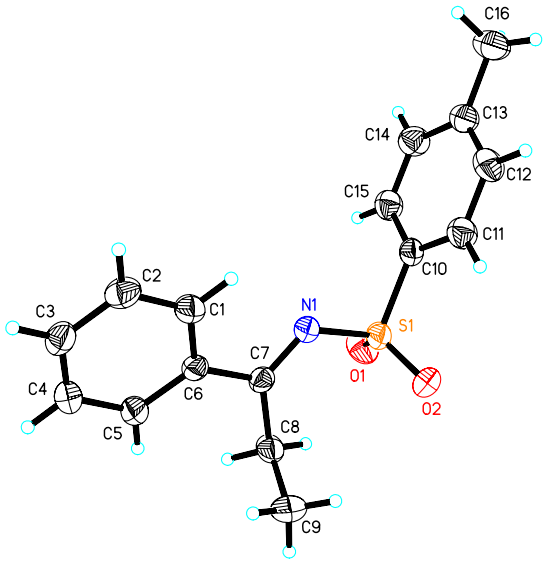
Supplementary Information for OBC paper b802867b



Molecular structure of **3o**

Table 1. Crystal data and structure refinement for complex **3o**

Identification code	complex 3q	
Empirical formula	C16 H17 N O2 S	
Formula weight	287.37	
Temperature	293(2) K	
Wavelength	0.71073 A	
Crystal system, space group	Monoclinic, P2(1)/c	
Unit cell dimensions	a = 8.6787(9) A	alpha = 90 deg.
	b = 13.9781(15) A	beta = 99.664(2) deg.
	c = 12.3242(13) A	gamma = 90 deg.
Volume	1473.9(3) A^3	
Z, Calculated density	4, 1.295 Mg/m^3	
Absorption coefficient	0.220 mm^-1	
F(000)	608	
Crystal size	0.496 x0.415x 0.347 mm	
Theta range for data collection	4.761 to 53.719 deg.	
Limiting indices	-11<=h<=11, -17<=k<=17, -15<=l<=7	
Reflections collected / unique	8462 / 3342 [R(int) = 0.0658]	
Absorption correction	empirical	
Max. and min. transmission	1.0000 and 0.73594	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3199 / 0 / 183	
Goodness-of-fit on F^2	0.970	
Final R indices [I>2sigma(I)]	R1 = 0.0498, wR2 = 0.1359	
R indices (all data)	R1 = 0.0617, wR2 = 0.1425	

Table 2. Atomic coordinates and equivalent isotropic displacement parameters for complex **3o**.

	x	y	z	U(eq)
S(1)	0.70189(5)	0.12908(3)	0.68264(4)	0.05215(19)
O(1)	0.82545(17)	0.17497(10)	0.75579(12)	0.0721(4)
O(2)	0.61536(19)	0.18363(10)	0.59503(11)	0.0727(4)
N(1)	0.57779(16)	0.07667(10)	0.75177(11)	0.0473(3)
C(1)	0.3540(2)	-0.02522(13)	0.83880(15)	0.0538(4)
H(1)	0.3919	-0.0510	0.7789	0.065
C(2)	0.2599(2)	-0.07962(14)	0.89330(17)	0.0618(5)
H(2)	0.2356	-0.1421	0.8708	0.074
C(3)	0.2011(2)	-0.04192(15)	0.98151(16)	0.0591(5)
H(3)	0.1370	-0.0788	1.0183	0.071
C(4)	0.2375(2)	0.04955(15)	1.01427(16)	0.0638(5)
H(4)	0.1976	0.0752	1.0734	0.077
C(5)	0.3330(2)	0.10438(13)	0.96039(15)	0.0561(5)
H(5)	0.3571	0.1667	0.9838	0.067
C(6)	0.39360(18)	0.06783(11)	0.87175(12)	0.0429(4)
C(7)	0.50276(19)	0.12406(11)	0.81540(12)	0.0434(4)
C(8)	0.5115(2)	0.23092(12)	0.83421(15)	0.0577(5)
H(8 A)	0.5202	0.2440	0.9123	0.069
H(8B)	0.6043	0.2559	0.8099	0.069
C(9)	0.3699(3)	0.28060(16)	0.7732(2)	0.0863(7)
H(9A)	0.3670	0.2733	0.6954	0.129
H(9B)	0.3744	0.3474	0.7917	0.129
H(9C)	0.2775	0.2529	0.7934	0.129
C(10)	0.7818(2)	0.02936(13)	0.62584(14)	0.0479(4)
C(11)	0.7207(2)	-0.00175(15)	0.52205(15)	0.0609(5)
H(11)	0.6355	0.0294	0.4812	0.073
C(12)	0.7864(2)	-0.07952(16)	0.47872(17)	0.0663(5)
H(12)	0.7442	-0.1003	0.4083	0.080
C(13)	0.9122(2)	-0.12721(13)	0.53634(17)	0.0568(5)
C(14)	0.9711(2)	-0.09485(15)	0.64091(18)	0.0643(5)
H(14)	1.0555	- 0.1266	0.6820	0.077
C(15)	0.9086(2)	-0.01733(15)	0.68565(15)	0.0601(5)
H(15)	0.9512	0.0038	0.7559	0.072
C(16)	0.9841(3)	-0.21283(16)	0.4900(2)	0.0794(7)
H(16A)	0.9543	-0.2699	0.5244	0.119
H(16B)	1.0959	-0.2068	0.5039	0.119
H(16C)	0.9480	-0.2163	0.4121	0.119

Table 3. Anisotropic displacement parameters (A^2 x 10^3) for complex **3o.**

	U11	U22	U33	U23	U13	U12
S(1)	0.0673(3)	0.0436(3)	0.0493(3)	0.00107(18)	0.0209(2)	-0.00358(19)
O(1)	0.0735(9)	0.0702(9)	0.0769(9)	-0.0212(7)	0.0253(7)	-0.0205(7)
O (2)	0.1041(11)	0.0571(8)	0.0621(9)	0.0195(6)	0.0288(8)	0.0168(7)
N(1)	0.0572(8)	0.0422(7)	0.0447(8)	0.0019(6)	0.0147(6)	0.0009(6)
C(1)	0.0607(10)	0.0460(9)	0.0564(11)	-0.0042(8)	0.0148(8)	-0.0010(8)
C(2)	0.0620(11)	0.0459(10)	0.0768(14)	0.0016(9)	0.0094(10)	-0.0075(8)
C(3)	0.0530(10)	0.0609(11)	0.0644(12)	0.0159(9)	0.0131(9)	-0.0017(9)
C(4)	0.0757(12)	0.0643(12)	0.0572(12)	0.0034(9)	0.0278(10)	0.0038(10)
C(5)	0.0712(12)	0.0483(9)	0.0522(11)	-0.0009(8)	0.0199(9)	0.0006(9)
C(6)	0.0471(8)	0.0418(8)	0.0386(8)	0.0032(7)	0.0039(7)	0.0054(7)
C(7)	0.0516(9)	0.0405(9)	0.0367(9)	0.0022(6)	0.0038(7)	0.0018(7)
C(8)	0.0784(12)	0.0412(9)	0.0588(11)	-0.0094(8)	0.0274(9)	-0.0081(9)
C(9)	0.1159(19)	0.0514(11)	0.0988(17)	0.0104(12)	0.0388(15)	0.0249(13)
C(10)	0.0545(9)	0.0485(9)	0.0438(9)	0.0023(7)	0.0172(7)	-0.0027(8)
C(11)	0.0641(11)	0.0665(12)	0.0506(11)	-0.0028(9)	0.0052(9)	0.0064(9)
C(12)	0.0763(12)	0.0696(13)	0.0528(11)	-0.0150(10)	0.0100(10)	-0.0030(11)
C(13)	0.0579(10)	0.0488(10)	0.0694(13)	-0.0017(8)	0.0266(10)	-0.0069(8)
C(14)	0.0592(11)	0.0654(12)	0.0671(13)	0.0004(10)	0.0077(9)	0.0067(10)
C(15)	0.0648(11)	0.0660(12)	0.0478(10)	-0.0018(9)	0.0050(9)	0.0035(9)
C(16)	0.0827(14)	0.0583(12)	0.1058(18)	-0.0139(12)	0.0403(13)	-0.0033(11)

Table 4. Bond lengths [A] and angles [deg] for complex **3o**.

S(1)-O(2)	1.4280(14
S(1)-O(1)	1.4316(15)
S(1)-N (1)	1.6525(13)
S(1)-C(10)	1.7543(18)
N(1)-C(7)	1.284(2)
C(1)-C(2)	1.371(2)
C(1)-C(6)	1.388(2)
C(1)-H(1)	0.9300
C(2)-C(3)	1.381(3)
C(2)-H(2)	0.9300
C(3)-C(4)	1.362(3)
C(3)-H(3)	0.9300
C(4)-C(5)	1.379(2)
C(4)-H(4)	0.9300
C(5)-C(6)	1.387(2)
C(5)-H(5)	0.9300
C(6)-C(7)	1.489(2)
C(7)-C(8)	1.512(2)
C(8)-C(9)	1.499(3)
C(8)-H(8A)	0.9700
C(8)-H(8B)	0.9700
C (9)-H(9A)	0.9600
C(9)-H(9B)	0.9600
C(9)-H(9C)	0.9600
C(10)-C(11)	1.371(3)
C(10)-C(15)	1.381(3)
C(11)-C(12)	1.376(3)
C(11)-H(11)	0.9300
C(12)-C(13)	1.371(3)
C(12)-H(12)	0.9300
C(13)-C(14)	1.380(3)
C(13)-C(16)	1.506(3)
C(14)-C(15)	1.369(3)
C(14)-H(14)	0.9300
C(15)-H(15)	0.9300
C(16)-H(16A)	0.9600
C(16)-H(16B)	0.9600
C(16)-H(16C)	0.9600
O(2)-S(1)-O(1)	118.69(10)
O(2)-S(1)-N(1)	108.73(8)
O(1)-S(1)-N(1)	110.99(8)
O(2)-S(1)-C(10)	108.40(8)
O(1)-S(1)-C(10)	107.61(8)

N(1)-S(1)-C(10)	100.90(7)
C(7)-N(1)-S(1)	121.82(11)
C(2)-C(1)-C(6)	120.97(17)
C(2)-C(1)-H(1)	119.5
C(6)-C(1)-H(1)	119.5
C(1)-C(2)-C(3)	120.21(17)
C(1)-C(2)-H(2)	119.9
C(3)-C(2)-H(2)	119.9
C(4)-C(3)-C(2)	119.60(17)
C(4)-C(3)-H(3)	120.2
C(2)-C(3)-H(3)	120.2
C(3)-C(4)-C(5)	120.48(18)
C(3)-C(4)-H(4)	119.8
C(5)-C (4)-H(4)	119.8
C(4)-C(5)-C(6)	120.85(18)
C(4)-C(5)-H(5)	119.6
C(6)-C(5)-H(5)	119.6 .
C(5)-C(6)-C(1)	117.87(16)
C(5)-C(6)-C(7)	121.86(15)
C(1)-C(6)-C(7)	120.23(15)
N(1)-C(7)-C(6)	116.10(14)
N(1)-C(7)-C(8)	125.87(15)
C(6)-C(7)-C(8)	118.00(14)
C(9)-C(8)-C(7)	111.40(16)
C(9)-C(8)-H(8A)	109.3
C(7)-C(8)-H(8A)	109.3
C(9)-C(8)-H(8B)	109.3
C(7)-C(8)-H(8B)	109.3
H(8A)-C(8)-H(8B)	108.0
C(8)-C(9)-H(9A)	109.5
C(8)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	109.5
C(8)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5
C(11)-C(10)-C(15)	119.80(17)
C(11)-C(10)-S(1)	120.49(14)
C(15)-C(10)-S(1)	119.71(14)
C(10)-C(11)-C(12)	119.48(18)
C(10)-C(11)-H(11)	120.3
C(12)-C(11)-H(11)	120.3
C(13)-C(12)-C(11)	121.92(18)
C(13)-C(12)-H(12)	119.0
C(11)-C(12)-H(12)	119.0
C(12)-C(13)-C(14)	117.51(18)
C(12)-C(13)-C(16)	122.3(2)

C(14)-C (13)-C(16)	120.17(19)
C(15)-C(14)-C(13)	121.73(18)
C(15)-C(14)-H(14)	119.1
C(13)-C(14)-H(14)	119.1
C(14)-C(15)-C(10)	119.56(18)
C(14)-C(15)-H(15)	120.2
C(10)-C(15)-H(15)	120.2
C(13)-C(16) -H (16A)	109.5
C(13)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5 .
C(13)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5