

Table 1: Bond angles of DSFS crystal

Atoms	Angles (°)
C(1)-C(2)-C(3)	120.5(2)
C(11)-C(12)-C(13)	121.3(2)
C(11)-C(12)-H(12)	119.3
C(11)-N(2)-C(15)	120.6(2)
C(11)-N(2)-C(16)	119.9(2)
C(12)-C(13)-H(13)	119
C(15)-N(2)-C(16)	117.9(2)
C(2)-C(1)-C(5)	115.5(2)
C(2)-C(1)-C(6)	119.5(2)
C(2)-C(1)-C(6)	119.9(2)
C(2)-C(3)-C(4)	120.5(2)
C(2)-C(3)-H(3)	119.7
C(2)-C(3)-H(3)	119.5
C(3)-C(4)-C(5)	119.5(2)
C(3)-C(4)-H(4)	120.3
C(3)-N(1)-C(14)	120.5(2)
C(3)-N(1)-C(4)	119.3(2)
C(4)-C(5)-C(6)	121.3(2)
C(4)-C(5)-H(5)	119.3
C(4)-C(5)-H(5)	119.5
C(4)-N(1)-C(14)	120.1(2)
C(5)-C(1)-C(6)	124.6(2)
C(5)-C(6)-C(7)	118.8(2)
C(6)-C(7)-C(8)	127.4(2)
C(6)-C(7)-H(7)	118.1
C(6)-C(7)-H(7)	116.3

C(7)-C(8)-C(13)	123.5(2)
Atoms	Angles (°)
C(7)-C(8)-C(9)	120.1(2)
C(8)-C(13)-C(12)	122.0(2)
C(8)-C(13)-H(13)	119
C(8)-C(9)-C(10)	122.7(2)
C(8)-C(9)-H(9)	118.7
C(9)-C(10)-C(11)	121.0(2)
C(9)-C(10)-H(10)	119.5
C(9)-C(8)-C(13)	116.3(2)
H(10)-C(10)-C(11)	119.5
H(12)-C(12)-C(13)	119.3
H(14A)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.4
H(15A)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.4
H(16A)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5
H(2)-C(2)-C(3)	119.3
H(2)-C(2)-C(3)	119.3
H(3)-C(3)-C(4)	119.8
H(4)-C(4)-C(5)	120.3
H(4)-C(4)-C(5)	119.2
H(5)-C(5)-C(6)	119.4
H(6)-C(6)-C(7)	117.3

H(7)-C(7)-C(8)	116.3
Atoms	Angles (°)
H(9)-C(9)-C(10)	118.7
N(1)-C(14)-H(14A)	109.5
N(1)-C(14)-H(14B)	109.5
N(1)-C(14)-H(14C)	109.5
N(1)-C(3)-C(2)	121.1(2)
N(1)-C(3)-H(3)	119.5
N(1)-C(4)-C(5)	121.5(2)
N(1)-C(4)-H(4)	119.3
N(2)-C(11)-C(10)	122.1(2)
N(2)-C(11)-C(12)	121.2(2)
N(2)-C(15)-H(15A)	109.5
N(2)-C(15)-H(15B)	109.5
N(2)-C(15)-H(15C)	109.5
N(2)-C(16)-H(16A)	109.4
N(2)-C(16)-H(16B)	109.5
N(2)-C(16)-H(16C)	109.5
O(1)-S(1)-C(1)	105.33(8)
O(1)-S(1)-O(3)	114.06(9)
O(1)-S(1)-O(4)	113.10(9)
O(2)-C(7)-C(6)	123.8(2)
O(2)-C(7)-H(7)	118.1
O(3)-S(1)-C(1)	105.01(9)
O(3)-S(1)-O(4)	113.03(9)
O(4)-S(1)-C(1)	105.21(8)
S(1)-C(1)-C(2)	118.3(1)
S(1)-C(1)-C(6)	122.2(1)

Table 2. Bond length of DSFS

Atoms	Length(Å)
S(1)-O(1)	1.443(1)
S(1)-O(3)	1.443(1)
S(1)-O(4)	1.443(2)
S(1)-C(1)	1.790(2)
O(2)-C(7)	1.182(3)
C(1)-C(2)	1.384(2)
C(1)-C(6)	1.397(2)
C(2)-H(2)	0.93
C(2)-C(3)	1.380(2)
C(3)-H(3)	0.93
C(3)-C(4)	1.373(3)
C(4)-H(4)	0.93
C(4)-C(5)	1.375(3)
C(5)-H(5)	0.93
C(5)-C(6)	1.396(2)
C(6)-C(7)	1.484(3)
C(7)-H(7)	0.93
N(1)-C(3)	1.337(3)
N(1)-C(4)	1.339(3)
N(1)-C(14)	1.478(3)
N(2)-C(11)	1.370(3)
N(2)-C(15)	1.437(3)
N(2)-C(16)	1.452(3)
C(1)-C(2)	1.392(3)
C(1)-C(5)	1.392(3)
C(1)-C(6)	1.449(3)
C(2)-H(2)	0.93
C(2)-C(3)	1.363(3)
C(3)-H(3)	0.93
C(4)-H(4)	0.93
C(4)-C(5)	1.361(3)
C(5)-H(5)	0.93
C(6)-H(6)	0.93
C(6)-C(7)	1.333(3)
C(7)-H(7)	0.93
C(7)-C(8)	1.451(3)
C(8)-C(9)	1.387(3)
C(8)-C(13)	1.393(3)

Atoms	Length(Å)
C(9)-H(9)	0.93
C(9)-C(10)	1.371(3)
C(10)-H(10)	0.93
C(10)-C(11)	1.396(3)
C(11)-C(12)	1.406(3)
C(12)-H(12)	0.93
C(12)-C(13)	1.371(3)
C(13)-H(13)	0.93
C(14)-H(14A)	0.96
C(14)-H(14B)	0.96
C(14)-H(14C)	0.96
C(15)-H(15A)	0.96
C(15)-H(15B)	0.96
C(15)-H(15C)	0.96
C(16)-H(16A)	0.96
C(16)-H(16B)	0.96
C(16)-H(16C)	0.96