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Theoretical Study on Hydrogen Transfer in the Dissociation of Dimethyl Disulfide Radical Cation

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Table S1 For each pathway, the involved sub-steps, free energy barriers of the rate-determining steps and sub-steps, and reaction free energy changes of sub-steps. The names and mechanisms of ten HT processes. Here, sub-steps going through transition states are all HT processes. The unit of energy is kcal•mol^{-1}.

Pathway for **R**	Sub-step	Free energy barrier		Reaction free energy change	HT name	HT mechanism
		RDS	Sub-step	Sub-step		
a	**R → TS1 → Int1**	52.5	52.5	23.1	1,3-C,S-HT	HAT
	Int1 → P1/P2		-	20.5/21.8	-	-
b	**R → TS1 → Int1**	52.5	52.5	23.1	1,3-C,S-HT	HAT
	Int1 → Int2		-	-2.3	-	-
	Int2 → TS2 → Int4		18.4	-9.7	1,3-S,S-HT	HAT
	Int4 → P3		-	33.3	-	-
c	**R → TS1 → Int1**	52.5	52.5	23.1	1,3-C,S-HT	HAT
	Int1 → Int2		-	-2.3	-	-
	Int2 → TS3 → Int5a		30.6	18.0	1,4-C,S-HT	HAT
	Int5a→ P4		-	14.7	-	-
d	**R → TS1 → Int1**	52.5	52.5	23.1	1,3-C,S-HT	HAT
	Int1 →Int3		-	11.3	-	-
	Int3 →TS4 → Int5b		15.1	4.4	1,1'-C,S-HT	HAT
	Int5b → P4		-	14.7	-	-
e	**R → TS5 → Int6**	63.4	63.4	40.0	1,2-C,S-HT	HAT
	Int6 → P3		-	4.4	-	-

Pathway for **R-w**	Sub-step	Free energy barrier		Reaction free energy change	HT name	HT mechanism
		RDS	Sub-step	Sub-step		
a-w	**R-w → TS1-w → Int1-w**	38.0	38.0	21.0	1,3-C,S-HT	cE2PT
	Int1-w → P1-w /P2-w		-	27.4/13.2	-	-

b-w	**R-w → TS1-w → Int1-w**	38.0	38.0	21.0	1,3-C,S-HT	cE2PT
	Int1-w → Int2-w		-	-7.5	-	-
	Int2-w → TS2-w → Int4-w		22.3	-3.0	1,3-S,S-HT	HAT
	Int4-w → P3-w		-	24.3	-	-
c-w	**R-w → TS1-w → Int1-w**	43.0	38.0	21.0	1,3-C,S-HT	cE2PT
	Int1-w → Int2-w		-	-7.5	-	-
	Int2-w → TS3-w → Int5a-w		29.5	17.3	1,4-C,S-HT	HAT
	Int5a-w→ P4-w		-	13.1	-	-
d-w	**R-w → TS1-w → Int1-w**	47.4	38.0	21.0	1,3-C,S-HT	cE2PT
	Int1-w →Int3-w		-	10.1	-	-
	Int3-w →TS4-w → Int5b-w		16.3	0.9	1,1’-C,S-HT	HAT
	Int5b-w → P4-w		-	11.9	-	-
e-w	**R-w → TS5-w → Int6-w**	43.7	43.7	31.6	1,2-C,S-HT	cE2PT
	Int6-w → P3-w		-	3.2	-	-

Table S2 The calculated NPA charge- and Hirshfeld spin-population of key moieties at transition states of all the ten HTs. The labels of atoms can be seen in Fig. 1 and 2.

	TS1 (1,3-C,S-HT in **R**)					**TS1-w** (1,3-C,S-HT in **R-w**)						
	H5	-C1H_2	S3	S2	-C4H_3	H9	H10	-C1H_2	-OH11-	S3	S2	-C4H_3
NPA charge	0.21	-0.05	0.50	0.27	0.06	0.54	0.46	-0.25	-0.27	0.15	0.33	0.04
Hirshfeld spin	0.04	0.56	0.31	0.07	0.03	0.06	0.01	0.58	0.04	0.02	0.30	0.01
	TS2 (1,3-S,S-HT in **R**)					**TS2-w** (1,3-S,S-HT in **R-w**)						
	H5	S3	S2	-C1H_2-	-C4H_3	H10	S3	S2	-C1H_2-	-C4H_3	H9OH11	
NPA charge	0.15	0.65	0.26	-0.15	0.08	0.18	0.67	0.21	-0.16	0.07	0.03	
Hirshfeld spin	0.01	0.31	0.64	0.02	0.02	0.01	0.35	0.59	0.02	0.03	0.00	
	TS3 (1,4-C,S-HT in **R**)					**TS3-w** (1,4-C,S-HT in **R-w**)						
	H6	-C4H_2	S2	-S3H5-	-C1H_2-	H6	-C4H_2	S2	-S3H10-	-C1H_2-	H9OH11	
NPA charge	0.13	-0.01	0.18	0.84	-0.14	0.13	-0.02	0.13	0.83	-0.15	0.08	
Hirshfeld spin	0.02	0.56	0.31	0.05	0.05	0.02	0.56	0.31	0.06	0.05	0.00	
	TS4 (1,1'-C,S-HT in **R**)					**TS4-w** (1,1'-C,S-HT in **R-w**)						
	H7	-C4H_2	S2	-S3H5	-C1H_2	H7	-C4H_2	S2	-S3H10	-C1H_2	H9OH11	
NPA charge	0.16	-0.13	0.44	0.39	0.13	0.16	-0.13	0.41	0.43	0.12	0.03	
Hirshfeld spin	0.04	0.49	0.10	0.20	0.18	0.04	0.45	0.14	0.19	0.19	0.00	
	TS5 (1,2-C,S-HT in **R**)					**TS5-w** (1,2-C,S-HT in **R-w**)						
	H8	-C1H_2	S2	S3	-C4H_3	H9	H11	-C1H_2	-OH10-	S2	S3	-C4H_3
NPA charge	0.28	0.03	0.43	0.23	0.04	0.55	0.53	-0.19	-0.21	0.19	0.12	0.01
Hirshfeld spin	0.01	0.68	0.24	0.07	0.00	0.05	0.02	0.67	0.04	0.21	0.01	0.01

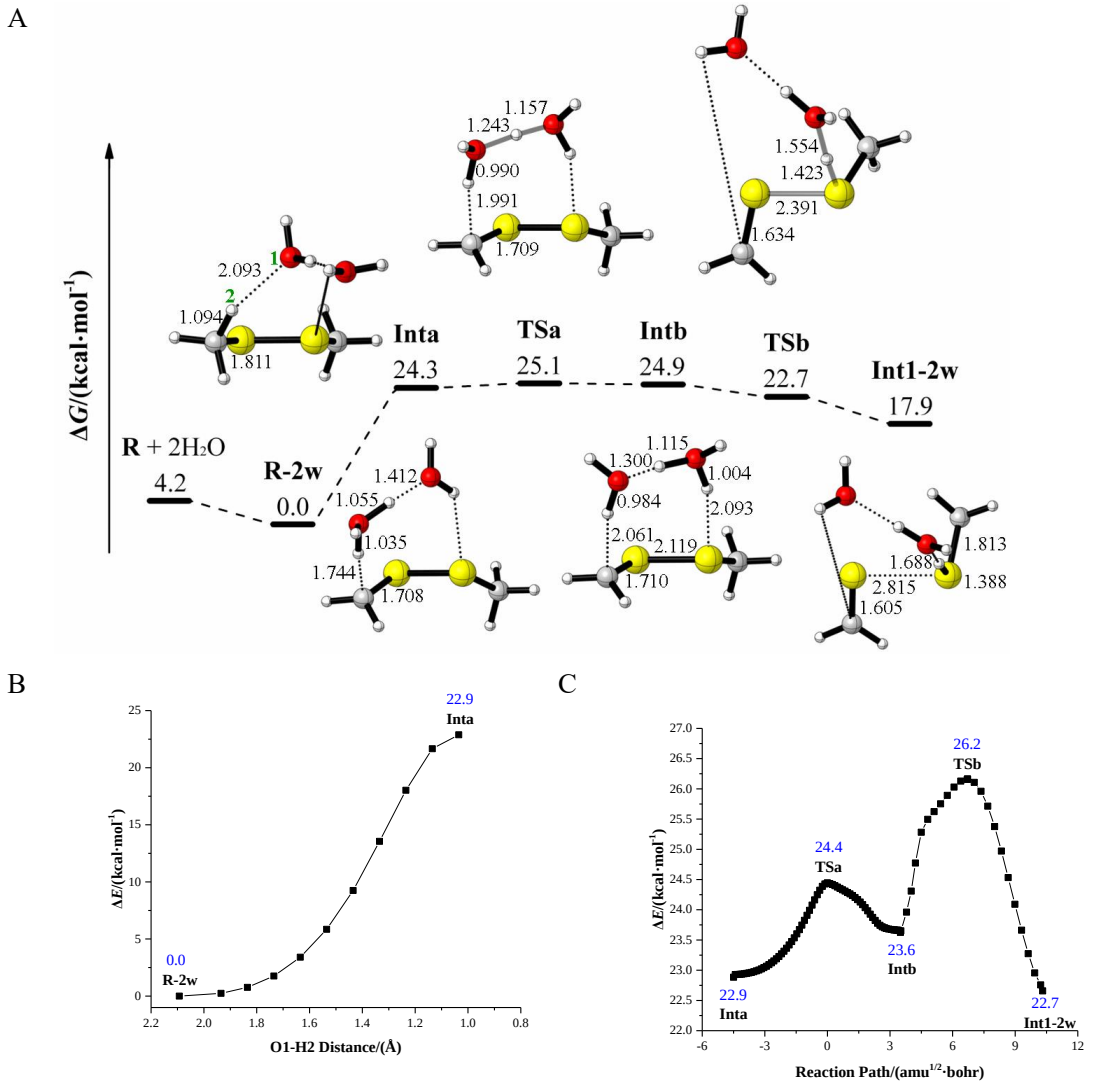
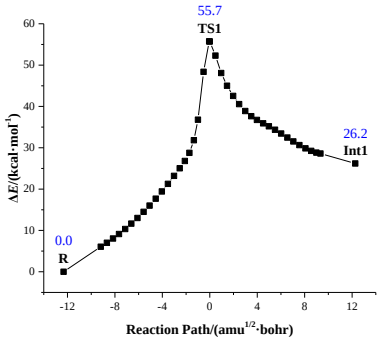
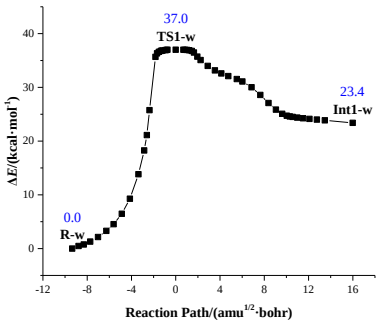


Fig. S1 A) Relative Δ*G* plot for the rate-determining step in pathway **b-w**, *i.e.* from **R-w** to **Int1-w** in Fig. 2, with the addition of a second water molecule. And key geometric parameters for each optimized stationary point in the gas phase computed at the UωB97X-D/6-311+G** level. Here, red, yellow, gray, and white balls represent oxygen, sulfur, carbon, and hydrogen atoms, respectively. The key atoms are labelled in dark green. The unit of bond distance is angstrom (Å). B) Flexible scanning profile for a barrierless sub-step from **R-2w** to **Inta**, and C) intrinsic reaction coordinate (IRC) profile for sub-steps from **Inta** to **Int1-2w**, and relative energies (Δ*E*) for the stationary points

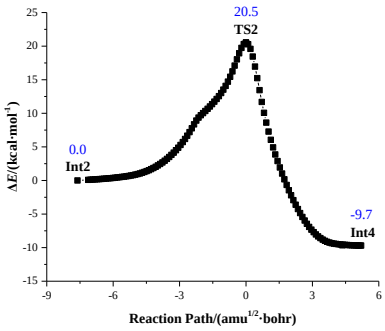
A 1,3-C,S-HT in **R**



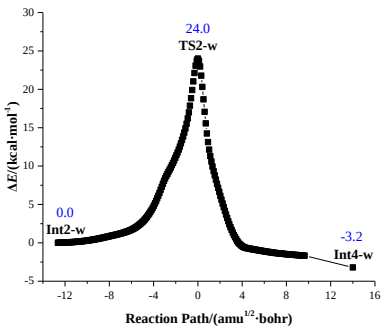
B 1,3-C,S-HT in **R-w**



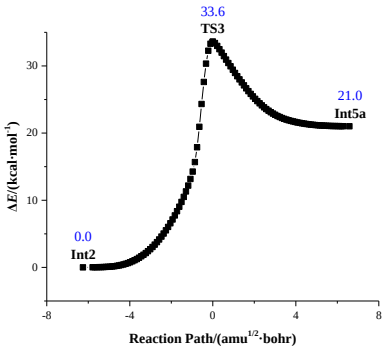
C 1,3-S,S-HT in **R**



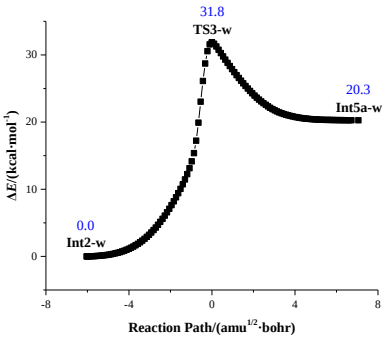
D 1,3-S,S-HT in **R-w**



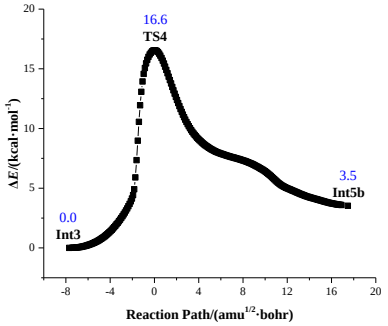
E 1,4-C,S-HT in **R**



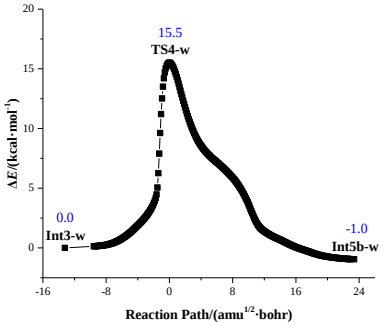
F 1,4-C,S-HT in **R-w**



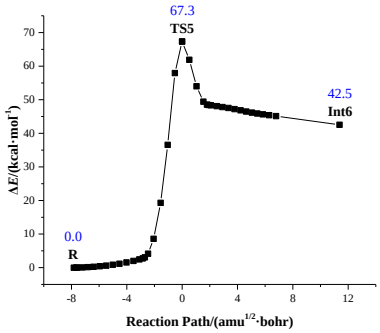
G 1,1'-C,S-HT in **R**



H 1,1'-C,S-HT in **R-w**



I 1,2-C,S-HT in **R**



J 1,2-C,S-HT in **R-w**

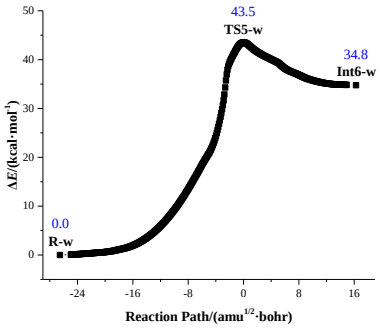
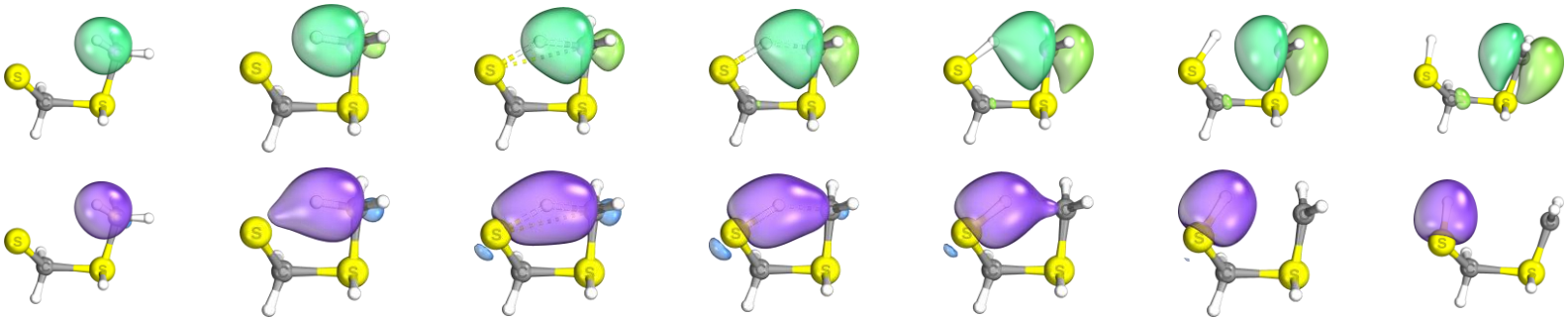


Fig. S2 In the gas phase, the predicted intrinsic reaction coordinate (IRC) profiles for five HTs in (A, C, E, G, I) **R** and (B, D, F, H, J) **R-w**, and relative energies (ΔE in kcal•mol^{-1}) for the stationary points at the UωB97X-D/6-311+G** level

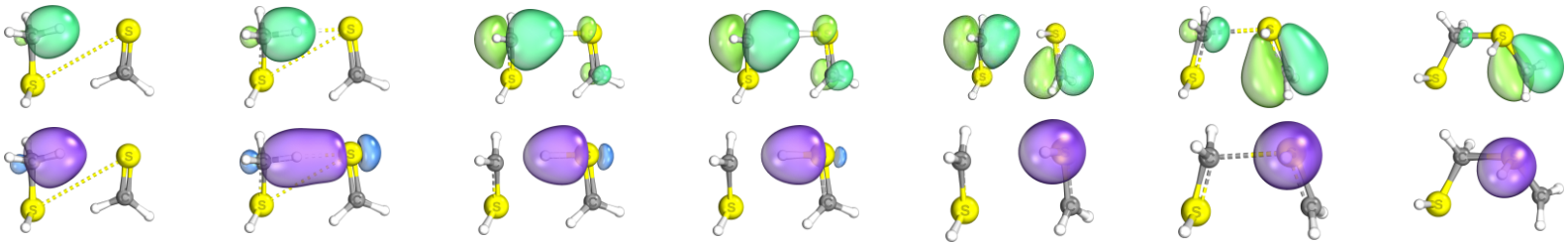
A 1,4-C,S-HT in **R**

Coordinate	-5.789	-0.755	-0.323	0.000	0.428	1.719	6.202



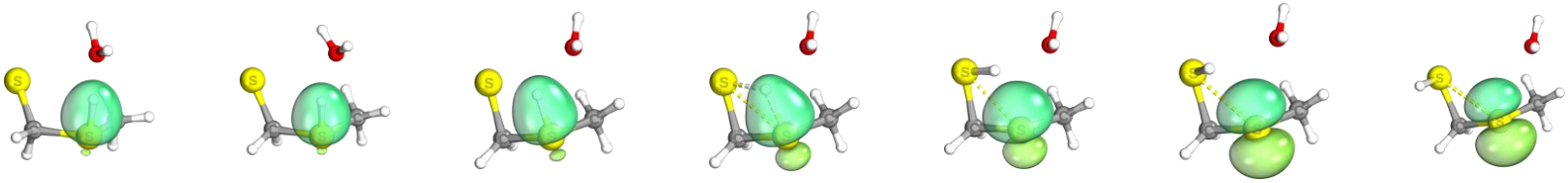
B 1,1'-C,S-HT in **R**

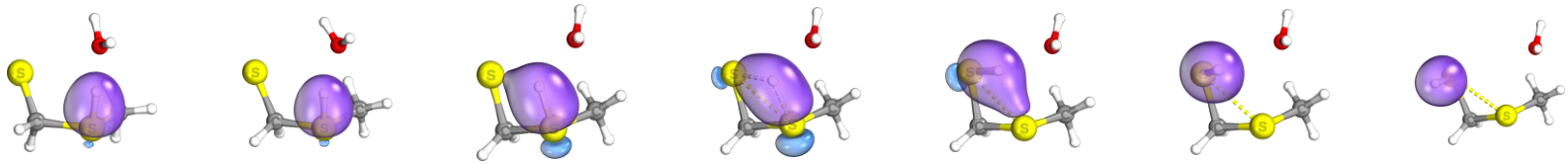
Coordinate	-7.427	-1.722	-0.430	0.000	2.681	9.114	16.791



C 1,3-S,S-HT in **R-w**

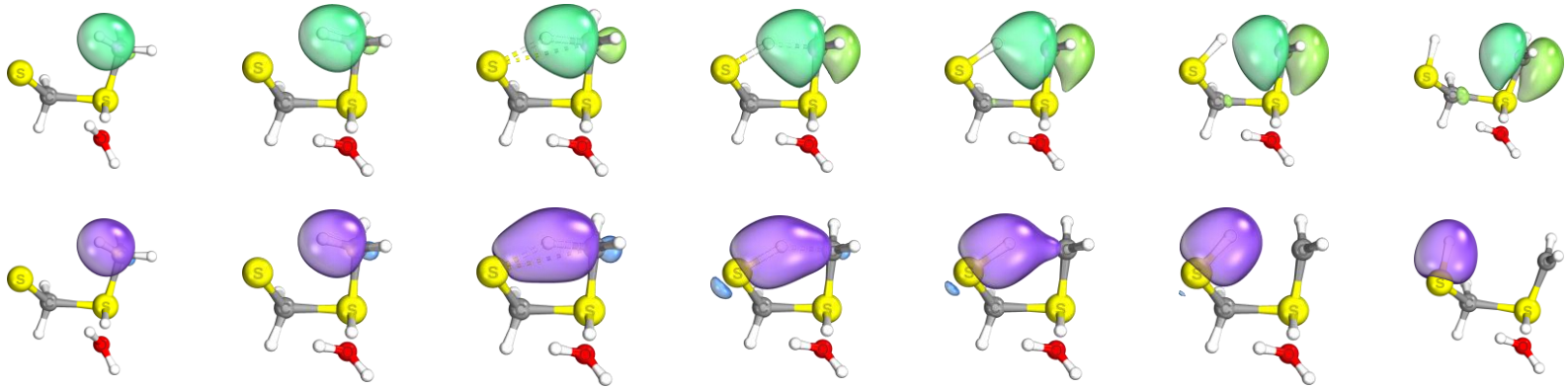
Coordinate	-12.627	-6.206	-0.510	0.000	1.019	2.239	9.544





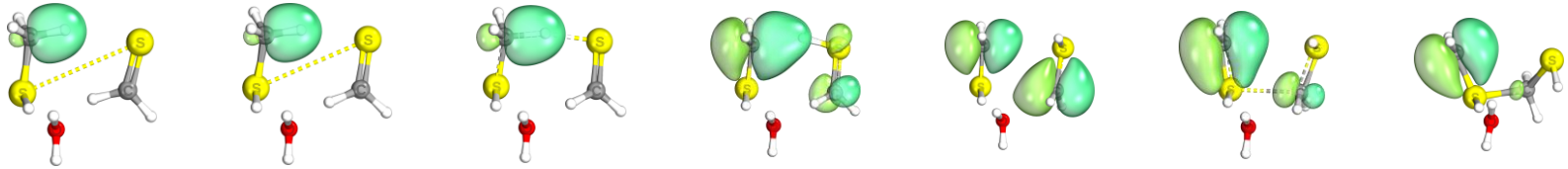
D 1,4-C,S-HT in **R-w**

Coordinate	-5.999	-1.406	-0.434	0.000	0.323	1.296	6.724



E 1,1'-C,S-HT in **R-w**

Coordinate	-9.568	-3.588	-1.282	0.000	4.186	8.381	22.910



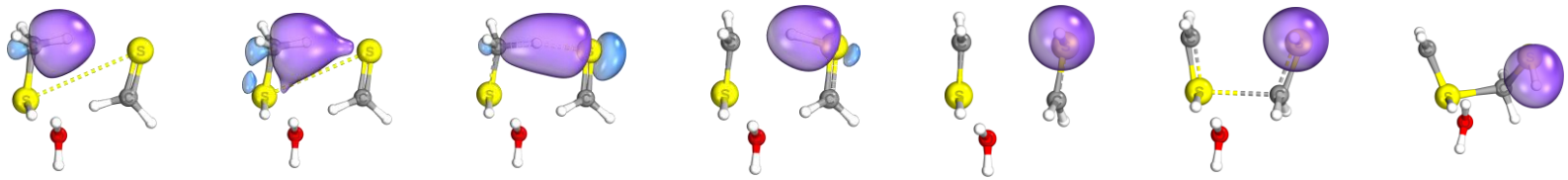
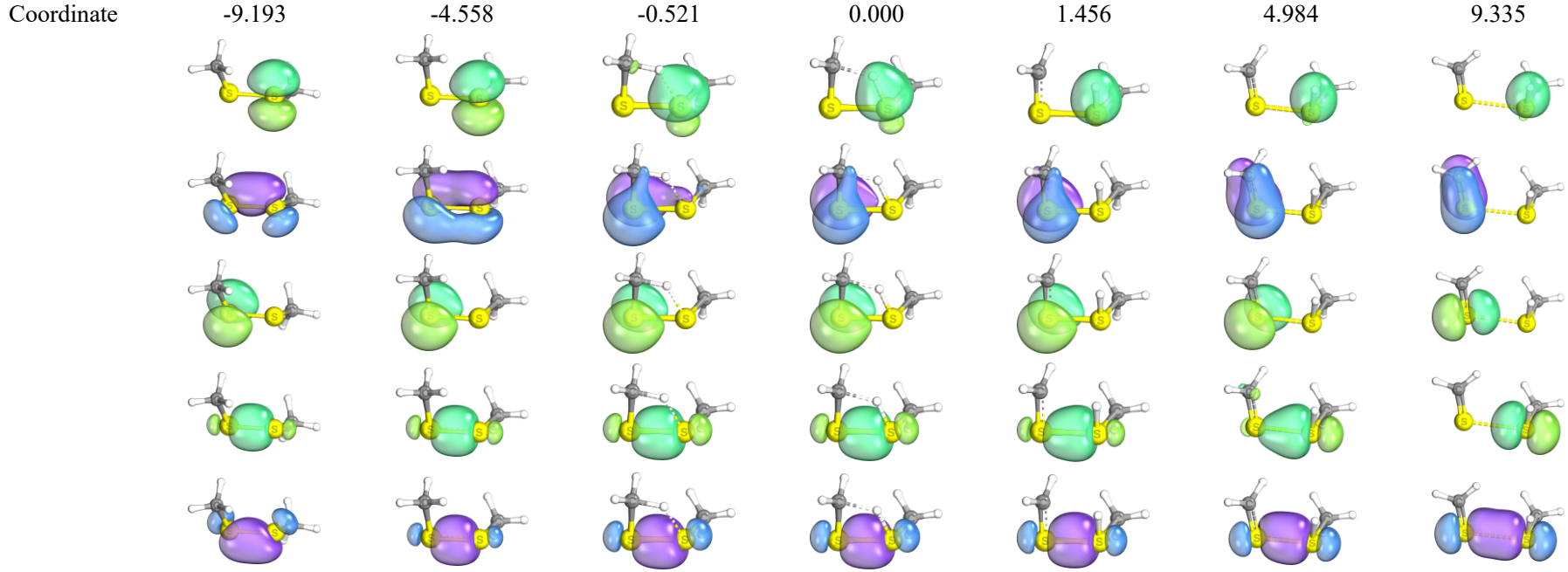
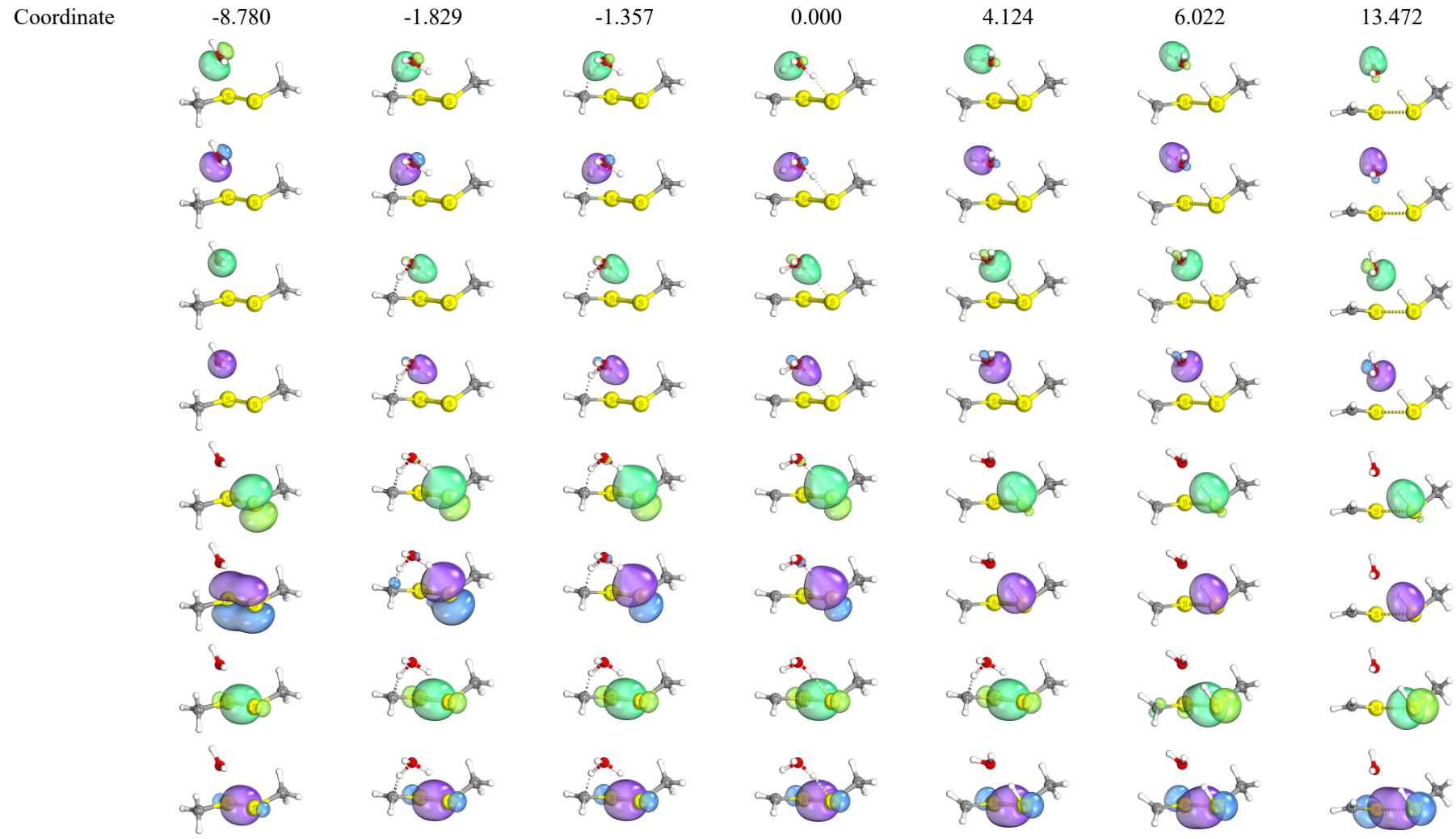


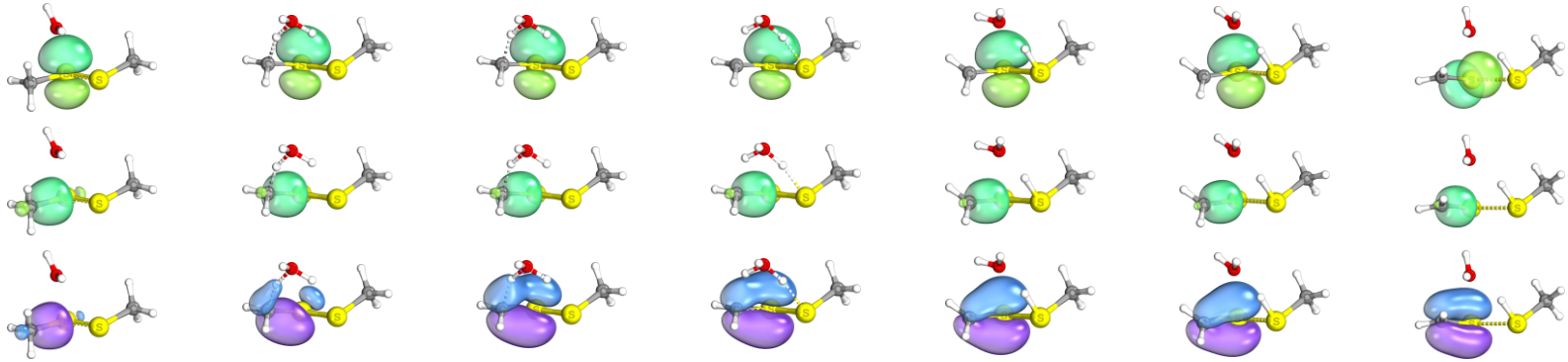
Fig. S3 The intrinsic bond orbital (IBO) transformations of the broken C-H bond along the intrinsic reaction coordinate (IRC) of 1,4-C,S- and 1,1'-C,S-HT in (A, B) **R** and (D, E) **R-w**. And the IBO transformation of the broken S-H bond along the IRC of 1,3-S,S-HT in (C) **R-w**. Here, the α- and β-IBOs are shown in green and purple, respectively. The unit of coordinate is amu$^{1/2}$•bohr.

A 1,3-C,S-HT in **R**



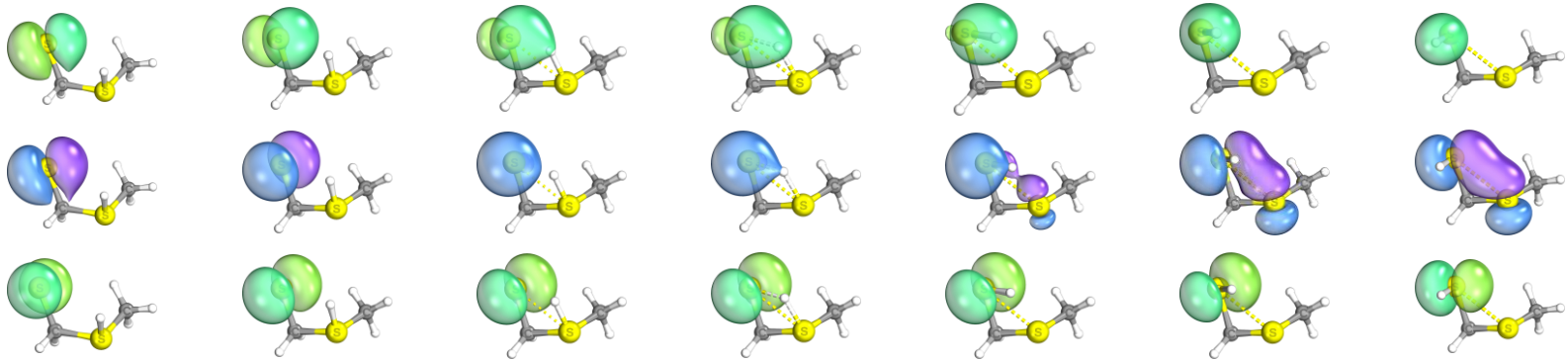
B 1,3-C,S-HT in **R-w**





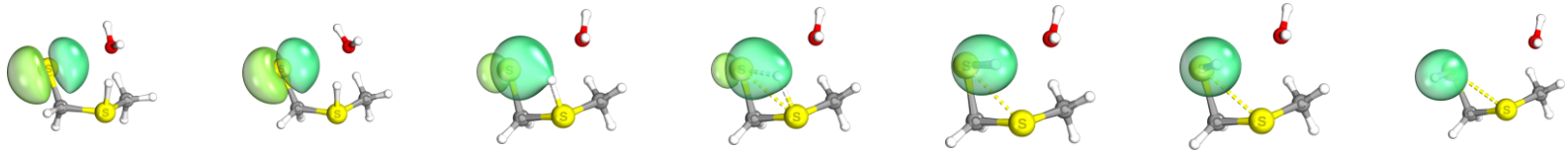
C 1,3-S,S-HT in **R**

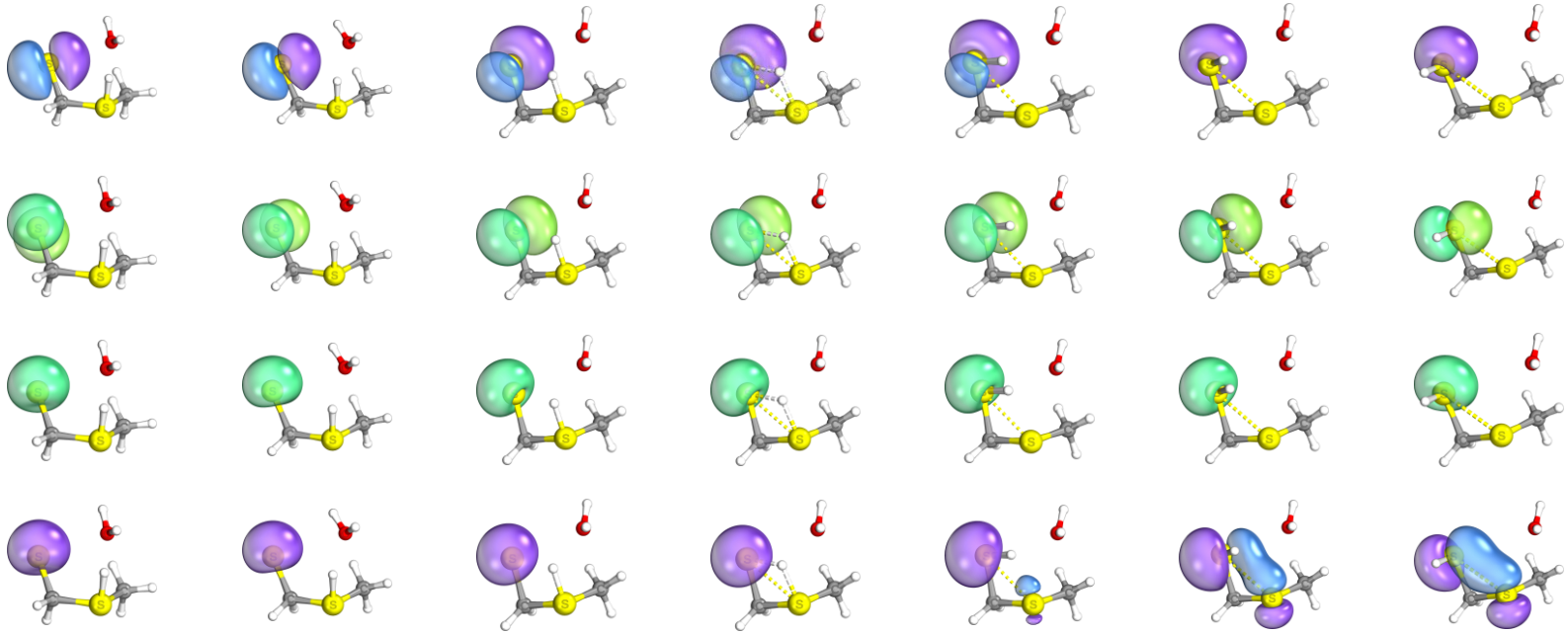
Coordinate	-7.126	-1.631	-0.408	0.000	0.714	1.939	5.204



D 1,3-S,S-HT in **R-w**

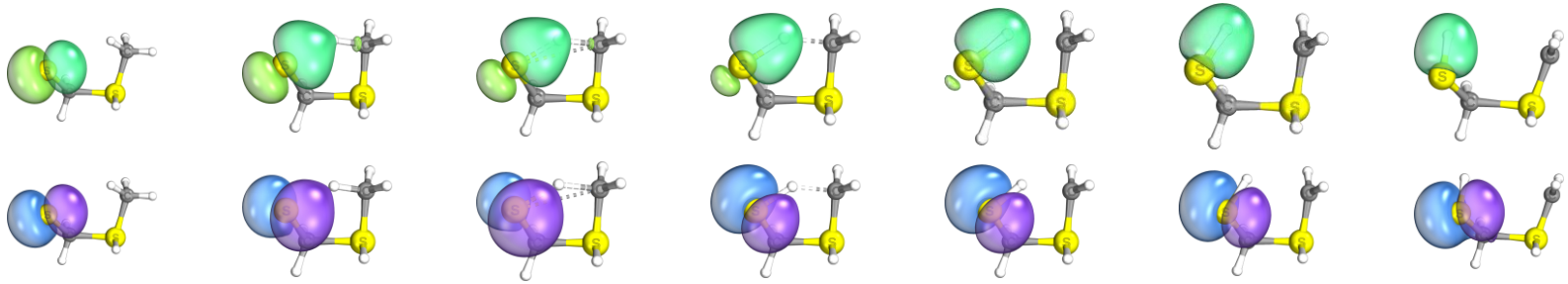
Coordinate	-12.627	-6.206	-0.510	0.000	1.019	2.239	9.544





E 1,4-C,S-HT in **R**

Coordinate	-5.789	-0.755	-0.323	0.000	0.428	1.719	6.202



F 1,4-C,S-HT in **R-w**

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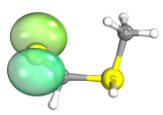
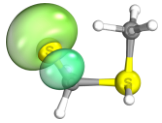
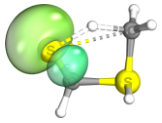
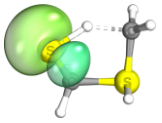
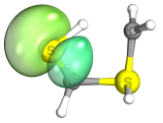
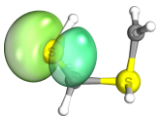
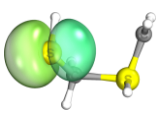
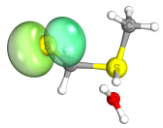
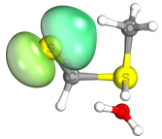
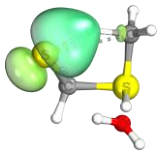
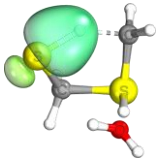
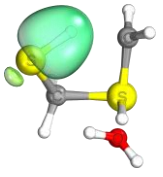
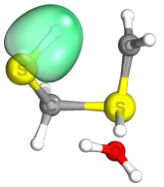
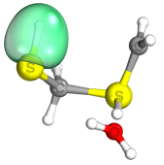
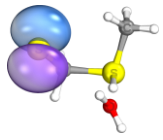
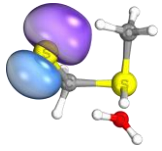
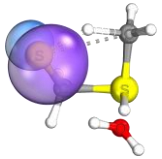
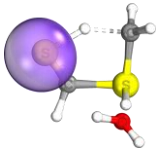
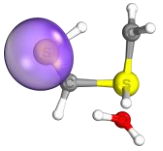
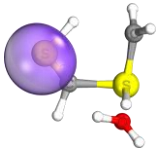
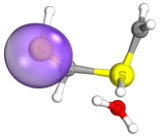
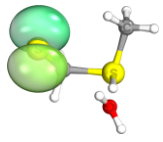
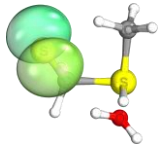
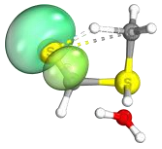
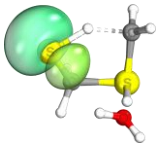
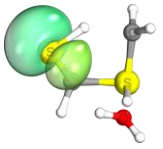
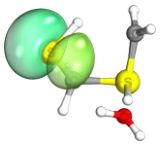
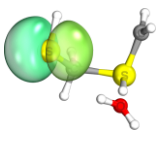
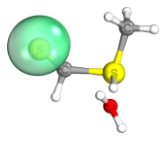
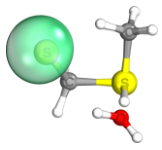
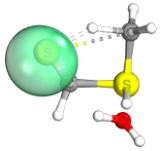
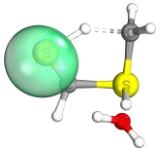
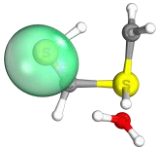
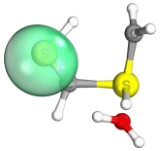
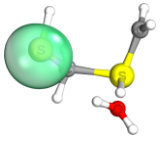
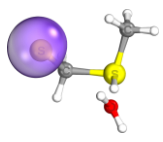
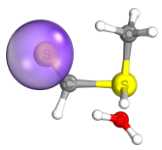
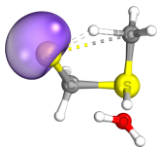
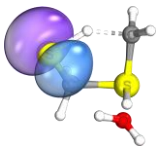
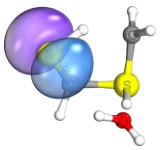
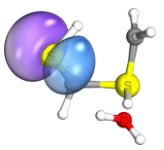
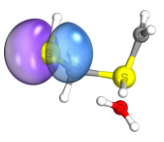
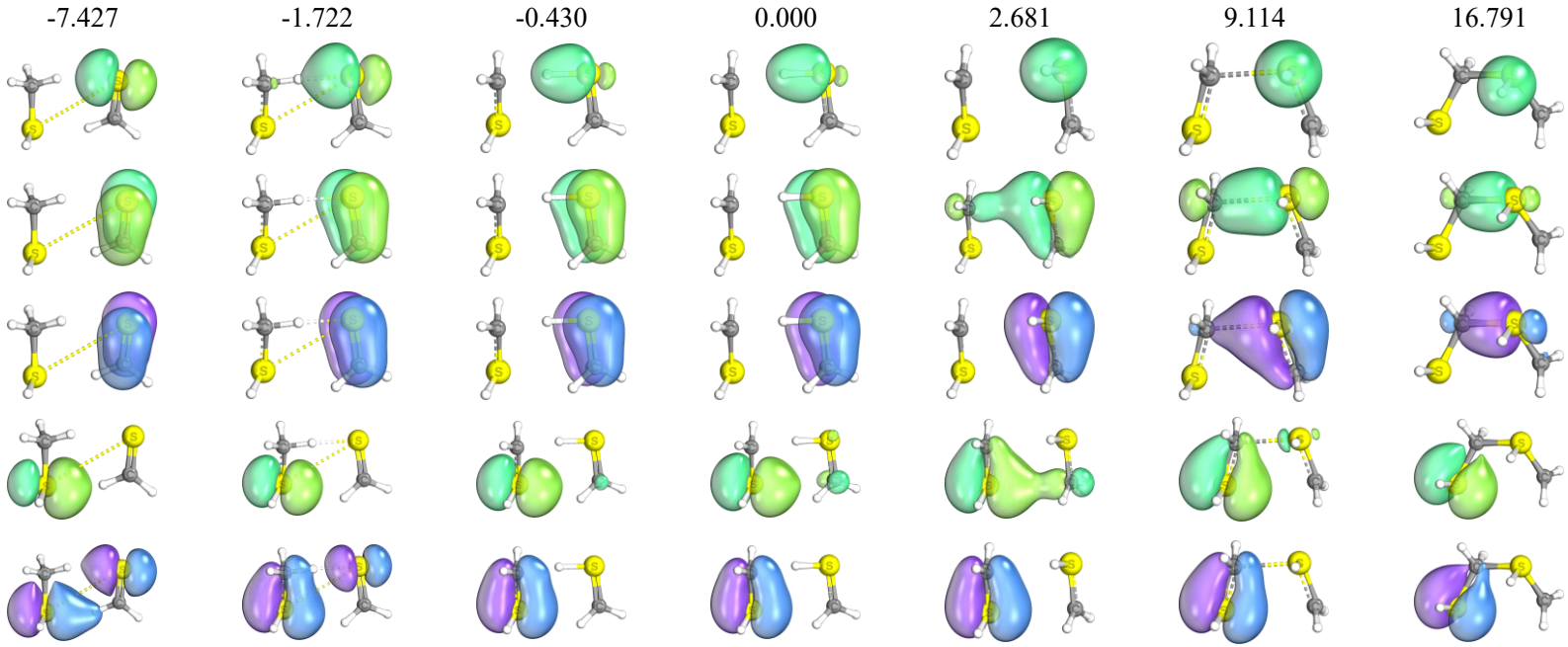
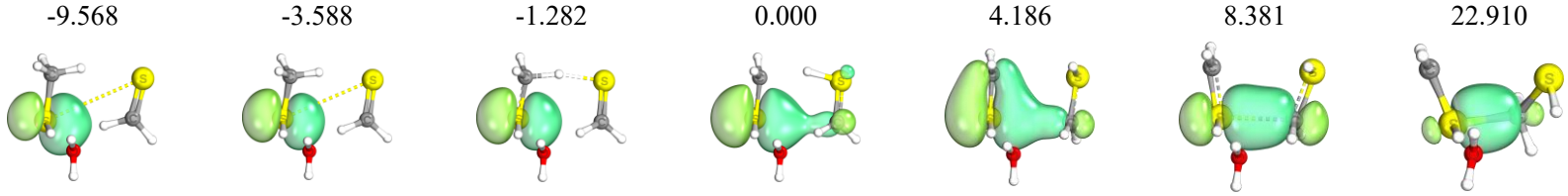
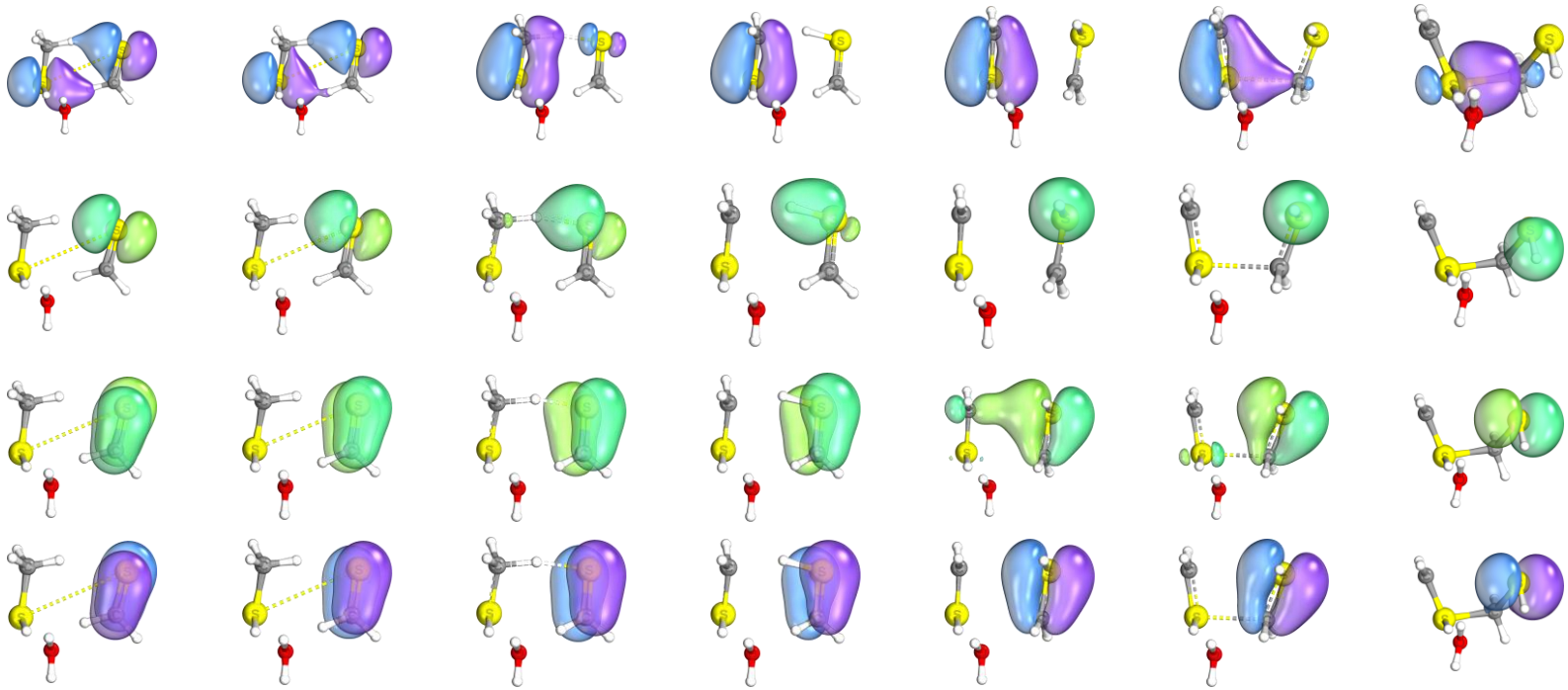
							
							
							
							
							
							

G 1,1'-C,S-HT in **R**



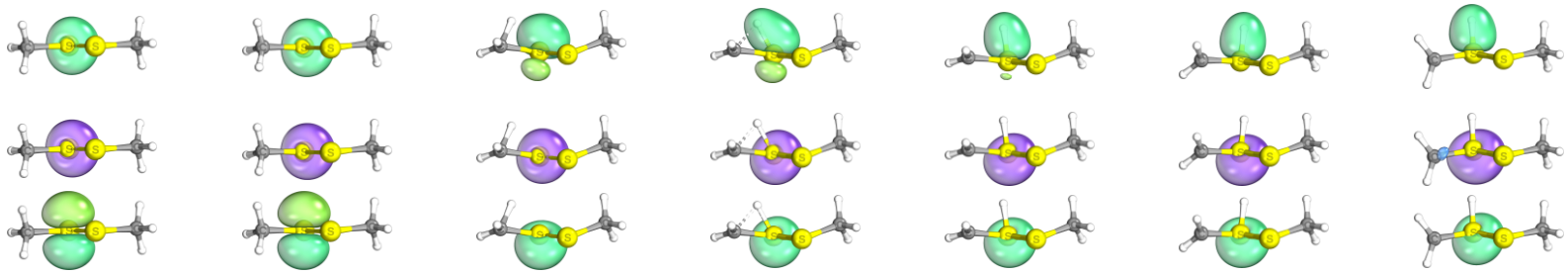
H 1,1'-C,S-HT in **R-w**

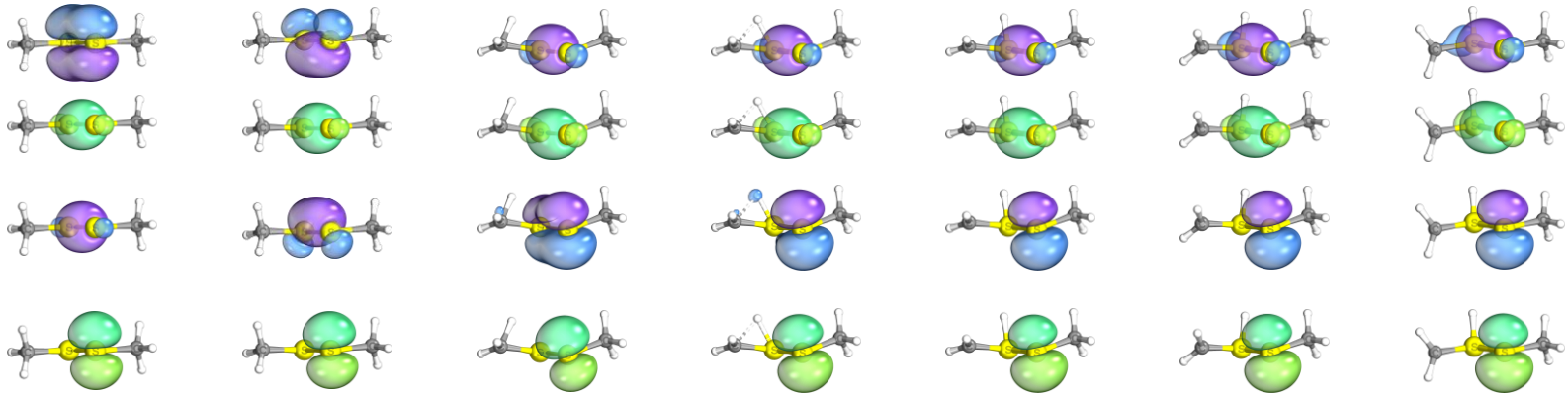




I 1,2-C,S-HT in **R**

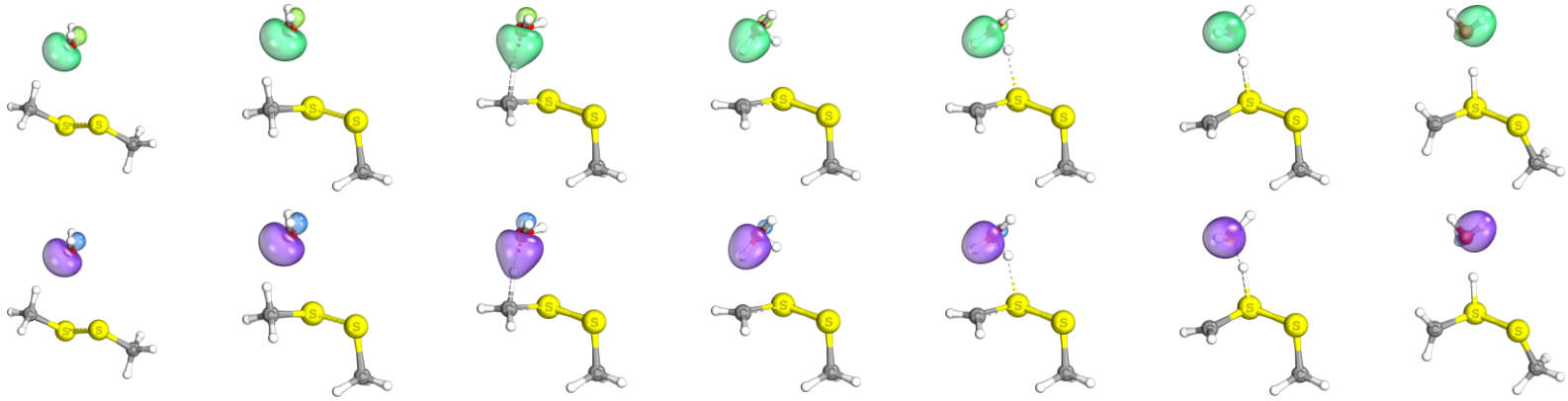
Coordinate	-7.828	-6.822	-1.043	0.000	1.043	2.920	6.794





J 1,2-C,S-HT in **R-w**

Coordinate	-24.965	-6.291	-2.542	0.000	1.212	5.184	14.911



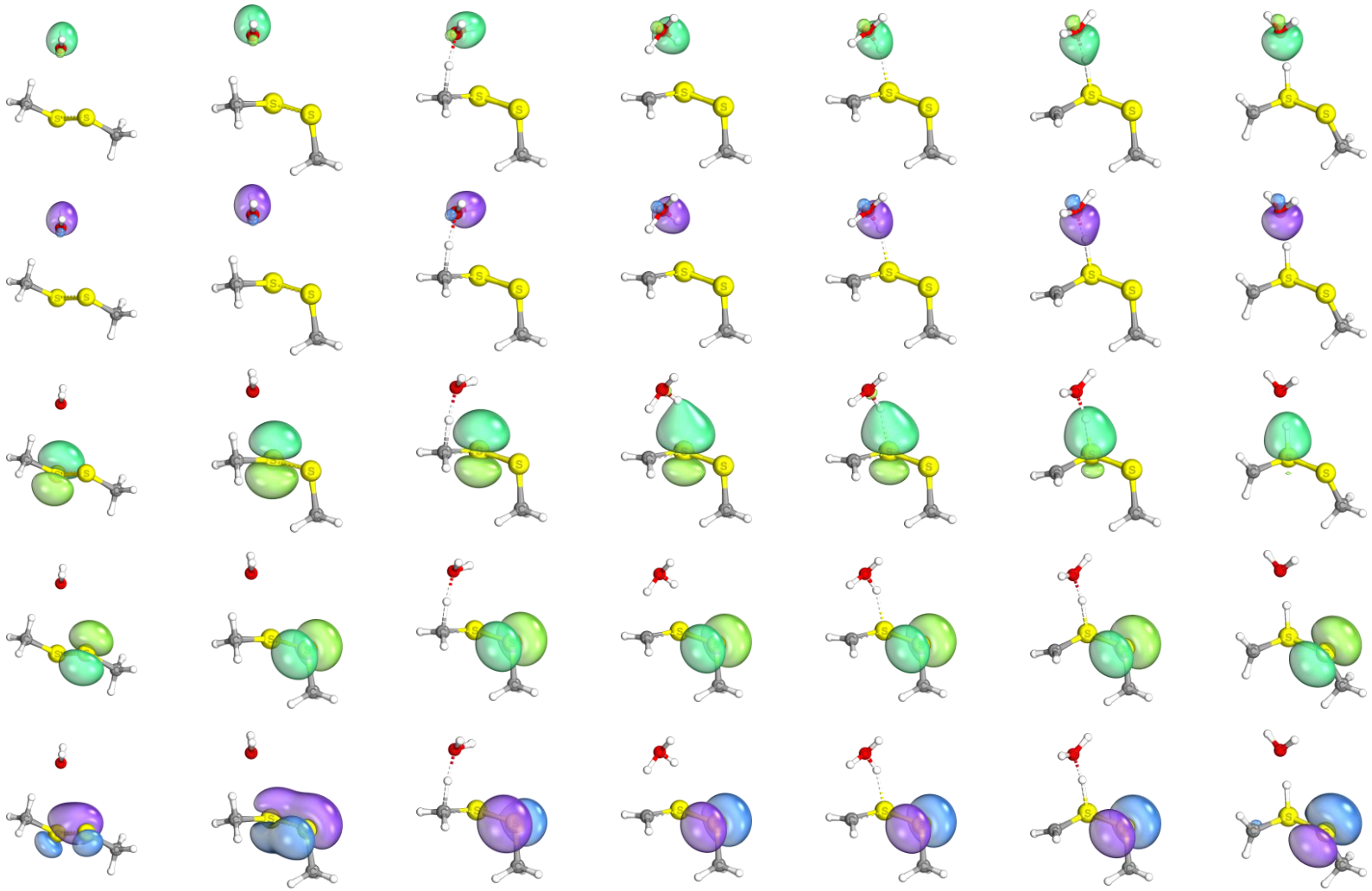
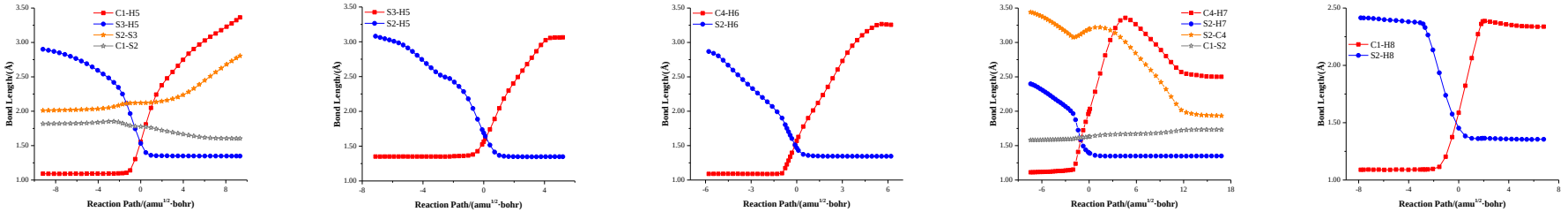


Fig. S4 The intrinsic bond orbital (IBO) transformations of the key bonds along the intrinsic reaction coordinate (IRC) of five HTs in (A, C, E, G, I) **R** and (B, D, F, H,

J) **R-w**. Here, the α- and β-IBOs are shown in green and purple, respectively. The unit of coordinate is amu$^{1/2}$•bohr.

A 1,3-C,S-HT in **R** C 1,3-S,S-HT in **R** E 1,4-C,S-HT in **R** G 1,1'-C,S-HT in **R** I 1,2-C,S-HT in **R**



B 1,3-C,S-HT in **R-w** D 1,3-S,S-HT in **R-w** F 1,4-C,S-HT in **R-w** H 1,1'-C,S-HT in **R-w** J 1,2-C,S-HT in **R-w**

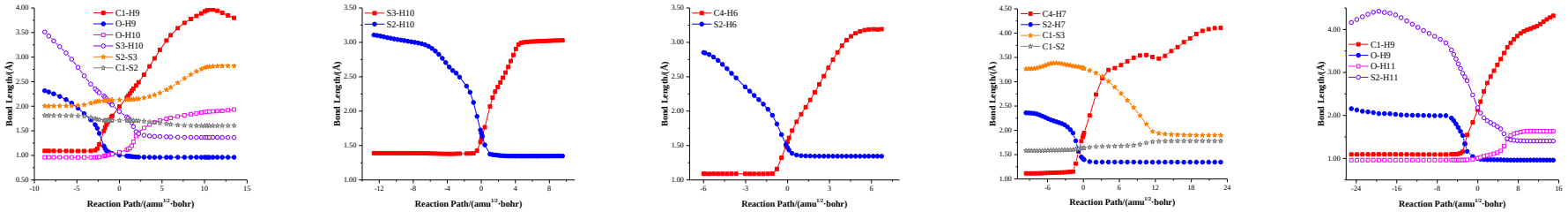
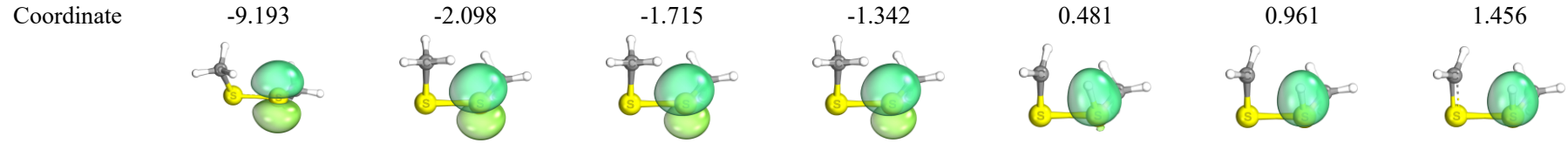
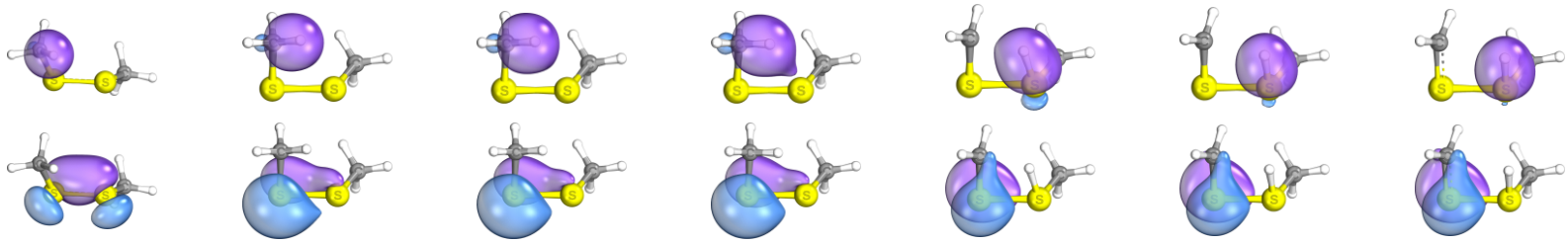


Fig. S5 The variations of key bond lengths along the intrinsic reaction coordinate (IRC) of five HTs in (A, C, E, G, I) **R** and (B, D, F, H, J) **R-w**. The labels of atoms can be seen in Fig. 1 and 2.

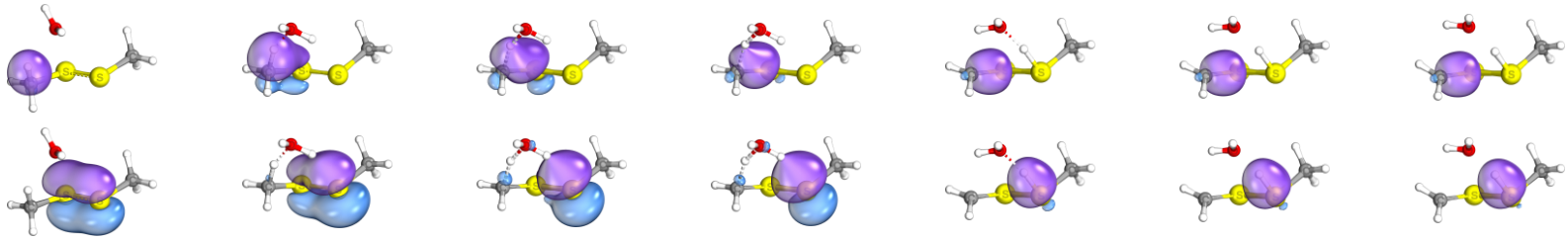
A 1,3-C,S-HT in **R**





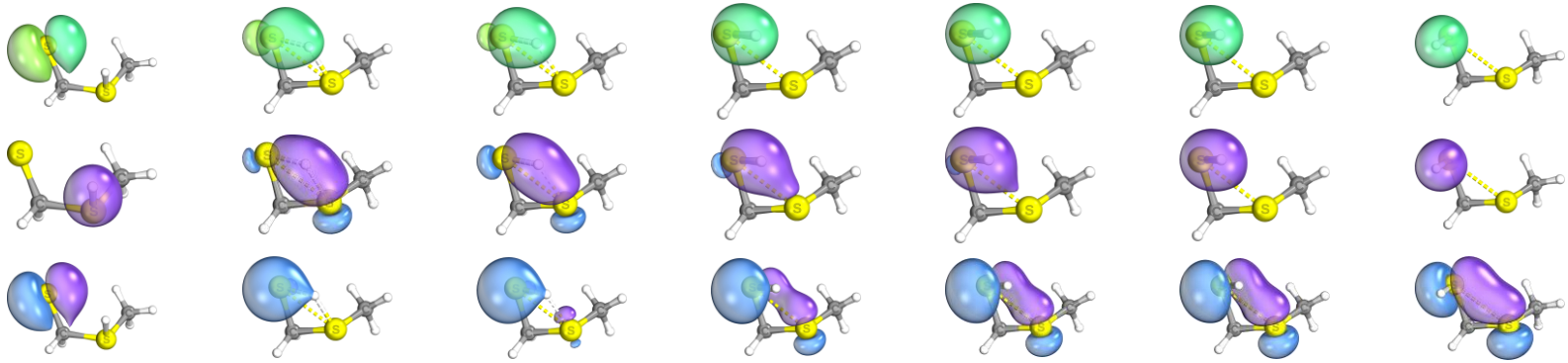
B 1,3-C,S-HT in **R-w**

Coordinate	-8.780	-2.373	-1.829	-1.682	2.250	2.890	3.537

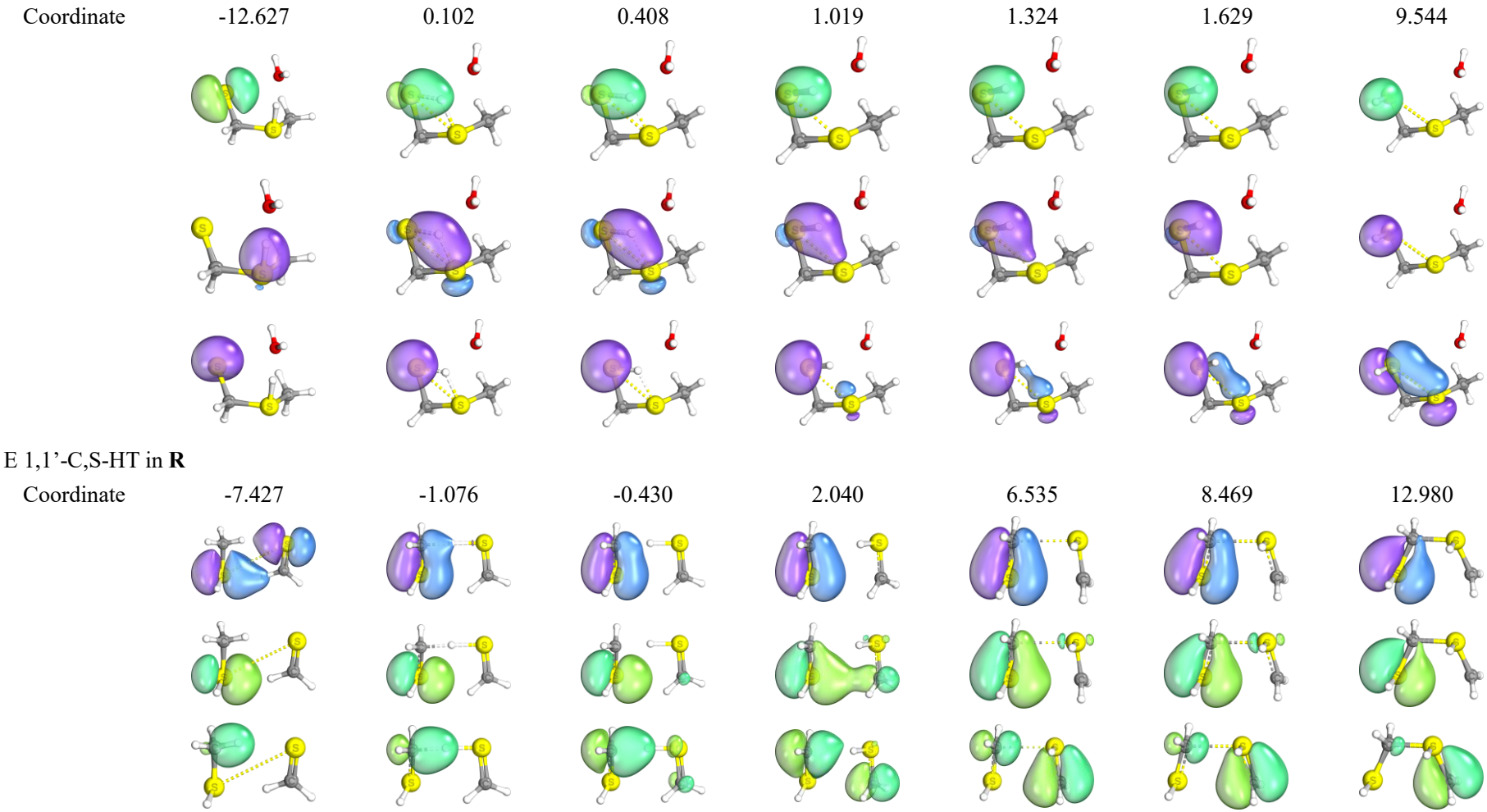


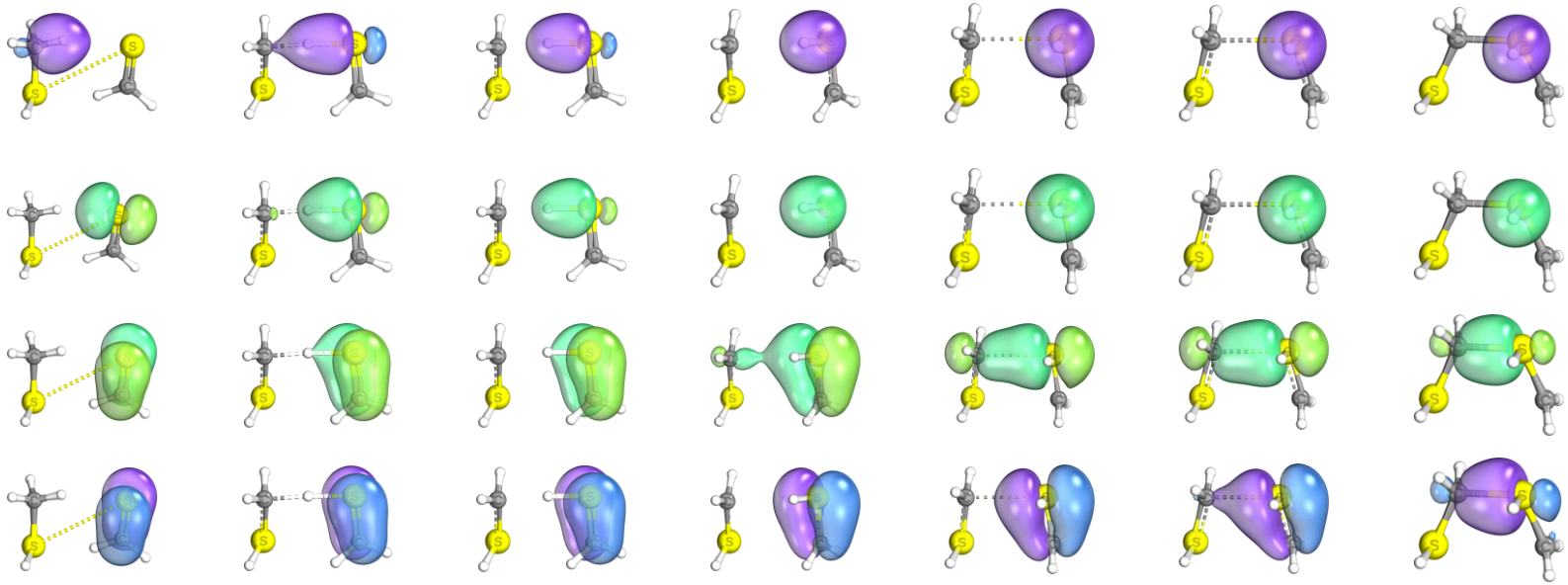
C 1,3-S,S-HT in **R**

Coordinate	-7.126	0.102	0.408	1.020	1.326	1.633	5.204



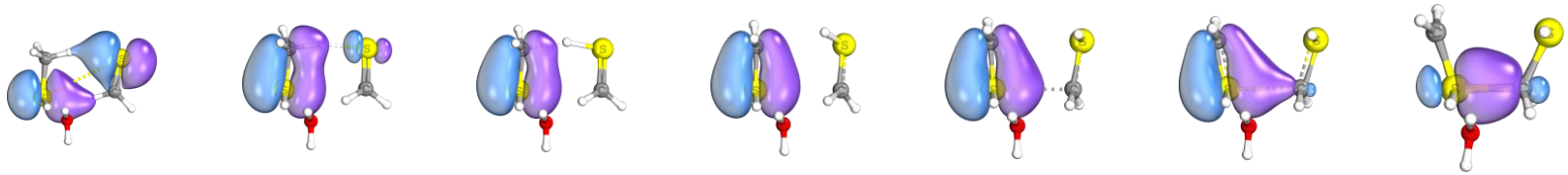
D 1,3-S,S-HT in **R-w**

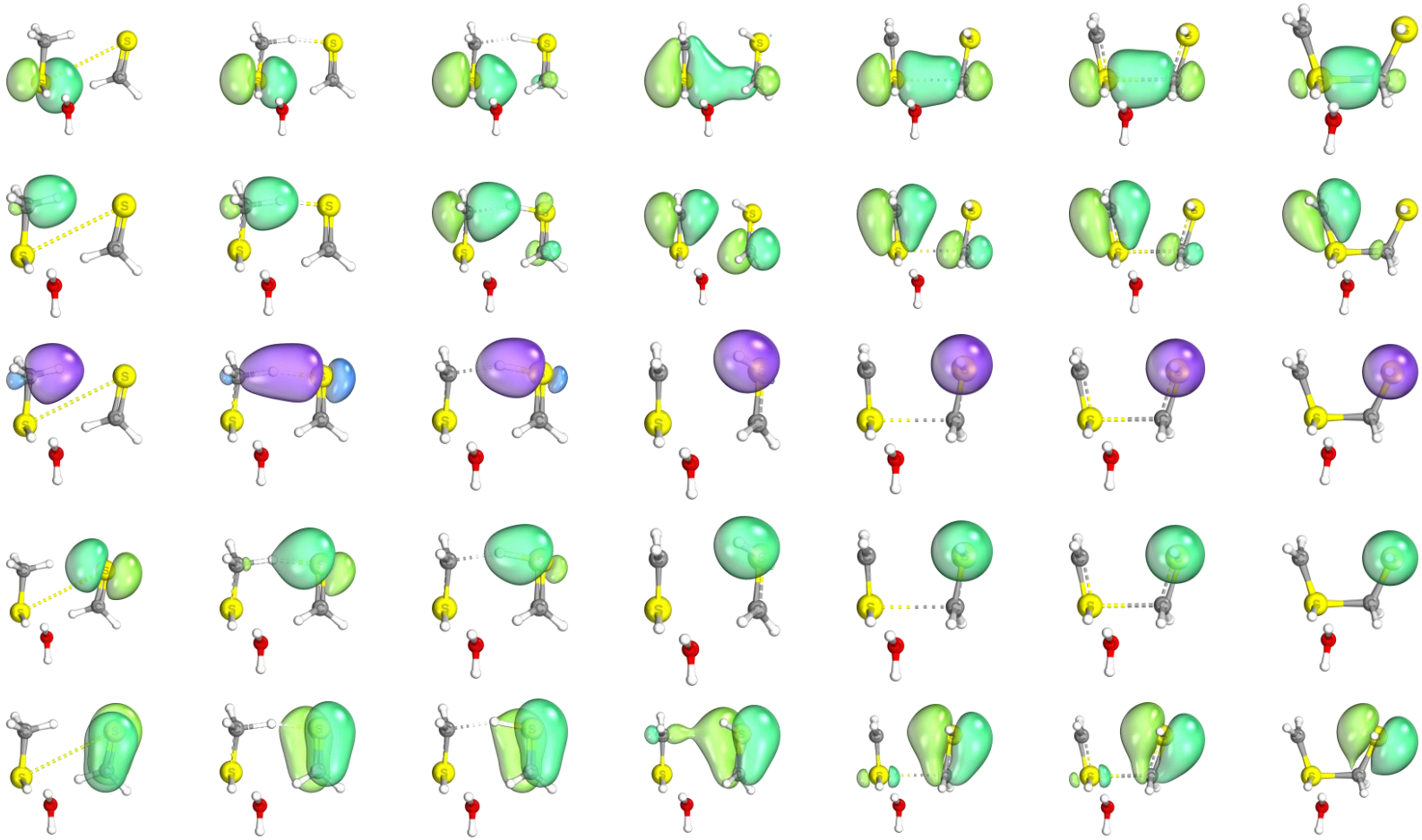

Coordinate
-12.627
0.102
0.408
1.019
1.324
1.629
9.544
E 1,1'-C,S-HT in **R**
Coordinate
-7.427
-1.076
-0.430
2.040
6.535
8.469
12.980



F 1,1'-C,S-HT in **R-w**

Coordinate	-9.568	-1.282	-0.348	2.098	6.282	8.381	12.581





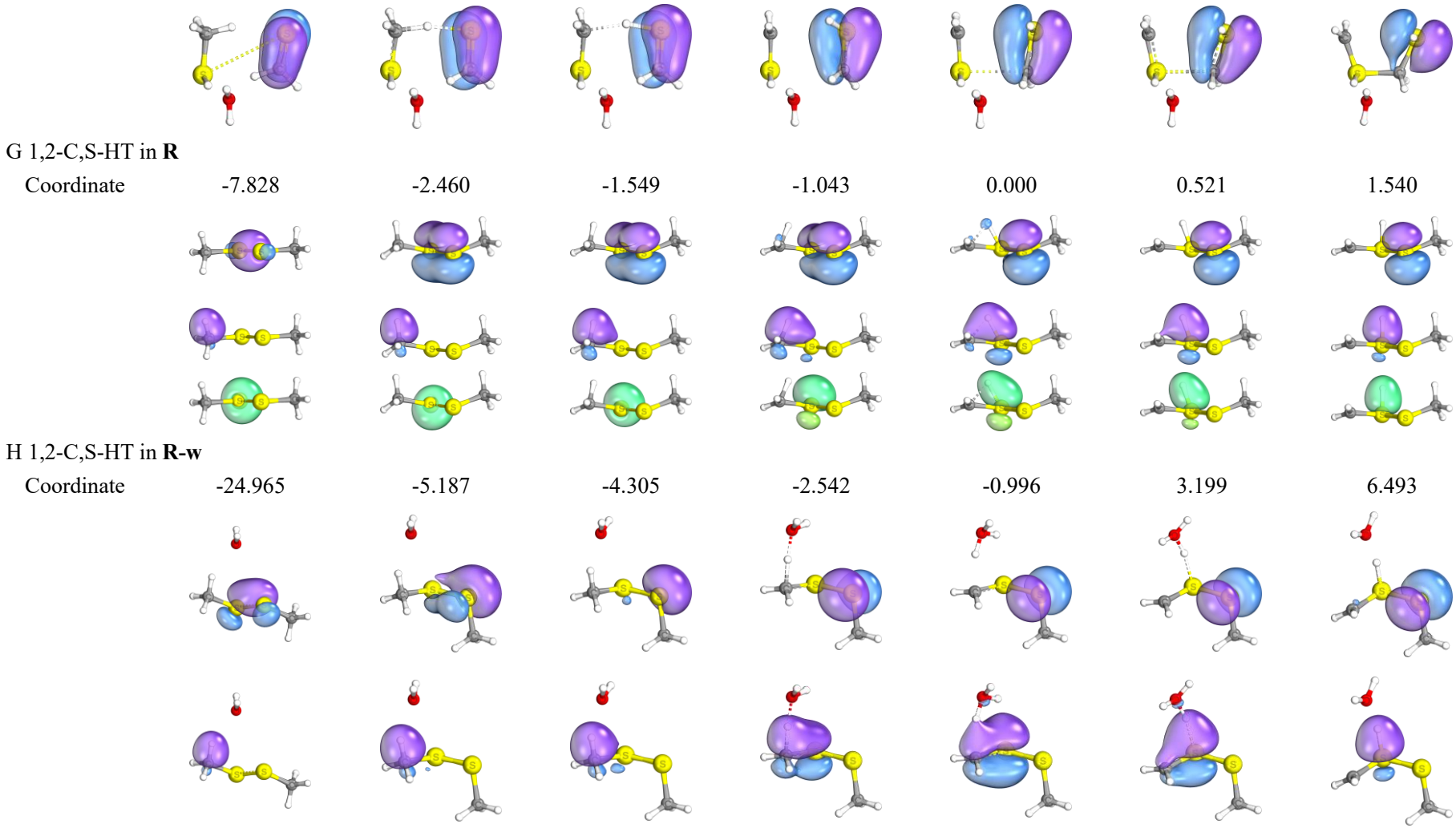


Fig. S6 The intrinsic bond orbital (IBO) transformations of the key bonds along the intrinsic reaction coordinate (IRC) of four HTs in (A, C, E, G) **R** and (B, D, F, H)

R-w. Here, the α- and β-IBOs are shown in green and purple, respectively. The unit of coordinate is $amu^{1/2}$•bohr.

The Cartesian coordinate (in Å) and Gibbs free energy (in a.u.) of each optimized stationary point

R

-875.872009

S	0.727607	0.690874	-0.000116
C	2.208071	-0.358279	0.000203
H	2.233197	-0.970825	-0.900924
H	3.044689	0.340982	-0.000062
H	2.233241	-0.970279	0.901693
S	-0.727597	-0.690834	-0.000129
C	-2.208088	0.358215	0.000191
H	-2.232793	0.971617	-0.900356
H	-3.044677	-0.341080	-0.001062
H	-2.233701	0.969335	0.902273

Int1

-875.835167

S	-1.160051	-0.690178	-0.161983
C	-2.173498	0.704442	0.409328
H	-1.862627	1.633132	-0.066104
H	-3.216175	0.490303	0.175030
H	-2.047138	0.767475	1.488590
S	1.362794	0.608313	-0.255405
C	2.206968	-0.558680	0.452143
H	-1.351252	-0.535034	-1.486914
H	1.756099	-1.493048	0.783825
H	3.276380	-0.427564	0.614955

Int2

-875.838831

S	-1.169569	-0.591330	-0.160631
S	1.798142	0.372071	-0.136666
H	-0.713495	1.774467	-0.136703
H	-0.904771	-0.485737	-1.480764
C	0.601737	-0.785370	0.440779
H	0.517957	-0.757806	1.531865
H	0.867579	-1.809666	0.162505
C	-1.543426	1.146893	0.187615
H	-1.715655	1.226736	1.260311
H	-2.458650	1.391022	-0.350827

Int3

-875.817126

S	2.062467	0.361801	0.045902
S	-1.882323	-0.480308	-0.043277
H	-1.997811	-0.622791	1.292461
H	-0.192209	1.232916	0.147224
C	-1.283692	1.207284	-0.062458
H	-1.786881	1.818018	0.686068
H	-1.449388	1.612851	-1.059315
C	1.355015	-1.046333	-0.080011
H	0.227970	-1.116031	-0.079010
H	1.888082	-1.994563	-0.174620

Int4

-875.854265

S	-0.892391	-0.571802	-0.402311
S	1.604356	0.445883	-0.126605
H	2.120607	-0.502375	-0.934291
C	0.467301	-0.642438	0.778331
H	0.215545	-0.207068	1.743127
H	0.838655	-1.658079	0.888877
C	-1.863439	0.825935	0.198254
H	-1.236885	1.712913	0.299783
H	-2.635181	1.008977	-0.548516
H	-2.317347	0.559354	1.154179

Int5a

-875.810153

S	-1.254408	-0.517218	-0.172741
S	1.789576	0.288853	-0.171524
H	1.575472	1.314287	0.673155
H	-0.934201	-0.388697	-1.478129
C	0.541656	-0.782483	0.483843
H	0.414807	-0.735430	1.564273
H	0.735841	-1.812255	0.181236
C	-1.660506	1.127061	0.181194
H	-2.109051	1.314638	1.147430
H	-1.532450	1.893821	-0.569940

Int5b

-875.810181

S	1.258123	-0.516173	-0.183428
S	-1.763269	0.381054	-0.052317

Int6

-875.808270

S	-0.887188	-0.727892	0.010953
C	-2.014600	0.674613	0.249823

H	-2.111579	-0.280112	-1.171651	H	-2.089367	1.287583	-0.646527
H	0.937424	-0.380785	-1.487391	H	-2.978424	0.188900	0.425501
C	-0.535577	-0.774967	0.490522	H	-1.752535	1.259404	1.129399
H	-0.735555	-1.814810	0.232224	S	0.902914	0.347907	-0.480144
H	-0.386062	-0.686539	1.565987	C	2.082343	-0.003014	0.725218
C	1.666685	1.126485	0.180162	H	1.351945	-0.450496	-1.473094
H	1.435886	1.916145	-0.520662	H	2.021044	0.574356	1.637934
H	2.155570	1.298894	1.129314	H	2.789243	-0.809591	0.583590

R-w

-952.302748

S	0.785039	0.484494	0.515876
C	2.415745	0.668659	-0.257131
H	2.305569	0.818378	-1.330865
H	2.845714	1.560134	0.199790
H	3.037517	-0.198933	-0.037582
S	0.112703	-1.158214	-0.417231
C	-1.495324	-1.387154	0.385928
H	-2.083820	-0.476400	0.252200
H	-1.950719	-2.229949	-0.134557
H	-1.348756	-1.631968	1.437816
O	-2.196315	1.635323	-0.255279
H	-2.568538	1.923190	-1.091955
H	-2.552844	2.243450	0.396277

Int1-w

-952.269281

S	-1.232312	-0.209404	-0.681805
C	-2.187039	-0.693522	0.784676
H	-1.611315	-0.543726	1.696011
H	-3.100312	-0.098804	0.812218
H	-2.444631	-1.744641	0.667907
S	1.291094	-1.268760	0.047889
C	2.181734	0.065633	0.110629
H	0.119927	3.132079	0.974271
H	3.260769	-0.018481	0.237682
H	1.745734	1.064899	0.035464
O	0.215742	2.658301	0.143547
H	-0.833221	1.022034	-0.264956
H	0.228438	3.338192	-0.536148

Int2-w

-952.281175

S	-0.654736	-0.939649	-0.577152
S	1.715386	0.842708	0.360567
H	-0.041416	-0.944857	1.750475
H	-1.277765	0.260578	-0.266288
C	1.052977	-0.253102	-0.860489
H	1.702702	-1.124506	-0.985752
H	0.992691	0.243488	-1.833139
C	-0.544387	-1.646692	1.085754
H	-0.002929	-2.588398	1.010676
H	-1.564303	-1.834885	1.418917
O	-1.928986	1.797725	0.071343
H	-1.695441	2.378760	0.799587
H	-2.703585	2.177843	-0.351449

Int3-w

-952.253129

S	2.363162	0.369529	-0.380218
S	-1.265627	-1.036626	0.601431
H	-1.813990	0.174150	0.267716
H	0.450747	-0.820548	-1.064250
C	-0.508067	-1.383682	-0.975646
H	-1.149479	-1.074451	-1.800116
H	-0.284063	-2.447381	-1.033540
C	1.619558	0.465289	1.014008
H	0.603971	-0.000401	1.149542
H	2.029523	0.962697	1.893965
O	-2.331008	1.853748	-0.296236
H	-2.664246	2.508426	0.322305
H	-2.753903	2.051425	-1.135314

Int4-w

-952.286018

S	-0.391680	-0.208732	0.326315

Int5a-w

-952.253712

S	-0.809286	-0.913095	-0.514702

S	2.204456	-0.246211	-0.521769	S	1.767207	0.674564	0.273612
H	2.289838	-1.572833	-0.301330	H	1.952695	-0.121047	1.342138
C	1.254116	0.156714	0.971411	H	-1.237403	0.408225	-0.345752
H	1.388911	1.206057	1.225053	C	1.027371	-0.560585	-0.782131
H	1.496023	-0.483773	1.815640	H	1.508719	-1.535271	-0.720977
C	-0.886013	1.391484	-0.341135	H	1.063208	-0.211986	-1.814877
H	-0.162099	1.730027	-1.083508	C	-0.938490	-1.448276	1.129901
H	-1.859647	1.224765	-0.798286	H	-0.692757	-2.480456	1.339614
H	-0.962858	2.108763	0.477885	H	-1.378122	-0.788225	1.864515
O	-3.235795	-0.570522	-0.198768	O	-1.687552	1.948481	0.002475
H	-3.964788	-0.415372	0.405935	H	-1.084947	2.609343	0.353734
H	-3.552040	-1.243558	-0.805644	H	-2.491003	2.401233	-0.267365

Int5b-w

-952.251746

S	-1.820806	0.401925	0.360485
S	0.918932	-0.855797	-0.497575
H	1.262818	0.452031	-0.202816
H	-1.375879	1.615375	-0.014767
C	0.962930	-1.543951	1.092296
H	1.217018	-0.927355	1.941959
H	0.779257	-2.606245	1.174803
C	-0.916764	-0.518029	-0.866663
H	-0.880573	-0.040072	-1.845509
H	-1.352063	-1.511242	-0.968685
O	1.396542	2.167253	0.045938
H	1.942260	2.720379	-0.520541
H	1.387814	2.592938	0.907685

Int6-w

-952.252466

S	1.069092	-0.659602	-0.550041
C	2.581536	-0.326942	0.397218
H	2.451125	-0.564576	1.451475
H	3.313479	-1.014878	-0.032779
H	2.930315	0.693577	0.251165
S	-0.305000	0.573371	0.531818
C	-0.735606	1.890733	-0.493286
H	-2.851915	-1.847783	-0.509989
H	-0.039317	2.715173	-0.561835
H	-1.646996	1.841814	-1.074045
O	-2.803873	-1.065772	0.046480
H	-1.446382	-0.228159	0.359330
H	-3.580381	-1.072047	0.612805

R-2w

-1028.735046

S	0.853400	-0.818231	-0.326778
C	2.302470	-1.817250	0.114230
H	2.536230	-1.691179	1.171144
H	2.007295	-2.848635	-0.078877
H	3.152243	-1.550063	-0.513543
S	1.539950	1.013314	0.116923
C	0.153752	2.054805	-0.404775
H	-0.752650	1.692273	0.089176
H	0.417012	3.058341	-0.069753
H	0.067645	2.031321	-1.491054
O	-1.793713	0.133311	1.019175
H	-4.747769	0.005747	-0.651496
H	-2.049490	0.138653	1.942856

Inta

-1028.696372

S	1.039162	-0.582771	-0.463409
C	2.814740	-0.719628	-0.102107
H	2.989043	-0.873284	0.961313
H	3.147608	-1.599709	-0.654206
H	3.340437	0.160233	-0.467739
S	0.517752	1.083646	0.706263
C	-0.513905	1.912361	-0.373375
H	-1.953872	0.927628	-0.364627
H	-0.919854	2.828493	0.049135
H	-0.270025	1.900952	-1.433107
O	-2.733328	0.249695	-0.296879
H	-0.854888	-2.027129	0.329178
H	-3.244743	0.219858	-1.115284

O	-4.038523	-0.602700	-0.435767	O	-1.818807	-1.941254	0.368335
H	-4.413900	-1.482970	-0.496822	H	-2.153330	-2.474878	1.094312
H	-2.589660	-0.145034	0.532056	H	-2.378939	-0.700083	-0.003401

Intb

-1028.695420

S	-1.079138	-0.423348	0.591725
C	-2.652305	-0.809473	-0.231648
H	-2.502767	-1.026536	-1.287917
H	-3.037812	-1.694882	0.274891
H	-3.348067	0.016317	-0.093730
S	-0.476681	1.240978	-0.572653
C	0.683454	1.930345	0.477869
H	2.312965	0.691159	0.238690
H	1.160431	2.813979	0.064657
H	0.541012	1.870306	1.552770
O	2.845605	-0.117153	0.063970
H	0.466237	-1.683402	-0.044465
H	3.564290	0.101104	-0.537760
O	1.382916	-1.997846	-0.307524
H	1.611381	-2.809979	0.160542
H	2.110371	-1.165379	-0.161717

Int1-2w

-1028.706511

S	-0.845596	1.322834	-0.460472
C	-0.600240	2.061521	1.176580
H	0.009373	1.411014	1.801763
H	-0.095501	3.018632	1.042606
H	-1.577510	2.222162	1.627167
S	-1.174636	-1.349355	0.360955
C	-2.503505	-1.638919	-0.491768
H	3.790132	-2.063130	0.008788
H	-2.962879	-2.625810	-0.466547
H	-2.978161	-0.878248	-1.109723
O	3.471978	-1.260342	0.427015
H	0.487110	1.046725	-0.731985
H	4.067920	-1.086115	1.158618
O	2.132545	0.717122	-0.909974
H	2.716549	1.164322	-1.524544
H	2.652967	0.024928	-0.459070

TS1

-875.788305

1399.1971i

S	-0.747369	-0.228264	-0.653846
C	-1.886073	0.330266	0.638923
H	-1.425965	1.104528	1.251187
H	-2.775096	0.705085	0.129283
H	-2.141494	-0.539218	1.245557
S	1.085079	-0.629030	0.336262
C	1.447225	1.061818	-0.075281
H	0.122900	1.010893	-0.890349
H	1.103214	1.827768	0.617840
H	2.346179	1.255141	-0.654021

TS2

-875.809474

1323.7334i

S	0.847495	0.524315	-0.441892
S	-1.585540	-0.461536	-0.107563
H	-0.301126	-0.236754	-1.182715
C	-0.560631	0.806603	0.691453
H	-0.298427	0.596348	1.726762
H	-0.914525	1.826025	0.553012
C	1.789854	-0.811747	0.348220
H	1.117323	-1.535521	0.805326
H	2.386947	-1.276532	-0.436155
H	2.443194	-0.347174	1.087012

TS3

-875.790020

1330.6418i

S	-1.277431	-0.432971	-0.127152
S	1.619973	0.248255	-0.134432
H	0.560558	1.242331	0.070703
H	-1.079918	-0.381850	-1.464879

TS4

-875.793178

389.8803i

S	-1.819690	-0.444754	-0.095449
S	1.825855	0.451673	-0.182349
H	2.201937	0.793544	1.065796
H	-0.668255	-0.957279	0.502448

C	0.430584	-1.006003	0.363474
H	0.352727	-1.146321	1.442406
H	0.614546	-1.966314	-0.118971
C	-1.000822	1.286271	0.224067
H	-1.169791	1.541913	1.266279
H	-1.337356	1.984096	-0.535446

TS5

-875.771032

1591.4301i

S	-0.788043	0.709922	-0.144028
C	-2.142090	-0.444496	0.234208
H	-2.048853	-0.853692	1.238305
H	-3.031126	0.188540	0.185493
H	-2.225187	-1.222476	-0.523182
S	0.810903	-0.632704	-0.189320
C	2.200569	0.416177	0.223347
H	1.408987	-0.614027	1.134266
H	3.170220	0.029317	-0.063142
H	2.009335	1.406775	0.616487

TS2-w

-952.245758

1404.1209i

S	-0.052790	0.902689	-0.645870
S	-0.969163	-1.360562	0.290390
H	0.369148	-0.609252	-0.390834
C	-1.681311	0.250927	-0.155244
H	-2.105305	0.810049	0.676359
H	-2.340554	0.232511	-1.019827
C	0.585867	1.645254	0.874616
H	0.292689	1.042901	1.733635
H	1.669798	1.659038	0.767335
H	0.189351	2.658411	0.942137
O	2.389067	-0.917832	-0.134661
H	2.968400	-1.117514	-0.874625
H	2.767843	-1.384606	0.614563

TS4-w

-952.227299

341.2419i

C	1.289952	-1.125466	0.152577
H	1.495480	-1.587412	1.111435
H	1.136060	-1.762142	-0.711131
C	-1.516765	1.135083	0.171321
H	-0.783470	1.478208	0.890942
H	-2.119509	1.866665	-0.358112

TS1-w

-952.242238

71.5840i

S	0.884457	0.088938	0.693345
C	2.253872	0.089702	-0.507682
H	1.923224	0.436259	-1.485146
H	2.999649	0.770925	-0.095952
H	2.681263	-0.909608	-0.568941
S	-0.464856	-1.224283	-0.305653
C	-1.965663	-0.565202	0.184597
H	-1.714602	1.337810	-0.355179
H	-2.808897	-1.030239	-0.317432
H	-2.107869	-0.269205	1.222781
O	-0.996309	2.037444	-0.357738
H	-0.172657	1.539484	0.094172
H	-1.272497	2.843536	0.103042

TS3-w

-952.234226

1343.6265i

S	0.413280	1.169261	-0.434575
S	-1.364708	-1.112882	0.246532
H	-0.906901	-0.114456	1.225365
H	1.369964	0.153044	-0.284863
C	-0.969549	0.093288	-1.040315
H	-1.790746	0.774444	-1.261959
H	-0.635699	-0.388203	-1.959293
C	-0.109575	1.218501	1.261596
H	-0.865119	1.967968	1.477331
H	0.674750	1.058163	1.993742
O	2.325862	-1.125793	0.046781
H	1.973870	-2.003027	0.222061
H	3.270587	-1.214380	-0.105632

TS5-w

-952.233196

327.7980i

S	-2.132366	0.022678	0.169424
S	1.265500	-1.095156	-0.602837
H	1.868348	0.031085	-0.153448
H	-1.093937	-0.539828	0.935789
C	0.523721	-1.541166	0.851789
H	0.852649	-1.107771	1.789824
H	0.050325	-2.516195	0.867963
C	-1.198159	1.067384	-0.671775
H	-0.220720	1.397274	-0.322685
H	-1.625329	1.517648	-1.562535
O	1.741725	2.031036	0.399085
H	2.244876	2.610947	-0.179416
H	1.906482	2.360891	1.286353

S	-1.103588	-0.842763	0.110483
C	-2.596833	0.189482	0.218070
H	-2.882829	0.556206	-0.766103
H	-3.371003	-0.484529	0.589620
H	-2.463299	1.007150	0.924325
S	0.259194	0.501764	-0.721662
C	0.935452	1.330558	0.645397
H	2.551842	-0.052347	0.805615
H	1.536392	2.203240	0.402223
H	0.427296	1.279715	1.602493
O	2.830172	-0.732148	0.130965
H	2.066553	-0.703588	-0.523859
H	2.972256	-1.612920	0.516024

TSa

-1028.694986

220.9657i

S	-1.062319	-0.438812	0.592678
C	-2.695066	-0.773662	-0.131436
H	-2.616497	-0.999892	-1.193420
H	-3.077329	-1.644808	0.401710
H	-3.353229	0.075475	0.043414
S	-0.463422	1.190730	-0.617789
C	0.661999	1.940252	0.427216
H	2.230545	0.728399	0.242631
H	1.144683	2.805382	-0.018038
H	0.483843	1.935475	1.498595
O	2.803911	-0.058109	0.063688
H	0.507124	-1.740076	-0.103666
H	3.569181	-0.052654	0.646567
O	1.431726	-1.964487	-0.392362
H	1.678094	-2.855456	-0.122142
H	2.158746	-1.101314	-0.139162

TSb

-1028.698808

189.8139i

S	-0.801193	1.092426	-0.486534
C	-0.632817	1.990325	1.081672
H	0.021132	1.449179	1.763167
H	-0.208936	2.967898	0.851907
H	-1.625503	2.109900	1.511292
S	-1.211047	-1.106288	0.358401
C	-2.578070	-1.594206	-0.392556
H	3.779091	-2.052515	0.139793
H	-2.626885	-2.613913	-0.762751
H	-3.437193	-0.945021	-0.532000
O	3.565107	-1.171815	0.455627
H	0.581562	0.854930	-0.725813
H	4.237827	-0.942904	1.099953
O	2.116521	0.670903	-0.879652
H	2.620969	1.026369	-1.613859
H	2.666068	-0.001554	-0.424054

$CH_2{=}S^{\bullet+}$

-437.118516

S	-0.576670	-0.000005	-0.000020
C	1.012338	-0.000006	0.000048
H	1.576439	-0.939759	0.000017
H	1.576246	0.939870	0.000017

CH_3SH

-438.684029

S	0.662401	-0.086850	-0.000037
C	-1.154822	0.019684	0.000050
H	-1.523837	0.521422	-0.893954
H	-1.522753	-1.006432	-0.000120
H	0.900874	1.235395	0.000119
H	-1.523775	0.521112	0.894253

$CH_3SH^{\bullet+}$

$CH_2{=}S$

-438.340265

S	0.645075	-0.090473	-0.000001
C	-1.132607	0.011604	-0.000008
H	-1.454783	0.569511	-0.888441
H	-1.532422	-1.000403	-0.000185
H	0.916397	1.239712	0.000007
H	-1.454746	0.569133	0.888688

-437.460128

S	-0.583927	-0.000032	0.000002
C	1.023745	-0.000028	-0.000022
H	1.600838	-0.924698	0.000048
H	1.599527	0.925376	0.000048

$CH_2=SH^+$

-437.751678

S	0.548185	-0.091265	0.000002
C	-1.065295	0.025712	-0.000007
H	-1.636192	-0.900495	0.000002
H	-1.593392	0.975909	0.000026
H	0.850393	1.230555	-0.000016

$CH_3S•$

-438.049569

S	-0.691427	0.000000	-0.001896
C	1.104640	0.000001	-0.008760
H	1.422078	-0.000050	1.040691
H	1.506453	-0.898397	-0.478934
H	1.506459	0.898438	-0.478855

$HSCH_2•$

-438.035133

C	-1.139476	0.021757	-0.013668
H	-1.643625	0.973205	0.055894
H	-1.687096	-0.908348	0.003097
S	0.582286	-0.088882	0.003707
H	0.851006	1.226712	-0.036298

$[CH_2=SH…H_2O]^+$

-514.197674

S	0.811913	-0.604350	-0.000071
C	1.215036	0.960489	0.000081
H	-2.702236	0.107461	-0.770933
H	2.267802	1.230840	0.000661
H	0.463271	1.745648	-0.000366
O	-2.128194	0.142324	-0.000063
H	-0.584473	-0.421020	-0.000843
H	-2.699642	0.105144	0.772629

$[CH_3SH…H_2O]^{•+}$

-514.788127

S	0.687935	-0.710030	-0.000001
C	1.372624	0.937649	-0.000027
H	1.003781	1.468750	-0.884692
H	1.005022	1.468131	0.885554
H	2.458012	0.873320	-0.000722
H	-2.759934	0.241636	0.773217
O	-2.188483	0.222930	-0.000013
H	-0.681614	-0.342247	0.000029
H	-2.760117	0.241564	-0.773108

$[CH_3SH…H_2O]$

-515.107091

S	-0.865052	-0.721354	-0.000006
C	-1.391105	1.022504	-0.000003
H	-1.039187	1.539121	0.892420
H	-1.038372	1.539352	-0.891970
H	-2.481138	1.024278	-0.000509
H	3.062919	0.017271	-0.763397
O	2.519988	0.218409	-0.000005
H	0.460162	-0.478151	0.000353
H	3.063181	0.017493	0.763258

H_2O

-76.428204

O	0.000000	0.000000	0.116318
H	0.000000	0.760737	-0.465272
H	0.000000	-0.760737	-0.465272