

Table ST1 Bond lengths [Å] and angles [°] for DACSC

C(1)-N(1)	1.418(15)	C(17)-H(17C)	0.9600
C(1)-H(1A)	0.9600	C(18)-N(2)	1.438(17)
C(1)-H(1B)	0.9600	C(18)-H(18A)	0.9600
C(1)-H(1C)	0.9600	C(18)-H(18B)	0.9600
C(2)-N(1)	1.285(14)	C(18)-H(18C)	0.9600
C(2)-C(3)	1.378(14)	C(19)-N(3)	1.541(13)
C(2)-H(2)	0.9300	C(19)-H(19A)	0.9600
C(3)-C(4)	1.406(13)	C(19)-H(19B)	0.9600
C(3)-H(3)	0.9300	C(19)-H(19C)	0.9600
C(4)-C(7)	1.412(14)	C(20)-N(3)	1.216(15)
C(4)-C(5)	1.438(14)	C(20)-C(21)	1.401(15)
C(5)-C(6)	1.323(15)	C(20)-H(20)	0.9300
C(5)-H(5)	0.9300	C(21)-C(22)	1.367(14)
C(6)-N(1)	1.434(14)	C(21)-H(21)	0.9300
C(6)-H(6)	0.9300	C(22)-C(23)	1.392(15)
C(7)-C(8)	1.365(14)	C(22)-C(25)	1.484(14)
C(7)-H(7)	0.9300	C(23)-C(24)	1.338(15)
C(8)-C(9)	1.441(13)	C(23)-H(23)	0.9300
C(8)-H(8)	0.9300	C(24)-N(3)	1.396(13)
C(9)-C(10)	1.344(16)	C(24)-H(24)	0.9300
C(9)-H(9)	0.9300	C(25)-C(26)	1.294(15)
C(10)-C(11)	1.468(16)	C(25)-H(25)	0.9300
C(10)-H(10)	0.9300	C(26)-C(27)	1.416(15)
C(11)-C(12)	1.354(15)	C(26)-H(26)	0.9300
C(11)-C(16)	1.384(16)	C(27)-C(28)	1.344(16)
C(12)-C(13)	1.406(14)	C(27)-H(27)	0.9300
C(12)-H(12)	0.9300	C(28)-C(29)	1.433(17)
C(13)-C(14)	1.357(15)	C(28)-H(28)	0.9300
C(13)-H(13)	0.9300	C(29)-C(34)	1.417(15)
C(14)-N(2)	1.352(14)	C(29)-C(30)	1.444(15)
C(14)-C(15)	1.460(14)	C(30)-C(31)	1.335(14)
C(15)-C(16)	1.345(16)	C(30)-H(30)	0.9300
C(15)-H(15)	0.9300	C(31)-C(32)	1.453(12)
C(16)-H(16)	0.9300	C(31)-H(31)	0.9300
C(17)-N(2)	1.466(14)	C(32)-C(33)	1.369(14)
C(17)-H(17A)	0.9600	C(32)-N(4)	1.376(13)
C(17)-H(17B)	0.9600		

C(33)-C(34)	1.380(14)	O(4)-S(2)	1.457(7)
C(33)-H(33)	0.9300	O(5)-S(2)	1.440(7)
C(34)-H(34)	0.9300	O(6)-S(2)	1.424(8)
C(35)-N(4)	1.432(14)	N(1)-C(1)-H(1A)	109.5
C(35)-H(35A)	0.9600	N(1)-C(1)-H(1B)	109.5
C(35)-H(35B)	0.9600	H(1A)-C(1)-H(1B)	109.5
C(35)-H(35C)	0.9600	N(1)-C(1)-H(1C)	109.5
C(36)-N(4)	1.444(15)	H(1A)-C(1)-H(1C)	109.5
C(36)-H(36A)	0.9600	H(1B)-C(1)-H(1C)	109.5
C(36)-H(36B)	0.9600	N(1)-C(2)-C(3)	124.2(10)
C(36)-H(36C)	0.9600	N(1)-C(2)-H(2)	117.9
C(37)-C(42)	1.377(14)	C(3)-C(2)-H(2)	117.9
C(37)-C(38)	1.379(14)	C(2)-C(3)-C(4)	120.2(10)
C(37)-Cl(1)	1.733(9)	C(2)-C(3)-H(3)	119.9
C(38)-C(39)	1.415(13)	C(4)-C(3)-H(3)	119.9
C(38)-H(38)	0.9300	C(3)-C(4)-C(7)	125.4(10)
C(39)-C(40)	1.369(11)	C(3)-C(4)-C(5)	116.0(10)
C(39)-H(39)	0.9300	C(7)-C(4)-C(5)	118.6(9)
C(40)-C(41)	1.393(11)	C(6)-C(5)-C(4)	119.9(10)
C(40)-S(1)	1.765(8)	C(6)-C(5)-H(5)	120.0
C(41)-C(42)	1.351(13)	C(4)-C(5)-H(5)	120.0
C(41)-H(41)	0.9300	C(5)-C(6)-N(1)	122.4(10)
C(42)-H(42)	0.9300	C(5)-C(6)-H(6)	118.8
C(43)-C(48)	1.371(11)	N(1)-C(6)-H(6)	118.8
C(43)-C(44)	1.379(11)	C(8)-C(7)-C(4)	126.3(10)
C(43)-S(2)	1.769(8)	C(8)-C(7)-H(7)	116.8
C(44)-C(45)	1.382(12)	C(4)-C(7)-H(7)	116.8
C(44)-H(44)	0.9300	C(7)-C(8)-C(9)	122.4(10)
C(45)-C(46)	1.380(14)	C(7)-C(8)-H(8)	118.8
C(45)-H(45)	0.9300	C(9)-C(8)-H(8)	118.8
C(46)-C(47)	1.363(14)	C(10)-C(9)-C(8)	120.9(11)
C(46)-Cl(2)	1.746(9)	C(10)-C(9)-H(9)	119.5
C(47)-C(48)	1.359(14)	C(8)-C(9)-H(9)	119.5
C(47)-H(47)	0.9300	C(9)-C(10)-C(11)	126.9(10)
C(48)-H(48)	0.9300	C(9)-C(10)-H(10)	116.6
O(1)-S(1)	1.430(8)	C(11)-C(10)-H(10)	116.6
O(2)-S(1)	1.461(6)	C(12)-C(11)-C(16)	115.1(11)
O(3)-S(1)	1.449(6)	C(12)-C(11)-C(10)	124.5(10)

C(16)-C(11)-C(10)	120.4(10)	C(22)-C(21)-H(21)	119.1
C(11)-C(12)-C(13)	124.5(11)	C(20)-C(21)-H(21)	119.1
C(11)-C(12)-H(12)	117.7	C(21)-C(22)-C(23)	114.9(10)
C(13)-C(12)-H(12)	117.7	C(21)-C(22)-C(25)	122.5(10)
C(14)-C(13)-C(12)	119.4(9)	C(23)-C(22)-C(25)	122.6(10)
C(14)-C(13)-H(13)	120.3	C(24)-C(23)-C(22)	121.7(11)
C(12)-C(13)-H(13)	120.3	C(24)-C(23)-H(23)	119.1
N(2)-C(14)-C(13)	123.0(9)	C(22)-C(23)-H(23)	119.1
N(2)-C(14)-C(15)	119.6(10)	C(23)-C(24)-N(3)	118.8(11)
C(13)-C(14)-C(15)	117.4(10)	C(23)-C(24)-H(24)	120.6
C(16)-C(15)-C(14)	119.2(11)	N(3)-C(24)-H(24)	120.6
C(16)-C(15)-H(15)	120.4	C(26)-C(25)-C(22)	127.0(10)
C(14)-C(15)-H(15)	120.4	C(26)-C(25)-H(25)	116.5
C(15)-C(16)-C(11)	124.3(11)	C(22)-C(25)-H(25)	116.5
C(15)-C(16)-H(16)	117.8	C(25)-C(26)-C(27)	125.0(11)
C(11)-C(16)-H(16)	117.8	C(25)-C(26)-H(26)	117.5
N(2)-C(17)-H(17A)	109.5	C(27)-C(26)-H(26)	117.5
N(2)-C(17)-H(17B)	109.5	C(28)-C(27)-C(26)	127.2(12)
H(17A)-C(17)-H(17B)	109.5	C(28)-C(27)-H(27)	116.4
N(2)-C(17)-H(17C)	109.5	C(26)-C(27)-H(27)	116.4
H(17A)-C(17)-H(17C)	109.5	C(27)-C(28)-C(29)	129.0(11)
H(17B)-C(17)-H(17C)	109.5	C(27)-C(28)-H(28)	115.5
N(2)-C(18)-H(18A)	109.5	C(29)-C(28)-H(28)	115.5
N(2)-C(18)-H(18B)	109.5	C(34)-C(29)-C(28)	120.0(10)
H(18A)-C(18)-H(18B)	109.5	C(34)-C(29)-C(30)	116.7(10)
N(2)-C(18)-H(18C)	109.5	C(28)-C(29)-C(30)	123.3(10)
H(18A)-C(18)-H(18C)	109.5	C(31)-C(30)-C(29)	120.6(9)
H(18B)-C(18)-H(18C)	109.5	C(31)-C(30)-H(30)	119.7
N(3)-C(19)-H(19A)	109.5	C(29)-C(30)-H(30)	119.7
N(3)-C(19)-H(19B)	109.5	C(30)-C(31)-C(32)	122.7(9)
H(19A)-C(19)-H(19B)	109.5	C(30)-C(31)-H(31)	118.6
N(3)-C(19)-H(19C)	109.5	C(32)-C(31)-H(31)	118.6
H(19A)-C(19)-H(19C)	109.5	C(33)-C(32)-N(4)	123.5(9)
H(19B)-C(19)-H(19C)	109.5	C(33)-C(32)-C(31)	115.9(9)
N(3)-C(20)-C(21)	120.6(12)	N(4)-C(32)-C(31)	120.5(10)
N(3)-C(20)-H(20)	119.7	C(32)-C(33)-C(34)	123.2(9)
C(21)-C(20)-H(20)	119.7	C(32)-C(33)-H(33)	118.4
C(22)-C(21)-C(20)	121.8(11)		

C(34)-C(33)-H(33)	118.4	C(43)-C(44)-H(44)	120.4
C(33)-C(34)-C(29)	120.8(10)	C(45)-C(44)-H(44)	120.4
C(33)-C(34)-H(34)	119.6	C(46)-C(45)-C(44)	119.5(8)
C(29)-C(34)-H(34)	119.6	C(46)-C(45)-H(45)	120.2
N(4)-C(35)-H(35A)	109.5	C(44)-C(45)-H(45)	120.2
N(4)-C(35)-H(35B)	109.5	C(47)-C(46)-C(45)	120.7(9)
H(35A)-C(35)-H(35B)	109.5	C(47)-C(46)-Cl(2)	120.0(8)
N(4)-C(35)-H(35C)	109.5	C(45)-C(46)-Cl(2)	119.2(7)
H(35A)-C(35)-H(35C)	109.5	C(48)-C(47)-C(46)	119.6(9)
H(35B)-C(35)-H(35C)	109.5	C(48)-C(47)-H(47)	120.2
N(4)-C(36)-H(36A)	109.5	C(46)-C(47)-H(47)	120.2
N(4)-C(36)-H(36B)	109.5	C(47)-C(48)-C(43)	120.9(8)
H(36A)-C(36)-H(36B)	109.5	C(47)-C(48)-H(48)	119.6
N(4)-C(36)-H(36C)	109.5	C(43)-C(48)-H(48)	119.6
H(36A)-C(36)-H(36C)	109.5	C(2)-N(1)-C(1)	124.8(10)
H(36B)-C(36)-H(36C)	109.5	C(2)-N(1)-C(6)	117.3(10)
C(42)-C(37)-C(38)	121.1(8)	C(1)-N(1)-C(6)	117.9(10)
C(42)-C(37)-Cl(1)	120.6(7)	C(14)-N(2)-C(18)	121.2(10)
C(38)-C(37)-Cl(1)	118.3(7)	C(14)-N(2)-C(17)	123.5(10)
C(37)-C(38)-C(39)	117.2(8)	C(18)-N(2)-C(17)	115.3(10)
C(37)-C(38)-H(38)	121.4	C(20)-N(3)-C(24)	122.2(11)
C(39)-C(38)-H(38)	121.4	C(20)-N(3)-C(19)	122.7(11)
C(40)-C(39)-C(38)	120.7(8)	C(24)-N(3)-C(19)	115.0(10)
C(40)-C(39)-H(39)	119.7	C(32)-N(4)-C(35)	123.2(9)
C(38)-C(39)-H(39)	119.7	C(32)-N(4)-C(36)	119.6(10)
C(39)-C(40)-C(41)	120.5(8)	C(35)-N(4)-C(36)	117.2(10)
C(39)-C(40)-S(1)	120.2(6)	O(1)-S(1)-O(3)	111.4(5)
C(41)-C(40)-S(1)	119.3(6)	O(1)-S(1)-O(2)	113.9(4)
C(42)-C(41)-C(40)	118.8(8)	O(3)-S(1)-O(2)	113.2(4)
C(42)-C(41)-H(41)	120.6	O(1)-S(1)-C(40)	107.0(4)
C(40)-C(41)-H(41)	120.6	O(3)-S(1)-C(40)	106.3(4)
C(41)-C(42)-C(37)	121.6(7)	O(2)-S(1)-C(40)	104.2(4)
C(41)-C(42)-H(42)	119.2	O(6)-S(2)-O(5)	114.0(5)
C(37)-C(42)-H(42)	119.2	O(6)-S(2)-O(4)	112.0(5)
C(48)-C(43)-C(44)	120.0(8)	O(5)-S(2)-O(4)	111.9(4)
C(48)-C(43)-S(2)	120.6(6)	O(6)-S(2)-C(43)	107.4(4)
C(44)-C(43)-S(2)	119.4(7)	O(5)-S(2)-C(43)	106.5(4)
C(43)-C(44)-C(45)	119.3(8)	O(4)-S(2)-C(43)	104.3(4)

Table ST2 Torsion angles [°] for DACSC

N(1)-C(2)-C(3)-C(4)	-0.8(11)	C(34)-C(29)-C(30)-C(31)	-0.7(9)
C(2)-C(3)-C(4)-C(7)	-179.4(6)	C(28)-C(29)-C(30)-C(31)	179.2(6)
C(2)-C(3)-C(4)-C(5)	-0.1(9)	C(29)-C(30)-C(31)-C(32)	-0.4(9)
C(3)-C(4)-C(5)-C(6)	0.3(10)	C(30)-C(31)-C(32)-C(33)	1.2(10)
C(7)-C(4)-C(5)-C(6)	179.6(7)	C(30)-C(31)-C(32)-N(4)	-179.3(6)
C(4)-C(5)-C(6)-N(1)	0.4(11)	N(4)-C(32)-C(33)-C(34)	179.6(7)
C(3)-C(4)-C(7)-C(8)	0.5(12)	C(31)-C(32)-C(33)-C(34)	-1.0(10)
C(5)-C(4)-C(7)-C(8)	-178.7(7)	C(32)-C(33)-C(34)-C(29)	0.0(11)
C(4)-C(7)-C(8)-C(9)	177.1(7)	C(28)-C(29)-C(34)-C(33)	-179.0(6)
C(7)-C(8)-C(9)-C(10)	-179.9(7)	C(30)-C(29)-C(34)-C(33)	0.9(10)
C(8)-C(9)-C(10)-C(11)	179.1(7)	C(42)-C(37)-C(38)-C(39)	-1.8(14)
C(9)-C(10)-C(11)-C(12)	0.5(12)	Cl(1)-C(37)-C(38)-C(39)	178.0(7)
C(9)-C(10)-C(11)-C(16)	179.2(7)	C(37)-C(38)-C(39)-C(40)	3.0(14)
C(16)-C(11)-C(12)-C(13)	1.3(10)	C(38)-C(39)-C(40)-C(41)	-3.1(12)
C(10)-C(11)-C(12)-C(13)	-180.0(7)	C(38)-C(39)-C(40)-S(1)	177.1(7)
C(11)-C(12)-C(13)-C(14)	-0.9(10)	C(39)-C(40)-C(41)-C(42)	1.9(12)
C(12)-C(13)-C(14)-N(2)	-179.5(6)	S(1)-C(40)-C(41)-C(42)	-178.2(6)
C(12)-C(13)-C(14)-C(15)	0.2(9)	C(40)-C(41)-C(42)-C(37)	-0.8(13)
N(2)-C(14)-C(15)-C(16)	179.7(6)	C(38)-C(37)-C(42)-C(41)	0.8(14)
C(13)-C(14)-C(15)-C(16)	0.0(9)	Cl(1)-C(37)-C(42)-C(41)	-179.1(7)
C(14)-C(15)-C(16)-C(11)	0.5(11)	C(48)-C(43)-C(44)-C(45)	-0.9(13)
C(12)-C(11)-C(16)-C(15)	-1.1(11)	S(2)-C(43)-C(44)-C(45)	178.9(7)
C(10)-C(11)-C(16)-C(15)	-179.9(7)	C(43)-C(44)-C(45)-C(46)	0.6(14)
N(3)-C(20)-C(21)-C(22)	0.2(11)	C(44)-C(45)-C(46)-C(47)	1.3(14)
C(20)-C(21)-C(22)-C(23)	-0.2(10)	C(44)-C(45)-C(46)-Cl(2)	178.6(7)
C(20)-C(21)-C(22)-C(25)	-179.2(6)	C(45)-C(46)-C(47)-C(48)	-2.8(16)
C(21)-C(22)-C(23)-C(24)	0.3(10)	Cl(2)-C(46)-C(47)-C(48)	179.9(8)
C(25)-C(22)-C(23)-C(24)	179.2(6)	C(46)-C(47)-C(48)-C(43)	2.5(17)
C(22)-C(23)-C(24)-N(3)	-0.3(11)	C(44)-C(43)-C(48)-C(47)	-0.6(14)
C(21)-C(22)-C(25)-C(26)	-176.4(7)	S(2)-C(43)-C(48)-C(47)	179.5(9)
C(23)-C(22)-C(25)-C(26)	4.7(11)	C(3)-C(2)-N(1)-C(1)	-179.8(7)
C(22)-C(25)-C(26)-C(27)	179.6(7)	C(3)-C(2)-N(1)-C(6)	1.4(10)
C(25)-C(26)-C(27)-C(28)	179.2(8)	C(5)-C(6)-N(1)-C(2)	-1.3(10)
C(26)-C(27)-C(28)-C(29)	179.5(7)	C(5)-C(6)-N(1)-C(1)	179.9(7)
C(27)-C(28)-C(29)-C(34)	178.0(8)	C(13)-C(14)-N(2)-C(18)	2.0(10)
C(27)-C(28)-C(29)-C(30)	-1.9(11)	C(15)-C(14)-N(2)-C(18)	-177.7(6)

C(13)-C(14)-N(2)-C(17)	-178.1(7)	
C(15)-C(14)-N(2)-C(17)	2.2(10)	
C(21)-C(20)-N(3)-C(24)	-0.2(11)	
C(21)-C(20)-N(3)-C(19)	-180.0(7)	
C(23)-C(24)-N(3)-C(20)	0.3(11)	
C(23)-C(24)-N(3)-C(19)	-179.9(7)	
C(33)-C(32)-N(4)-C(35)	178.9(7)	
C(31)-C(32)-N(4)-C(35)	-0.5(11)	
C(33)-C(32)-N(4)-C(36)	-1.9(12)	
C(31)-C(32)-N(4)-C(36)	178.7(7)	
C(39)-C(40)-S(1)-O(1)	37.7(8)	
C(41)-C(40)-S(1)-O(1)	-142.1(7)	
C(39)-C(40)-S(1)-O(3)	156.9(7)	
C(41)-C(40)-S(1)-O(3)	-23.0(7)	
C(39)-C(40)-S(1)-O(2)	-83.3(7)	
C(41)-C(40)-S(1)-O(2)	96.9(7)	
C(48)-C(43)-S(2)-O(6)	-35.5(8)	
C(44)-C(43)-S(2)-O(6)	144.7(7)	
C(48)-C(43)-S(2)-O(5)	-158.0(7)	
C(44)-C(43)-S(2)-O(5)	22.2(8)	
C(48)-C(43)-S(2)-O(4)	83.5(7)	
C(44)-C(43)-S(2)-O(4)	-96.3(7)	

Table ST3: Comparison of melting points of commercialized crystals

Crystal	Melting point
DAST ²¹	256±1
DSTMS ²¹	258±1
OH1 ²³	212

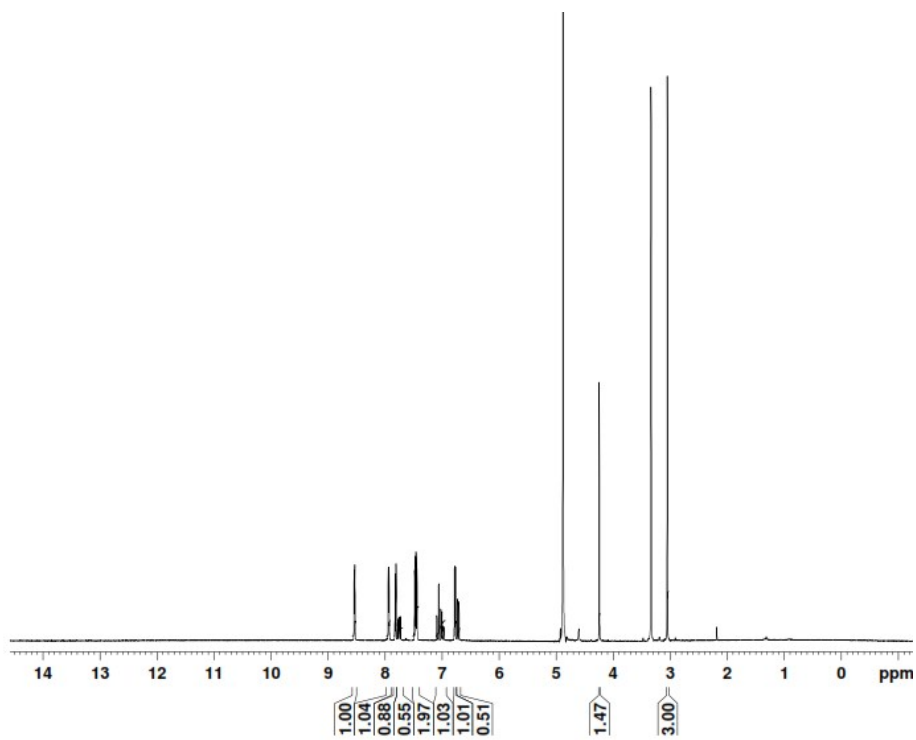


Figure SF1 NMR spectrum of DACSC.H₂O (supplimentary)