

SUPPLEMENTARY DATA

1. Bond lengths for structures 8, 9.HCl, 10, 11 and 12

	8 X = O	9 X = NHMe	10 X = S	11 X = SO	12 X = SO ₂
C(1)-O(1)	1.3740(16)	1.368(2)	1.3809(14)	1.382(2)	1.368(2)
C(2)-O(2)	1.3799(16)	1.382(2)	1.3792(14)	1.375(2)	1.378(2)
C(3)-O(3)	1.3654(18)	1.370(2)	1.3644(15)	1.366(2)	1.365(2)
C(4)-H(4)	0.948(17)	0.91(2)	0.947(17)	0.96(2)	0.97(2)
C(4A)-C(5)	1.5101(19)	1.503(3)	1.5046(17)	1.500(2)	1.507(2)
C(5)-X(6)	1.4395(16)	1.512(2)	1.8267(13)	1.8289(19)	1.7886(19)
C(5)-H(5A)	0.966(17)	1.01(2)	0.980(16)	0.99(2)	0.95(2)
C(5)-H(5B)	0.990(15)	0.95(2)	0.958(17)	0.97(2)	0.99(2)
C(11A)-C(11B)	1.479(3)	1.485(3)	1.489(2)	1.489(3)	1.490(2)
C(7)-C(7A)	1.5101(19)	1.500(3)	1.5046(17)	1.500(2)	1.497(2)
C(7)-X(6)	1.4395(16)	1.514(3)	1.8267(13)	1.8289(19)	1.7830(18)
C(7)-H(7A)	0.966(17)	0.95(2)	0.980(16)	0.99(2)	1.00(2)
C(7)-H(7B)	0.990(15)	0.98(2)	0.958(17)	0.97(2)	0.94(2)
C(8)-H(8)	0.948(17)	0.93(2)	0.947(17)	0.96(2)	0.98(2)
C(9)-O(9)	1.3654(18)	1.367(2)	1.3644(15)	1.366(2)	1.372(2)
C(10)-O(10)	1.3799(16)	1.383(2)	1.3792(14)	1.375(2)	1.381(2)
C(11)-O(11)	1.3740(16)	1.377(2)	1.3809(14)	1.382(2)	1.378(2)
C(12)-O(1)	1.4359(17)	1.446(2)	1.4323(17)	1.421(3)	1.446(2)
C(13)-O(2)	1.4414(18)	1.427(3)	1.4218(16)	1.425(2)	1.405(3)
C(14)-O(3)	1.4337(19)	1.435(3)	1.4318(16)	1.425(2)	1.435(2)
C(15)-O(9)	1.4337(19)	1.429(3)	1.4318(16)	1.425(2)	1.418(3)
C(16)-O(10)	1.4414(18)	1.426(3)	1.4218(16)	1.425(2)	1.433(3)
C(17)-O(11)	1.4359(17)	1.433(3)	1.4323(17)	1.421(3)	1.437(3)
C(18)-N(6)		1.492(3)			
N(6)-H(6)		0.94(2)			
O(12)-H(12D)		1.13(10)			
O(12)-H(12E)		0.89(7)			
O(6)-S(6)				1.378(3)	
O(6')-S(6)				1.378(3)	
O(6A)-S(6)					1.4425(13)
O(6B)-S(6)					1.4472(13)

2. Bond angles for structures 8, 9.HCl, 10, 11 and 12

	8 X = O	9 X = NHMe	10 X = S	11 X = SO	12 X = SO ₂
O(1)-C(1)-C(2)	121.96(12)	122.52(16)	118.19(10)	118.59(15)	121.41(15)
O(1)-C(1)-C(11B)	117.51(12)	117.25(16)	120.61(11)	119.94(15)	118.02(15)
O(2)-C(2)-C(1)	119.42(12)	121.44(17)	119.81(11)	118.48(15)	119.35(15)
O(2)-C(2)-C(3)	120.51(13)	118.88(16)	120.63(11)	122.16(16)	120.41(15)
O(3)-C(3)-C(4)	124.91(13)	124.38(18)	123.97(11)	123.96(16)	124.29(16)
O(3)-C(3)-C(2)	115.19(12)	115.34(15)	116.31(11)	116.40(15)	116.03(15)
C(3)-C(4)-H(4)	121.3(10)	121.3(12)	119.1(10)	122.0(13)	119.8(11)
C(4A)-C(4)-H(4)	118.5(10)	119.0(12)	120.4(10)	117.3(13)	120.2(11)
C(4)-C(4A)-C(5)	120.10(12)	119.31(18)	119.85(11)	120.05(16)	118.22(16)
C(11B)-C(4A)-C(5)	119.01(13)	119.75(17)	119.63(11)	119.39(15)	120.18(15)
C(4A)-C(5)-X(6)	113.55(11)	112.92(16)	113.36(9)	114.13(13)	112.05(13)
C(4A)-C(5)-H(5A)	111.8(9)	108.9(10)	112.6(10)	112.2(12)	114.2(12)
X(6)-C(5)-H(5A)	104.4(9)	106.4(11)	104.0(10)	103.8(13)	103.2(12)
C(4A)-C(5)-H(5B)	109.4(8)	109.4(12)	110.3(9)	110.1(13)	113.0(11)
X(6)-C(5)-H(5B)	110.0(9)	107.5(12)	106.6(9)	106.5(13)	104.1(11)
H(5A)-C(5)-H(5B)	107.4(12)	111.8(16)	109.7(13)	109.8(18)	109.4(16)
C(5)-X(6)-C(7)	<i>114.24(14)</i>	113.86(15)	<i>100.25(8)</i>	<i>98.93(12)</i>	102.71(9)
C(7A)-C(7)-X(6)	<i>113.55(11)</i>	113.30(16)	<i>113.36(9)</i>	<i>114.13(13)</i>	111.40(13)
C(7A)-C(7)-H(7A)	<i>111.8(9)</i>	111.5(12)	<i>112.6(10)</i>	<i>112.2(12)</i>	112.0(11)
X(6)-C(7)-H(7A)	<i>104.4(9)</i>	104.5(12)	<i>104.0(10)</i>	<i>103.8(13)</i>	105.0(11)
C(7A)-C(7)-H(7B)	<i>109.4(8)</i>	108.5(11)	<i>110.3(9)</i>	<i>110.1(13)</i>	111.6(12)
X(6)-C(7)-H(7B)	<i>110.0(9)</i>	106.8(11)	<i>106.6(9)</i>	<i>106.5(13)</i>	106.6(12)
H(7A)-C(7)-H(7B)	<i>107.4(12)</i>	112.0(16)	<i>109.7(13)</i>	<i>109.8(18)</i>	110.0(17)
C(8)-C(7A)-C(7)	<i>120.10(12)</i>	120.47(17)	<i>119.85(11)</i>	<i>120.05(16)</i>	119.63(16)
C(9)-C(8)-H(8)	<i>121.3(10)</i>	121.3(13)	<i>119.1(10)</i>	<i>122.0(13)</i>	120.3(13)
C(7A)-C(8)-H(8)	<i>118.5(10)</i>	118.4(13)	<i>120.4(10)</i>	<i>117.3(13)</i>	119.8(13)
O(9)-C(9)-C(8)	<i>124.91(13)</i>	125.35(18)	<i>123.97(11)</i>	<i>123.96(16)</i>	123.73(18)
O(9)-C(9)-C(10)	<i>115.19(12)</i>	115.15(17)	<i>116.31(11)</i>	<i>116.40(15)</i>	116.37(17)
C(18)-N(6)-C(5)		111.63(16)			
C(18)-N(6)-C(7)		110.15(16)			
C(18)-N(6)-H(6)		106.0(13)			
C(5)-N(6)-H(6)		106.7(13)			
C(7)-N(6)-H(6)		108.2(13)			
H(12D)-O(12)-H(12E)		107(6)			
O(6)-S(6)-O(6')				<i>115.5(2)</i>	
O(6)-S(6)-C(5)				109.07(13)	
O(6')-S(6)-C(5)				<i>111.52(13)</i>	
O(6A)-S(6)-O(6B)					117.37(8)
O(6A)-S(6)-C(7)					107.69(8)
O(6B)-S(6)-C(7)					109.37(9)
O(6A)-S(6)-C(5)					110.55(9)
O(6B)-S(6)-C(5)					108.15(9)

3. Dihedral angles for structures 8, 9.HCl, 10, 11 and 12

	8 X = O	9 X = NHMe	10 X = S	11 X = SO	12 X = SO ₂
C(5)-C(4A)-C(11B)-C(1)	-175.72(12)	-176.93(17)	-177.70(11)	-176.77(16)	-175.74(15)
C(5)-C(4A)-C(11B)-C(11A)	0.8(2)	7.7(3)	1.38(19)	0.9(3)	0.8(3)
C(3)-C(4)-C(4A)-C(5)	-179.56(13)	-178.07(18)	179.54(11)	178.45(16)	177.24(16)
X(6)-C(5)-C(4A)-C(4)	-108.00(14)	-114.1(2)	-104.20(12)	-102.63(17)	-104.21(17)
X(6)-C(7)-C(7A)-C(8)	-108.00(14)	-109.0(2)	-104.20(12)	-102.63(17)	-99.79(18)
X(6)-C(5)-C(4A)-C(11B)	72.78(16)	68.6(2)	76.23(13)	77.04(19)	75.08(19)
X(6)-C(7)-C(7A)-C(11A)	72.78(16)	73.1(2)	76.23(13)	77.04(19)	80.52(18)
C(4A)-C(5)-X(6)-C(7)	-43.57(9)	-50.4(2)	-44.52(7)	-44.99(11)	-44.62(15)
C(7A)-C(7)-X(6)-C(5)	-43.57(9)	-35.2(2)	-44.52(7)	-44.99(11)	-44.36(15)
C(7)-C(7A)-C(8)-C(9)	-179.56(13)	-177.77(19)	179.54(11)	178.45(16)	-177.14(17)
C(7)-C(7A)-C(11A)-C(11)	-175.72(12)	-179.67(18)	-177.70(11)	-176.77(16)	176.87(16)
C(7)-C(7A)-C(11A)-C(11B)	0.8(2)	-6.7(3)	1.38(19)	0.9(3)	-6.0(2)
C(7A)-C(11A)-C(11B)-C(4A)	-49.8	-51.1(3)	-59.9	-58.8	-54.9(2)
C(11)-C(11A)-C(11B)-C(4A)	126.6	121.7(2)	119.0	118.8	122.14(19)
C(7A)-C(11A)-C(11B)-C(1)	126.6	133.6(2)	119.0	118.8	121.53(19)
C(11)-C(11A)-C(11B)-C(1)	-57.0	-53.6(3)	-61.9	-63.6	-61.4(2)
O(1)-C(1)-C(2)-O(2)	4.15(18)	6.5(3)	4.46(17)	4.9(2)	3.4(2)
O(1)-C(1)-C(2)-C(3)	179.30(12)	-175.10(17)	-178.70(10)	-179.16(15)	-177.05(16)
O(1)-C(1)-C(11B)-C(4A)	176.34(11)	169.95(16)	177.17(10)	176.92(15)	173.71(15)
O(1)-C(1)-C(11B)-C(11A)	-0.1(2)	-14.8(3)	-1.89(19)	-0.7(3)	-2.8(2)
O(2)-C(2)-C(3)-O(3)	0.43(18)	1.0(2)	-3.94(17)	-4.1(3)	1.3(2)
O(3)-C(3)-C(4)-C(4A)	174.07(12)	178.09(17)	-179.48(11)	-179.52(16)	-179.51(17)
O(3)-C(3)-C(2)-C(1)	-174.67(11)	-177.41(16)	179.25(10)	-179.84(15)	-178.30(15)
C(1)-C(2)-C(3)-C(4)	3.6(2)	5.2(3)	0.38(18)	1.6(3)	3.6(3)
C(2)-C(3)-C(4)-C(4A)	-4.0(2)	-4.7(3)	-0.70(19)	-1.1(3)	-1.6(3)
C(3)-C(4)-C(4A)-C(11B)	-0.4(2)	-0.8(3)	-0.89(19)	-1.2(3)	-2.0(3)
C(4)-C(4A)-C(11B)-C(1)	5.07(19)	5.8(3)	2.73(18)	2.9(3)	3.5(3)
C(4A)-C(11B)-C(1)-C(2)	-5.46(19)	-5.3(3)	-3.07(18)	-2.4(3)	-1.5(3)
C(4)-C(4A)-C(11B)-C(11A)	-178.37(13)	-169.61(17)	-178.19(12)	-179.43(17)	-179.91(16)
C(2)-C(1)-C(11B)-C(11A)	178.10(13)	169.96(17)	177.87(12)	180.00(17)	-177.97(16)
O(11)-C(11)-C(10)-O(10)	4.15(18)	-1.1(3)	4.46(17)	4.9(2)	0.3(3)
O(10)-C(10)-C(9)-O(9)	0.43(18)	3.1(3)	-3.94(17)	-4.1(3)	1.4(3)
C(11)-C(10)-C(9)-C(8)	3.6(2)	1.1(3)	0.38(18)	1.6(3)	-2.7(3)
C(10)-C(9)-C(8)-C(7A)	-4.0(2)	-1.9(3)	-0.70(19)	-1.1(3)	0.3(3)
C(9)-C(8)-C(7A)-C(11A)	-0.4(2)	0.1(3)	-0.89(19)	-1.2(3)	2.5(3)
C(8)-C(7A)-C(11A)-C(11)	5.07(19)	2.4(3)	2.73(18)	2.9(3)	-2.8(3)
C(7A)-C(11A)-C(11)-C(10)	-5.46(19)	-3.2(3)	-3.07(18)	-2.4(3)	0.3(3)
C(4A)-C(5)-N(6)-C(18)		75.0(2)			
C(7A)-C(7)-N(6)-C(18)		-161.48(17)			
C(4A)-C(5)-S(6)-O(6)				71.57(19)	
C(4A)-C(5)-S(6)-O(6')				-159.66(17)	
C(4A)-C(5)-S(6)-O(6A)					70.03(14)
C(4A)-C(5)-S(6)-O(6B)					-160.20(12)
C(7A)-C(7)-S(6)-O(6A)					-161.07(12)
C(7A)-C(7)-S(6)-O(6B)					70.34(15)