-C24	119.9(2)	C26-C25-H25	122(2)	C24-C25-H25	119(2)
C27-C26-C25	120.5(2)	C27-C26-H26	121(2)	C25-C26-H26	119(2)
C26-C27-C28	120.2(2)	C26-C27-H27	121(2)	C28-C27-H27	119(2)
C23-C28-C27	119.0(2)	C23-C28-H28	119(2)	C27-C28-H28	122(2)
C14-N1-C9	110.3(2)	C14-N1-H1	107(2)	C9-N1-H1	107(2)
C11-N2-C12	112.8(2)	C11-N2-C23	123.6(2)	C12-N2-C23	123.6(2)
C22-O5-H22a	50.45(13)	C22-O5-H22b	50.94(13)	H22a-O5-H22b	101.4(2)
C8-O5'-H8a	54(2)	C8-O5'-H8b	58(2)	H8a-O5'-H8b	112(3)

Table 1. Summary of Structure Determination of Compound 25

Formula:	$C_{18}H_{12}N_2$
Formula weight:	256.30
Crystal class:	monoclinic
Space group:	$P2_1/c$ (#14)
Z	2
Cell constants:	
a	13.546(2)Å
b	3.9888(5)Å
c	11.508(1)Å
β	98.376(6)°
V	615.17(14)Å^3
μ	0.82 cm^{-1}
crystal size, mm	0.40 x 0.28 x 0.15
D_{calc}	1.384 g/cm^3
F(000)	268
Radiation:	Mo-K_α (λ=0.71069Å)
2θ range	6.08–50.64°
hkl collected:	-16≤ h ≤16; -4≤ k ≤4; -13≤ l ≤13
No. reflections measured:	4202
No. unique reflections:	1102 (R_{int}=0.0292)
No. observed reflections	1023 (F>4σ)
No. reflections used in refinement	1102
No. parameters	116
R indices (F>4σ)	R_1=0.0415
	wR_2=0.0955
R indices (all data)	R1=0.0463
	wR2=0.0982
GOF:	1.152
Final Difference Peaks, e/Å^3	+0.148, -0.107

Table 2. Refined Positional Parameters for Compound 25

Atom	x	y	z	U_{eq}, Å^2
N1	1.04351(8)	-0.1626(3)	0.90732(9)	0.0433(4)
C1	0.86618(11)	-0.2066(4)	0.80385(12)	0.0458(4)
C2	0.77200(11)	-0.0945(4)	0.84881(12)	0.0441(4)
C3	0.67374(12)	-0.1189(4)	0.7970(2)	0.0526(4)
C4	0.59945(12)	0.0050(4)	0.8569(2)	0.0576(5)
C5	0.62317(12)	0.1531(4)	0.9666(2)	0.0565(5)
C6	0.72105(11)	0.1787(4)	1.01948(14)	0.0511(4)
C7	0.79545(11)	0.0540(4)	0.95985(12)	0.0436(4)
C8	0.90339(10)	0.0447(3)	0.99317(11)	0.0409(4)
C9	0.94583(10)	-0.1126(3)	0.90291(12)	0.0410(4)
H1a	0.8666(11)	-0.451(5)	0.7852(13)	0.056(4)
H1b	0.8786(12)	-0.086(4)	0.729(2)	0.059(5)
H3	0.6554(12)	-0.228(5)	0.719(2)	0.063(5)
H4	0.5258(14)	-0.010(5)	0.821(2)	0.068(5)
H5	0.5687(13)	0.237(5)	1.007(2)	0.069(5)
H6	0.7402(12)	0.279(5)	1.098(2)	0.059(5)

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

Table 3. Refined Thermal Parameters (U's) for Compound 25

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
N1	0.0466(7)	0.0456(7)	0.0397(7)	0.0012(5)	0.0123(5)	0.0008(5)
C1	0.0498(9)	0.0482(8)	0.0408(8)	-0.0014(6)	0.0117(6)	-0.0009(7)
C2	0.0469(8)	0.0434(8)	0.0435(8)	0.0054(6)	0.0118(6)	-0.0017(6)
C3	0.0512(9)	0.0567(9)	0.0499(9)	0.0042(7)	0.0076(7)	-0.0063(7)
C4	0.0438(9)	0.0655(10)	0.0638(10)	0.0088(8)	0.0087(7)	-0.0025(8)
C5	0.0470(9)	0.0623(10)	0.0633(10)	0.0029(8)	0.0189(8)	0.0034(7)
C6	0.0478(9)	0.0565(9)	0.0515(9)	0.0004(7)	0.0158(7)	0.0023(7)
C7	0.0452(8)	0.0436(8)	0.0441(8)	0.0052(6)	0.0136(6)	0.0007(6)
C8	0.0455(8)	0.0400(7)	0.0392(7)	0.0033(6)	0.0132(6)	0.0009(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 25, Å

N1-C9	1.332(2)	N1-C8#1	1.345(2)	C1-C9	1.499(2)
C1-C2	1.512(2)	C2-C3	1.380(2)	C2-C7	1.402(2)
C3-C4	1.391(2)	C4-C5	1.388(2)	C5-C6	1.380(2)
C6-C7	1.391(2)	C7-C8	1.457(2)	C8-N1#1	1.345(2)
C8-C9	1.406(2)				

Table 5. Bond Angles in Compound 25, °

C9-N1-C8#1	112.65(12)	C9-C1-C2	102.45(11)	C3-C2-C7	119.97(14)
C3-C2-C1	129.78(14)	C7-C2-C1	110.26(13)	C2-C3-C4	118.9(2)
C5-C4-C3	120.9(2)	C6-C5-C4	120.9(2)	C5-C6-C7	118.3(2)
C6-C7-C2	121.08(14)	C6-C7-C8	130.59(14)	C2-C7-C8	108.33(12)
N1#1-C8-C9	124.01(13)	N1#1-C8-C7	127.35(12)	C9-C8-C7	108.64(12)
N1-C9-C8	123.34(13)	N1-C9-C1	126.35(12)	C8-C9-C1	110.30(12)

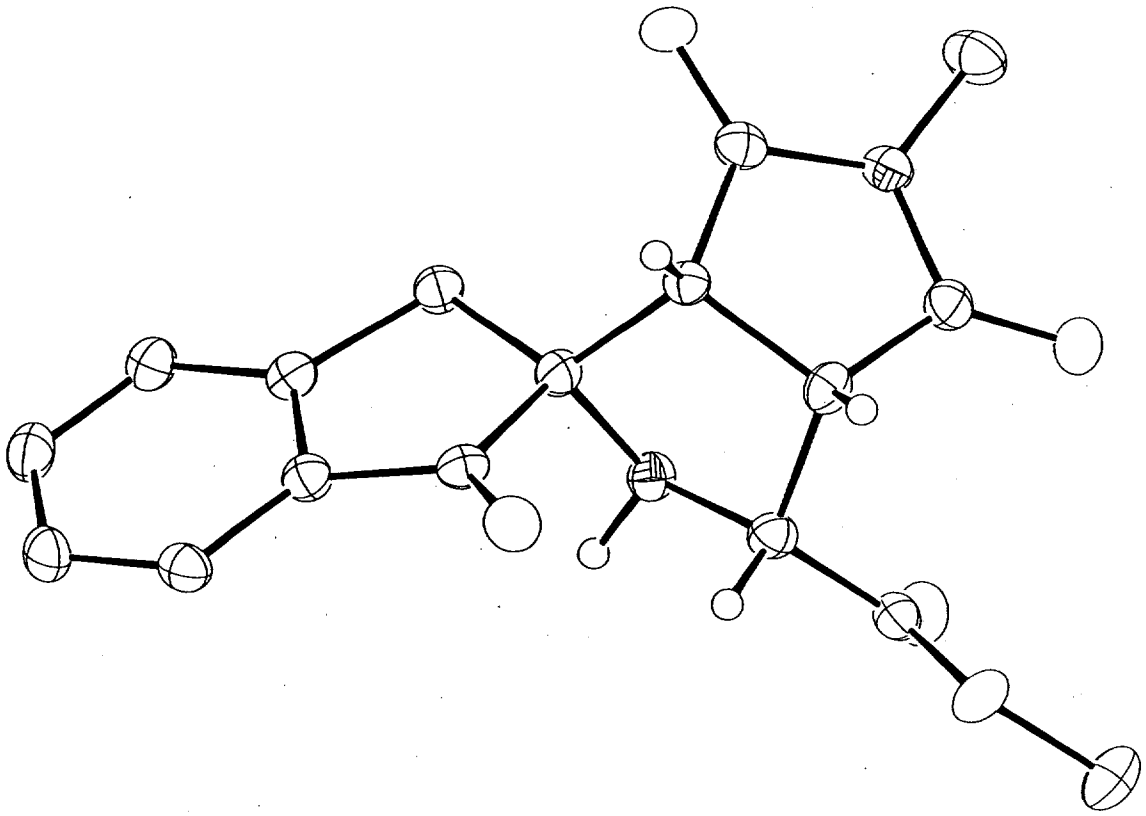

Figure S1. ORTEP drawing of Compound 11 with 30% probability thermal eppisoids.

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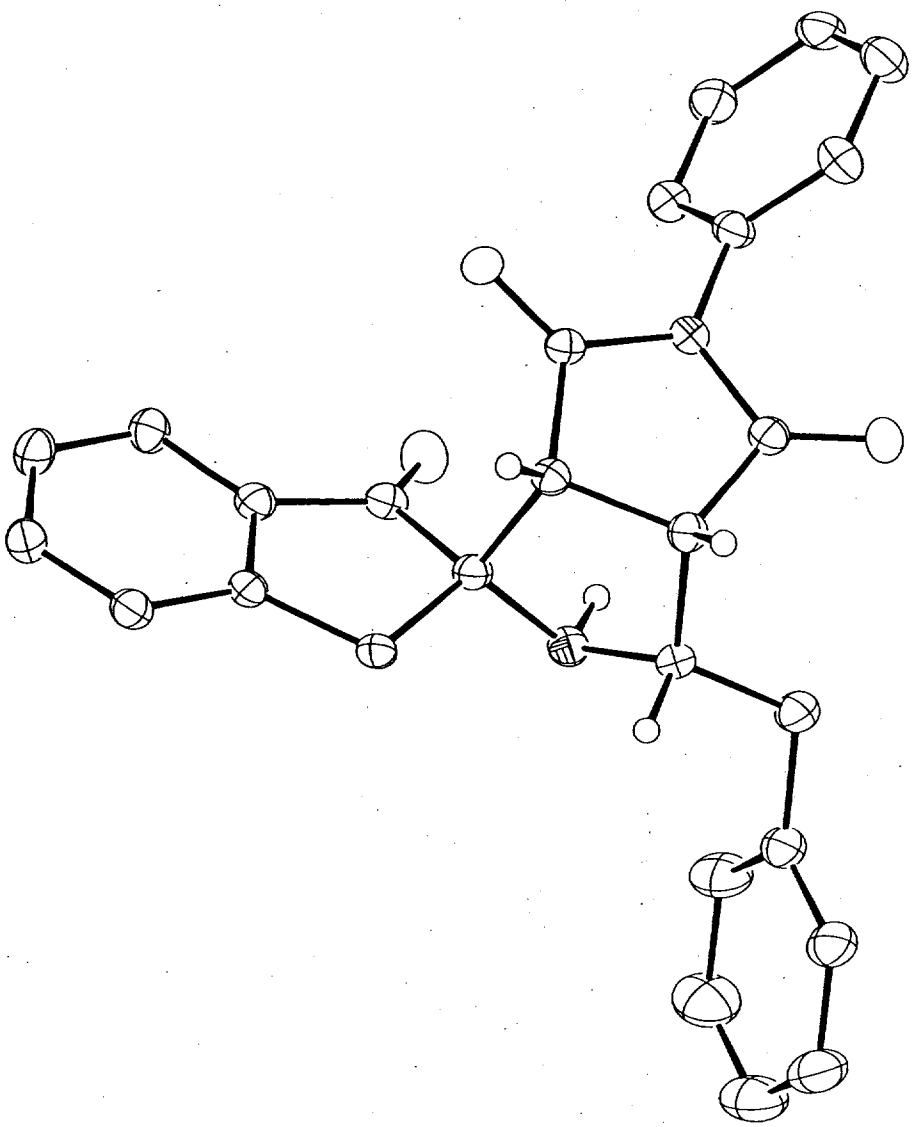

Figure S2. ORTEP drawing of Compound 13 with 30% probability thermal eppisoids.

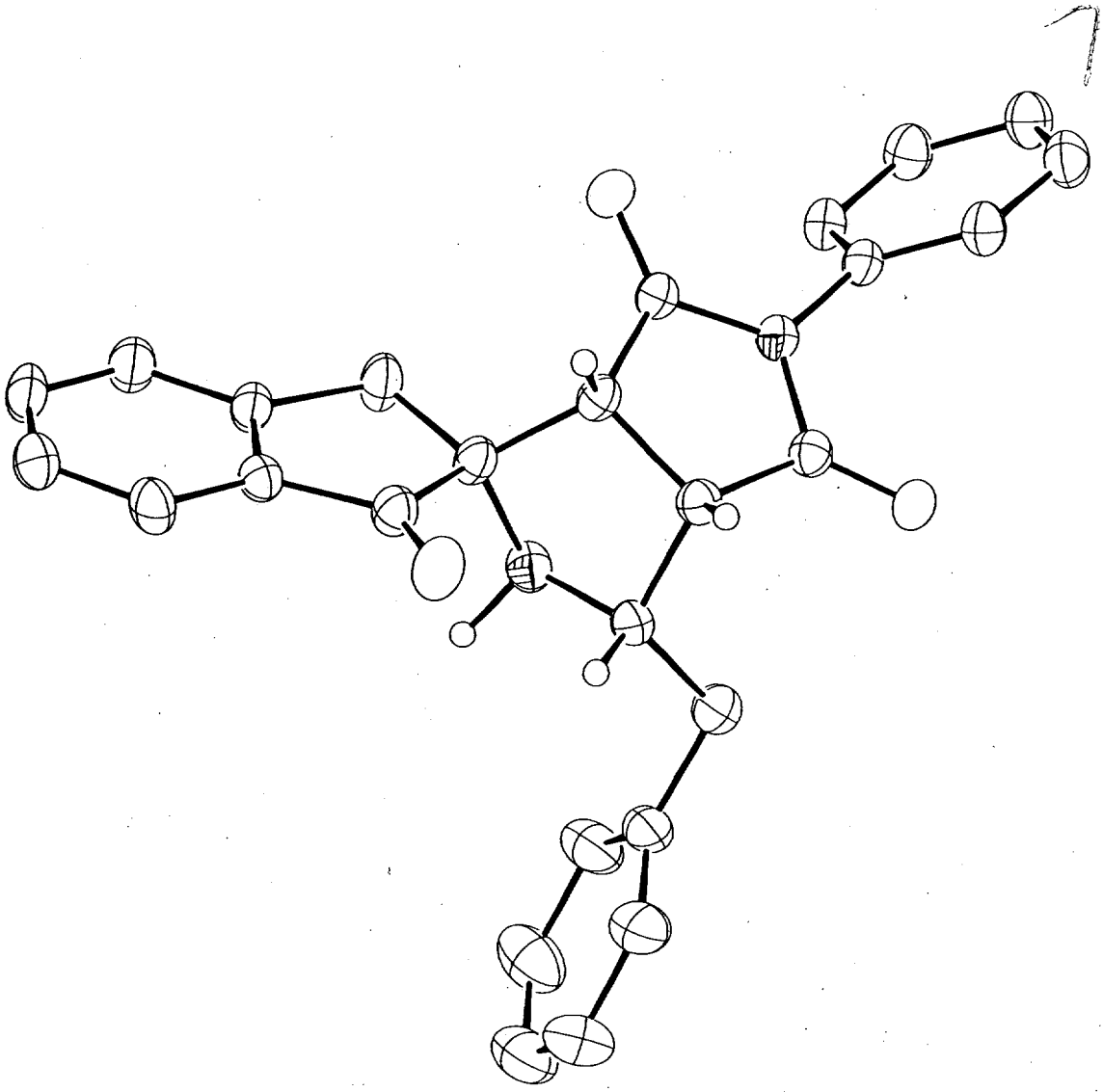

Figure S3. ORTEP drawing of Compound 14 with 30% probability thermal eppisoids.

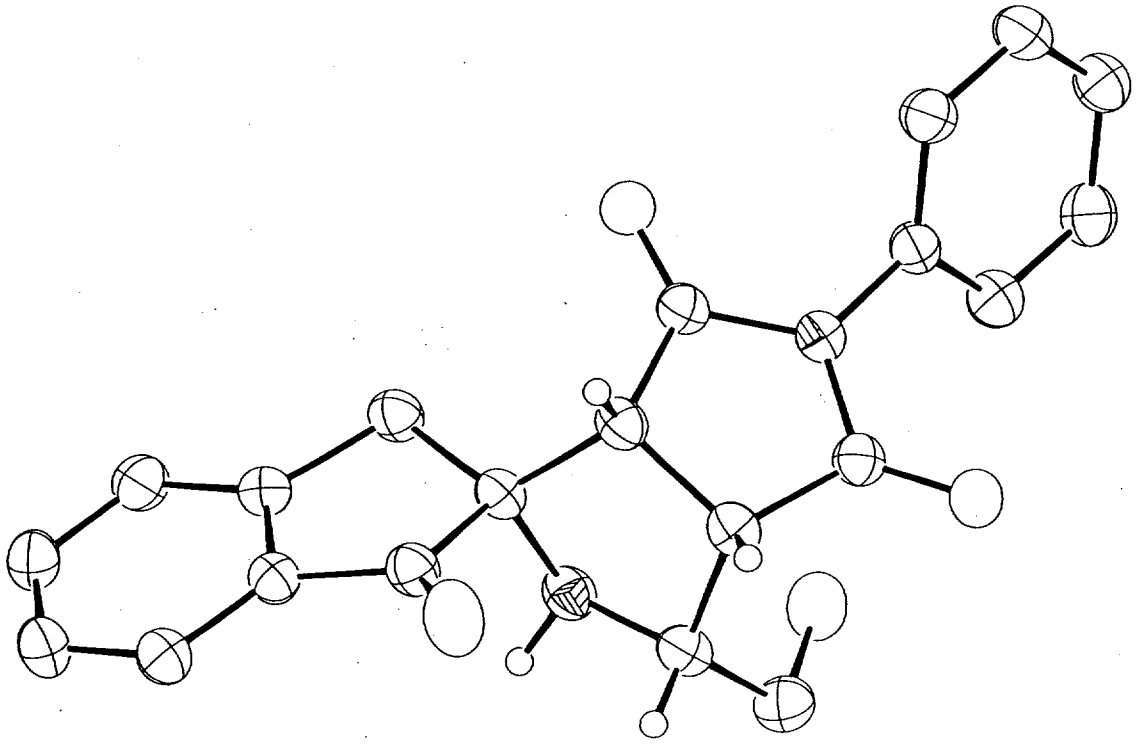

Figure S4. ORTEP drawing of Compound 15 with 30% probability thermal eppisoids.

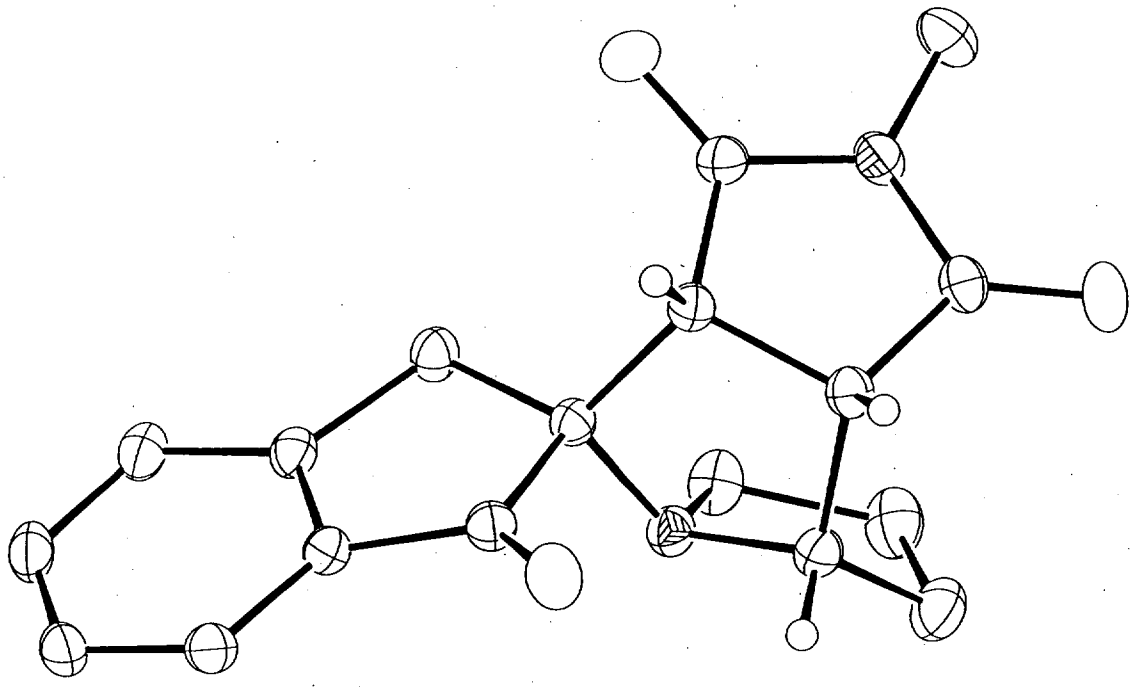

Figure S5. ORTEP drawing of Compound 17 with 30% probability thermal eppisoids.

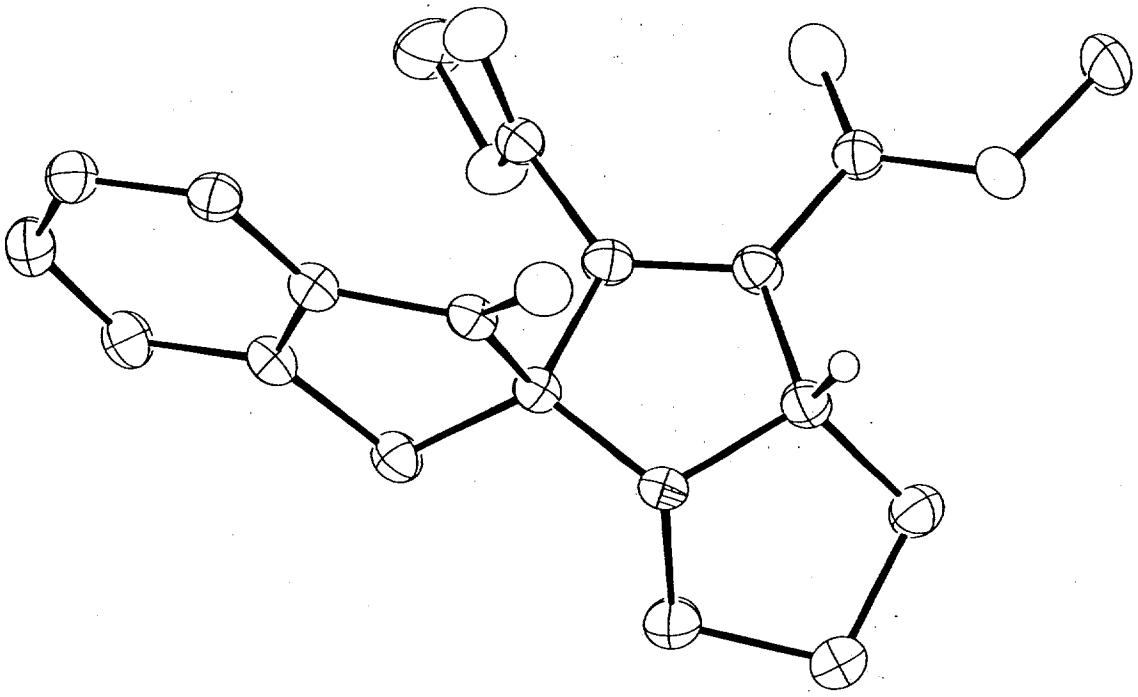

Figure S6. ORTEP drawing of Compound 18 with 30% probability thermal eppisoids.

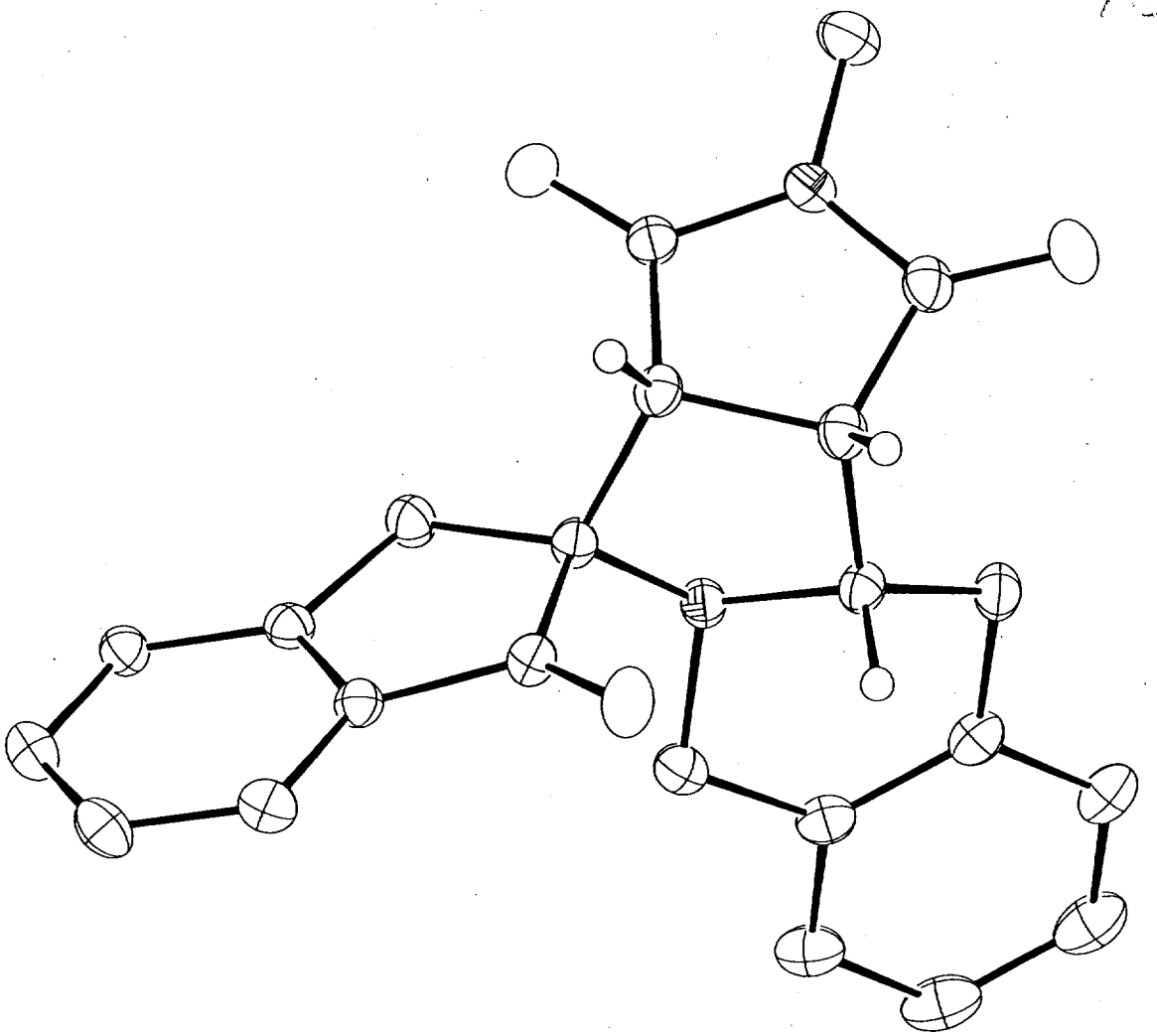

Figure S7. ORTEP drawing of Compound 19 with 30% probability thermal eppisoids.

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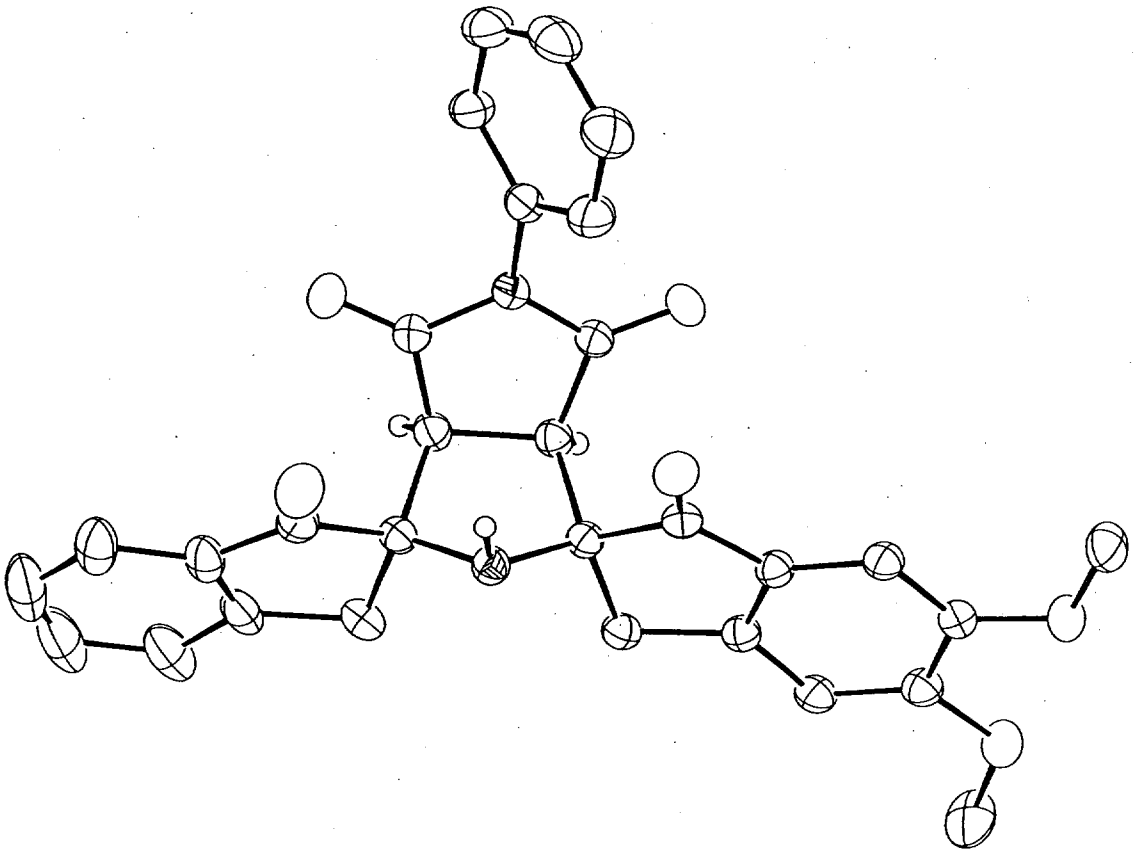

Figure S8. ORTEP drawing of Compound 23 with 30% probability thermal eppisoids.

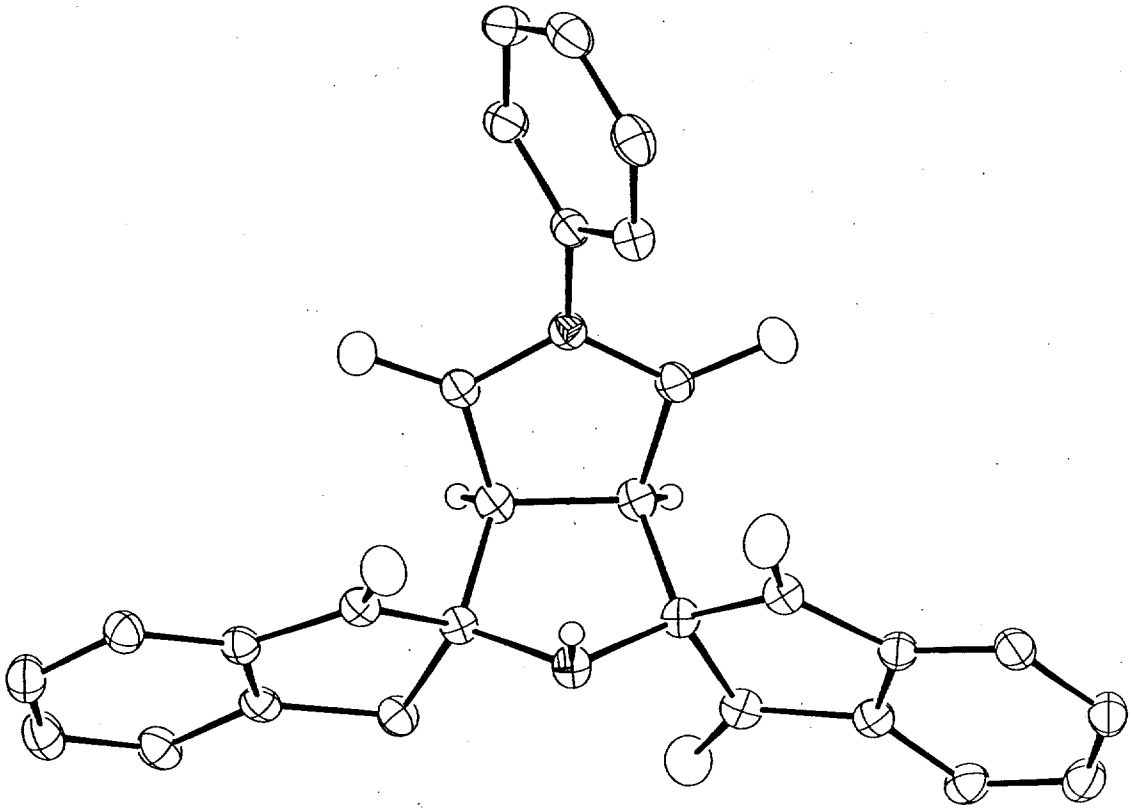

Figure S9. ORTEP drawing of Compound 24 with 30% probability thermal eppisoids.

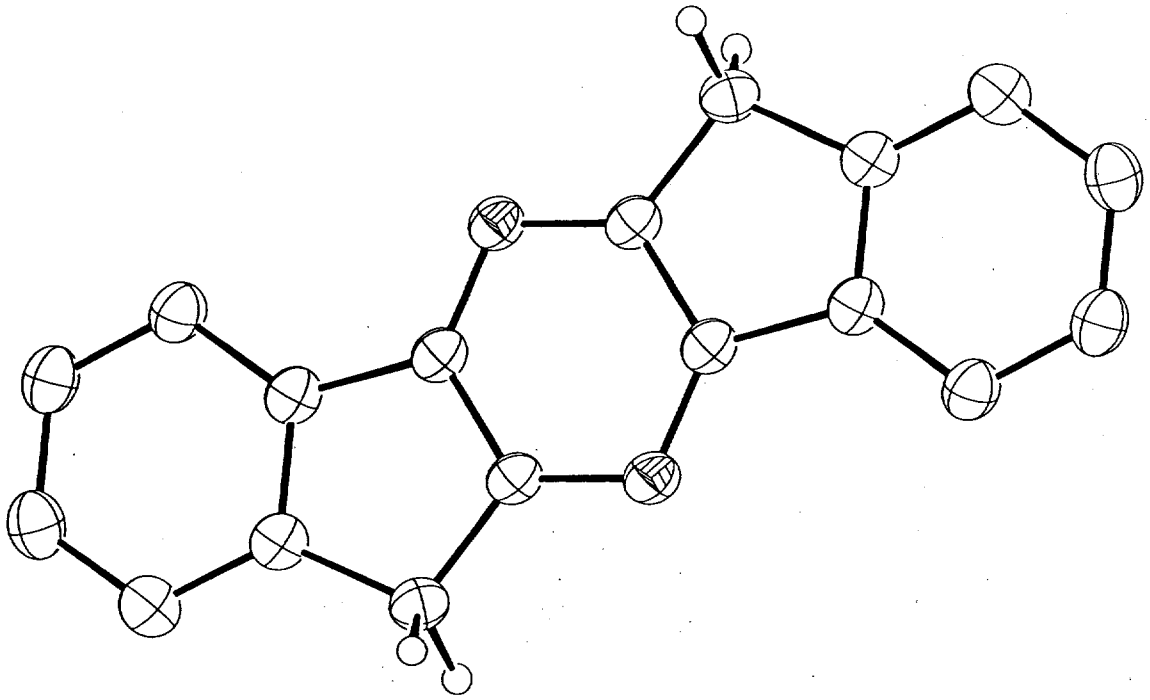

Figure S10. ORTEP drawing of Compound 25 with 30% probability thermal eppisoids.