

O(1')	-1914(1)	1411(1)	1910(1)	20(1)
N(1')	-1293(1)	439(1)	3335(1)	18(1)
N(2')	-2271(1)	1381(1)	4520(1)	19(1)
N(3')	-3700(2)	2851(1)	4094(1)	18(1)
N(4')	-3635(2)	2876(1)	2577(1)	19(1)
C(1')	-690(2)	-155(1)	2882(1)	19(1)
C(2')	-288(2)	-972(2)	3301(1)	22(1)
C(3')	-660(2)	-862(2)	3998(1)	22(1)
C(4')	-1278(2)	25(1)	4020(1)	19(1)
C(5')	-1803(2)	481(1)	4605(1)	19(1)
C(6')	-1920(2)	100(2)	5330(1)	25(1)
C(7')	-2457(2)	796(2)	5694(1)	24(1)
C(8')	-2694(2)	1603(1)	5191(1)	19(1)
C(9')	-3344(2)	2462(1)	5307(1)	19(1)
C(10')	-3511(2)	2740(1)	6017(1)	20(1)
C(11')	-2534(2)	2608(2)	6364(1)	25(1)
C(12')	-2622(2)	2897(2)	7008(1)	30(1)
C(13')	-3673(2)	3339(2)	7315(1)	32(1)
C(14')	-4655(2)	3474(2)	6986(1)	29(1)
C(15')	-4577(2)	3165(2)	6349(1)	24(1)
C(16')	-3838(2)	3067(1)	4768(1)	18(1)
C(17')	-4610(2)	3905(2)	4770(1)	20(1)
C(18')	-4953(2)	4158(2)	4120(1)	22(1)
C(19')	-4364(2)	3493(1)	3695(1)	18(1)
C(20')	-4398(2)	3459(1)	2981(1)	19(1)
C(21')	-5185(2)	3986(2)	2559(1)	23(1)
C(22')	-4874(2)	3724(2)	1901(1)	22(1)
C(23')	-3888(2)	3038(1)	1903(1)	19(1)
C(24')	-3223(2)	2628(1)	1320(1)	20(1)
C(25')	-3602(2)	3018(1)	624(1)	20(1)
C(26')	-3371(2)	3879(2)	281(1)	25(1)
C(27')	-3765(2)	4246(2)	-348(1)	26(1)
C(28')	-4398(2)	3747(2)	-642(1)	27(1)
C(29')	-4623(2)	2882(2)	-310(1)	28(1)
C(30')	-4239(2)	2519(2)	320(1)	24(1)
C(31')	-2298(2)	1931(1)	1307(1)	19(1)
C(32')	-1578(2)	1581(2)	716(1)	23(1)
C(33')	-810(2)	858(2)	946(1)	23(1)
C(34')	-1020(2)	721(1)	1691(1)	20(1)
C(35')	-508(2)	18(1)	2136(1)	20(1)
C(36')	302(2)	-728(1)	1790(1)	21(1)
C(37')	-163(2)	-1460(2)	1641(1)	27(1)
C(38')	562(2)	-2179(2)	1349(1)	31(1)
C(39')	1755(2)	-2169(2)	1195(1)	30(1)
C(40')	2229(2)	-1437(2)	1332(1)	34(1)
C(41')	1509(2)	-720(2)	1631(1)	29(1)
C(1S)	1451(2)	1084(2)	2954(1)	26(1)
O(1S)	1856(1)	1797(1)	3219(1)	23(1)
C(2S)	-515(2)	3099(2)	4494(1)	30(1)
O(2S)	-257(1)	2318(1)	4119(1)	29(1)
C(3S)	-786(2)	3134(2)	2364(1)	36(1)
O(3S)	-1350(1)	2561(1)	2945(1)	27(1)

Table 3. Bond lengths [Å] and angles [°] for OSMAR.

O(1)-C(34)	1.399(2)	O(1)-C(31)	1.406(2)
N(1)-C(1)	1.378(3)	N(1)-C(4)	1.380(2)
N(1)-H(1N)	0.87(2)	N(2)-C(5)	1.353(3)
N(2)-C(8)	1.386(2)	N(2)-H(2N)	0.95(3)
N(3)-C(19)	1.346(3)	N(3)-C(16)	1.391(2)
N(4)-C(20)	1.376(3)	N(4)-C(23)	1.387(3)
N(4)-H(4N)	0.96(2)	C(1)-C(2)	1.411(3)
C(1)-C(35)	1.421(3)	C(2)-C(3)	1.384(3)
C(2)-H(2)	1.01(2)	C(3)-C(4)	1.394(3)
C(3)-H(3)	0.99(2)	C(4)-C(5)	1.421(3)
C(5)-C(6)	1.414(3)	C(6)-C(7)	1.370(3)
C(6)-H(6)	0.97(2)	C(7)-C(8)	1.421(3)
C(7)-H(7)	0.95(2)	C(8)-C(9)	1.411(3)
C(9)-C(16)	1.404(3)	C(9)-C(10)	1.502(3)
C(10)-C(11)	1.389(3)	C(10)-C(15)	1.392(3)
C(11)-C(12)	1.396(3)	C(11)-H(11)	0.95(2)
C(12)-C(13)	1.381(3)	C(12)-H(12)	0.96(2)
C(13)-C(14)	1.379(3)	C(13)-H(13)	1.01(2)
C(14)-C(15)	1.396(3)	C(14)-H(14)	0.98(2)
C(15)-H(15)	0.98(2)	C(16)-C(17)	1.440(3)
C(17)-C(18)	1.358(3)	C(17)-H(17)	0.99(2)
C(18)-C(19)	1.438(3)	C(18)-H(18)	1.00(2)
C(19)-C(20)	1.432(3)	C(20)-C(21)	1.392(3)
C(21)-C(22)	1.389(3)	C(21)-H(21)	0.96(2)
C(22)-C(23)	1.398(3)	C(22)-H(22)	1.00(2)
C(23)-C(24)	1.422(3)	C(24)-C(31)	1.369(3)
C(24)-C(25)	1.507(3)	C(25)-C(30)	1.389(3)
C(25)-C(26)	1.392(3)	C(26)-C(27)	1.391(3)
C(26)-H(26)	1.04(2)	C(27)-C(28)	1.385(3)
C(27)-H(27)	0.98(2)	C(28)-C(29)	1.382(3)
C(28)-H(28)	1.00(2)	C(29)-C(30)	1.396(3)
C(29)-H(29)	1.00(2)	C(30)-H(30)	1.00(2)
C(31)-C(32)	1.413(3)	C(32)-C(33)	1.354(3)
C(32)-H(32)	0.99(2)	C(33)-C(34)	1.419(3)
C(33)-H(33)	0.975(19)	C(34)-C(35)	1.378(3)
C(35)-C(36)	1.500(3)	C(36)-C(37)	1.391(3)
C(36)-C(41)	1.393(3)	C(37)-C(38)	1.385(3)
C(37)-H(37)	1.02(2)	C(38)-C(39)	1.379(3)
C(38)-H(38)	1.00(2)	C(39)-C(40)	1.382(3)
C(39)-H(39)	0.96(2)	C(40)-C(41)	1.389(3)
C(40)-H(40)	0.98(3)	C(41)-H(41)	1.01(2)
O(1')-C(34')	1.399(2)	O(1')-C(31')	1.403(2)
N(1')-C(1')	1.376(3)	N(1')-C(4')	1.382(3)
N(1')-H(1N')	0.94(2)	N(2')-C(5')	1.352(2)
N(2')-C(8')	1.393(2)	N(3')-C(19')	1.361(3)
N(3')-C(16')	1.389(2)	N(3')-H(3N')	0.93(2)
N(4')-C(20')	1.376(3)	N(4')-C(23')	1.383(2)
N(4')-H(4N')	0.90(2)	C(1')-C(2')	1.409(3)
C(1')-C(35')	1.427(3)	C(2')-C(3')	1.385(3)
C(2')-H(2')	0.973(19)	C(3')-C(4')	1.397(3)
C(3')-H(3')	0.99(2)	C(4')-C(5')	1.423(3)
C(5')-C(6')	1.429(3)	C(6')-C(7')	1.359(3)

C(7')-H(7')	0.94(2)	C(8')-C(9')	1.405(3)
C(9')-C(16')	1.412(3)	C(9')-C(10')	1.490(3)
C(10')-C(15')	1.400(3)	C(10')-C(11')	1.407(3)
C(11')-C(12')	1.385(3)	C(11')-H(11')	1.00(2)
C(12')-C(13')	1.379(3)	C(12')-H(12')	0.98(2)
C(13')-C(14')	1.391(3)	C(13')-H(13')	0.95(2)
C(14')-C(15')	1.388(3)	C(14')-H(14')	0.98(2)
C(15')-H(15')	1.01(2)	C(16')-C(17')	1.413(3)
C(17')-C(18')	1.382(3)	C(17')-H(17')	1.00(2)
C(18')-C(19')	1.410(3)	C(18')-H(18')	1.01(2)
C(19')-C(20')	1.420(3)	C(20')-C(21')	1.404(3)
C(21')-C(22')	1.381(3)	C(21')-H(21')	0.97(2)
C(22')-C(23')	1.408(3)	C(22')-H(22')	0.98(2)
C(23')-C(24')	1.427(3)	C(24')-C(31')	1.370(3)
C(24')-C(25')	1.508(3)	C(25')-C(26')	1.382(3)
C(25')-C(30')	1.398(3)	C(26')-C(27')	1.390(3)
C(26')-H(26')	0.98(2)	C(27')-C(28')	1.385(3)
C(27')-H(27')	0.97(2)	C(28')-C(29')	1.378(3)
C(28')-H(28')	1.00(2)	C(29')-C(30')	1.388(3)
C(29')-H(29')	0.94(2)	C(30')-H(30')	0.97(2)
C(31')-C(32')	1.424(3)	C(32')-C(33')	1.353(3)
C(32')-H(32')	0.97(2)	C(33')-C(34')	1.423(3)
C(33')-H(33')	1.00(2)	C(34')-C(35')	1.375(3)
C(35')-C(36')	1.503(3)	C(36')-C(37')	1.385(3)
C(36')-C(41')	1.390(3)	C(37')-C(38')	1.386(3)
C(37')-H(37')	0.96(2)	C(38')-C(39')	1.374(3)
C(38')-H(38')	1.00(2)	C(39')-C(40')	1.383(3)
C(39')-H(39')	0.93(2)	C(40')-C(41')	1.387(3)
C(40')-H(40')	0.96(2)	C(41')-H(41')	0.99(2)
C(1S)-O(1S)	1.433(3)	C(1S)-H(1SA)	1.03(2)
C(1S)-H(1SB)	0.99(2)	C(1S)-H(1SC)	0.96(2)
O(1S)-H(1SD)	0.92(3)	C(2S)-O(2S)	1.438(3)
C(2S)-H(2SA)	0.97(2)	C(2S)-H(2SB)	0.99(2)
C(2S)-H(2SC)	1.07(3)	O(2S)-H(2SD)	0.88(3)
C(3S)-O(3S)	1.425(3)	C(3S)-H(3SA)	0.98(3)
C(3S)-H(3SC)	0.99(3)	C(3S)-H(3SB)	1.03(3)
O(3S)-H(3SD)	0.88(3)		

C(34)-O(1)-C(31)	107.10(15)	C(1)-N(1)-C(4)	109.57(17)
C(1)-N(1)-H(1N)	126.0(15)	C(4)-N(1)-H(1N)	123.7(15)
C(5)-N(2)-C(8)	110.48(18)	C(5)-N(2)-H(2N)	132.9(15)
C(8)-N(2)-H(2N)	114.9(15)	C(19)-N(3)-C(16)	105.81(17)
C(20)-N(4)-C(23)	109.65(17)	C(20)-N(4)-H(4N)	124.0(13)
C(23)-N(4)-H(4N)	123.8(13)	N(1)-C(1)-C(2)	106.82(18)
N(1)-C(1)-C(35)	126.78(18)	C(2)-C(1)-C(35)	126.36(19)
C(3)-C(2)-C(1)	107.91(19)	C(3)-C(2)-H(2)	128.8(12)
C(1)-C(2)-H(2)	123.3(12)	C(2)-C(3)-C(4)	108.23(19)
C(2)-C(3)-H(3)	125.5(12)	C(4)-C(3)-H(3)	126.1(12)
N(1)-C(4)-C(3)	107.41(18)	N(1)-C(4)-C(5)	124.00(18)
C(3)-C(4)-C(5)	128.59(18)	N(2)-C(5)-C(6)	107.59(18)
N(2)-C(5)-C(4)	123.85(18)	C(6)-C(5)-C(4)	128.56(19)
C(7)-C(6)-C(5)	107.59(19)	C(7)-C(6)-H(6)	127.9(11)
C(5)-C(6)-H(6)	124.5(11)	C(6)-C(7)-C(8)	108.58(19)
C(6)-C(7)-H(7)	129.6(13)	C(8)-C(7)-H(7)	121.8(13)
N(2)-C(8)-C(9)	121.58(19)	N(2)-C(8)-C(7)	105.65(18)
C(9)-C(8)-C(7)	132.02(19)	C(16)-C(9)-C(8)	122.16(18)
C(16)-C(9)-C(10)	120.27(18)	C(8)-C(9)-C(10)	117.45(18)

C(11)-C(10)-C(15)	118.8(2)	C(11)-C(10)-C(9)	120.64(19)
C(15)-C(10)-C(9)	120.6(2)	C(10)-C(11)-C(12)	120.5(2)
C(10)-C(11)-H(11)	120.7(13)	C(12)-C(11)-H(11)	118.9(13)
C(13)-C(12)-C(11)	120.2(2)	C(13)-C(12)-H(12)	121.3(14)
C(11)-C(12)-H(12)	118.5(14)	C(14)-C(13)-C(12)	119.9(2)
C(14)-C(13)-H(13)	116.4(14)	C(12)-C(13)-H(13)	123.7(14)
C(13)-C(14)-C(15)	120.0(2)	C(13)-C(14)-H(14)	121.5(14)
C(15)-C(14)-H(14)	118.5(14)	C(10)-C(15)-C(14)	120.6(2)
C(10)-C(15)-H(15)	120.7(12)	C(14)-C(15)-H(15)	118.7(12)
N(3)-C(16)-C(9)	121.50(19)	N(3)-C(16)-C(17)	109.36(18)
C(9)-C(16)-C(17)	129.14(19)	C(18)-C(17)-C(16)	107.14(19)
C(18)-C(17)-H(17)	123.8(13)	C(16)-C(17)-H(17)	129.1(13)
C(17)-C(18)-C(19)	106.20(19)	C(17)-C(18)-H(18)	128.2(12)
C(19)-C(18)-H(18)	125.6(12)	N(3)-C(19)-C(20)	121.62(19)
N(3)-C(19)-C(18)	111.49(18)	C(20)-C(19)-C(18)	126.86(19)
N(4)-C(20)-C(21)	107.62(18)	N(4)-C(20)-C(19)	122.84(19)
C(21)-C(20)-C(19)	129.5(2)	C(22)-C(21)-C(20)	107.6(2)
C(22)-C(21)-H(21)	126.4(12)	C(20)-C(21)-H(21)	126.0(12)
C(21)-C(22)-C(23)	108.7(2)	C(21)-C(22)-H(22)	126.3(12)
C(23)-C(22)-H(22)	125.0(12)	N(4)-C(23)-C(22)	106.35(18)
N(4)-C(23)-C(24)	126.40(19)	C(22)-C(23)-C(24)	127.20(19)
C(31)-C(24)-C(23)	130.15(19)	C(31)-C(24)-C(25)	114.75(18)
C(23)-C(24)-C(25)	115.06(18)	C(30)-C(25)-C(26)	118.8(2)
C(30)-C(25)-C(24)	119.86(18)	C(26)-C(25)-C(24)	121.38(19)
C(27)-C(26)-C(25)	120.3(2)	C(27)-C(26)-H(26)	118.3(12)
C(25)-C(26)-H(26)	121.4(12)	C(28)-C(27)-C(26)	120.5(2)
C(28)-C(27)-H(27)	121.8(13)	C(26)-C(27)-H(27)	117.7(14)
C(29)-C(28)-C(27)	119.8(2)	C(29)-C(28)-H(28)	116.9(13)
C(27)-C(28)-H(28)	123.3(13)	C(28)-C(29)-C(30)	119.8(2)
C(28)-C(29)-H(29)	121.8(14)	C(30)-C(29)-H(29)	118.4(14)
C(25)-C(30)-C(29)	120.9(2)	C(25)-C(30)-H(30)	121.0(13)
C(29)-C(30)-H(30)	118.0(13)	C(24)-C(31)-O(1)	123.90(18)
C(24)-C(31)-C(32)	128.5(2)	O(1)-C(31)-C(32)	107.52(18)
C(33)-C(32)-C(31)	109.1(2)	C(33)-C(32)-H(32)	127.1(13)
C(31)-C(32)-H(32)	123.8(13)	C(32)-C(33)-C(34)	108.1(2)
C(32)-C(33)-H(33)	129.3(11)	C(34)-C(33)-H(33)	122.6(11)
C(35)-C(34)-O(1)	122.91(18)	C(35)-C(34)-C(33)	128.9(2)
O(1)-C(34)-C(33)	108.12(18)	C(34)-C(35)-C(1)	128.11(19)
C(34)-C(35)-C(36)	116.46(18)	C(1)-C(35)-C(36)	115.39(18)
C(37)-C(36)-C(41)	118.4(2)	C(37)-C(36)-C(35)	119.8(2)
C(41)-C(36)-C(35)	121.7(2)	C(38)-C(37)-C(36)	121.0(2)
C(38)-C(37)-H(37)	119.0(12)	C(36)-C(37)-H(37)	120.1(12)
C(39)-C(38)-C(37)	120.3(2)	C(39)-C(38)-H(38)	120.3(12)
C(37)-C(38)-H(38)	119.3(12)	C(38)-C(39)-C(40)	119.4(2)
C(38)-C(39)-H(39)	119.8(13)	C(40)-C(39)-H(39)	120.9(13)
C(39)-C(40)-C(41)	120.6(2)	C(39)-C(40)-H(40)	119.8(15)
C(41)-C(40)-H(40)	119.6(15)	C(40)-C(41)-C(36)	120.3(2)
C(40)-C(41)-H(41)	122.4(12)	C(36)-C(41)-H(41)	117.3(12)
C(34')-O(1')-C(31')	107.39(15)	C(1')-N(1')-C(4')	110.02(17)
C(1')-N(1')-H(1N')	125.3(13)	C(4')-N(1')-H(1N')	124.3(13)
C(5')-N(2')-C(8')	106.16(17)	C(19')-N(3')-C(16')	110.72(17)
C(19')-N(3')-H(3N')	131.0(13)	C(16')-N(3')-H(3N')	118.2(13)
C(20')-N(4')-C(23')	109.73(17)	C(20')-N(4')-H(4N')	123.9(15)
C(23')-N(4')-H(4N')	125.0(15)	N(1')-C(1')-C(2')	106.52(19)
N(1')-C(1')-C(35')	127.02(19)	C(2')-C(1')-C(35')	126.46(19)
C(3')-C(2')-C(1')	108.33(19)	C(3')-C(2')-H(2')	129.1(11)
C(1')-C(2')-H(2')	122.3(11)	C(2')-C(3')-C(4')	108.0(2)

C(2')-C(3')-H(3')	126.7(13)	C(4')-C(3')-H(3')	125.3(13)
N(1')-C(4')-C(3')	107.12(18)	N(1')-C(4')-C(5')	122.91(18)
C(3')-C(4')-C(5')	129.96(19)	N(2')-C(5')-C(4')	121.26(19)
N(2')-C(5')-C(6')	111.10(18)	C(4')-C(5')-C(6')	127.6(2)
C(7')-C(6')-C(5')	106.6(2)	C(7')-C(6')-H(6')	127.0(13)
C(5')-C(6')-H(6')	126.3(13)	C(6')-C(7')-C(8')	107.32(19)
C(6')-C(7')-H(7')	129.6(13)	C(8')-C(7')-H(7')	122.6(13)
N(2')-C(8')-C(9')	122.29(19)	N(2')-C(8')-C(7')	108.84(18)
C(9')-C(8')-C(7')	128.56(19)	C(8')-C(9')-C(16')	121.56(18)
C(8')-C(9')-C(10')	119.04(18)	C(16')-C(9')-C(10')	119.40(18)
C(15')-C(10')-C(11')	117.70(19)	C(15')-C(10')-C(9')	123.68(19)
C(11')-C(10')-C(9')	118.56(19)	C(12')-C(11')-C(10')	121.1(2)
C(12')-C(11')-H(11')	122.7(13)	C(10')-C(11')-H(11')	116.2(13)
C(13')-C(12')-C(11')	120.1(2)	C(13')-C(12')-H(12')	121.3(13)
C(11')-C(12')-H(12')	118.5(13)	C(12')-C(13')-C(14')	120.1(2)
C(12')-C(13')-H(13')	121.1(14)	C(14')-C(13')-H(13')	118.8(14)
C(15')-C(14')-C(13')	119.9(2)	C(15')-C(14')-H(14')	119.5(13)
C(13')-C(14')-H(14')	120.5(13)	C(14')-C(15')-C(10')	121.0(2)
C(14')-C(15')-H(15')	118.8(12)	C(10')-C(15')-H(15')	120.1(12)
N(3')-C(16')-C(9')	122.07(18)	N(3')-C(16')-C(17')	105.53(18)
C(9')-C(16')-C(17')	132.14(18)	C(18')-C(17')-C(16')	108.86(18)
C(18')-C(17')-H(17')	126.3(12)	C(16')-C(17')-H(17')	124.8(12)
C(17')-C(18')-C(19')	107.52(19)	C(17')-C(18')-H(18')	127.1(11)
C(19')-C(18')-H(18')	125.3(11)	N(3')-C(19')-C(18')	107.32(18)
N(3')-C(19')-C(20')	123.59(18)	C(18')-C(19')-C(20')	129.09(19)
N(4')-C(20')-C(21')	107.52(18)	N(4')-C(20')-C(19')	124.49(18)
C(21')-C(20')-C(19')	127.99(19)	C(22')-C(21')-C(20')	107.57(19)
C(22')-C(21')-H(21')	127.6(13)	C(20')-C(21')-H(21')	124.7(13)
C(21')-C(22')-C(23')	108.69(19)	C(21')-C(22')-H(22')	126.5(13)
C(23')-C(22')-H(22')	124.8(12)	N(4')-C(23')-C(22')	106.44(17)
N(4')-C(23')-C(24')	126.01(18)	C(22')-C(23')-C(24')	127.44(19)
C(31')-C(24')-C(23')	129.10(19)	C(31')-C(24')-C(25')	115.81(17)
C(23')-C(24')-C(25')	115.08(18)	C(26')-C(25')-C(30')	118.3(2)
C(26')-C(25')-C(24')	121.62(18)	C(30')-C(25')-C(24')	120.06(19)
C(25')-C(26')-C(27')	121.1(2)	C(25')-C(26')-H(26')	118.4(13)
C(27')-C(26')-H(26')	120.4(13)	C(28')-C(27')-C(26')	120.0(2)
C(28')-C(27')-H(27')	119.7(13)	C(26')-C(27')-H(27')	120.3(13)
C(29')-C(28')-C(27')	119.6(2)	C(29')-C(28')-H(28')	122.5(12)
C(27')-C(28')-H(28')	117.9(12)	C(28')-C(29')-C(30')	120.4(2)
C(28')-C(29')-H(29')	120.7(14)	C(30')-C(29')-H(29')	118.9(15)
C(29')-C(30')-C(25')	120.6(2)	C(29')-C(30')-H(30')	120.9(12)
C(25')-C(30')-H(30')	118.4(12)	C(24')-C(31')-O(1')	123.90(18)
C(24')-C(31')-C(32')	128.52(19)	O(1')-C(31')-C(32')	107.57(17)
C(33')-C(32')-C(31')	108.6(2)	C(33')-C(32')-H(32')	127.8(12)
C(31')-C(32')-H(32')	123.5(12)	C(32')-C(33')-C(34')	108.5(2)
C(32')-C(33')-H(33')	130.0(12)	C(34')-C(33')-H(33')	121.5(12)
C(35')-C(34')-O(1')	124.36(18)	C(35')-C(34')-C(33')	127.70(19)
O(1')-C(34')-C(33')	107.84(18)	C(34')-C(35')-C(1')	129.98(19)
C(34')-C(35')-C(36')	115.62(18)	C(1')-C(35')-C(36')	114.22(18)
C(37')-C(36')-C(41')	118.9(2)	C(37')-C(36')-C(35')	119.05(19)
C(41')-C(36')-C(35')	121.99(19)	C(36')-C(37')-C(38')	120.6(2)
C(36')-C(37')-H(37')	120.9(13)	C(38')-C(37')-H(37')	118.4(13)
C(39')-C(38')-C(37')	120.2(2)	C(39')-C(38')-H(38')	119.0(13)
C(37')-C(38')-H(38')	120.8(13)	C(38')-C(39')-C(40')	119.7(2)
C(38')-C(39')-H(39')	118.8(13)	C(40')-C(39')-H(39')	121.4(13)
C(39')-C(40')-C(41')	120.3(2)	C(39')-C(40')-H(40')	121.3(13)
C(41')-C(40')-H(40')	118.3(13)	C(40')-C(41')-C(36')	120.2(2)

C(40')-C(41')-H(41')	118.7(13)	C(36')-C(41')-H(41')	121.0(13)
O(1S)-C(1S)-H(1SA)	108.9(13)	O(1S)-C(1S)-H(1SB)	110.0(13)
H(1SA)-C(1S)-H(1SB)	106.8(18)	O(1S)-C(1S)-H(1SC)	112.1(13)
H(1SA)-C(1S)-H(1SC)	113.6(19)	H(1SB)-C(1S)-H(1SC)	105.2(18)
C(1S)-O(1S)-H(1SD)	106.4(16)	O(2S)-C(2S)-H(2SA)	109.6(14)
O(2S)-C(2S)-H(2SB)	106.4(13)	H(2SA)-C(2S)-H(2SB)	108.8(19)
O(2S)-C(2S)-H(2SC)	108.6(14)	H(2SA)-C(2S)-H(2SC)	114(2)
H(2SB)-C(2S)-H(2SC)	109(2)	C(2S)-O(2S)-H(2SD)	104.7(18)
O(3S)-C(3S)-H(3SA)	109.9(16)	O(3S)-C(3S)-H(3SC)	115.6(16)
H(3SA)-C(3S)-H(3SC)	105(2)	O(3S)-C(3S)-H(3SB)	109.3(16)
H(3SA)-C(3S)-H(3SB)	110(2)	H(3SC)-C(3S)-H(3SB)	107(2)
C(3S)-O(3S)-H(3SD)	109(2)		

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters [$\text{\AA}^2 \times 10^3$] for OSMAR.

The anisotropic displacement factor exponent takes the form:

$$-2\pi^2 [(ha^*)^2 U_{11} + \dots + 2hka^* b^* U_{12}]$$

	U11	U22	U33	U23	U13	U12
O(1)	22(1)	24(1)	20(1)	-3(1)	-1(1)	1(1)
N(1)	19(1)	24(1)	19(1)	-4(1)	-9(1)	1(1)
N(2)	21(1)	21(1)	18(1)	-5(1)	-7(1)	-1(1)
N(3)	20(1)	23(1)	19(1)	-4(1)	-6(1)	-2(1)
N(4)	21(1)	21(1)	18(1)	-1(1)	-7(1)	-2(1)
C(1)	19(1)	21(1)	20(1)	-4(1)	-4(1)	0(1)
C(2)	18(1)	26(1)	23(1)	-5(1)	-5(1)	0(1)
C(3)	18(1)	27(1)	21(1)	-1(1)	-7(1)	-2(1)
C(4)	20(1)	21(1)	17(1)	-1(1)	-7(1)	-4(1)
C(5)	19(1)	20(1)	21(1)	-3(1)	-6(1)	-5(1)
C(6)	23(1)	22(1)	22(1)	-2(1)	-12(1)	-4(1)
C(7)	26(1)	24(1)	21(1)	-3(1)	-8(1)	-5(1)
C(8)	21(1)	22(1)	18(1)	-5(1)	-5(1)	-6(1)
C(9)	18(1)	22(1)	22(1)	-6(1)	-4(1)	-6(1)
C(10)	20(1)	24(1)	21(1)	-6(1)	-6(1)	-1(1)
C(11)	29(1)	26(1)	28(1)	-6(1)	-6(1)	-5(1)
C(12)	35(1)	40(2)	21(1)	-3(1)	-2(1)	-2(1)
C(13)	34(1)	46(2)	24(1)	-14(1)	-6(1)	-2(1)
C(14)	27(1)	34(2)	30(1)	-14(1)	-7(1)	-4(1)
C(15)	20(1)	29(1)	25(1)	-6(1)	-6(1)	-2(1)
C(16)	18(1)	24(1)	20(1)	-7(1)	-4(1)	-5(1)
C(17)	19(1)	25(1)	23(1)	-8(1)	-4(1)	-2(1)
C(18)	22(1)	22(1)	23(1)	-4(1)	-6(1)	0(1)
C(19)	18(1)	25(1)	21(1)	-2(1)	-5(1)	-3(1)
C(20)	16(1)	24(1)	23(1)	-6(1)	-4(1)	-1(1)
C(21)	23(1)	22(1)	25(1)	-2(1)	-6(1)	3(1)
C(22)	23(1)	26(1)	21(1)	-2(1)	-5(1)	2(1)
C(23)	16(1)	24(1)	18(1)	-1(1)	-6(1)	-1(1)
C(24)	18(1)	26(1)	16(1)	0(1)	-6(1)	-3(1)
C(25)	21(1)	21(1)	18(1)	-6(1)	-7(1)	1(1)
C(26)	23(1)	45(2)	21(1)	0(1)	-6(1)	-5(1)
C(27)	22(1)	48(2)	25(1)	-5(1)	-12(1)	1(1)
C(28)	32(1)	30(1)	21(1)	-4(1)	-9(1)	5(1)
C(29)	29(1)	26(1)	19(1)	-4(1)	-3(1)	0(1)
C(30)	22(1)	26(1)	21(1)	-5(1)	-8(1)	-1(1)
C(31)	21(1)	29(1)	16(1)	-1(1)	-7(1)	-3(1)
C(32)	27(1)	26(1)	20(1)	-3(1)	-9(1)	-4(1)
C(33)	28(1)	23(1)	20(1)	-4(1)	-7(1)	-4(1)
C(34)	20(1)	21(1)	20(1)	-6(1)	-2(1)	0(1)
C(35)	20(1)	22(1)	22(1)	-5(1)	-4(1)	-3(1)
C(36)	22(1)	25(1)	21(1)	-7(1)	-1(1)	0(1)
C(37)	27(1)	25(1)	31(1)	-7(1)	-4(1)	-3(1)
C(38)	28(1)	32(2)	31(1)	-10(1)	-4(1)	-1(1)
C(39)	33(1)	28(1)	28(1)	-13(1)	-12(1)	4(1)
C(40)	50(2)	22(1)	29(1)	-4(1)	-1(1)	-1(1)
C(41)	38(1)	26(1)	25(1)	-2(1)	-4(1)	-4(1)

O(1')	20(1)	21(1)	18(1)	-4(1)	-7(1)	3(1)
N(1')	18(1)	16(1)	21(1)	-4(1)	-7(1)	3(1)
N(2')	19(1)	22(1)	18(1)	-5(1)	-6(1)	0(1)
N(3')	20(1)	19(1)	14(1)	-3(1)	-5(1)	1(1)
N(4')	17(1)	21(1)	18(1)	-1(1)	-9(1)	2(1)
C(1')	17(1)	20(1)	23(1)	-6(1)	-5(1)	-1(1)
C(2')	22(1)	20(1)	24(1)	-7(1)	-9(1)	3(1)
C(3')	24(1)	22(1)	21(1)	-5(1)	-9(1)	1(1)
C(4')	17(1)	21(1)	19(1)	-2(1)	-8(1)	-1(1)
C(5')	16(1)	20(1)	23(1)	-2(1)	-9(1)	-2(1)
C(6')	30(1)	23(1)	21(1)	0(1)	-10(1)	1(1)
C(7')	27(1)	29(1)	15(1)	-4(1)	-5(1)	0(1)
C(8')	18(1)	24(1)	17(1)	-5(1)	-6(1)	-3(1)
C(9')	18(1)	21(1)	18(1)	-5(1)	-3(1)	-3(1)
C(10')	24(1)	19(1)	18(1)	-3(1)	-5(1)	-4(1)
C(11')	26(1)	29(1)	21(1)	-8(1)	-5(1)	-1(1)
C(12')	35(1)	34(1)	23(1)	-8(1)	-11(1)	-2(1)
C(13')	45(2)	32(1)	18(1)	-8(1)	-6(1)	-2(1)
C(14')	35(1)	26(1)	22(1)	-6(1)	1(1)	4(1)
C(15')	28(1)	24(1)	19(1)	-2(1)	-3(1)	-1(1)
C(16')	16(1)	22(1)	16(1)	-5(1)	-1(1)	-4(1)
C(17')	20(1)	23(1)	18(1)	-5(1)	-2(1)	-3(1)
C(18')	20(1)	21(1)	23(1)	-2(1)	-2(1)	-1(1)
C(19')	15(1)	21(1)	19(1)	-1(1)	-4(1)	-3(1)
C(20')	16(1)	20(1)	22(1)	-5(1)	-4(1)	0(1)
C(21')	20(1)	24(1)	23(1)	-4(1)	-5(1)	2(1)
C(22')	21(1)	26(1)	21(1)	-4(1)	-8(1)	1(1)
C(23')	19(1)	21(1)	18(1)	-3(1)	-6(1)	-4(1)
C(24')	21(1)	22(1)	18(1)	-3(1)	-5(1)	-5(1)
C(25')	18(1)	22(1)	19(1)	-4(1)	-4(1)	2(1)
C(26')	28(1)	24(1)	22(1)	-5(1)	-7(1)	-1(1)
C(27')	28(1)	24(1)	22(1)	1(1)	-2(1)	3(1)
C(28')	26(1)	35(2)	17(1)	-3(1)	-6(1)	7(1)
C(29')	24(1)	37(2)	25(1)	-9(1)	-10(1)	0(1)
C(30')	23(1)	24(1)	24(1)	-3(1)	-6(1)	-2(1)
C(31')	20(1)	21(1)	16(1)	-1(1)	-7(1)	-3(1)
C(32')	26(1)	25(1)	19(1)	-3(1)	-5(1)	-4(1)
C(33')	24(1)	24(1)	21(1)	-6(1)	-4(1)	0(1)
C(34')	17(1)	21(1)	22(1)	-7(1)	-4(1)	-1(1)
C(35')	18(1)	23(1)	21(1)	-6(1)	-4(1)	-3(1)
C(36')	24(1)	22(1)	17(1)	-3(1)	-7(1)	2(1)
C(37')	26(1)	30(1)	27(1)	-9(1)	-5(1)	-3(1)
C(38')	38(2)	29(1)	29(1)	-10(1)	-6(1)	-2(1)
C(39')	40(2)	28(1)	20(1)	-8(1)	-6(1)	11(1)
C(40')	19(1)	44(2)	37(2)	-12(1)	-2(1)	5(1)
C(41')	25(1)	29(1)	34(1)	-10(1)	-6(1)	-2(1)
C(1S)	26(1)	27(1)	26(1)	-4(1)	-8(1)	-6(1)
O(1S)	23(1)	24(1)	24(1)	-6(1)	-6(1)	-3(1)
C(2S)	28(1)	29(2)	35(2)	-10(1)	-3(1)	-3(1)
O(2S)	27(1)	33(1)	29(1)	-12(1)	-2(1)	-7(1)
C(3S)	33(2)	43(2)	32(2)	6(1)	-8(1)	-12(1)
O(3S)	23(1)	38(1)	23(1)	-1(1)	-9(1)	-6(1)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for OSMAR.

	x	y	z	U(eq)
H(1N)	3690(20)	1476(16)	3058(12)	36(7)
H(2N)	3130(20)	2595(17)	3930(13)	51(8)
H(4N)	2217(19)	2993(16)	2611(12)	31(6)
H(2)	6632(18)	-329(14)	2772(11)	26(6)
H(3)	6341(19)	138(15)	4012(11)	33(6)
H(6)	5133(17)	762(13)	5166(10)	15(5)
H(7)	3795(19)	1955(15)	5870(12)	32(6)
H(11)	1641(19)	2487(15)	6292(11)	29(6)
H(12)	1320(20)	2942(16)	7389(13)	37(7)
H(13)	1730(20)	4454(16)	7523(13)	42(7)
H(14)	2460(20)	5413(16)	6515(12)	40(7)
H(15)	2786(18)	4949(14)	5411(11)	25(6)
H(17)	1047(19)	5223(15)	4839(12)	35(7)
H(18)	704(18)	5740(14)	3592(11)	23(6)
H(21)	1040(18)	5720(15)	2213(11)	23(6)
H(22)	1339(19)	5059(15)	1067(12)	34(6)
H(26)	31(19)	3082(15)	847(12)	31(6)
H(27)	-620(20)	3628(15)	-226(11)	37(7)
H(28)	650(20)	4369(15)	-1230(12)	41(7)
H(29)	2600(20)	4471(16)	-1121(13)	43(7)
H(30)	3294(19)	3914(14)	-64(11)	30(6)
H(32)	2660(20)	1746(16)	302(13)	45(7)
H(33)	4043(16)	325(14)	749(10)	15(5)
H(37)	6595(19)	517(16)	911(12)	35(7)
H(38)	7888(19)	-723(14)	460(11)	29(6)
H(39)	7594(18)	-2264(15)	912(11)	26(6)
H(40)	6070(20)	-2586(18)	1852(13)	47(8)
H(41)	4780(20)	-1339(15)	2356(12)	33(6)
H(1N')	-1589(18)	1058(15)	3203(11)	23(6)
H(3N')	-3233(19)	2305(15)	3995(11)	30(7)
H(4N')	-2980(20)	2540(16)	2707(12)	38(7)
H(2')	118(16)	-1518(13)	3103(10)	14(5)
H(3')	-510(20)	-1323(16)	4411(12)	39(7)
H(6')	-1692(19)	-551(16)	5524(12)	33(6)
H(7')	-2734(18)	780(14)	6174(11)	26(6)
H(11')	-1780(20)	2308(15)	6116(12)	34(6)
H(12')	-1930(20)	2762(15)	7243(12)	37(7)
H(13')	-3751(19)	3534(15)	7761(12)	36(7)
H(14')	-5390(20)	3813(15)	7190(11)	31(6)
H(15')	-5303(19)	3247(14)	6128(11)	26(6)
H(17')	-4884(18)	4241(14)	5185(11)	28(6)
H(18')	-5493(18)	4726(14)	3962(10)	21(6)
H(21')	-5850(20)	4431(15)	2722(11)	31(6)
H(22')	-5280(19)	3953(15)	1499(12)	33(6)
H(26')	-2958(18)	4244(14)	506(11)	24(6)
H(27')	-3585(19)	4844(16)	-586(12)	32(6)
H(28')	-4678(18)	4036(15)	-1091(12)	31(6)

H(30)	-4336(17)	1910(17)	558(10)	17(5)
H(32')	-1660(18)	1833(14)	235(11)	25(6)
H(33')	-186(18)	453(14)	676(11)	23(6)
H(37')	-990(20)	-1490(15)	1751(12)	37(7)
H(38')	230(19)	-2710(15)	1247(11)	30(6)
H(39')	2229(19)	-2669(15)	1012(11)	26(6)
H(40')	3060(20)	-1413(14)	1229(11)	28(6)
H(41')	1867(19)	-188(15)	1703(11)	32(6)
H(1SA)	1010(20)	1379(16)	2547(13)	42(7)
H(1SB)	2130(20)	655(16)	2761(12)	37(7)
H(1SC)	1000(20)	708(15)	3315(12)	30(6)
H(1SD)	1240(20)	2026(17)	3538(13)	50(8)
H(2SA)	-1360(20)	3290(16)	4577(12)	43(7)
H(2SB)	-140(20)	3603(16)	4185(12)	36(7)
H(2SC)	-130(20)	2921(18)	4961(15)	67(9)
H(2SD)	-800(30)	1970(20)	4313(15)	65(10)
H(3SA)	-1320(20)	3363(18)	2023(14)	60(9)
H(3SC)	-550(20)	3700(20)	2474(14)	59(9)
H(3SB)	-40(30)	2761(19)	2135(14)	65(9)
H(3SD)	-970(30)	2510(20)	3302(15)	70(10)

Table 1. Crystal data and structure refinement for OCORR.

Identification code	OCORR
Empirical formula	$C_{37}H_{25}N_3O$
Crystal color, habit	deep purple rod
Crystal size	0.70 x 0.15 x 0.10 mm
Crystal system	Orthorhombic
Space group	$P2_1^2_1^2_1$
Unit cell dimensions	$a = 6.48810(10) \text{ \AA}$ $\alpha = 90^\circ$ $b = 18.0075(2) \text{ \AA}$ $\beta = 90^\circ$ $c = 22.7207(3) \text{ \AA}$ $\gamma = 90^\circ$
Volume	$2654.56(6) \text{ \AA}^3$
Peaks to determine cell	7340 with $I > 10\sigma(I)$
Z	4
Formula weight	527.60
Density (calculated)	1.320 g/cm^3
Absorption coefficient	0.080 mm^{-1}
F(000)	1104

Solution and Refinement

Solution	direct methods
Refinement method	Full-matrix least-squares on F^2
Hydrogen atoms	mixed

Hydrogen atoms were placed geometrically and refined with a riding model (including free rotation about C---C bonds for methyl groups), and with U_{iso} constrained to be 1.2 (1.5 for methyl groups) times U_{eq} of the carrier atom. Hydrogens at nitrogens were detected in difference Fourier maps and refined with a distance constraint.

Weighting scheme

$$w = 1/[\sigma^2(F_o^2) + (0.1054P)^2 + 0.0P]$$

$$\text{where } P = [F_o^2 + 2F_c^2]/3$$

Data / restraints / parameters	4659 / 2 / 380
Goodness-of-fit on F^2	0.975
Final R indices [$I > 2\sigma(I)$]	R1 = 0.0762, wR2 = 0.1721
R indices (all data)	R1 = 0.1094, wR2 = 0.1870
Observed data [$I > 2\sigma(I)$]	3247
Absolute structure parameter	0(3)
Extinction coefficient	0.0031(12)
Largest diff. peak and hole	0.364 and -0.377 $e\text{\AA}^{-3}$
Largest and mean Δ / esd	0.000 and 0.000

$$wR2 = [\sum[w(F_o^2 - F_c^2)^2] / \sum[w(F_o^2)^2]]^{1/2}$$

$$R1 = \sum||F_o| - |F_c|| / \sum|F_o|$$

Data Collection

Diffractometer	CCD area detector
θ range for data collection	1.44 to 25.00 $^{\circ}$
Index ranges	$-7 \leq h \leq 7, -18 \leq k \leq 21, -27 \leq l \leq 26$
Scan Type	phi and omega scans
Scan Time	30sec / frame
Scan Range	0.3 $^{\circ}$ in phi and omega scans
Temperature	98(2) K
Wavelength	0.71073 Å
Detector-to-sample distance	4.956 cm
Reflections collected	17980
Independent reflections	4659 ($R_{int} = 0.1272$)
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9920 and 0.9460

The data collection nominally covered over a hemisphere of reciprocal space, by a combination of three sets of exposures; each set had a different ϕ angle for the crystal and each exposure covered 0.3 $^{\circ}$ in ω . The crystal-to-detector distance was 4.956 cm. Coverage of the unique set is over 97% complete to at least 26 $^{\circ}$ in θ . Crystal decay was monitored by repeating the initial frames at the end of data collection and analyzing the duplicate reflections. No decay was observed.

References

Data Collection:

SMART Software Reference Manual (1994). Siemens Analytical
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Data Reduction:

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Structure Solution, Refinement and Graphics:

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4.2.6.8, and 4.2.4.2, Kluwer: Boston.

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H. D. Flack (1983). Acta Cryst. A39, 876-881.

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University, and the W.M.Keck Foundation for the purchase of
the X-ray instrument and computers.

Table 2. Atomic coordinates [$\times 10^4$] and equivalent isotropic displacement parameters [$\text{\AA}^2 \times 10^3$] for OCORR. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	$U(\text{eq})$
O(1)	9429(5)	638(2)	930(1)	30(1)
N(1)	13015(6)	1313(2)	857(2)	26(1)
N(2)	13120(5)	1209(2)	-263(2)	25(1)
N(3)	9619(6)	506(2)	-381(2)	22(1)
C(1)	12808(7)	1502(2)	1432(2)	26(1)
C(2)	14496(7)	1981(2)	1557(2)	30(1)
C(3)	15614(7)	2078(2)	1046(2)	32(1)
C(4)	14647(7)	1660(2)	600(2)	27(1)
C(5)	14724(7)	1591(2)	-25(2)	29(1)
C(6)	16001(7)	1880(2)	-489(2)	33(1)
C(7)	15137(6)	1656(2)	-1008(2)	27(1)
C(8)	13322(7)	1230(2)	-866(2)	27(1)
C(9)	11797(7)	891(3)	-1216(2)	27(1)
C(10)	11948(7)	952(2)	-1874(2)	26(1)
C(11)	13778(8)	777(2)	-2163(2)	32(1)
C(12)	13941(8)	878(2)	-2770(2)	36(1)
C(13)	12266(8)	1141(3)	-3088(2)	32(1)
C(14)	10457(8)	1316(2)	-2802(2)	31(1)
C(15)	10287(7)	1221(2)	-2199(2)	27(1)
C(16)	10071(7)	509(2)	-977(2)	25(1)
C(17)	8640(7)	27(2)	-1245(2)	26(1)
C(18)	7407(7)	-274(2)	-820(2)	26(1)
C(19)	7993(6)	30(2)	-263(2)	24(1)
C(20)	7187(6)	-123(2)	298(2)	24(1)
C(21)	5584(7)	-735(2)	324(2)	22(1)
C(22)	3654(7)	-655(2)	83(2)	28(1)
C(23)	2226(7)	-1234(3)	98(2)	28(1)
C(24)	2757(7)	-1904(2)	364(2)	27(1)
C(25)	4677(7)	-1990(2)	609(2)	27(1)
C(26)	6112(7)	-1412(2)	593(2)	26(1)
C(27)	7705(6)	186(2)	844(2)	24(1)
C(28)	6670(7)	119(2)	1386(2)	25(1)
C(29)	7724(7)	526(2)	1802(2)	26(1)
C(30)	9476(7)	847(2)	1528(2)	26(1)
C(31)	11097(7)	1255(3)	1765(2)	26(1)
C(32)	11026(7)	1453(2)	2404(2)	26(1)
C(33)	9429(7)	1878(3)	2638(2)	35(1)
C(34)	9387(8)	2059(3)	3233(2)	34(1)
C(35)	10946(8)	1817(3)	3602(2)	35(1)
C(36)	12543(8)	1393(3)	3379(2)	37(1)
C(37)	12569(7)	1213(3)	2782(2)	33(1)

Table 3. Bond lengths [Å] and angles [°] for OCORR.

O(1)-C(27)	1.397(5)	O(1)-C(30)	1.412(5)
N(1)-C(1)	1.356(6)	N(1)-C(4)	1.362(6)
N(2)-C(5)	1.360(6)	N(2)-C(8)	1.376(5)
N(3)-C(16)	1.385(5)	N(3)-C(19)	1.386(5)
C(1)-C(31)	1.415(6)	C(1)-C(2)	1.423(6)
C(2)-C(3)	1.381(6)	C(3)-C(4)	1.410(6)
C(4)-C(5)	1.426(6)	C(5)-C(6)	1.438(6)
C(6)-C(7)	1.366(6)	C(7)-C(8)	1.442(6)
C(8)-C(9)	1.409(6)	C(9)-C(16)	1.421(6)
C(9)-C(10)	1.503(6)	C(10)-C(11)	1.393(6)
C(10)-C(15)	1.394(6)	C(11)-C(12)	1.393(6)
C(12)-C(13)	1.389(7)	C(13)-C(14)	1.377(6)
C(14)-C(15)	1.385(6)	C(16)-C(17)	1.410(6)
C(17)-C(18)	1.367(6)	C(18)-C(19)	1.430(6)
C(19)-C(20)	1.404(6)	C(20)-C(27)	1.402(6)
C(20)-C(21)	1.516(5)	C(21)-C(22)	1.374(6)
C(21)-C(26)	1.407(6)	C(22)-C(23)	1.394(6)
C(23)-C(24)	1.393(6)	C(24)-C(25)	1.373(6)
C(25)-C(26)	1.397(6)	C(27)-C(28)	1.407(6)
C(28)-C(29)	1.377(6)	C(29)-C(30)	1.418(6)
C(30)-C(31)	1.390(6)	C(31)-C(32)	1.496(6)
C(32)-C(37)	1.389(6)	C(32)-C(33)	1.393(6)
C(33)-C(34)	1.390(6)	C(34)-C(35)	1.384(7)
C(35)-C(36)	1.384(7)	C(36)-C(37)	1.394(6)
C(27)-O(1)-C(30)	107.8(3)	C(1)-N(1)-C(4)	112.0(4)
C(5)-N(2)-C(8)	107.9(4)	C(16)-N(3)-C(19)	110.6(4)
N(1)-C(1)-C(31)	120.8(4)	N(1)-C(1)-C(2)	105.6(4)
C(31)-C(1)-C(2)	133.5(4)	C(3)-C(2)-C(1)	108.2(4)
C(2)-C(3)-C(4)	107.7(4)	N(1)-C(4)-C(3)	106.4(4)
N(1)-C(4)-C(5)	114.5(4)	C(3)-C(4)-C(5)	138.3(4)
N(2)-C(5)-C(4)	114.4(4)	N(2)-C(5)-C(6)	109.5(4)
C(4)-C(5)-C(6)	135.9(4)	C(7)-C(6)-C(5)	106.8(4)
C(6)-C(7)-C(8)	107.4(4)	N(2)-C(8)-C(9)	118.8(4)
N(2)-C(8)-C(7)	108.4(4)	C(9)-C(8)-C(7)	132.7(4)
C(8)-C(9)-C(16)	123.2(4)	C(8)-C(9)-C(10)	118.9(4)
C(16)-C(9)-C(10)	117.8(4)	C(11)-C(10)-C(15)	119.1(4)
C(11)-C(10)-C(9)	120.6(4)	C(15)-C(10)-C(9)	120.2(4)
C(10)-C(11)-C(12)	120.2(5)	C(13)-C(12)-C(11)	119.9(5)
C(14)-C(13)-C(12)	120.0(4)	C(13)-C(14)-C(15)	120.4(5)
C(14)-C(15)-C(10)	120.4(4)	N(3)-C(16)-C(17)	106.3(4)
N(3)-C(16)-C(9)	122.8(4)	C(17)-C(16)-C(9)	130.6(4)
C(18)-C(17)-C(16)	108.9(4)	C(17)-C(18)-C(19)	108.6(4)
N(3)-C(19)-C(20)	125.5(4)	N(3)-C(19)-C(18)	105.6(4)
C(20)-C(19)-C(18)	128.9(4)	C(27)-C(20)-C(19)	129.5(4)
C(27)-C(20)-C(21)	114.8(4)	C(19)-C(20)-C(21)	115.7(4)
C(22)-C(21)-C(26)	119.0(4)	C(22)-C(21)-C(20)	122.3(4)
C(26)-C(21)-C(20)	118.7(4)	C(21)-C(22)-C(23)	121.3(4)
C(24)-C(23)-C(22)	119.5(4)	C(25)-C(24)-C(23)	119.9(4)
C(24)-C(25)-C(26)	120.6(4)	C(25)-C(26)-C(21)	119.7(4)
O(1)-C(27)-C(20)	123.2(4)	O(1)-C(27)-C(28)	108.1(4)
C(20)-C(27)-C(28)	128.8(4)	C(29)-C(28)-C(27)	108.5(4)
C(28)-C(29)-C(30)	108.3(4)	C(31)-C(30)-O(1)	121.9(4)

C(31)-C(30)-C(29)	130.7(4)	O(1)-C(30)-C(29)	107.2(4)
C(30)-C(31)-C(1)	123.6(4)	C(30)-C(31)-C(32)	118.5(4)
C(1)-C(31)-C(32)	117.8(4)	C(37)-C(32)-C(33)	118.1(4)
C(37)-C(32)-C(31)	120.3(4)	C(33)-C(32)-C(31)	121.6(4)
C(34)-C(33)-C(32)	120.9(4)	C(35)-C(34)-C(33)	120.1(5)
C(36)-C(35)-C(34)	120.0(4)	C(35)-C(36)-C(37)	119.5(5)
C(32)-C(37)-C(36)	121.4(5)		

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters [$\text{\AA}^2 \times 10^3$] for OCORR.

The anisotropic displacement factor exponent takes the form:

$$-2\pi^2 [(ha^*)^2 U_{11} + \dots + 2hka^* b^* U_{12}]$$

	U11	U22	U33	U23	U13	U12
O(1)	37(2)	19(2)	34(2)	-1(2)	-5(2)	0(1)
N(1)	29(2)	14(2)	36(2)	-5(2)	-2(2)	1(2)
N(2)	28(2)	16(2)	32(2)	4(2)	-2(2)	0(2)
N(3)	26(2)	15(2)	26(2)	1(2)	0(2)	-2(2)
C(1)	33(3)	11(2)	33(3)	-6(2)	-5(2)	5(2)
C(2)	39(3)	12(2)	38(3)	1(2)	-1(2)	-2(2)
C(3)	32(3)	12(2)	53(3)	2(2)	-9(2)	-4(2)
C(4)	31(2)	12(2)	38(3)	2(2)	3(2)	1(2)
C(5)	30(2)	13(2)	46(3)	6(2)	0(2)	-1(2)
C(6)	33(3)	17(3)	49(3)	9(2)	-1(2)	-2(2)
C(7)	32(3)	13(2)	36(3)	2(2)	5(2)	1(2)
C(8)	31(2)	15(3)	36(3)	5(2)	4(2)	3(2)
C(9)	29(3)	19(3)	32(3)	1(2)	6(2)	4(2)
C(10)	34(3)	8(2)	35(3)	1(2)	3(2)	-6(2)
C(11)	47(3)	12(3)	38(3)	7(2)	7(2)	-3(2)
C(12)	56(4)	13(3)	39(3)	-2(2)	16(3)	-4(2)
C(13)	54(3)	13(3)	29(3)	1(2)	1(2)	-8(2)
C(14)	45(3)	15(3)	33(3)	1(2)	-2(2)	-6(2)
C(15)	37(3)	14(2)	31(3)	-1(2)	2(2)	-3(2)
C(16)	35(3)	18(3)	22(2)	0(2)	3(2)	1(2)
C(17)	36(3)	17(3)	25(2)	-3(2)	0(2)	3(2)
C(18)	31(2)	12(2)	36(3)	0(2)	-3(2)	-4(2)
C(19)	29(2)	13(2)	31(2)	-3(2)	5(2)	-1(2)
C(20)	31(2)	1(2)	30(2)	4(2)	-1(2)	-3(2)
C(21)	31(2)	11(2)	22(2)	-4(2)	6(2)	-5(2)
C(22)	35(3)	11(2)	37(3)	1(2)	0(2)	3(2)
C(23)	39(3)	19(3)	27(3)	-1(2)	1(2)	-5(2)
C(24)	45(3)	15(3)	22(2)	-5(2)	6(2)	-12(2)
C(25)	46(3)	9(2)	26(2)	1(2)	2(2)	-4(2)
C(26)	34(2)	20(3)	22(2)	0(2)	4(2)	0(2)
C(27)	23(2)	12(2)	37(3)	3(2)	-2(2)	-1(2)
C(28)	34(3)	9(2)	33(3)	2(2)	3(2)	-3(2)
C(29)	37(3)	17(3)	24(2)	-3(2)	2(2)	4(2)
C(30)	35(3)	20(3)	22(2)	-6(2)	-4(2)	8(2)
C(31)	33(3)	15(3)	31(3)	-6(2)	-4(2)	3(2)
C(32)	35(3)	9(2)	34(3)	-7(2)	-2(2)	-2(2)
C(33)	38(3)	29(3)	37(3)	-2(2)	-4(2)	8(2)
C(34)	47(3)	22(3)	34(3)	-1(2)	-2(2)	3(2)
C(35)	57(3)	19(3)	28(3)	-7(2)	-6(2)	-1(2)
C(36)	51(3)	27(3)	33(3)	-4(2)	-9(2)	7(2)
C(37)	38(3)	23(3)	38(3)	-13(2)	-5(2)	6(2)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for OCORR.

	x	y	z	U(eq)
H(1N)	12060 (60)	1120 (30)	679 (19)	37 (15)
H(3N)	10530 (80)	630 (40)	-150 (20)	80 (20)
H(2A)	14802	2196	1929	35
H(3A)	16817	2374	1003	39
H(6A)	17212	2171	-444	39
H(7A)	15639	1762	-1392	33
H(11A)	14917	589	-1947	39
H(12A)	15198	766	-2966	43
H(13A)	12367	1201	-3502	38
H(14A)	9320	1502	-3020	37
H(15A)	9031	1340	-2006	33
H(17A)	8548	-72	-1655	31
H(18A)	6340	-626	-884	32
H(22A)	3285	-198	-96	33
H(23A)	901	-1171	-73	34
H(24A)	1792	-2300	376	33
H(25A)	5033	-2447	791	33
H(26A)	7437	-1475	764	31
H(28A)	5449	-160	1453	30
H(29A)	7343	582	2203	31
H(33A)	8353	2046	2387	42
H(34A)	8287	2348	3386	41
H(35A)	10919	1943	4008	41
H(36A)	13615	1225	3631	44
H(37A)	13665	919	2632	40