Electronic supplementary information for the paper:

Energy Framework Approach to the Supramolecular Reactions: Interplay of the Secondary Bonding Interaction in Ph2E2 (E=Se, Te) / p-I-C6F4-I Co-crystals.

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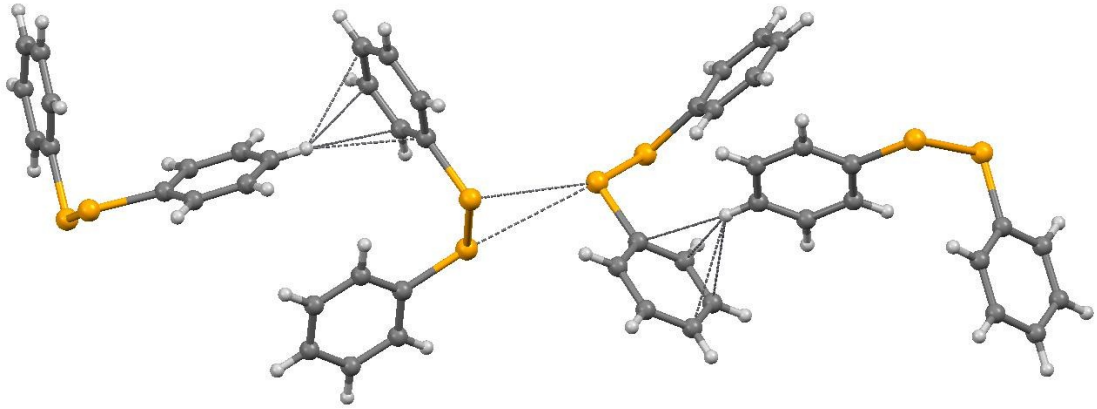
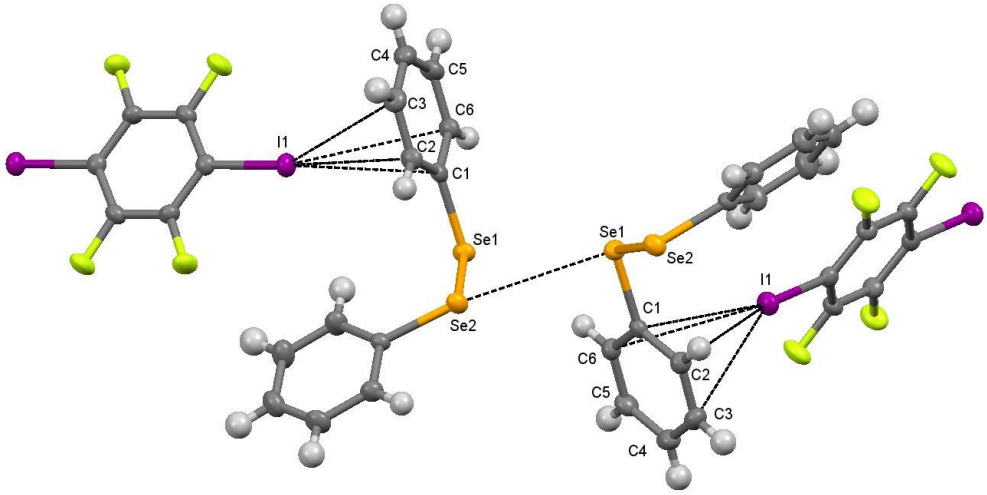


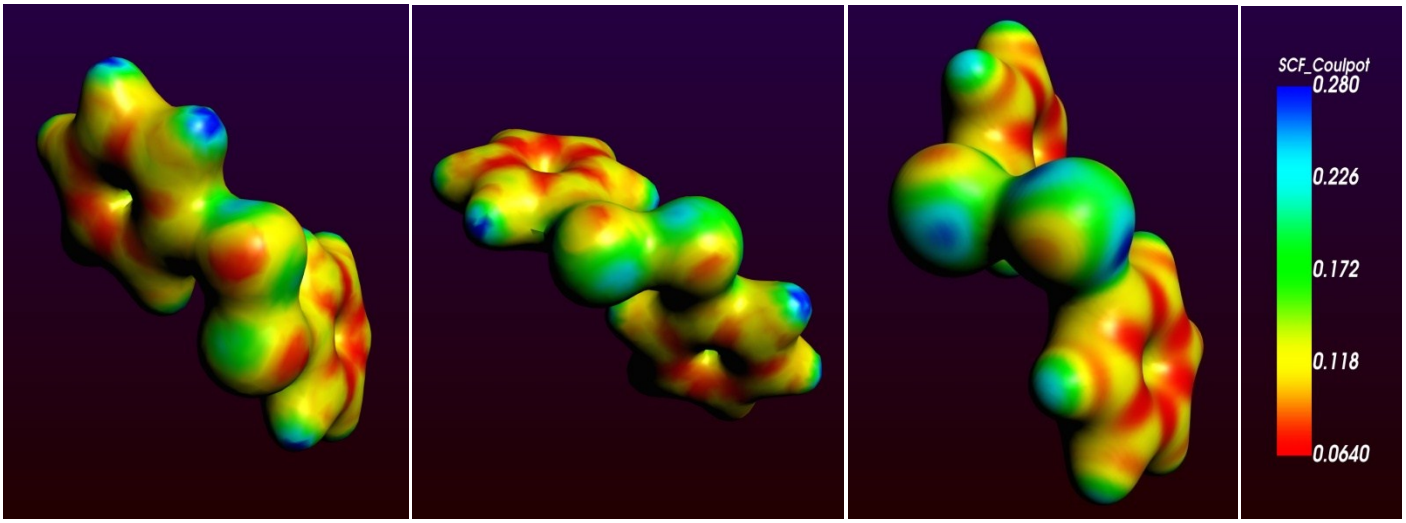
,

a



b

Figure 1_esi. a) Fragment of the packing diagram of **2** showing the H---πPh hydrogen bonds in parent Ph_2Se_2 substituted by **b)** I---πPh halogen bonds in the Ph2Se2-DITFB cocrystal



a **b** **c**

Figure 2_esi ESP maps for Ph_2E_2

a) E = S (in the native Ph_2S_2);

b) E = Se (in the native Ph_2Se_2);

c) E = Te (in Ph_2Te_2-DITFB cocrystal **1**)

Computations

Crystal Explorer 17.5 and QTAIM

General remarks for Tables(1-4_esi) and relevant Figures (4-7_esi).
Intermolecular interaction energies were calculated in CrystalExplorer B3LYP-DGDZVP

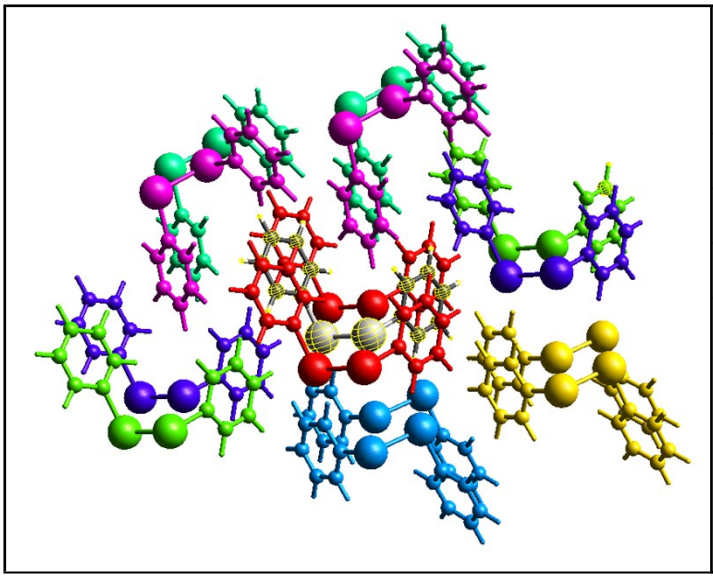
Total energies, only reported a benchmarked B3LYP-DGDZVP energy model, is the sum of the four energy components, scaled appropriately

Scale factors for benchmarked B3LYP-DGDZVP energy model [1].

Energy Model	k_ele	k_pol	k_disp	k_rep
CE-B3LYP DGDZVP	1.057	0.740	0.871	0.618

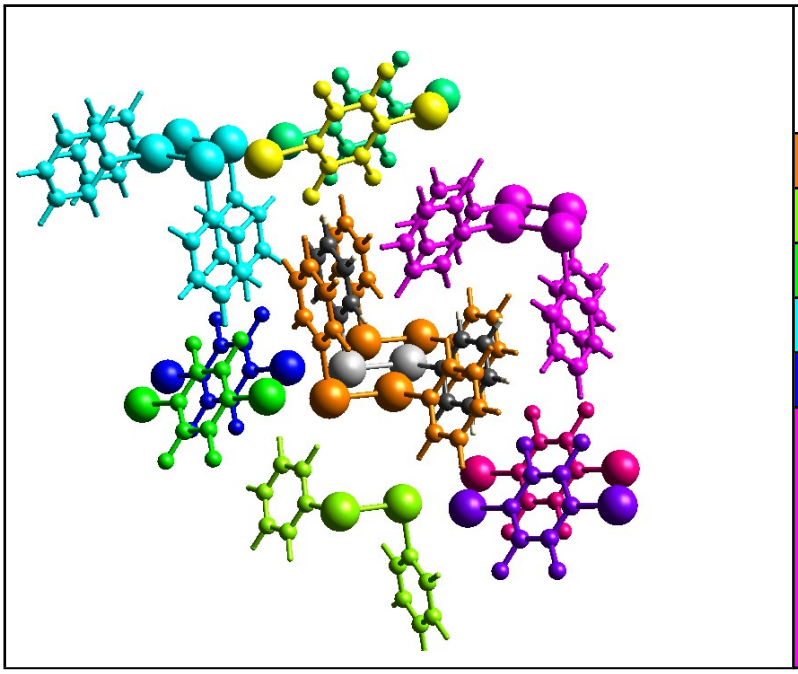
1. C. F. Mackenzie, P. R. Spackman, D. Jayatilaka and M. A. Spackman, *IUCrJ,* **2017**, *4*, 575.

Table 1_esi. Interaction Energies in Ph_2Te_2 (DPHTE01) crystal (kJ/mol)



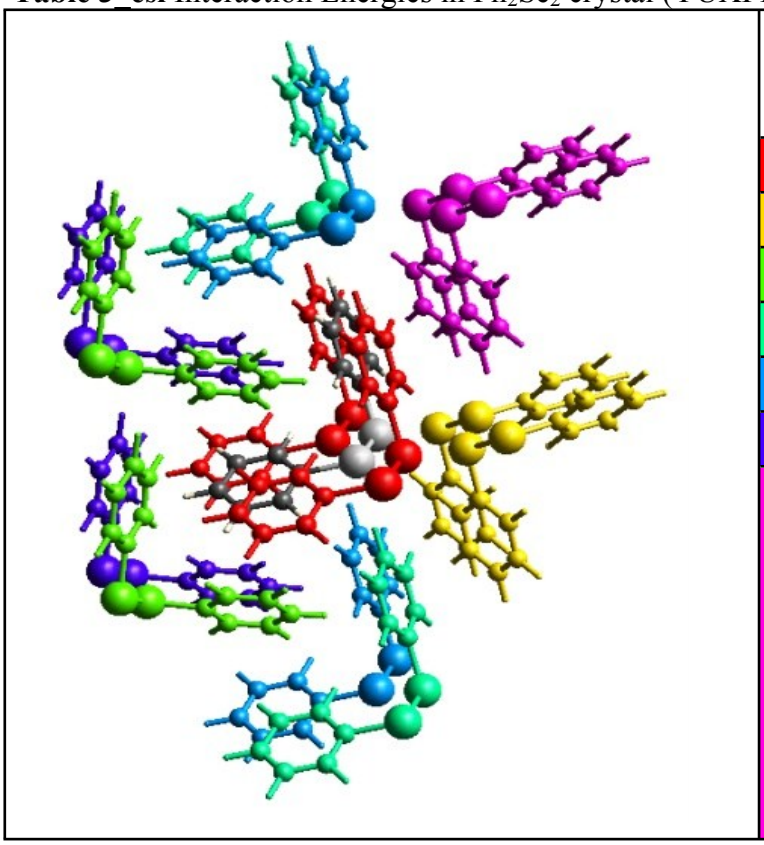
	E_{tot}, CE kJ/mol	E_{tot}, QTAIM, kJ/mol
	-35.4	-14,48
	-6.9	-5,94
	-15.0	-9.33
	-15.5	-6,82

Table 2_esi Interaction Energies (kJ/mol) in Ph_2Te_2 _DITFB crystal (**1**)
Total energies, only reported for two benchmarked energy models, are the sum of the four energy components, scaled appropriately (see the scale factor table below)



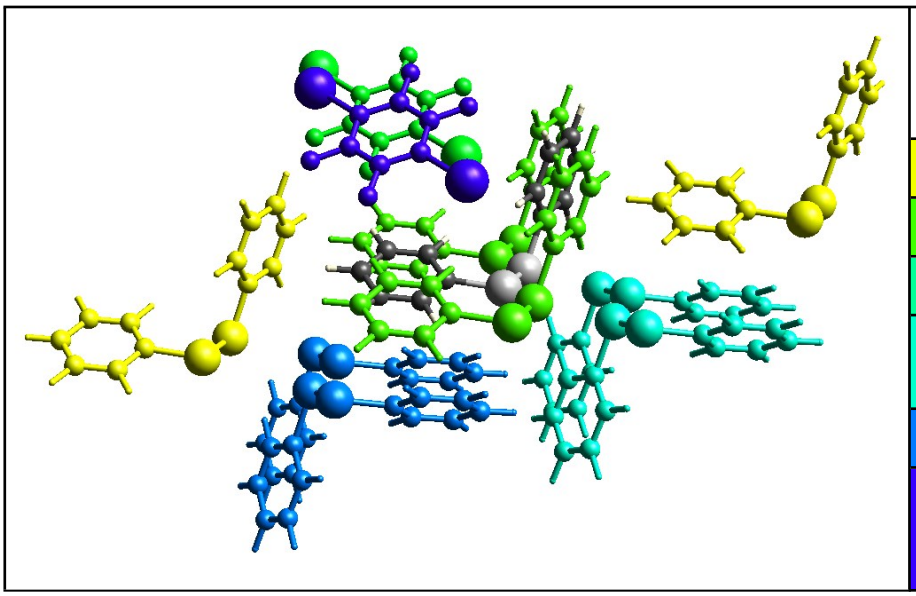
	E_{tot}, CE kJ/mol	E_{tot}, QTAIM, kJ/mol
	-32.1	-16.1
	-11.5	
	-10.4	-13.2
	-11.5	
	-11.1	-4.2
	-23.8	

Table 3_esi Interaction Energies in Ph_2Se_2 crystal (YUXPIR)



	E_{tot}, CE kJ/mol	E_{tot}, QTAIM, kJ/mol
	-22.7	-14,73
	-8.8	-8,37
	-16.8	-9.25
	-6.1	-3,68
	-11.2	-12,17
	-20.5	-10.21
	-12.3	

Table 4_esi Interaction Energies in Ph_2Se_2 _DITFB crystal (**2**)



	E_{tot}, CE kJ/mol	E_{tot}, QTAIM, kJ/mol
	-10.4	-11,09
	-21.8	-12.55
	-22.3	
	-11.5	-8,33 -8,16
	-18.3	
	-24.1	13.72

Table 5_esi

Interaction Energies (CE-B3LYP-DGDZVP) between *p*-DITFB molecules in their stacks in cocrystals **1**-**2**.

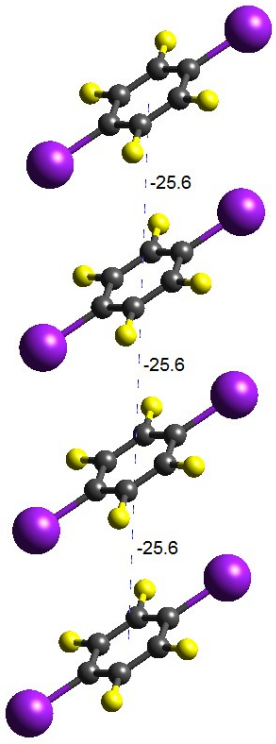
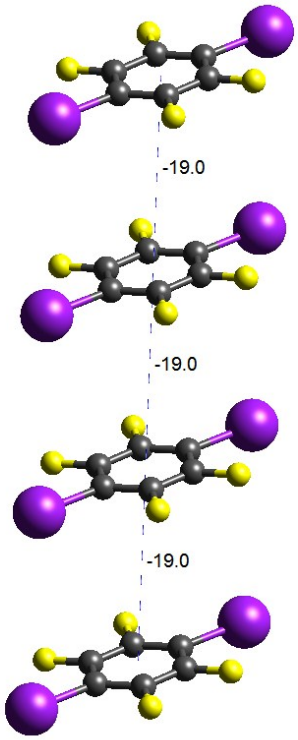
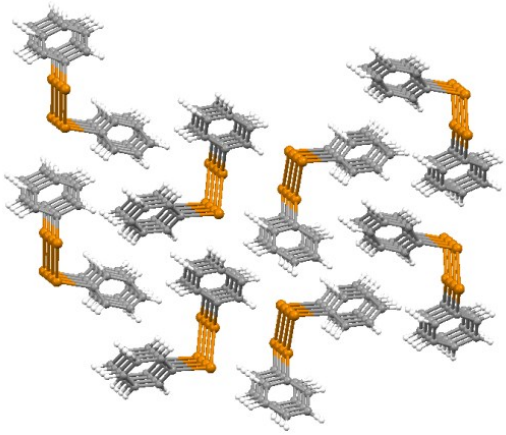
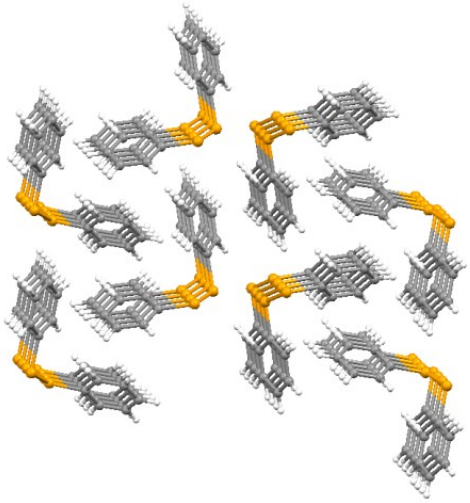
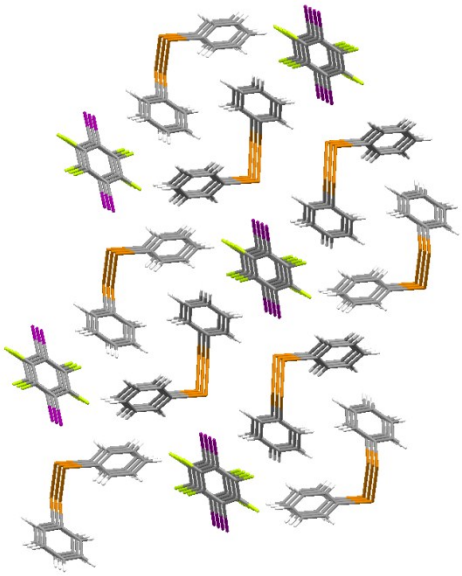
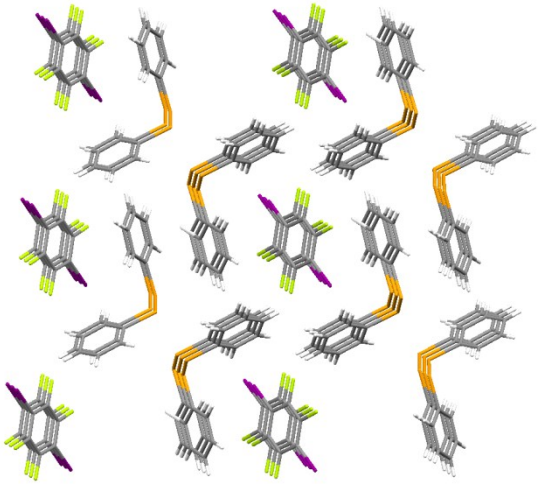
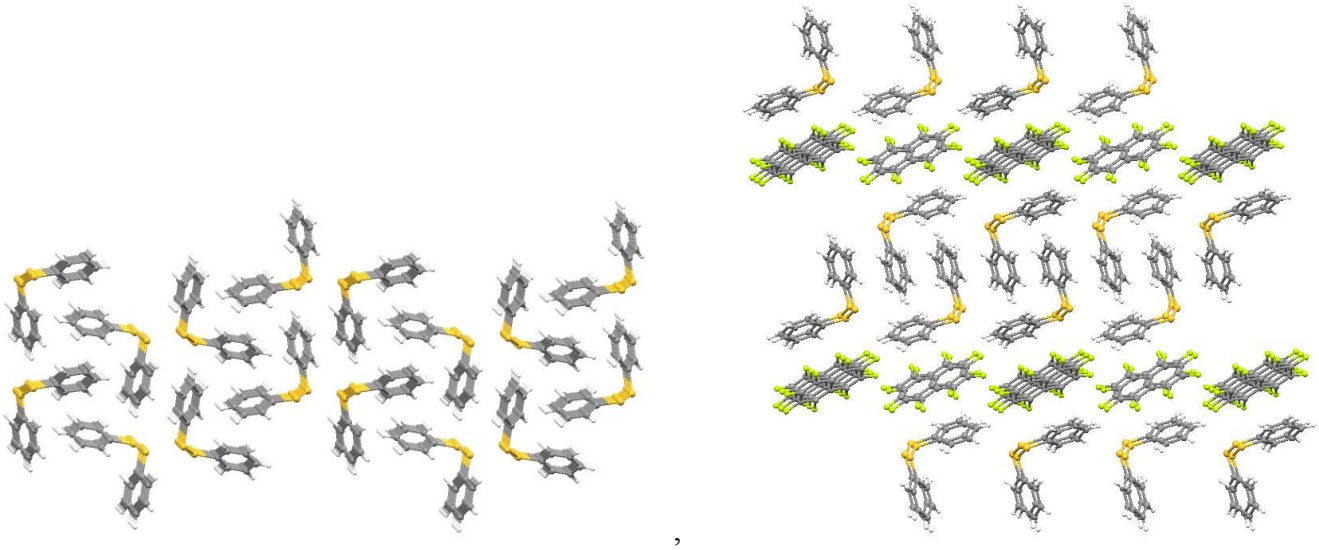
1	**2**
	
-25.6 kJ/mol	-19.0 kJ/mol
5.4 Å	5.67 Å

Table 6_esi. Packing of the native Ph_2Te_2, Ph_2Se_2 and their co-crystals **1** and **2**

	Ph_2Te_2	Ph_2Se_2
Unit cell	$P2_12_12_1$ (YUXQEO) a 5.1563(8) b 8.5809(13) c 26.784(4)	$P2_12_12_1$ (YUXPIR) a 5.5699(19) b 8.238(3) c 23.826(7)
Packing View along *a* axis		
	1 Ph_2Te_2 *p*-DITFB	**2** Ph_2Se_2 *p*-DITFB
Packing View along *b* axis		
	$P\ 2_1/n$ a 13.2557(10) b 5.3985(4) c 23.3604(18)	$P\ 2_1/c$ a 10.1178(7) b 5.6743(4) c 26.6419(18) \



a) , **b)**

Figure 3_esi. Packing of Ph_2S_2 molecules in the native crystal (a) and Ph_2S_2 / $C_{10}F_8$ cocrystal (b)

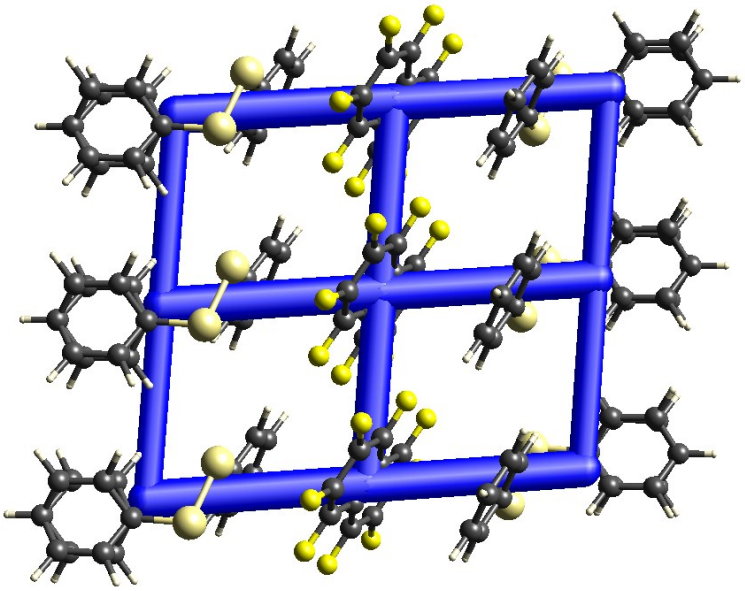


Figure 4_esi. Fragment of the energy framework in Ph_2S_2 - OFNp cocrystal.

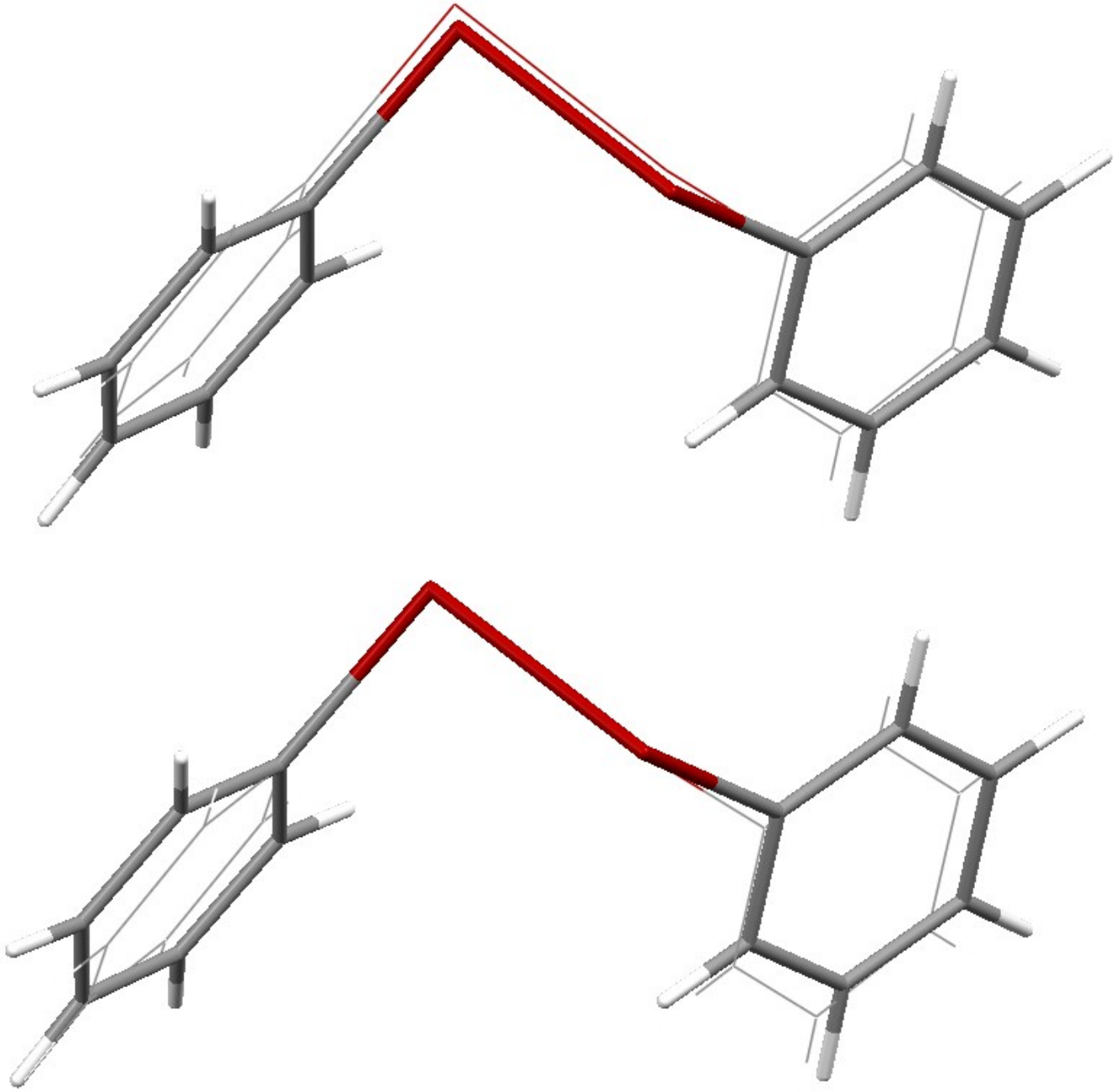


Figure 5_esi. Structure overlay of the Ph_2Te_2 chain fragments in the parent Ph_2Te_2 crystal (YUXQEO) and co-crystal **1** (wireframe).

Figure 6_esi. Structure overlay of the Ph_2Se_2 chain fragments in the parent Ph_2Se_2 crystal (YUXPIR) and co-crystal **2** (wireframe).

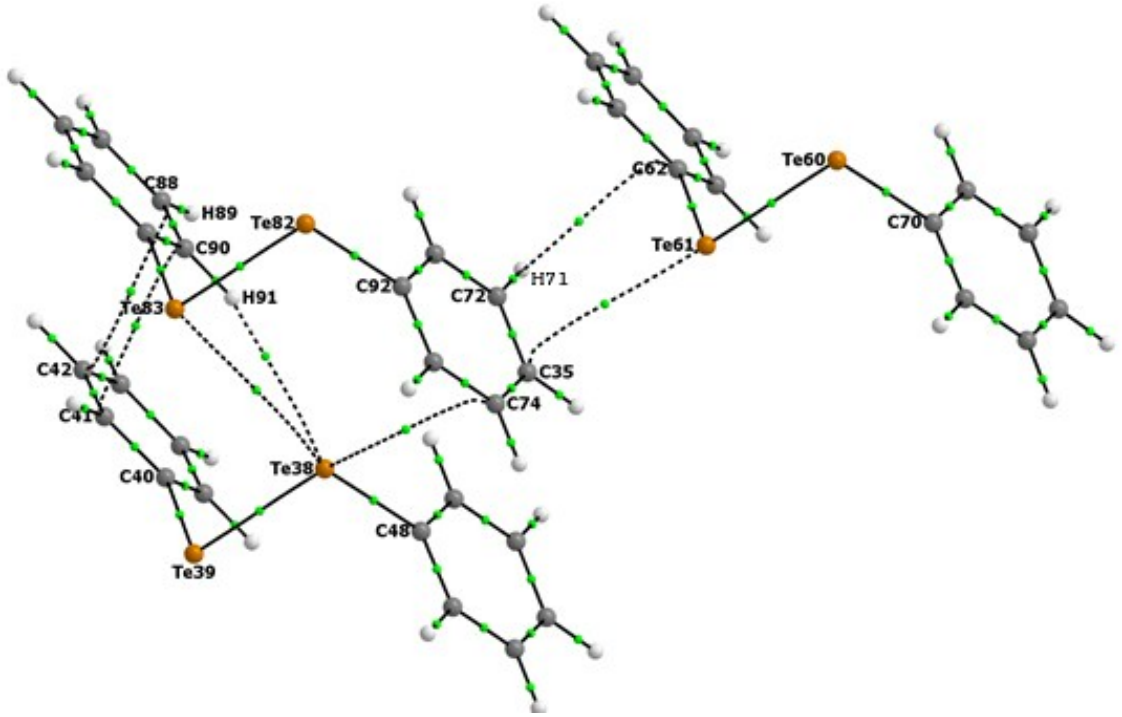


Figure 7_esi. Selected critical points (BCP) [3, -1] in the native Ph_2Te_2

Table 7. Selected critical points [3, -1] in the native Ph_2Te_2

Type	Name	Atoms	Rho, e·Å-3	V, a.e.	L, e·Å-5	Ellip	E, kcal/mol
(3,-1)	BCP	C88 C42	0,03	-0,002	0,31	2,24	-0,51
(3,-1)	BCP	C90 C41	0,03	-0,002	0,31	2,05	-0,51
(3,-1)	BCP	Te83 Te38	0,04	-0,002	0,32	0,18	-0,62
(3,-1)	BCP	Te38 H91	0,04	-0,002	0,36	0,04	-0,78
(3,-1)	BCP	H71 C62	0,04	-0,003	0,42	0,31	-0,80
(3,-1)	BCP	C35 Te61	0,04	-0,003	0,41	0,95	-0,82
(3,-1)	BCP	Te38 C74	0,05	-0,003	0,49	1,61	-1,05
(3,-1)	BCP	C90 C88	2,17	-0,459	-23,21	0,19	
(3,-1)	BCP	C72 H71	1,86	-0,309	-23,10	0,01	
(3,-1)	BCP	C88 H89	1,86	-0,308	-22,98	0,01	
(3,-1)	BCP	Te38 C48	0,81	-0,126	1,10	0,03	
(3,-1)	BCP	Te60 C70	0,81	-0,125	1,03	0,03	
(3,-1)	BCP	Te82 C92	0,81	-0,125	0,98	0,03	
(3,-1)	BCP	Te39 C40	0,79	-0,118	0,82	0,03	
(3,-1)	BCP	Te61 C62	0,80	-0,118	0,73	0,03	
(3,-1)	BCP	Te39 Te38	0,48	-0,049	-0,12	0,01	
(3,-1)	BCP	Te61 Te60	0,48	-0,049	-0,12	0,00	
(3,-1)	BCP	Te83 Te82	0,48	-0,048	-0,11	0,00	

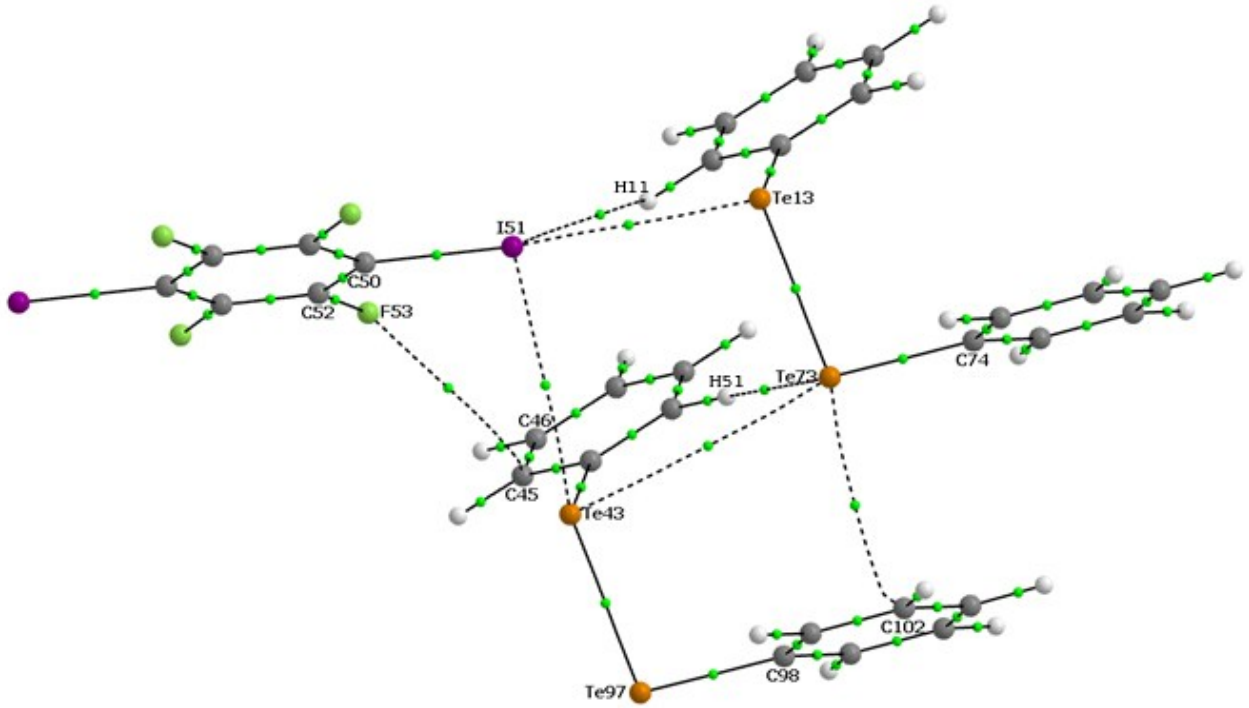


Figure 8_esi. Selected critical points (BCP) [3, -1] in **1**

Table 8_esi. Selected critical points [3, -1] in **1.**

Type	Name	Atoms	Rho, e·Å-3	V, a.e.	L, e·Å-5	Ellip	E, kcal/mol
(3,-1)	BCP	Te13 I51	0,11	-0,007	0,73	0,04	-2,28
(3,-1)	BCP	C102 Te73	0,06	-0,004	0,54	0,63	-1,29
(3,-1)	BCP	I51 H11	0,05	-0,003	0,48	0,07	-1,00
(3,-1)	BCP	H54 Te73	0,05	-0,003	0,43	0,03	-0,95
(3,-1)	BCP	I51 H42	0,05	-0,003	0,47	0,44	-0,93
(3,-1)	BCP	H24 I51	0,04	-0,003	0,43	0,12	-0,89

(3,-1)	BCP	Te43 I51	0,05	-0,002	0,39	0,06	-0,76
(3,-1)	BCP	H96 C67	0,03	-0,002	0,33	0,56	-0,55
(3,-1)	BCP	Te43 Te73	0,03	-0,002	0,26	0,23	-0,48
(3,-1)	BCP	C45 F53	0,01	-0,001	0,18	0,88	-0,26
(3,-1)	BCP	F53 C52	1,81	-0,810	-1,79	0,02	
(3,-1)	BCP	I51 C50	0,84	-0,130	0,30	0,07	
(3,-1)	BCP	Te73 C74	0,80	-0,121	0,79	0,06	
(3,-1)	BCP	Te97 C98	0,80	-0,120	0,81	0,06	
(3,-1)	BCP	Te73 Te13	0,48	-0,048	-0,12	0,04	
(3,-1)	BCP	Te97 Te43	0,47	-0,047	-0,10	0,02	

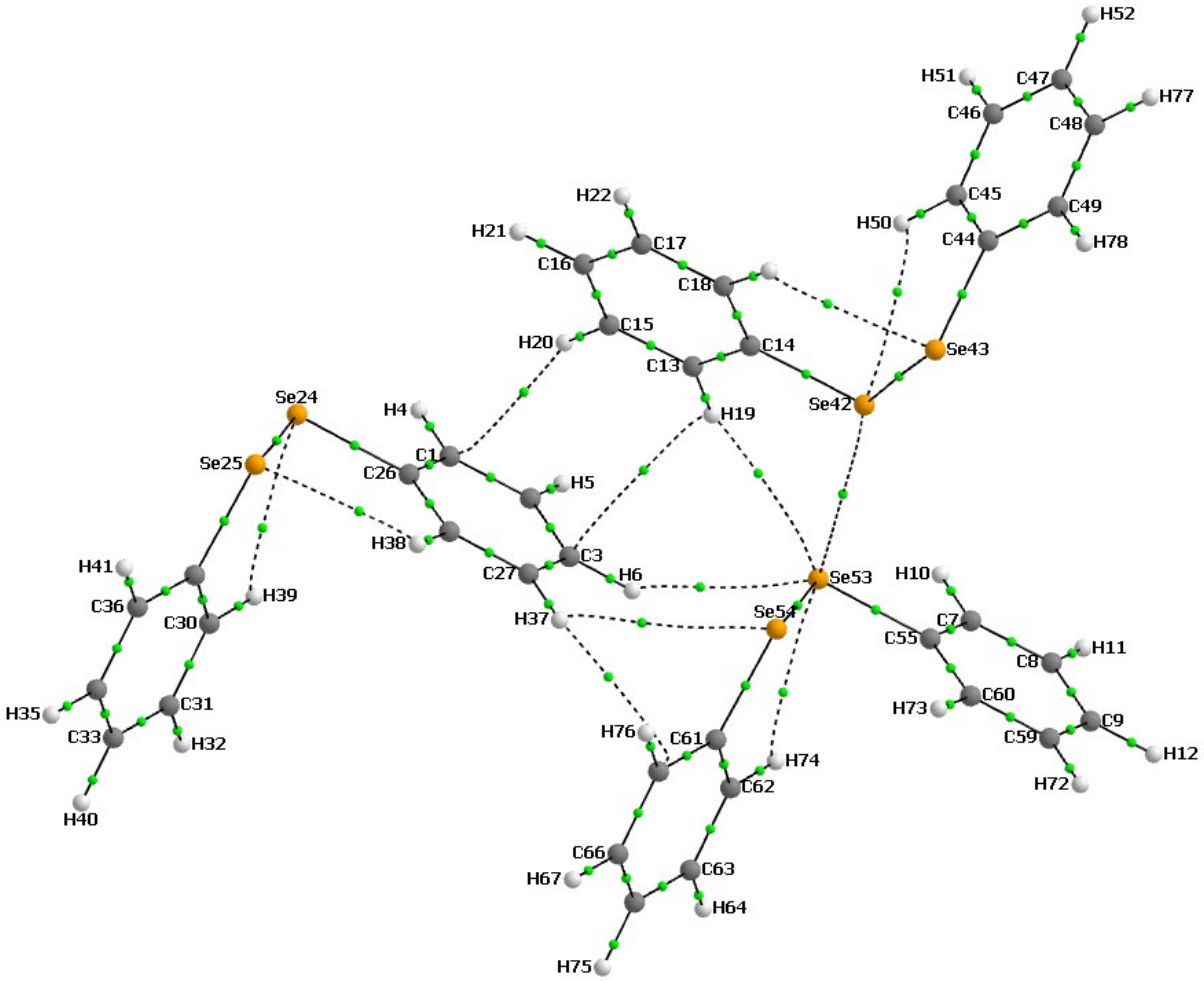


Figure 9_esi. Selected critical points (BCP) [3, -1] in the native Ph_2Se_2

Table 9_esi. Selected critical points [3, -1] for Ph_2Se_2**.**

Type	Name	Atoms	Rho, e·Å-3	V, a.e.	L, e·Å-5	Ellip	E, kcal/mol
(3,-1)	BCP	Se43 H23	0,09	-0,007	0,84	0,44	-2,15
(3,-1)	BCP	H73 Se54	0,09	-0,007	0,83	0,42	-2,15
(3,-1)	BCP	H38 Se25	0,09	-0,007	0,84	0,43	-2,14
(3,-1)	BCP	Se53 H74	0,08	-0,006	0,81	0,72	-2
(3,-1)	BCP	Se79 H94	0,08	-0,006	0,8	0,65	-1,99
(3,-1)	BCP	Se24 H39	0,08	-0,006	0,81	0,67	-1,98
(3,-1)	BCP	H50 Se42	0,08	-0,006	0,81	0,71	-1,97
(3,-1)	BCP	Se53 H6	0,06	-0,004	0,58	0,04	-1,36
(3,-1)	BCP	Se42 Se54	0,05	-0,004	0,52	0,3	-1,18
(3,-1)	BCP	Se42 Se53	0,05	-0,003	0,44	0,99	-0,98
(3,-1)	BCP	C68 H37	0,04	-0,003	0,41	1,06	-0,82
(3,-1)	BCP	Se53 H19	0,04	-0,003	0,37	0,08	-0,8
(3,-1)	BCP	H69 Se42	0,04	-0,003	0,37	0,07	-0,8
(3,-1)	BCP	Se54 H37	0,03	-0,002	0,38	2,44	-0,71
(3,-1)	BCP	C56 H73	0,03	-0,002	0,35	0,76	-0,62
(3,-1)	BCP	H70 C59	0,03	-0,002	0,34	0,76	-0,58
(3,-1)	BCP	H69 Se54	0,03	-0,002	0,28	0,19	-0,5
(3,-1)	BCP	C85 H76	0,02	-0,001	0,29	1,56	-0,45

(3,-1)	BCP	H87 C68	0,02	-0,001	0,28	2,33	-0,43
(3,-1)	BCP	H19 C3	0,02	-0,001	0,25	0,21	-0,4
(3,-1)	BCP	C2 C1	2,09	-0,429	-21,52	0,2	
(3,-1)	BCP	C3 C2	2,26	-0,493	-25	0,2	
(3,-1)	BCP	C1 H4	1,85	-0,308	-22,85	0,02	
(3,-1)	BCP	C2 H5	1,86	-0,308	-22,93	0,01	
(3,-1)	BCP	H6 C3	1,86	-0,31	-23,17	0,02	
(3,-1)	BCP	C8 C7	2,09	-0,429	-21,53	0,2	
(3,-1)	BCP	C9 C8	2,26	-0,493	-25,03	0,2	
(3,-1)	BCP	C7 H10	1,85	-0,308	-22,94	0,02	
(3,-1)	BCP	C8 H11	1,86	-0,308	-23	0,01	
(3,-1)	BCP	H12 C9	1,86	-0,309	-23,06	0,02	
(3,-1)	BCP	C14 C13	2,09	-0,434	-21,36	0,2	
(3,-1)	BCP	H20 C1	0,04	-0,003	0,42	0,95	
(3,-1)	BCP	C13 C15	2,09	-0,429	-21,57	0,19	
(3,-1)	BCP	C16 C15	2,26	-0,493	-25,04	0,2	
(3,-1)	BCP	C17 C16	2,05	-0,41	-20,76	0,18	
(3,-1)	BCP	C18 C14	2,19	-0,473	-23,53	0,19	
(3,-1)	BCP	C18 C17	2,17	-0,46	-23,05	0,2	
(3,-1)	BCP	C13 H19	1,86	-0,31	-23,12	0,02	
(3,-1)	BCP	C15 H20	1,86	-0,309	-23,21	0,01	
(3,-1)	BCP	C16 H21	1,86	-0,309	-23,06	0,02	
(3,-1)	BCP	H22 C17	1,86	-0,31	-23,16	0,02	
(3,-1)	BCP	H23 C18	1,85	-0,306	-22,91	0,02	
(3,-1)	BCP	C26 C1	2,09	-0,434	-21,33	0,2	
(3,-1)	BCP	Se25 Se24	0,74	-0,092	-1,05	0,01	
(3,-1)	BCP	C26 Se24	1,04	-0,157	-3,97	0,19	
(3,-1)	BCP	C27 C3	2,05	-0,41	-20,81	0,18	
(3,-1)	BCP	C28 C26	2,19	-0,473	-23,57	0,18	
(3,-1)	BCP	C27 C28	2,17	-0,46	-23,09	0,2	
(3,-1)	BCP	C29 C30	2,13	-0,448	-22,28	0,19	
(3,-1)	BCP	Se25 C29	1,04	-0,154	-3,96	0,17	
(3,-1)	BCP	C30 C31	2,17	-0,46	-23,15	0,19	
(3,-1)	BCP	C33 C31	2,25	-0,487	-24,89	0,19	
(3,-1)	BCP	C30 H39	1,86	-0,309	-23,25	0,02	
(3,-1)	BCP	C31 H32	1,86	-0,309	-23,06	0,01	
(3,-1)	BCP	C36 C29	2,17	-0,464	-23,05	0,2	
(3,-1)	BCP	C34 C33	2,2	-0,469	-23,86	0,19	
(3,-1)	BCP	C33 H40	1,86	-0,309	-22,9	0,02	
(3,-1)	BCP	C36 C34	2,13	-0,444	-22,3	0,2	
(3,-1)	BCP	H35 C34	1,86	-0,309	-23,08	0,02	
(3,-1)	BCP	H41 C36	1,85	-0,308	-22,89	0,02	
(3,-1)	BCP	H37 C27	1,88	-0,311	-23,51	0,01	
(3,-1)	BCP	H38 C28	1,86	-0,307	-22,99	0,02	
(3,-1)	BCP	Se42 C14	1,04	-0,156	-4,02	0,18	
(3,-1)	BCP	C44 C45	2,13	-0,448	-22,29	0,19	
(3,-1)	BCP	C49 C44	2,17	-0,464	-23,05	0,2	
(3,-1)	BCP	Se43 Se42	0,74	-0,092	-1,04	0,02	
(3,-1)	BCP	C44 Se43	1,04	-0,154	-3,91	0,17	

(3,-1)	BCP	C46 C45	2,17	-0,46	-23,16	0,19
(3,-1)	BCP	C47 C46	2,25	-0,487	-24,88	0,19
(3,-1)	BCP	C48 C47	2,2	-0,469	-23,86	0,19
(3,-1)	BCP	C48 C49	2,13	-0,444	-22,31	0,2
(3,-1)	BCP	C45 H50	1,87	-0,309	-23,25	0,02
(3,-1)	BCP	C46 H51	1,86	-0,309	-23,04	0,01
(3,-1)	BCP	H52 C47	1,85	-0,309	-22,88	0,02
(3,-1)	BCP	C55 C7	2,1	-0,434	-21,38	0,2
(3,-1)	BCP	Se54 Se53	0,74	-0,092	-1,04	0,02
(3,-1)	BCP	C55 Se53	1,04	-0,156	-3,97	0,18
(3,-1)	BCP	C57 C56	2,09	-0,429	-21,54	0,19
(3,-1)	BCP	C58 C57	2,26	-0,493	-25,01	0,2
(3,-1)	BCP	C59 C9	2,05	-0,41	-20,76	0,18
(3,-1)	BCP	C60 C55	2,19	-0,473	-23,55	0,18
(3,-1)	BCP	C59 C60	2,17	-0,46	-23,07	0,2
(3,-1)	BCP	Se54 C61	1,04	-0,154	-3,9	0,17
(3,-1)	BCP	C61 C62	2,13	-0,448	-22,29	0,19
(3,-1)	BCP	C62 C63	2,17	-0,46	-23,16	0,19
(3,-1)	BCP	C63 H64	1,86	-0,309	-23,07	0,01
(3,-1)	BCP	C65 C63	2,25	-0,487	-24,9	0,19
(3,-1)	BCP	C68 C61	2,17	-0,464	-23,02	0,19
(3,-1)	BCP	C66 C65	2,2	-0,469	-23,87	0,19
(3,-1)	BCP	C68 C66	2,13	-0,444	-22,32	0,19
(3,-1)	BCP	H67 C66	1,86	-0,309	-23,14	0,01
(3,-1)	BCP	C56 H69	1,86	-0,31	-23,19	0,02
(3,-1)	BCP	C57 H70	1,86	-0,309	-23,09	0,01
(3,-1)	BCP	H71 C58	1,86	-0,309	-22,98	0,02
(3,-1)	BCP	H72 C59	1,87	-0,31	-23,25	0,02
(3,-1)	BCP	H73 C60	1,86	-0,307	-23,06	0,02
(3,-1)	BCP	C62 H74	1,86	-0,309	-23,23	0,02
(3,-1)	BCP	C65 H75	1,86	-0,309	-22,92	0,02
(3,-1)	BCP	H76 C68	1,86	-0,308	-22,99	0,02
(3,-1)	BCP	H77 C48	1,86	-0,309	-23,07	0,02
(3,-1)	BCP	H78 C49	1,85	-0,308	-22,89	0,02
(3,-1)	BCP	C81 C56	2,09	-0,434	-21,38	0,19
(3,-1)	BCP	Se80 Se79	0,74	-0,092	-1,03	0,01
(3,-1)	BCP	C81 Se79	1,04	-0,157	-3,98	0,19
(3,-1)	BCP	C82 C58	2,05	-0,41	-20,76	0,18
(3,-1)	BCP	C83 C81	2,19	-0,472	-23,57	0,18
(3,-1)	BCP	C82 C83	2,17	-0,46	-23,05	0,2
(3,-1)	BCP	Se80 C84	1,03	-0,154	-3,92	0,17
(3,-1)	BCP	C84 C85	2,13	-0,448	-22,28	0,19
(3,-1)	BCP	H92 C82	1,86	-0,31	-23,16	0,02
(3,-1)	BCP	C85 C86	2,17	-0,46	-23,14	0,19
(3,-1)	BCP	C86 H87	1,86	-0,309	-23,14	0,01
(3,-1)	BCP	C88 C86	2,25	-0,487	-24,87	0,19
(3,-1)	BCP	C91 C84	2,17	-0,464	-23,07	0,2
(3,-1)	BCP	C89 C88	2,2	-0,469	-23,86	0,19
(3,-1)	BCP	C91 C89	2,13	-0,444	-22,3	0,2

(3,-1)	BCP	H90 C89	1,86	-0,309	-23,08	0,01
(3,-1)	BCP	C85 H94	1,86	-0,308	-23,19	0,02
(3,-1)	BCP	H93 C83	1,85	-0,306	-22,93	0,02
(3,-1)	BCP	C88 H95	1,85	-0,309	-22,86	0,02
(3,-1)	BCP	H96 C91	1,85	-0,308	-22,91	0,02

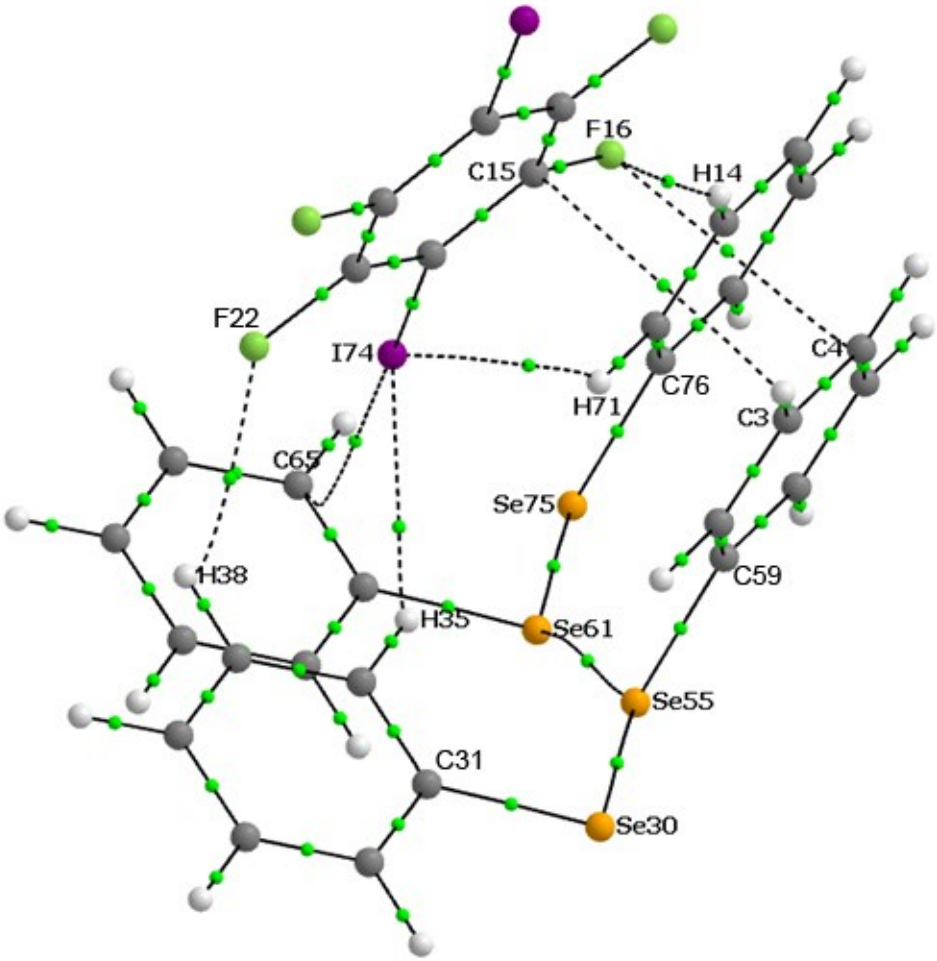
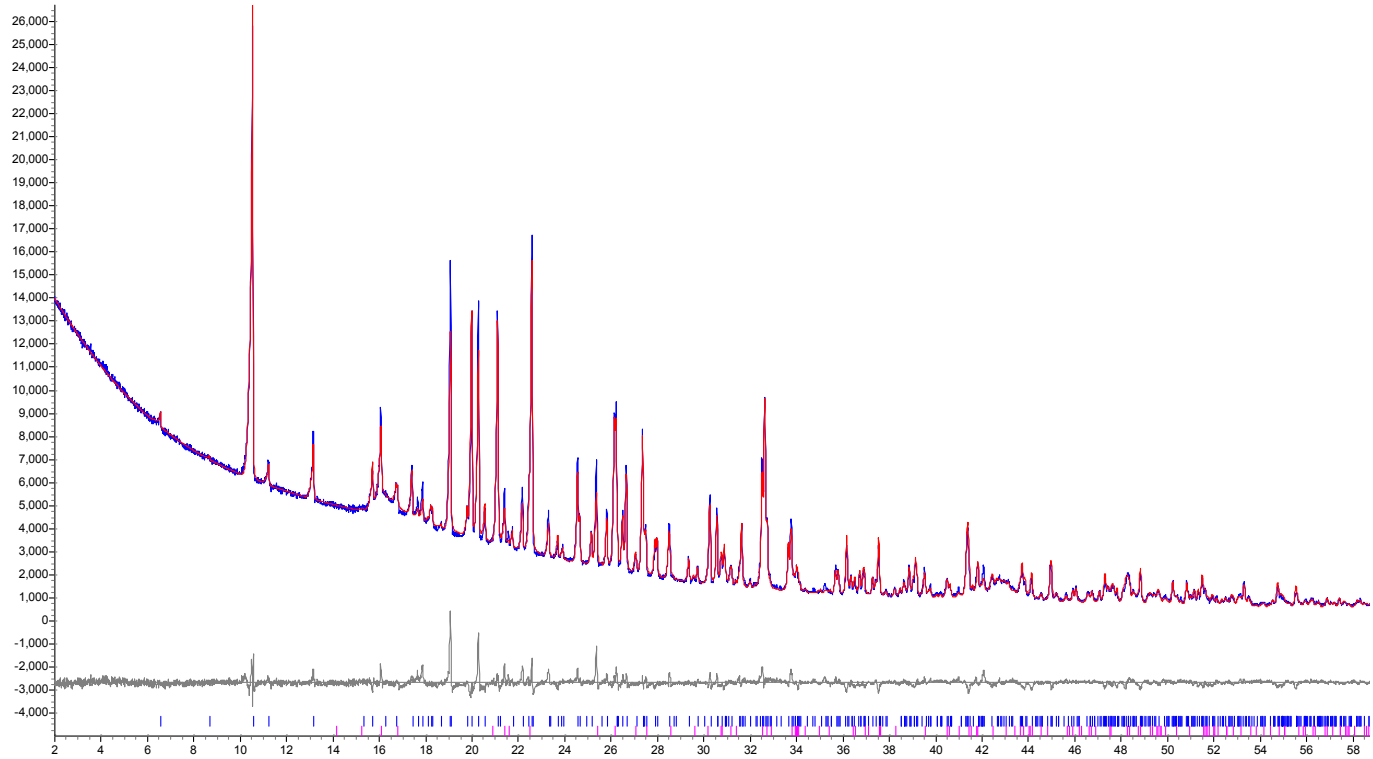


Figure 10_esi. Selected critical points (BCP) [3, -1] in **2**.

Table 10_esi. Selected critical points [3, -1] for **2.**

Type	Name	Atoms	Rho, e·Å-3	V, a.e.	L, e·Å-5	Ellip	E, kcal/mol
(3,-1)	BCP	C3 C15	0,02	-0,001	0,19	0,38	-0,28
(3,-1)	BCP	C4 F16	0,02	-0,001	0,27	1,16	-0,41
(3,-1)	BCP	I74 H35	0,05	-0,003	0,46	0,10	-0,96
(3,-1)	BCP	H71 I74	0,05	-0,003	0,49	0,14	-0,99
(3,-1)	BCP	H38 F22	0,04	-0,003	0,59	0,25	-1,00
(3,-1)	BCP	Se41 Se55	0,05	-0,003	0,45	0,02	-1,00
(3,-1)	BCP	H14 F16	0,04	-0,004	0,68	0,04	-1,16
(3,-1)	BCP	Se61 Se55	0,06	-0,004	0,53	0,11	-1,26
(3,-1)	BCP	Se30 H39	0,08	-0,006	0,82	0,64	-2,03
(3,-1)	BCP	Se61 H71	0,08	-0,007	0,81	0,61	-2,05
(3,-1)	BCP	C4 C3	2,19	-0,462	-23,56	0,19	
(3,-1)	BCP	F16 C15	1,80	-0,806	-1,63	0,02	
(3,-1)	BCP	Se55 Se30	0,73	-0,090	-1,00	0,03	
(3,-1)	BCP	Se30 C31	1,04	-0,155	-4,00	0,18	
(3,-1)	BCP	Se75 Se61	0,73	-0,090	-1,00	0,03	
(3,-1)	BCP	Se75 H66	0,09	-0,007	0,86	0,43	
(3,-1)	BCP	Se75 C76	1,04	-0,155	-4,01	0,17	

The powder pattern of **2** was measured on a Bruker D8 Advance Vario diffractometer at room temperature with LynxEye detector and Ge(111) monochromator, λ(Cu Kα 1) = 1.54060 Å, θ/2θ scan from 2° to 90°, step size 0.0104788°. The measurement was performed in transmission mode, with the sample deposited between two Kapton films. Quantitative phase analysis was performed with Rietveld method as implemented in Bruker TOPAS5 (TOPAS 5 UserManual; BrukerAXS GmbH: Karlsruhe, Germany, 2015.). According to the analysis the sample contains 98% of **2** and 2% of p-DITFB.



Experimental and calculated powder patterns for **2**.

Refined lattice parameters for **2**

a (Å)	10.18697(17)
b (Å)	5.75575(7)
c (Å)	26.9217(4)
beta (°)	93.7761(11)

Lattice parameters for **2** from single crystal experiment

a (Å)	10.1178(7)
b (Å)	5.6743(4)
c (Å)	26.6419(18)
beta (°)	94.6130(10)

Refined lattice parameters for *p*-DITFB

a (Å)	6.2528(2)
b (Å)	11.6093(5)
c (Å)	5.9208(3)
beta (°)	92.621(3)

Lattice parameters for *p*-DITFB single crystal (ZZZAVM02, Se Ye Oh, C.W.Nickels, F.Garcia, W.Jones, T.Friscic, *CrystEngComm* (2012), **14**, 6110)

a (Å)	6.268(3)
b (Å)	11.639(5)
c (Å)	5.929(2)
beta (°)	92.70(3)

Rexp : 1.98 Rwp : 4.46 Rp : 2.85 GOF : 2.2.

Table 11_esi. Intramolelular distances and angles in cocrystal **1.**

Distances, Å

Te1 Te2 2.7161(3) .
Te1 C1 2.1257(12) .
Te2 C7 2.124(3) .
C1 C6 1.3900 .
C1 C2 1.3900 .
C4 C3 1.3900 .
C4 C5 1.3900 .
C4 H4 0.9300 .
C3 C2 1.3900 .
C6 C5 1.3900 .
C7 C8 1.387(4) .
C7 C12 1.393(4) .
C11 C10 1.380(4) .
C11 C12 1.385(4) .
C8 C9 1.391(4) .
I1 C13 2.099(2) .
F4 C18 1.344(3) .
F1 C14 1.346(3) .
C14 C13 1.384(3) .
C14 C18 1.381(4)
C13 C18 1.383(4) .

Angles, °

C1 Te1 Te2 95.97(5) .
C7 Te2 Te1 100.54(6) .
C6 C1 Te1 119.0 .
C2 C1 Te1 121.0 .
C2 C1 C6 120.0 .
C5 C4 C3 120.0 .
H4 C4 C3 120.00(6) .
H4 C4 C5 120.00(6) .
C2 C3 C4 120.0 .
H3 C3 C4 120.00(6) .
H3 C3 C2 120.00(6) .
C5 C6 C1 120.0 .
H6 C6 C1 120.00(6) .
H6 C6 C5 120.00(6) .
C6 C5 C4 120.0 .
H5 C5 C4 120.00(6) .
H5 C5 C6 120.00(6) .
C8 C7 Te2 120.32(18) .
C12 C7 Te2 120.22(19) .
C12 C7 C8 119.4(2) .
C12 C11 C10 120.1(2) .
C9 C8 C7 119.9(2) .
C3 C2 C1 120.0 .
C10 C9 C8 120.3(2) .
C9 C10 C11 120.1(3) .
C11 C12 C7 120.2(2) .
C13 C14 F1 120.1(2) .
C18 C14 F1 118.7(2)
C18 C14 C13 121.2(2)
C14 C13 I1 120.94(19) .
C18 C13 I1 121.46(17) .
C18 C13 C14 117.6(2) .
C14 C18 F4 118.4(2)
C13 C18 F4 120.3(2) .
C13 C18 C14 121.2(2) .

Table 12_esi. Intramolelular distances and angles in cocrystal **2.**

Distances, Å	**Angles, °**
Se2 Se1 2.31335(15) .	C7 Se2 Se1 102.189(2) . .
Se2 C7 1.93399(14) .	C1 Se1 Se2 103.036(4) . .
Se1 C1 1.93392(17) .	C3 C4 C5 119.390(9) . .
F1 C14 1.34545(12) .	H4 C4 C5 120.305(4) . .
F4 C18 1.34546(11) .	H4 C4 C3 120.305(6) . .
C4 C5 1.38609(13) .	C6 C5 C4 120.630(4) . .
C4 C3 1.38548(9) .	H5 C5 C4 119.685(4) . .
C5 C6 1.38465(16) .	H5 C5 C6 119.685(2) . .
C10 C11 1.38195(9) .	C9 C10 C11 119.186(4) . .
C10 C9 1.37708(11) .	H10 C10 C11 120.407(3) . .
C3 C2 1.39173(16) .	H10 C10 C9 120.407(2) . .
C7 C8 1.38353(9) .	C2 C3 C4 120.462(7) . .
C7 C12 1.38162(11) .	C8 C7 Se2 115.833(5) . .
C11 C12 1.37767(11) .	C12 C7 Se2 123.773(3) . .
C1 C6 1.38998(9) .	C12 C7 C8 120.389(5) . .
C1 C2 1.38195(13) .	C12 C11 C10 120.810(6) .
C13 C18 1.38474(12) .	C6 C1 Se1 116.370(7) . .
C13 C14 1.37566(11) .	C2 C1 Se1 123.298(4) . .
C8 C9 1.39426(11) .	C2 C1 C6 120.331(9) . .
C18 C14 1.38165(10)	C18 C13 I1 121.244(4) . .
	C14 C13 I1 121.266(6) . .
	C14 C13 C18 117.488(5) . .
	C9 C8 C7 119.036(5) . .
	C11 C12 C7 119.756(4) . .
	C13 C18 F4 120.532(5) . .
	C14 C18 F4 118.415(7)
	C14 C18 C13 121.053(5)
	C1 C6 C5 119.575(7) . .
	C1 C2 C3 119.608(4) . .
	C8 C9 C10 120.807(4) . .
	C13 C14 F1 120.471(5) . .
	C18 C14 F1 118.068(5)
	C18 C14 C13 121.459(7)