Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting information for

DFT Investigations of Phenyldithiafulvene Dimers at Different Oxidation States

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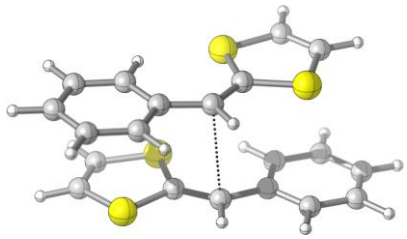
1. Optimized geometries and energies of Ph-DTF dimers in the gas phase

π-1



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#p m062x/def2svp opt freq empiricaldispersion=gd3
nosymm geom=connectivity
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Charge = 1, Multiplicity = 2, Point group = C1
Electronic Energy = -2362.797651 Hartree
$\hat{S}^2$ = 0.7603

Number of imaginary frequencies = 0

Sum of electronic and zero-point Energies = -2362.495494 Hartree

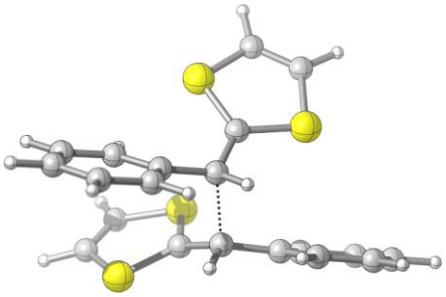
Sum of electronic and thermal Energies = -2362.473716 Hartree

Sum of electronic and thermal Enthalpies = -2362.472772 Hartree

Sum of electronic and thermal Free Energies = -2362.547946 Hartree

	Cartesian Coordinates				Cartesian Coordinates		
Atoms	***X***	***Y***	***Z***	**Atoms**	***X***	***Y***	***Z***
C	-2.352929	1.322251	-0.466517	C	-3.729748	1.190477	-0.607338
C	-4.556058	1.099252	0.515668	C	-3.993146	1.141455	1.791749
C	-2.617630	1.270960	1.938284	C	-1.764797	1.368040	0.815231
C	0.716242	1.684832	0.231179	C	3.117283	2.142303	-0.620094
C	2.370096	2.019453	-1.731687	S	2.311518	1.944779	0.894217
S	0.686846	1.663910	-1.512642	C	-0.348366	1.512659	1.081970
H	-1.752562	1.408006	-1.370482	H	-4.166248	1.171851	-1.607038
H	-5.636478	1.009653	0.394923	H	-4.629038	1.080130	2.675554
H	-2.182784	1.311122	2.939334	H	4.185093	2.361055	-0.608487
H	2.740729	2.124080	-2.751162	H	-0.089206	1.556392	2.144420
C	2.617670	-1.272815	1.937189	C	3.993182	-1.143159	1.790741
C	4.556067	-1.099781	0.514688	C	3.729733	-1.189967	-0.608385
C	2.352918	-1.321862	-0.467653	C	1.764815	-1.368852	0.814063
C	-0.716222	-1.685121	0.229741	C	-2.370134	-2.017714	-1.733421
C	-3.117307	-2.141610	-0.621933	S	-0.686839	-1.662583	-1.514060
S	-2.311492	-1.945661	0.892554	C	0.348389	-1.513724	1.080683
H	2.182850	-1.313907	2.938212	H	4.629092	-1.082642	2.674588
H	5.636484	-1.010067	0.394005	H	4.166208	-1.170404	-1.608077
H	1.752521	-1.406723	-1.371684	H	-2.740799	-2.121299	-2.752991
H	-4.185134	-2.360285	-0.610519	H	0.089232	-1.558437	2.143093

TS-1



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empiricaldispersion=gd3 nosymm geom=connectivity
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Charge = 1, Multiplicity = 2, Point group = C1
Electronic Energy = -2362.777498 Hartree
$\hat{S}^2$ = 0.7657

Number of imaginary frequencies = 1, vi = -318.02

Sum of electronic and zero-point Energies = -2362.474707 Hartree

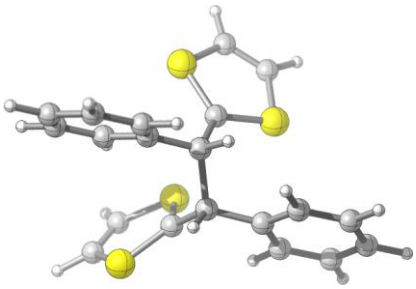
Sum of electronic and thermal Energies = -2362.453870 Hartree

Sum of electronic and thermal Enthalpies = -2362.452926 Hartree

Sum of electronic and thermal Free Energies = -2362.527298 Hartree

	Cartesian Coordinates				Cartesian Coordinates		
Atoms	***X***	***Y***	***Z***	**Atoms**	***X***	***Y***	***Z***
C	-2.557132	0.701540	0.075296	C	-3.929238	0.742570	0.314050
C	-4.411998	0.860510	1.616235	C	-3.515114	0.929294	2.682249
C	-2.144040	0.893848	2.443792	C	-1.644403	0.794837	1.137218
C	0.468283	1.520659	-0.068763	C	2.231341	2.827449	-1.414187
C	1.057881	3.103153	-2.010785	S	2.183120	1.766331	-0.048077
S	-0.357568	2.379837	-1.327343	C	-0.169617	0.741414	0.946414
H	-2.206190	0.565165	-0.950529	H	-4.624772	0.676303	-0.523698
H	-5.486139	0.895126	1.801332	H	-3.884309	1.017108	3.704575
H	-1.447870	0.958517	3.283485	H	3.199439	3.217995	-1.727623
H	0.933182	3.752415	-2.877371	H	0.369586	0.822579	1.895009
C	2.362419	-0.815746	2.125047	C	3.742607	-0.757256	2.279786
C	4.578740	-1.083295	1.210185	C	4.020519	-1.492510	0.001951
C	2.635252	-1.547519	-0.154538	C	1.785622	-1.187122	0.898521
C	-0.431626	-1.668651	-0.308727	C	-1.548337	-1.916822	-2.609368
C	-2.409209	-2.468853	-1.734672	S	-0.063281	-1.294607	-1.955003
S	-1.925545	-2.491140	-0.074317	C	0.295538	-1.157962	0.802860
H	1.719293	-0.577411	2.976729	H	4.168521	-0.466351	3.240664
H	5.662007	-1.039369	1.327876	H	4.665264	-1.780432	-0.829217
H	2.236755	-1.899526	-1.105566	H	-1.698236	-1.863701	-3.687570
H	-3.363694	-2.922199	-2.002450	H	-0.175546	-1.451003	1.749266

σ-1



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#p m062x/def2svp opt freq empiricaldispersion=gd3
nosymm geom=connectivity
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Charge = 1, Multiplicity = 2, Point group = C1
Electronic Energy = -2362.784206 Hartree
$\hat{S}^2$ = 0.7592

Number of imaginary frequencies = 0

Sum of electronic and zero-point Energies = -2362.479856 Hartree

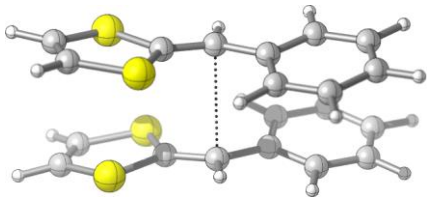
Sum of electronic and thermal Energies = -2362.458918 Hartree

Sum of electronic and thermal Enthalpies = -2362.457974 Hartree

Sum of electronic and thermal Free Energies = -2362.531983 Hartree

	Cartesian Coordinates				Cartesian Coordinates		
Atoms	***X***	***Y***	***Z***	**Atoms**	***X***	***Y***	***Z***
C	-2.645853	0.241222	0.123014	C	-4.012659	0.215148	0.391805
C	-4.484875	0.536587	1.663919	C	-3.584074	0.888553	2.667009
C	-2.217000	0.917875	2.396956	C	-1.731431	0.596040	1.125218
C	0.218296	1.476523	-0.223689	C	1.625543	2.928338	-1.793285
C	0.352721	3.319321	-1.992792	S	1.884120	1.698696	-0.600936
S	-0.856429	2.547767	-1.028957	C	-0.232032	0.600480	0.896721
H	-2.298544	-0.009191	-0.881951	H	-4.712923	-0.058135	-0.398492
H	-5.555184	0.515162	1.871900	H	-3.944601	1.144792	3.663740
H	-1.517590	1.197272	3.188713	H	2.494588	3.330555	-2.314264
H	0.036669	4.086683	-2.699707	H	0.231364	1.012682	1.805642
C	2.431659	-0.243900	2.141722	C	3.810016	-0.174864	2.321160
C	4.666345	-0.752858	1.382984	C	4.131240	-1.421181	0.285084
C	2.748791	-1.492387	0.107821	C	1.883310	-0.882240	1.020151
C	-0.154353	-1.625580	-0.323571	C	-1.075585	-2.077500	-2.666807
C	-1.704793	-2.950648	-1.855870	S	0.093116	-1.027175	-1.918791
S	-1.267777	-2.919265	-0.184914	C	0.363608	-0.895744	0.853354
H	1.779645	0.195950	2.900711	H	4.216923	0.324341	3.201294
H	5.746873	-0.697257	1.519419	H	4.791151	-1.898937	-0.440035
H	2.354335	-2.034942	-0.751357	H	-1.226725	-2.004022	-3.743433
H	-2.439829	-3.684940	-2.186053	H	-0.068201	-1.367448	1.750528

π-2



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nosymm geom=connectivity
```

Charge = 1, Multiplicity = 2, Point group = C1
Electronic Energy = -2362.790900 Hartree
$\hat{S}^2$ = 0.7585

Number of imaginary frequencies = 0

Sum of electronic and zero-point Energies = -2362.489215 Hartree

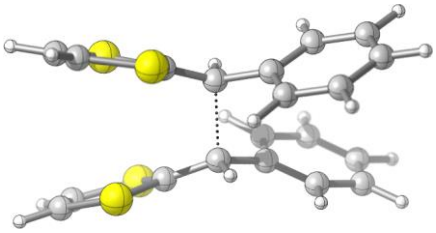
Sum of electronic and thermal Energies = -2362.467167 Hartree

Sum of electronic and thermal Enthalpies = -2362.466222 Hartree

Sum of electronic and thermal Free Energies = -2362.543474 Hartree

	Cartesian Coordinates				Cartesian Coordinates		
Atoms	***X***	***Y***	***Z***	**Atoms**	***X***	***Y***	***Z***
C	1.685247	2.282145	0.667015	C	2.958912	2.656368	1.078761
C	4.081866	2.288919	0.332006	C	3.926073	1.529978	-0.828143
C	2.656253	1.145614	-1.239198	C	1.509712	1.525114	-0.509986
C	-1.050659	1.451504	-0.725237	C	-3.629866	1.673956	-0.854332
C	-3.249893	2.531562	0.106987	S	-2.380716	0.738777	-1.610196
S	-1.555237	2.602805	0.483877	C	0.233313	1.072463	-1.026303
H	0.835903	2.573084	1.285061	H	3.078954	3.242346	1.990702
H	5.076842	2.593841	0.658687	H	4.797944	1.233655	-1.412390
H	2.536942	0.545651	-2.143852	H	-4.655354	1.536327	-1.197178
H	-3.921174	3.186903	0.662130	H	0.311127	0.347858	-1.844257
C	2.656368	-1.145466	1.239268	C	3.926174	-1.529840	0.828177
C	4.081937	-2.288713	-0.332022	C	2.958970	-2.656075	-1.078803
C	1.685320	-2.281844	-0.667022	C	1.509821	-1.524898	0.510034
C	-1.050507	-1.451511	0.725290	C	-3.249545	-2.531856	-0.107030
C	-3.629676	-1.674297	0.854273	S	-1.554865	-2.602893	-0.483835
S	-2.380688	-0.738954	1.610196	C	0.233410	-1.072310	1.026364
H	2.537076	-0.545554	2.143959	H	4.798058	-1.233580	1.412436
H	5.076903	-2.593641	-0.658727	H	3.078992	-3.241980	-1.990794
H	0.835946	-2.572656	-1.285095	H	-3.920717	-3.187282	-0.662205
H	-4.655200	-1.536800	1.197068	H	0.311166	-0.347667	1.844290

TS-2



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#p m062x/def2svp opt=(calcfc,ts,noeigen) freq
empiricaldispersion=gd3 nosymm geom=connectivity
```

Charge = 1, Multiplicity = 2, Point group = C1
Electronic Energy = -2362.779979 Hartree
$\hat{S}^2$ = 0.7644

Number of imaginary frequencies = 1, vi = -305.01

Sum of electronic and zero-point Energies = -2362.477407 Hartree

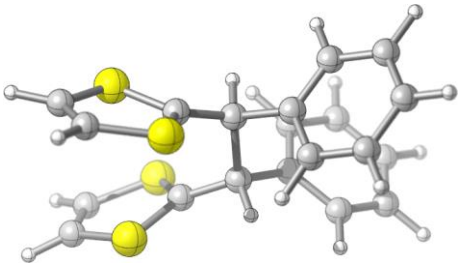
Sum of electronic and thermal Energies = -2362.456443 Hartree

Sum of electronic and thermal Enthalpies = -2362.455499 Hartree

Sum of electronic and thermal Free Energies = -2362.529969 Hartree

	Cartesian Coordinates				Cartesian Coordinates		
Atoms	***X***	***Y***	***Z***	**Atoms**	***X***	***Y***	***Z***
C	1.616553	2.195782	0.926085	C	2.818516	2.819580	1.253501
C	3.915087	2.721521	0.397414	C	3.807462	1.991655	-0.785757
C	2.606926	1.367929	-1.114934	C	1.494658	1.474631	-0.270505
C	-1.018915	1.383945	-0.649618	C	-3.534729	1.767144	-1.009645
C	-3.141247	2.732863	-0.159586	S	-2.301650	0.687182	-1.574812
S	-1.461644	2.776409	0.269587	C	0.250977	0.744505	-0.643021
H	0.784209	2.258256	1.631492	H	2.900522	3.378320	2.186486
H	4.855672	3.208551	0.656923	H	4.663725	1.902670	-1.455100
H	2.531324	0.784294	-2.035028	H	-4.549521	1.642819	-1.387334
H	-3.794011	3.502259	0.253391	H	0.387633	0.112484	-1.527761
C	2.606915	-1.367953	1.114943	C	3.807447	-1.991687	0.785768
C	3.915069	-2.721555	-0.397402	C	2.818498	-2.819606	-1.253490
C	1.616539	-2.195800	-0.926077	C	1.494648	-1.474648	0.270513
C	-1.018925	-1.383945	0.649623	C	-3.141265	-2.732848	0.159588
C	-3.534743	-1.767127	1.009646	S	-1.461662	-2.776406	-0.269582
S	-2.301657	-0.687173	1.574815	C	0.250971	-0.744514	0.643027
H	2.531316	-0.784318	2.035038	H	4.663710	-1.902708	1.455113
H	4.855651	-3.208591	-0.656910	H	2.900502	-3.378347	-2.186475
H	0.784196	-2.258268	-1.631485	H	-3.794035	-3.502239	-0.253390
H	-4.549534	-1.642795	1.387334	H	0.387631	-0.112493	1.527768

σ-2



```
#p m062x/def2svp opt freq
empiricaldispersion=gd3 nosymm
geom=connectivity
```

Charge = 1, Multiplicity = 2, Point group = C1
Electronic Energy = -2362.783032 Hartree
$\hat{S}^2$ = 0.7575

Number of imaginary frequencies = 0

Sum of electronic and zero-point Energies = -2362.479173 Hartree

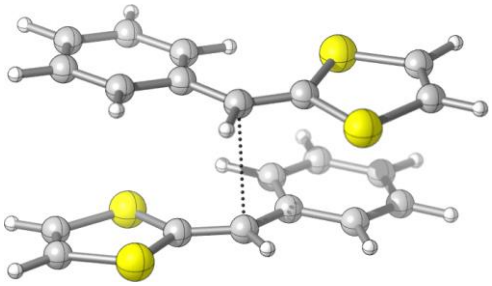
Sum of electronic and thermal Energies = -2362.457953 Hartree

Sum of electronic and thermal Enthalpies = -2362.457009 Hartree

Sum of electronic and thermal Free Energies = -2362.532945 Hartree

	Cartesian Coordinates				Cartesian Coordinates		
Atoms	***X***	***Y***	***Z***	**Atoms**	***X***	***Y***	***Z***
C	1.677782	2.052854	1.074426	C	2.812952	2.816607	1.340169
C	3.769655	3.016392	0.345900	C	3.587903	2.449150	-0.914206
C	2.450705	1.689436	-1.181948	C	1.483514	1.490893	-0.193444
C	-1.010079	1.390269	-0.516638	C	-3.489542	1.894917	-0.876209
C	-3.059462	2.799409	0.025863	S	-2.291930	0.808406	-1.501222
S	-1.381329	2.759113	0.449492	C	0.261620	0.654347	-0.508917
H	0.948883	1.896952	1.874702	H	2.952938	3.251216	2.330564
H	4.659876	3.610204	0.555798	H	4.336157	2.594927	-1.693991
H	2.316574	1.240971	-2.168692	H	-4.506640	1.834872	-1.263210
H	-3.683466	3.573560	0.473227	H	0.389689	0.201448	-1.502947
C	2.451415	-1.688333	1.181903	C	3.588957	-2.447536	0.914175
C	3.771033	-3.014605	-0.345964	C	2.814307	-2.815154	-1.340278
C	1.678790	-2.051914	-1.074547	C	1.484196	-1.490139	0.193356
C	-1.009449	-1.390656	0.516521	C	-3.058176	-2.800746	-0.025992
C	-3.488691	-1.896428	0.876045	S	-1.380053	-2.759691	-0.449586
S	-2.291591	-0.809350	1.501054	C	0.261914	-0.654153	0.508815
H	2.317028	-1.240002	2.168673	H	4.337226	-2.593049	1.693995
H	4.661523	-3.608016	-0.555851	H	2.954545	-3.249622	-2.330699
H	0.949876	-1.896262	-1.874857	H	-3.681815	-3.575196	-0.473349
H	-4.505825	-1.836839	1.263023	H	0.389762	-0.201196	1.502847

π-3



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#p m062x/def2svp opt freq
empiricaldispersion=gd3 nosymm
geom=connectivity
```

Charge = 1, Multiplicity = 2, Point group = C1
Electronic Energy = -2362.796197 Hartree
$\hat{S}^2$ = 0.7615

Number of imaginary frequencies = 0

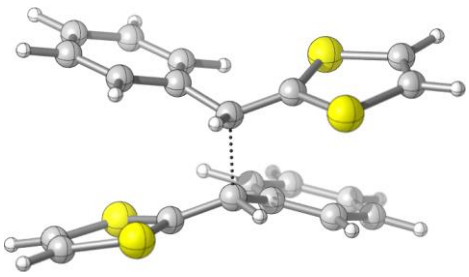
Sum of electronic and zero-point Energies = -2362.493912 Hartree

Sum of electronic and thermal Energies = -2362.472224 Hartree

Sum of electronic and thermal Enthalpies = -2362.471280 Hartree
Sum of electronic and thermal Free Energies = -2362.546170 Hartree

	Cartesian Coordinates				Cartesian Coordinates		
Atoms	***X***	***Y***	***Z***	**Atoms**	***X***	***Y***	***Z***
C	-0.713607	1.609592	-1.527056	C	-1.777302	1.853315	-2.392072
C	-3.042710	2.161065	-1.892655	C	-3.244688	2.220032	-0.511412
C	-2.187697	1.981477	0.356759	C	-0.895686	1.679251	-0.128621
C	1.497703	1.317895	0.727905	C	4.004338	1.037387	1.315464
C	3.966899	1.180034	-0.020734	S	2.485730	1.059270	2.144578
S	2.406892	1.371280	-0.751649	C	0.132814	1.435477	0.863170
H	0.253155	1.359343	-1.961065	H	-1.612851	1.805787	-3.469250
H	-3.867169	2.362944	-2.577643	H	-4.228647	2.468959	-0.111456
H	-2.345500	2.049912	1.435296	H	4.912212	0.914933	1.905954
H	4.839170	1.188124	-0.674269	H	-0.227857	1.422630	1.896796
C	2.187705	-1.981878	0.355080	C	3.244646	-2.219826	-0.513319
C	3.042613	-2.159772	-1.894509	C	1.777211	-1.851537	-2.393640
C	0.713569	-1.608402	-1.528392	C	0.895700	-1.679185	-0.130022
C	-1.497663	-1.318479	0.726718	C	-3.966771	-1.179856	-0.022019
C	-4.004320	-1.038339	1.314300	S	-2.406714	-1.370563	-0.752963
S	-2.485787	-1.061000	2.143528	C	-0.132783	-1.436172	0.861961
H	2.345541	-2.051172	1.433557	H	4.228604	-2.469136	-0.113597
H	3.867030	-2.361182	-2.579686	H	1.612723	-1.803156	-3.470775
H	-0.253199	-1.357725	-1.962154	H	-4.838989	-1.187355	-0.675632
H	-4.912242	-0.916341	1.904810	H	0.227859	-1.424184	1.895608

TS-3



```
#p m062x/def2svp opt=(calcfc,ts,noeigen) freq
empiricaldispersion=gd3 nosymm
geom=connectivity
```

Charge = 1, Multiplicity = 2, Point group = C1
Electronic Energy = -2362.782721 Hartree
$\hat{S}^2$ = 0.7635

Number of imaginary frequencies = 1, vi = -208.91

Sum of electronic and zero-point Energies = -2362.479380 Hartree

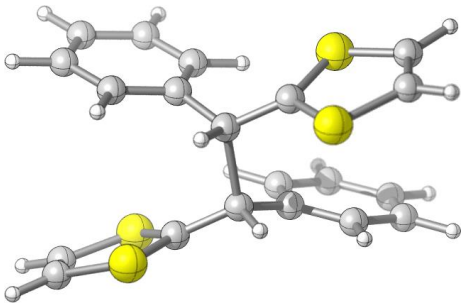
Sum of electronic and thermal Energies = -2362.458649 Hartree

Sum of electronic and thermal Enthalpies = -2362.457704 Hartree

Sum of electronic and thermal Free Energies = -2362.531032 Hartree

	Cartesian Coordinates				Cartesian Coordinates		
Atoms	***X***	***Y***	***Z***	**Atoms**	***X***	***Y***	***Z***
C	-0.496349	1.545652	-1.638743	C	-1.433674	2.051876	-2.539677
C	-2.653323	2.549665	-2.086133	C	-2.930368	2.550356	-0.719252
C	-1.995248	2.047324	0.180654	C	-0.767206	1.532194	-0.263312
C	1.551228	1.120914	0.761387	C	4.005329	0.974951	1.524778
C	4.053137	1.194441	0.199099	S	2.425304	0.885057	2.230782
S	2.538808	1.344970	-0.628689	C	0.126808	0.917936	0.766273
H	0.434649	1.142769	-2.035940	H	-1.203936	2.056685	-3.605916
H	-3.380895	2.946766	-2.794856	H	-3.874195	2.953754	-0.350090
H	-2.217409	2.058513	1.250419	H	4.872811	0.876952	2.177086
H	4.967801	1.297730	-0.384743	H	-0.275345	1.117332	1.769444
C	1.995226	-2.047283	0.181192	C	2.930291	-2.550603	-0.718609
C	2.653167	-2.550341	-2.085475	C	1.433495	-2.052686	-2.539106
C	0.496226	-1.546173	-1.638277	C	0.767161	-1.532285	-0.262865
C	-1.551210	-1.120675	0.761841	C	-4.053153	-1.194392	0.199722
C	-4.005267	-0.974458	1.525325	S	-2.538871	-1.345196	-0.628103
S	-2.425201	-0.884329	2.231207	C	-0.126790	-0.917698	0.766576
H	2.217449	-2.058133	1.250948	H	3.874138	-2.953890	-0.349375
H	3.380695	-2.947671	-2.794114	H	1.203697	-2.057829	-3.605329
H	-0.434791	-1.143403	-2.035545	H	-4.967850	-1.297873	-0.384032
H	-4.872712	-0.876240	2.177650	H	0.275423	-1.116771	1.769787

σ-3



```
#p m062x/def2svp opt freq
empiricaldispersion=gd3 nosymm
geom=connectivity
```

Charge = 1, Multiplicity = 2, Point group = C1
Electronic Energy = -2362.782815 Hartree
$\hat{S}^2$ = 0.7607

Number of imaginary frequencies = 0

Sum of electronic and zero-point Energies = -2362.478772 Hartree

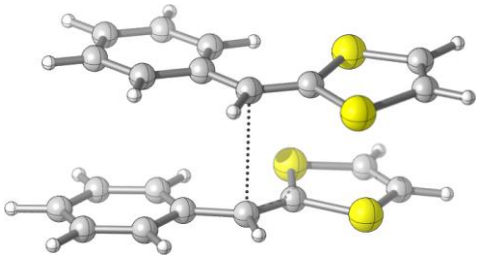
Sum of electronic and thermal Energies = -2362.457568 Hartree

Sum of electronic and thermal Enthalpies = -2362.456624 Hartree

Sum of electronic and thermal Free Energies = -2362.531229 Hartree

	Cartesian Coordinates				Cartesian Coordinates		
Atoms	***X***	***Y***	***Z***	**Atoms**	***X***	***Y***	***Z***
C	-0.449922	1.554891	-1.651291	C	-1.355718	2.111469	-2.555089
C	-2.559822	2.650433	-2.107388	C	-2.852320	2.641607	-0.744017
C	-1.947424	2.089242	0.158378	C	-0.736716	1.532535	-0.280026
C	1.564207	1.091016	0.769672	C	4.006649	0.936503	1.560926
C	4.070051	1.166714	0.237337	S	2.417786	0.842939	2.245861
S	2.565623	1.326222	-0.605566	C	0.127777	0.866753	0.754987
H	0.469412	1.121467	-2.043821	H	-1.113531	2.122802	-3.618516
H	-3.263168	3.086221	-2.817840	H	-3.783992	3.075799	-0.379023
H	-2.182061	2.092869	1.225642	H	4.866217	0.832748	2.222749
H	4.991697	1.274518	-0.334634	H	-0.274610	1.112450	1.749459
C	1.947121	-2.089734	0.155777	C	2.852144	-2.640909	-0.747217
C	2.560011	-2.647584	-2.110677	C	1.356148	-2.107666	-2.557872
C	0.450221	-1.552293	-1.653465	C	0.736628	-1.532134	-0.282081
C	-1.564397	-1.092103	0.768277	C	-4.070333	-1.167182	0.236210
C	-4.006748	-0.938852	1.560114	S	-2.566018	-1.325419	-0.607133
S	-2.417787	-0.846196	2.244940	C	-0.127960	-0.867779	0.753785
H	2.181468	-2.095055	1.223098	H	3.783629	-3.075851	-0.382640
H	3.263461	-3.082422	-2.821609	H	1.114259	-2.117288	-3.621383
H	-0.468876	-1.118028	-2.045601	H	-4.992058	-1.274228	-0.335777
H	-4.866222	-0.836094	2.222214	H	0.274435	-1.114838	1.747916

π-4



```
#p m062x/def2svp opt freq
empiricaldispersion=gd3 nosymm
geom=connectivity
```

Charge = 1, Multiplicity = 2, Point group = C1
Electronic Energy = -2362.795099 Hartree
$\hat{S}^2$ = 0.7604

Number of imaginary frequencies = 0

Sum of electronic and zero-point Energies = -2362.493020 Hartree

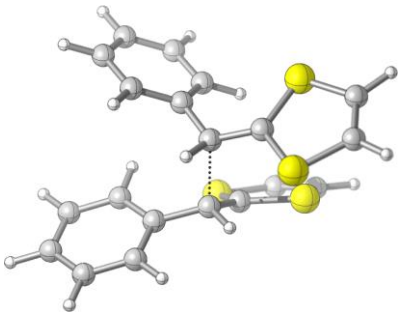
Sum of electronic and thermal Energies = -2362.471203 Hartree

Sum of electronic and thermal Enthalpies = -2362.470258 Hartree

Sum of electronic and thermal Free Energies = -2362.545622 Hartree

	Cartesian Coordinates				Cartesian Coordinates		
Atoms	***X***	***Y***	***Z***	**Atoms**	***X***	***Y***	***Z***
C	0.958527	1.572372	1.461403	C	2.096766	1.733048	2.245155
C	3.332451	1.998497	1.654102	C	3.431369	2.094666	0.263341
C	2.302537	1.928684	-0.523643	C	1.037724	1.673836	0.054563
C	-1.423570	1.434553	-0.628977	C	-3.839409	1.342347	0.296756
C	-3.979563	1.295966	-1.038420	S	-2.219276	1.412424	0.922288
S	-2.526282	1.304845	-1.980283	C	-0.073326	1.528464	-0.860067
C	2.532808	-1.128017	-2.031476	C	3.914897	-1.005736	-1.990037
C	4.582737	-1.082275	-0.766237	C	3.855633	-1.278965	0.410061
C	2.472300	-1.399912	0.374086	C	1.779302	-1.329151	-0.852815
C	-0.649347	-1.660562	-0.087868	C	-2.976500	-2.165601	0.939049
C	-2.145106	-2.057772	1.988765	S	-2.292824	-1.919264	-0.633716
S	-0.486745	-1.669972	1.649505	C	0.346195	-1.462275	-1.012933
H	0.014204	1.373858	1.964855	H	2.015569	1.661245	3.330358
H	4.217282	2.135735	2.277118	H	4.394100	2.301034	-0.205666
H	2.383076	2.007356	-1.609574	H	-4.662173	1.357097	1.011635
H	-4.933130	1.260803	-1.565392	H	0.206064	1.555165	-1.918223
H	2.014431	-1.082416	-2.991971	H	4.475840	-0.860842	-2.913912
H	5.669519	-0.996113	-0.729137	H	4.374105	-1.344087	1.367382
H	1.949828	-1.565152	1.314379	H	-4.036248	-2.412088	1.005739
H	-2.431378	-2.196817	3.031274	H	0.003415	-1.465966	-2.052816

TS-4



```
#p m062x/def2svp opt=(calcfc,ts,noeigen) freq
empiricaldispersion=gd3 nosymm geom=connectivity
```

Charge = 1, Multiplicity = 2, Point group = C1
Electronic Energy = -2362.780699 Hartree
$\hat{S}^2$ = 0.7661

Number of imaginary frequencies = 1, vi = -301.53

Sum of electronic and zero-point Energies = -2362.477803 Hartree

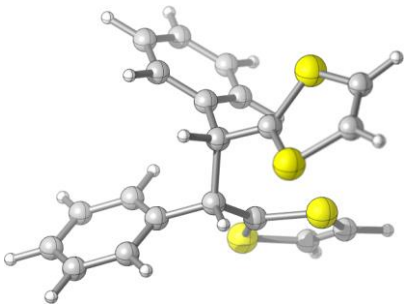
Sum of electronic and thermal Energies = -2362.456977 Hartree

Sum of electronic and thermal Enthalpies = -2362.456033 Hartree

Sum of electronic and thermal Free Energies = -2362.529950 Hartree

	Cartesian Coordinates				Cartesian Coordinates		
Atoms	***X***	***Y***	***Z***	**Atoms**	***X***	***Y***	***Z***
C	0.097373	-1.515681	-1.537483	C	0.792617	-2.215735	-2.521719
C	1.838304	-3.068514	-2.168427	C	2.189775	-3.217933	-0.826596
C	1.501111	-2.514324	0.157251	C	0.442087	-1.662169	-0.184580
C	-1.647174	-0.865361	0.995974	C	-4.185455	-0.977991	0.638714
C	-4.030978	-0.347392	1.816141	S	-2.748665	-1.505751	-0.176502
S	-2.402267	-0.138901	2.376424	C	-0.227697	-0.887958	0.889697
C	2.343497	1.266210	2.300592	C	3.696209	1.196445	2.619744
C	4.613499	0.742345	1.672012	C	4.168907	0.350866	0.410249
C	2.815095	0.419223	0.087159	C	1.886724	0.893843	1.027310
C	-0.083571	1.551399	-0.436478	C	-1.736891	2.454600	-2.188158
C	-0.545494	2.398600	-2.810611	S	-1.761288	1.953903	-0.527734
S	0.804063	1.829978	-1.886726	C	0.427049	0.980184	0.758808
H	-0.706012	-0.837030	-1.834257	H	0.516912	-2.093522	-3.569902
H	2.379289	-3.617469	-2.940072	H	3.007446	-3.882161	-0.544863
H	1.790723	-2.618664	1.205048	H	-5.147302	-1.200561	0.176303
H	-4.844563	0.012732	2.445671	H	0.264586	-0.995967	1.862364
H	1.630564	1.628996	3.044866	H	4.035367	1.500773	3.610444
H	5.674299	0.688537	1.919296	H	4.878874	-0.020446	-0.329630
H	2.490154	0.062419	-0.891879	H	-2.664293	2.806927	-2.639068
H	-0.368024	2.696913	-3.844073	H	-0.139150	1.317857	1.636325

σ-4



```
#p m062x/def2svp opt freq empiricaldispersion=gd3
nosymm geom=connectivity
```

Charge = 1, Multiplicity = 2, Point group = C1
Electronic Energy = -2362.785687 Hartree
$\hat{S}^2$ = 0.7580

Number of imaginary frequencies = 0

Sum of electronic and zero-point Energies = -2362.481184 Hartree

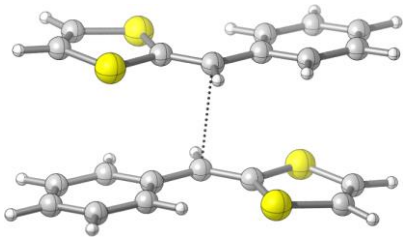
Sum of electronic and thermal Energies = -2362.460270 Hartree

Sum of electronic and thermal Enthalpies = -2362.459325 Hartree

Sum of electronic and thermal Free Energies = -2362.533249 Hartree

	Cartesian Coordinates				Cartesian Coordinates		
Atoms	***X***	***Y***	***Z***	**Atoms**	***X***	***Y***	***Z***
C	-0.180223	-1.868514	-1.025439	C	0.277649	-3.020510	-1.662537
C	1.037401	-3.955485	-0.959260	C	1.330025	-3.738847	0.386303
C	0.875077	-2.585254	1.022127	C	0.122050	-1.636145	0.324056
C	-1.767683	-0.150283	1.061431	C	-4.309909	-0.326221	0.902873
C	-4.085615	0.819566	1.570718	S	-2.929225	-1.283026	0.471643
S	-2.427023	1.197240	1.924784	C	-0.299792	-0.367688	1.030068
C	2.503340	1.749090	1.777061	C	3.855679	1.705658	2.109957
C	4.696637	0.785236	1.487120	C	4.179179	-0.090812	0.534045
C	2.825857	-0.052169	0.202260	C	1.974311	0.875340	0.820823
C	0.172796	1.280438	-0.897427	C	-1.153282	1.763031	-3.026598
C	0.120435	1.568424	-3.425403	S	-1.442043	1.652827	-1.320797
S	1.281532	1.240212	-2.193364	C	0.494271	0.955933	0.507481
H	-0.785462	-1.154433	-1.588785	H	0.036062	-3.190970	-2.712392
H	1.394693	-4.856381	-1.459393	H	1.917765	-4.468534	0.944247
H	1.122393	-2.410782	2.071546	H	-5.298284	-0.704763	0.641354
H	-4.859340	1.498778	1.927973	H	0.066461	-0.420155	2.068080
H	1.850706	2.476066	2.266382	H	4.252012	2.394899	2.856301
H	5.755778	0.749846	1.744696	H	4.831140	-0.816482	0.046463
H	2.440836	-0.758973	-0.535269	H	-1.989988	1.996975	-3.684607
H	0.466250	1.623262	-4.458022	H	0.070066	1.764049	1.129293

π-5



```
#p m062x/def2svp opt freq empiricaldispersion=gd3
nosymm geom=connectivity
```

Charge = 1, Multiplicity = 2, Point group = C1
Electronic Energy = -2362.792111 Hartree
S^2 = 0.7595

Number of imaginary frequencies = 1, vi = -3.42

Sum of electronic and zero-point Energies = -2362.490376 Hartree

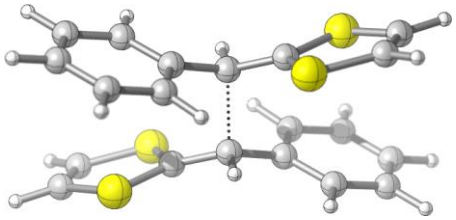
Sum of electronic and thermal Energies = -2362.469291 Hartree

Sum of electronic and thermal Enthalpies = -2362.468347 Hartree

Sum of electronic and thermal Free Energies = -2362.541970 Hartree

	Cartesian Coordinates				Cartesian Coordinates		
Atoms	***X***	***Y***	***Z***	**Atoms**	***X***	***Y***	***Z***
C	1.756965	-2.341956	-0.436925	C	3.079499	-2.683220	-0.701129
C	4.114689	-2.181506	0.090152	C	3.819817	-1.322356	1.150376
C	2.501272	-0.975179	1.416839	C	1.439144	-1.485855	0.638858
C	-1.135540	-1.503361	0.603493	C	-3.214206	-2.589619	-0.485866
C	-3.702996	-1.791028	0.478416	S	-1.489176	-2.620220	-0.686096
S	-2.555991	-0.888201	1.404781	C	0.103752	-1.068883	1.014244
C	-2.500893	0.974586	-1.417296	C	-3.819571	1.321494	-1.151150
C	-4.114835	2.180915	-0.091252	C	-3.079900	2.683181	0.700012
C	-1.757234	2.342175	0.436133	C	-1.439020	1.485779	-0.639300
C	1.135652	1.503645	-0.603197	C	3.703035	1.791584	-0.477301
C	3.213872	2.589908	0.487009	S	2.556406	0.888836	-1.404215
S	1.488774	2.620278	0.686727	C	-0.103467	1.069034	-1.014338
H	0.981264	-2.754033	-1.081199	H	3.304116	-3.352494	-1.532392
H	5.147303	-2.465178	-0.116880	H	4.621040	-0.929968	1.778213
H	2.273860	-0.312090	2.254976	H	-3.814094	-3.219818	-1.142310
H	-4.760416	-1.676050	0.716426	H	0.074669	-0.341178	1.832436
H	-2.273173	0.311302	-2.255195	H	-4.620591	0.928698	-1.778989
H	-5.147555	2.464389	0.115522	H	-3.304819	3.352703	1.530992
H	-0.981737	2.754750	1.080334	H	4.760540	1.676773	-0.715020
H	3.813493	3.220033	1.143768	H	-0.074048	0.341371	-1.832555

TS-5



```
#p m062x/def2svp opt=(calcfc,ts,noeigen) freq
empiricaldispersion=gd3 nosymm
geom=connectivity
```

Charge = 1, Multiplicity = 2, Point group = C1
Electronic Energy = -2362.781574 Hartree
$\hat{S}^2$ = 0.7607

Number of imaginary frequencies = 1, vi = -291.39

Sum of electronic and zero-point Energies = -2362.478911 Hartree

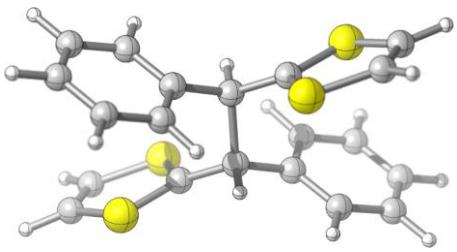
Sum of electronic and thermal Energies = -2362.457970 Hartree

Sum of electronic and thermal Enthalpies = -2362.457026 Hartree

Sum of electronic and thermal Free Energies = -2362.531973 Hartree

	Cartesian Coordinates				Cartesian Coordinates		
Atoms	***X***	***Y***	***Z***	**Atoms**	***X***	***Y***	***Z***
C	1.527041	-2.267230	-0.612446	C	2.781334	-2.862005	-0.740468
C	3.763140	-2.650124	0.225914	C	3.484189	-1.839044	1.325813
C	2.229455	-1.249353	1.458249	C	1.231062	-1.462263	0.497199
C	-1.319460	-1.350536	0.469635	C	-3.362407	-2.640147	-0.414835
C	-3.850857	-1.805428	0.519367	S	-1.651540	-2.584093	-0.692134
S	-2.709550	-0.782206	1.318856	C	-0.051196	-0.722939	0.655943
C	-2.229477	1.249291	-1.458338	C	-3.484208	1.838985	-1.325892
C	-3.763153	2.650055	-0.225985	C	-2.781344	2.861924	0.740396
C	-1.527053	2.267145	0.612365	C	-1.231081	1.462189	-0.497288
C	1.319438	1.350463	-0.469752	C	3.850829	1.805386	-0.519534
C	3.362379	2.640139	0.414638	S	2.709527	0.782112	-1.318963
S	1.651516	2.584074	0.691961	C	0.051175	0.722860	-0.656038
H	0.800759	-2.417449	-1.413070	H	2.993785	-3.487535	-1.608300
H	4.743112	-3.117366	0.122659	H	4.244751	-1.669089	2.089013
H	2.017487	-0.616541	2.323363	H	-3.952333	-3.351453	-0.992586
H	-4.899215	-1.736020	0.809327	H	-0.050152	-0.092541	1.554128
H	-2.017513	0.616487	-2.323459	H	-4.244773	1.669040	-2.089092
H	-4.743124	3.117298	-0.122722	H	-2.993791	3.487445	1.608236
H	-0.800768	2.417351	1.412989	H	4.899184	1.735978	-0.809503
H	3.952303	3.351476	0.992352	H	0.050122	0.092451	-1.554216

σ-5



```
#p m062x/def2svp opt freq
empiricaldispersion=gd3 nosymm
geom=connectivity
```

Charge = 1, Multiplicity = 2, Point group = C1
Electronic Energy = -2362.783675 Hartree
$\hat{S}^2$ = 0.7573

Number of imaginary frequencies = 1, vi = -12.81

Sum of electronic and zero-point Energies = -2362.479874 Hartree

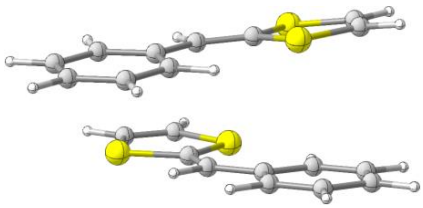
Sum of electronic and thermal Energies = -2362.459517 Hartree

Sum of electronic and thermal Enthalpies = -2362.458573 Hartree

Sum of electronic and thermal Free Energies = -2362.531928 Hartree

	Cartesian Coordinates				Cartesian Coordinates		
Atoms	***X***	***Y***	***Z***	**Atoms**	***X***	***Y***	***Z***
C	1.587249	-2.127014	-0.744009	C	2.805304	-2.796554	-0.845070
C	3.706060	-2.777613	0.219284	C	3.381299	-2.088439	1.386335
C	2.158442	-1.426385	1.490301	C	1.247503	-1.442881	0.430173
C	-1.283917	-1.373551	0.404929	C	-3.249941	-2.759611	-0.487236
C	-3.763807	-2.020874	0.513154	S	-1.560618	-2.555294	-0.814138
S	-2.672090	-0.955033	1.325644	C	-0.022539	-0.632598	0.549619
C	-2.155763	1.422378	-1.489140	C	-3.379003	2.083860	-1.385577
C	-3.705201	2.771537	-0.218058	C	-2.805639	2.789393	0.847342
C	-1.587300	2.120339	0.746729	C	-1.245959	1.437987	-0.428047
C	1.285026	1.372321	-0.403458	C	3.763152	2.026486	-0.511876
C	3.243273	2.776876	0.476679	S	2.678065	0.945607	-1.313241
S	1.553651	2.571228	0.800571	C	0.024958	0.628975	-0.546794
H	0.922724	-2.122300	-1.611608	H	3.055381	-3.327029	-1.764671
H	4.660075	-3.299727	0.138090	H	4.079804	-2.068850	2.223791
H	1.910259	-0.888852	2.408466	H	-3.806918	-3.480521	-1.085408
H	-4.801944	-2.050791	0.843699	H	-0.031984	-0.129495	1.528650
H	-1.906314	0.886218	-2.407760	H	-4.076619	2.065089	-2.223793
H	-4.659474	3.293242	-0.137258	H	-3.056934	3.318547	1.767375
H	-0.923550	2.114476	1.614949	H	4.802388	2.055247	-0.839056
H	3.795755	3.507542	1.067149	H	0.034915	0.124397	-1.525182

π-6



```
#p m062x/def2svp opt freq empiricaldispersion=gd3
nosymm geom=connectivity
```

Charge = 1, Multiplicity = 2, Point group = C1
Electronic Energy = -2362.793834 Hartree
$\hat{S}^2$ = 0.7592

Number of imaginary frequencies = 0

Sum of electronic and zero-point Energies = -2362.491647 Hartree

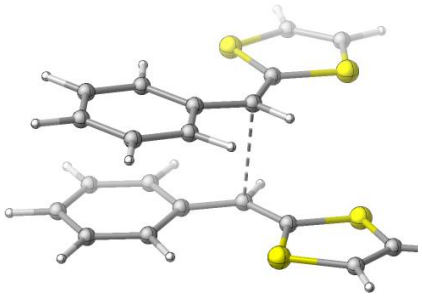
Sum of electronic and thermal Energies = -2362.469734 Hartree

Sum of electronic and thermal Enthalpies = -2362.468790 Hartree

Sum of electronic and thermal Free Energies = -2362.545319 Hartree

	Cartesian Coordinates				Cartesian Coordinates		
Atoms	***X***	***Y***	***Z***	**Atoms**	***X***	***Y***	***Z***
C	1.950873	-1.088366	1.346262	C	3.280175	-0.750410	1.573535
C	3.616951	0.486926	2.129741	C	2.608778	1.392043	2.462885
C	1.278027	1.062827	2.233789	C	0.916916	-0.183034	1.669949
C	-1.167248	-1.475790	0.910557	C	-1.982630	-3.658579	-0.219496
C	-3.100262	-2.956775	0.026739	S	-0.472810	-2.944288	0.267964
S	-2.915829	-1.415832	0.800649	C	-0.495195	-0.408849	1.451467
C	-2.779883	1.621909	-0.935164	C	-3.584075	2.627511	-0.411653
C	-3.002032	3.719572	0.231214	C	-1.610847	3.799996	0.341744
C	-0.801082	2.799839	-0.181935	C	-1.373218	1.684222	-0.831137
C	0.719178	0.361845	-1.522610	C	2.971342	-0.745598	-2.146009
C	3.293575	0.464482	-1.649591	S	1.293882	-1.152607	-2.177245
S	1.995728	1.472687	-1.113831	C	-0.631097	0.559232	-1.364937
H	1.734831	-2.073522	0.935955	H	4.064435	-1.468773	1.330216
H	4.662079	0.735566	2.318917	H	2.860447	2.353809	2.911300
H	0.488685	1.767890	2.504023	H	-1.952540	-4.644095	-0.683873
H	-4.108990	-3.294630	-0.211185	H	-1.139961	0.414108	1.776129
H	-3.236599	0.773539	-1.448232	H	-4.668072	2.562992	-0.510481
H	-3.628667	4.512402	0.641184	H	-1.153451	4.655765	0.839632
H	0.276852	2.897246	-0.062219	H	3.687405	-1.475170	-2.523936
H	4.308059	0.855381	-1.569197	H	-1.256566	-0.264710	-1.724732

π-7



```
#p m062x/def2svp opt freq empiricaldispersion=gd3
nosymm geom=connectivity
```

Charge = 2, Multiplicity = 1, Point group = C1

Electronic Energy = -2362.432691 Hartree

Number of imaginary frequencies = 0

Sum of electronic and zero-point Energies = -2362.129432 Hartree

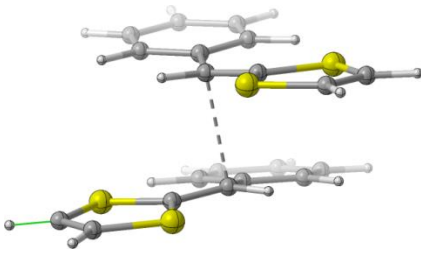
Sum of electronic and thermal Energies = -2362.108035 Hartree

Sum of electronic and thermal Enthalpies = -2362.107091 Hartree

Sum of electronic and thermal Free Energies = -2362.180648 Hartree

	Cartesian Coordinates				Cartesian Coordinates		
Atoms	***X***	***Y***	***Z***	**Atoms**	***X***	***Y***	***Z***
C	2.094126	0.192365	-1.288268	C	3.454208	0.062838	-1.510188
C	4.027159	0.537629	-2.698907	C	3.233684	1.151707	-3.673053
C	1.871017	1.287401	-3.460046	C	1.265401	0.808128	-2.262755
C	-1.021777	0.735979	-1.074908	C	-3.170146	0.691514	0.332075
C	-2.245947	0.034683	1.064758	S	-2.638740	1.321628	-1.181189
S	-0.662427	-0.093214	0.388311	C	-0.145471	0.977785	-2.154971
H	1.695075	-0.167678	-0.341938	H	4.085943	-0.393552	-0.747320
H	5.104133	0.449436	-2.853122	H	3.688462	1.545182	-4.582571
H	1.255922	1.811852	-4.194640	H	-4.201907	0.872756	0.639345
H	-2.419134	-0.395850	2.053185	H	-0.605212	1.540629	-2.973678
C	0.613729	-2.777113	-1.598812	C	1.816996	-3.401521	-1.310860
C	2.866914	-3.335540	-2.232177	C	2.708645	-2.645929	-3.443143
C	1.511392	-2.017811	-3.739733	C	0.430983	-2.066299	-2.819996
C	-1.382218	-0.781493	-4.127121	C	-1.913116	0.436410	-6.318562
C	-3.083681	0.397961	-5.647176	S	-0.552449	-0.303869	-5.555921
S	-3.061136	-0.394664	-4.117298	C	-0.837011	-1.442731	-3.005376
H	-0.225528	-2.869129	-0.905863	H	1.935366	-3.963222	-0.383839
H	3.808338	-3.845196	-2.019113	H	3.526393	-2.620247	-4.164250
H	1.423168	-1.515098	-4.701018	H	-1.771554	0.875852	-7.308102
H	-4.030487	0.800367	-6.012484	H	-1.571612	-1.651725	-2.221077

TS-6



```
#p m062x/def2svp opt=(calcfc,ts,noeigen) freq
empiricaldispersion=gd3 nosymm geom=connectivity
```

Charge = 2, Multiplicity = 1, Point group = C1

Electronic Energy = -2362.432488 Hartree

Number of imaginary frequencies = 1, vi = -75.41

Sum of electronic and zero-point Energies = -2362.129261 Hartree

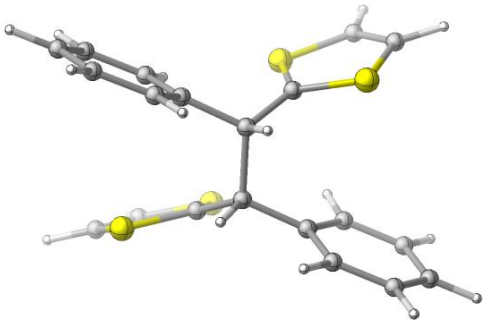
Sum of electronic and thermal Energies = -2362.108658 Hartree

Sum of electronic and thermal Enthalpies = -2362.107714 Hartree

Sum of electronic and thermal Free Energies = -2362.179393 Hartree

	Cartesian Coordinates				Cartesian Coordinates		
Atoms	***X***	***Y***	***Z***	**Atoms**	***X***	***Y***	***Z***
C	2.100532	0.180475	-1.331839	C	3.466379	0.129931	-1.563035
C	4.006988	0.677323	-2.733104	C	3.175591	1.285265	-3.677466
C	1.807489	1.342760	-3.452591	C	1.238793	0.789217	-2.275642
C	-1.018699	0.674379	-1.020601	C	-3.093970	0.687123	0.487633
C	-2.138087	0.045823	1.193308	S	-2.629653	1.266193	-1.066816
S	-0.594637	-0.114957	0.437341	C	-0.191348	0.857952	-2.164618
H	1.725136	-0.256759	-0.408369	H	4.122934	-0.328636	-0.822882
H	5.085309	0.647064	-2.897924	H	3.602216	1.735427	-4.574291
H	1.163117	1.863146	-4.164952	H	-4.108727	0.886024	0.838079
H	-2.261970	-0.354334	2.201767	H	-0.676933	1.446830	-2.948817
C	0.532041	-2.790365	-1.611093	C	1.697127	-3.482100	-1.311800
C	2.774653	-3.439402	-2.200415	C	2.682007	-2.705606	-3.389547
C	1.522918	-2.009266	-3.694923	C	0.419680	-2.035895	-2.808334
C	-1.342575	-0.733436	-4.180588	C	-1.822402	0.365041	-6.441707
C	-3.009433	0.355641	-5.798424	S	-0.481114	-0.323750	-5.601320
S	-3.016947	-0.357005	-4.230161	C	-0.809793	-1.318121	-2.996897
H	-0.328846	-2.865183	-0.942702	H	1.761608	-4.077020	-0.400291
H	3.685451	-3.997471	-1.977140	H	3.520775	-2.690136	-4.086267
H	1.495548	-1.454344	-4.631043	H	-1.655337	0.752001	-7.449092
H	-3.949645	0.732592	-6.205888	H	-1.578671	-1.536202	-2.249347

σ-6



```
#p m062x/def2svp opt freq
empiricaldispersion=gd3 nosymm geom=connecti
vity
```

Charge = 2, Multiplicity = 1, Point group = C1

Electronic Energy = -2362.463446 Hartree

Number of imaginary frequencies = 0

Sum of electronic and zero-point Energies = -2362.157286 Hartree

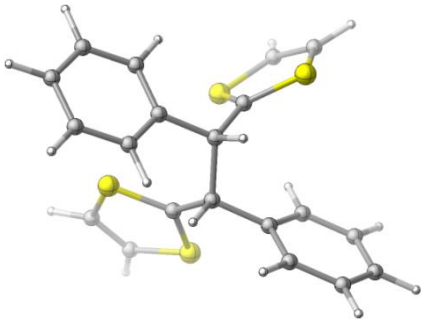
Sum of electronic and thermal Energies = -2362.136668 Hartree

Sum of electronic and thermal Enthalpies = -2362.135723 Hartree

Sum of electronic and thermal Free Energies = -2362.209997 Hartree

	Cartesian Coordinates				Cartesian Coordinates		
Atoms	***X***	***Y***	***Z***	**Atoms**	***X***	***Y***	***Z***
C	1.504774	1.839838	-3.251677	C	1.767115	3.056533	-3.876749
C	0.753603	4.007612	-4.010592	C	-0.520839	3.737037	-3.517882
C	-0.781192	2.522481	-2.882047	C	0.227864	1.564887	-2.739089
C	0.727195	-0.112694	-0.880128	C	2.568821	-0.615345	0.802053
C	1.409576	-0.928682	1.431118	S	2.409798	-0.009627	-0.796898
S	-0.017977	-0.685649	0.515968	C	-0.126145	0.245357	-2.073937
H	2.314901	1.107126	-3.188156	H	2.766781	3.265772	-4.259611
H	0.961346	4.961645	-4.496512	H	-1.316384	4.476392	-3.616370
H	-1.780717	2.329073	-2.484669	H	3.567673	-0.689902	1.237476
H	1.325907	-1.300909	2.454610	H	-1.137411	0.360361	-1.656389
C	-1.998079	-2.703029	-2.429866	C	-2.357792	-3.895434	-1.800516
C	-1.386574	-4.677429	-1.179812	C	-0.054140	-4.260126	-1.179243
C	0.303579	-3.064703	-1.798057	C	-0.665900	-2.278040	-2.438690
C	0.702241	-1.027385	-4.194570	C	2.742899	-1.418922	-5.663164
C	1.910658	-0.643161	-6.400310	S	2.168248	-1.859124	-4.106009
S	0.433728	-0.216343	-5.644783	C	-0.341979	-0.951660	-3.105692
H	-2.766868	-2.107010	-2.927909	H	-3.399944	-4.216487	-1.807271
H	-1.664666	-5.615671	-0.698330	H	0.709466	-4.870885	-0.695957
H	1.352150	-2.755198	-1.754659	H	3.713118	-1.798675	-5.990789
H	2.105979	-0.293888	-7.416651	H	-1.253307	-0.627914	-3.630040

σ-7



```
#p m062x/def2svp opt freq empiricaldispersion=gd3
nosymm geom=connectivity
```

Charge = 2, Multiplicity = 1, Point group = C1

Electronic Energy = -2362.466199 Hartree

Number of imaginary frequencies = 0

Sum of electronic and zero-point Energies = -2362.160133 Hartree

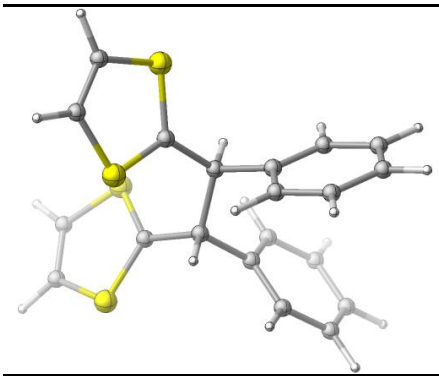
Sum of electronic and thermal Energies = -2362.139586 Hartree

Sum of electronic and thermal Enthalpies = -2362.138642 Hartree

Sum of electronic and thermal Free Energies = -2362.212709 Hartree

	Cartesian Coordinates				Cartesian Coordinates		
Atoms	***X***	***Y***	***Z***	**Atoms**	***X***	***Y***	***Z***
C	1.284036	2.440890	-2.212511	C	1.438690	3.690639	-2.817943
C	0.483257	4.161859	-3.713576	C	-0.651305	3.391829	-3.981088
C	-0.807783	2.148111	-3.377826	C	0.173470	1.644862	-2.509084
C	0.958672	-0.233670	-0.943499	C	2.003368	-1.212060	1.154337
C	3.021362	-1.101514	0.266165	S	0.467228	-0.696232	0.592722
S	2.602714	-0.447183	-1.267039	C	-0.053854	0.239783	-1.951785
H	2.041364	2.126504	-1.495147	H	2.308996	4.300884	-2.573953
H	0.606919	5.137525	-4.184936	H	-1.423566	3.767532	-4.653407
H	-1.717574	1.577575	-3.581831	H	2.093884	-1.589954	2.175208
H	4.062458	-1.370614	0.457233	H	-1.017326	0.248879	-1.416759
C	-2.070400	-2.476267	-2.417171	C	-2.509660	-3.665735	-1.835994
C	-1.585713	-4.576406	-1.327157	C	-0.220337	-4.294873	-1.398100
C	0.219133	-3.103761	-1.972004	C	-0.704576	-2.183659	-2.493184
C	0.783960	-0.934005	-4.145292	C	2.420525	-0.477151	-6.039197
C	2.205091	-1.814355	-6.064462	S	1.563578	0.402935	-4.838812
S	1.125062	-2.417963	-4.878193	C	-0.289109	-0.841357	-3.075795
H	-2.804455	-1.773759	-2.820460	H	-3.577299	-3.883029	-1.790064
H	-1.927850	-5.510937	-0.880975	H	0.505528	-5.010715	-1.010249
H	1.294706	-2.912475	-2.023561	H	3.078320	0.072393	-6.716202
H	2.660176	-2.518090	-6.764915	H	-1.164188	-0.456210	-3.625301

σ-8



```
#p m062x/def2svp opt freq empiricaldispersion=gd3
nosymm geom=connectivity
```

Charge = 2, Multiplicity = 1, Point group = C1

Electronic Energy = -2362.464768 Hartree

Number of imaginary frequencies = 0

Sum of electronic and zero-point Energies = -2362.159714 Hartree

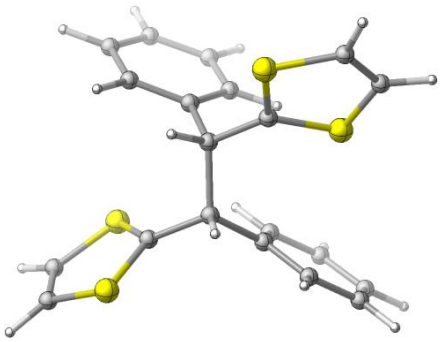
Sum of electronic and thermal Energies = -2362.138787 Hartree

Sum of electronic and thermal Enthalpies = -2362.137842 Hartree

Sum of electronic and thermal Free Energies = -2362.213431 Hartree

	Cartesian Coordinates				Cartesian Coordinates		
Atoms	***X***	***Y***	***Z***	**Atoms**	***X***	***Y***	***Z***
C	1.433000	-0.209492	-0.300290	C	2.648847	-0.236033	0.378930
C	3.783113	0.336519	-0.198968	C	3.701447	0.934149	-1.456124
C	2.487049	0.961019	-2.140482	C	1.353049	0.384292	-1.564388
C	-1.017376	1.052012	-1.537904	C	-2.355930	2.821068	-0.296937
C	-2.853306	1.636313	0.128460	S	-1.082151	2.734143	-1.448568
S	-2.125023	0.237589	-0.560221	C	0.044805	0.357024	-2.355028
H	0.554564	-0.660001	0.171881	H	2.710874	-0.700765	1.363428
H	4.733792	0.318136	0.335078	H	4.587455	1.379000	-1.910285
H	2.432864	1.415404	-3.132596	H	-2.698161	3.804620	0.033259
H	-3.657021	1.507367	0.856489	H	0.204583	0.957302	-3.266588
C	1.604816	-2.749579	-2.911888	C	2.719966	-3.285563	-3.554542
C	3.105967	-2.803450	-4.804652	C	2.376438	-1.783288	-5.417181
C	1.260290	-1.246344	-4.779658	C	0.877369	-1.725621	-3.522440
C	-1.535292	-1.238619	-3.629968	C	-3.499571	-2.211635	-4.916807
C	-3.382224	-0.937457	-5.358069	S	-2.364734	-2.703357	-3.722340
S	-2.112955	-0.020644	-4.644169	C	-0.299206	-1.097660	-2.775057
H	1.317026	-3.119492	-1.924963	H	3.290765	-4.080388	-3.073320
H	3.977627	-3.225339	-5.306221	H	2.675437	-1.407940	-6.396361
H	0.699512	-0.450140	-5.278748	H	-4.246147	-2.932156	-5.258885
H	-4.013861	-0.464057	-6.112729	H	-0.460192	-1.696715	-1.862946

σ-9



```
#p m062x/def2svp opt freq empiricaldispersion=gd3
nosymm geom=connectivity
```

Charge = 2, Multiplicity = 1, Point group = C1

Electronic Energy = -2362.471586 Hartree

Number of imaginary frequencies = 0

Sum of electronic and zero-point Energies = -2362.165049 Hartree

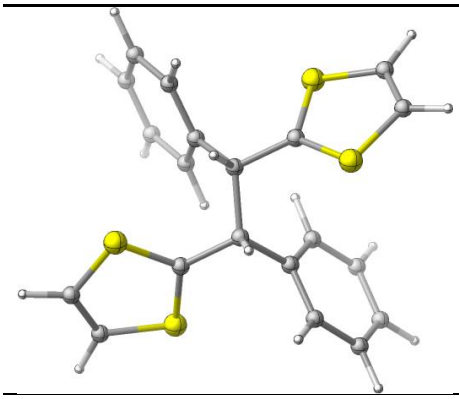
Sum of electronic and thermal Energies = -2362.144576 Hartree

Sum of electronic and thermal Enthalpies = -2362.143632 Hartree

Sum of electronic and thermal Free Energies = -2362.217021 Hartree

	Cartesian Coordinates				Cartesian Coordinates		
Atoms	***X***	***Y***	***Z***	**Atoms**	***X***	***Y***	***Z***
C	2.099625	0.655148	-2.128004	C	3.260276	1.335794	-2.493596
C	3.178101	2.545447	-3.185219	C	1.930231	3.083209	-3.499579
C	0.769192	2.399920	-3.142549	C	0.843889	1.169484	-2.474876
C	-0.580891	0.211592	-0.670364	C	-1.079888	0.616044	1.792024
C	-0.306348	-0.496032	1.752022	S	-1.431437	1.322075	0.271110
S	0.180758	-1.023653	0.192029	C	-0.466597	0.451285	-2.160925
H	2.192881	-0.276292	-1.566314	H	4.234310	0.926962	-2.222354
H	4.088754	3.079206	-3.460117	H	1.858675	4.041063	-4.016299
H	-0.204602	2.829234	-3.393602	H	-1.484672	1.077478	2.695257
H	0.009595	-1.077516	2.620733	H	-1.263362	1.172706	-2.398997
C	-0.903517	-3.115710	-1.994632	C	-0.324741	-4.315250	-1.584128
C	1.029963	-4.549826	-1.818569	C	1.796958	-3.592250	-2.484195
C	1.217542	-2.395340	-2.903355	C	-0.132794	-2.136283	-2.636504
C	-0.699507	-0.588187	-4.502933	C	0.054442	-0.188714	-6.893625
C	-1.195302	-0.702795	-6.996143	S	0.659290	0.018730	-5.299721
S	-1.960937	-1.076047	-5.509654	C	-0.819491	-0.825131	-3.012321
H	-1.966242	-2.940616	-1.805938	H	-0.935656	-5.070552	-1.088251
H	1.485366	-5.488955	-1.501739	H	2.849874	-3.784996	-2.693241
H	1.834632	-1.674706	-3.443364	H	0.684905	0.111801	-7.733160
H	-1.732946	-0.887128	-7.928643	H	-1.892825	-0.990974	-2.832062

σ-10



#p m062x/def2svp opt freq empiricaldispersion=gd3 nosymm geom=connectivity

Charge = 2, Multiplicity = 1, Point group = C1

Electronic Energy = -2362.469365 Hartree

Number of imaginary frequencies = 0

Sum of electronic and zero-point Energies = -2362.163159 Hartree

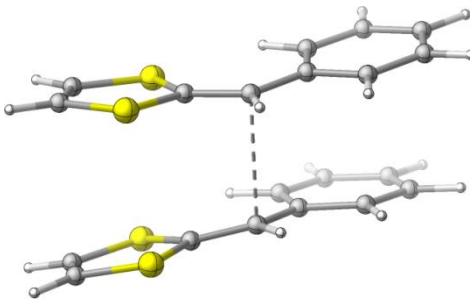
Sum of electronic and thermal Energies = -2362.142640 Hartree

Sum of electronic and thermal Enthalpies = -2362.141695 Hartree

Sum of electronic and thermal Free Energies = -2362.214950 Hartree

Atoms	Cartesian Coordinates			Atoms	Cartesian Coordinates		
	X	***Y***	***Z***		***X***	***Y***	***Z***
C	1.856468	0.735394	-3.250648	C	2.891242	1.587195	-3.637587
C	2.760663	2.967457	-3.486844	C	1.583700	3.499556	-2.960671
C	0.545804	2.650735	-2.580980	C	0.677132	1.260787	-2.707656
C	-0.492151	0.219436	-0.732776	C	0.018878	0.402782	1.742672
C	-1.048293	-0.427990	1.660118	S	0.618634	1.013640	0.254380
S	-1.618740	-0.742197	0.072205	C	-0.494377	0.403105	-2.239590
H	1.980903	-0.339317	-3.390711	H	3.805720	1.167578	-4.058403
H	3.573372	3.629371	-3.788239	H	1.467374	4.578743	-2.854967
H	-0.378601	3.081125	-2.183977	H	0.508342	0.709244	2.669622
H	-1.555502	-0.900928	2.503721	H	-1.399359	1.011069	-2.426779
C	-0.760912	-3.430636	-2.580289	C	-0.203607	-4.621952	-2.119738
C	1.030956	-4.607657	-1.471007	C	1.699948	-3.399090	-1.279425
C	1.147492	-2.206514	-1.747038	C	-0.084864	-2.214037	-2.412438
C	-0.526847	-0.826517	-4.469441	C	0.097531	-1.257028	-6.887534
C	-0.532792	-0.057669	-6.890912	S	0.244863	-2.029727	-5.361498
S	-1.071590	0.497908	-5.359000	C	-0.750358	-0.961560	-2.974088
H	-1.737402	-3.452869	-3.073600	H	-0.740717	-5.560872	-2.258657
H	1.467976	-5.537931	-1.106227	H	2.660600	-3.382082	-0.763381
H	1.686806	-1.274291	-1.573488	H	0.503021	-1.757999	-7.769199
H	-0.715270	0.564938	-7.769364	H	-1.838539	-1.140976	-2.888366

π-8



```
#p m062x/def2svp opt freq
empiricaldispersion=gd3 nosymm geom=connecti
vity
```

Charge = 2, Multiplicity = 1, Point group = C1

Electronic Energy = -2362.431983 Hartree

Number of imaginary frequencies = 0

Sum of electronic and zero-point Energies = -2362.129015 Hartree

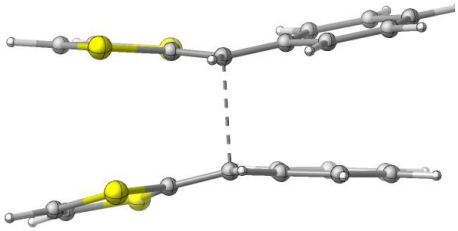
Sum of electronic and thermal Energies = -2362.107528 Hartree

Sum of electronic and thermal Enthalpies = -2362.106583 Hartree

Sum of electronic and thermal Free Energies = -2362.180847 Hartree

	Cartesian Coordinates				Cartesian Coordinates		
Atoms	***X***	***Y***	***Z***	**Atoms**	***X***	***Y***	***Z***
C	-1.186993	-1.888185	1.020714	C	-2.394383	-2.260101	1.587054
C	-3.558998	-2.303625	0.806944	C	-3.516080	-1.962646	-0.548771
C	-2.313275	-1.590400	-1.124970	C	-1.112691	-1.562983	-0.363280
C	1.419985	-1.303546	-0.693930	C	3.986637	-1.249988	-0.807854
C	3.690478	-1.671045	0.443385	S	2.652749	-0.891874	-1.828284
S	2.020813	-1.817656	0.839436	C	0.074232	-1.208950	-1.072512
C	-2.703522	1.623541	-1.532512	C	-4.068281	1.557339	-1.317060
C	-4.550849	1.306667	-0.026751	C	-3.663671	1.125558	1.044827
C	-2.297407	1.202885	0.840721	C	-1.781456	1.461204	-0.457089
C	0.738116	1.652233	0.031755	C	3.165610	2.081286	0.767199
C	2.509755	1.715212	1.889076	S	2.236767	2.139119	-0.683962
S	0.835527	1.326199	1.724733	C	-0.403096	1.606647	-0.781788
H	-0.307643	-1.867641	1.662754	H	-2.437487	-2.529128	2.642926
H	-4.500920	-2.618703	1.259714	H	-4.421787	-2.006474	-1.154825
H	-2.272194	-1.356533	-2.190863	H	4.995326	-1.144618	-1.212379
H	4.426619	-1.960718	1.196095	H	-0.075442	-0.957234	-2.127509
H	-2.321983	1.833867	-2.534414	H	-4.762488	1.709123	-2.143997
H	-5.627282	1.265810	0.150679	H	-4.053186	0.943508	2.047064
H	-1.642562	1.083732	1.702340	H	4.214125	2.382554	0.726200
H	2.952065	1.666313	2.886128	H	-0.204001	1.851239	-1.831279

TS-7



```
#p m062x/def2svp opt=(calcfc,ts,noeigen) freq
empiricaldispersion=gd3 nosymm geom=connectivity
```

Charge = 2, Multiplicity = 1, Point group = C1

Electronic Energy = -2362.430980 Hartree

Number of imaginary frequencies = 1, vi = -76.82

Sum of electronic and zero-point Energies = -2362.127974 Hartree

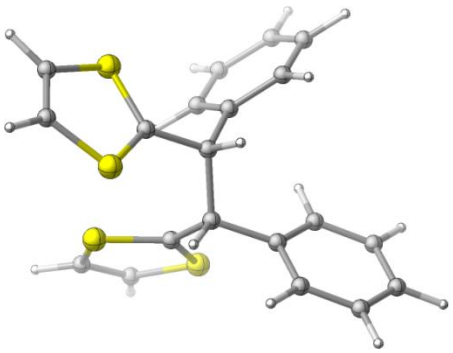
Sum of electronic and thermal Energies = -2362.107358 Hartree

Sum of electronic and thermal Enthalpies = -2362.106414 Hartree

Sum of electronic and thermal Free Energies = -2362.177725 Hartree

Atoms	Cartesian Coordinates			Atoms	Cartesian Coordinates		
	X	***Y***	***Z***		***X***	***Y***	***Z***
C	-0.906813	-1.670464	1.387709	C	-2.019165	-2.043515	2.129104
C	-3.229271	-2.337278	1.489561	C	-3.329969	-2.253921	0.098146
C	-2.226045	-1.874650	-0.649949	C	-0.988295	-1.581573	-0.025137
C	1.478487	-1.223012	-0.679720	C	4.009512	-1.200535	-1.118249
C	3.877388	-1.426452	0.206096	S	2.546323	-1.000497	-2.003293
S	2.264050	-1.493577	0.817981	C	0.076960	-1.162585	-0.896287
C	-2.515539	1.118206	-1.973104	C	-3.900627	1.091918	-1.940225
C	-4.564841	1.136561	-0.709799	C	-3.837581	1.209368	0.483795
C	-2.451416	1.245254	0.457642	C	-1.759327	1.203847	-0.775803
C	0.659169	1.584598	0.031252	C	2.893761	2.361791	1.033617
C	2.099464	2.095134	2.091733	S	2.195531	2.118984	-0.523114
S	0.509351	1.524897	1.736368	C	-0.328826	1.224783	-0.924297
H	0.018789	-1.465211	1.924487	H	-1.944528	-2.124133	3.213985
H	-4.091855	-2.648424	2.081067	H	-4.268331	-2.499252	-0.400424
H	-2.299243	-1.829963	-1.738325	H	4.956091	-1.156270	-1.660986
H	4.701106	-1.599334	0.901730	H	-0.190964	-1.139196	-1.957190
H	-1.998089	1.098347	-2.935654	H	-4.468702	1.047741	-2.869874
H	-5.655714	1.126325	-0.680621	H	-4.361438	1.254871	1.439043
H	-1.928468	1.320683	1.409572	H	3.911563	2.752658	1.092955
H	2.376577	2.227552	3.139560	H	0.020939	1.319542	-1.958202

σ-11



```
#p m062x/def2svp opt freq
empiricaldispersion=gd3 nosymm geom=connecti
vity
```

Charge = 2, Multiplicity = 1, Point group = C1

Electronic Energy = -2362.464684 Hartree

Number of imaginary frequencies = 0

Sum of electronic and zero-point Energies = -2362.158867 Hartree

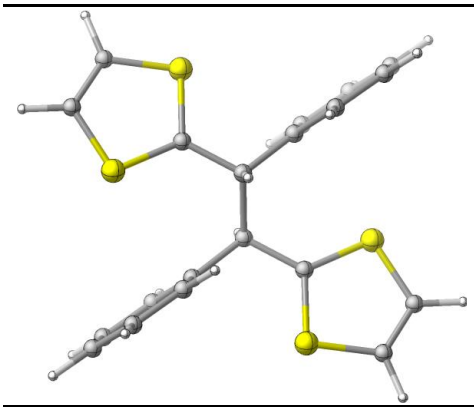
Sum of electronic and thermal Energies = -2362.138281 Hartree

Sum of electronic and thermal Enthalpies = -2362.137337 Hartree

Sum of electronic and thermal Free Energies = -2362.211223 Hartree

	Cartesian Coordinates				Cartesian Coordinates		
Atoms	***X***	***Y***	***Z***	**Atoms**	***X***	***Y***	***Z***
C	-0.415738	-0.784086	2.235748	C	-0.811320	-1.105491	3.533491
C	-1.975478	-1.841446	3.753968	C	-2.746625	-2.263177	2.672109
C	-2.352748	-1.950329	1.372329	C	-1.189359	-1.207452	1.143877
C	0.447591	-1.642292	-0.722625	C	2.282809	-2.775985	-2.085482
C	2.641646	-2.914809	-0.786697	S	0.799862	-1.949047	-2.347806
S	1.567553	-2.249389	0.376615	C	-0.803700	-0.900619	-0.296725
C	0.146691	2.308374	1.088446	C	1.190782	3.012928	1.686267
C	2.501501	2.822365	1.250644	C	2.767911	1.932839	0.208200
C	1.725744	1.227548	-0.390391	C	0.405429	1.404070	0.052707
C	-0.939898	1.025480	-2.031135	C	-1.842477	1.298112	-4.399269
C	-0.946194	2.299544	-4.227496	S	-2.056397	0.261680	-3.046602
S	-0.162328	2.363007	-2.700255	C	-0.753578	0.650703	-0.572618
H	0.494089	-0.197720	2.093776	H	-0.206989	-0.772642	4.378046
H	-2.281361	-2.086881	4.771584	H	-3.657002	-2.840123	2.837549
H	-2.962073	-2.291591	0.531586	H	2.835776	-3.158356	-2.946100
H	3.539134	-3.428376	-0.434272	H	-1.615028	-1.312241	-0.920189
H	-0.876447	2.453262	1.443661	H	0.977598	3.713680	2.494170
H	3.318110	3.374597	1.717274	H	3.790952	1.795339	-0.143898
H	1.954382	0.555976	-1.223376	H	-2.425214	1.109164	-5.303702
H	-0.690774	3.050454	-4.978880	H	-1.676628	1.012936	-0.085869

σ-12



```
#p m062x/def2svp opt freq
empiricaldispersion=gd3 nosymm geom=connecti
vity
```

Charge = 2, Multiplicity = 1, Point group = C1

Electronic Energy = -2362.479811 Hartree

Number of imaginary frequencies = 0

Sum of electronic and zero-point Energies = -2362.173714 Hartree

Sum of electronic and thermal Energies = -2362.153328 Hartree

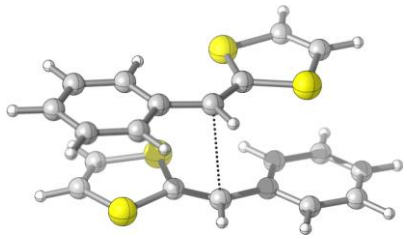
Sum of electronic and thermal Enthalpies = -2362.152384 Hartree

Sum of electronic and thermal Free Energies = -2362.225067 Hartree

	Cartesian Coordinates				Cartesian Coordinates		
Atoms	***X***	***Y***	***Z***	**Atoms**	***X***	***Y***	***Z***
C	-1.694284	-0.990593	1.876837	C	-2.878051	-1.521721	2.383621
C	-3.592973	-2.466064	1.642455	C	-3.115873	-2.888565	0.401809
C	-1.929719	-2.358477	-0.107604	C	-1.218999	-1.399589	0.621157
C	1.274762	-1.279534	0.787010	C	3.613252	-1.873573	1.592131
C	2.779455	-2.702159	2.266848	S	2.866961	-0.782366	0.499515
S	1.113341	-2.525818	1.917849	C	0.039678	-0.782059	0.038215
C	1.929638	2.358603	0.107506	C	3.115781	2.888724	-0.401899
C	3.592958	2.466156	-1.642491	C	2.878121	1.521712	-2.383616
C	1.694368	0.990549	-1.876841	C	1.219011	1.399610	-0.621207
C	-1.274728	1.279518	-0.787057	C	-3.613226	1.873545	-1.592152
C	-2.779415	2.701948	-2.267078	S	-2.866937	0.782495	-0.499381
S	-1.113291	2.525552	-1.918164	C	-0.039651	0.782057	-0.038258
H	-1.145425	-0.254112	2.471953	H	-3.245145	-1.199246	3.358745
H	-4.521064	-2.879724	2.039247	H	-3.667178	-3.634085	-0.172501
H	-1.564338	-2.688241	-1.083524	H	4.700128	-1.844962	1.695498
H	3.085184	-3.451634	2.999938	H	0.156829	-1.155441	-0.993464
H	1.564200	2.688423	1.083385	H	3.667016	3.634320	0.172380
H	4.521038	2.879844	-2.039279	H	3.245274	1.199187	-3.358702
H	1.145586	0.253980	-2.471918	H	-4.700112	1.844998	-1.695436
H	-3.085140	3.451310	-3.000286	H	-0.156829	1.155437	0.993420

2. Optimized geometries and energies of Ph-DTF dimers in CH_2Cl_2

π-1



```
#p m062x/def2svp nosymm opt freq
empiricaldispersion=gd3 scrf=(smd,sol
vent=dichloromethane) geom=connectivity
```

Charge = 1, Multiplicity = 2, Point group = C1
Electronic Energy = -2362.874570 Hartree
$\hat{S}^2$ = 0.7602

Number of imaginary frequencies = 0

Sum of electronic and zero-point Energies = -2362.572796 Hartree

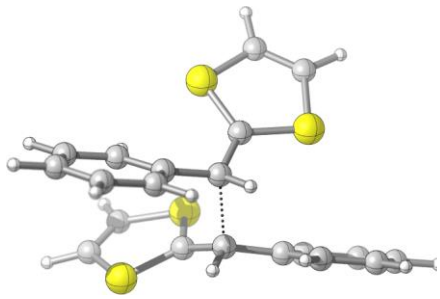
Sum of electronic and thermal Energies = -2362.550992 Hartree

Sum of electronic and thermal Enthalpies = -2362.550048 Hartree

Sum of electronic and thermal Free Energies = -2362.625332 Hartree

	Cartesian Coordinates				Cartesian Coordinates		
Atoms	***X***	***Y***	***Z***	**Atoms**	***X***	***Y***	***Z***
C	-2.347776	1.320995	-0.474093	C	-3.723128	1.179072	-0.625262
C	-4.557875	1.091009	0.491842	C	-4.004516	1.146802	1.772163
C	-2.630410	1.283714	1.929552	C	-1.769492	1.377478	0.812021
C	0.714254	1.683977	0.246841	C	3.124834	2.130819	-0.595536
C	2.383359	2.005079	-1.709939	S	2.307645	1.945351	0.915467
S	0.696714	1.660004	-1.497495	C	-0.354851	1.519812	1.092981
H	-1.743992	1.395286	-1.376894	H	-4.148416	1.138878	-1.629471
H	-5.636085	0.983623	0.362678	H	-4.646418	1.081483	2.651971
H	-2.197870	1.324720	2.931436	H	4.195340	2.341972	-0.579804
H	2.761036	2.095137	-2.729470	H	-0.107540	1.559897	2.158599
C	2.630421	-1.285487	1.928386	C	4.004531	-1.148487	1.771115
C	4.557891	-1.091565	0.490844	C	3.723138	-1.178569	-0.626339
C	2.347780	-1.320558	-0.475295	C	1.769500	-1.378197	0.810768
C	-0.714257	-1.684144	0.245320	C	-2.383388	-2.003466	-1.711718
C	-3.124834	-2.130295	-0.597415	S	-0.696761	-1.658488	-1.498990
S	-2.307616	-1.946218	0.913738	C	0.354858	-1.520745	1.091597
H	2.197887	-1.327407	2.930236	H	4.646440	-1.083997	2.650981
H	5.636106	-0.984112	0.361777	H	4.148422	-1.137465	-1.630512
H	1.743982	-1.393961	-1.378159	H	-2.761082	-2.092606	-2.731322
H	-4.195328	-2.341522	-0.581861	H	0.107547	-1.561773	2.157178

TS-1



```
#p m062x/def2svp opt=(calcfc,ts,noeigen) nosymm
freq empiricaldispersi on=gd3
scrf=(smd,solvent=dichloromethane)
geom=connectivity
```

Charge = 1, Multiplicity = 2, Point group = C1
Electronic Energy = -2362.854742 Hartree
$\hat{S}^2$ = 0.7651

Number of imaginary frequencies = 1, vi = -312.24

Sum of electronic and zero-point Energies = -2362.551979 Hartree

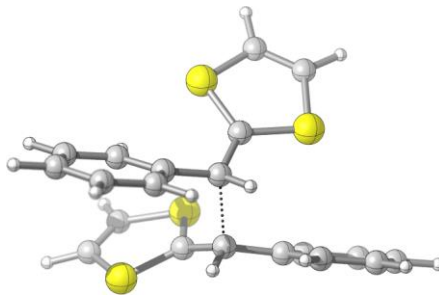
Sum of electronic and thermal Energies = -2362.531180 Hartree

Sum of electronic and thermal Enthalpies = -2362.530235 Hartree

Sum of electronic and thermal Free Energies = -2362.604053 Hartree

	Cartesian Coordinates				Cartesian Coordinates		
Atoms	***X***	***Y***	***Z***	**Atoms**	***X***	***Y***	***Z***
C	-2.583791	0.678605	0.121384	C	-3.950943	0.721165	0.392467
C	-4.402878	0.865857	1.703271	C	-3.480154	0.956943	2.746872
C	-2.114855	0.916626	2.477333	C	-1.646484	0.794563	1.159968
C	0.434097	1.512544	-0.096043	C	2.165074	2.786148	-1.522040
C	0.976764	3.057248	-2.087938	S	2.151047	1.756430	-0.129139
S	-0.423038	2.358990	-1.345508	C	-0.176128	0.748472	0.941309
H	-2.261728	0.523823	-0.911794	H	-4.664623	0.630351	-0.427994
H	-5.473072	0.900003	1.913299	H	-3.825334	1.061912	3.776636
H	-1.394250	0.989535	3.295585	H	3.126581	3.161309	-1.875186
H	0.829631	3.686818	-2.966848	H	0.377610	0.823465	1.880970
C	2.339671	-0.809535	2.149124	C	3.717843	-0.759411	2.328078
C	4.572786	-1.112342	1.281401	C	4.034212	-1.539521	0.069892
C	2.651438	-1.586227	-0.111947	C	1.783817	-1.198419	0.917593
C	-0.400974	-1.649251	-0.348287	C	-1.459059	-1.817519	-2.686439
C	-2.341466	-2.401311	-1.856099	S	0.008442	-1.222936	-1.970985
S	-1.895443	-2.488205	-0.186278	C	0.296131	-1.173247	0.793929
H	1.678761	-0.546127	2.979128	H	4.127163	-0.449096	3.290705
H	5.654450	-1.070719	1.418199	H	4.691010	-1.844355	-0.746289
H	2.270041	-1.952200	-1.064918	H	-1.582925	-1.716013	-3.765575
H	-3.292357	-2.839181	-2.163347	H	-0.195563	-1.470018	1.728248

σ-1



```
#p m062x/def2svp nosymm opt freq
empiricaldispersion=gd3 scrf=(smd,sol
vent=dichloromethane) geom=connectivity
```

Charge = 1, Multiplicity = 2, Point group = C1
Electronic Energy = -2362.862064 Hartree
$\hat{S}^2$ = 0.7588

Number of imaginary frequencies = 0

Sum of electronic and zero-point Energies = -2362.558365 Hartree

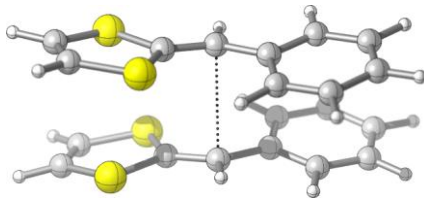
Sum of electronic and thermal Energies = -2362.537275 Hartree

Sum of electronic and thermal Enthalpies = -2362.536331 Hartree

Sum of electronic and thermal Free Energies = -2362.611182 Hartree

	Cartesian Coordinates				Cartesian Coordinates		
Atoms	***X***	***Y***	***Z***	**Atoms**	***X***	***Y***	***Z***
C	-2.640275	0.200800	0.141973	C	-4.007486	0.183933	0.414443
C	-4.478088	0.552907	1.674731	C	-3.575481	0.944361	2.662925
C	-2.208200	0.963756	2.390550	C	-1.725824	0.592049	1.130521
C	0.221254	1.491572	-0.203604	C	1.611178	2.924974	-1.801375
C	0.333669	3.302398	-2.004226	S	1.869335	1.715637	-0.595855
S	-0.855457	2.524459	-1.028397	C	-0.225895	0.591895	0.903330
H	-2.297611	-0.088797	-0.854023	H	-4.706942	-0.122643	-0.364808
H	-5.548642	0.536894	1.885385	H	-3.934664	1.237497	3.650659
H	-1.502176	1.270467	3.166235	H	2.480198	3.321859	-2.329087
H	0.004807	4.054789	-2.722618	H	0.230623	1.009828	1.812826
C	2.424817	-0.268403	2.162862	C	3.802105	-0.205985	2.357752
C	4.668704	-0.763385	1.415294	C	4.144157	-1.402842	0.294556
C	2.762654	-1.468236	0.101634	C	1.887485	-0.881403	1.020964
C	-0.128329	-1.630960	-0.353437	C	-1.103839	-2.063986	-2.692774
C	-1.706060	-2.952210	-1.883745	S	0.094721	-1.025195	-1.964013
S	-1.222372	-2.959194	-0.216682	C	0.369328	-0.893580	0.833188
H	1.761725	0.160016	2.918943	H	4.200229	0.275962	3.252165
H	5.748458	-0.709935	1.563317	H	4.810880	-1.858681	-0.439242
H	2.374352	-1.984001	-0.777124	H	-1.290074	-1.967979	-3.763113
H	-2.450565	-3.679217	-2.211360	H	-0.062844	-1.373648	1.725187

π-2



```
#p m062x/def2svp nosymm opt freq
empiricaldispersion=gd3 scrf=(smd,sol
vent=dichloromethane) geom=connectivity
```

Charge = 1, Multiplicity = 2, Point group = C1
Electronic Energy = -2362.868666 Hartree
S^2 = 0.7585

Number of imaginary frequencies = 0

Sum of electronic and zero-point Energies = -2362.567850 Hartree

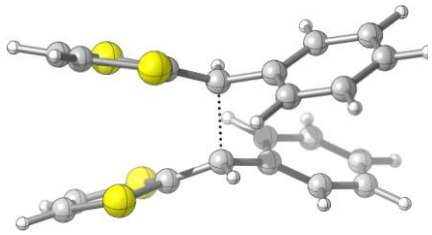
Sum of electronic and thermal Energies = -2362.545620 Hartree

Sum of electronic and thermal Enthalpies = -2362.544676 Hartree

Sum of electronic and thermal Free Energies = -2362.622740 Hartree

	Cartesian Coordinates				Cartesian Coordinates		
Atoms	***X***	***Y***	***Z***	**Atoms**	***X***	***Y***	***Z***
C	1.648734	2.334380	0.696729	C	2.900881	2.756961	1.131847
C	4.051273	2.430076	0.408870	C	3.944550	1.662476	-0.751938
C	2.696906	1.228715	-1.185618	C	1.523521	1.569045	-0.480480
C	-1.025958	1.423491	-0.763193	C	-3.611287	1.555478	-0.936740
C	-3.275045	2.455726	0.001849	S	-2.318201	0.654840	-1.657468
S	-1.588941	2.602425	0.392021	C	0.272651	1.062622	-1.018303
H	0.780060	2.586418	1.304993	H	2.979728	3.343709	2.048265
H	5.028920	2.768095	0.756060	H	4.838327	1.392652	-1.316755
H	2.615038	0.619402	-2.088601	H	-4.629171	1.361540	-1.278507
H	-3.979094	3.094766	0.537043	H	0.394290	0.319825	-1.814079
C	2.696850	-1.228511	1.185609	C	3.944538	-1.662255	0.752035
C	4.051373	-2.429839	-0.408773	C	2.901051	-2.756719	-1.131861
C	1.648861	-2.334156	-0.696848	C	1.523532	-1.568845	0.480364
C	-1.025980	-1.423380	0.762979	C	-3.274972	-2.456139	-0.001670
C	-3.611272	-1.555863	0.936869	S	-1.588899	-2.602456	-0.392127
S	-2.318279	-0.654817	1.657257	C	0.272611	-1.062430	1.018088
H	2.614894	-0.619209	2.088590	H	4.838262	-1.392429	1.316935
H	5.029055	-2.767843	-0.755879	H	2.979988	-3.343443	-2.048287
H	0.780248	-2.586155	-1.305213	H	-3.978960	-3.095402	-0.536679
H	-4.629146	-1.362123	1.278779	H	0.394197	-0.319574	1.813816

TS-2



```
#p m062x/def2svp opt=(calcfc,ts,noeigen) nosymm
freq empiricaldispersi on=gd3
scrf=(smd,solvent=dichloromethane)
geom=connectivity
```

Charge = 1, Multiplicity = 2, Point group = C1
Electronic Energy = -2362.859275 Hartree
$\hat{S}^2$ = 0.7635

Number of imaginary frequencies = 1, vi = -291.55

Sum of electronic and zero-point Energies = -2362.556514 Hartree

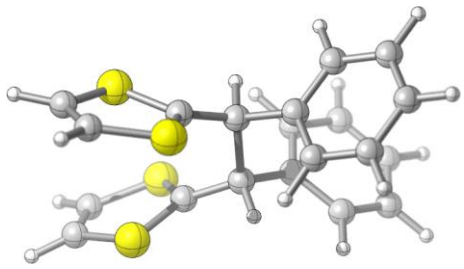
Sum of electronic and thermal Energies = -2362.535674 Hartree

Sum of electronic and thermal Enthalpies = -2362.534730 Hartree

Sum of electronic and thermal Free Energies = -2362.608471 Hartree

	Cartesian Coordinates				Cartesian Coordinates		
Atoms	***X***	***Y***	***Z***	**Atoms**	***X***	***Y***	***Z***
C	1.646352	2.200729	0.897748	C	2.854785	2.828023	1.197799
C	3.932743	2.736664	0.316940	C	3.799418	2.009038	-0.866191
C	2.592765	1.382313	-1.168771	C	1.498706	1.481023	-0.297343
C	-1.020737	1.383217	-0.625952	C	-3.554192	1.734523	-0.914446
C	-3.160758	2.671913	-0.034512	S	-2.312734	0.706850	-1.552881
S	-1.471712	2.727857	0.359165	C	0.250230	0.755130	-0.655739
H	0.833421	2.252237	1.625377	H	2.955628	3.382454	2.132113
H	4.878207	3.225859	0.556548	H	4.639992	1.924816	-1.556801
H	2.491544	0.805845	-2.090976	H	-4.576762	1.597559	-1.269582
H	-3.819515	3.406208	0.431863	H	0.373834	0.118446	-1.539015
C	2.592836	-1.382409	1.168836	C	3.799496	-2.009079	0.866170
C	3.932791	-2.736644	-0.317002	C	2.854796	-2.827996	-1.197814
C	1.646356	-2.200756	-0.897676	C	1.498737	-1.481114	0.297456
C	-1.020719	-1.383314	0.626068	C	-3.160816	-2.671734	0.034311
C	-3.554201	-1.734501	0.914434	S	-1.471765	-2.727711	-0.359351
S	-2.312686	-0.707041	1.553101	C	0.250262	-0.755261	0.655937
H	2.491641	-0.805982	2.091070	H	4.640101	-1.924859	1.556742
H	4.878260	-3.225796	-0.556678	H	2.955611	-3.382379	-2.132161
H	0.833403	-2.252261	-1.625278	H	-3.819617	-3.405883	-0.432228
H	-4.576767	-1.597545	1.269584	H	0.373882	-0.118664	1.539278

σ-2



```
#p m062x/def2svp nosymm opt freq
empiricaldispersion=gd3 scrf=(smd,sol
vent=dichloromethane) geom=connectivity
```

Charge = 1, Multiplicity = 2, Point group = C1
Electronic Energy = -2362.863171 Hartree
$\hat{S}^2$ = 0.7572

Number of imaginary frequencies = 0

Sum of electronic and zero-point Energies = -2362.559273 Hartree

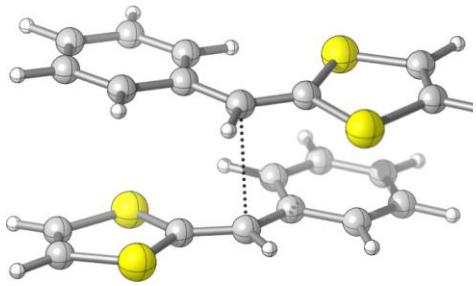
Sum of electronic and thermal Energies = -2362.538069 Hartree

Sum of electronic and thermal Enthalpies = -2362.537125 Hartree

Sum of electronic and thermal Free Energies = -2362.612445 Hartree

	Cartesian Coordinates				Cartesian Coordinates		
Atoms	***X***	***Y***	***Z***	**Atoms**	***X***	***Y***	***Z***
C	1.714980	2.041757	1.049024	C	2.848180	2.817729	1.292061
C	3.773476	3.045625	0.273644	C	3.561154	2.494060	-0.989862
C	2.426157	1.722167	-1.235288	C	1.490782	1.494152	-0.220584
C	-1.003905	1.382873	-0.512284	C	-3.499744	1.852064	-0.819634
C	-3.072033	2.746375	0.092568	S	-2.292209	0.803708	-1.488782
S	-1.385584	2.726476	0.485229	C	0.269239	0.648164	-0.515689
H	1.013190	1.861408	1.867557	H	3.009913	3.239038	2.285523
H	4.662479	3.648078	0.466977	H	4.283928	2.661541	-1.789956
H	2.264383	1.286338	-2.224013	H	-4.524380	1.774040	-1.185872
H	-3.702391	3.497330	0.571889	H	0.388136	0.193927	-1.510500
C	2.426860	-1.721145	1.235251	C	3.562215	-2.492515	0.989839
C	3.774903	-3.043821	-0.273720	C	2.849622	-2.816176	-1.292207
C	1.716059	-2.040733	-1.049180	C	1.491476	-1.493427	0.220488
C	-1.003286	-1.383304	0.512168	C	-3.070825	-2.747704	-0.092672
C	-3.498925	-1.853563	0.819511	S	-1.384384	-2.727093	-0.485327
S	-2.291845	-0.804678	1.488654	C	0.269529	-0.648020	0.515578
H	2.264785	-1.285504	2.224008	H	4.284983	-2.659788	1.789982
H	4.664187	-3.645862	-0.467042	H	3.011651	-3.237264	-2.285715
H	1.014286	-1.860543	-1.867764	H	-3.700863	-3.498929	-0.571983
H	-4.523601	-1.775976	1.185725	H	0.388195	-0.193750	1.510397

π-3



```
#p m062x/def2svp nosymm opt freq
empiricaldispersion=gd3 scrf=(smd,sol
vent=dichloromethane) geom=connectivity
```

Charge = 1, Multiplicity = 2, Point group = C1
Electronic Energy = -2362.872781 Hartree
$\hat{S}^2$ = 0.7614

Number of imaginary frequencies = 0

Sum of electronic and zero-point Energies = -2362.570901 Hartree

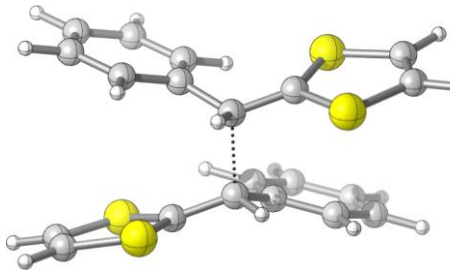
Sum of electronic and thermal Energies = -2362.549273 Hartree

Sum of electronic and thermal Enthalpies = -2362.548329 Hartree

Sum of electronic and thermal Free Energies = -2362.622847 Hartree

	Cartesian Coordinates				Cartesian Coordinates		
Atoms	***X***	***Y***	***Z***	**Atoms**	***X***	***Y***	***Z***
C	-0.716641	1.610013	-1.524748	C	-1.783761	1.848516	-2.388141
C	-3.049739	2.151379	-1.886911	C	-3.248239	2.212713	-0.504813
C	-2.187488	1.982370	0.361934	C	-0.894934	1.683441	-0.125874
C	1.497304	1.315950	0.728022	C	4.007893	1.018455	1.304174
C	3.967714	1.172137	-0.030126	S	2.492233	1.049102	2.139118
S	2.405944	1.385602	-0.752169	C	0.133180	1.434690	0.867080
H	0.245551	1.352389	-1.964839	H	-1.620799	1.790597	-3.465444
H	-3.879310	2.338829	-2.570491	H	-4.234904	2.447320	-0.101756
H	-2.343270	2.046953	1.441109	H	4.917220	0.875121	1.889627
H	4.837484	1.171483	-0.688820	H	-0.228841	1.413359	1.899678
C	2.187542	-1.982592	0.360396	C	3.248221	-2.212284	-0.506611
C	3.049612	-2.149855	-1.888648	C	1.783612	-1.846537	-2.389551
C	0.716565	-1.608677	-1.525891	C	0.894962	-1.683257	-0.127097
C	-1.497231	-1.316531	0.727015	C	-3.967551	-1.172423	-0.031316
C	-4.007929	-1.019887	1.303110	S	-2.405665	-1.385069	-0.753356
S	-2.492368	-1.051078	2.138238	C	-0.133119	-1.435259	0.866069
H	2.343395	-2.047995	1.439515	H	4.234911	-2.447236	-0.103817
H	3.879124	-2.336784	-2.572441	H	1.620589	-1.787706	-3.466797
H	-0.245641	-1.350547	-1.965673	H	-4.837237	-1.171368	-0.690121
H	-4.917355	-0.877215	1.888572	H	0.228900	-1.414672	1.898687

TS-3



```
#p m062x/def2svp opt=(calcfc,ts,noeigen) nosymm
freq empiricaldispersi on=gd3
scrf=(smd,solvent=dichloromethane)
geom=connectivity
```

Charge = 1, Multiplicity = 2, Point group = C1
Electronic Energy = -2362.859125 Hartree
$\hat{S}^2$ = 0.7627

Number of imaginary frequencies = 1, vi = -150.50

Sum of electronic and zero-point Energies = -2362.556496 Hartree

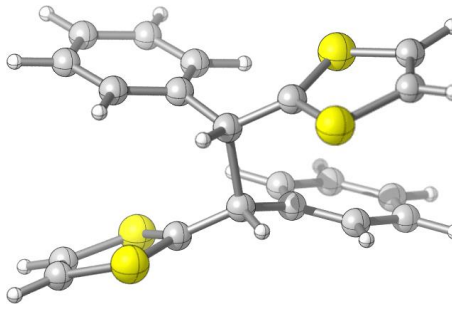
Sum of electronic and thermal Energies = -2362.535656 Hartree

Sum of electronic and thermal Enthalpies = -2362.534712 Hartree

Sum of electronic and thermal Free Energies = -2362.608439 Hartree

Atoms	Cartesian Coordinates			Atoms	Cartesian Coordinates		
	X	***Y***	***Z***		***X***	***Y***	***Z***
C	-0.521735	1.555164	-1.629742	C	-1.472510	2.063518	-2.516159
C	-2.686776	2.557943	-2.043689	C	-2.943006	2.555151	-0.672108
C	-1.993038	2.052764	0.213536	C	-0.771302	1.538156	-0.250106
C	1.559042	1.112005	0.739219	C	4.026165	0.967645	1.470490
C	4.058493	1.175519	0.143224	S	2.454786	0.893518	2.197302
S	2.531954	1.328416	-0.663683	C	0.132250	0.908539	0.765382
H	0.400724	1.150961	-2.045224	H	-1.258664	2.065023	-3.586140
H	-3.428558	2.949615	-2.741507	H	-3.885298	2.948703	-0.287333
H	-2.199668	2.058486	1.286170	H	4.901991	0.866083	2.113028
H	4.966341	1.266499	-0.454959	H	-0.250195	1.114890	1.774265
C	1.992993	-2.052677	0.214135	C	2.942931	-2.555326	-0.671391
C	2.686653	-2.558525	-2.042962	C	1.472367	-2.064250	-2.515536
C	0.521618	-1.555636	-1.629240	C	0.771242	-1.538204	-0.249618
C	-1.559037	-1.111766	0.739717	C	-4.058521	-1.175589	0.143922
C	-4.026109	-0.967342	1.471128	S	-2.532032	-1.328627	-0.663054
S	-2.454680	-0.892930	2.197809	C	-0.132253	-0.908252	0.765715
H	2.199656	-2.058077	1.286764	H	3.885237	-2.948762	-0.286530
H	3.428415	-2.950395	-2.740690	H	1.258484	-2.066076	-3.585510
H	-0.400863	-1.151572	-2.044813	H	-4.966408	-1.266792	-0.454169
H	-4.901895	-0.865646	2.113697	H	0.250258	-1.114244	1.774647

σ-3



```
#p m062x/def2svp nosymm opt freq
empiricaldispersion=gd3 scrf=(smd,sol
vent=dichloromethane) geom=connectivity
```

Charge = 1, Multiplicity = 2, Point group = C1
Electronic Energy = -2362.859222 Hartree
S^2 = 0.7604

Number of imaginary frequencies = 0

Sum of electronic and zero-point Energies = -2362.554646 Hartree

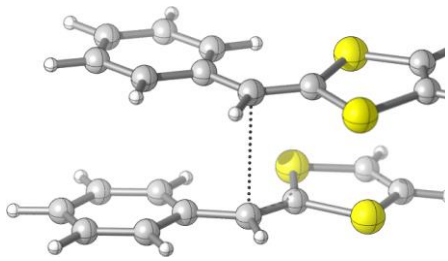
Sum of electronic and thermal Energies = -2362.533935 Hartree

Sum of electronic and thermal Enthalpies = -2362.532990 Hartree

Sum of electronic and thermal Free Energies = -2362.605347 Hartree

	Cartesian Coordinates				Cartesian Coordinates		
Atoms	***X***	***Y***	***Z***	**Atoms**	***X***	***Y***	***Z***
C	-0.419911	1.559835	-1.665035	C	-1.318190	2.117421	-2.576832
C	-2.529788	2.649822	-2.140187	C	-2.837594	2.633423	-0.779497
C	-1.939852	2.081616	0.130957	C	-0.721110	1.531577	-0.296650
C	1.565556	1.089585	0.783363	C	3.999029	0.954660	1.611628
C	4.082836	1.182596	0.289663	S	2.399827	0.854832	2.272576
S	2.588582	1.333574	-0.575382	C	0.130335	0.864100	0.749393
H	0.502442	1.128338	-2.053061	H	-1.065181	2.128093	-3.638158
H	-3.230267	3.080380	-2.857511	H	-3.778937	3.054501	-0.422655
H	-2.185441	2.076146	1.195739	H	4.849090	0.852948	2.287873
H	5.013176	1.292242	-0.269503	H	-0.287518	1.113841	1.735554
C	1.939218	-2.082661	0.128992	C	2.837289	-2.632633	-0.782255
C	2.530157	-2.645906	-2.143132	C	1.318825	-2.112409	-2.579186
C	0.420167	-1.556743	-1.666586	C	0.720808	-1.531450	-0.298018
C	-1.565752	-1.090985	0.782852	C	-4.082963	-1.184542	0.289114
C	-3.999219	-0.957439	1.611224	S	-2.588669	-1.334496	-0.576074
S	-2.400033	-0.857465	2.272328	C	-0.130618	-0.865218	0.748827
H	2.184331	-2.079432	1.193896	H	3.778404	-3.054639	-0.425905
H	3.230973	-3.074881	-2.861077	H	1.066371	-2.120649	-3.640667
H	-0.501964	-1.124220	-2.054028	H	-5.013274	-1.294119	-0.270117
H	-4.849352	-0.856474	2.287489	H	0.287480	-1.115624	1.734722

π-4



```
#p m062x/def2svp opt freq nosymm
scrf=(smd,solvent=dichloromethane)
```

Charge = 1, Multiplicity = 2, Point group = C1
Electronic Energy = -2362.869072 Hartree
$\hat{S}^2$ = 0.7595

Number of imaginary frequencies = 0

Sum of electronic and zero-point Energies = -2362.567874 Hartree

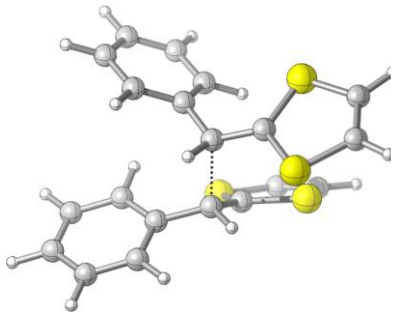
Sum of electronic and thermal Energies = -2362.545969 Hartree

Sum of electronic and thermal Enthalpies = -2362.545025 Hartree

Sum of electronic and thermal Free Energies = -2362.620655 Hartree

	Cartesian Coordinates				Cartesian Coordinates		
Atoms	***X***	***Y***	***Z***	**Atoms**	***X***	***Y***	***Z***
C	0.971041	1.579435	1.455637	C	2.115498	1.747573	2.231369
C	3.344547	2.025055	1.632603	C	3.430072	2.125259	0.240602
C	2.295446	1.951607	-0.538417	C	1.036795	1.686381	0.048975
C	-1.426174	1.432392	-0.615637	C	-3.831640	1.294628	0.340318
C	-3.987428	1.250720	-0.992972	S	-2.206330	1.409626	0.943546
S	-2.546237	1.298435	-1.951515	C	-0.078985	1.529409	-0.862161
C	2.549462	-1.128371	-2.021118	C	3.933124	-1.016410	-1.968627
C	4.593912	-1.109274	-0.741813	C	3.856894	-1.313288	0.427227
C	2.471689	-1.425884	0.380642	C	1.786953	-1.337829	-0.849840
C	-0.650725	-1.657012	-0.106776	C	-3.001803	-2.118946	0.894429
C	-2.181283	-2.025057	1.953856	S	-2.289288	-1.904461	-0.669628
S	-0.510199	-1.680071	1.631768	C	0.352194	-1.455569	-1.023483
H	0.037054	1.363394	1.971400	H	2.042225	1.663499	3.316672
H	4.234966	2.161750	2.248471	H	4.388498	2.335733	-0.236831
H	2.363118	2.029685	-1.625430	H	-4.645869	1.276502	1.066511
H	-4.946689	1.185162	-1.508486	H	0.195419	1.549232	-1.921816
H	2.034091	-1.058471	-2.981541	H	4.499720	-0.858543	-2.887556
H	5.680817	-1.024035	-0.695630	H	4.367175	-1.386957	1.388869
H	1.944194	-1.596051	1.317731	H	-4.071193	-2.329950	0.948393
H	-2.485256	-2.140234	2.995428	H	0.020008	-1.440052	-2.066512

TS-4



```
#p m062x/def2svp opt=(calcfc,ts,noeigen) freq nosymm
scrf=(smd,solvent=dichloromethane)
```

Charge = 1, Multiplicity = 2, Point group = C1
Electronic Energy = -2362.854667 Hartree
$\hat{S}^2$ = 0.7642

Number of imaginary frequencies = 1, vi = -294.40

Sum of electronic and zero-point Energies = -2362.551975 Hartree

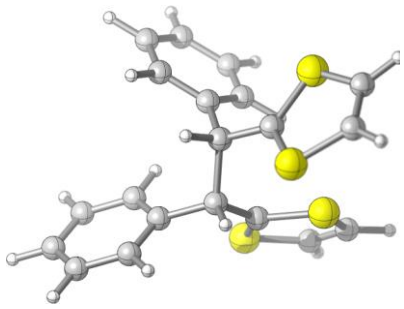
Sum of electronic and thermal Energies = -2362.531176 Hartree

Sum of electronic and thermal Enthalpies = -2362.530231 Hartree

Sum of electronic and thermal Free Energies = -2362.603906 Hartree

	Cartesian Coordinates				Cartesian Coordinates		
Atoms	***X***	***Y***	***Z***	**Atoms**	***X***	***Y***	***Z***
C	0.124218	-1.535456	-1.533174	C	0.833425	-2.239593	-2.505864
C	1.879482	-3.085508	-2.137134	C	2.218731	-3.223014	-0.790007
C	1.516344	-2.515712	0.182015	C	0.454854	-1.671345	-0.175511
C	-1.644876	-0.866832	0.986005	C	-4.183049	-0.899008	0.581236
C	-4.032009	-0.310415	1.779581	S	-2.744865	-1.446053	-0.220137
S	-2.409382	-0.174042	2.378677	C	-0.226012	-0.898427	0.893546
C	2.348440	1.228292	2.298636	C	3.702970	1.156750	2.612675
C	4.622019	0.733096	1.651270	C	4.175579	0.373635	0.380144
C	2.819651	0.444828	0.062024	C	1.889892	0.889515	1.015616
C	-0.101364	1.549293	-0.424095	C	-1.796698	2.456416	-2.136959
C	-0.627060	2.381299	-2.795688	S	-1.772886	1.979987	-0.469874
S	0.743288	1.809715	-1.903465	C	0.428034	0.975559	0.760673
H	-0.675625	-0.861754	-1.849121	H	0.568306	-2.120805	-3.557626
H	2.431982	-3.635819	-2.900482	H	3.038912	-3.879421	-0.495140
H	1.791814	-2.608840	1.234985	H	-5.141554	-1.071984	0.089530
H	-4.846640	0.061223	2.402942	H	0.259380	-1.007205	1.869492
H	1.630186	1.560475	3.052256	H	4.041907	1.433761	3.612213
H	5.684114	0.676460	1.895150	H	4.884413	0.023574	-0.371885
H	2.497634	0.112929	-0.926678	H	-2.736728	2.808259	-2.563969
H	-0.477687	2.660835	-3.839867	H	-0.123432	1.304572	1.649629

σ-4



```
#p m062x/def2svp opt freq nosymm
scrf=(smd,solvent=dichloromethane)
```

Charge = 1, Multiplicity = 2, Point group = C1
Electronic Energy = -2362.859759 Hartree
$\hat{S}^2$ = 0.7566

Number of imaginary frequencies = 0

Sum of electronic and zero-point Energies = -2362.555441 Hartree

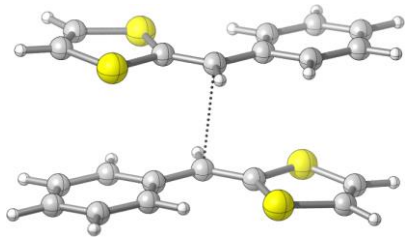
Sum of electronic and thermal Energies = -2362.534490 Hartree

Sum of electronic and thermal Enthalpies = -2362.533546 Hartree

Sum of electronic and thermal Free Energies = -2362.607679 Hartree

	Cartesian Coordinates				Cartesian Coordinates		
Atoms	***X***	***Y***	***Z***	**Atoms**	***X***	***Y***	***Z***
C	-0.168663	-1.888510	-1.008912	C	0.300890	-3.039400	-1.641198
C	1.066148	-3.966537	-0.932882	C	1.352910	-3.742359	0.413493
C	0.886809	-2.589518	1.043797	C	0.127600	-1.647787	0.340776
C	-1.770132	-0.153272	1.055805	C	-4.318129	-0.288020	0.839700
C	-4.090849	0.844081	1.525251	S	-2.942835	-1.276792	0.446050
S	-2.435422	1.184567	1.946142	C	-0.300635	-0.378635	1.044664
C	2.509454	1.730911	1.776912	C	3.865702	1.693014	2.097155
C	4.708083	0.782409	1.459964	C	4.186575	-0.089923	0.505009
C	2.829077	-0.056294	0.186161	C	1.976203	0.861255	0.817995
C	0.150985	1.266665	-0.881879	C	-1.188024	1.787796	-2.991187
C	0.081309	1.596439	-3.406919	S	-1.457093	1.648150	-1.289304
S	1.241246	1.243098	-2.184566	C	0.491852	0.937022	0.522121
H	-0.777748	-1.185063	-1.581473	H	0.064838	-3.212012	-2.692426
H	1.433713	-4.865848	-1.429836	H	1.946043	-4.465161	0.975975
H	1.126126	-2.406438	2.093823	H	-5.306207	-0.639964	0.539004
H	-4.863149	1.537693	1.860093	H	0.059078	-0.435509	2.084496
H	1.853324	2.447786	2.276030	H	4.264055	2.379805	2.845665
H	5.770468	0.751871	1.707320	H	4.837604	-0.808461	0.004621
H	2.444245	-0.759958	-0.554502	H	-2.034232	2.030557	-3.635944
H	0.422320	1.663812	-4.441586	H	0.079030	1.749000	1.144372

π-5



```
#p m062x/def2svp opt freq nosymm
scrf=(smd,solvent=dichloromethane)
```

Charge = 1, Multiplicity = 2, Point group = C1
Electronic Energy = -2362.865229 Hartree
$\hat{S}^2$ = 0.7601

Number of imaginary frequencies = 0

Sum of electronic and zero-point Energies = -2362.564341 Hartree

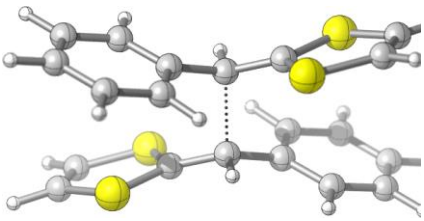
Sum of electronic and thermal Energies = -2362.542268 Hartree

Sum of electronic and thermal Enthalpies = -2362.541324 Hartree

Sum of electronic and thermal Free Energies = -2362.618650 Hartree

	Cartesian Coordinates				Cartesian Coordinates		
Atoms	***X***	***Y***	***Z***	**Atoms**	***X***	***Y***	***Z***
C	1.758393	-2.339988	-0.446109	C	3.078401	-2.682944	-0.723443
C	4.121823	-2.191465	0.063811	C	3.837632	-1.341109	1.134536
C	2.521655	-0.994893	1.416693	C	1.451446	-1.495474	0.642177
C	-1.122691	-1.490472	0.620955	C	-3.222755	-2.552820	-0.457893
C	-3.697954	-1.747541	0.506914	S	-1.498352	-2.608775	-0.661491
S	-2.533982	-0.863181	1.430700	C	0.121555	-1.070434	1.030642
C	-2.498372	0.961821	-1.432837	C	-3.822186	1.292633	-1.170069
C	-4.130503	2.157206	-0.117354	C	-3.102929	2.679426	0.670756
C	-1.775031	2.351155	0.413503	C	-1.444114	1.490744	-0.655100
C	1.129594	1.509372	-0.595852	C	3.701058	1.783410	-0.438664
C	3.204740	2.585240	0.517972	S	2.558362	0.892979	-1.384110
S	1.476192	2.632925	0.690796	C	-0.104645	1.076491	-1.021237
H	0.979598	-2.734069	-1.098145	H	3.294011	-3.339170	-1.567987
H	5.153297	-2.468392	-0.159639	H	4.645816	-0.946664	1.752751
H	2.300987	-0.333627	2.258097	H	-3.834448	-3.170222	-1.117071
H	-4.754426	-1.614160	0.744861	H	0.106716	-0.348647	1.854393
H	-2.258667	0.290959	-2.261394	H	-4.617853	0.875596	-1.789711
H	-5.168368	2.422276	0.090408	H	-3.336821	3.348516	1.500192
H	-1.009068	2.770843	1.064673	H	4.762292	1.656636	-0.658094
H	3.801431	3.206012	1.187688	H	-0.071953	0.349038	-1.839236

TS-5



```
#p m062x/def2svp opt=(calcfc,ts,noeigen) freq
nosymm scrf=(smd,solvent=dichloromethane)
```

Charge = 1, Multiplicity = 2, Point group = C1
Electronic Energy = -2362.854707 Hartree
$\hat{S}^2$ = 0.7665

Number of imaginary frequencies = 1, vi = -275.22

Sum of electronic and zero-point Energies = -2362.551468 Hartree

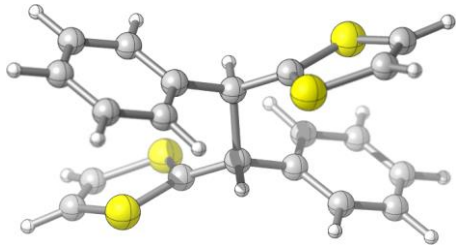
Sum of electronic and thermal Energies = -2362.530697 Hartree

Sum of electronic and thermal Enthalpies = -2362.529753 Hartree

Sum of electronic and thermal Free Energies = -2362.603464 Hartree

Atoms	Cartesian Coordinates			Atoms	Cartesian Coordinates		
	X	***Y***	***Z***		***X***	***Y***	***Z***
C	1.526651	-2.260894	-0.630269	C	2.773864	-2.872826	-0.751264
C	3.744316	-2.695567	0.234188	C	3.461939	-1.899509	1.344911
C	2.213814	-1.293802	1.471332	C	1.225675	-1.475605	0.492583
C	-1.317433	-1.361853	0.464559	C	-3.345836	-2.711526	-0.374844
C	-3.847354	-1.851296	0.527397	S	-1.634997	-2.641780	-0.652491
S	-2.719369	-0.785408	1.292224	C	-0.053437	-0.731811	0.656252
C	-2.213943	1.293518	-1.471321	C	-3.462167	1.898973	-1.344687
C	-3.744497	2.695021	-0.233943	C	-2.773884	2.872533	0.751301
C	-1.526569	2.260841	0.630104	C	-1.225654	1.475546	-0.492760
C	1.317513	1.362016	-0.464844	C	3.847456	1.851427	-0.527483
C	3.345794	2.712028	0.374323	S	2.719592	0.785211	-1.292030
S	1.634911	2.642398	0.651730	C	0.053549	0.731945	-0.656600
H	0.814107	-2.369390	-1.450156	H	2.991735	-3.478723	-1.632179
H	4.720979	-3.171559	0.133426	H	4.216513	-1.748856	2.118748
H	1.995980	-0.668985	2.340723	H	-3.925690	-3.449144	-0.931459
H	-4.898704	-1.783243	0.811145	H	-0.047810	-0.106350	1.557175
H	-1.996147	0.668749	-2.340756	H	-4.216854	1.748142	-2.118380
H	-4.721235	3.170823	-0.133018	H	-2.991692	3.478454	1.632214
H	-0.813872	2.369649	1.449820	H	4.898856	1.783227	-0.811012
H	3.925564	3.449857	0.930742	H	0.047934	0.106588	-1.557600

σ-5



```
#p m062x/def2svp opt freq nosymm
scrf=(smd,solvent=dichloromethane)
```

Charge = 1, Multiplicity = 2, Point group = C1
Electronic Energy = -2362.857236 Hartree
$\hat{S}^2$ = 0.7578

Number of imaginary frequencies = 0

Sum of electronic and zero-point Energies = -2362.553557 Hartree

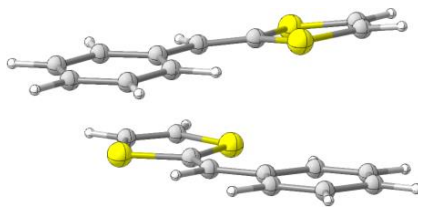
Sum of electronic and thermal Energies = -2362.532214 Hartree

Sum of electronic and thermal Enthalpies = -2362.531270 Hartree

Sum of electronic and thermal Free Energies = -2362.607360 Hartree

	Cartesian Coordinates				Cartesian Coordinates		
Atoms	***X***	***Y***	***Z***	**Atoms**	***X***	***Y***	***Z***
C	1.606497	-2.139161	-0.737659	C	2.811071	-2.836226	-0.822567
C	3.689401	-2.855096	0.261178	C	3.357069	-2.172884	1.431090
C	2.148380	-1.482312	1.518895	C	1.258786	-1.463673	0.439759
C	-1.266328	-1.388131	0.409420	C	-3.258525	-2.720298	-0.520665
C	-3.744193	-2.059373	0.544209	S	-1.578498	-2.482865	-0.885022
S	-2.630107	-1.049545	1.402917	C	-0.006616	-0.642489	0.558026
C	-2.125224	1.457911	-1.494783	C	-3.338472	2.139737	-1.397226
C	-3.678265	2.797395	-0.215636	C	-2.804458	2.761641	0.871511
C	-1.597074	2.071129	0.777965	C	-1.241211	1.422481	-0.412099
C	1.279536	1.376152	-0.406824	C	3.736581	2.107736	-0.561656
C	3.186316	2.912266	0.365483	S	2.689278	0.934635	-1.279468
S	1.504960	2.669824	0.699716	C	0.029657	0.610911	-0.534794
H	0.962773	-2.100830	-1.620397	H	3.068935	-3.356378	-1.746505
H	4.634159	-3.396599	0.191221	H	4.040731	-2.176551	2.281725
H	1.892306	-0.944368	2.434727	H	-3.832730	-3.397592	-1.154156
H	-4.773155	-2.120272	0.901647	H	-0.012940	-0.154121	1.543442
H	-1.861878	0.940801	-2.420518	H	-4.019110	2.156482	-2.250090
H	-4.626254	3.332275	-0.138756	H	-3.068959	3.261875	1.804500
H	-0.954501	2.015884	1.660919	H	4.777445	2.144084	-0.886361
H	3.710846	3.703049	0.903713	H	0.033563	0.110869	-1.515362

π-6



```
#p m062x/def2svp opt nosymm freq
empiricaldispersion=gd3 scrf=(smd,sol
vent=dichloromethane) geom=connectivity
```

Charge = 1, Multiplicity = 2, Point group = C1
Electronic Energy = -2362.870313 Hartree
$\hat{S}^2$ = 0.7596

Number of imaginary frequencies = 0

Sum of electronic and zero-point Energies = -2362.568569 Hartree

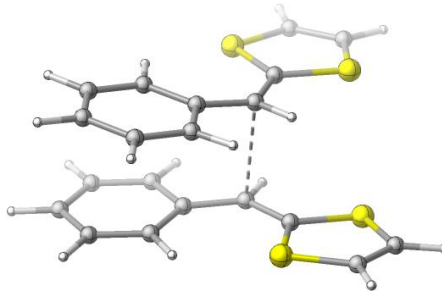
Sum of electronic and thermal Energies = -2362.546676 Hartree

Sum of electronic and thermal Enthalpies = -2362.545732 Hartree

Sum of electronic and thermal Free Energies = -2362.621945 Hartree

	Cartesian Coordinates				Cartesian Coordinates		
Atoms	***X***	***Y***	***Z***	**Atoms**	***X***	***Y***	***Z***
C	1.975985	-1.105790	1.350119	C	3.315281	-0.779493	1.536885
C	3.679716	0.452945	2.086534	C	2.688781	1.363863	2.456128
C	1.348434	1.047441	2.265987	C	0.959718	-0.192499	1.706521
C	-1.154940	-1.440606	0.962708	C	-2.018472	-3.574075	-0.233482
C	-3.121618	-2.863787	0.045012	S	-0.492587	-2.907313	0.278054
S	-2.905860	-1.358035	0.880919	C	-0.461243	-0.396091	1.516495
C	-2.805266	1.598614	-1.008643	C	-3.624609	2.608344	-0.514644
C	-3.065052	3.688711	0.167432	C	-1.680256	3.751853	0.351461
C	-0.855050	2.749466	-0.144089	C	-1.404458	1.649960	-0.839111
C	0.711246	0.353702	-1.498535	C	2.985657	-0.718577	-2.103983
C	3.285809	0.499670	-1.612536	S	1.316405	-1.149400	-2.147415
S	1.967193	1.488605	-1.094079	C	-0.644480	0.529335	-1.358517
H	1.743441	-2.086179	0.937409	H	4.084956	-1.500152	1.255412
H	4.733164	0.696286	2.234003	H	2.961545	2.325406	2.893674
H	0.572031	1.759751	2.554826	H	-2.007051	-4.539598	-0.740839
H	-4.138254	-3.171843	-0.204376	H	-1.083564	0.431587	1.871185
H	-3.243143	0.755530	-1.546665	H	-4.703921	2.551493	-0.662919
H	-3.704310	4.482076	0.557929	H	-1.238740	4.591083	0.890950
H	0.214349	2.826307	0.048643	H	3.716733	-1.442836	-2.466103
H	4.295192	0.904669	-1.523109	H	-1.255595	-0.299661	-1.732851

π-7



```
#p m062x/def2svp opt freq empiricaldispersion=gd3
nosymm geom=connecti vity
scrf=(smd,solvent=dichloromethane)
```

Charge = 2, Multiplicity = 1, Point group = C1

Electronic Energy = -2362.655555 Hartree

Number of imaginary frequencies = 0

Sum of electronic and zero-point Energies = -2362.351565 Hartree

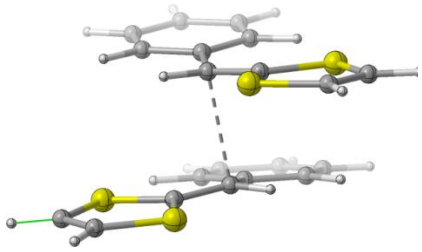
Sum of electronic and thermal Energies = -2362.330405 Hartree

Sum of electronic and thermal Enthalpies = -2362.329461 Hartree

Sum of electronic and thermal Free Energies = -2362.401778 Hartree

	Cartesian Coordinates				Cartesian Coordinates		
Atoms	***X***	***Y***	***Z***	**Atoms**	***X***	***Y***	***Z***
C	2.106962	0.210437	-1.279628	C	3.463308	0.044123	-1.501293
C	4.044533	0.477867	-2.700414	C	3.264786	1.092846	-3.682917
C	1.905272	1.266512	-3.471321	C	1.292630	0.824115	-2.265934
C	-1.004068	0.754028	-1.106191	C	-3.184235	0.639688	0.243524
C	-2.269997	-0.027293	0.977921	S	-2.622135	1.330384	-1.230362
S	-0.666691	-0.103491	0.345328	C	-0.117808	1.015008	-2.169518
H	1.705481	-0.121875	-0.324355	H	4.081212	-0.421476	-0.732681
H	5.116329	0.347656	-2.859931	H	3.722565	1.446441	-4.607108
H	1.296400	1.778161	-4.218926	H	-4.229253	0.787668	0.523199
H	-2.464655	-0.500724	1.942817	H	-0.560759	1.599666	-2.983046
C	0.621409	-2.755285	-1.576290	C	1.838824	-3.357205	-1.293905
C	2.879787	-3.282561	-2.222026	C	2.699521	-2.609829	-3.438261
C	1.490814	-2.001335	-3.729416	C	0.420299	-2.057177	-2.799828
C	-1.402226	-0.781167	-4.095777	C	-1.956303	0.445843	-6.274757
C	-3.114363	0.422102	-5.582635	S	-0.596567	-0.322555	-5.544685
S	-3.075800	-0.381162	-4.061264	C	-0.851876	-1.435624	-2.974550
H	-0.209365	-2.850471	-0.873782	H	1.975076	-3.897406	-0.356707
H	3.835253	-3.764356	-2.007167	H	3.512929	-2.567185	-4.163497
H	1.393879	-1.500301	-4.690529	H	-1.825030	0.895038	-7.261398
H	-4.059334	0.847931	-5.924852	H	-1.579304	-1.636814	-2.179639

TS-6



```
#p m062x/def2svp opt=(calcfc,ts,noeigen) freq
empiricaldispersion=gd3 nosymm geom=connectivity
scrf=(smd,solvent=dichloromethane)
```

Charge = 2, Multiplicity = 1, Point group = C1

Electronic Energy = -2362.655517 Hartree

Number of imaginary frequencies = 1, vi = -48.47

Sum of electronic and zero-point Energies = -2362.351697 Hartree

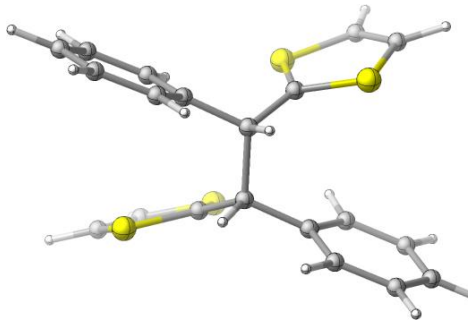
Sum of electronic and thermal Energies = -2362.331202 Hartree

Sum of electronic and thermal Enthalpies = -2362.330258 Hartree

Sum of electronic and thermal Free Energies = -2362.401276 Hartree

	Cartesian Coordinates				Cartesian Coordinates		
Atoms	***X***	***Y***	***Z***	**Atoms**	***X***	***Y***	***Z***
C	2.095509	0.179870	-1.260866	C	3.458996	0.039940	-1.463206
C	4.052192	0.508239	-2.642211	C	3.277021	1.127906	-3.625057
C	1.910179	1.270774	-3.434354	C	1.288461	0.798411	-2.247750
C	-1.017275	0.747803	-1.092155	C	-3.186798	0.725573	0.276955
C	-2.280715	0.063527	1.025623	S	-2.621539	1.351611	-1.223822
S	-0.687078	-0.070633	0.378689	C	-0.131743	0.955828	-2.174214
H	1.683104	-0.187892	-0.323069	H	4.070837	-0.433803	-0.694670
H	5.128428	0.399517	-2.786695	H	3.742984	1.507275	-4.534873
H	1.304339	1.780972	-4.186133	H	-4.225504	0.907861	0.559627
H	-2.475600	-0.373309	2.007376	H	-0.569236	1.539885	-2.990266
C	0.643516	-2.761888	-1.611589	C	1.850644	-3.396445	-1.355259
C	2.885539	-3.320122	-2.289655	C	2.708705	-2.612729	-3.485415
C	1.507323	-1.976683	-3.752248	C	0.444901	-2.036351	-2.816487
C	-1.397146	-0.772768	-4.102995	C	-1.989792	0.374583	-6.313319
C	-3.142865	0.347112	-5.613210	S	-0.610302	-0.339248	-5.565470
S	-3.075925	-0.406959	-4.067977	C	-0.820261	-1.383973	-2.964875
H	-0.180334	-2.849953	-0.899780	H	1.983723	-3.960553	-0.431762
H	3.833437	-3.824552	-2.094442	H	3.517698	-2.563026	-4.215187
H	1.416079	-1.444026	-4.696866	H	-1.873469	0.792880	-7.315223
H	-4.099463	0.740375	-5.961909	H	-1.541069	-1.594811	-2.167060

σ-6



```
#p m062x/def2svp opt freq
empiricaldispersion=gd3 nosymm
geom=connectivity
scrf=(smd,solvent=dichloromethane)
```

Charge = 2, Multiplicity = 1, Point group = C1

Electronic Energy = -2362.691479 Hartree

Number of imaginary frequencies = 0

Sum of electronic and zero-point Energies = -2362.384318 Hartree

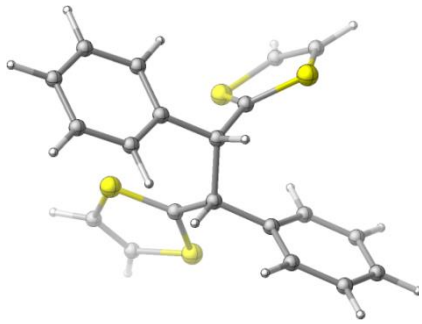
Sum of electronic and thermal Energies = -2362.364060 Hartree

Sum of electronic and thermal Enthalpies = -2362.363116 Hartree

Sum of electronic and thermal Free Energies = -2362.434838 Hartree

	Cartesian Coordinates				Cartesian Coordinates		
Atoms	***X***	***Y***	***Z***	**Atoms**	***X***	***Y***	***Z***
C	1.498157	1.894078	-3.192055	C	1.713293	3.098152	-3.860222
C	0.648533	3.966514	-4.100896	C	-0.632767	3.625404	-3.671381
C	-0.847621	2.424702	-2.995939	C	0.215479	1.550012	-2.744344
C	0.761915	-0.166474	-0.916446	C	2.626323	-0.833409	0.685134
C	1.473638	-1.068704	1.355525	S	2.448225	-0.197346	-0.897274
S	0.035949	-0.700776	0.504223	C	-0.112779	0.224509	-2.078895
H	2.357170	1.231365	-3.058098	H	2.718857	3.352898	-4.197437
H	0.818968	4.908554	-4.624120	H	-1.471572	4.297856	-3.856290
H	-1.852691	2.165628	-2.654543	H	3.634082	-0.994832	1.073718
H	1.402212	-1.454432	2.374820	H	-1.122989	0.320899	-1.655993
C	-2.024247	-2.586760	-2.316889	C	-2.426090	-3.732193	-1.631010
C	-1.473451	-4.577784	-1.065100	C	-0.118284	-4.268943	-1.180191
C	0.284111	-3.119536	-1.858822	C	-0.666592	-2.272356	-2.443809
C	0.752723	-1.011275	-4.180876	C	2.871591	-1.277343	-5.566639
C	2.048859	-0.501540	-6.311560	S	2.241538	-1.792965	-4.057466
S	0.524899	-0.158898	-5.614544	C	-0.321220	-0.960999	-3.127529
H	-2.772933	-1.928421	-2.763886	H	-3.488436	-3.964854	-1.545163
H	-1.785495	-5.477406	-0.532653	H	0.634730	-4.921105	-0.735781
H	1.354670	-2.902905	-1.892995	H	3.872383	-1.605524	-5.854984
H	2.281690	-0.098199	-7.299424	H	-1.225321	-0.635370	-3.661965

σ-7



```
#p m062x/def2svp opt freq empiricaldispersion=gd3
nosymm geom=connectivity
scrf=(smd,solvent=dichloromethane)
```

Charge = 2, Multiplicity = 1, Point group = C1

Electronic Energy = -2362.694716 Hartree

Number of imaginary frequencies = 0

Sum of electronic and zero-point Energies = -2362.387660 Hartree

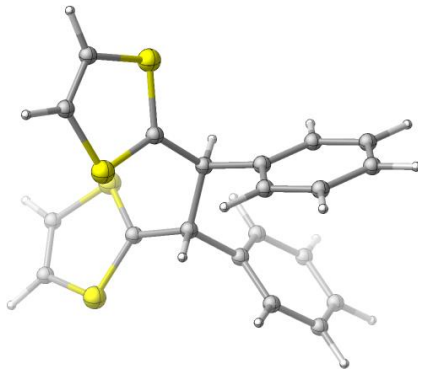
Sum of electronic and thermal Energies = -2362.367401 Hartree

Sum of electronic and thermal Enthalpies = -2362.366456 Hartree

Sum of electronic and thermal Free Energies = -2362.438176 Hartree

	Cartesian Coordinates				Cartesian Coordinates		
Atoms	***X***	***Y***	***Z***	**Atoms**	***X***	***Y***	***Z***
C	1.232195	2.452871	-2.176760	C	1.354705	3.716603	-2.758859
C	0.384019	4.183086	-3.640281	C	-0.731974	3.390696	-3.916752
C	-0.857574	2.132085	-3.337133	C	0.138745	1.636407	-2.482161
C	1.061043	-0.237387	-1.016474	C	2.317898	-1.129639	1.003042
C	3.235198	-1.071994	0.008696	S	0.737319	-0.618494	0.583685
S	2.661481	-0.482702	-1.497754	C	-0.039283	0.217877	-1.936543
H	2.003052	2.137878	-1.473808	H	2.218595	4.335579	-2.513041
H	0.486989	5.166789	-4.100443	H	-1.512222	3.754402	-4.586814
H	-1.745519	1.536399	-3.559049	H	2.510146	-1.468065	2.023618
H	4.287085	-1.353431	0.095599	H	-0.966442	0.206458	-1.341992
C	-2.143195	-2.485281	-2.564191	C	-2.636971	-3.667601	-2.015785
C	-1.771313	-4.561055	-1.386390	C	-0.410157	-4.268325	-1.308309
C	0.084390	-3.084410	-1.853357	C	-0.779378	-2.179720	-2.488732
C	0.781140	-0.970548	-4.098184	C	2.488117	-0.536548	-5.936297
C	2.379037	-1.882707	-5.857505	S	1.499595	0.361423	-4.860073
S	1.277692	-2.472319	-4.684572	C	-0.314860	-0.848542	-3.061091
H	-2.824053	-1.788222	-3.058256	H	-3.702607	-3.890584	-2.084184
H	-2.156220	-5.487864	-0.958587	H	0.275392	-4.963424	-0.821994
H	1.157994	-2.894377	-1.779564	H	3.141858	0.009496	-6.620358
H	2.927495	-2.601481	-6.470052	H	-1.171912	-0.443103	-3.621102

σ-8



```
#p m062x/def2svp opt freq empiricaldispersion=gd3
nosymm geom=connectivity
scrf=(smd,solvent=dichloromethane)
```

Charge = 2, Multiplicity = 1, Point group = C1

Electronic Energy = -2362.694867 Hartree

Number of imaginary frequencies = 0

Sum of electronic and zero-point Energies = -2362.388739 Hartree

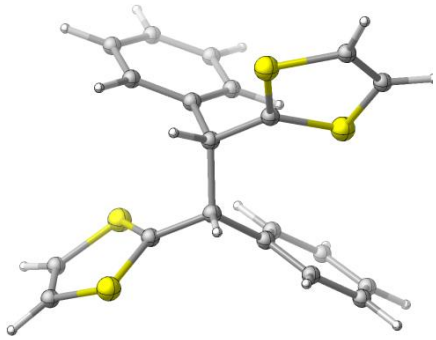
Sum of electronic and thermal Energies = -2362.368139 Hartree

Sum of electronic and thermal Enthalpies = -2362.367195 Hartree

Sum of electronic and thermal Free Energies = -2362.440837 Hartree

	Cartesian Coordinates				Cartesian Coordinates		
Atoms	***X***	***Y***	***Z***	**Atoms**	***X***	***Y***	***Z***
C	1.444775	-0.165576	-0.244872	C	2.652249	-0.188582	0.450382
C	3.807434	0.330080	-0.136006	C	3.753178	0.873319	-1.419212
C	2.546529	0.898621	-2.117440	C	1.390541	0.375818	-1.533164
C	-1.006319	1.031168	-1.567263	C	-2.463359	2.779011	-0.436406
C	-2.946922	1.586754	-0.018107	S	-1.130324	2.708901	-1.514719
S	-2.140727	0.203446	-0.636843	C	0.096061	0.355241	-2.346099
H	0.551432	-0.578428	0.231691	H	2.688136	-0.612389	1.454925
H	4.751545	0.311722	0.410462	H	4.653568	1.278362	-1.883151
H	2.503764	1.314493	-3.126338	H	-2.855350	3.756722	-0.147070
H	-3.785988	1.443017	0.666397	H	0.277214	0.964391	-3.248034
C	1.625103	-2.780390	-2.983138	C	2.726692	-3.316394	-3.649840
C	3.120204	-2.795554	-4.881853	C	2.409716	-1.737212	-5.450595
C	1.308543	-1.199521	-4.787614	C	0.917913	-1.717260	-3.548716
C	-1.509957	-1.221771	-3.592533	C	-3.574664	-2.156019	-4.743134
C	-3.425645	-0.905479	-5.237393	S	-2.406435	-2.646567	-3.585689
S	-2.086907	-0.022644	-4.624542	C	-0.245845	-1.098821	-2.775325
H	1.322250	-3.179905	-2.012793	H	3.280244	-4.141710	-3.199889
H	3.982862	-3.214939	-5.401773	H	2.713148	-1.327201	-6.414794
H	0.767796	-0.365991	-5.245335	H	-4.369289	-2.853674	-5.016581
H	-4.076578	-0.428703	-5.973957	H	-0.389085	-1.706114	-1.865436

σ-9



```
#p m062x/def2svp opt freq empiricaldispersion=gd3
nosymm geom=connectivity
scrf=(smd,solvent=dichloromethane)
```

Charge = 2, Multiplicity = 1, Point group = C1

Electronic Energy = -2362.695517 Hartree

Number of imaginary frequencies = 0

Sum of electronic and zero-point Energies = -2362.387904 Hartree

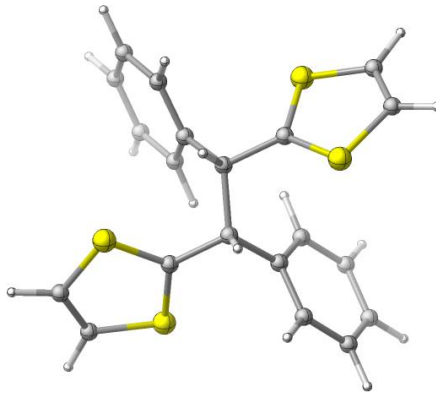
Sum of electronic and thermal Energies = -2362.367691 Hartree

Sum of electronic and thermal Enthalpies = -2362.366747 Hartree

Sum of electronic and thermal Free Energies = -2362.438458 Hartree

Atoms	Cartesian Coordinates			Atoms	Cartesian Coordinates		
	X	***Y***	***Z***		***X***	***Y***	***Z***
C	2.123558	0.650575	-2.002011	C	3.305995	1.298446	-2.357882
C	3.271057	2.425737	-3.178496	C	2.047354	2.912090	-3.637617
C	0.865273	2.262972	-3.287587	C	0.893217	1.116146	-2.481249
C	-0.615131	0.222989	-0.692919	C	-1.275387	0.623794	1.732004
C	-0.484778	-0.474913	1.746089	S	-1.541299	1.318161	0.189348
S	0.106061	-0.995910	0.222033	C	-0.438993	0.437024	-2.176275
H	2.186553	-0.221966	-1.349166	H	4.258233	0.921672	-1.982588
H	4.198353	2.932682	-3.449752	H	2.010128	3.801367	-4.268294
H	-0.092019	2.643203	-3.652878	H	-1.744011	1.081130	2.605772
H	-0.213986	-1.050438	2.634132	H	-1.220151	1.156238	-2.462916
C	-0.790601	-3.157335	-1.997465	C	-0.165078	-4.335190	-1.593312
C	1.197999	-4.515111	-1.825523	C	1.927613	-3.521457	-2.478653
C	1.302412	-2.344677	-2.889289	C	-0.059606	-2.143952	-2.632191
C	-0.758341	-0.598758	-4.480080	C	-0.131273	-0.151224	-6.900904
C	-1.458076	-0.421737	-6.919914	S	0.618993	-0.189370	-5.359996
S	-2.158883	-0.769354	-5.397477	C	-0.799094	-0.860642	-2.994398
H	-1.857272	-3.017475	-1.806151	H	-0.746476	-5.113327	-1.096891
H	1.691634	-5.434975	-1.508415	H	2.990732	-3.662072	-2.678358
H	1.902993	-1.594128	-3.405972	H	0.479809	0.093512	-7.772548
H	-2.092345	-0.433828	-7.808660	H	-1.857666	-1.039675	-2.755349

σ-10



```
#p m062x/def2svp opt freq empiricaldispersion=gd3
nosymm geom=connectivity
scrf=(smd,solvent=dichloromethane)
```

Charge = 2, Multiplicity = 1, Point group = C1

Electronic Energy = -2362.693939 Hartree

Number of imaginary frequencies = 0

Sum of electronic and zero-point Energies = -2362.387182 Hartree

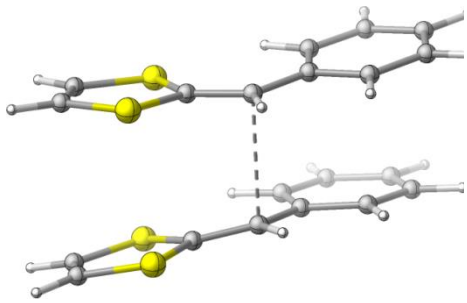
Sum of electronic and thermal Energies = -2362.366883 Hartree

Sum of electronic and thermal Enthalpies = -2362.365939 Hartree

Sum of electronic and thermal Free Energies = -2362.437480 Hartree

	Cartesian Coordinates				Cartesian Coordinates		
Atoms	***X***	***Y***	***Z***	**Atoms**	***X***	***Y***	***Z***
C	1.840125	0.741705	-3.289857	C	2.875796	1.596506	-3.668467
C	2.759620	2.971844	-3.475010	C	1.595790	3.496050	-2.912359
C	0.556644	2.645189	-2.544073	C	0.673084	1.258949	-2.716282
C	-0.502000	0.222536	-0.753092	C	0.035458	0.366088	1.723017
C	-1.062976	-0.419517	1.642199	S	0.643991	0.962570	0.234592
S	-1.660906	-0.692815	0.057736	C	-0.502587	0.401397	-2.256473
H	1.961992	-0.328081	-3.462308	H	3.777248	1.178387	-4.118159
H	3.572981	3.636234	-3.770241	H	1.490056	4.572121	-2.768139
H	-0.359064	3.061033	-2.114738	H	0.547317	0.644695	2.646582
H	-1.582293	-0.880018	2.485030	H	-1.410500	1.003437	-2.444793
C	-0.761386	-3.431102	-2.564719	C	-0.205369	-4.614748	-2.084729
C	1.028391	-4.591910	-1.434420	C	1.700595	-3.382303	-1.266280
C	1.150928	-2.197480	-1.756078	C	-0.083812	-2.213242	-2.415423
C	-0.526780	-0.835901	-4.475529	C	0.109556	-1.258703	-6.895431
C	-0.525315	-0.064069	-6.897834	S	0.253670	-2.030703	-5.370002
S	-1.074294	0.484580	-5.367899	C	-0.753055	-0.966394	-2.984880
H	-1.736756	-3.450531	-3.059101	H	-0.743781	-5.555036	-2.210535
H	1.462661	-5.516341	-1.051111	H	2.660835	-3.354108	-0.749729
H	1.698655	-1.266520	-1.604451	H	0.522669	-1.756134	-7.775316
H	-0.708092	0.560112	-7.775141	H	-1.841591	-1.147553	-2.908359

π-8



```
#p m062x/def2svp opt freq
empiricaldispersion=gd3 nosymm
geom=connectivity
scrf=(smd,solvent=dichloromethane)
```

Charge = 2, Multiplicity = 1, Point group = C1

Electronic Energy = -2362.658833 Hartree

Number of imaginary frequencies = 0

Sum of electronic and zero-point Energies = -2362.355409 Hartree

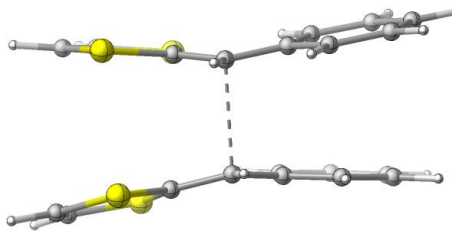
Sum of electronic and thermal Energies = -2362.334252 Hartree

Sum of electronic and thermal Enthalpies = -2362.333308 Hartree

Sum of electronic and thermal Free Energies = -2362.405335 Hartree

	Cartesian Coordinates				Cartesian Coordinates		
Atoms	***X***	***Y***	***Z***	**Atoms**	***X***	***Y***	***Z***
C	-1.200927	-1.911165	1.007873	C	-2.417979	-2.257047	1.572936
C	-3.582661	-2.268768	0.795734	C	-3.530469	-1.926618	-0.558039
C	-2.319228	-1.578325	-1.133314	C	-1.121532	-1.579379	-0.371489
C	1.405706	-1.294623	-0.687474	C	3.970770	-1.149777	-0.752168
C	3.664908	-1.570179	0.497097	S	2.647803	-0.856442	-1.801750
S	1.997823	-1.786853	0.857815	C	0.067100	-1.215004	-1.079655
C	-2.696889	1.562701	-1.529407	C	-4.062416	1.484650	-1.312231
C	-4.544225	1.280852	-0.015871	C	-3.657301	1.164587	1.062932
C	-2.291158	1.259175	0.858375	C	-1.779475	1.465017	-0.447594
C	0.743520	1.644595	0.022227	C	3.200089	1.987550	0.708865
C	2.557535	1.623845	1.839229	S	2.238426	2.111237	-0.713145
S	0.869103	1.300271	1.710200	C	-0.399023	1.599088	-0.783821
H	-0.327048	-1.909346	1.657252	H	-2.464725	-2.517938	2.630601
H	-4.534395	-2.548448	1.250688	H	-4.438996	-1.931330	-1.161462
H	-2.267725	-1.320096	-2.192767	H	4.982840	-0.991198	-1.130794
H	4.396952	-1.808750	1.271293	H	-0.085182	-0.951973	-2.131174
H	-2.307042	1.712762	-2.538595	H	-4.756019	1.575156	-2.148575
H	-5.619368	1.215737	0.160688	H	-4.042945	1.009589	2.071151
H	-1.637585	1.192014	1.727199	H	4.262894	2.229919	0.643405
H	3.027424	1.516270	2.819107	H	-0.207453	1.820232	-1.839627

TS-7



```
#p m062x/def2svp opt=(calcfc,ts,noeigen) freq
empiricaldispersion=gd3 nosymm geom=connectivity
scrf=(smd,solvent=dichloromethane)
```

Charge = 2, Multiplicity = 1, Point group = C1

Electronic Energy = -2362.658198 Hartree

Number of imaginary frequencies = 1, vi = -81.53

Sum of electronic and zero-point Energies = -2362.355069 Hartree

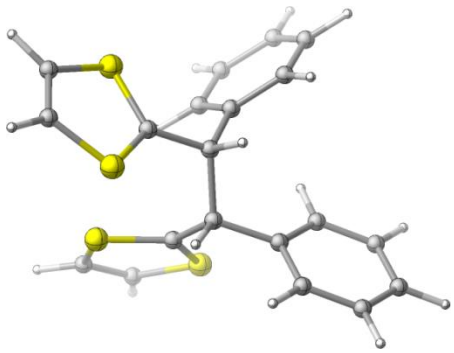
Sum of electronic and thermal Energies = -2362.334452 Hartree

Sum of electronic and thermal Enthalpies = -2362.333508 Hartree

Sum of electronic and thermal Free Energies = -2362.404855 Hartree

	Cartesian Coordinates				Cartesian Coordinates		
Atoms	***X***	***Y***	***Z***	**Atoms**	***X***	***Y***	***Z***
C	-0.996966	-1.669995	1.320993	C	-2.150262	-2.022999	2.008766
C	-3.329586	-2.307440	1.313933	C	-3.357932	-2.236337	-0.081357
C	-2.212385	-1.882331	-0.777503	C	-1.003626	-1.601638	-0.094743
C	1.483979	-1.229452	-0.612240	C	4.037076	-1.079351	-0.857406
C	3.817079	-1.313016	0.454514	S	2.640808	-0.953837	-1.849673
S	2.172922	-1.486016	0.938167	C	0.106304	-1.207397	-0.920229
C	-2.588506	1.096244	-1.886289	C	-3.969329	1.032101	-1.777484
C	-4.565786	1.058256	-0.514176	C	-3.777053	1.159174	0.637144
C	-2.396159	1.241510	0.536314	C	-1.773018	1.212719	-0.732673
C	0.684287	1.609859	-0.071337	C	3.011513	2.285304	0.786973
C	2.280377	2.032998	1.893024	S	2.196379	2.113302	-0.719404
S	0.649092	1.536003	1.642927	C	-0.356667	1.275909	-0.965595
H	-0.108031	-1.450082	1.910623	H	-2.130117	-2.075341	3.097782
H	-4.228820	-2.589021	1.864351	H	-4.277389	-2.459012	-0.624359
H	-2.225339	-1.838259	-1.868110	H	5.019106	-0.966333	-1.321983
H	4.593623	-1.426866	1.214421	H	-0.112411	-1.158786	-1.991955
H	-2.114600	1.074234	-2.869882	H	-4.583852	0.958209	-2.675183
H	-5.651872	1.003730	-0.423501	H	-4.246630	1.181567	1.621072
H	-1.825913	1.338179	1.458852	H	4.050621	2.620649	0.781101
H	2.639905	2.117337	2.920851	H	-0.070807	1.339442	-2.021577

σ-11



```
#p m062x/def2svp opt freq
empiricaldispersion=gd3 nosymm geom=connectivity
scrf=(smd,solvent=dichloromethane)
```

Charge = 2, Multiplicity = 1, Point group = C1

Electronic Energy = -2362.693397 Hartree

Number of imaginary frequencies = 0

Sum of electronic and zero-point Energies = -2362.386530 Hartree

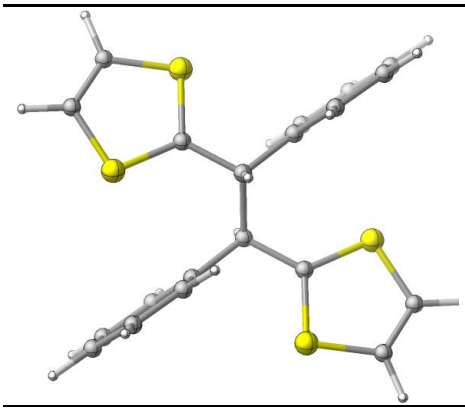
Sum of electronic and thermal Energies = -2362.366240 Hartree

Sum of electronic and thermal Enthalpies = -2362.365296 Hartree

Sum of electronic and thermal Free Energies = -2362.437368 Hartree

	Cartesian Coordinates				Cartesian Coordinates		
Atoms	***X***	***Y***	***Z***	**Atoms**	***X***	***Y***	***Z***
C	-0.301038	-0.792208	2.216245	C	-0.627377	-1.115430	3.533181
C	-1.804368	-1.806061	3.819252	C	-2.658271	-2.178859	2.781981
C	-2.333741	-1.862685	1.464175	C	-1.155592	-1.167314	1.168460
C	0.364599	-1.605036	-0.801267	C	2.144352	-2.665827	-2.290904
C	2.530548	-2.916155	-1.018709	S	0.674325	-1.795773	-2.451960
S	1.497785	-2.322818	0.214817	C	-0.854364	-0.864893	-0.292860
C	0.008642	2.344728	1.110654	C	1.023258	3.024823	1.781590
C	2.357101	2.806566	1.437692	C	2.674193	1.915625	0.412263
C	1.660803	1.234783	-0.260888	C	0.318259	1.437601	0.091819
C	-0.923893	1.011426	-2.053685	C	-1.704390	1.191311	-4.472178
C	-0.673177	2.059936	-4.354207	S	-2.113008	0.334510	-3.044050
S	0.060472	2.150923	-2.806687	C	-0.813860	0.684688	-0.580119
H	0.625470	-0.246593	2.028993	H	0.045989	-0.820193	4.338954
H	-2.054713	-2.055103	4.851576	H	-3.580269	-2.721193	2.996392
H	-3.001154	-2.160446	0.652540	H	2.673476	-2.979676	-3.193610
H	3.428550	-3.466063	-0.727417	H	-1.705550	-1.269859	-0.864209
H	-1.034888	2.506532	1.390418	H	0.769151	3.724974	2.578458
H	3.152079	3.336120	1.964773	H	3.714726	1.749181	0.130681
H	1.941417	0.556122	-1.070906	H	-2.282526	1.004864	-5.380321
H	-0.283721	2.689315	-5.157840	H	-1.759093	1.048165	-0.144436

σ-12



```
#p m062x/def2svp opt freq
empiricaldispersion=gd3 nosymm geom=connectivity
scrf=(smd,solvent=dichloromethane)
```

Charge = 2, Multiplicity = 1, Point group = C1

Electronic Energy = -2362.702522 Hartree

Number of imaginary frequencies = 0

Sum of electronic and zero-point Energies = -2362.395221 Hartree

Sum of electronic and thermal Energies = -2362.375122 Hartree

Sum of electronic and thermal Enthalpies = -2362.374178 Hartree

Sum of electronic and thermal Free Energies = -2362.445139 Hartree

	Cartesian Coordinates				Cartesian Coordinates		
Atoms	***X***	***Y***	***Z***	**Atoms**	***X***	***Y***	***Z***
C	1.635214	-1.911917	-1.048438	C	2.816057	-2.631330	-1.216041
C	3.609677	-2.940194	-0.109555	C	3.214368	-2.541541	1.167272
C	2.031396	-1.823140	1.339150	C	1.241943	-1.496275	0.232297
C	-1.255470	-1.494275	0.181525	C	-2.790103	-3.506146	-0.123715
C	-3.613754	-2.443513	0.028511	S	-1.115223	-3.159550	-0.062130
S	-2.846498	-0.926999	0.255725	C	-0.009047	-0.656876	0.426268
C	-2.031346	1.823101	-1.339273	C	-3.214339	2.541474	-1.167423
C	-3.609686	2.940121	0.109394	C	-2.816082	2.631280	1.215898
C	-1.635218	1.911895	1.048323	C	-1.241909	1.496257	-0.232402
C	1.255500	1.494313	-0.181557	C	3.613752	2.443608	-0.028425
C	2.790069	3.506221	0.123762	S	2.846544	0.927074	-0.255672
S	1.115200	3.159583	0.062101	C	0.009104	0.656886	-0.426345
H	1.023916	-1.672728	-1.923322	H	3.120140	-2.946535	-2.215143
H	4.538427	-3.496664	-0.244329	H	3.830378	-2.785758	2.033770
H	1.726060	-1.495963	2.336006	H	-3.105520	-4.539819	-0.280692
H	-4.705554	-2.475935	0.010776	H	-0.055410	-0.368646	1.489592
H	-1.725980	1.495929	-2.336122	H	-3.830334	2.785674	-2.033937
H	-4.538452	3.496567	0.244146	H	-3.120194	2.946481	2.214992
H	-1.023932	1.672728	1.923223	H	4.705550	2.476056	-0.010636
H	3.105454	4.539901	0.280755	H	0.055504	0.368664	-1.489669

3. Results of Intrinsic Reaction Coordinate (IRC) Analysis

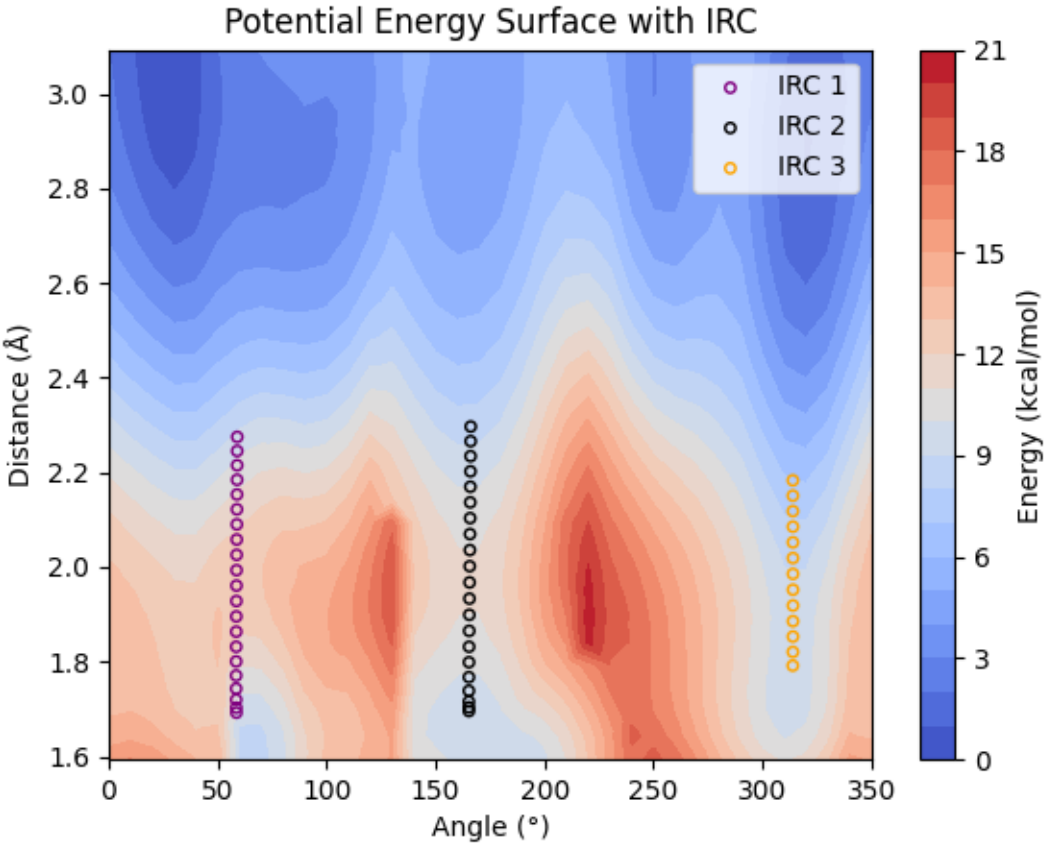


Figure S-1: 2D-countour plot of the PES of anti-MV-dimer (in vacuo) and the IRC trajectories calculated from **TS-1** (IRC 1), **TS-2** (IRC 2) and **TS-3** (IRC 3).

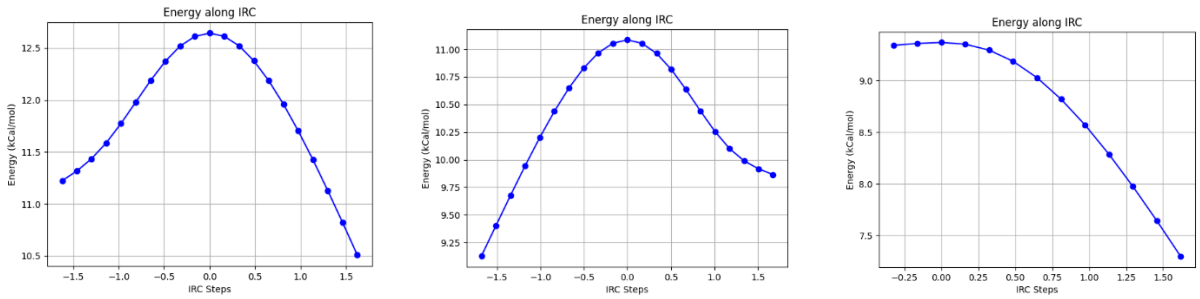


Figure S-2: IRC trajectories (in vacuo) calculated from **TS-1** (left), **TS-2** (middle) and **TS-3** (right).

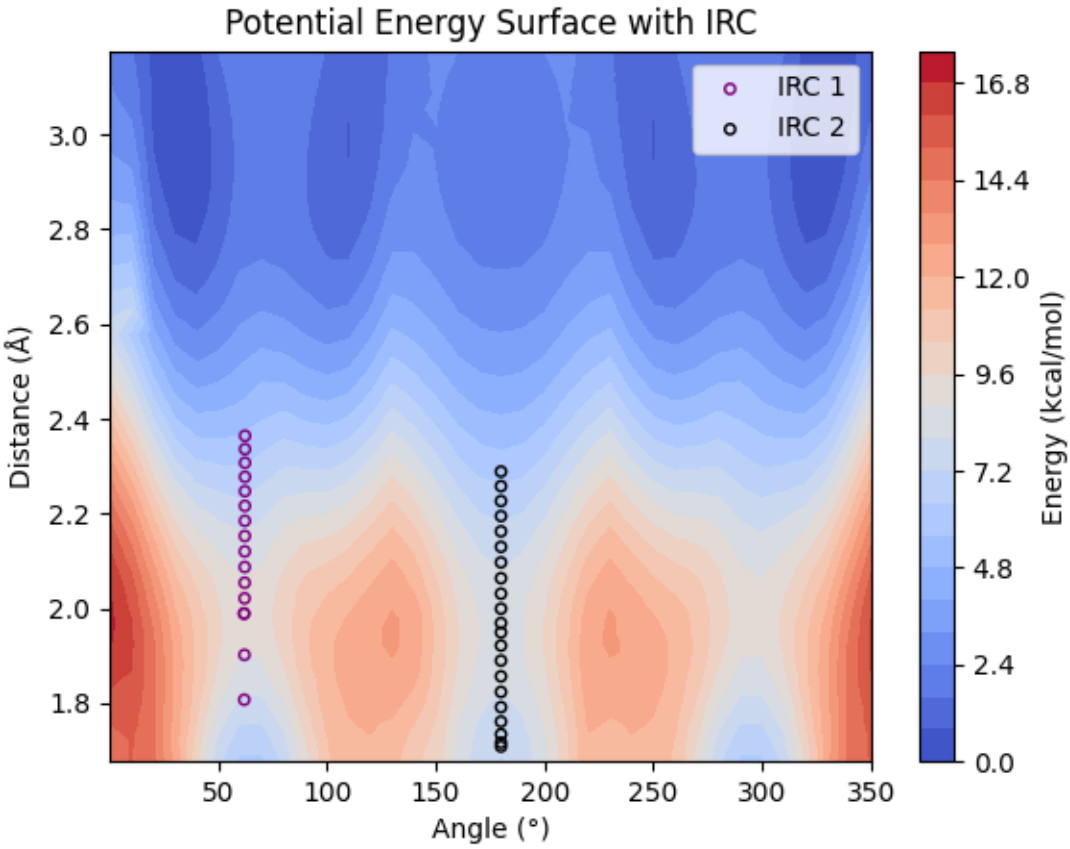


Figure S-3: 2D-countour plot of the PES of syn-MV-dimer (in vacuo) and the IRC trajectories calculated from **TS-4** (IRC 1) and **TS-5** (IRC 2).

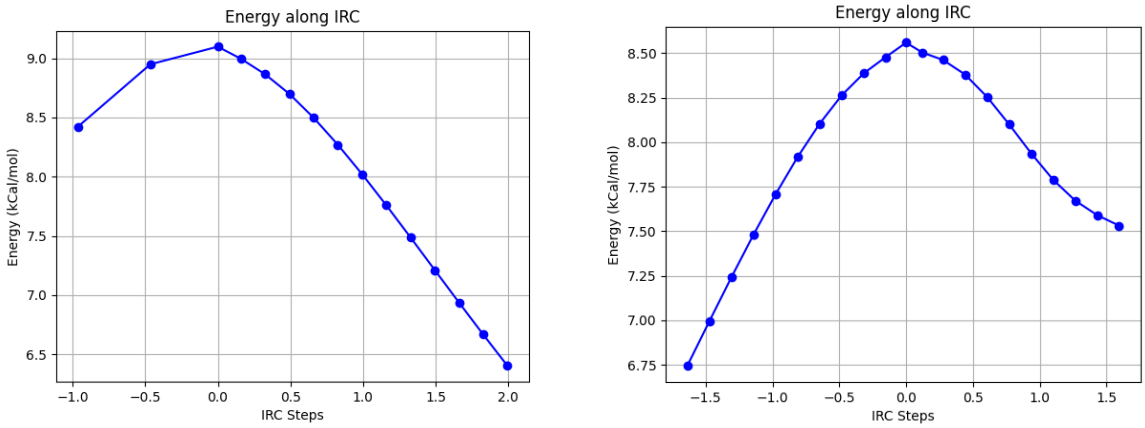


Figure S-4: IRC trajectories (in vacuo) calculated from **TS-4** (left) and **TS-5** (right).

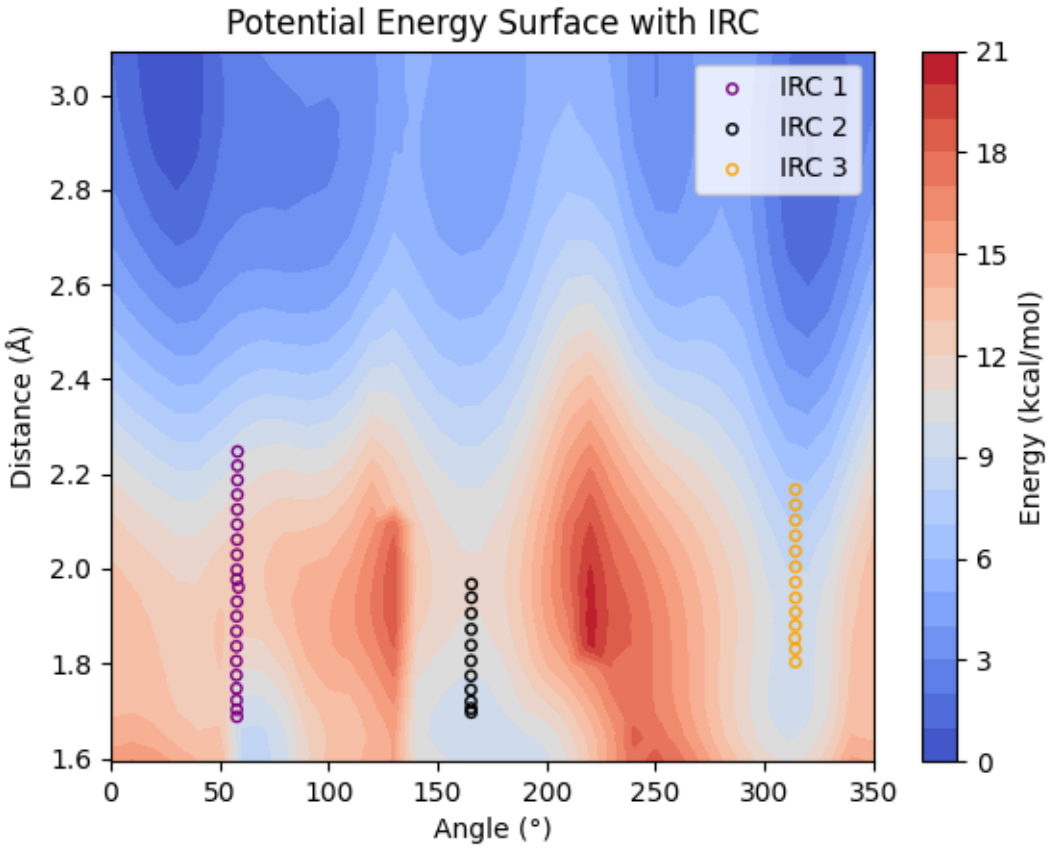


Figure S-5: 2D-countour plot of the PES of anti-MV-dimer (in CH_2Cl_2) and the IRC trajectories calculated from **TS-1** (IRC 1), **TS-2** (IRC 2), and **TS-3** (IRC 3).

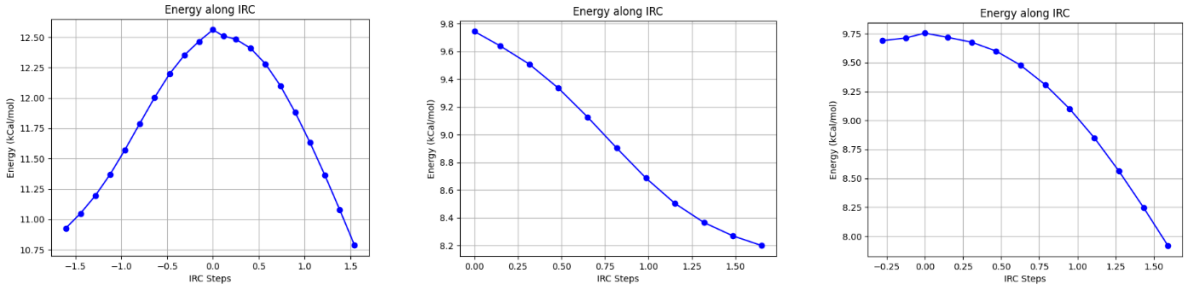


Figure S-6: IRC trajectories (in CH_2Cl_2) calculated from **TS-1** (left), **TS-2** (middle), and **TS-3** (right).

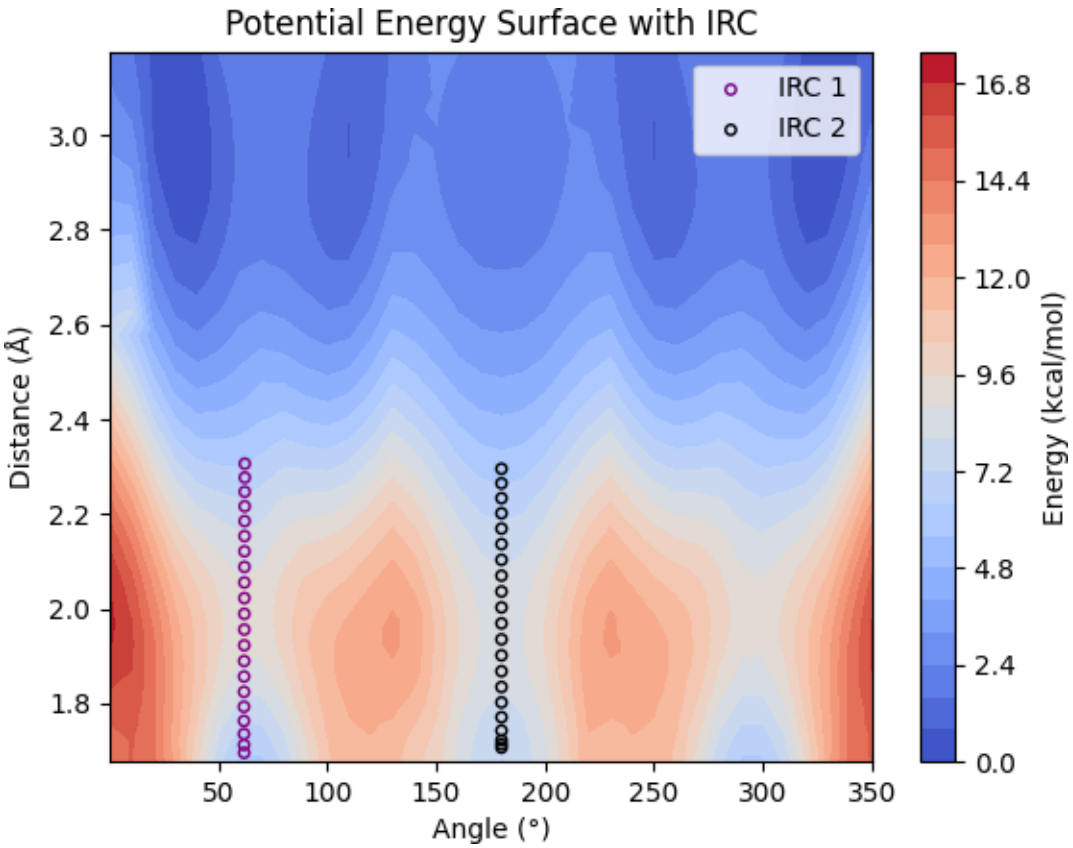


Figure S-7: 2D-countour plot of the PES of syn-MV-dimer (in CH_2Cl_2) and the IRC trajectories calculated from **TS-4** (IRC 1) and **TS-5** (IRC 2).

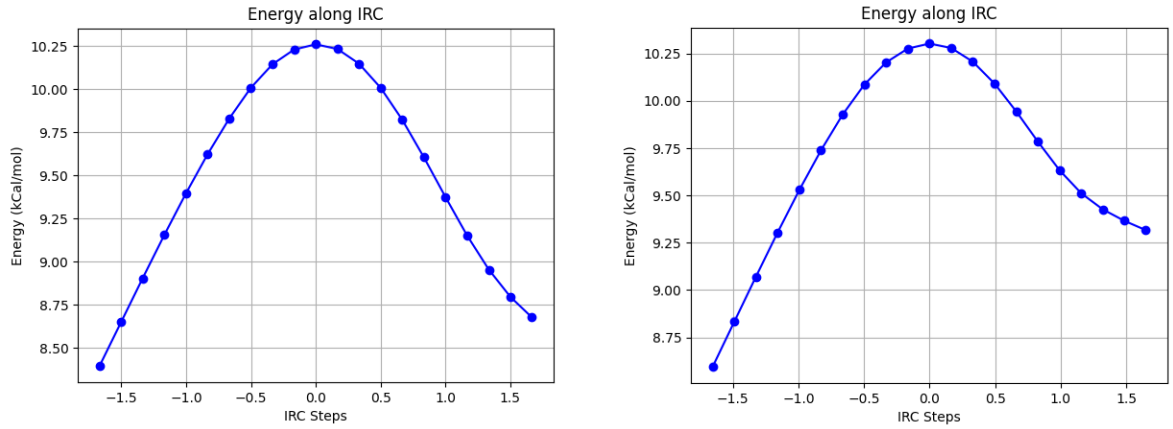


Figure S-8: IRC trajectories (in CH_2Cl_2) calculated from **TS-4** (left) and **TS-5** (right).

4. Results of QTAIM Analysis of π-MV-dimers

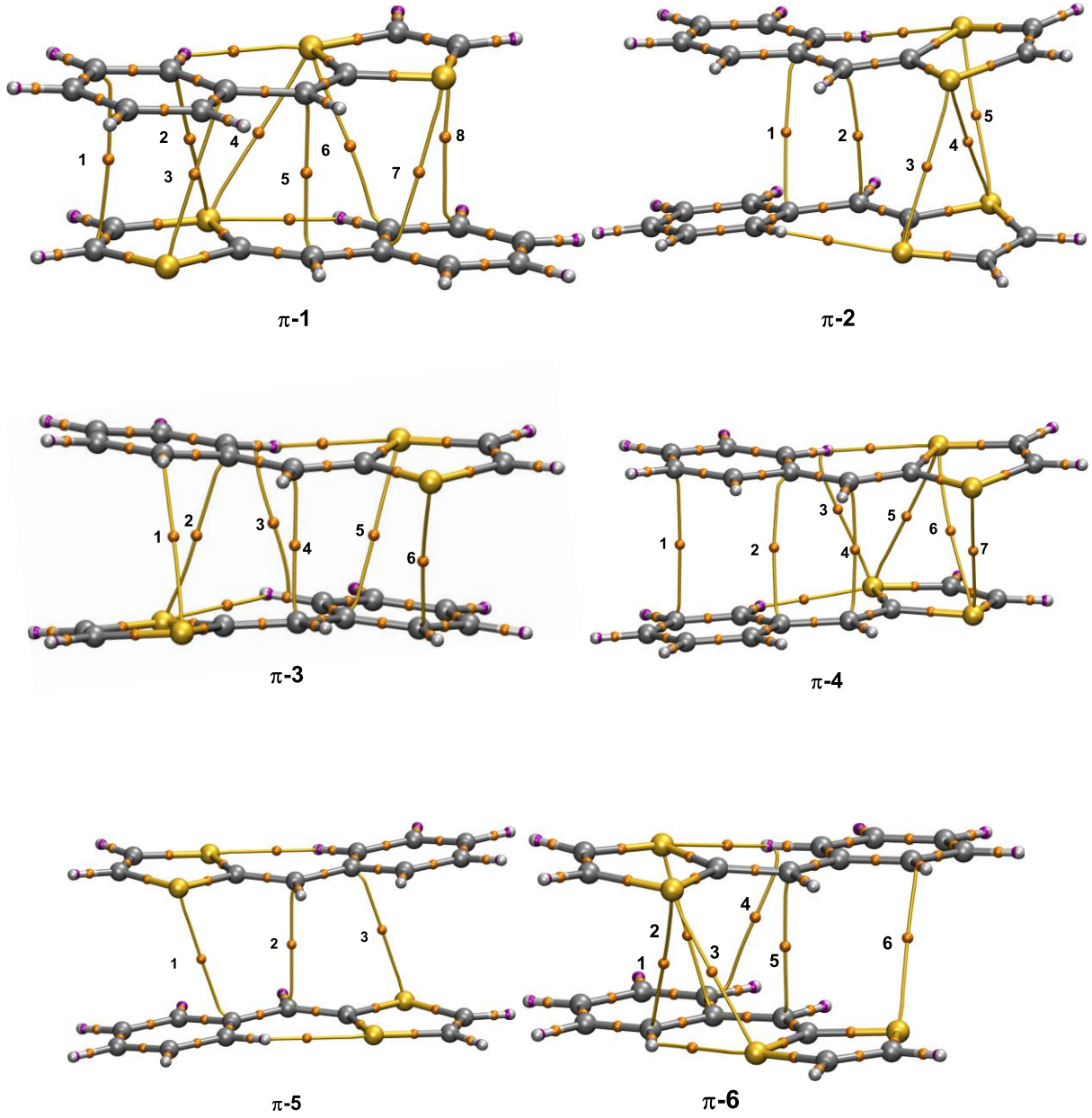


Figure S-9: QTAIM diagrams of the π-MV-dimers (in vacuo) with the intermolecular bond paths (orange lines) and (3,-1) critical points (orange spheres) highlighted.

Table S-1 Summary of the properties of (3,-1) critical points obtained from the QTAIM analysis of **π-1**

CP	Connected atoms	ρ(r)	s(r)	G(r)	V(r)	E(r)	$\Delta^2\rho(r)$
1	C-C	0.006561	-3.68E-05	0.003667	-0.00305	0.000617	0.017138
2	C-S	0.006524	-5.48E-05	0.003856	-0.00322	0.000633	0.017954
3	C-S	0.00986	-6.26E-05	0.00587	-0.0052	0.00067	0.026159
4	S-S	0.009139	-3.90E-05	0.004703	-0.00465	4.90E-05	0.019007
5	C-C*	0.011113	-0.0003	0.005429	-0.00446	0.000971	0.025602
6	C-S	0.006524	-5.48E-05	0.003856	-0.00322	0.000633	0.017955
7	C-S	0.00986	-6.26E-05	0.00587	-0.0052	0.00067	0.026158
8	C-C	0.006559	-3.69E-05	0.003667	-0.00305	0.000617	0.017134

ρ(r) = Total electron density , s(r) = spin density, G(r) = Lagrangian kinetic energy Potential energy density V(r), Energy density E(r), Laplacian of electron density $\Delta^2\rho(r)$. ρ in (a.u.). C-C* represents the C-C bond formed after dimerization.

Table S-2 Summary of the properties of critical points (CPs) obtained from the QTAIM analysis of **π-2**

CP	Connected atoms	ρ(r)	s(r)	G(r)	V(r)	E(r)	$\Delta^2\rho(r)$
1	C-C	0.00827	-9.37E-05	0.005152	-0.00415	0.001003	0.024621
2	C-C*	0.013198	-0.00038	0.006881	-0.00567	0.001207	0.032351
3	S-S	0.009027	-5.93E-05	0.004967	-0.00495	1.83E-05	0.019942
4	S-S	0.009027	-5.93E-05	0.004967	-0.00495	1.82E-05	0.019942
5	S-S	0.010271	-9.68E-05	0.005971	-0.00603	-6.22E-05	0.023636

ρ(r) = Total electron density , s(r) = spin density, G(r) = Lagrangian kinetic energy Potential energy density V(r), Energy density E(r), Laplacian of electron density $\Delta^2\rho(r)$. ρ in (a.u.). C-C* represents the C-C bond formed after dimerization.

Table S-3 Summary of the properties of critical points (CPs) obtained from the QTAIM analysis of **π-3**

CP	Connected atoms	ρ(r)	s(r)	G(r)	V(r)	E(r)	$\Delta^2\rho(r)$
1	C-S	0.006889	-4.12E-05	0.004151	-0.00342	0.000729	0.019522
2	C-S	0.008675	-6.41E-05	0.005319	-0.00473	0.000587	0.023623
3	C-C	0.005179	-1.69E-05	0.003168	-0.00198	0.001192	0.01744
4	C-C*	0.015791	-0.00075	0.008199	-0.007	0.001198	0.037587
5	C-S	0.008673	-6.41E-05	0.005318	-0.00473	0.000587	0.023618
6	C-S	0.006887	-4.12E-05	0.004149	-0.00342	0.000729	0.019515

ρ(r) = Total electron density , s(r) = spin density, G(r) = Lagrangian kinetic energy Potential energy density V(r), Energy density E(r), Laplacian of electron density $\Delta^2\rho(r)$. ρ in (a.u.). C-C* represents the C-C bond formed after dimerization.

Table S-4 Summary of the properties of critical points (CPs) obtained from the QTAIM analysis of **π-4**

CP	Connected atoms	ρ(r)	s(r)	G(r)	V(r)	E(r)	$\Delta^2\rho(r)$
1	C-C	0.006365	-7.76E-05	0.003397	-0.00281	0.000591	0.01595
2	C-C	0.008316	-8.06E-05	0.004966	-0.00398	0.000981	0.023787
3	C-S	0.007039	1.47E-05	0.004361	-0.0034	0.000958	0.021275
4	C-C*	0.012083	-0.00034	0.006168	-0.00506	0.001109	0.029109
5	S-S	0.009206	-5.98E-05	0.005048	-0.00506	-1.46E-05	0.020133
6	S-S	0.008293	-6.99E-05	0.005143	-0.00503	0.000111	0.021018
7	S-S	0.011041	-0.0001	0.005923	-0.006	-7.72E-05	0.023385

ρ(r) = Total electron density , s(r) = spin density, G(r) = Lagrangian kinetic energy Potential energy density V(r), Energy density E(r), Laplacian of electron density $\Delta^2\rho(r)$. ρ in (a.u.). C-C* represents the C-C bond formed after dimerization.

Table S-5 Summary of the properties of critical points (CPs) obtained from the QTAIM analysis of **π-5**

CP	Connected atoms	ρ(r)	s(r)	G(r)	V(r)	E(r)	$\Delta^2\rho(r)$
1	C-S	1.04E-02	-6.65E-05	6.32E-03	-5.62E-03	6.99E-04	2.81E-02
2	C-C*	1.42E-02	-5.94E-04	7.23E-03	-6.02E-03	1.21E-03	3.37E-02
3	C-S	1.04E-02	-6.65E-05	6.32E-03	-5.62E-03	6.99E-04	2.81E-02

ρ(r) = Total electron density , s(r) = spin density, G(r) = Lagrangian kinetic energy Potential energy density V(r), Energy density E(r), Laplacian of electron density $\Delta^2\rho(r)$. ρ in (a.u.). C-C* represents the C-C bond formed after dimerization.

Table S-6 Summary of the properties of critical points (CPs) obtained from the QTAIM analysis of **π-6**

CP	Connected atoms	ρ(r)	s(r)	G(r)	V(r)	E(r)	$\Delta^2\rho(r)$
1	C-S	0.006443	-6.42E-05	0.003764	-0.00321	0.000556	0.017279
2	C-S	0.009099	-5.66E-05	0.005439	-0.00486	0.000578	0.024067
3	S-S	0.010725	-6.52E-05	0.005452	-0.00547	-1.85E-05	0.021732
4	C-H	0.004323	-9.57E-07	0.002622	-0.00166	0.000963	0.014339
5	C-C*	0.01333	-0.00028	0.00733	-0.00589	0.001443	0.035092
6	C-S	0.007196	7.06E-06	0.004296	-0.00333	0.000964	0.021038

ρ(r) = Total electron density , s(r) = spin density, G(r) = Lagrangian kinetic energy Potential energy density V(r), Energy density E(r), Laplacian of electron density $\Delta^2\rho(r)$. ρ in (a.u.). C-C* represents the C-C bond formed after dimerization.

5. Results of Spin Density Analysis

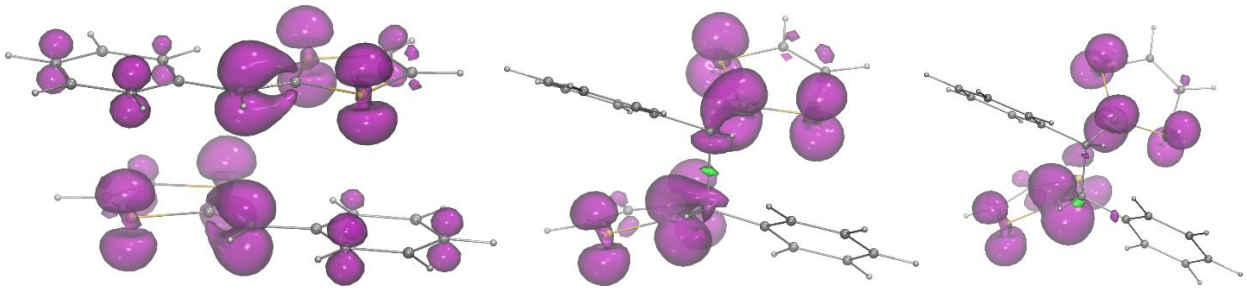


Figure S-10: Spin density plots of **π-1** (left), **TS-1** (middle), and **σ-1** (right)**.** Isovalue of 0.003 a.u.

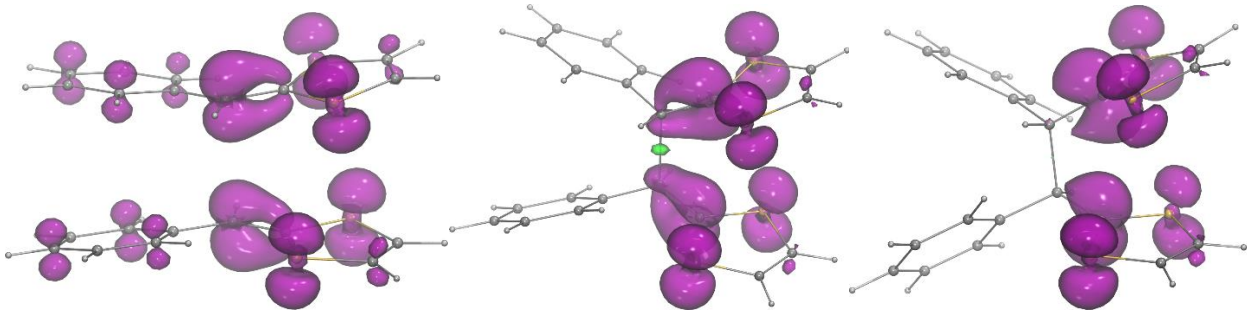


Figure S-11: Spin density plots of **π-2** (left), **TS-2** (middle), and **σ-2** (right)**.** Isovalue of 0.003 a.u.

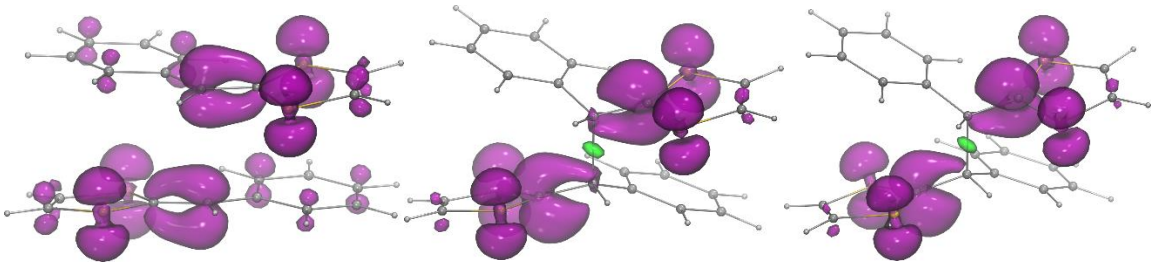


Figure S-12: Spin density plots of **π-3** (left), **TS-3** (middle), and **σ-3** (right)**.** Isovalue of 0.003 a.u.

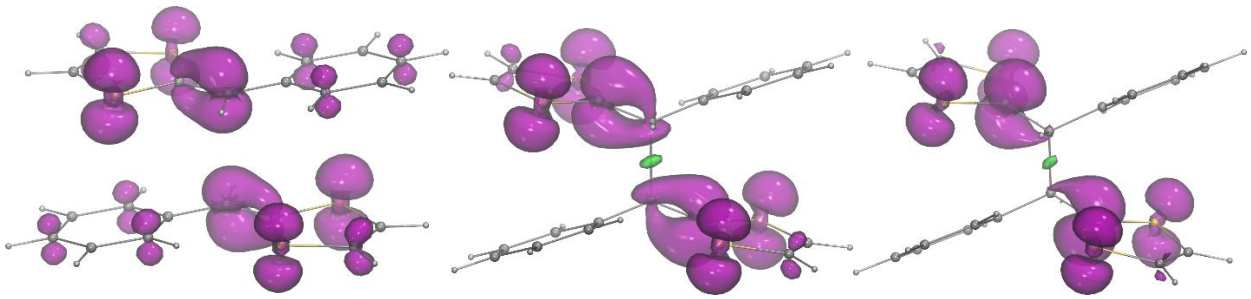


Figure S-13: Spin density plots of **π-4** (left), **TS-4** (middle), and **σ-4** (right)**.** Isovalue of 0.003 a.u.

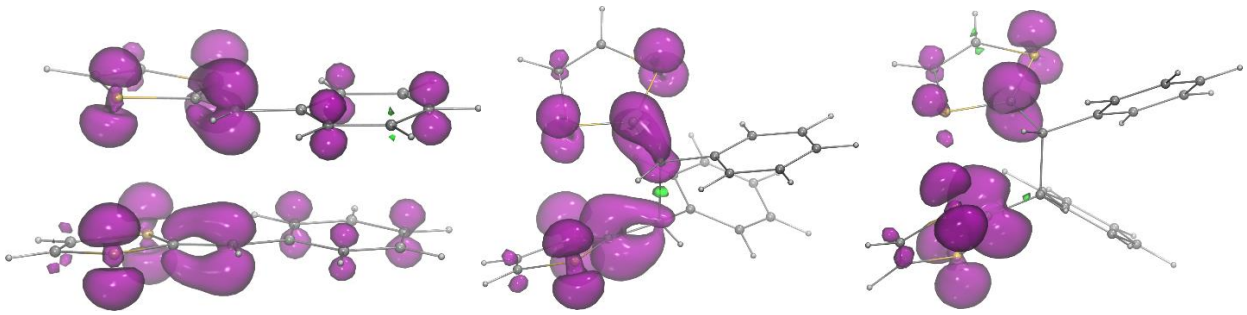


Figure S-14: Spin density plots of **π-5** (left), **TS-5** (middle), and **σ-5** (right)**.** Isovalue of 0.003 a.u.