Co-crystals of an organic tris-selenocyanate with ditopic Lewis bases: recurrent chalcogen bond (ChB) interactions motifs

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SUPPLEMENTARY INFORMATION

Table S1. Atomic coordinates of tris(selenocyanatomethyl)-2,4,6-trimethylbenzene **1** after optimization.

Atom	Coordinates		
C	−0.29828600	1.26654000	−0.69880800
C	−1.01864700	0.13005900	−1.11398700
C	−0.53104800	−1.16279000	−0.80489400
C	0.65031600	−1.31763500	−0.05004700
C	1.35278200	−0.16479000	0.38107300
C	0.89977600	1.12879500	0.04540000
C	−0.76171600	2.64535800	−1.07802000
H	0.03149800	3.38482900	−1.03543600
H	−1.19965400	2.68674200	−2.07711500
C	−2.29945900	0.26167400	−1.91346000
H	−2.14683400	−0.02302900	−2.96324300
H	−3.08655400	−0.37964400	−1.50646700
H	−2.70189900	1.27236200	−1.90556100
C	−1.27262900	−2.36154000	−1.32436900
H	−1.76496100	−2.16454100	−2.27821200
H	−0.64544400	−3.23800300	−1.45582200
C	1.20166600	−2.68090000	0.31804800
H	1.16042400	−2.84202300	1.40065100
H	0.64999900	−3.50600800	−0.12685700
H	2.24471300	−2.77938600	−0.00070000
C	2.58098300	−0.33792700	1.22561700
H	2.77199500	0.50324600	1.88464600
H	2.54202000	−1.24073400	1.83542100
C	1.67775500	2.37329100	0.43224800
H	2.01702700	2.90962900	−0.46020300
H	1.07151600	3.05507700	1.03492600
H	2.57506800	2.15526700	1.00683000
C	−1.58714600	3.14644700	1.71299100
C	−2.00989000	−3.21682800	1.39977700
C	4.05584500	0.52097300	−1.19099200
N	−1.18781600	2.99313500	2.79918600
N	−1.51618600	−3.37709400	2.44516000
N	3.92090100	1.23746200	−2.10281100
Se	−2.28289400	3.42219500	0.02700900
Se	−2.86192100	−2.98643300	−0.22066200
Se	4.32484300	−0.64613300	0.21168000

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 1 2 1.5 6 1.5 7 1.0
 2 3 1.5 10 1.0
 3 4 1.5 14 1.0
 4 5 1.5 17 1.0
 5 6 1.5 21 1.0
 6 24 1.0
 7 8 1.0 9 1.0 34 1.0
 8
 9
 10 11 1.0 12 1.0 13 1.0
 11
 12
 13
 14 15 1.0 16 1.0 35 1.0
 15
 16
 17 18 1.0 19 1.0 20 1.0
 18
 19
 20
 21 22 1.0 23 1.0 36 1.0
 22
 23
 24 25 1.0 26 1.0 27 1.0
 25
 26
 27
 28 31 3.0 34 1.0
 29 32 3.0 35 1.0
 30 33 3.0 36 1.0
 31
 32
 33
 34
 35
 36

C H N O
6-31+G**
****
Se     0
S   2   1.00
      1.0330000             -3.3224095
      0.6521000              3.6003462
S   1   1.00
      0.1660000              1.0000000
P   2   1.00
      2.3660000             -0.1185522
      0.3833000              1.0414320
P   1   1.00
      0.1186000              1.0000000
P   1   1.00
      0.0328000              1.0000000
D   1   1.00
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      0.3630000              1.0000000
****

SE     0
SE-ECP     3     28
f-ul potential
  5
1    433.1931336            -28.0000000
2     83.8952157           -214.3841762
2     18.5839139            -65.6918782
2      5.3955286            -24.6153932
2      1.7474326             -2.4481497
s-ul potential
  5
0    202.8986193              3.0000000
1     78.3820487             62.0295390
2     35.0753037            258.8555984
2     10.8769543            118.7800153
2      2.8005941             38.2355279
p-ul potential
  5
0     44.3011875              5.0000000
1     20.3874206             24.7973458
2     23.1889948             63.7575640
2      7.9777664             79.0512831
2      2.2988146             22.9520183
d-ul potential
  5
0     73.3628263              3.0000000
1     48.3835618             22.4705907
2     25.6297211            140.5492887
2      7.1705822             63.5781835
2      1.3639538              7.075361
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