Hydrogen- and halogen-bond cooperativity in determining the crystal packing of dihalogen Charge-Transfer adducts: a study case from heterocyclic pentatomic chalcogenone donors

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Electronic Supplementary Information (ESI)

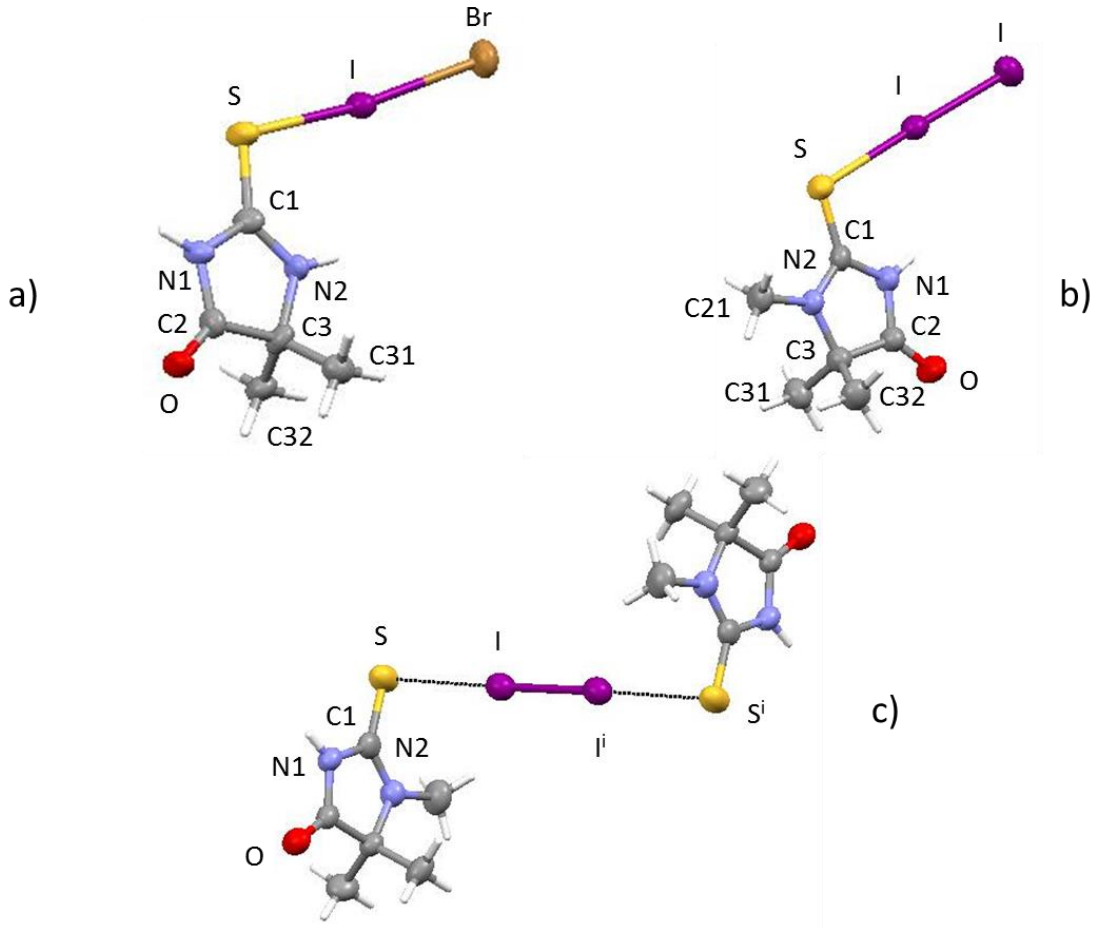

Figure 1S. a) ORTEP view of the asymmetric unit in **1** [S···I 2.587(3), I–Br 2.744(2), C1–S 1.694(8), N1–C1 1.362(10), N2–C1 1.319(11), C2–O 1.201(10) Å, S–I–Br 173.43(6), C1–S–I 104.5(3), N1–C1–S 120.9(6), N2–C1–S 130.1(7)°]; b) ORTEP view of the asymmetric unit in **2** [S···I 2.818(2), I–I 2.795(1), C1–S 1.679(4), N1–C1 1.371(5), N2–C1 1.327(5), C2–O 1.203(5) Å, S–I–I 178.03(3), C1–S–I 103.51(14), N1–C1–S 125.8(3), N2–C1–S 125.5(3)°]; c) ORTEP view of the bridging adduct in **3** [S···I 3.171(1), I–I^i 2.751(1), C1–S 1.672(3), N1–C1 1.380(3), N2–C1 1.324(3), C2–O 1.220(3) Å, S–I–I^i 175.83(2), C1–S–I 88.25(9), N1–C1–S 123.8(2), N2–C1–S 128.3(2)°, i = 1-x, 1-y, 2-z. Displacement parameters are drawn at 30% probability level.

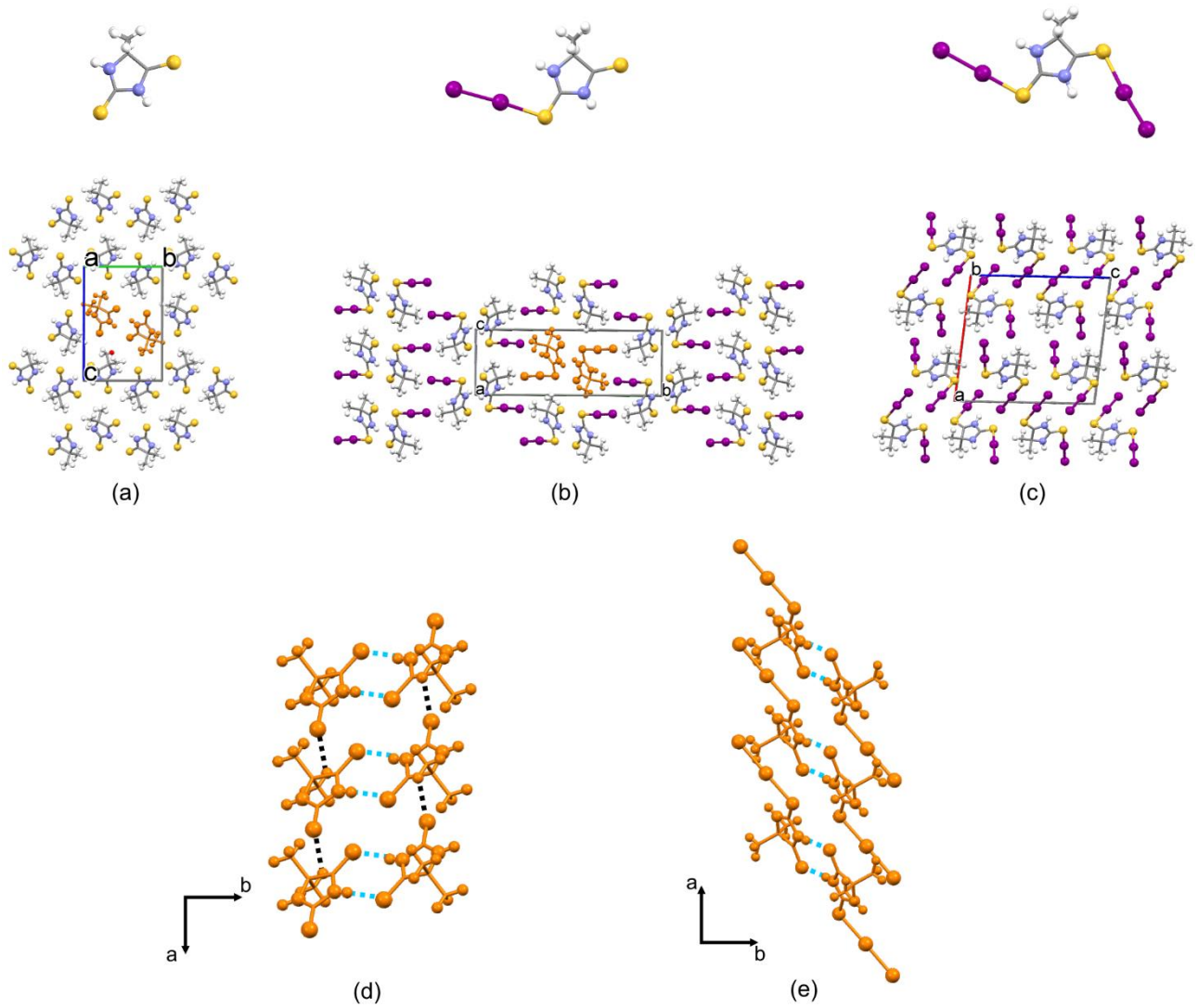

Figure 2S. Crystal packing comparison of the structures FILXED (a), **4** (KUWDEL) (b) and **5** (KUWDIP) (c). Instances of the stack of centrosymmetric dimers for FILXED (d) and **4** (e). The common stack of centrosymmetric N–H···S bonded dimers is indicated as orange. N–H···S hydrogen bonds are indicated as blue dashed lines, other interactions as black dashed lines.

Table 1S. Unit cell parameters for the compounds **1**-**7**.

	1	**2**	**3**	**4**[a]	**5**[a]	**6**[a]	**7**[a]
Formula	$C_5H_8BrIN_2OS$	$C_6H_{10}I_2N_2OS$	$C_6H_{10}IN_2OS$	$C_5H_8I_2N_2S_2$	$C_5H_8I_4N_2S_2$	$C_5H_8I_2N_2OS_1$	$C_5H_8I_2N_2OSe$
L / XY ratio	1:1	1:1	2:1	1:1	1:2	1:1	1:1
M	351.00	412.02	285.12				
Crystal System	triclinic	monoclinic	monoclinic	monoclinic	monoclinic	monoclinic	triclinic
Space Group	P-1 (No. 2)	$P2_1/c$ (No. 14)	$P2_1/n$ (No. 14)	$P2_1/n$	$P2_1/c$	$P2_1/n$	P-1
a/ Å	7.786(3)	7.900(2)	8.8008(10)	6.681(1)	14.757(2)	13.183(3)	8.034(3)
b/ Å	8.719(4)	11.379(3)	10.319(2)	22.212(4)	6.136(1)	6.106(1)	8.769(4)
c/ Å	9.403(4)	12.977(5)	11.1239(10)	7.854(1)	16.284(3)	14.550(2)	9.805(5)
α / º	62.62(4)	90.00	90.00	90.00	90.00	90.00	63.44(1)
β / º	89.52(4)	95.60(3)	96.590(10)	98.89(1)	96.33(1)	113.29(1)	67.56(4)
γ / º	66.88(4)	90.00	90.00	90.00	90.00	90.00	67.01(4)
V /Å^3	509.6(4)	1161.0(6)	1003.5(2)	1151.519	1465.510	1075.773	550.510
Z	2	4	4	4	4	4	2
$\rho_{calcd.}$	2.288	2.357	1.887				
T/K	293(2)	293(2)	293(2)				
μ(Mo-Kα)/mm^{-1}	7.221	5.560	3.352				
Reflections collected	1588	2524	1756				
Uniq. Reflections	1588	2524	1756				
Reflections with I > 2σ(I)	1413	2080	1562				
R_{int}	0.000	0.012	0.011				
$R1$ (I > 2σ(I))	0.0307	0.0258	0.0191				
$wR2$ (all data)	01864	0.0721	0.0523				

[a] **4**, **5**, **6** and **7** refer to previously published structures (CSD ref codes: KUWDEL, KUWDIP, KUWDOV and KUWDUB) and their cell parameters are here reported only for comparison purposes with those of **1**-**3**.

Table 2S. Intermolecular interactions for structures **1-7**.

Structure		D–H···A	d(D–H)	d(H···A)	d(D···A)	∠(DHA)	Symmetry	Fig.
1	●	N(1)–H(1)···O	0.86	2.00	2.848(11)	169	-x,2-y,1-z	Fig. 2a, 3a
	●	N(2)–H(2)···I	0.86	3.04	3.533(9)	119	-	Fig. 1a
	●	N(2)–H(2)···Br	0.86	2.79	3.480(9)	139	1-x,1-y,-z	Fig. 2a, 3a
	●	C(32) –H(32B)···O	0.96	2.55	3.413(15)	149	1-x,2-y,1-z	Fig. 2a, 3a
	●	C(32) –H(32A)···Br	0.96	3.19	3.749(12)	143	x,y,1+z	Fig. 2b
2	●	N(1)–H(1)···O	0.86	2.15	2.935(5)	151	1-x,-y,2-z	Fig. 7
	●	N(1)–H(1)···I(1)	0.86	2.99	3.547(4)	125	-	Fig. 1b
	●	C(31)-H(31B)···I(2)	0.96	3.35	4.275(5)*	161	1-x,-y,2-z	Fig. 7
	●	C(21)-H(21C)···I(2)	0.96	3.22	4.159(5)*	166	x,1/2-y,-1/2+z	Fig. 7
	●	C(21)-H(21C)···I(1)	0.96	3.35	4.125(4)	139	x,1/2-y,-1/2+z	Fig. 7
	●	S···I(2)	-	-	3.751(2)	143	2-x,-1/2+y,3/2-z	Fig. 7
3	●	N(1)–H(1)···O	0.86	2.04	2.872(3)	163	-x,1-y,1-z	Fig. 8
	●	C(31)–H(31C)···S	0.96	3.14	3.907(3)*	138	-1+x,y,z	Fig.8
	●	C(21)–H(21B)···I	0.96	3.21	3.959(3)*	137	-	Fig. 1c, 8b
	●	C(21)–H(21B)···O	0.96	2.85	3.399(4)	118	-1/2+x,1/2-y,-1/2+z	Fig. 8c
	●	C(31)–H(31A)···O	0.96	2.70	3.553(4)	148	-1/2-x,-1/2+y,3/2-z	Fig. 8c
	●	C(21)–H(21C)···I	0.96	3.21	3.973(3)*	138	1/2-x,-1/2+y,3/2-z	Fig. 8c
	●	C(32)–H(32A)···S	0.96	3.01	3.952(4)*	167	-1/2+x,1/2-y,1/2+z	Fig. 8c
4	●	N(2)–H(2)···S(2)	0.79(3)	2.58(3)	3.362(3)	173(3)	2-x,-y,-z	Fig. 5
	●	C(5) –H(8)···I(2)	1.09(6)	2.98(6)	3.634(4)	119(4)	3/2+x,1/2-y,1/2+z	Fig. 5b
	●	N(1)–H(1)···I(1)	0.85(5)	3.16(5)	3.598(3)	114(4)	-	Fig. 1d
	●	C(4) –H(3)···S(1)	0.95(4)	3.09(4)	3.570(4)	113(3)	x,y,1+z	-
	●	C(4) –H(5)···S(1)	0.87(4)	3.18(4)	3.998(5)*	158(4)	1-x,-y,-z	Fig 5c
	●	C(5) –H(7)···I(2)	0.89(5)	3.32(5)	4.154(4)*	158(4)	-1+x,y,z	Fig 5c
	●	C(4) –H(4)···I(1)	0.92(4)	3.36(4)	4.217(4)*	157(4)	1+x,y,1+z	Fig 5c
	●	C(5) –H(8)···I(1)	1.09(6)	3.32(6)	4.177(4) *	137(4)	-1+x,y,-1+z	Fig. 5a
5	●	N(1)–H(1)···I(2)	1.03(6)	2.85(6)	3.748(5)	146(5)'	1-x,-1/2+y,3/2-z	Fig 6b
	●	N(2)–H(2)···I(4)	1.09(6)	2.97(6)	3.903(5)	144(4)	-x,1/2+y,3/2-z	Fig 6b
	●	N(1)–H(1)···I(1)	1.03(6)	2.89(6)	3.474(5)	117(4)	-	Fig 1e
	●	N(2)–H(2)···I(3)	1.09(6)	3.13(6)	3.697(6)	114(4)	-	Fig 1e
	●	C(4)–H(3)···I(2)	0.81(8)	3.35(7)	3.894(7)*	127(6)	1-x,3/2+y,3/2-z	Fig 6b
	●	C(4)–H(5)···I(2)	0.87(6)	3.31(6)	4.058(7)*	146(5)	1-x,-1/2+y,3/2-z	Fig 6b
	●	C(5)–H(6)···S(2)	1.08(7)	3.01(6)	3.951(7)*	146(5)	x,-1+y,z	Fig 6a
	●	C(5)–H(8)···S(1)	0.94(8)	3.19(8)	4.110(8)*	167(6)	x,-1/2-y,1/2+z	Fig 6a
6	●	N(2)–H(2)···O(1)	0.81(4)	2.13(4)	2.874(4)	154(4)	1-x,2-y,-z	Fig. 4
	●	N(1)–H(1)···I(1)	0.96(5)	2.93(4)	3.621(3)	130(3)	-	Fig. 1f
	●	C(4)–H(5)···O(1)	1.01(3)	2.90(3)	3.559(6)	123(2)	3/2-x,1/2+y,1/2-z	Fig. 4
	●	C(5)–H(8)···I(2)	1.00(5)	3.23(5)	3.682(5)	109(3)	1/2-x,-3/2+y,1/2-z	Fig. 4
7	●	N(2)–H(2)···O(1)	0.75(7)	2.12(7)	2.868(7)	176(7)	1-x,-1-y,2-z	Fig 3b
	●	N(1)–H(1)···I(2)	1.01(8)	2.81(9)	3.752(5)	156(6)	-x,1-y,1-z	Fig 3b
	●	N(1)–H(1)···I(1)	1.01(8)	3.18(8)	3.579(5)	105(6)	-	Fig 1g
	●	C(5) –H(8)···O(1)	0.81(5)	2.74(5)	3.076(7)	154(4)	-x,-1-y,2-z	Fig 3b
	●	C(4) –H(3)···I(1)	0.90(6)	3.35(7)	4.148(5)*	149(5)	1-x,-y,1-z	-
	●	C(5) –H(6)···I(2)	0.99(8)	3.23(8)	4.124(7)*	152(5)	x,1+y,-1+z	-

[a] **4**, **5**, **6** and **7** refer to previously published structures (CSD ref codes: KUWDEL, KUWDIP, KUWDOV and KUWDUB). ●hydrogen bond, ●intramolecular interactions, ●weak interactions. *ESD values calculated using Olex[2] (V 1.2.8) software[1].

1. Dolomanov O. V, Blake A. J., Champness N. R. and Schröder, M. (2003). *J. Appl. Cryst.*, **36**, 1283-1284.

Table 3S. Cartesian coordinates of the optimised structures

1: dth·IBr (Binary adduct)

I	-1.9708376	-2.8884398	-2.0938633
Br	-0.8472601	-4.7175355	-3.4920905
S	-3.1120795	-0.8353241	-0.5306988
O	-0.0382518	2.3568384	1.7404330
N	-0.4446447	-0.4363220	-0.3048120
H	-0.2366550	-1.2328970	-0.8990228
N	-1.6681445	1.0046766	0.7875824
H	-2.5025443	1.4544612	1.1400410
C	-1.7065649	-0.1061493	-0.0294971
C	-0.3725253	1.4180125	1.0579799
C	0.5375984	0.4419428	0.3152779
C	1.3584243	1.1907345	-0.7266279
H	0.7087683	1.7100934	-1.4326959
H	1.9904910	0.4920056	-1.2779767
H	1.9935405	1.9229183	-0.2261062
C	1.4132698	-0.3083061	1.3103632
H	0.8022397	-0.8442107	2.0382105
H	2.0490726	0.4036869	1.8383845
H	2.0461033	-1.0261856	0.7851188

1: $(dth)_2$·IBr (Ternary assembly)

S	-0.8425274	-3.8213313	-2.7497426
O	1.8242937	-0.3724306	-0.3340448
N	1.7480474	-3.1851567	-2.3764555
H	2.0614443	-3.9564435	-2.9467291
N	0.3514290	-1.8448720	-1.3540425
H	-0.5355576	-1.4446502	-1.0324983

C	0.4284441	-2.9732725	-2.1768968
C	1.5733987	-1.3467441	-1.0336157
C	2.6127909	-2.2293635	-1.7103826
C	3.4271287	-1.4003741	-2.6969751
H	2.7776054	-0.9418835	-3.4442011
H	4.1552494	-2.0349980	-3.2064261
H	3.9609302	-0.6144303	-2.1607432
C	3.4955510	-2.8854197	-0.6548779
H	2.8942748	-3.4748481	0.0390175
H	4.0301913	-2.1160561	-0.0959147
H	4.2246154	-3.5424918	-1.1335792
I	-0.2144262	4.9877343	3.6375109
Br	-1.4497376	6.7880414	4.9988508
S	1.0409751	2.9920124	2.1346778
O	-1.8280992	-0.3424229	-0.1850001
N	-1.5980954	2.4721964	1.8486354
H	-1.8568642	3.2618507	2.4320519
N	-0.2783943	1.0789476	0.7916104
H	0.5860750	0.6350803	0.4396678
C	-0.3163335	2.1953801	1.6033400
C	-1.5377596	0.6207027	0.5033986
C	-2.5198346	1.5460592	1.2092470
C	-3.3316891	0.7604619	2.2314941
H	-2.6768041	0.2779637	2.9586479
H	-4.0132748	1.4289874	2.7608278
H	-3.9149259	-0.0047387	1.7172555
C	-3.4038928	2.2455134	0.1843497
H	-2.7997807	2.8079618	-0.5291827
H	-3.9881637	1.4995839	-0.3563566
H	-4.0862838	2.9334502	0.6870816

2: mdth·I_2 (Binary adduct)

I	3.5582696	-1.5509002	-2.7677496
I	4.4737600	-3.7747669	-4.0588806
S	2.5201199	0.7777928	-1.3677484
O	-1.1183724	-2.4216093	-0.1394878
N	0.7029076	-1.1635193	-0.8404068

H	1.1990127	-1.8423914	-1.4101439
N	0.3079816	0.7597160	0.1468525
C	1.1603088	0.1270894	-0.6709706
C	-0.4816953	-1.3939937	-0.1721290
C	-0.8317274	-0.0793343	0.5195568
C	0.4157705	2.1635392	0.4775640
H	-0.1468885	2.3526802	1.3904053
H	0.0261830	2.7910831	-0.3276121
H	1.4635523	2.4133046	0.6403363
C	-2.1356569	0.4630224	-0.0526832
H	-2.3993796	1.4083808	0.4256614
H	-2.9329982	-0.2581715	0.1331963
H	-2.0516652	0.6219734	-1.1295167
C	-0.9115587	-0.3019446	2.0233485
H	-1.1898450	0.6188269	2.5390828
H	0.0444935	-0.6539336	2.4143959
H	-1.6725724	-1.0568439	2.2269288

2: $(mdth)_2 \cdot I_2$ (Ternary assembly)

S	2.7426667	3.7268784	-0.3744777
O	-0.8283263	0.5850468	1.1022301
N	0.9530484	1.8271421	0.2964672
H	1.4107620	1.1011149	-0.2534867
N	0.5740271	3.7810020	1.2315552
C	1.4200761	3.1407156	0.3984343
C	-0.1913301	1.6234225	0.9964503
C	-0.5581199	2.9507702	1.6370260
C	0.6500001	5.1992833	1.4894111
H	0.1781729	5.4123570	2.4480766
H	0.1536833	5.7758710	0.7039045
H	1.6982084	5.4919192	1.5242578
C	-1.8694548	3.4502695	1.0379687
H	-2.1375047	4.4165941	1.4707451
H	-2.6621192	2.7349203	1.2647167
H	-1.7842533	3.5600780	-0.0454483
C	-0.6558378	2.7846732	3.1471107
H	-0.9337628	3.7280659	3.6211026

H	0.2950693	2.4452394	3.5618960
H	-1.4283183	2.0463032	3.3703026
I	-3.4750315	-1.4500927	1.5352493
I	-4.4825585	0.6679241	2.9575331
S	-2.3846269	-3.6207637	0.0512497
O	1.5305606	-0.6905989	-1.0486090
N	-0.4022842	-1.7882762	-0.3684987
H	-0.7725241	-1.0506181	0.2481453
N	-0.2007694	-3.6883925	-1.4689022
C	-0.9813093	-3.0229860	-0.6055435
C	0.7805040	-1.6495652	-1.0464928
C	1.0042746	-2.9413450	-1.8176549
C	-0.4620567	-5.0474628	-1.8896891
H	0.1741832	-5.2748784	-2.7432788
H	-0.2576182	-5.7552917	-1.0830649
H	-1.5078080	-5.1447166	-2.1811071
C	2.2630027	-3.6289455	-1.3017723
H	2.4327590	-4.5656099	-1.8362948
H	3.1193704	-2.9726673	-1.4642236
H	2.1801971	-3.8403699	-0.2339324
C	1.0830259	-2.6391806	-3.3080467
H	1.2621707	-3.5515641	-3.8796440
H	0.1592659	-2.1758246	-3.6586940
H	1.9105854	-1.9504409	-3.4849714

3: mdth·I_2 (Binary adduct, orthogonal conformation)

I	3.2952307	1.0181649	0.9904554
I	3.5116110	2.8359874	2.9870000
S	2.8550718	-0.9583270	-1.2184815
O	-1.2138154	1.8150982	-1.9828640
N	0.7601517	0.5975109	-1.8739676
H	1.2888132	1.0272813	-2.6214611
N	0.3674021	-0.7356462	-0.1763118
C	1.2997453	-0.3874164	-1.0688476
C	-0.5072575	0.9715772	-1.4801621
C	-0.8341219	0.0976966	-0.2734664
C	0.5943345	-1.6632996	0.9092906

H	-0.3077948	-2.2521315	1.0752951
H	0.8621154	-1.1303313	1.8243887
H	1.4159270	-2.3202333	0.6300098
C	-2.0803209	-0.7271214	-0.5611930
H	-2.3510819	-1.3346176	0.3039449
H	-1.9243249	-1.3805254	-1.4214127
H	-2.9063872	-0.0491840	-0.7812633
C	-0.9959550	0.9797605	0.9598008
H	-1.2528252	0.3738533	1.8308559
H	-1.8012369	1.6936838	0.7795306
H	-0.0752812	1.5282198	1.1688591

3: $(mdth)_2 \cdot I_2$ (Ternary assembly, orthogonal conformation)

I	0.7235346	0.2596192	1.8091144
I	-1.1446467	1.8213461	3.0121556
S	2.6251974	-1.5484736	0.4133828
O	-1.2999398	-1.9293548	-2.6259586
N	0.6700487	-1.6408149	-1.4366981
H	1.1202528	-0.9248988	-2.0305065
N	0.3452825	-2.9911564	0.2710878
C	1.1969865	-2.0957337	-0.2419090
C	-0.5681414	-2.1611468	-1.6767459
C	-0.8830611	-3.0943260	-0.5181646
C	0.4924396	-3.5868422	1.5801326
H	0.0835631	-4.5969811	1.5628085
H	-0.0236687	-2.9917064	2.3374398
H	1.5527984	-3.6227989	1.8227915
C	-1.1146991	-4.5057817	-1.0388905
H	-1.3644636	-5.1829545	-0.2203141
H	-0.2279188	-4.8802103	-1.5533530
H	-1.9486115	-4.4890161	-1.7423470
C	-2.0848696	-2.5568277	0.2521352
H	-2.3321300	-3.2211806	1.0824760
H	-2.9412849	-2.5035382	-0.4219985
H	-1.8792349	-1.5591245	0.6453422
S	-2.3908290	0.2258312	-6.3075535
O	1.5371877	0.3062028	-3.2434643

N	-0.4011505	0.0757300	-4.4956604
H	-0.8530957	-0.6829594	-3.9743973
N	-0.1484157	1.6875491	-5.9750331
C	-0.9805803	0.6873284	-5.6143209
C	0.7915344	0.6251908	-4.1628650
C	1.0627447	1.7360882	-5.1637618
C	-0.3418428	2.4812939	-7.1652181
H	0.1476625	3.4460148	-7.0347791
H	0.0658742	1.9833727	-8.0493236
H	-1.4100664	2.6309750	-7.3138477
C	1.2132773	3.0597934	-4.4245335
H	1.4254186	3.8701429	-5.1243701
H	0.3033304	3.2981625	-3.8712854
H	2.0430504	2.9829584	-3.7201746
C	2.3061239	1.3953304	-5.9783183
H	2.5077576	2.1812931	-6.7089325
H	3.1634635	1.3110581	-5.3087149
H	2.1763214	0.4482138	-6.5058874

4: ddth·I_2 (Binary adduct)

I	-2.9788026	0.8370235	-2.6994439
I	-4.9829264	2.6521456	-2.2919189
S	-0.8067308	-1.0543407	-3.0074149
S	2.7406900	-1.6202011	0.9650429
N	-0.4419966	0.0381203	-0.5516152
N	1.0470168	-1.4470285	-1.1030897
C	-0.0936982	-0.7897012	-1.5353732
C	1.4562637	-1.0684633	0.1443643
C	0.4509249	-0.0180391	0.6022263
C	-0.2938156	-0.4902679	1.8454315
C	1.1375817	1.3242321	0.8259822
H	-1.2585410	0.6351712	-0.6361405
H	1.5213095	-2.1393853	-1.6698268
H	-1.0496565	0.2453100	2.1291448
H	0.4163827	-0.6071545	2.6652106
H	-0.7820695	-1.4483325	1.6608665
H	0.3980127	2.0805008	1.0979649

H	1.6584314	1.6452417	-0.0773073
H	1.8616238	1.2251687	1.6358967

4: (ddth)$_2$·I$_2$ (Ternary assembly)

I	-5.2549226	3.3183216	-1.1859616
I	-7.2336423	5.1357923	-0.6289038
S	-3.1320628	1.4439069	-1.6536480
S	0.5858380	0.7198410	2.1373894
N	-2.6522350	2.4376578	0.8242687
N	-1.1940962	0.9666590	0.1410639
C	-2.3516314	1.6481764	-0.2059360
C	-0.7357138	1.2960069	1.3732170
C	-1.7058117	2.3302219	1.9286480
C	-2.3907564	1.8085690	3.1869346
C	-0.9985931	3.6584978	2.1737160
H	-3.4680783	3.0415070	0.8016260
H	-0.7481224	0.2848948	-0.4921872
H	-3.1283116	2.5341945	3.5367100
H	-1.6427350	1.6559395	3.9662007
H	-2.8921816	0.8605355	2.9866573
H	-1.7190940	4.4066411	2.5114737
H	-0.5198405	4.0134309	1.2598187
H	-0.2369382	3.5234060	2.9429971
S	3.9567126	-2.0189114	1.7354538
S	0.1535565	-1.1979749	-1.9667420
N	3.4036726	-2.9535515	-0.7398505
N	1.9703993	-1.4849266	-0.0064705
C	3.1428568	-2.1770819	0.3293653
C	1.4890493	-1.7902981	-1.2246371
C	2.4375070	-2.8234895	-1.8200355
C	3.0885077	-2.2845270	-3.0896379
C	1.7060171	-4.1371136	-2.0761211
H	4.2076166	-3.5639650	-0.7524282
H	1.5441143	-0.8129576	0.6421613
H	3.8115191	-3.0087731	-3.4721100
H	2.3227773	-2.1139243	-3.8475695
H	3.6023641	-1.3436603	-2.8871532

H	2.4091150	-4.8878183	-2.4445161
H	1.2442917	-4.5040378	-1.1582111
H	0.9288517	-3.9811894	-2.8255825

5: ddth·I_2 (same as above)

5: ddth·$(I_2)_2$ (Ternary assembly)

I	0.6990770	2.9396563	3.2027935
I	2.5824929	4.8878724	3.4902932
I	-3.2752104	-3.3407511	-0.4252200
I	-5.4034501	-4.3982730	0.8675620
S	-1.2581023	0.8107304	2.7564065
S	-0.9065136	-2.0814672	-1.7449540
N	0.3710993	0.7617742	0.5876312
N	-1.2180771	-0.7266844	0.5543509
C	-0.6646892	0.3156274	1.2986391
C	-0.5688915	-0.9577077	-0.6075921
C	0.5704156	0.0494096	-0.6690769
C	1.9199817	-0.6607326	-0.6871084
C	0.4009998	0.9855081	-1.8611722
H	0.9417822	1.5317542	0.9236592
H	-2.0313641	-1.2539118	0.8656051
H	2.0174560	-1.3244519	0.1732425
H	2.0065971	-1.2496271	-1.6013891
H	2.7254309	0.0763125	-0.6608946
H	-0.5706365	1.4805240	-1.8272120
H	1.1870172	1.7435958	-1.8499876
H	0.4745851	0.4108420	-2.7855760

6: dth·I_2 (Binary adduct)

I	-2.4984942	-2.8667658	-1.5014641
I	-3.7854777	-4.7637725	-0.0058789
S	-1.0881335	-0.8199199	-2.9764048
O	1.7906666	2.3040070	-0.3774085
N	-0.3899077	-0.4150487	-0.3931786
N	0.5236284	0.9792196	-1.8027510
C	-0.3272148	-0.1026908	-1.6895536

C	1.0279213	1.3888809	-0.5792823
C	0.4203596	0.4453826	0.4567767
C	1.5255293	-0.3346829	1.1568083
C	-0.4366092	1.2364835	1.4365045
H	-0.9663401	-1.1868631	-0.0741161
H	0.7419710	1.4107122	-2.6908982
H	1.0934052	-1.0296284	1.8794683
H	2.1178580	-0.8999761	0.4357768
H	2.1798556	0.3614274	1.6835183
H	-0.8947119	0.5620948	2.1626022
H	0.1913879	1.9534524	1.9671887
H	-1.2256939	1.7776878	0.9122922

6: $(dth)_2 \cdot I_2$ (Ternary assembly)

I	-3.6832962	-4.9390445	0.8813329
I	-4.9141893	-6.8198538	2.4637294
S	-2.3551392	-2.9379876	-0.6715541
O	0.5373494	0.3023719	1.7521169
N	-1.5885288	-2.4497124	1.8757686
N	-0.7418098	-1.0753211	0.3950208
C	-1.5682575	-2.1696901	0.5697991
C	-0.2207267	-0.6377808	1.5838169
C	-0.7681699	-1.5511660	2.6722969
C	0.3764163	-2.2871781	3.3575571
C	-1.6049702	-0.7431572	3.6563457
H	-2.1391726	-3.2235350	2.2333354
H	-0.5364576	-0.6344452	-0.5160412
H	-0.0172224	-2.9664980	4.1160765
H	0.9539408	-2.8645790	2.6339924
H	1.0345775	-1.5624494	3.8390009
H	-2.0248327	-1.4020855	4.4187849
H	-0.9723128	0.0014070	4.1417003
H	-2.4219831	-0.2337616	3.1430541
S	2.9536364	3.7441135	0.3665718
O	0.0239222	0.3858410	-1.8655582
N	2.0935877	3.1679193	-2.1197903
N	1.3240152	1.8137482	-0.5814247

C	2.1387297	2.9308261	-0.7901120
C	0.7750025	1.3444815	-1.7317873
C	1.2646002	2.2379077	-2.8631861
C	0.0764353	2.9246521	-3.5266593
C	2.0714303	1.4113241	-3.8579446
H	2.6140676	3.9340958	-2.5201939
H	1.1644877	1.3996434	0.3426590
H	0.4242579	3.5888545	-4.3205914
H	-0.4855069	3.5119287	-2.7987931
H	-0.5838935	2.1730373	-3.9617033
H	2.4494781	2.0526665	-4.6568510
H	1.4334069	0.6428934	-4.2968925
H	2.9171274	0.9305330	-3.3638765

7: dsh·I_2 (Binary adduct)

I	1.8759482	2.9581657	-2.0780509
I	0.4263266	4.8233570	-3.5142561
Se	3.2653117	0.8972656	-0.5014868
O	0.0379832	-2.3784642	1.7415982
N	0.4796234	0.4232001	-0.2854474
N	1.6832981	-1.0171564	0.8251542
C	1.7308183	0.0929259	0.0150514
C	0.3815189	-1.4362140	1.0692715
C	-0.5147784	-0.4587708	0.3119648
C	-1.3123603	-1.2028291	-0.7510634
C	-1.4098297	0.2899594	1.2907716
H	0.2830120	1.2236191	-0.8812198
H	2.5118226	-1.4666521	1.1920329
H	-0.6474102	-1.7186544	-1.4453527
H	-1.9572814	-1.9376557	-0.2670849
H	-1.9328824	-0.5017706	-1.3124013
H	-0.8134446	0.8238855	2.0321367
H	-2.0315330	1.0092277	0.7543257
H	-2.0561431	-0.4234386	1.8040563

7: $(dsh)_2·I_2$ (Ternary assembly)

I	-0.4015337	5.0580283	-3.6596083

I	-2.0067567	6.8458895	-5.0533413
Se	1.1432060	3.0977706	-2.1467237
O	-1.8018115	-0.3772411	0.1683026
N	-1.5980317	2.4529357	-1.8474535
N	-0.2674552	1.0794013	-0.7834566
C	-0.3201457	2.1956270	-1.5869907
C	-1.5233615	0.5946741	-0.5116830
C	-2.5124158	1.5062779	-1.2250653
C	-3.2954872	0.7142766	-2.2647225
C	-3.4213278	2.1869118	-0.2092729
H	-1.8625980	3.2422233	-2.4318604
H	0.6004484	0.6494216	-0.4232264
H	-2.6218494	0.2482515	-2.9854172
H	-3.8722337	-0.0644362	-1.7634648
H	-3.9808334	1.3748510	-2.7990347
H	-2.8362427	2.7559016	0.5148788
H	-4.1080610	2.8655776	-0.7184903
H	-3.9998814	1.4283604	0.3199606
Se	-0.8990395	-3.9329680	2.7601119
O	1.8448235	-0.3420562	0.3613156
N	1.7901443	-3.1744532	2.3775152
N	0.3854004	-1.8502483	1.3509195
C	0.4756153	-2.9794883	2.1612275
C	1.6039301	-1.3266666	1.0490936
C	2.6489657	-2.1979358	1.7313432
C	3.4354657	-1.3665753	2.7381807
C	3.5551005	-2.8322614	0.6824475
H	2.1080655	-3.9460944	2.9456842
H	-0.5050903	-1.4628472	1.0223723
H	2.7682183	-0.9268961	3.4810184
H	3.9625250	-0.5661928	2.2167130
H	4.1675793	-1.9941525	3.2505033
H	2.9721611	-3.4253239	-0.0238969
H	4.2886083	-3.4811730	1.1653127
H	4.0838990	-2.0493695	0.1368080

AIM analysis of compounds 1-3 and KUWDIP

In the following Tables the AIM BCP parameters for compounds **1**-**3**, their assemblies (see Figure 10) and for published structure KUWDIP, **5** (see Figure 11) are summarised.

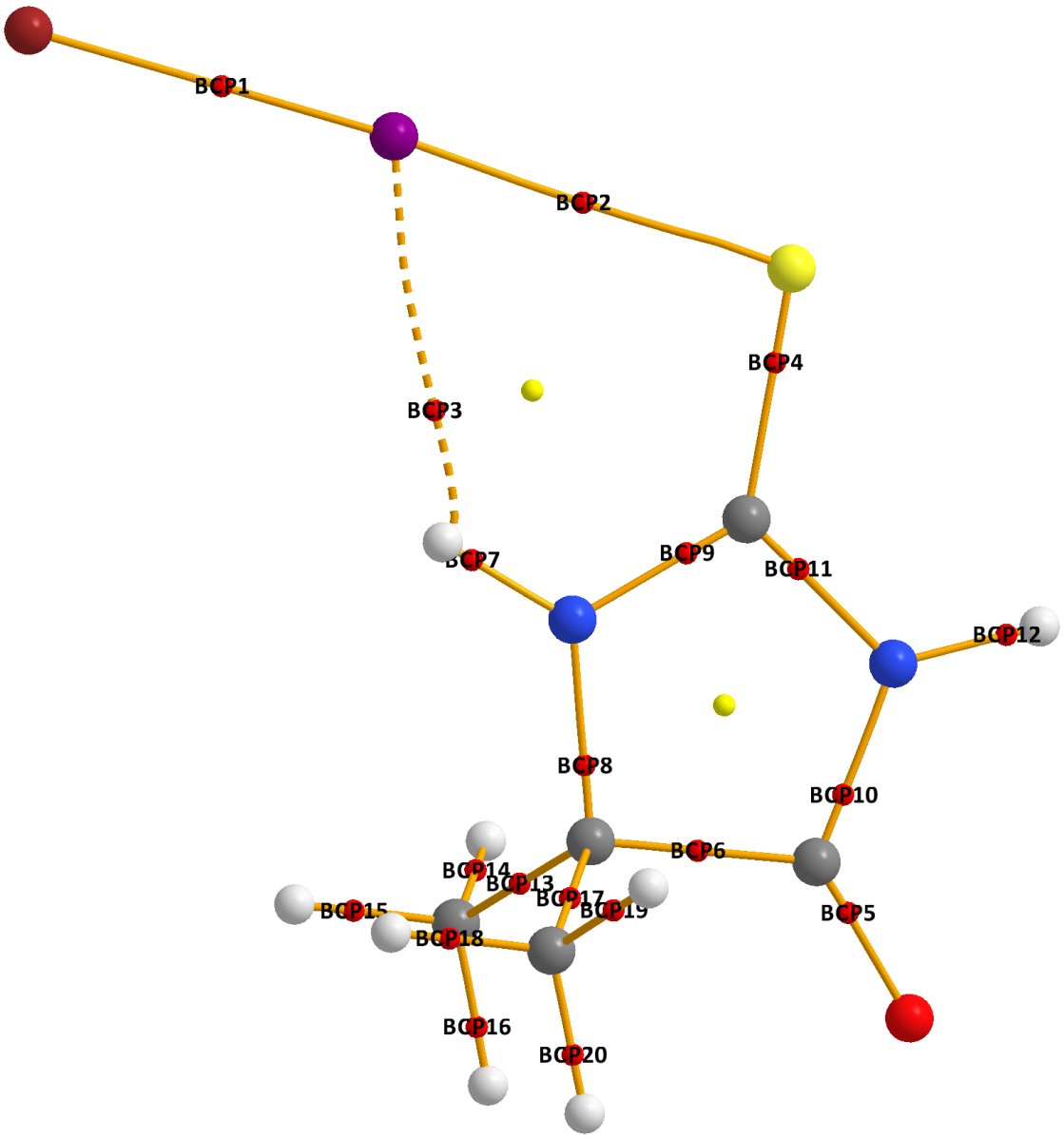

Table 4S. AIM parameters for binary adduct of compound **1** in a.u.*

BCP#	Atoms	ρ(r)[au]	$\nabla^2\rho(r)$[au]	ε	H[au]
BCP1	I1 - Br2	0.079	0.022	0.008	-0.029
BCP2	I1 - S3	0.042	0.066	0.047	**-0.007**
BCP3	I1 - H6	0.015	0.045	0.014	0.001
BCP4	S3 - C9	0.222	0.219	0.320	-0.257
BCP5	O4 - C10	0.433	-0.080	0.107	-0.801
BCP6	C10 - C11	0.276	-0.851	0.074	-0.265
BCP7	N5 - H6	0.337	-2.072	0.040	-0.561
BCP8	N5 - C11	0.266	-0.753	0.012	-0.389
BCP9	N5 - C9	0.361	-1.271	0.099	-0.628
BCP10	N7 - C10	0.316	-1.052	0.003	-0.517
BCP11	N7 - C9	0.329	-1.219	0.008	-0.532
BCP12	N7 - H8	0.340	-2.100	0.039	-0.566
BCP13	C11 - C12	0.263	-0.767	0.031	-0.247
BCP14	C12 - H13	0.286	-1.049	0.010	-0.301
BCP15	C12 - H14	0.284	-1.040	0.010	-0.299

BCP16	C12 - H15	0.286	-1.055	0.007	-0.301
BCP17	C11 - C16	0.263	-0.767	0.031	-0.247
BCP18	C16 - H19	0.284	-1.040	0.010	-0.299
BCP19	C16 - H17	0.286	-1.049	0.010	-0.301
BCP20	C16 - H18	0.286	-1.055	0.007	-0.301

* $\rho(r)$ Electron density at the Bond Critical Point (BCP); $\nabla^2\rho(r)$ Laplacian of the electron density; *H* local electronic energy density at BCP; ε ellipticity at BCP.

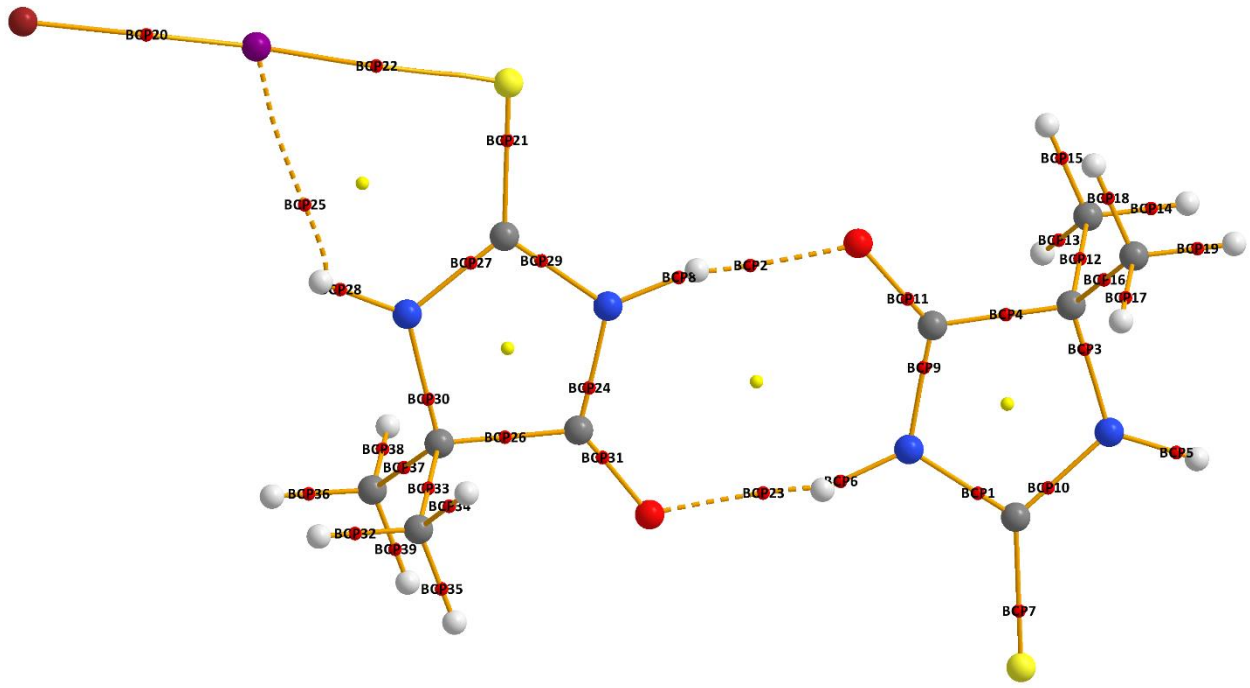

Table 5S. AIM parameters for the ternary assembly of compound **1** in a.u.*

BCP#	Atoms	ρ(r)[au]	$\nabla^2\rho(r)$[au]	ε	H[au]
BCP1	N5 - C7	0.315	-1.166	0.002	-0.491
BCP2	O2 - H25	0.035	0.129	0.028	-0.001
BCP3	N3 - C9	0.271	-0.808	0.011	-0.395
BCP4	C8 - C9	0.278	-0.868	0.071	-0.271
BCP5	N3 - H4	0.343	-2.028	0.048	-0.553
BCP6	N5 - H6	0.325	-2.144	0.031	-0.571
BCP7	S1 - C7	0.227	0.375	0.179	-0.261
BCP8	N24 - H25	0.315	-2.099	0.029	-0.560
BCP9	N5 - C8	0.340	-1.156	0.030	-0.580
BCP10	N3 - C7	0.346	-1.232	0.084	-0.588
BCP11	O2 - C8	0.416	-0.240	0.058	-0.762
BCP12	C9 - C10	0.262	-0.764	0.033	-0.246
BCP13	C10 - H11	0.286	-1.048	0.009	-0.301
BCP14	C10 - H12	0.284	-1.035	0.009	-0.298
BCP15	C10 - H13	0.286	-1.054	0.007	-0.301
BCP16	C9 - C14	0.262	-0.764	0.033	-0.246
BCP17	C14 - H15	0.286	-1.048	0.009	-0.301
BCP18	C14 - H16	0.286	-1.054	0.007	-0.301

BCP19	C14 - H17	0.284	-1.035	0.009	-0.298
BCP20	I18 - Br19	0.077	0.026	0.008	-0.027
BCP21	S20 - C26	0.222	0.208	0.335	-0.259
BCP22	I18 - S20	0.045	0.065	0.047	**-0.008**
BCP23	H6 - O21	0.025	0.107	0.029	0.002
BCP24	N24 - C27	0.331	-1.154	0.020	-0.553
BCP25	I18 - H23	0.015	0.046	0.010	0.001
BCP26	C27 - C28	0.278	-0.867	0.073	-0.270
BCP27	N22 - C26	0.360	-1.259	0.095	-0.627
BCP28	N22 - H23	0.336	-2.072	0.040	-0.561
BCP29	N24 - C26	0.330	-1.249	0.014	-0.526
BCP30	N22 - C28	0.267	-0.765	0.011	-0.391
BCP31	O21 - C27	0.423	-0.180	0.075	-0.776
BCP32	C29 - H31	0.284	-1.040	0.010	-0.299
BCP33	C28 - C29	0.262	-0.764	0.031	-0.247
BCP34	C29 - H30	0.286	-1.049	0.010	-0.301
BCP35	C29 - H32	0.286	-1.055	0.007	-0.301
BCP36	C33 - H36	0.284	-1.041	0.010	-0.299
BCP37	C28 - C33	0.262	-0.764	0.031	-0.247
BCP38	C33 - H34	0.286	-1.049	0.010	-0.301
BCP39	C33 - H35	0.286	-1.055	0.007	-0.301

* $\rho(r)$ Electron density at the Bond Critical Point (BCP); $\nabla^2\rho(r)$ Laplacian of the electron density; H local electronic energy density at BCP; ε ellipticity at BCP.

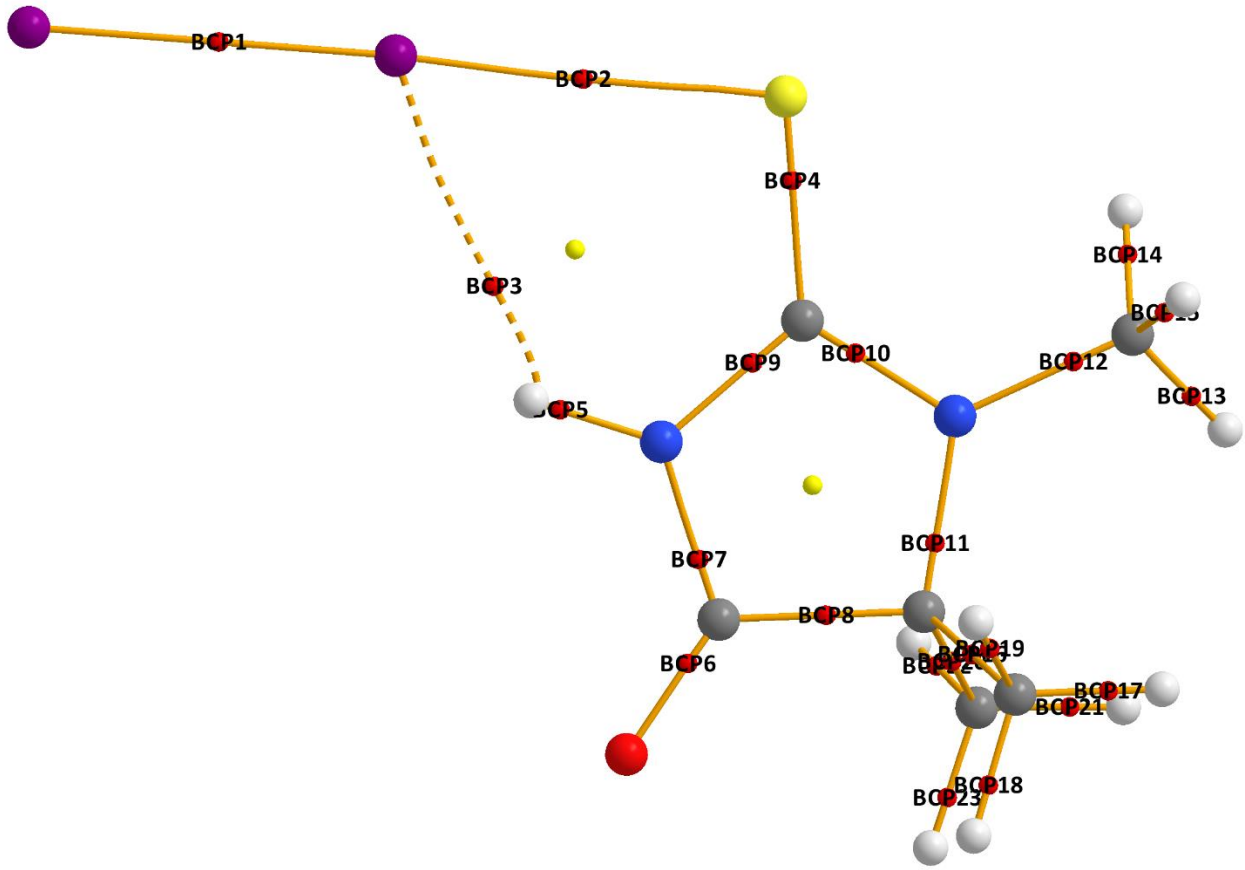

Table 6S. AIM parameters for the binary adducts of compound **2** in a.u.*

BCP#	Atoms	ρ(r)[au]	$\nabla^2\rho(r)$[au]	ε	H[au]
BCP1	I1 - I2	0.073	-0.005	0.006	-0.024
BCP2	I1 - S3	0.036	0.064	0.051	**-0.004**
BCP3	I1 - H6	0.013	0.040	0.010	0.001
BCP4	S3 - C8	0.221	0.223	0.265	-0.257
BCP5	N5 - H6	0.336	-2.115	0.036	-0.568
BCP6	O4 - C9	0.432	-0.096	0.104	-0.798
BCP7	N5 - C9	0.321	-1.065	0.008	-0.532
BCP8	C9 - C10	0.276	-0.856	0.073	-0.266
BCP9	N5 - C8	0.329	-1.229	0.019	-0.531
BCP10	N7 - C8	0.356	-1.252	0.114	-0.614
BCP11	N7 - C10	0.266	-0.792	0.017	-0.375
BCP12	N7 - C11	0.264	-0.653	0.024	-0.399
BCP13	C11 - H12	0.291	-1.095	0.036	-0.309
BCP14	C11 - H14	0.293	-1.110	0.031	-0.310
BCP15	C11 - H13	0.290	-1.084	0.039	-0.305
BCP16	C10 - C15	0.262	-0.763	0.029	-0.246
BCP17	C15 - H16	0.284	-1.037	0.011	-0.299
BCP18	C15 - H17	0.286	-1.052	0.006	-0.300
BCP19	C15 - H18	0.285	-1.044	0.010	-0.300
BCP20	C10 - C19	0.263	-0.768	0.029	-0.248
BCP21	C19 - H20	0.284	-1.038	0.011	-0.299

BCP22	C19 - H21	0.285	-1.047	0.010	-0.300
BCP23	C19 - H22	0.286	-1.052	0.006	-0.300

* ρ(r) Electron density at the Bond Critical Point (BCP); $\nabla^2\rho$(r) Laplacian of the electron density; *H* local electronic energy density at BCP; ε ellipticity at BCP.

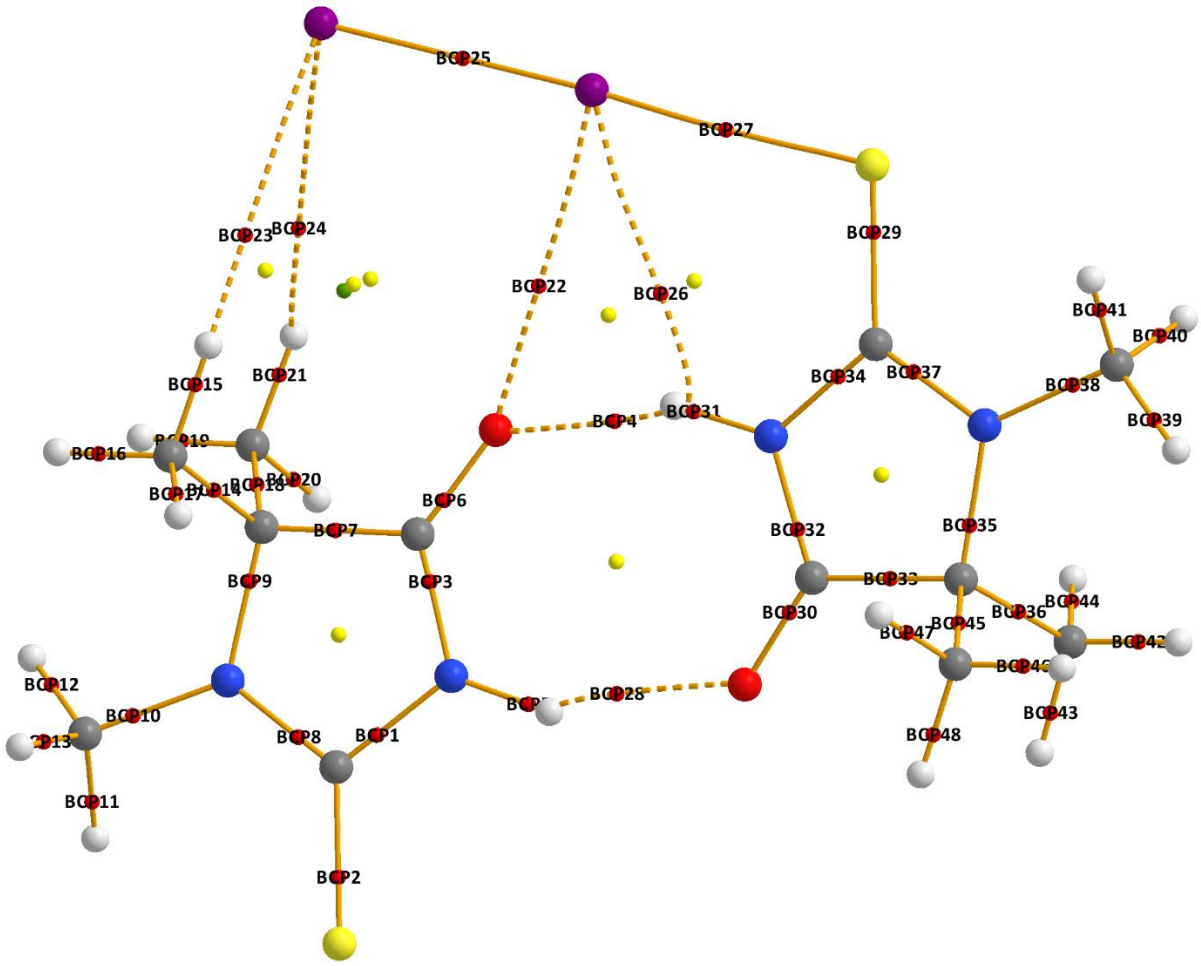

Table 7S. AIM parameters for the ternary assembly of compound **2** in a.u.*

BCP#	Atoms	ρ(r)[au]	$\nabla^2\rho$(r)[au]	ε	H[au]
BCP1	N3 - C6	0.316	-1.164	0.007	-0.494
BCP2	S1 - C6	0.225	0.334	0.162	-0.259
BCP3	N3 - C7	0.340	-1.137	0.025	-0.582
BCP4	O2 - H26	0.028	0.117	0.013	0.002
BCP5	N3 - H4	0.331	-2.172	0.033	-0.579
BCP6	O2 - C7	0.419	-0.216	0.059	-0.767
BCP7	C7 - C8	0.280	-0.879	0.073	-0.274
BCP8	N5 - C6	0.349	-1.244	0.113	-0.593
BCP9	N5 - C8	0.268	-0.817	0.021	-0.375
BCP10	N5 - C9	0.267	-0.687	0.025	-0.403
BCP11	C9 - H12	0.294	-1.113	0.029	-0.310
BCP12	C9 - H10	0.291	-1.089	0.037	-0.308

BCP13	C9 - H11	0.289	-1.076	0.040	-0.304
BCP14	C8 - C13	0.261	-0.755	0.030	-0.244
BCP15	C13 - H15	0.287	-1.061	0.006	-0.301
BCP16	C13 - H14	0.284	-1.033	0.011	-0.298
BCP17	C13 - H16	0.284	-1.038	0.010	-0.299
BCP18	C8 - C17	0.263	-0.767	0.029	-0.248
BCP19	C17 - H18	0.284	-1.034	0.012	-0.299
BCP20	C17 - H19	0.285	-1.042	0.010	-0.300
BCP21	C17 - H20	0.287	-1.058	0.006	-0.301
BCP22	O2 - I21	0.009	0.035	0.030	0.002
BCP23	H15 - I22	0.006	0.015	0.065	0.001
BCP24	H20 - I22	0.004	0.012	0.089	0.001
BCP25	I21 - I22	0.070	0.002	0.006	-0.023
BCP26	I21 - H26	0.007	0.026	0.609	0.001
BCP27	I21 - S23	0.040	0.068	0.039	-0.006
BCP28	H4 - O24	0.021	0.097	0.018	0.003
BCP29	S23 - C28	0.222	0.212	0.286	-0.258
BCP30	O24 - C29	0.423	-0.160	0.076	-0.778
BCP31	N25 - H26	0.318	-2.127	0.029	-0.566
BCP32	N25 - C29	0.332	-1.160	0.025	-0.554
BCP33	C29 - C30	0.279	-0.874	0.072	-0.272
BCP34	N25 - C28	0.327	-1.236	0.026	-0.517
BCP35	N27 - C30	0.268	-0.800	0.016	-0.380
BCP36	C30 - C35	0.262	-0.761	0.030	-0.246
BCP37	N27 - C28	0.356	-1.246	0.114	-0.613
BCP38	N27 - C31	0.264	-0.653	0.028	-0.399
BCP39	C31 - H32	0.291	-1.095	0.034	-0.309
BCP40	C31 - H33	0.290	-1.087	0.038	-0.305
BCP41	C31 - H34	0.293	-1.106	0.033	-0.309
BCP42	C35 - H36	0.284	-1.038	0.011	-0.299
BCP43	C35 - H37	0.286	-1.053	0.006	-0.300
BCP44	C35 - H38	0.285	-1.045	0.010	-0.300
BCP45	C30 - C39	0.263	-0.766	0.030	-0.247
BCP46	C39 - H40	0.284	-1.038	0.011	-0.299
BCP47	C39 - H41	0.285	-1.047	0.010	-0.300
BCP48	C39 - H42	0.286	-1.053	0.006	-0.300

* $\rho(r)$ Electron density at the Bond Critical Point (BCP); $\nabla^2\rho(r)$ Laplacian of the electron density; H local electronic energy density at BCP; ε ellipticity at BCP.

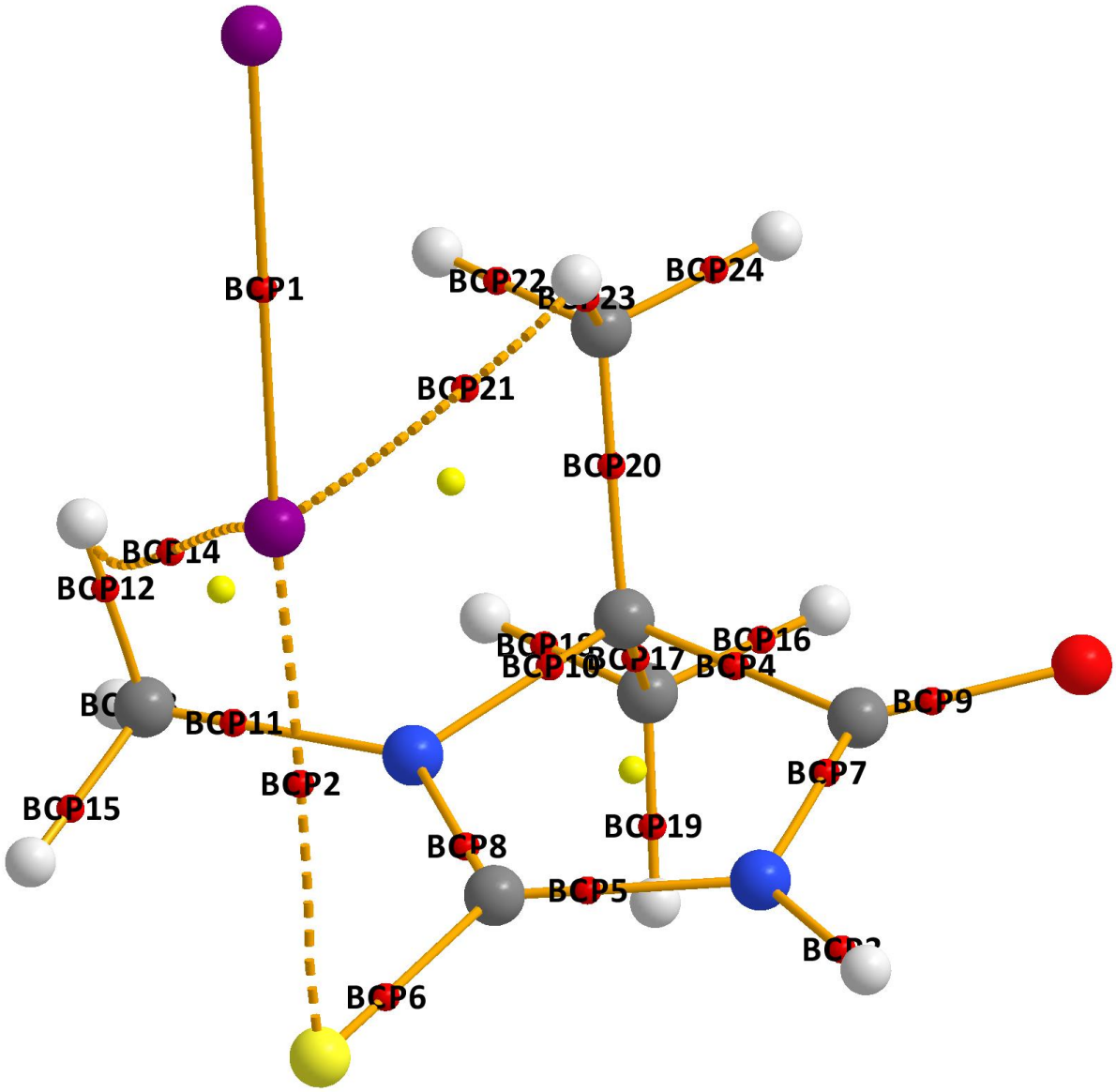

Table 8S. AIM parameters for the binary adduct of compound **3** in a.u.*

BCP#	Atoms	ρ(r)[au]	$\nabla^2\rho(r)$[au]	ε	H[au]
BCP21	I1 - H22	0.004	0.013	0.100	0.001
BCP14	I1 - H13	0.006	0.019	0.540	0.001
BCP2	I1 - S3	0.029	0.059	0.073	**-0.002**
BCP1	I1 - I2	0.075	-0.010	0.002	-0.026
BCP20	C10 - C19	0.261	-0.757	0.028	-0.245
BCP17	C10 - C15	0.263	-0.769	0.028	-0.248
BCP4	C9 - C10	0.277	-0.858	0.074	-0.267
BCP24	C19 - H21	0.286	-1.050	0.007	-0.300
BCP16	C15 - H18	0.286	-1.052	0.006	-0.300
BCP23	C19 - H22	0.286	-1.051	0.010	-0.300
BCP22	C19 - H20	0.284	-1.038	0.011	-0.299
BCP19	C15 - H17	0.285	-1.045	0.010	-0.300
BCP18	C15 - H16	0.285	-1.040	0.011	-0.300

BCP12	C11 - H13	0.290	-1.088	0.039	-0.306
BCP13	C11 - H12	0.291	-1.089	0.039	-0.308
BCP15	C11 - H14	0.294	-1.118	0.028	-0.311
BCP10	N7 - C10	0.265	-0.793	0.019	-0.372
BCP6	S3 - C8	0.219	0.244	0.083	-0.252
BCP3	N5 - H6	0.340	-2.101	0.039	-0.566
BCP11	N7 - C11	0.263	-0.621	0.020	-0.399
BCP5	N5 - C8	0.327	-1.206	0.012	-0.529
BCP7	N5 - C9	0.322	-1.060	0.005	-0.533
BCP8	N7 - C8	0.358	-1.234	0.119	-0.621
BCP9	O4 - C9	0.432	-0.101	0.102	-0.797

* $\rho(r)$ Electron density at the Bond Critical Point (BCP); $\nabla^2\rho(r)$ Laplacian of the electron density; *H* local electronic energy density at BCP; ε ellipticity at BCP.

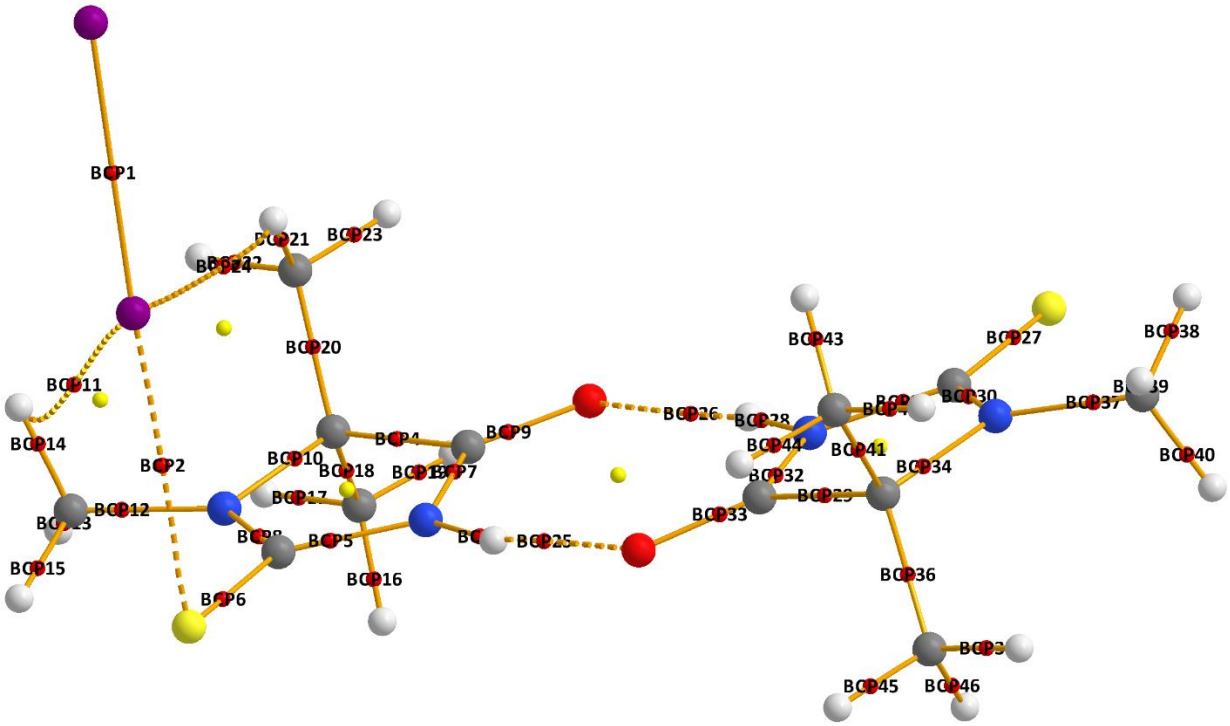

Table 9S. AIM parameters for the ternary assembly of compound **3** in a.u.*

BCP#	Atoms	ρ(r)[au]	$\nabla^2\rho(r)$[au]	ε	H[au]
BCP1	I1 - I2	0.074	-0.008	0.001	-0.026
BCP2	I1 - S3	0.031	0.060	0.079	**-0.003**
BCP3	N5 - H6	0.316	-2.102	0.029	-0.560
BCP4	C9 - C10	0.279	-0.874	0.073	-0.272
BCP5	N5 - C8	0.328	-1.237	0.018	-0.525
BCP6	S3 - C8	0.219	0.237	0.070	-0.253
BCP7	N5 - C9	0.336	-1.160	0.022	-0.568
BCP8	N7 - C8	0.357	-1.225	0.113	-0.619

BCP9	O4 - C9	0.421	-0.198	0.070	-0.772
BCP10	N7 - C10	0.267	-0.804	0.018	-0.374
BCP11	I1 - H13	0.005	0.018	0.717	0.001
BCP12	N7 - C11	0.263	-0.630	0.022	-0.399
BCP13	C11 - H12	0.291	-1.089	0.039	-0.308
BCP14	C11 - H13	0.290	-1.086	0.039	-0.305
BCP15	C11 - H14	0.294	-1.117	0.029	-0.311
BCP16	C15 - H17	0.285	-1.045	0.010	-0.300
BCP17	C15 - H16	0.284	-1.039	0.011	-0.299
BCP18	C10 - C15	0.263	-0.768	0.029	-0.248
BCP19	C15 - H18	0.286	-1.052	0.006	-0.300
BCP20	C10 - C19	0.261	-0.755	0.028	-0.245
BCP21	C19 - H22	0.286	-1.052	0.010	-0.300
BCP22	C19 - H20	0.284	-1.037	0.011	-0.299
BCP23	C19 - H21	0.286	-1.050	0.007	-0.300
BCP24	I1 - H22	0.005	0.013	0.073	0.001
BCP25	H6 - O24	0.035	0.128	0.028	-0.001
BCP26	O4 - H26	0.026	0.108	0.031	0.002
BCP27	S23 - C28	0.226	0.345	0.161	-0.259
BCP28	N25 - H26	0.325	-2.140	0.031	-0.570
BCP29	C29 - C30	0.280	-0.877	0.071	-0.273
BCP30	N27 - C28	0.348	-1.234	0.111	-0.590
BCP31	N25 - C28	0.314	-1.162	0.008	-0.487
BCP32	N25 - C29	0.342	-1.149	0.031	-0.587
BCP33	O24 - C29	0.416	-0.249	0.057	-0.762
BCP34	N27 - C30	0.271	-0.834	0.020	-0.379
BCP35	C39 - H40	0.284	-1.037	0.010	-0.299
BCP36	C30 - C39	0.262	-0.759	0.031	-0.245
BCP37	N27 - C31	0.267	-0.682	0.026	-0.403
BCP38	C31 - H34	0.294	-1.114	0.029	-0.311
BCP39	C31 - H32	0.290	-1.088	0.037	-0.308
BCP40	C31 - H33	0.289	-1.076	0.040	-0.304
BCP41	C30 - C35	0.262	-0.765	0.031	-0.246
BCP42	C35 - H36	0.284	-1.037	0.011	-0.299
BCP43	C35 - H37	0.285	-1.047	0.010	-0.300
BCP44	C35 - H38	0.286	-1.051	0.006	-0.300
BCP45	C39 - H41	0.286	-1.051	0.006	-0.300
BCP46	C39 - H42	0.285	-1.043	0.009	-0.300

* $\rho(r)$ Electron density at the Bond Critical Point (BCP); $\nabla^2\rho(r)$ Laplacian of the electron density; H local electronic energy density at BCP; ε ellipticity at BCP.

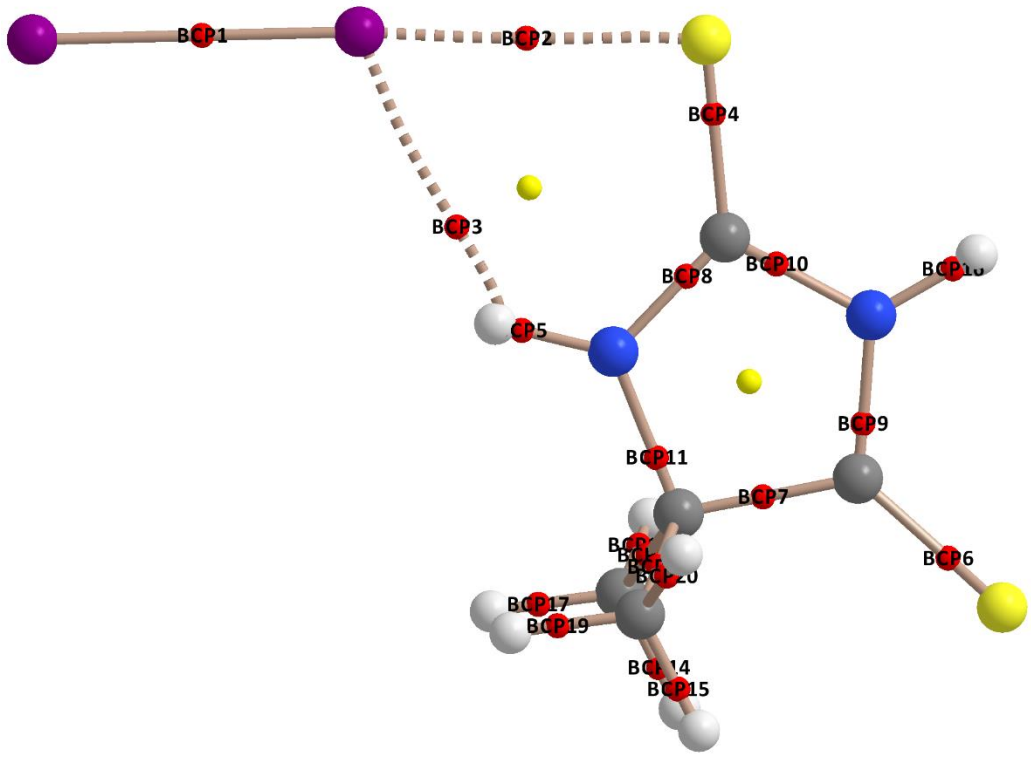

Table 10S. AIM parameters for the binary adduct of compound **KUWDIP** in a.u.*

BCP#	Atoms	ρ(r)[au]	$\nabla^2\rho(r)$[au]	ε	H[au]
BCP1	I1 - I2	0.072	-0.004	0.005	-0.024
BCP2	I1 - S3	0.037	0.064	0.050	-0.005
BCP3	I1 - H12	0.015	0.043	0.019	0.001
BCP4	S3 - C7	0.222	0.247	0.279	-0.256
BCP5	N5 - H12	0.337	-2.068	0.040	-0.559
BCP6	S4 - C8	0.234	0.340	0.198	-0.275
BCP7	C8 - C9	0.273	-0.834	0.054	-0.264
BCP8	N5 - C7	0.361	-1.252	0.101	-0.631
BCP9	N6 - C8	0.327	-0.976	0.055	-0.552
BCP10	N6 - C7	0.324	-1.193	0.007	-0.520
BCP11	N5 - C9	0.264	-0.757	0.026	-0.382
BCP12	C9 - C10	0.262	-0.766	0.026	-0.247
BCP13	C9 - C11	0.262	-0.766	0.026	-0.247
BCP14	C10 - H15	0.287	-1.058	0.007	-0.301
BCP15	C11 - H19	0.287	-1.058	0.007	-0.301
BCP16	N6 - H13	0.341	-2.118	0.038	-0.569
BCP17	C10 - H14	0.284	-1.038	0.010	-0.299
BCP18	C10 - H16	0.286	-1.051	0.010	-0.301
BCP19	C11 - H17	0.284	-1.038	0.010	-0.299
BCP20	C11 - H18	0.286	-1.051	0.010	-0.301

* $\rho(r)$ Electron density at the Bond Critical Point (BCP); $\nabla^2\rho(r)$ Laplacian of the electron density; *H* local electronic energy density at BCP; ε ellipticity at BCP.

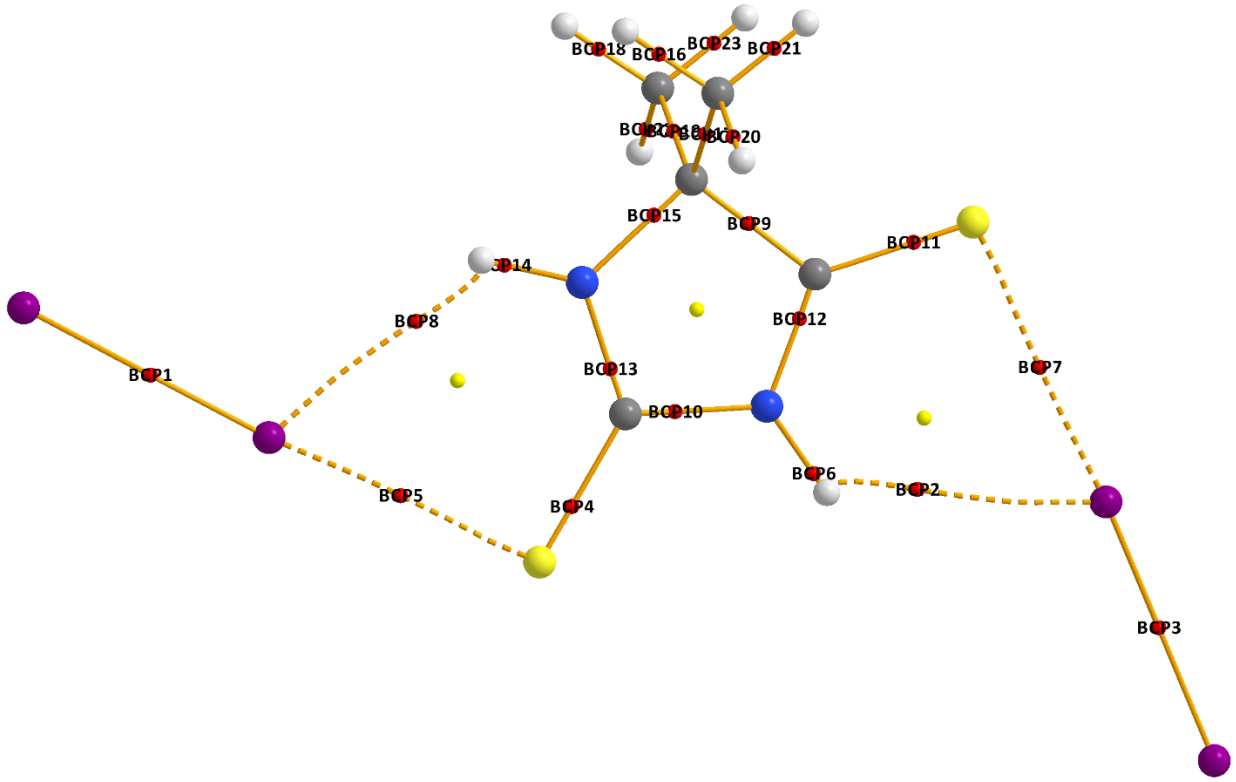

Table 11S. AIM parameters for the ternary assembly of compound **KUWDIP**, **5**, in a.u.*

BCP#	Atoms	ρ(r)[au]	$\nabla^2\rho(r)$[au]	ε	H[au]
BCP1	I1 - I2	0.074	-0.007	0.004	-0.025
BCP2	I3 - H15	0.013	0.039	0.004	0.001
BCP3	I3 - I4	0.076	-0.012	0.004	-0.027
BCP4	S5 - C9	0.223	0.280	0.270	-0.258
BCP5	I1 - S5	0.035	0.064	0.048	**-0.004**
BCP6	N8 - H15	0.335	-2.137	0.034	-0.572
BCP7	I3 - S6	0.031	0.062	0.039	**-0.003**
BCP8	I1 - H14	0.015	0.044	0.024	0.001
BCP9	C10 - C11	0.274	-0.840	0.053	-0.266
BCP10	N8 - C9	0.318	-1.167	0.001	-0.500
BCP11	S6 - C10	0.231	0.269	0.273	-0.272
BCP12	N8 - C10	0.339	-1.002	0.044	-0.583
BCP13	N7 - C9	0.360	-1.248	0.106	-0.628
BCP14	N7 - H14	0.336	-2.068	0.040	-0.559
BCP15	N7 - C11	0.266	-0.773	0.030	-0.384
BCP16	C12 - H18	0.284	-1.040	0.010	-0.299
BCP17	C11 - C12	0.261	-0.762	0.026	-0.246
BCP18	C13 - H20	0.284	-1.040	0.010	-0.299
BCP19	C11 - C13	0.261	-0.762	0.026	-0.246
BCP20	C12 - H16	0.286	-1.052	0.010	-0.301
BCP21	C12 - H17	0.287	-1.057	0.007	-0.301
BCP22	C13 - H19	0.286	-1.052	0.010	-0.301

* $\rho(r)$ Electron density at the Bond Critical Point (BCP); $\nabla^2\rho(r)$ Laplacian of the electron density; *H* local electronic energy density at BCP; ε ellipticity at BCP.