Supporting Information

Table S1: Topological parameters at bond critical points (BCPs) for noncovalent interactions in EDT–(HF), EDT–(H_2O), and EDT–(NH_3) clusters calculated at the MP2/aug-cc-pVTZ level of theory. Electron density (ρ), Laplacian of electron density ($\nabla^2\rho$), kinetic energy density (G_{BCP}), potential energy density (V_{BCP}), and the ratio $|V|/G$ are reported in atomic units (a.u.) unless stated otherwise.

BCP	Interaction	ρ	$\nabla^2\rho$	G_{BCP}	V_{BCP}	$\lvert V\rvert/G$
EDT–$(HF)_1$–I						
22	F11–H12←S7	0.0319	0.0436	0.0173	−0.0238	1.37
27	S9–H10←F11	0.0082	0.0296	0.0064	−0.0054	0.84
EDT–$(HF)_2$–I						
29	F13–H14←S9	0.0334	0.0434	0.0180	−0.0252	1.40
25	F11–H12←S7	0.0333	0.0434	0.0180	−0.0252	1.40
36	S9–H10←F11	0.0127	0.0484	0.0105	−0.0088	0.84
19	S7–H8←F13	0.0127	0.0484	0.0105	−0.0088	0.84
EDT–$(HF)_3$–I						
18	F13–H14←S9	0.0332	0.0436	0.0179	−0.0250	1.39
28	F15–H16←S7	0.0241	0.0467	0.0144	−0.0171	1.18
38	F11–H12←S7	0.0291	0.0461	0.0165	−0.0214	1.29
37	S9–H10←F11	0.0124	0.0473	0.0102	−0.0087	0.85
EDT–$(H_2O)_1$–I						
26	O11–H12←S7	0.0193	0.0428	0.0115	−0.0124	1.07
28	S9–H10←O11	0.0126	0.0458	0.0095	−0.0077	0.81
EDT–$(H_2O)_2$–I						
38	O11–H12←S7	0.0212	0.0448	0.0126	−0.0140	1.11
23	S9–H10←O11	0.0157	0.0601	0.0129	−0.0108	0.84
20	O14–H15←S9	0.0213	0.0448	0.0126	−0.0140	1.11
34	S7–H8←O14	0.0158	0.0603	0.0129	−0.0108	0.84
EDT–$(H_2O)_3$–I						

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BCP	Interaction	ρ	$\nabla^2\rho$	G_{BCP}	V_{BCP}	$\lvert V\rvert/G$
26	O11–H12←S7	0.0198	0.0442	0.0120	−0.0129	1.07
27	S9–H10←O11	0.0156	0.0598	0.0128	−0.0107	0.83
40	O14–H15←S9	0.0212	0.0447	0.0126	−0.0139	1.10
41	S7–H8←O14	0.0176	0.0673	0.0147	−0.0126	0.85
34	O17–H19←S7	0.0162	0.0419	0.0103	−0.0102	0.99
EDT–$(NH_3)_1$–I						
23	S9–H10←N11	0.0208	0.0573	0.0138	−0.0133	0.96
26	N11–H14←S7	0.0099	0.0277	0.0060	−0.0052	0.86
EDT–$(NH_3)_2$–I						
33	S9–H10←N11	0.0220	0.0597	0.0147	−0.0146	0.99
26	N11–H13←S7	0.0119	0.0323	0.0073	−0.0065	0.89
20	S7–H8←N15	0.0221	0.0597	0.0147	−0.0146	0.99
27	N15–H18←S9	0.0123	0.0324	0.0073	−0.0066	0.90
EDT–$(NH_3)_3$–I						
24	N11–H13←S7	0.0109	0.0296	0.0066	−0.0058	0.87
23	S9–H10←N11	0.0199	0.0560	0.0133	−0.0125	0.93
39	C4–H6←N19	0.0088	0.0282	0.0058	−0.0046	0.79
28	N15–H17←S9	0.0105	0.0307	0.0067	−0.0058	0.86
35	S7←N19	0.0068	0.0282	0.0056	−0.0041	0.73

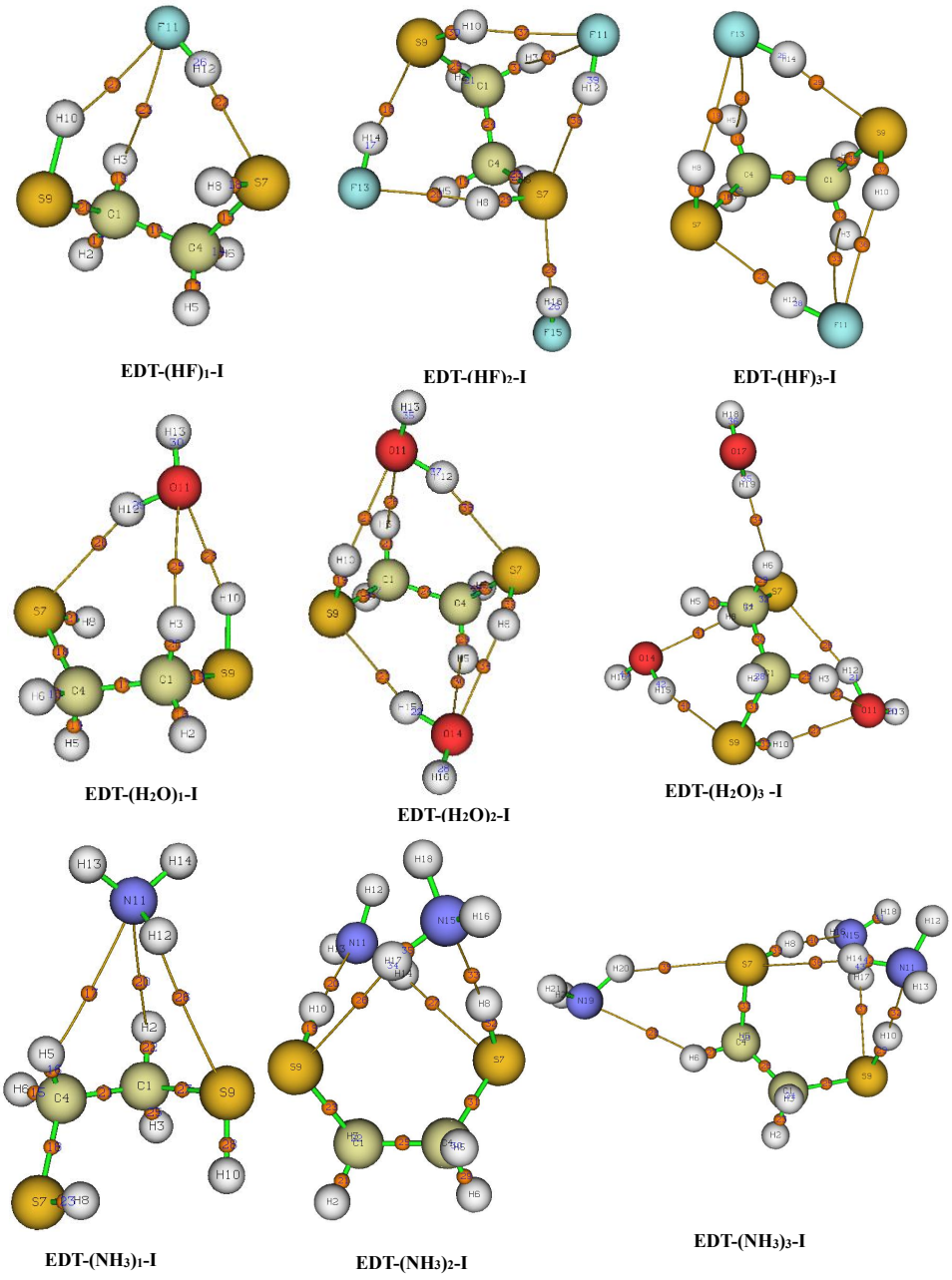

Figure S1: Bond critical points (BCPs) for noncovalent interactions in EDT–(HF), EDT–(H_2O), and EDT–(NH_3) clusters at the MP2/aug-cc-pVTZ level of theory.

Table S2. Optimized Geometries

All geometries are optimized at the MP2/aug-cc-pVTZ level of theory. Cartesian coordinates are given in Å.

EDT

C	-0.25647	-0.45918	0.54547
H	-0.84553	-0.73472	1.42202
H	-0.53707	-1.11883	-0.27370
C	1.22328	-0.59198	0.86522
H	1.49993	0.05379	1.69671
H	1.44497	-1.62311	1.14613
S	2.31851	-0.25102	-0.54380
H	2.14910	1.07623	-0.53355
S	-0.77932	1.23565	0.15126
H	-0.22677	1.27171	-1.06683

HF

F	3.50754	0.55538	-0.63624
H	2.84739	-0.01359	-0.33582

H_2O

O	-3.33165	-0.94358	-0.41817
H	-2.91756	-0.07647	-0.38768
H	-4.23695	-0.76136	-0.68573

NH_3

N	2.87939	-1.28721	-0.27329
H	2.52929	-0.67687	-1.00083
H	3.04007	-2.18990	-0.70193
H	3.78559	-0.92761	-0.00154

EDT–$(HF)_1$–I

C	0.88566	-0.44126	0.95076
H	1.59685	-0.98595	1.59493
H	0.5256	0.43712	1.50637
C	-0.26713	-1.38666	0.58817
H	0.10637	-2.27879	0.06205
H	-0.77953	-1.71777	1.50809
S	-1.59871	-0.63289	-0.44324
H	-0.84367	-0.47895	-1.55881
S	1.87038	0.14164	-0.49542

H	1.14155	1.25758	-0.73263
F	-0.94673	2.3439	0.36321
H	-1.28448	1.49923	0.13614

EDT–$(HF)_1$–II

C	-1.35912	0.72752	0.72047
H	-1.71553	1.76987	0.78613
H	-1.58794	0.22796	1.67423
C	0.14922	0.7345	0.44958
H	0.38163	1.24245	-0.49852
H	0.67133	1.26672	1.26334
S	0.91652	-0.94387	0.4247
H	0.42584	-1.31722	-0.78199
S	-2.36885	-0.03452	-0.6189
H	-2.12934	-1.32298	-0.27827
F	3.51196	0.5592	-0.63825
H	2.84296	-0.0174	-0.33381

EDT–$(HF)_2$–I

C	0	0.87546	-0.43087	1.18553
H	0	1.48301	-0.93357	1.9392
H	0	0.37745	0.41185	1.66124
C	0	-0.12898	-1.42422	0.62062
H	0	0.36898	-2.25905	0.13114
H	0	-0.73001	-1.82227	1.43925
S	0	-1.33426	-0.73478	-0.55968
H	0	-0.56195	-0.84998	-1.64853
S	0	2.07086	0.2429	-0.01371
H	0	1.29195	1.23739	-0.4605
F	0	-0.69419	2.23575	-0.08978
H	0	-1.02466	1.36901	-0.26722
F	0	1.42324	-1.66739	-2.33427
H	0	1.75576	-1.07491	-1.67828

EDT–$(HF)_2$–II

C	0.76438	0.76805	-0.04553
H	1.16019	1.67085	0.44989
H	1.10544	0.77498	-1.09157
C	-0.76437	0.76804	0.04562
H	-1.10544	0.77489	1.09166

H	-1.16019	1.67088	-0.44974
S	-1.57156	-0.6405	-0.83361
H	-1.31924	-1.57996	0.10979
S	1.57157	-0.64055	0.83359
H	1.31924	-1.57994	-0.10988
F	-4.21162	0.52373	0.52181
H	-3.56013	0.06056	0.04007
F	4.21159	0.52376	-0.52184
H	3.56012	0.06057	-0.0401

EDT–$(HF)_3$–I

C	0	-0.00141	0.71729	1.36534
H	0	0.46705	0.81949	2.34483
H	0	-0.80741	1.44572	1.30103
C	0	-0.52101	-0.70427	1.2223
H	0	0.28407	-1.43504	1.26789
H	0	-1.21734	-0.91826	2.03406
S	0	-1.46429	-1.0298	-0.30676
H	0	-0.41433	-1.35632	-1.07506
S	0	1.28278	1.20822	0.16835
H	0	0.44518	1.61977	-0.79301
F	0	-1.74707	1.91885	-1.25799
H	0	-1.8188	1.00273	-1.06399
F	0	1.73511	-1.55334	-1.10361
H	0	1.75279	-0.67937	-0.74555
F	0	-2.32944	-3.67338	1.19896
H	0	-2.14351	-3.01173	0.56808

EDT–$(HF)_3$–II

C	-0.70845	-0.58506	-0.6131
H	-1.15327	-1.50415	-1.02914
H	-1.00883	0.25781	-1.25224
C	0.81434	-0.75178	-0.57021
H	1.10864	-1.61658	0.04335
H	1.2005	-0.90948	-1.59139
S	1.73674	0.72373	0.05424
H	1.37348	0.5951	1.35396
S	-1.4848	-0.35671	1.04923
H	-1.51022	0.99736	1.02214
F	4.21924	-1.32888	-0.03397

H	3.6808	-0.57604	0.0581
F	-4.12133	-1.09402	-0.5885
H	-3.49827	-0.80653	0.0432
F	-0.65657	2.79522	-0.36367
H	0.16865	2.36029	-0.32845

EDT–$(H_2O)_1$–I

C	0.74121	-0.62778	0.94529
H	1.33548	-1.28961	1.59831
H	0.55999	0.31413	1.48327
C	-0.57375	-1.33839	0.59758
H	-0.37806	-2.28685	0.07321
H	-1.12622	-1.56738	1.52559
S	-1.75346	-0.3498	-0.4176
H	-0.97266	-0.29996	-1.52477
S	1.80961	-0.26191	-0.51426
H	1.37302	1.00716	-0.69439
O	-0.15744	2.54621	0.34602
H	-0.87297	1.91971	0.15467
H	-0.56217	3.41744	0.26851

EDT–$(H_2O)_1$–II

C	-0.26476	-0.4673	0.5488
H	-0.85929	-0.75197	1.43386
H	-0.55568	-1.1298	-0.27967
C	1.22833	-0.59309	0.868
H	1.51147	0.06325	1.70516
H	1.44692	-1.63489	1.15996
S	2.34484	-0.26213	-0.56002
H	2.23254	1.08698	-0.5309
S	-0.81088	1.25109	0.15524
H	-0.28285	1.29642	-1.09149
O	-3.3331	-0.94421	-0.41851
H	-2.91193	-0.07292	-0.38646
H	-4.24114	-0.76429	-0.6866

EDT–$(H_2O)_2$–I

C	0.72724	-0.64344	0.93555
H	1.31542	-1.31597	1.56124
H	0.56511	0.2817	1.48445
C	-0.58892	-1.32231	0.58699
H	-0.41253	-2.26064	0.06337

H	-1.14595	-1.54187	1.49944
S	-1.7183	-0.3115	-0.41884
H	-0.89872	-0.23513	-1.47712
S	1.76157	-0.26551	-0.51469
H	1.35057	1.00268	-0.64461
O	-0.11781	2.48515	0.35829
H	-0.83279	1.85914	0.16168
H	-0.52093	3.35548	0.28662
O	0.42191	-1.78752	-2.36418
H	1.17581	-1.28941	-2.03995
H	0.09381	-1.38346	-3.17083

EDT–$(H_2O)_2$–II

C	-0.76481	-0.62554	0.03137
H	-1.10929	-1.5291	0.56263
H	-1.21237	-0.63531	-0.97326
C	0.76484	-0.62553	-0.03136
H	1.21239	-0.6353	0.97327
H	1.10933	-1.52908	-0.56263
S	1.48363	0.78	-0.98836
H	1.30408	1.72412	-0.03342
S	-1.48363	0.77997	0.98838
H	-1.30407	1.7241	0.03346
O	-3.93752	-0.90539	-0.64039
H	-3.57695	-0.23855	-0.03805
H	-4.89332	-0.80451	-0.56938
O	3.93749	-0.90541	0.64035
H	3.57695	-0.23852	0.03804
H	4.8933	-0.80461	0.56931

EDT–$(H_2O)_3$–I

C	0	0.41715	-0.41175	1.40258
H	0	0.09558	-0.73321	2.39425
H	0	1.49556	-0.54549	1.33796
C	0	0.02484	1.04462	1.21294
H	0	-1.05575	1.17421	1.2317
H	0	0.44626	1.64428	2.02081
S	0	0.63845	1.81497	-0.32354
H	0	-0.4111	1.48211	-1.09158
S	0	-0.35288	-1.58637	0.24099
H	0	0.59622	-1.50041	-0.70258
O	0	2.57282	-0.7159	-1.19986
H	0	2.19642	0.17414	-1.11109

H	0	3.24519	-0.63783	-1.88321
O	0	-2.34429	0.60568	-1.19897
H	0	-1.94895	-0.21239	-0.85356
H	0	-3.05693	0.3172	-1.77694
O	0	-0.09336	4.2208	1.83014
H	0	-0.25393	5.15607	1.67634
H	0	0.04373	3.84948	0.94756

EDT–$(H_2O)_3$–II

C	-0.69944	-0.51712	-0.56042
H	-1.15544	-1.45092	-0.91448
H	-1.01262	0.28713	-1.23345
C	0.81654	-0.68778	-0.54751
H	1.12602	-1.50758	0.10985
H	1.16726	-0.92332	-1.56159
S	1.78186	0.81782	-0.0673
H	1.39174	0.83652	1.23313
S	-1.44956	-0.19176	1.1016
H	-1.51891	1.15899	0.97833
O	4.09765	-1.65783	0.04145
H	3.71942	-0.76597	0.0975
H	5.03845	-1.54429	0.2183
O	-0.83864	2.94049	-0.35588
H	-0.79567	3.87786	-0.57684
H	0.07024	2.60696	-0.43842
O	-3.96722	-1.60533	-0.62971
H	-4.87267	-1.69742	-0.31234
H	-3.51169	-1.08409	0.05205

EDT–$(NH_3)_1$–I

C	0.14408	0.28272	1.0517
H	1.06278	-0.09938	1.525
H	-0.45673	0.81529	1.80485
C	-0.63113	-0.89906	0.46165
H	-0.01332	-1.4381	-0.27085
H	-0.88857	-1.60249	1.27267
S	-2.2491	-0.45658	-0.30186
H	-1.73884	0.10398	-1.42396
S	0.74565	1.49728	-0.19665
H	-0.45153	2.07943	-0.44421
N	2.87155	-1.28837	-0.26497
H	2.52907	-0.67209	-1.00544
H	3.0433	-2.1948	-0.70439

H	3.79043	-0.92634	-0.00279

EDT–$(NH_3)_1$–II

C	-0.30584	-1.12388	0.86049
H	-0.57437	-2.07962	1.34264
H	0.2167	-0.50216	1.60391
C	-1.58972	-0.43724	0.37711
H	-2.1004	-1.05657	-0.3769
H	-2.27773	-0.29696	1.22939
S	-1.3484	1.25376	-0.31196
H	-0.60165	0.86039	-1.37257
S	0.87944	-1.55023	-0.48708
H	1.60366	-0.40312	-0.40673
N	2.26596	1.64923	0.29483
H	2.68998	2.31573	-0.3525
H	2.75498	1.76614	1.18388
H	1.30383	1.9618	0.44411

EDT–$(NH_3)_2$–I

C	0	-0.33543	-0.57954	-1.83918
H	0	-0.13866	-1.17396	-2.73346
H	0	-1.32885	-0.14458	-1.93991
C	0	0.71951	0.50981	-1.72415
H	0	1.70563	0.07565	-1.56507
H	0	0.75048	1.07659	-2.65668
S	0	0.41372	1.7496	-0.42812
H	0	0.90789	1.03155	0.60388
S	0	-0.3616	-1.77906	-0.47137
H	0	-1.09137	-1.03241	0.38583
N	0	-2.26391	0.3888	1.46414
H	0	-2.10823	0.61041	2.44023
H	0	-3.25953	0.4751	1.29888
H	0	-1.79883	1.10909	0.91905
N	0	1.7715	-0.35181	1.98115
H	0	2.77683	-0.43896	2.06914
H	0	1.45297	-1.0894	1.35925
H	0	1.37927	-0.54609	2.89468

EDT–$(NH_3)_2$–II

C	1.56529	0.98154	-0.16374
H	1.66775	1.96717	0.31226
H	1.53181	1.13492	-1.24842
C	0.28302	0.32538	0.33699

H	-0.5759	0.97773	0.11524
H	0.32336	0.15966	1.41974
S	-0.13366	-1.27411	-0.48886
H	0.75686	-2.05321	0.17424
S	3.13051	0.10156	0.26892
H	2.99278	-0.91614	-0.61761
N	-3.73319	-0.96499	0.45394
H	-2.78783	-1.3289	0.32432
H	-4.33804	-1.488	-0.17646
H	-4.01738	-1.21282	1.39977
N	-2.73171	2.03097	-0.23527
H	-3.06965	2.7333	0.42011
H	-3.22168	1.15719	-0.01699
H	-3.04727	2.32655	-1.15731

EDT–$(NH_3)_3$–I

C	0	-0.09248	1.71568	-0.31183
H	0	0.09858	2.58932	-0.93779
H	0	-0.03882	2.03515	0.72803
C	0	0.9593	0.65899	-0.60608
H	0	0.86416	0.29417	-1.62809
H	0	1.95627	1.08809	-0.49037
S	0	0.93785	-0.77624	0.51527
H	0	0.01587	-1.49919	-0.15835
S	0	-1.80894	1.2342	-0.68222
H	0	-2.04368	0.57005	0.46958
N	0	-2.04403	-0.34533	2.41029
H	0	-2.46994	-1.2346	2.6421
H	0	-2.12941	0.24323	3.23022
H	0	-1.0541	-0.51759	2.25947
N	0	-1.47501	-2.21558	-1.48274
H	0	-1.26481	-2.5889	-2.40062
H	0	-1.76704	-1.24954	-1.60465
H	0	-2.27816	-2.72627	-1.13581
N	0	4.32179	0.09434	0.04598
H	0	3.62186	-0.63328	0.15051
H	0	4.87836	0.08808	0.89201
H	0	4.93657	-0.19342	-0.70555

EDT–$(NH_3)_3$–II

C	0.38314	-0.54453	-0.13686
H	0.69052	-1.59862	-0.10682

H	0.19961	-0.21946	0.89343
C	-0.87962	-0.41794	-0.98359
H	-0.68912	-0.73406	-2.01626
H	-1.66492	-1.06282	-0.56231
S	-1.64004	1.2649	-1.02549
H	-0.62688	1.87174	-1.6959
S	1.85433	0.3781	-0.77941
H	1.66651	1.51415	-0.04237
N	0.74048	3.06135	1.23413
H	0.76895	3.02398	2.25111
H	-0.19656	2.7788	0.94509
H	0.85428	4.03819	0.97105
N	3.15865	-2.79067	0.55343
H	3.38989	-2.84612	1.54377
H	3.20692	-1.80405	0.29497
H	3.90876	-3.26405	0.05289
N	-3.48885	-2.50495	0.4338
H	-3.83433	-2.23458	1.35288
H	-3.24075	-3.49086	0.49438
H	-4.28069	-2.44256	-0.20364