

ORGANOMETALLICS

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

atom	x	y	z	B_{eq}
Y()	0.16465(3)	-0.20531(3)	-0.18178(5)	3.08(1)
O(1)	0.3553(2)	-0.2147(2)	-0.2641(3)	3.58(6)
O(2)	0.2232(3)	-0.0728(2)	-0.3018(4)	4.84(8)
N(1)	0.2678(3)	-0.3314(2)	-0.1734(4)	3.14(7)
N(2)	0.4766(3)	-0.3179(2)	-0.2358(4)	3.58(8)
C(1)	0.3665(3)	-0.2910(3)	-0.2260(5)	3.20(9)
C(2)	0.5123(4)	-0.3792(3)	-0.1383(6)	4.6(1)
C(3)	0.5659(5)	-0.4590(4)	-0.2389(7)	6.7(2)
C(4)	0.5987(5)	-0.3286(4)	0.0052(7)	6.8(2)
C(5)	0.5728(4)	-0.2706(3)	-0.3165(6)	4.6(1)
C(6)	0.6189(4)	-0.1716(4)	-0.2284(8)	6.5(1)
C(7)	0.5393(5)	-0.2782(4)	-0.4900(7)	6.3(2)
C(8)	0.2381(3)	-0.4259(3)	-0.1784(5)	3.10(9)
C(9)	0.2528(3)	-0.4936(3)	-0.3138(5)	3.8(1)
C(10)	0.2115(4)	-0.5847(3)	-0.3198(6)	4.6(1)
C(11)	0.1545(4)	-0.6098(3)	-0.1930(7)	5.1(1)
C(12)	0.1395(4)	-0.5437(4)	-0.0587(6)	5.0(1)
C(13)	0.1800(4)	-0.4525(3)	-0.0520(5)	4.1(1)
C(14)	0.0023(4)	-0.3500(3)	-0.3257(6)	4.5(1)
C(15)	-0.0645(4)	-0.2847(4)	-0.2432(6)	5.2(1)
C(16)	-0.0507(4)	-0.2116(4)	-0.3203(6)	5.2(1)
C(17)	0.0232(4)	-0.2335(3)	-0.4499(5)	4.6(1)
C(18)	0.0562(4)	-0.3184(3)	-0.4535(5)	4.1(1)
C(19)	0.1306(5)	-0.3695(4)	-0.5746(6)	6.1(1)

Table 1. Atomic coordinates and B_{iso}/B_{eq} (continued)

atom	x	y	z	B_{eq}
C(20)	0.1303(7)	-0.1937(4)	0.1311(6)	6.4(2)
C(21)	0.0636(6)	-0.1347(6)	0.0891(7)	7.7(2)
C(22)	0.136(1)	-0.0642(5)	0.0588(8)	8.6(2)
C(23)	0.2522(8)	-0.0762(6)	0.0828(8)	8.8(2)
C(24)	0.2485(6)	-0.1576(6)	0.1303(6)	7.3(2)
C(25)	0.3646(9)	-0.184(1)	0.177(1)	21.3(5)
C(26)	0.1516(6)	-0.0051(5)	-0.319(1)	12.0(3)
C(27)	0.2068(7)	0.0515(6)	-0.406(1)	13.0(3)
C(28)	0.3223(7)	0.0279(5)	-0.4413(10)	9.8(2)
C(29)	0.3275(6)	-0.0539(5)	-0.378(1)	10.5(3)
H(1)	0.4422	-0.4041	-0.0957	5.4073
H(2)	0.5858	-0.4970	-0.1726	7.9838
H(3)	0.5049	-0.4948	-0.3205	7.9838
H(4)	0.6330	-0.4376	-0.2910	7.9838
H(5)	0.6200	-0.3710	0.0623	8.0726
H(6)	0.6701	-0.2995	-0.0335	8.0726
H(7)	0.5615	-0.2839	0.0736	8.0726
H(8)	0.6394	-0.3024	-0.3159	5.4630
H(9)	0.6401	-0.1686	-0.1191	7.5373
H(10)	0.6880	-0.1487	-0.2792	7.5373
H(11)	0.5580	-0.1353	-0.2340	7.5373
H(12)	0.4698	-0.2510	-0.4978	7.4401
H(13)	0.6043	-0.2468	-0.5370	7.4401
H(14)	0.5244	-0.3405	-0.5459	7.4401

Table 1. Atomic coordinates and B_{iso}/B_{eq} (continued)

atom	x	y	z	B_{eq}
H(15)	0.2926	-0.4770	-0.4033	4.5258
H(16)	0.2222	-0.6299	-0.4127	5.5132
H(17)	0.1255	-0.6727	-0.1983	6.0821
H(18)	0.1019	-0.5609	0.0309	6.0419
H(19)	0.1673	-0.4071	0.0417	4.7819
H(20)	-0.0014	-0.4100	-0.3103	5.3510
H(21)	-0.1215	-0.2943	-0.1663	6.0848
H(22)	-0.0972	-0.1638	-0.3039	6.0962
H(23)	0.0358	-0.2014	-0.5329	5.4019
H(24)	0.0814	-0.4251	-0.6327	7.3080
H(25)	0.1564	-0.3335	-0.6486	7.3080
H(26)	0.1965	-0.3833	-0.5219	7.3080
H(27)	0.1007	-0.2438	0.1762	7.7464
H(28)	-0.0221	-0.1390	0.1016	8.8994
H(29)	0.1116	-0.0093	0.0456	10.4479
H(30)	0.3228	-0.0311	0.0895	10.3513
H(31)	0.3631	-0.2279	0.2044	40.9661
H(32)	0.4167	-0.1726	0.0832	40.9661
H(33)	0.4025	-0.1228	0.2609	40.9661
H(34)	0.0756	-0.0375	-0.3816	14.4116
H(35)	0.1292	0.0261	-0.2183	14.4116
H(36)	0.1611	0.0524	-0.4983	15.4390
H(37)	0.2187	0.1141	-0.3356	15.4390
H(38)	0.3291	0.0134	-0.5591	11.4977

Table 1. Atomic coordinates and B_{iso}/B_{eq} (continued)

atom	x	y	z	B_{eq}
H(39)	0.3865	0.0745	-0.3957	11.4977
H(40)	0.3955	-0.0457	-0.3106	12.7356
H(41)	0.3316	-0.1064	-0.4704	12.7356

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

Table 2. Anisotropic Displacement Parameters

atom	U ₁₁	U ₂₂	U ₃₃	U ₁₂	U ₁₃	U ₂₃
Y()	0.0335(3)	0.0384(3)	0.0462(3)	0.0113(2)	0.0050(2)	0.0083(2)
O(1)	0.037(1)	0.037(2)	0.068(2)	0.012(1)	0.010(1)	0.018(1)
O(2)	0.057(2)	0.050(2)	0.088(2)	0.021(2)	0.023(2)	0.031(2)
N(1)	0.033(2)	0.040(2)	0.048(2)	0.009(2)	0.005(1)	0.010(2)
N(2)	0.032(2)	0.042(2)	0.067(2)	0.013(2)	0.005(2)	0.018(2)
C(1)	0.035(2)	0.038(2)	0.046(2)	0.009(2)	-0.001(2)	0.004(2)
C(2)	0.040(2)	0.061(3)	0.080(3)	0.013(2)	-0.001(2)	0.029(3)
C(3)	0.085(4)	0.061(3)	0.122(5)	0.033(3)	0.004(3)	0.035(3)
C(4)	0.061(3)	0.113(5)	0.085(4)	0.021(3)	-0.019(3)	0.023(4)
C(5)	0.040(2)	0.052(3)	0.093(4)	0.020(2)	0.020(2)	0.026(3)
C(6)	0.050(3)	0.058(3)	0.134(5)	-0.002(3)	0.005(3)	0.024(3)
C(7)	0.083(4)	0.074(4)	0.095(4)	0.034(3)	0.038(3)	0.030(3)
C(8)	0.028(2)	0.041(2)	0.051(2)	0.009(2)	-0.002(2)	0.013(2)
C(9)	0.042(2)	0.045(3)	0.058(3)	0.009(2)	0.003(2)	0.012(2)
C(10)	0.049(3)	0.046(3)	0.076(3)	0.014(2)	-0.013(2)	0.002(2)
C(11)	0.046(3)	0.046(3)	0.108(4)	0.006(2)	-0.010(3)	0.031(3)
C(12)	0.047(3)	0.069(4)	0.089(4)	0.014(3)	0.010(2)	0.044(3)
C(13)	0.044(2)	0.054(3)	0.063(3)	0.015(2)	0.010(2)	0.021(2)
C(14)	0.044(3)	0.054(3)	0.069(3)	-0.005(2)	-0.015(2)	0.016(2)
C(15)	0.031(2)	0.087(4)	0.080(3)	0.001(2)	0.005(2)	0.026(3)
C(16)	0.039(3)	0.080(4)	0.082(3)	0.021(2)	-0.006(2)	0.023(3)
C(17)	0.049(3)	0.072(3)	0.061(3)	0.012(2)	-0.009(2)	0.028(3)
C(18)	0.041(2)	0.061(3)	0.051(3)	0.005(2)	-0.010(2)	0.010(2)
C(19)	0.086(4)	0.090(4)	0.051(3)	0.023(3)	-0.011(3)	0.004(3)

Table 2. Anisotropic Displacement Parameters (continued)

atom	U ₁₁	U ₂₂	U ₃₃	U ₁₂	U ₁₃	U ₂₃
C(20)	0.124(5)	0.070(4)	0.053(3)	0.029(4)	0.028(3)	0.012(3)
C(21)	0.083(4)	0.127(6)	0.072(4)	0.049(5)	0.019(3)	-0.019(4)
C(22)	0.196(9)	0.057(4)	0.076(4)	0.058(5)	0.015(5)	-0.002(3)
C(23)	0.124(6)	0.097(6)	0.070(4)	-0.037(5)	0.015(4)	-0.030(4)
C(24)	0.085(5)	0.135(6)	0.051(3)	0.057(5)	-0.016(3)	-0.018(4)
C(25)	0.194(10)	0.46(2)	0.126(7)	0.21(1)	-0.080(7)	-0.094(9)
C(26)	0.110(5)	0.115(6)	0.30(1)	0.083(5)	0.098(6)	0.135(7)
C(27)	0.119(6)	0.168(8)	0.29(1)	0.079(6)	0.079(7)	0.174(9)
C(28)	0.119(6)	0.112(6)	0.182(7)	0.042(5)	0.045(5)	0.097(6)
C(29)	0.101(5)	0.139(6)	0.221(8)	0.062(5)	0.086(5)	0.135(6)

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
Y	O(1)	2.285(2)	Y	O(2)	2.473(3)
Y	N(1)	2.401(3)	Y	C(1)	2.776(4)
Y	C(14)	2.673(4)	Y	C(15)	2.666(4)
Y	C(16)	2.657(4)	Y	C(17)	2.673(4)
Y	C(18)	2.689(4)	Y	C(20)	2.668(5)
Y	C(21)	2.662(5)	Y	C(22)	2.667(6)
Y	C(23)	2.683(6)	Y	C(24)	2.701(5)
O(1)	C(1)	1.297(4)	O(2)	C(26)	1.432(6)
O(2)	C(29)	1.374(6)	N(1)	C(1)	1.323(5)
N(1)	C(8)	1.416(5)	N(2)	C(1)	1.362(5)
N(2)	C(2)	1.475(5)	N(2)	C(5)	1.477(5)
C(2)	C(3)	1.527(7)	C(2)	C(4)	1.526(7)
C(5)	C(6)	1.525(7)	C(5)	C(7)	1.493(7)
C(8)	C(9)	1.388(5)	C(8)	C(13)	1.378(5)
C(9)	C(10)	1.382(6)	C(10)	C(11)	1.365(7)
C(11)	C(12)	1.368(7)	C(12)	C(13)	1.380(6)
C(14)	C(15)	1.403(6)	C(14)	C(18)	1.400(6)
C(15)	C(16)	1.407(7)	C(16)	C(17)	1.402(6)
C(17)	C(18)	1.390(6)	C(18)	C(19)	1.492(7)
C(20)	C(21)	1.355(8)	C(20)	C(24)	1.361(8)
C(21)	C(22)	1.324(9)	C(22)	C(23)	1.366(10)
C(23)	C(24)	1.384(10)	C(24)	C(25)	1.494(10)
C(26)	C(27)	1.345(9)	C(27)	C(28)	1.421(9)
C(28)	C(29)	1.474(8)			

Table 4. Bond Lengths($\text{\AA}$)

atom	atom	distance	atom	atom	distance
C(2)	H(1)	0.94	C(3)	H(2)	0.94
C(3)	H(3)	0.97	C(3)	H(4)	0.94
C(4)	H(5)	0.95	C(4)	H(6)	0.96
C(4)	H(7)	0.94	C(5)	H(8)	0.95
C(6)	H(9)	0.95	C(6)	H(10)	0.95
C(6)	H(11)	0.95	C(7)	H(12)	0.95
C(7)	H(13)	0.96	C(7)	H(14)	0.95
C(9)	H(15)	0.95	C(10)	H(16)	0.94
C(11)	H(17)	0.95	C(12)	H(18)	0.95
C(13)	H(19)	0.96	C(14)	H(20)	0.95
C(15)	H(21)	0.94	C(16)	H(22)	0.94
C(17)	H(23)	0.95	C(19)	H(24)	0.96
C(19)	H(25)	0.95	C(19)	H(26)	0.94
C(20)	H(27)	0.95	C(21)	H(28)	0.97
C(22)	H(29)	0.95	C(23)	H(30)	0.96
C(25)	H(31)	0.76	C(25)	H(32)	1.03
C(25)	H(33)	1.06	C(26)	H(34)	1.00
C(26)	H(35)	0.94	C(27)	H(36)	0.94
C(27)	H(37)	0.99	C(28)	H(38)	0.98
C(28)	H(39)	0.94	C(29)	H(40)	0.92
C(29)	H(41)	0.99			

Table 5. Bond Angles(°)

atom	atom	atom	angle	atom	atom	atom	angle
O(1)	Y	O(2)	74.18(9)	O(1)	Y	N(1)	55.96(9)
O(1)	Y	C(1)	27.58(10)	O(1)	Y	C(14)	113.6(1)
O(1)	Y	C(15)	143.4(1)	O(1)	Y	C(16)	136.8(1)
O(1)	Y	C(17)	106.5(1)	O(1)	Y	C(18)	94.7(1)
O(1)	Y	C(20)	117.1(2)	O(1)	Y	C(21)	136.8(2)
O(1)	Y	C(22)	117.4(3)	O(1)	Y	C(23)	90.4(2)
O(1)	Y	C(24)	90.4(2)	O(2)	Y	N(1)	129.80(10)
O(2)	Y	C(1)	101.7(1)	O(2)	Y	C(14)	122.8(1)
O(2)	Y	C(15)	114.9(1)	O(2)	Y	C(16)	84.2(1)
O(2)	Y	C(17)	73.2(1)	O(2)	Y	C(18)	95.9(1)
O(2)	Y	C(20)	124.7(1)	O(2)	Y	C(21)	103.8(2)
O(2)	Y	C(22)	77.5(2)	O(2)	Y	C(23)	79.4(2)
O(2)	Y	C(24)	108.1(2)	N(1)	Y	C(1)	28.4(1)
N(1)	Y	C(14)	77.5(1)	N(1)	Y	C(15)	103.1(1)
N(1)	Y	C(16)	127.7(1)	N(1)	Y	C(17)	113.2(1)
N(1)	Y	C(18)	83.6(1)	N(1)	Y	C(20)	86.6(2)
N(1)	Y	C(21)	115.7(2)	N(1)	Y	C(22)	128.5(2)
N(1)	Y	C(23)	104.4(3)	N(1)	Y	C(24)	79.8(2)
C(1)	Y	C(14)	97.4(1)	C(1)	Y	C(15)	126.9(1)
C(1)	Y	C(16)	140.9(1)	C(1)	Y	C(17)	113.9(1)
C(1)	Y	C(18)	90.6(1)	C(1)	Y	C(20)	102.0(2)
C(1)	Y	C(21)	130.1(2)	C(1)	Y	C(22)	126.3(2)
C(1)	Y	C(23)	96.8(3)	C(1)	Y	C(24)	83.1(1)
C(14)	Y	C(15)	30.5(1)	C(14)	Y	C(16)	50.3(1)

Table 5. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C(14)	Y	C(17)	49.8(1)	C(14)	Y	C(18)	30.3(1)
C(14)	Y	C(20)	102.5(2)	C(14)	Y	C(21)	103.6(2)
C(14)	Y	C(22)	128.7(3)	C(14)	Y	C(23)	150.1(2)
C(14)	Y	C(24)	127.6(2)	C(15)	Y	C(16)	30.6(1)
C(15)	Y	C(17)	50.2(1)	C(15)	Y	C(18)	50.3(1)
C(15)	Y	C(20)	87.8(2)	C(15)	Y	C(21)	77.7(2)
C(15)	Y	C(22)	99.2(3)	C(15)	Y	C(23)	125.7(2)
C(15)	Y	C(24)	117.2(2)	C(16)	Y	C(17)	30.5(1)
C(16)	Y	C(18)	50.3(1)	C(16)	Y	C(20)	106.0(2)
C(16)	Y	C(21)	84.1(2)	C(16)	Y	C(22)	92.8(3)
C(16)	Y	C(23)	122.2(3)	C(16)	Y	C(24)	132.3(2)
C(17)	Y	C(18)	30.1(1)	C(17)	Y	C(20)	135.7(2)
C(17)	Y	C(21)	114.2(2)	C(17)	Y	C(22)	116.8(2)
C(17)	Y	C(23)	142.1(3)	C(17)	Y	C(24)	162.6(2)
C(18)	Y	C(20)	132.8(2)	C(18)	Y	C(21)	127.9(2)
C(18)	Y	C(22)	143.1(2)	C(18)	Y	C(23)	172.0(3)
C(18)	Y	C(24)	155.9(2)	C(20)	Y	C(21)	29.5(2)
C(20)	Y	C(22)	48.4(2)	C(20)	Y	C(23)	48.7(2)
C(20)	Y	C(24)	29.4(2)	C(21)	Y	C(22)	28.8(2)
C(21)	Y	C(23)	48.2(2)	C(21)	Y	C(24)	48.4(2)
C(22)	Y	C(23)	29.6(2)	C(22)	Y	C(24)	48.8(2)
C(23)	Y	C(24)	29.8(2)	Y	O(1)	C(1)	97.8(2)
Y	O(2)	C(26)	127.2(3)	Y	O(2)	C(29)	126.5(3)
C(26)	O(2)	C(29)	106.1(4)	Y	N(1)	C(1)	91.7(2)

Table 5. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
Y	N(1)	C(8)	138.0(2)	C(1)	N(1)	C(8)	126.2(3)
C(1)	N(2)	C(2)	121.7(3)	C(1)	N(2)	C(5)	119.9(3)
C(2)	N(2)	C(5)	117.1(3)	Y	C(1)	O(1)	54.6(2)
Y	C(1)	N(1)	59.8(2)	Y	C(1)	N(2)	169.8(3)
O(1)	C(1)	N(1)	114.3(3)	O(1)	C(1)	N(2)	118.1(3)
N(1)	C(1)	N(2)	127.5(4)	N(2)	C(2)	C(3)	112.6(4)
N(2)	C(2)	C(4)	112.8(4)	C(3)	C(2)	C(4)	109.8(4)
N(2)	C(5)	C(6)	114.5(4)	N(2)	C(5)	C(7)	112.2(4)
C(6)	C(5)	C(7)	111.4(4)	N(1)	C(8)	C(9)	122.6(3)
N(1)	C(8)	C(13)	119.2(4)	C(9)	C(8)	C(13)	117.8(4)
C(8)	C(9)	C(10)	120.8(4)	C(9)	C(10)	C(11)	120.5(4)
C(10)	C(11)	C(12)	119.3(4)	C(11)	C(12)	C(13)	120.5(4)
C(8)	C(13)	C(12)	121.1(4)	Y	C(14)	C(15)	74.5(3)
Y	C(14)	C(18)	75.5(2)	C(15)	C(14)	C(18)	108.7(4)
Y	C(15)	C(14)	75.0(2)	Y	C(15)	C(16)	74.3(2)
C(14)	C(15)	C(16)	107.4(4)	Y	C(16)	C(15)	75.0(2)
Y	C(16)	C(17)	75.4(2)	C(15)	C(16)	C(17)	107.6(4)
Y	C(17)	C(16)	74.1(2)	Y	C(17)	C(18)	75.6(2)
C(16)	C(17)	C(18)	108.9(4)	Y	C(18)	C(14)	74.2(2)
Y	C(18)	C(17)	74.4(3)	Y	C(18)	C(19)	119.3(3)
C(14)	C(18)	C(17)	107.4(4)	C(14)	C(18)	C(19)	125.6(4)
C(17)	C(18)	C(19)	126.9(4)	Y	C(20)	C(21)	75.0(3)
Y	C(20)	C(24)	76.7(3)	C(21)	C(20)	C(24)	108.0(6)
Y	C(21)	C(20)	75.5(3)	Y	C(21)	C(22)	75.8(4)

Table 5. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C(20)	C(21)	C(22)	109.4(6)	Y	C(22)	C(21)	75.4(4)
Y	C(22)	C(23)	75.9(4)	C(21)	C(22)	C(23)	108.3(7)
Y	C(23)	C(22)	74.6(4)	Y	C(23)	C(24)	75.8(3)
C(22)	C(23)	C(24)	107.4(6)	Y	C(24)	C(20)	74.0(3)
Y	C(24)	C(23)	74.4(3)	Y	C(24)	C(25)	120.0(4)
C(20)	C(24)	C(23)	106.9(6)	C(20)	C(24)	C(25)	134(1)
C(23)	C(24)	C(25)	118(1)	O(2)	C(26)	C(27)	111.2(5)
C(26)	C(27)	C(28)	108.5(6)	C(27)	C(28)	C(29)	105.3(6)
O(2)	C(29)	C(28)	108.8(5)				

Table 6. Bond Angles(°)

atom	atom	atom	angle	atom	atom	atom	angle
N(2)	C(2)	H(1)	107.1	C(3)	C(2)	H(1)	107.3
C(4)	C(2)	H(1)	106.9	C(2)	C(3)	H(2)	109.8
C(2)	C(3)	H(3)	108.1	C(2)	C(3)	H(4)	110.7
H(2)	C(3)	H(3)	108.2	H(2)	C(3)	H(4)	111.3
H(3)	C(3)	H(4)	108.6	C(2)	C(4)	H(5)	109.4
C(2)	C(4)	H(6)	109.3	C(2)	C(4)	H(7)	109.5
H(5)	C(4)	H(6)	108.9	H(5)	C(4)	H(7)	110.3
H(6)	C(4)	H(7)	109.4	N(2)	C(5)	H(8)	106.1
C(6)	C(5)	H(8)	105.8	C(7)	C(5)	H(8)	106.1
C(5)	C(6)	H(9)	109.8	C(5)	C(6)	H(10)	109.4
C(5)	C(6)	H(11)	109.5	H(9)	C(6)	H(10)	109.4
H(9)	C(6)	H(11)	109.8	H(10)	C(6)	H(11)	109.0
C(5)	C(7)	H(12)	109.6	C(5)	C(7)	H(13)	109.2
C(5)	C(7)	H(14)	109.7	H(12)	C(7)	H(13)	109.1
H(12)	C(7)	H(14)	110.1	H(13)	C(7)	H(14)	109.2
C(8)	C(9)	H(15)	119.5	C(10)	C(9)	H(15)	119.7
C(9)	C(10)	H(16)	119.7	C(11)	C(10)	H(16)	119.8
C(10)	C(11)	H(17)	120.1	C(12)	C(11)	H(17)	120.6
C(11)	C(12)	H(18)	119.7	C(13)	C(12)	H(18)	119.8
C(8)	C(13)	H(19)	119.4	C(12)	C(13)	H(19)	119.6
Y	C(14)	H(20)	125.5	C(15)	C(14)	H(20)	125.0
C(18)	C(14)	H(20)	125.3	Y	C(15)	H(21)	126.6
C(14)	C(15)	H(21)	125.4	C(16)	C(15)	H(21)	125.9
Y	C(16)	H(22)	126.4	C(15)	C(16)	H(22)	125.6

Table 6. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C(17)	C(16)	H(22)	125.3	Y	C(17)	H(23)	125.6
C(16)	C(17)	H(23)	125.0	C(18)	C(17)	H(23)	125.1
C(18)	C(19)	H(24)	108.4	C(18)	C(19)	H(25)	109.2
C(18)	C(19)	H(26)	109.8	H(24)	C(19)	H(25)	108.8
H(24)	C(19)	H(26)	109.7	H(25)	C(19)	H(26)	110.9
Y	C(20)	H(27)	124.9	C(21)	C(20)	H(27)	125.8
C(24)	C(20)	H(27)	124.9	Y	C(21)	H(28)	124.8
C(20)	C(21)	H(28)	123.3	C(22)	C(21)	H(28)	126.2
Y	C(22)	H(29)	125.0	C(21)	C(22)	H(29)	125.0
C(23)	C(22)	H(29)	125.4	Y	C(23)	H(30)	125.8
C(22)	C(23)	H(30)	126.4	C(24)	C(23)	H(30)	124.9
C(24)	C(25)	H(31)	118.8	C(24)	C(25)	H(32)	101.8
C(24)	C(25)	H(33)	100.1	H(31)	C(25)	H(32)	119.8
H(31)	C(25)	H(33)	116.1	H(32)	C(25)	H(33)	96.1
O(2)	C(26)	H(34)	107.7	O(2)	C(26)	H(35)	111.1
C(27)	C(26)	H(34)	107.0	C(27)	C(26)	H(35)	113.0
H(34)	C(26)	H(35)	106.4	C(26)	C(27)	H(36)	113.3
C(26)	C(27)	H(37)	107.4	C(28)	C(27)	H(36)	112.6
C(28)	C(27)	H(37)	107.6	H(36)	C(27)	H(37)	107.1
C(27)	C(28)	H(38)	109.0	C(27)	C(28)	H(39)	114.0
C(29)	C(28)	H(38)	110.6	C(29)	C(28)	H(39)	110.4
H(38)	C(28)	H(39)	107.5	O(2)	C(29)	H(40)	112.6
O(2)	C(29)	H(41)	108.1	C(28)	C(29)	H(40)	110.9
C(28)	C(29)	H(41)	108.2	H(40)	C(29)	H(41)	108.1

Table 6. Bond Angles($^{\circ}$) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
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Table 7. Torsion Angles(°)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
Y	O(1)	C(1)	N(1)	5.1(3)	Y	O(1)	C(1)	N(2)	-171.6(3)
Y	O(2)	C(26)	C(27)	-173.3(6)	Y	O(2)	C(29)	C(28)	176.0(4)
Y	N(1)	C(1)	O(1)	-4.8(3)	Y	N(1)	C(1)	N(2)	171.5(4)
Y	N(1)	C(8)	C(9)	105.8(4)	Y	N(1)	C(8)	C(13)	-66.9(5)
Y	C(1)	N(1)	C(8)	160.6(4)	Y	C(1)	N(2)	C(2)	112(1)
Y	C(1)	N(2)	C(5)	-53(1)	Y	C(14)	C(15)	C(16)	67.9(3)
Y	C(14)	C(18)	C(17)	-67.5(3)	Y	C(14)	C(18)	C(19)	115.0(4)
Y	C(15)	C(14)	C(18)	-68.4(3)	Y	C(15)	C(16)	C(17)	69.0(3)
Y	C(16)	C(15)	C(14)	-68.4(3)	Y	C(16)	C(17)	C(18)	68.2(3)
Y	C(17)	C(16)	C(15)	-68.7(3)	Y	C(17)	C(18)	C(14)	67.4(3)
Y	C(17)	C(18)	C(19)	-115.1(4)	Y	C(18)	C(14)	C(15)	67.7(3)
Y	C(18)	C(17)	C(16)	-67.2(3)	Y	C(20)	C(21)	C(22)	-68.9(5)
Y	C(20)	C(24)	C(23)	67.6(4)	Y	C(20)	C(24)	C(25)	-116.5(8)
Y	C(21)	C(20)	C(24)	70.3(4)	Y	C(21)	C(22)	C(23)	-69.4(5)
Y	C(22)	C(21)	C(20)	68.8(4)	Y	C(22)	C(23)	C(24)	-69.4(4)
Y	C(23)	C(22)	C(21)	69.1(5)	Y	C(23)	C(24)	C(20)	-67.4(4)
Y	C(23)	C(24)	C(25)	116.0(6)	Y	C(24)	C(20)	C(21)	-69.1(4)
Y	C(24)	C(23)	C(22)	68.5(4)	O(1)	Y	O(2)	C(26)	178.8(6)
O(1)	Y	O(2)	C(29)	4.9(5)	O(1)	Y	N(1)	C(1)	3.0(2)
O(1)	Y	N(1)	C(8)	-153.3(4)	O(1)	Y	C(1)	N(1)	-174.6(4)
O(1)	Y	C(1)	N(2)	46(1)	O(1)	Y	C(14)	C(15)	-169.7(3)
O(1)	Y	C(14)	C(18)	-55.1(3)	O(1)	Y	C(15)	C(14)	16.0(4)
O(1)	Y	C(15)	C(16)	-97.3(3)	O(1)	Y	C(16)	C(15)	120.1(3)
O(1)	Y	C(16)	C(17)	7.0(4)	O(1)	Y	C(17)	C(16)	-175.0(3)

Table 7. Torsion Angles(°) (continued)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
O(1)	Y	C(17)	C(18)	70.1(3)	O(1)	Y	C(18)	C(14)	131.1(3)
O(1)	Y	C(18)	C(17)	-115.2(3)	O(1)	Y	C(18)	C(19)	8.7(4)
O(1)	Y	C(20)	C(21)	139.5(5)	O(1)	Y	C(20)	C(24)	26.4(5)
O(1)	Y	C(21)	C(20)	-57.7(6)	O(1)	Y	C(21)	C(22)	57.1(7)
O(1)	Y	C(22)	C(21)	-139.7(5)	O(1)	Y	C(22)	C(23)	-26.1(6)
O(1)	Y	C(23)	C(22)	157.0(6)	O(1)	Y	C(23)	C(24)	-90.1(5)
O(1)	Y	C(24)	C(20)	-156.7(4)	O(1)	Y	C(24)	C(23)	90.1(5)
O(1)	Y	C(24)	C(25)	-23.8(9)	O(1)	C(1)	Y	O(2)	2.9(2)
O(1)	C(1)	Y	N(1)	174.6(4)	O(1)	C(1)	Y	C(14)	128.7(2)
O(1)	C(1)	Y	C(15)	136.8(2)	O(1)	C(1)	Y	C(16)	98.2(3)
O(1)	C(1)	Y	C(17)	79.6(2)	O(1)	C(1)	Y	C(18)	99.1(2)
O(1)	C(1)	Y	C(20)	-126.8(2)	O(1)	C(1)	Y	C(21)	-116.6(3)
O(1)	C(1)	Y	C(22)	-80.0(3)	O(1)	C(1)	Y	C(23)	-77.6(3)
O(1)	C(1)	Y	C(24)	-104.2(3)	O(1)	C(1)	N(1)	C(8)	155.7(3)
O(1)	C(1)	N(2)	C(2)	155.1(4)	O(1)	C(1)	N(2)	C(5)	-11.3(5)
O(2)	Y	O(1)	C(1)	-177.0(2)	O(2)	Y	N(1)	C(1)	10.6(3)
O(2)	Y	N(1)	C(8)	-145.7(3)	O(2)	Y	C(1)	N(1)	-171.7(2)
O(2)	Y	C(1)	N(2)	49(1)	O(2)	Y	C(14)	C(15)	-83.8(3)
O(2)	Y	C(14)	C(18)	30.8(3)	O(2)	Y	C(15)	C(14)	112.9(3)
O(2)	Y	C(15)	C(16)	-0.5(3)	O(2)	Y	C(16)	C(15)	179.6(3)
O(2)	Y	C(16)	C(17)	66.5(3)	O(2)	Y	C(17)	C(16)	-107.7(3)
O(2)	Y	C(17)	C(18)	137.4(3)	O(2)	Y	C(18)	C(14)	-154.4(3)
O(2)	Y	C(18)	C(17)	-40.7(3)	O(2)	Y	C(18)	C(19)	83.3(4)
O(2)	Y	C(20)	C(21)	50.5(6)	O(2)	Y	C(20)	C(24)	-62.5(5)

Table 7. Torsion Angles($^{\circ}$) (continued)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
O(2)	Y	C(21)	C(20)	-139.2(5)	O(2)	Y	C(21)	C(22)	-24.4(6)
O(2)	Y	C(22)	C(21)	155.7(6)	O(2)	Y	C(22)	C(23)	-90.6(6)
O(2)	Y	C(23)	C(22)	83.2(6)	O(2)	Y	C(23)	C(24)	-163.9(5)
O(2)	Y	C(24)	C(20)	129.9(4)	O(2)	Y	C(24)	C(23)	16.7(5)
O(2)	Y	C(24)	C(25)	-97.3(9)	O(2)	C(26)	C(27)	C(28)	-3(1)
O(2)	C(29)	C(28)	C(27)	-3(1)	N(1)	Y	O(1)	C(1)	-3.1(2)
N(1)	Y	O(2)	C(26)	172.2(6)	N(1)	Y	O(2)	C(29)	-1.7(6)
N(1)	Y	C(1)	N(2)	-138(1)	N(1)	Y	C(14)	C(15)	146.6(3)
N(1)	Y	C(14)	C(18)	-98.8(3)	N(1)	Y	C(15)	C(14)	-33.5(3)
N(1)	Y	C(15)	C(16)	-146.8(3)	N(1)	Y	C(16)	C(15)	42.3(4)
N(1)	Y	C(16)	C(17)	-70.8(3)	N(1)	Y	C(17)	C(16)	125.5(3)
N(1)	Y	C(17)	C(18)	10.7(3)	N(1)	Y	C(18)	C(14)	76.1(3)
N(1)	Y	C(18)	C(17)	-170.2(3)	N(1)	Y	C(18)	C(19)	-46.2(4)
N(1)	Y	C(20)	C(21)	-171.9(5)	N(1)	Y	C(20)	C(24)	75.1(4)
N(1)	Y	C(21)	C(20)	9.0(5)	N(1)	Y	C(21)	C(22)	123.8(6)
N(1)	Y	C(22)	C(21)	-72.9(7)	N(1)	Y	C(22)	C(23)	40.8(7)
N(1)	Y	C(23)	C(22)	-148.2(6)	N(1)	Y	C(23)	C(24)	-35.3(5)
N(1)	Y	C(24)	C(20)	-101.4(4)	N(1)	Y	C(24)	C(23)	145.4(5)
N(1)	Y	C(24)	C(25)	31.4(9)	N(1)	C(1)	Y	C(14)	-45.9(2)
N(1)	C(1)	Y	C(15)	-37.8(3)	N(1)	C(1)	Y	C(16)	-76.4(3)
N(1)	C(1)	Y	C(17)	-95.0(2)	N(1)	C(1)	Y	C(18)	-75.5(2)
N(1)	C(1)	Y	C(20)	58.6(3)	N(1)	C(1)	Y	C(21)	68.8(3)
N(1)	C(1)	Y	C(22)	105.4(3)	N(1)	C(1)	Y	C(23)	107.8(3)
N(1)	C(1)	Y	C(24)	81.2(3)	N(1)	C(1)	N(2)	C(2)	-21.1(6)

Table 7. Torsion Angles(°) (continued)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
N(1)	C(1)	N(2)	C(5)	172.5(4)	N(1)	C(8)	C(9)	C(10)	-173.4(4)
N(1)	C(8)	C(13)	C(12)	174.0(4)	N(2)	C(1)	Y	C(14)	175(1)
N(2)	C(1)	Y	C(15)	-176(1)	N(2)	C(1)	Y	C(16)	145(1)
N(2)	C(1)	Y	C(17)	126(1)	N(2)	C(1)	Y	C(18)	145(1)
N(2)	C(1)	Y	C(20)	-79(1)	N(2)	C(1)	Y	C(21)	-69(1)
N(2)	C(1)	Y	C(22)	-33(1)	N(2)	C(1)	Y	C(23)	-30(1)
N(2)	C(1)	Y	C(24)	-57(1)	N(2)	C(1)	N(1)	C(8)	-27.9(6)
C(1)	Y	O(2)	C(26)	177.4(6)	C(1)	Y	O(2)	C(29)	3.4(6)
C(1)	Y	N(1)	C(8)	-156.4(5)	C(1)	Y	C(14)	C(15)	167.1(3)
C(1)	Y	C(14)	C(18)	-78.3(3)	C(1)	Y	C(15)	C(14)	-16.1(3)
C(1)	Y	C(15)	C(16)	-129.4(3)	C(1)	Y	C(16)	C(15)	78.1(4)
C(1)	Y	C(16)	C(17)	-35.0(4)	C(1)	Y	C(17)	C(16)	156.6(3)
C(1)	Y	C(17)	C(18)	41.8(3)	C(1)	Y	C(18)	C(14)	103.8(3)
C(1)	Y	C(18)	C(17)	-142.5(3)	C(1)	Y	C(18)	C(19)	-18.6(4)
C(1)	Y	C(20)	C(21)	164.1(5)	C(1)	Y	C(20)	C(24)	51.1(4)
C(1)	Y	C(21)	C(20)	-20.5(6)	C(1)	Y	C(21)	C(22)	94.3(6)
C(1)	Y	C(22)	C(21)	-108.8(6)	C(1)	Y	C(22)	C(23)	4.8(7)
C(1)	Y	C(23)	C(22)	-176.1(6)	C(1)	Y	C(23)	C(24)	-63.2(5)
C(1)	Y	C(24)	C(20)	-130.0(4)	C(1)	Y	C(24)	C(23)	116.8(5)
C(1)	Y	C(24)	C(25)	2.8(9)	C(1)	O(1)	Y	C(14)	-57.7(2)
C(1)	O(1)	Y	C(15)	-66.4(3)	C(1)	O(1)	Y	C(16)	-114.1(3)
C(1)	O(1)	Y	C(17)	-110.4(2)	C(1)	O(1)	Y	C(18)	-82.2(2)
C(1)	O(1)	Y	C(20)	61.7(3)	C(1)	O(1)	Y	C(21)	89.5(4)
C(1)	O(1)	Y	C(22)	116.6(3)	C(1)	O(1)	Y	C(23)	104.1(3)

Table 7. Torsion Angles(°) (continued)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
C(1)	O(1)	Y	C(24)	74.3(3)	C(1)	N(1)	Y	C(14)	133.2(2)
C(1)	N(1)	Y	C(15)	149.8(2)	C(1)	N(1)	Y	C(16)	129.2(2)
C(1)	N(1)	Y	C(17)	97.7(2)	C(1)	N(1)	Y	C(18)	103.1(2)
C(1)	N(1)	Y	C(20)	-123.2(3)	C(1)	N(1)	Y	C(21)	-127.6(3)
C(1)	N(1)	Y	C(22)	-96.9(4)	C(1)	N(1)	Y	C(23)	-77.5(3)
C(1)	N(1)	Y	C(24)	-94.4(3)	C(1)	N(1)	C(8)	C(9)	-44.5(6)
C(1)	N(1)	C(8)	C(13)	142.9(4)	C(1)	N(2)	C(2)	C(3)	131.3(4)
C(1)	N(2)	C(2)	C(4)	-103.8(4)	C(1)	N(2)	C(5)	C(6)	67.4(5)
C(1)	N(2)	C(5)	C(7)	-60.9(5)	C(2)	N(2)	C(5)	C(6)	-99.6(5)
C(2)	N(2)	C(5)	C(7)	132.2(4)	C(3)	C(2)	N(2)	C(5)	-62.0(5)
C(4)	C(2)	N(2)	C(5)	63.0(5)	C(8)	N(1)	Y	C(14)	-23.2(4)
C(8)	N(1)	Y	C(15)	-6.5(4)	C(8)	N(1)	Y	C(16)	-27.2(4)
C(8)	N(1)	Y	C(17)	-58.6(4)	C(8)	N(1)	Y	C(18)	-53.3(4)
C(8)	N(1)	Y	C(20)	80.4(4)	C(8)	N(1)	Y	C(21)	76.0(4)
C(8)	N(1)	Y	C(22)	106.7(5)	C(8)	N(1)	Y	C(23)	126.2(4)
C(8)	N(1)	Y	C(24)	109.2(4)	C(8)	C(9)	C(10)	C(11)	0.5(6)
C(8)	C(13)	C(12)	C(11)	-1.1(7)	C(9)	C(8)	C(13)	C(12)	1.0(6)
C(9)	C(10)	C(11)	C(12)	-0.6(7)	C(10)	C(9)	C(8)	C(13)	-0.7(6)
C(10)	C(11)	C(12)	C(13)	0.9(7)	C(14)	Y	O(2)	C(26)	70.5(6)
C(14)	Y	O(2)	C(29)	-103.4(6)	C(14)	Y	C(15)	C(16)	-113.3(4)
C(14)	Y	C(16)	C(15)	37.3(3)	C(14)	Y	C(16)	C(17)	-75.9(3)
C(14)	Y	C(17)	C(16)	77.7(3)	C(14)	Y	C(17)	C(18)	-37.2(3)
C(14)	Y	C(18)	C(17)	113.7(4)	C(14)	Y	C(18)	C(19)	-122.3(5)
C(14)	Y	C(20)	C(21)	-95.4(5)	C(14)	Y	C(20)	C(24)	151.5(4)

Table 7. Torsion Angles(°) (continued)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
C(14)	Y	C(21)	C(20)	91.5(5)	C(14)	Y	C(21)	C(22)	-153.6(5)
C(14)	Y	C(22)	C(21)	33.6(6)	C(14)	Y	C(22)	C(23)	147.2(5)
C(14)	Y	C(23)	C(22)	-58.2(10)	C(14)	Y	C(23)	C(24)	54.7(9)
C(14)	Y	C(24)	C(20)	-36.0(5)	C(14)	Y	C(24)	C(23)	-149.2(5)
C(14)	Y	C(24)	C(25)	96.9(9)	C(14)	C(15)	Y	C(16)	113.3(4)
C(14)	C(15)	Y	C(17)	75.9(3)	C(14)	C(15)	Y	C(18)	36.5(3)
C(14)	C(15)	Y	C(20)	-119.5(3)	C(14)	C(15)	Y	C(21)	-147.4(3)
C(14)	C(15)	Y	C(22)	-166.7(3)	C(14)	C(15)	Y	C(23)	-152.3(4)
C(14)	C(15)	Y	C(24)	-118.6(3)	C(14)	C(15)	C(16)	C(17)	0.6(5)
C(14)	C(18)	Y	C(15)	-36.8(3)	C(14)	C(18)	Y	C(16)	-77.0(3)
C(14)	C(18)	Y	C(17)	-113.7(4)	C(14)	C(18)	Y	C(20)	-3.2(4)
C(14)	C(18)	Y	C(21)	-41.7(4)	C(14)	C(18)	Y	C(22)	-77.4(4)
C(14)	C(18)	Y	C(23)	-99(1)	C(14)	C(18)	Y	C(24)	29.6(5)
C(14)	C(18)	C(17)	C(16)	0.2(5)	C(15)	Y	O(2)	C(26)	36.8(6)
C(15)	Y	O(2)	C(29)	-137.1(6)	C(15)	Y	C(14)	C(18)	114.6(4)
C(15)	Y	C(16)	C(17)	-113.1(4)	C(15)	Y	C(17)	C(16)	37.6(3)
C(15)	Y	C(17)	C(18)	-77.3(3)	C(15)	Y	C(18)	C(17)	76.9(3)
C(15)	Y	C(18)	C(19)	-159.1(4)	C(15)	Y	C(20)	C(21)	-68.6(5)
C(15)	Y	C(20)	C(24)	178.4(5)	C(15)	Y	C(21)	C(20)	107.8(5)
C(15)	Y	C(21)	C(22)	-137.3(6)	C(15)	Y	C(22)	C(21)	42.1(6)
C(15)	Y	C(22)	C(23)	155.8(6)	C(15)	Y	C(23)	C(22)	-29.9(7)
C(15)	Y	C(23)	C(24)	83.0(6)	C(15)	Y	C(24)	C(20)	-1.8(5)
C(15)	Y	C(24)	C(23)	-115.0(6)	C(15)	Y	C(24)	C(25)	131.0(9)
C(15)	C(14)	Y	C(16)	-37.5(3)	C(15)	C(14)	Y	C(17)	-77.7(3)

Table 7. Torsion Angles(°) (continued)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
C(15)	C(14)	Y	C(18)	-114.6(4)	C(15)	C(14)	Y	C(20)	63.0(3)
C(15)	C(14)	Y	C(21)	32.7(3)	C(15)	C(14)	Y	C(22)	16.9(4)
C(15)	C(14)	Y	C(23)	49.4(6)	C(15)	C(14)	Y	C(24)	80.1(3)
C(15)	C(14)	C(18)	C(17)	0.2(5)	C(15)	C(14)	C(18)	C(19)	-177.3(4)
C(15)	C(16)	Y	C(17)	113.1(4)	C(15)	C(16)	Y	C(18)	76.9(3)
C(15)	C(16)	Y	C(20)	-55.9(3)	C(15)	C(16)	Y	C(21)	-75.8(4)
C(15)	C(16)	Y	C(22)	-103.3(3)	C(15)	C(16)	Y	C(23)	-106.8(4)
C(15)	C(16)	Y	C(24)	-71.2(4)	C(15)	C(16)	C(17)	C(18)	-0.5(5)
C(16)	Y	O(2)	C(26)	36.6(6)	C(16)	Y	O(2)	C(29)	-137.4(6)
C(16)	Y	C(14)	C(18)	77.1(3)	C(16)	Y	C(17)	C(18)	-114.9(4)
C(16)	Y	C(18)	C(17)	36.8(3)	C(16)	Y	C(18)	C(19)	160.7(4)
C(16)	Y	C(20)	C(21)	-43.6(5)	C(16)	Y	C(20)	C(24)	-156.6(4)
C(16)	Y	C(21)	C(20)	138.2(5)	C(16)	Y	C(21)	C(22)	-107.0(6)
C(16)	Y	C(22)	C(21)	72.3(5)	C(16)	Y	C(22)	C(23)	-174.1(6)
C(16)	Y	C(23)	C(22)	7.0(7)	C(16)	Y	C(23)	C(24)	119.9(5)
C(16)	Y	C(24)	C(20)	31.0(6)	C(16)	Y	C(24)	C(23)	-82.2(6)
C(16)	Y	C(24)	C(25)	163.9(9)	C(16)	C(15)	Y	C(17)	-37.4(3)
C(16)	C(15)	Y	C(18)	-76.8(3)	C(16)	C(15)	Y	C(20)	127.2(3)
C(16)	C(15)	Y	C(21)	99.2(4)	C(16)	C(15)	Y	C(22)	79.9(3)
C(16)	C(15)	Y	C(23)	94.4(4)	C(16)	C(15)	Y	C(24)	128.1(3)
C(16)	C(15)	C(14)	C(18)	-0.5(5)	C(16)	C(17)	Y	C(18)	114.9(4)
C(16)	C(17)	Y	C(20)	15.2(4)	C(16)	C(17)	Y	C(21)	-9.8(4)
C(16)	C(17)	Y	C(22)	-41.6(4)	C(16)	C(17)	Y	C(23)	-62.0(4)
C(16)	C(17)	Y	C(24)	-10.7(9)	C(16)	C(17)	C(18)	C(19)	177.6(4)

Table 7. Torsion Angles(°) (continued)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
C(17)	Y	O(2)	C(26)	65.6(6)	C(17)	Y	O(2)	C(29)	-108.3(6)
C(17)	Y	C(14)	C(18)	36.9(3)	C(17)	Y	C(18)	C(19)	123.9(5)
C(17)	Y	C(20)	C(21)	-51.5(5)	C(17)	Y	C(20)	C(24)	-164.6(4)
C(17)	Y	C(21)	C(20)	143.2(4)	C(17)	Y	C(21)	C(22)	-102.0(5)
C(17)	Y	C(22)	C(21)	92.0(5)	C(17)	Y	C(22)	C(23)	-154.3(5)
C(17)	Y	C(23)	C(22)	39.0(7)	C(17)	Y	C(23)	C(24)	151.9(4)
C(17)	Y	C(24)	C(20)	38(1)	C(17)	Y	C(24)	C(23)	-74(1)
C(17)	Y	C(24)	C(25)	171.2(8)	C(17)	C(16)	Y	C(18)	-36.2(3)
C(17)	C(16)	Y	C(20)	-169.0(3)	C(17)	C(16)	Y	C(21)	171.0(4)
C(17)	C(16)	Y	C(22)	143.6(3)	C(17)	C(16)	Y	C(23)	140.1(3)
C(17)	C(16)	Y	C(24)	175.7(3)	C(17)	C(18)	Y	C(20)	110.5(3)
C(17)	C(18)	Y	C(21)	72.0(4)	C(17)	C(18)	Y	C(22)	36.4(5)
C(17)	C(18)	Y	C(23)	13(1)	C(17)	C(18)	Y	C(24)	143.3(4)
C(18)	Y	O(2)	C(26)	85.6(6)	C(18)	Y	O(2)	C(29)	-88.4(6)
C(18)	Y	C(20)	C(21)	-93.8(5)	C(18)	Y	C(20)	C(24)	153.2(4)
C(18)	Y	C(21)	C(20)	111.7(4)	C(18)	Y	C(21)	C(22)	-133.5(5)
C(18)	Y	C(22)	C(21)	72.6(5)	C(18)	Y	C(22)	C(23)	-173.8(4)
C(18)	Y	C(23)	C(22)	27(1)	C(18)	Y	C(23)	C(24)	140(1)
C(18)	Y	C(24)	C(20)	-54.2(6)	C(18)	Y	C(24)	C(23)	-167.5(5)
C(18)	Y	C(24)	C(25)	78(1)	C(18)	C(14)	Y	C(20)	177.6(3)
C(18)	C(14)	Y	C(21)	147.3(3)	C(18)	C(14)	Y	C(22)	131.4(3)
C(18)	C(14)	Y	C(23)	163.9(6)	C(18)	C(14)	Y	C(24)	-165.3(3)
C(18)	C(17)	Y	C(20)	-99.7(3)	C(18)	C(17)	Y	C(21)	-124.7(3)
C(18)	C(17)	Y	C(22)	-156.5(3)	C(18)	C(17)	Y	C(23)	-176.9(3)

Table 7. Torsion Angles(°) (continued)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
C(18)	C(17)	Y	C(24)	-125.5(8)	C(19)	C(18)	Y	C(20)	-125.6(4)
C(19)	C(18)	Y	C(21)	-164.1(4)	C(19)	C(18)	Y	C(22)	160.3(4)
C(19)	C(18)	Y	C(23)	137(1)	C(19)	C(18)	Y	C(24)	-92.8(5)
C(20)	Y	O(2)	C(26)	-68.9(6)	C(20)	Y	O(2)	C(29)	117.2(6)
C(20)	Y	C(21)	C(22)	114.8(6)	C(20)	Y	C(22)	C(21)	-36.7(4)
C(20)	Y	C(22)	C(23)	77.0(5)	C(20)	Y	C(23)	C(22)	-76.0(5)
C(20)	Y	C(23)	C(24)	36.9(4)	C(20)	Y	C(24)	C(23)	-113.2(6)
C(20)	Y	C(24)	C(25)	132(1)	C(20)	C(21)	Y	C(22)	-114.8(6)
C(20)	C(21)	Y	C(23)	-77.4(5)	C(20)	C(21)	Y	C(24)	-37.1(4)
C(20)	C(21)	C(22)	C(23)	-0.6(8)	C(20)	C(24)	Y	C(21)	37.3(4)
C(20)	C(24)	Y	C(22)	76.0(4)	C(20)	C(24)	Y	C(23)	113.2(6)
C(20)	C(24)	C(23)	C(22)	1.1(7)	C(21)	Y	O(2)	C(26)	-45.9(6)
C(21)	Y	O(2)	C(29)	140.2(6)	C(21)	Y	C(20)	C(24)	-113.0(6)
C(21)	Y	C(22)	C(23)	113.6(7)	C(21)	Y	C(23)	C(22)	-36.3(4)
C(21)	Y	C(23)	C(24)	76.6(4)	C(21)	Y	C(24)	C(23)	-75.9(4)
C(21)	Y	C(24)	C(25)	170(1)	C(21)	C(20)	Y	C(22)	35.8(4)
C(21)	C(20)	Y	C(23)	75.6(5)	C(21)	C(20)	Y	C(24)	113.0(6)
C(21)	C(20)	C(24)	C(23)	-1.5(6)	C(21)	C(20)	C(24)	C(25)	174.3(7)
C(21)	C(22)	Y	C(23)	-113.6(7)	C(21)	C(22)	Y	C(24)	-76.1(5)
C(21)	C(22)	C(23)	C(24)	-0.3(7)	C(22)	Y	O(2)	C(26)	-57.6(6)
C(22)	Y	O(2)	C(29)	128.4(6)	C(22)	Y	C(20)	C(24)	-77.3(4)
C(22)	Y	C(23)	C(24)	112.9(6)	C(22)	Y	C(24)	C(23)	-37.2(4)
C(22)	Y	C(24)	C(25)	-151(1)	C(22)	C(21)	Y	C(23)	37.4(4)
C(22)	C(21)	Y	C(24)	77.7(5)	C(22)	C(21)	C(20)	C(24)	1.3(7)

Table 7. Torsion Angles(°) (continued)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
C(22)	C(23)	Y	C(24)	-112.9(6)	C(22)	C(23)	C(24)	C(25)	-175.5(6)
C(23)	Y	O(2)	C(26)	-87.8(6)	C(23)	Y	O(2)	C(29)	98.3(6)
C(23)	Y	C(20)	C(24)	-37.5(4)	C(23)	Y	C(24)	C(25)	-113(1)
C(23)	C(22)	Y	C(24)	37.5(4)	C(24)	Y	O(2)	C(26)	-96.1(6)
C(24)	Y	O(2)	C(29)	89.9(6)	C(26)	O(2)	C(29)	C(28)	1.1(9)
C(26)	C(27)	C(28)	C(29)	4(1)	C(27)	C(26)	O(2)	C(29)	1(1)

Table 8. Least Squares Planes

Plane number 1

Atoms defining plane	Distance
C(14)	0.002(4)
C(15)	-0.004(4)
C(16)	0.004(4)
C(17)	-0.002(4)
C(18)	0.000(4)
Additional Atoms	Distance
Y	2.391
C(19)	-0.054

Plane number 2

Atoms defining plane	Distance
C(20)	0.007(5)
C(21)	-0.006(5)
C(22)	0.001(6)
C(23)	0.005(6)
C(24)	-0.007(5)
Additional Atoms	Distance
Y	2.414
C(25)	-0.109

Plane number 3

Atoms defining plane	Distance
O(2)	0.000(3)
C(26)	0.01(1)
C(27)	-0.03(1)
C(28)	0.016(9)
C(29)	-0.013(10)

Plane number 4

Atoms defining plane	Distance
O(1)	0.003(3)
N(1)	0.005(3)
N(2)	0.006(3)
C(1)	-0.019(4)

Plane number 5

Atoms defining plane	Distance
C(8)	0.003(3)
C(9)	-0.002(4)
C(10)	0.001(4)
C(11)	-0.002(4)
C(12)	0.004(4)
C(13)	-0.005(4)

Additional Atoms	Distance
C(25)	1.369

Summary

plane	mean deviation	χ^2
1	0.0021	1.6
2	0.0053	5.4
3	0.0142	12.0
4	0.0083	33.1
5	0.0027	3.2

Dihedral angles between planes (°)

plane	1	2	3	4
2	126.00			
3	29.53	154.58		
4	38.55	164.55	11.06	
5	32.60	104.23	57.12	61.95

