Supplementary Material (ESI) for New Journal of Chemistry

Supplementary Information

Table 1. Bond lengths [A] and angles [deg] for AMPH-SULPH.

phase II 120K		**phase I 336K**	
C(1A)-C(2A)	1.3834(12)	S(1)-O(4)#1	1.337(3)
C(1A)-C(6A)	1.3918(11)	S(1)-O(4)	1.337(3)
C(1A)-H(1A)	0.943(8)	S(1)-O(1)	1.365(2)
C(2A)-C(3A)	1.3701(14)	S(1)-O(1)#1	1.365(2)
C(2A)-H(2A)	0.975(8)	S(1)-O(3)#1	1.437(2)
C(3A)-C(4A)	1.3802(15)	S(1)-O(3)	1.437(2)
C(3A)-H(3A)	0.962(8)	S(1)-O(2)	1.489(3)
C(4A)-C(5A)	1.3860(12)	S(1)-O(2)#1	1.489(3)
C(4A)-H(4A)	0.945(8)	O(1)-O(1)#1	1.419(5)
C(5A)-C(6A)	1.3836(12)	O(1)-O(3)	1.770(4)
C(5A)-H(5A)	0.914(7)	O(2)-O(4)	1.344(5)
C(6A)-C(7A)	1.5022(10)	O(2)-O(3)#1	1.810(5)
C(7A)-C(8A)	1.5271(11)	O(3)-O(4)	1.576(4)
C(7A)-H(7A1)	0.909(9)	O(3)-O(2)#1	1.810(5)
C(7A)-H(7A2)	0.934(8)	O(4)-O(4)#1	1.617(7)
C(8A)-N(1A)	1.5006(9)	N(1)-C(8)	1.5073(17)
C(8A)-C(9A)	1.5126(11)	N(1)-H(1A)	0.8900
C(8A)-H(8A)	0.964(8)	N(1)-H(1B)	0.8900
C(9A)-H(9A1)	0.890(8)	N(1)-H(1C)	0.8900
C(9A)-H(9A2)	0.990(6)	C(9)-C(8)	1.4942
C(9A)-H(9A3)	0.919(8)	C(9)-H(9A)	0.9600
N(1A)-H(1A1)	0.870(8)	C(9)-H(9B)	0.9600
N(1A)-H(1A2)	0.945(9)	C(9)-H(9C)	0.9600
N(1A)-H(1A3)	0.872(8)	C(8)-C(7)	1.498(2)
C(1B)-C(2B)	1.3839(12)	C(8)-H(8)	1.0483
C(1B)-C(6B)	1.3837(11)	C(6)-C(5)	1.341(3)
C(1B)-H(1B)	0.896(8)	C(6)-C(1)	1.335(3)
C(2B)-C(3B)	1.3719(14)	C(6)-C(7)	1.482(2)
C(2B)-H(2B)	0.967(7)	C(1)-C(2)	1.391(4)
C(3B)-C(4B)	1.3806(14)	C(1)-H(1)	0.9100
C(3B)-H(3B)	0.936(7)	C(7)-H(7A)	0.9600
C(4B)-C(5B)	1.3928(12)	C(7)-H(7B)	0.9600
C(4B)-H(4B)	0.965(8)	C(3)-C(4)	1.328(5)
C(5B)-C(6B)	1.3933(12)	C(3)-C(2)	1.341(5)
C(5B)-H(5B)	0.953(7)	C(3)-H(3)	0.9100
C(6B)-C(7B)	1.5059(11)	C(2)-H(2)	0.9100
C(7B)-C(8B)	1.5300(11)	C(4)-C(5)	1.397(3)
C(7B)-H(7B1)	0.972(9)	C(4)-H(4)	0.9100
C(7B)-H(7B2)	0.956(9)	C(5)-H(5)	0.9100
C(8B)-N(1B)	1.5013(9)		
C(8B)-C(9B)	1.5138(11)		
C(8B)-H(8B)	0.936(7)		
C(9B)-H(9B1)	0.912(8)		
C(9B)-H(9B2)	1.014(6)		

C(9B)-H(9B3)	0.936(8)		
N(1B)-H(1B1)	0.925(7)		
N(1B)-H(1B2)	0.888(8)		
N(1B)-H(1B3)	0.898(9)		
C(1C)-C(6C)	1.3844(11)		
C(1C)-C(2C)	1.3893(12)		
C(1C)-H(1C)	1.066(8)		
C(2C)-C(3C)	1.3853(13)		
C(2C)-H(2C)	1.080(8)		
C(3C)-C(4C)	1.3776(12)		
C(3C)-H(3C)	0.984(9)		
C(4C)-C(5C)	1.3921(13)		
C(4C)-H(4C)	1.052(8)		
C(5C)-C(6C)	1.3832(12)		
C(5C)-H(5C)	1.072(8)		
C(6C)-C(7C)	1.5208(11)		
C(7C)-C(8C)	1.5210(12)		
C(7C)-H(7C1)	0.983(8)		
C(7C)-H(7C2)	0.946(8)		
C(8C)-N(1C)	1.5031(9)		
C(8C)-C(9C)	1.5050(13)		
C(8C)-H(8C)	1.054(7)		
C(9C)-H(9C1)	0.985(9)		
C(9C)-H(9C2)	0.993(8)		
C(9C)-H(9C3)	0.998(9)		
N(1C)-H(1C1)	0.866(8)		
N(1C)-H(1C2)	0.851(9)		
N(1C)-H(1C3)	0.929(8)		
C(1D)-C(2D)	1.3911(11)		
C(1D)-C(6D)	1.3944(12)		
C(1D)-H(1D)	1.094(8)		
C(2D)-C(3D)	1.3941(14)		
C(2D)-H(2D)	1.083(9)		
C(3D)-C(4D)	1.3845(13)		
C(3D)-H(3D)	1.019(7)		
C(4D)-C(5D)	1.3969(12)		
C(4D)-H(4D)	1.117(9)		
C(5D)-C(6D)	1.3898(12)		
C(5D)-H(5D)	1.086(7)		
C(6D)-C(7D)	1.5141(11)		
C(7D)-C(8D)	1.5160(10)		
C(7D)-H(7D1)	1.031(9)		
C(7D)-H(7D2)	0.980(9)		
C(8D)-N(1D)	1.5008(9)		
C(8D)-C(9D)	1.5264(12)		
C(8D)-H(8D)	1.109(8)		
C(9D)-H(9D1)	1.045(8)		
C(9D)-H(9D2)	1.043(9)		
C(9D)-H(9D3)	0.996(8)		
N(1D)-H(1D1)	0.926(9)		

N(1D)-H(1D2)	0.924(7)		
N(1D)-H(1D3)	0.938(9)		
O(1A)-S(1A)	1.4840(6)		
O(2A)-S(1A)	1.4663(6)		
O(3A)-S(1A)	1.4808(6)		
O(4A)-S(1A)	1.4592(6)		
O(2B)-S(1B)	1.4697(6)		
O(3B)-S(1B)	1.4649(6)		
O(4B)-S(1B)	1.4822(5)		
O(1B)-S(1B)	1.4455(6)		

phase II 120K		**phase I 336K**	
C(2A)-C(1A)-C(6A)	121.12(8)	O(4)#1-S(1)-O(4)	74.4(3)
C(2A)-C(1A)-H(1A)	121.2(5)	O(4)#1-S(1)-O(1)	159.9(2)
C(6A)-C(1A)-H(1A)	117.7(5)	O(4)-S(1)-O(1)	114.95(17)
C(3A)-C(2A)-C(1A)	119.90(9)	O(4)#1-S(1)-O(1)#1	114.95(17)
C(3A)-C(2A)-H(2A)	121.8(5)	O(4)-S(1)-O(1)#1	159.9(2)
C(1A)-C(2A)-H(2A)	118.3(5)	O(1)-S(1)-O(1)#1	62.6(2)
C(2A)-C(3A)-C(4A)	120.08(8)	O(4)#1-S(1)-O(3)#1	69.1(2)
C(2A)-C(3A)-H(3A)	117.7(5)	O(4)-S(1)-O(3)#1	89.6(2)
C(4A)-C(3A)-H(3A)	121.8(5)	O(1)-S(1)-O(3)#1	126.35(17)
C(3A)-C(4A)-C(5A)	119.85(9)	O(1)#1-S(1)-O(3)#1	78.31(17)
C(3A)-C(4A)-H(4A)	123.6(5)	O(4)#1-S(1)-O(3)	89.6(2)
C(5A)-C(4A)-H(4A)	116.4(5)	O(4)-S(1)-O(3)	69.1(2)
C(6A)-C(5A)-C(4A)	121.00(8)	O(1)-S(1)-O(3)	78.31(17)
C(6A)-C(5A)-H(5A)	118.5(5)	O(1)#1-S(1)-O(3)	126.35(17)
C(4A)-C(5A)-H(5A)	120.4(5)	O(3)#1-S(1)-O(3)	153.6(3)
C(5A)-C(6A)-C(1A)	118.02(7)	O(4)#1-S(1)-O(2)	119.2(3)
C(5A)-C(6A)-C(7A)	121.65(7)	O(4)-S(1)-O(2)	56.5(2)
C(1A)-C(6A)-C(7A)	120.29(7)	O(1)-S(1)-O(2)	79.4(2)
C(6A)-C(7A)-C(8A)	113.31(6)	O(1)#1-S(1)-O(2)	104.6(2)
C(6A)-C(7A)-H(7A1)	107.5(5)	O(3)#1-S(1)-O(2)	76.44(19)
C(8A)-C(7A)-H(7A1)	107.8(6)	O(3)-S(1)-O(2)	102.47(18)
C(6A)-C(7A)-H(7A2)	108.2(5)	O(4)#1-S(1)-O(2)#1	56.5(2)
C(8A)-C(7A)-H(7A2)	111.4(5)	O(4)-S(1)-O(2)#1	119.2(3)
H(7A1)-C(7A)-H(7A2)	108.4(7)	O(1)-S(1)-O(2)#1	104.6(2)
N(1A)-C(8A)-C(9A)	109.07(6)	O(1)#1-S(1)-O(2)#1	79.4(2)
N(1A)-C(8A)-C(7A)	107.82(6)	O(3)#1-S(1)-O(2)#1	102.47(18)
C(9A)-C(8A)-C(7A)	113.82(6)	O(3)-S(1)-O(2)#1	76.44(19)
N(1A)-C(8A)-H(8A)	106.8(5)	O(2)-S(1)-O(2)#1	175.4(5)

C(9A)-C(8A)-H(8A)	110.0(5)	S(1)-O(1)-O(1)#1	58.69(10)
C(7A)-C(8A)-H(8A)	109.1(5)	S(1)-O(1)-O(3)	52.65(12)
C(8A)-C(9A)-H(9A1)	112.9(6)	O(1)#1-O(1)-O(3)	102.73(17)
C(8A)-C(9A)-H(9A2)	109.6(5)	O(4)-O(2)-S(1)	56.07(18)
H(9A1)-C(9A)-H(9A2)	105.3(7)	O(4)-O(2)-O(3)#1	75.0(3)
C(8A)-C(9A)-H(9A3)	110.7(6)	S(1)-O(2)-O(3)#1	50.49(13)
H(9A1)-C(9A)-H(9A3)	107.1(8)	S(1)-O(3)-O(4)	52.45(15)
H(9A2)-C(9A)-H(9A3)	111.2(7)	S(1)-O(3)-O(1)	49.04(11)
C(8A)-N(1A)-H(1A1)	107.4(5)	O(4)-O(3)-O(1)	85.62(18)
C(8A)-N(1A)-H(1A2)	111.6(5)	S(1)-O(3)-O(2)#1	53.07(14)
H(1A1)-N(1A)-H(1A2)	106.1(8)	O(4)-O(3)-O(2)#1	91.9(2)
C(8A)-N(1A)-H(1A3)	111.7(5)	O(1)-O(3)-O(2)#1	78.3(2)
H(1A1)-N(1A)-H(1A3)	110.5(8)	S(1)-O(4)-O(2)	67.5(2)
H(1A2)-N(1A)-H(1A3)	109.4(8)	S(1)-O(4)-O(3)	58.41(15)
C(2B)-C(1B)-C(6B)	121.22(8)	O(2)-O(4)-O(3)	102.5(3)
C(2B)-C(1B)-H(1B)	119.0(5)	S(1)-O(4)-O(4)#1	52.80(15)
C(6B)-C(1B)-H(1B)	119.7(5)	O(2)-O(4)-O(4)#1	110.6(3)
C(3B)-C(2B)-C(1B)	120.04(8)	O(3)-O(4)-O(4)#1	75.5(3)
C(3B)-C(2B)-H(2B)	122.3(5)	C(8)-N(1)-H(1A)	109.5
C(1B)-C(2B)-H(2B)	117.6(5)	C(8)-N(1)-H(1B)	109.5
C(2B)-C(3B)-C(4B)	119.94(8)	H(1A)-N(1)-H(1B)	109.5
C(2B)-C(3B)-H(3B)	120.3(6)	C(8)-N(1)-H(1C)	109.5
C(4B)-C(3B)-H(3B)	119.4(6)	H(1A)-N(1)-H(1C)	109.5
C(3B)-C(4B)-C(5B)	120.11(9)	H(1B)-N(1)-H(1C)	109.5
C(3B)-C(4B)-H(4B)	123.6(4)	C(8)-C(9)-H(9A)	109.5
C(5B)-C(4B)-H(4B)	116.2(5)	C(8)-C(9)-H(9B)	109.5
C(4B)-C(5B)-C(6B)	120.28(8)	H(9A)-C(9)-H(9B)	109.5
C(4B)-C(5B)-H(5B)	118.8(5)	C(8)-C(9)-H(9C)	109.5
C(6B)-C(5B)-H(5B)	120.8(5)	H(9A)-C(9)-H(9C)	109.5
C(1B)-C(6B)-C(5B)	118.39(7)	H(9B)-C(9)-H(9C)	109.5
C(1B)-C(6B)-C(7B)	121.03(7)	C(9)-C(8)-C(7)	113.64(9)
C(5B)-C(6B)-C(7B)	120.55(7)	C(9)-C(8)-N(1)	106.65(8)
C(6B)-C(7B)-C(8B)	112.79(6)	C(7)-C(8)-N(1)	108.86(13)
C(6B)-C(7B)-H(7B1)	107.1(5)	C(9)-C(8)-H(8)	104.3

C(8B)-C(7B)-H(7B1)	110.4(5)	C(7)-C(8)-H(8)	114.4
C(6B)-C(7B)-H(7B2)	109.2(5)	N(1)-C(8)-H(8)	108.6
C(8B)-C(7B)-H(7B2)	111.5(6)	C(5)-C(6)-C(1)	116.5(2)
H(7B1)-C(7B)-H(7B2)	105.6(7)	C(5)-C(6)-C(7)	121.51(19)
N(1B)-C(8B)-C(9B)	108.76(6)	C(1)-C(6)-C(7)	121.94(19)
N(1B)-C(8B)-C(7B)	108.39(6)	C(6)-C(1)-C(2)	121.3(3)
C(9B)-C(8B)-C(7B)	113.81(6)	C(6)-C(1)-H(1)	119.4
N(1B)-C(8B)-H(8B)	106.6(4)	C(2)-C(1)-H(1)	119.4
C(9B)-C(8B)-H(8B)	108.1(5)	C(6)-C(7)-C(8)	114.76(14)
C(7B)-C(8B)-H(8B)	110.9(5)	C(6)-C(7)-H(7A)	108.6
C(8B)-C(9B)-H(9B1)	113.1(5)	C(8)-C(7)-H(7A)	108.6
C(8B)-C(9B)-H(9B2)	106.4(5)	C(6)-C(7)-H(7B)	108.6
H(9B1)-C(9B)-H(9B2)	105.9(7)	C(8)-C(7)-H(7B)	108.6
C(8B)-C(9B)-H(9B3)	110.1(6)	H(7A)-C(7)-H(7B)	107.6
H(9B1)-C(9B)-H(9B3)	109.0(8)	C(4)-C(3)-C(2)	119.5(3)
H(9B2)-C(9B)-H(9B3)	112.4(6)	C(4)-C(3)-H(3)	120.2
C(8B)-N(1B)-H(1B1)	109.1(4)	C(2)-C(3)-H(3)	120.2
C(8B)-N(1B)-H(1B2)	111.1(5)	C(3)-C(2)-C(1)	120.7(3)
H(1B1)-N(1B)-H(1B2)	105.9(7)	C(3)-C(2)-H(2)	119.7
C(8B)-N(1B)-H(1B3)	112.3(5)	C(1)-C(2)-H(2)	119.7
H(1B1)-N(1B)-H(1B3)	112.2(8)	C(3)-C(4)-C(5)	118.5(3)
H(1B2)-N(1B)-H(1B3)	106.0(8)	C(3)-C(4)-H(4)	120.7
C(6C)-C(1C)-C(2C)	121.37(8)	C(5)-C(4)-H(4)	120.7
C(6C)-C(1C)-H(1C)	115.7(4)	C(6)-C(5)-C(4)	123.4(3)
C(2C)-C(1C)-H(1C)	122.9(4)	C(6)-C(5)-H(5)	118.3
C(3C)-C(2C)-C(1C)	119.45(7)	C(4)-C(5)-H(5)	118.3
C(3C)-C(2C)-H(2C)	127.0(5)		
C(1C)-C(2C)-H(2C)	113.3(5)		
C(4C)-C(3C)-C(2C)	119.90(8)		
C(4C)-C(3C)-H(3C)	120.2(5)		
C(2C)-C(3C)-H(3C)	119.8(5)		
C(3C)-C(4C)-C(5C)	120.03(8)		
C(3C)-C(4C)-H(4C)	119.6(4)		
C(5C)-C(4C)-H(4C)	120.0(4)		

C(6C)-C(5C)-C(4C)	120.86(8)		
C(6C)-C(5C)-H(5C)	121.3(5)		
C(4C)-C(5C)-H(5C)	117.8(5)		
C(5C)-C(6C)-C(1C)	118.37(7)		
C(5C)-C(6C)-C(7C)	121.04(7)		
C(1C)-C(6C)-C(7C)	120.55(7)		
C(8C)-C(7C)-C(6C)	113.02(7)		
C(8C)-C(7C)-H(7C1)	108.6(5)		
C(6C)-C(7C)-H(7C1)	110.1(5)		
C(8C)-C(7C)-H(7C2)	107.3(5)		
C(6C)-C(7C)-H(7C2)	112.1(5)		
H(7C1)-C(7C)-H(7C2)	105.4(7)		
N(1C)-C(8C)-C(9C)	109.29(7)		
N(1C)-C(8C)-C(7C)	108.03(6)		
C(9C)-C(8C)-C(7C)	113.94(7)		
N(1C)-C(8C)-H(8C)	111.2(4)		
C(9C)-C(8C)-H(8C)	103.8(4)		
C(7C)-C(8C)-H(8C)	110.6(5)		
C(8C)-C(9C)-H(9C1)	108.5(5)		
C(8C)-C(9C)-H(9C2)	110.2(6)		
H(9C1)-C(9C)-H(9C2)	108.7(8)		
C(8C)-C(9C)-H(9C3)	109.8(6)		
H(9C1)-C(9C)-H(9C3)	107.3(8)		
H(9C2)-C(9C)-H(9C3)	112.2(7)		
C(8C)-N(1C)-H(1C1)	109.7(5)		
C(8C)-N(1C)-H(1C2)	106.2(6)		
H(1C1)-N(1C)-H(1C2)	111.8(9)		
C(8C)-N(1C)-H(1C3)	113.0(5)		
H(1C1)-N(1C)-H(1C3)	107.6(8)		
H(1C2)-N(1C)-H(1C3)	108.6(7)		
C(2D)-C(1D)-C(6D)	120.62(8)		
C(2D)-C(1D)-H(1D)	123.6(4)		
C(6D)-C(1D)-H(1D)	115.6(4)		

C(1D)-C(2D)-C(3D)	120.05(8)		
C(1D)-C(2D)-H(2D)	121.2(5)		
C(3D)-C(2D)-H(2D)	118.7(5)		
C(4D)-C(3D)-C(2D)	119.63(8)		
C(4D)-C(3D)-H(3D)	119.0(5)		
C(2D)-C(3D)-H(3D)	121.2(5)		
C(3D)-C(4D)-C(5D)	120.15(9)		
C(3D)-C(4D)-H(4D)	117.3(5)		
C(5D)-C(4D)-H(4D)	122.1(5)		
C(6D)-C(5D)-C(4D)	120.59(8)		
C(6D)-C(5D)-H(5D)	115.8(4)		
C(4D)-C(5D)-H(5D)	123.4(4)		
C(5D)-C(6D)-C(1D)	118.92(7)		
C(5D)-C(6D)-C(7D)	119.42(7)		
C(1D)-C(6D)-C(7D)	121.62(7)		
C(6D)-C(7D)-C(8D)	110.27(6)		
C(6D)-C(7D)-H(7D1)	108.1(5)		
C(8D)-C(7D)-H(7D1)	107.1(5)		
C(6D)-C(7D)-H(7D2)	112.2(5)		
C(8D)-C(7D)-H(7D2)	109.3(5)		
H(7D1)-C(7D)-H(7D2)	109.7(7)		
N(1D)-C(8D)-C(7D)	110.11(5)		
N(1D)-C(8D)-C(9D)	108.56(6)		
C(7D)-C(8D)-C(9D)	113.42(7)		
N(1D)-C(8D)-H(8D)	108.8(4)		
C(7D)-C(8D)-H(8D)	100.2(4)		
C(9D)-C(8D)-H(8D)	115.5(4)		
C(8D)-C(9D)-H(9D1)	113.3(5)		
C(8D)-C(9D)-H(9D2)	106.8(6)		
H(9D1)-C(9D)-H(9D2)	118.5(7)		
C(8D)-C(9D)-H(9D3)	104.3(4)		
H(9D1)-C(9D)-H(9D3)	106.0(7)		
H(9D2)-C(9D)-H(9D3)	106.9(7)		
C(8D)-N(1D)-H(1D1)	110.9(5)		
C(8D)-N(1D)-H(1D2)	108.8(4)		
H(1D1)-N(1D)-H(1D2)	112.2(8)		

C(8D)-N(1D)-H(1D3)	106.1(6)		
H(1D1)-N(1D)-H(1D3)	106.3(7)		
H(1D2)-N(1D)-H(1D3)	112.4(8)		
O(4A)-S(1A)-O(2A)	111.93(4)		
O(4A)-S(1A)-O(3A)	109.09(3)		
O(2A)-S(1A)-O(3A)	109.85(4)		
O(4A)-S(1A)-O(1A)	110.30(4)		
O(2A)-S(1A)-O(1A)	108.04(3)		
O(3A)-S(1A)-O(1A)	107.54(3)		
O(1B)-S(1B)-O(3B)	110.62(4)		
O(1B)-S(1B)-O(2B)	110.99(4)		
O(3B)-S(1B)-O(2B)	109.17(3)		
O(1B)-S(1B)-O(4B)	108.12(3)		
O(3B)-S(1B)-O(4B)	109.98(3)		
O(2B)-S(1B)-O(4B)	107.91(3)		

Symmetry transformations used to generate equivalent atoms: #1 -x+2,y,-z+1

Table 2. Torsion angles [deg] for AMPH-SULPH.

phase II 120K		**phase I 336K**	
C(6A)-C(1A)-C(2A)-C(3A)	-0.19(14)	O(4)#1-S(1)-O(1)-O(1)#1	88.1(5)
C(1A)-C(2A)-C(3A)-C(4A)	1.49(15)	O(4)-S(1)-O(1)-O(1)#1	-157.8(2)
C(2A)-C(3A)-C(4A)-C(5A)	-1.73(15)	O(3)#1-S(1)-O(1)-O(1)#1	-48.4(3)
C(3A)-C(4A)-C(5A)-C(6A)	0.68(14)	O(3)-S(1)-O(1)-O(1)#1	142.1(2)
C(4A)-C(5A)-C(6A)-C(1A)	0.60(13)	O(2)-S(1)-O(1)-O(1)#1	-112.7(2)
C(4A)-C(5A)-C(6A)-C(7A)	-176.87(8)	O(2)#1-S(1)-O(1)-O(1)#1	69.6(3)
C(2A)-C(1A)-C(6A)-C(5A)	-0.84(13)	O(4)#1-S(1)-O(1)-O(3)	-53.9(5)
C(2A)-C(1A)-C(6A)-C(7A)	176.65(8)	O(4)-S(1)-O(1)-O(3)	60.2(2)
C(5A)-C(6A)-C(7A)-C(8A)	-76.39(10)	O(1)#1-S(1)-O(1)-O(3)	-142.1(2)
C(1A)-C(6A)-C(7A)-C(8A)	106.21(9)	O(3)#1-S(1)-O(1)-O(3)	169.56(13)
C(6A)-C(7A)-C(8A)-N(1A)	177.40(6)	O(2)-S(1)-O(1)-O(3)	105.24(19)
C(6A)-C(7A)-C(8A)-C(9A)	-61.46(9)	O(2)#1-S(1)-O(1)-O(3)	-72.5(2)
C(6B)-C(1B)-C(2B)-C(3B)	0.21(14)	O(4)#1-S(1)-O(2)-O(4)	42.3(4)
C(1B)-C(2B)-C(3B)-C(4B)	0.70(15)	O(1)-S(1)-O(2)-O(4)	-129.7(2)
C(2B)-C(3B)-C(4B)-C(5B)	-0.67(15)	O(1)#1-S(1)-O(2)-O(4)	172.5(2)
C(3B)-C(4B)-C(5B)-C(6B)	-0.25(14)	O(3)#1-S(1)-O(2)-O(4)	98.6(3)
C(2B)-C(1B)-C(6B)-C(5B)	-1.11(13)	O(3)-S(1)-O(2)-O(4)	-54.3(3)
C(2B)-C(1B)-C(6B)-C(7B)	176.99(8)	O(2)#1-S(1)-O(2)-O(4)	21.7(2)
C(4B)-C(5B)-C(6B)-C(1B)	1.12(13)	O(4)#1-S(1)-O(2)-O(3)#1	-56.3(3)
C(4B)-C(5B)-C(6B)-C(7B)	-176.99(8)	O(4)-S(1)-O(2)-O(3)#1	-98.6(3)
C(1B)-C(6B)-C(7B)-C(8B)	103.63(9)	O(1)-S(1)-O(2)-O(3)#1	131.70(19)
C(5B)-C(6B)-C(7B)-C(8B)	-78.30(10)	O(1)#1-S(1)-O(2)-O(3)#1	73.84(19)
C(6B)-C(7B)-C(8B)-N(1B)	175.62(6)	O(3)-S(1)-O(2)-O(3)#1	-152.9(3)

C(6B)-C(7B)-C(8B)-C(9B)	-63.24(9)	O(2)#1-S(1)-O(2)-O(3)#1	-76.98(16)
C(6C)-C(1C)-C(2C)-C(3C)	0.76(14)	O(4)#1-S(1)-O(3)-O(4)	-73.5(3)
C(1C)-C(2C)-C(3C)-C(4C)	0.04(15)	O(1)-S(1)-O(3)-O(4)	122.67(19)
C(2C)-C(3C)-C(4C)-C(5C)	-1.02(16)	O(1)#1-S(1)-O(3)-O(4)	165.3(2)
C(3C)-C(4C)-C(5C)-C(6C)	1.24(16)	O(3)#1-S(1)-O(3)-O(4)	-38.17(16)
C(4C)-C(5C)-C(6C)-C(1C)	-0.45(14)	O(2)-S(1)-O(3)-O(4)	46.4(3)
C(4C)-C(5C)-C(6C)-C(7C)	-178.39(9)	O(2)#1-S(1)-O(3)-O(4)	-129.0(3)
C(2C)-C(1C)-C(6C)-C(5C)	-0.55(13)	O(4)#1-S(1)-O(3)-O(1)	163.9(2)
C(2C)-C(1C)-C(6C)-C(7C)	177.40(8)	O(4)-S(1)-O(3)-O(1)	-122.67(19)
C(5C)-C(6C)-C(7C)-C(8C)	-67.50(10)	O(1)#1-S(1)-O(3)-O(1)	42.7(3)
C(1C)-C(6C)-C(7C)-C(8C)	114.60(9)	O(3)#1-S(1)-O(3)-O(1)	-160.84(12)
C(6C)-C(7C)-C(8C)-N(1C)	169.43(6)	O(2)-S(1)-O(3)-O(1)	-76.3(3)
C(6C)-C(7C)-C(8C)-C(9C)	-68.93(9)	O(2)#1-S(1)-O(3)-O(1)	108.4(3)
C(6D)-C(1D)-C(2D)-C(3D)	-1.02(13)	O(4)#1-S(1)-O(3)-O(2)#1	55.5(3)
C(1D)-C(2D)-C(3D)-C(4D)	-0.35(13)	O(4)-S(1)-O(3)-O(2)#1	129.0(3)
C(2D)-C(3D)-C(4D)-C(5D)	0.91(13)	O(1)-S(1)-O(3)-O(2)#1	-108.4(3)
C(3D)-C(4D)-C(5D)-C(6D)	-0.11(13)	O(1)#1-S(1)-O(3)-O(2)#1	-65.7(3)
C(4D)-C(5D)-C(6D)-C(1D)	-1.23(12)	O(3)#1-S(1)-O(3)-O(2)#1	90.8(2)
C(4D)-C(5D)-C(6D)-C(7D)	176.56(7)	O(2)-S(1)-O(3)-O(2)#1	175.4(5)
C(2D)-C(1D)-C(6D)-C(5D)	1.80(12)	O(1)#1-O(1)-O(3)-S(1)	-32.58(17)
C(2D)-C(1D)-C(6D)-C(7D)	-175.94(7)	S(1)-O(1)-O(3)-O(4)	-42.02(15)
C(5D)-C(6D)-C(7D)-C(8D)	-79.22(9)	O(1)#1-O(1)-O(3)-O(4)	-74.6(2)
C(1D)-C(6D)-C(7D)-C(8D)	98.51(9)	S(1)-O(1)-O(3)-O(2)#1	50.80(15)
C(6D)-C(7D)-C(8D)-N(1D)	162.22(7)	O(1)#1-O(1)-O(3)-O(2)#1	18.2(2)
C(6D)-C(7D)-C(8D)-C(9D)	-75.92(9)	O(4)#1-S(1)-O(4)-O(2)	-142.4(4)
		O(1)-S(1)-O(4)-O(2)	56.6(3)
		O(1)#1-S(1)-O(4)-O(2)	-21.6(6)
		O(3)#1-S(1)-O(4)-O(2)	-74.0(3)
		O(3)-S(1)-O(4)-O(2)	122.0(3)
		O(2)#1-S(1)-O(4)-O(2)	-178.0(2)
		O(4)#1-S(1)-O(4)-O(3)	95.6(3)
		O(1)-S(1)-O(4)-O(3)	-65.4(2)
		O(1)#1-S(1)-O(4)-O(3)	-143.6(5)
		O(3)#1-S(1)-O(4)-O(3)	164.05(18)
		O(2)-S(1)-O(4)-O(3)	-122.0(3)
		O(2)#1-S(1)-O(4)-O(3)	60.0(3)

		O(1)-S(1)-O(4)-O(4)#1	-161.01(19)
		O(1)#1-S(1)-O(4)-O(4)#1	120.8(5)
		O(3)#1-S(1)-O(4)-O(4)#1	68.4(2)
		O(3)-S(1)-O(4)-O(4)#1	-95.6(3)
		O(2)-S(1)-O(4)-O(4)#1	142.4(4)
		O(2)#1-S(1)-O(4)-O(4)#1	-35.6(3)
		O(3)#1-O(2)-O(4)-S(1)	52.16(14)
		S(1)-O(2)-O(4)-O(3)	47.73(18)
		O(3)#1-O(2)-O(4)-O(3)	99.9(2)
		S(1)-O(2)-O(4)-O(4)#1	-31.3(3)
		O(3)#1-O(2)-O(4)-O(4)#1	20.9(3)
		O(1)-O(3)-O(4)-S(1)	39.61(13)
		O(2)#1-O(3)-O(4)-S(1)	-38.5(2)
		S(1)-O(3)-O(4)-O(2)	-53.4(2)
		O(1)-O(3)-O(4)-O(2)	-13.7(3)
		O(2)#1-O(3)-O(4)-O(2)	-91.8(3)
		S(1)-O(3)-O(4)-O(4)#1	54.96(16)
		O(1)-O(3)-O(4)-O(4)#1	94.57(16)
		O(2)#1-O(3)-O(4)-O(4)#1	16.5(2)
		C(5)-C(6)-C(1)-C(2)	0.1(4)
		C(7)-C(6)-C(1)-C(2)	177.7(2)
		C(5)-C(6)-C(7)-C(8)	-65.3(2)
		C(1)-C(6)-C(7)-C(8)	117.3(2)
		C(9)-C(8)-C(7)-C(6)	-63.78(17)
		N(1)-C(8)-C(7)-C(6)	177.54(14)
		C(4)-C(3)-C(2)-C(1)	-3.5(5)
		C(6)-C(1)-C(2)-C(3)	2.4(5)
		C(2)-C(3)-C(4)-C(5)	2.2(5)
		C(1)-C(6)-C(5)-C(4)	-1.4(4)
		C(7)-C(6)-C(5)-C(4)	-179.0(2)
		C(3)-C(4)-C(5)-C(6)	0.2(5)

Symmetry transformations used to generate equivalent atoms: #1 -x+2,y,-z+1

Table 3a. Hydrogen bonds for AMPH-SULPH phase II at 120K [A and deg.].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(1A)-H(1A2)...O(1A)	0.945(9)	1.828(9)	2.7636(9)	169.9(8)
N(1A)-H(1A3)...O(2A)#1	0.872(8)	1.888(8)	2.7568(9)	174.4(8)
N(1A)-H(1A1)...O(4B)#1	0.870(8)	1.904(8)	2.7567(8)	166.2(8)
N(1B)-H(1B2)...O(2B)	0.888(8)	1.900(8)	2.7856(9)	175.0(8)
N(1B)-H(1B3)...O(3B)#1	0.898(9)	1.899(9)	2.7847(9)	168.4(7)
N(1B)-H(1B1)...O(3A)#2	0.925(7)	1.897(7)	2.8063(9)	166.9(8)
N(1C)-H(1C2)...O(2B)	0.851(9)	1.999(8)	2.8299(9)	165.2(9)
N(1C)-H(1C3)...O(4B)#1	0.929(8)	1.884(8)	2.7984(9)	167.9(7)
N(1C)-H(1C1)...O(4A)	0.866(8)	1.898(8)	2.7638(8)	179.3(10)
N(1D)-H(1D2)...O(1B)#3	0.924(7)	1.806(7)	2.7180(8)	168.7(7)
N(1D)-H(1D3)...O(1A)#4	0.938(9)	1.831(9)	2.7586(8)	169.3(8)
N(1D)-H(1D1)...O(3A)	0.926(9)	1.902(9)	2.8022(9)	163.6(8)

Table 3b. Hydrogen bonds for AMPH-SULPH phase I at 336K [A and deg.] .

D-H	d(D-H)	d(H..A)	d(D..A)	<DHA
N1-H1A ...O1	0.89	1.91	2.770(1)	161
N1-H1A ...O1#5	0.89	2.45	3.181(1)	139
N1-H1B ...O4#6	0.89	2.06	2.950(2)	176
N1-H1B ...O3#7	0.89	2.34	3.003(2)	130
N1-H1B ...O4#7	0.89	2.39	3.144(2)	142
N1-H1C ...O3#8	0.89	1.95	2.668(2)	135
N1-H1C ...O1#8	0.89	2.31	3.202(1)	172
N1-H1C ...O4#8	0.89	2.62	3.297 (2)	132

Symmetry transformations used to generate equivalent atoms:
#1 x,y-1,z #2 x+1,y,z #3 x-1,y,z #4 x,y+1,z #5 -x+2, y, -z+1
#6 -x+2, y-1, -z+1 #7 x, y-1, z #8 -x+3/2, y-1/2, -z+1

Table 4. Selected the C-H…π interactions at 120K and 336K

T. [K]	C-H…π	d (πo-H)	<H πo
120	C3A-H3A-RING A	3.22(1)	72.7(6)
	C3B-H3B-RING B	3.25(1)	73.5(6)
	C1C-H1C-RING D	2.52(1)	87.4(7)
	C4C-H4C-RING D	3.43(1)	76.5(6)
	C9A-H9A2-RING A	3.36(1)	78.8(5)
	C9B-H9B2-RING B	3.38(1)	77.1(6)
	C9C-H9C2-RING C	3.51(2)	80.3(5)
336	C3-H3-RING A	3.56	63
	C9-H9B-RING A	3.53	78