

Electronic Supplementary Information

Mechanistic Insights into Benzyne Formation via 1,2-di-iodobenzene Photolysis

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Overview of Bonding evolution theory (BET)

Silvi and co-workers introduced the Bonding evolution theory (BET)⁵⁵ as an alternative framework for approaching a very elusive concept: the chemical bond concept. Within this methodology, the modeling of a chemical reaction takes the form of a gradient dynamical system, wherein the electron localization function (ELF)⁵⁶ plays the role of a time-independent potential function. ELF serves as a quantum tool for visualizing the Pauli exclusion principle. The nullity condition of a potential, such as the ELF, defined over the 3D real space, yields four types of equilibria: attractors, saddles of index one and two, and repellers, each surrounded by its associated basin. The collection of these singular solutions is often referred to as the topographic map, molecular graph (MG), or phase-space portrait of the function or, more precisely, of its gradient.⁵⁷⁻⁵⁹

It is pertinent to mention that ELF maxima align closely with predictions stemming from the valence-shell electron pair repulsion theory (VSEPR),⁶⁰ establishing a robust connection between Lewis bonding concepts encompassing valence, bonds, core, and lone pairs.⁶¹⁻⁶⁸ The topographical analysis of ELF remains invariant

concerning the computational level;^{69,70} moreover, this function can also be derived from X-ray diffraction data.⁷¹⁻⁷²

Within the BET framework, the spatial arrangement of chemical bonding is conceptually elucidated through the interplay of electron localization pairs and electron density distributions, effectively delineated by basin populations. Particularly key molecular bonding events, including bond formation, cleavage, and the dynamic redistribution of electrons during chemical transformations, find adept representation through a succession of molecular configurations guided by the ELF (ELF-MG). This sequence is punctuated by sharp transitions in the spatial extent of electron pair localization, marking substantial shifts in the prevailing bonding interactions underlying the molecular system.

Optimized Cartesian coordinates for reactants (Min1), transition structures (Min2 and Min3), products (P), and minimum energy conical intersection (MECI) points of functionalized 1,2-di-iodobenzenes at WB97X using the def2-TZVP basis set and including the CPCM solvation model (solvent=benzene).

Min1(S₀)

1,2-di-chloro benzene

C	-5.224888	1.758818	0.043193
C	-3.837096	1.759340	0.028774
C	-3.146194	2.965973	-0.013993
C	-3.848495	4.162630	-0.043792
C	-5.232483	4.157625	-0.030665
C	-5.921397	2.954365	0.013171
H	-5.748619	0.812131	0.077751
H	-3.296332	5.093039	-0.077167
H	-5.771654	5.096457	-0.054454
H	-7.004260	2.942980	0.024059
Cl	-1.421792	3.008026	-0.030907
Cl	-3.000204	0.251350	0.063861

Min1(S₀)

1,2-di-bromo benzene

C	-5.241470	1.769478	0.042718
C	-3.852395	1.767999	0.028950
C	-3.161811	2.973953	-0.014349
C	-3.865875	4.170827	-0.043628
C	-5.249530	4.167226	-0.030357
C	-5.938495	2.964463	0.012653
H	-5.770714	0.825886	0.076797
H	-3.318502	5.103926	-0.076852
H	-5.787064	5.106965	-0.053606
H	-7.021340	2.952082	0.023090
Br	-1.279327	3.054435	-0.036136
Br	-2.966890	0.105495	0.070550

Min1(S₀)

1,2-di-iodo benzene

C	-5.261133	1.784151	0.042735
C	-3.869117	1.776444	0.028605
C	-3.177261	2.984269	-0.014476
C	-3.887492	4.181089	-0.044211
C	-5.271053	4.179863	-0.030904
C	-5.959788	2.977926	0.012969
H	-5.799030	0.845343	0.076979
H	-3.348660	5.119374	-0.078063
H	-5.807218	5.120478	-0.054651
H	-7.042668	2.963941	0.024108
I	-1.095627	3.118181	-0.037297
I	-2.934366	-0.088324	0.074037

Min2(S₁)

1,2-di-chloro benzene

C	-5.239695	1.779809	0.041958
C	-3.855829	1.872148	0.023968
C	-3.264501	3.087955	-0.019847
C	-3.939977	4.274944	-0.048116
C	-5.334546	4.196654	-0.030034
C	-5.969786	2.961772	0.013870
H	-5.730481	0.814021	0.076832
H	-3.433148	5.232092	-0.082799
H	-5.922843	5.106887	-0.050117
H	-7.051697	2.915179	0.026737
Cl	-0.852012	2.293355	-0.009818
Cl	-2.858898	0.427920	0.057198

Min2(S₁)

1,2-di-bromo benzene

C	-5.362583	1.795125	0.051727
C	-3.989426	1.801805	0.043311
C	-3.271563	2.944615	-0.002619
C	-3.887726	4.185293	-0.043901
C	-5.276553	4.209667	-0.036686
C	-6.009626	3.029363	0.011344
H	-5.931501	0.873012	0.088221
H	-3.309899	5.101879	-0.081102
H	-5.790855	5.162297	-0.069820
H	-7.093118	3.066352	0.016895
Br	-1.348788	2.804159	-0.011205
Br	-2.181775	-0.010833	0.033667

Min2(S₁)

1,2-di-iodo benzene

C	-5.351396	1.801772	0.047894
C	-3.971817	1.816498	0.035775
C	-3.286217	2.971600	-0.007922
C	-3.907340	4.209170	-0.044052
C	-5.296148	4.218107	-0.034224
C	-6.013743	3.026103	0.012078
H	-5.913248	0.873946	0.083545
H	-3.340227	5.132938	-0.079641

H	-5.821685	5.164996	-0.063600
H	-7.097776	3.050377	0.019640
I	-1.128862	2.829664	-0.022709
I	-2.324956	-0.132435	0.053047

Min3(T₁)

1,2-di-chloro benzene

C	-5.376777	1.767792	0.044014
C	-3.986340	1.748808	0.026041
C	-3.334300	2.949891	-0.017671
C	-3.941972	4.175265	-0.047517
C	-5.336459	4.184932	-0.029954
C	-6.039365	2.987807	0.015737
H	-5.926756	0.834959	0.079855
H	-3.372047	5.096322	-0.082385
H	-5.868715	5.128546	-0.051895
H	-7.122390	2.999760	0.029710
Cl	-0.030431	2.838385	-0.024630
Cl	-3.117861	0.250268	0.058526

Min3(T₁)

1,2-di-bromo benzene

C	-5.238727	1.836478	0.084814
C	-3.875662	1.965072	0.091818
C	-3.198602	3.147966	0.028283
C	-3.941550	4.321201	-0.049530
C	-5.328128	4.242505	-0.059609
C	-5.977710	3.016061	0.006553
H	-5.723032	0.868342	0.136574
H	-3.438639	5.279459	-0.101473
H	-5.908020	5.155329	-0.120020
H	-7.060546	2.973475	-0.003027
Br	-1.308995	3.191910	0.046793
Br	-2.453804	-1.035061	-0.061344

Min3(T₁)

1,2-di-iodo benzene

C	-5.251316	1.866668	0.252025
C	-3.888553	2.003387	0.294427
C	-3.206283	3.171627	0.127999
C	-3.949491	4.327695	-0.102014
C	-5.334515	4.243641	-0.152728
C	-5.986032	3.028534	0.022312
H	-5.737593	0.907810	0.388536
H	-3.450615	5.279837	-0.240110
H	-5.910914	5.142894	-0.333192
H	-7.067891	2.980904	-0.020980
I	-1.122430	3.218743	0.215964
I	-2.547779	-1.209003	-0.452408

P(S₀)

Benzynes + Cl₂

C	-5.984938	1.886287	0.025068
C	-4.620481	1.672781	0.029960
C	-3.737862	2.536488	0.009874
C	-3.887683	3.906206	-0.017527

C	-5.249738	4.232417	-0.022850
C	-6.259773	3.258948	-0.002620
H	-6.764004	1.136070	0.040666
H	-3.104546	4.652188	-0.033582
H	-5.533940	5.278876	-0.043515
H	-7.295108	3.582026	-0.008765
Cl	-0.342352	2.374263	-0.131198
Cl	-0.672975	0.446249	0.154388

P(S₀)

Benzyne + Br₂

C	-5.898729	1.889644	0.081655
C	-4.523907	1.760734	0.120821
C	-3.697757	2.678149	0.080229
C	-3.929630	4.033008	-0.011859
C	-5.308871	4.272775	-0.058371
C	-6.257181	3.239895	-0.012614
H	-6.629475	1.092769	0.116025
H	-3.194184	4.825400	-0.046239
H	-5.656888	5.297330	-0.132136
H	-7.309953	3.497828	-0.051660
Br	-0.194930	2.276186	-0.043194
Br	-0.851897	0.099084	-0.042756

P(S₀)

Benzyne + I₂

C	-5.613892	1.898683	0.046887
C	-4.239630	2.020461	0.015074
C	-3.581285	3.064882	-0.035604
C	-4.059777	4.358274	-0.068400
C	-5.459773	4.351200	-0.039787
C	-6.208474	3.166023	0.016077
H	-6.190637	0.984829	0.091607
H	-3.480038	5.270226	-0.112748
H	-5.985944	5.299277	-0.062444
H	-7.290807	3.233341	0.036902
I	-0.006122	1.800532	0.161239
I	-1.337021	-0.484927	-0.048902

Min1(S₀)

1,2,4-di-iodo methyl benzene

C	-5.283564	1.877876	0.053764
C	-3.890807	1.869499	0.035541
C	-3.195349	3.071542	-0.018462
C	-3.913133	4.264702	-0.053828
C	-5.293968	4.258985	-0.036680
C	-6.003382	3.062284	0.016067
H	-5.816653	0.935555	0.098315
H	-3.379918	5.206112	-0.094583
H	-5.828445	5.202263	-0.064007
I	-1.114759	3.208420	-0.047722
I	-2.961023	0.002091	0.093170
C	-7.505943	3.056041	0.018940
H	-7.896645	3.728010	0.784841
H	-7.892614	3.396191	-0.944129

H	-7.897295	2.056331	0.206273
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Min2(S₁)

1,2,4-di-iodo methyl benzene

C	-5.266333	1.822465	0.083797
C	-3.887066	1.820358	0.073126
C	-3.184211	2.962058	-0.010863
C	-3.802415	4.199746	-0.094166
C	-5.188602	4.219668	-0.086308
C	-5.938541	3.043377	0.005566
H	-5.834988	0.898810	0.148712
H	-3.232000	5.119631	-0.166813
H	-5.702178	5.172557	-0.156958
I	-1.033374	2.804700	-0.024181
I	-2.251557	-0.148587	0.125280
C	-7.441593	3.099073	0.037099
H	-7.876131	2.118257	-0.156914
H	-7.793769	3.433675	1.015654
H	-7.825366	3.799375	-0.706355

Min3(T₁)

1,2,4-di-iodo methyl benzene

C	-5.381592	1.853583	0.175183
C	-4.013434	1.843275	0.186822
C	-3.217039	2.936851	0.045533
C	-3.838028	4.170507	-0.124436
C	-5.223448	4.229278	-0.138634
C	-6.014414	3.089874	0.011113
H	-5.962289	0.944197	0.286036
H	-3.249297	5.072318	-0.247815
H	-5.703548	5.191776	-0.276042
I	-1.136000	2.768857	0.076823
I	-1.298207	-0.573476	-0.019414
C	-7.514078	3.188989	0.020313
H	-7.972141	2.269782	-0.345054
H	-7.878965	3.360954	1.035814
H	-7.855648	4.018399	-0.599567

P(S₀)

4-methyl benzyne + I₂

C	-6.512742	1.841054	0.063050
C	-5.134558	1.753647	0.042637
C	-4.331715	2.689218	-0.012447
C	-4.622097	4.037775	-0.065727
C	-6.004835	4.231689	-0.048900
C	-6.938983	3.176397	0.013538
H	-7.216226	1.019268	0.109586
H	-3.915934	4.856285	-0.114197
H	-6.382473	5.248898	-0.086993
I	-0.655268	2.901411	-0.198556
I	-1.028279	0.313654	0.253377
C	-8.412731	3.491600	0.029268
H	-8.676147	4.080836	0.909814
H	-8.697977	4.070220	-0.851204
H	-9.009137	2.579448	0.042953

Min1(S₀)

1,2,4-di-iodo formyl benzene

C	-5.296907	1.862875	0.033297
C	-3.906325	1.839557	0.016915
C	-3.208585	3.044541	-0.020923
C	-3.908173	4.252493	-0.044717
C	-5.286320	4.265548	-0.029542
C	-5.985882	3.064524	0.010834
H	-5.850315	0.930833	0.063643
H	-3.357766	5.183823	-0.074629
H	-5.834106	5.199675	-0.047444
I	-1.129532	3.161524	-0.043404
I	-2.986512	-0.030822	0.051870
C	-7.467883	3.046296	0.032907
O	-8.157312	4.034432	0.011527
H	-7.920181	2.037002	0.071165

Min2(S₁)

1,2,4-di-iodo formyl benzene

C	-5.429665	1.882337	0.036489
C	-4.051599	1.812277	0.028921
C	-3.310225	2.935854	-0.003726
C	-3.865846	4.209292	-0.031905
C	-5.245627	4.298103	-0.028333
C	-6.028034	3.141887	0.006518
H	-6.050027	0.989882	0.063267
H	-3.247985	5.099885	-0.056449
H	-5.736638	5.263383	-0.052263
I	-1.170972	2.697811	-0.015027
I	-2.493000	-0.216186	0.048470
C	-7.507060	3.238196	0.010726
O	-8.124248	4.273286	-0.034743
H	-8.034988	2.266336	0.059620

Min3(T₁)

1,2,4-di-iodo formyl benzene

C	-5.533815	1.910543	0.034228
C	-4.166542	1.846737	0.027162
C	-3.338068	2.926058	-0.004693
C	-3.904392	4.201206	-0.035000
C	-5.282418	4.317945	-0.031357
C	-6.097653	3.187256	0.004101
H	-6.157887	1.023119	0.060877
H	-3.275007	5.082714	-0.060429
H	-5.748384	5.295335	-0.055922
I	-1.265612	2.678770	-0.008335
I	-1.662573	-0.660134	0.058685
C	-7.575504	3.327034	0.011835
O	-8.154066	4.383471	-0.015759
H	-8.133994	2.372287	0.046170

P(S₀)4-formyl benzyne + I₂

C	-6.551121	1.857663	0.076787
C	-5.176409	1.749758	0.069684

C	-4.379202	2.690993	0.020737
C	-4.635825	4.045582	-0.039530
C	-6.013788	4.260405	-0.039317
C	-6.944823	3.204873	0.016631
H	-7.271931	1.049776	0.120002
H	-3.913018	4.848576	-0.081028
H	-6.397829	5.273143	-0.083394
I	-0.669731	2.920321	-0.008312
I	-1.104438	0.302495	-0.015129
C	-8.398121	3.501543	0.011598
O	-8.874286	4.608400	-0.036502
H	-9.050477	2.608271	0.055873

Min1(S₀)

1,2,4-di-iodo cyano benzene

C	-5.320104	2.433516	0.993859
C	-3.958480	2.176395	0.898730
C	-3.233081	2.705442	-0.168704
C	-3.881534	3.480300	-1.127219
C	-5.235314	3.733100	-1.036565
C	-5.955647	3.207211	0.031136
H	-5.893241	2.031663	1.819212
H	-3.316860	3.889239	-1.954840
H	-5.730916	4.333873	-1.788101
I	-1.190197	2.401544	-0.427914
I	-3.115243	0.999154	2.395992
C	-7.366835	3.459272	0.146224
N	-8.493249	3.661391	0.236790

Min2(S₁)

1,2,4-di-iodo cyano benzene

C	-5.416994	1.856106	0.050009
C	-4.041077	1.808481	0.034042
C	-3.308441	2.939608	-0.014230
C	-3.876892	4.203192	-0.050113
C	-5.259449	4.281945	-0.037162
C	-6.024977	3.114781	0.013078
H	-6.028670	0.960947	0.088793
H	-3.272252	5.102142	-0.087904
H	-5.749856	5.246512	-0.066603
I	-1.169579	2.717497	-0.040032
I	-2.474644	-0.203884	0.062993
C	-7.460885	3.208619	0.026439
N	-8.607215	3.276045	0.039327

Min3(T₁)

1,2,4-di-iodo cyano benzene

C	-5.516758	1.893439	0.047290
C	-4.151415	1.852389	0.030270
C	-3.331625	2.939098	-0.016542
C	-3.912495	4.203926	-0.050971
C	-5.293582	4.310652	-0.037235
C	-6.092601	3.168005	0.011755
H	-6.130082	1.001596	0.085254
H	-3.296577	5.094311	-0.087842

H	-5.758256	5.287693	-0.065227
I	-1.258494	2.704329	-0.037228
I	-1.754413	-0.632729	0.072424
C	-7.525382	3.296498	0.026737
N	-8.669252	3.392782	0.039950

P(S₀)

4-cyano benzyne + I₂

C	-6.376195	1.904368	-0.286643
C	-5.001706	1.871202	-0.197362
C	-4.288168	2.850376	0.045756
C	-4.620437	4.162150	0.283583
C	-6.008423	4.301679	0.213883
C	-6.855113	3.209187	-0.061677
H	-7.043241	1.078777	-0.496453
H	-3.956374	4.988433	0.494673
H	-6.452884	5.276747	0.375685
I	-0.756084	2.547473	0.168696
I	-1.275125	-0.031813	-0.165251
C	-8.275001	3.441902	-0.115156
N	-9.407849	3.624719	-0.158034

Min1(S₀)

1,2,4-di-iodo nitro benzene

C	-5.282368	1.841827	0.033359
C	-3.893523	1.838550	0.017148
C	-3.204574	3.051418	-0.020638
C	-3.913070	4.250703	-0.041669
C	-5.293826	4.259170	-0.024704
C	-5.953199	3.046383	0.012434
H	-5.843669	0.918816	0.062038
H	-3.375137	5.188909	-0.071649
H	-5.850179	5.185315	-0.040126
I	-1.127952	3.183620	-0.048083
I	-2.958266	-0.022136	0.051621
N	-7.426185	3.032140	0.030007
O	-7.996639	4.099675	0.026459
O	-7.980612	1.956510	0.046501

Min2(S₁)

1,2,4-di-iodo nitro benzene

C	-5.416598	1.861525	0.049284
C	-4.039651	1.810814	0.035251
C	-3.303280	2.941071	-0.012808
C	-3.867692	4.207244	-0.051623
C	-5.249954	4.292237	-0.041611
C	-5.994418	3.122654	0.009880
H	-6.041667	0.977842	0.087602
H	-3.260193	5.104165	-0.089102
H	-5.750315	5.249517	-0.072950
I	-1.169495	2.712624	-0.032330
I	-2.479740	-0.210129	0.070184
N	-7.466187	3.227338	0.023452
O	-7.956034	4.333257	-0.036196
O	-8.104039	2.200754	0.093582

Min3(T₁)

1,2,4-di-iodo nitro benzene

C	-5.506548	1.892123	0.048496
C	-4.140526	1.852762	0.032235
C	-3.321293	2.940632	-0.017907
C	-3.900943	4.206137	-0.056414
C	-5.282350	4.314859	-0.042890
C	-6.055806	3.166606	0.009136
H	-6.132077	1.010429	0.088482
H	-3.284937	5.096191	-0.096244
H	-5.760979	5.283200	-0.073229
I	-1.249397	2.703684	-0.038009
I	-1.769723	-0.633547	0.098827
N	-7.525047	3.299252	0.023111
O	-7.989843	4.416478	0.008004
O	-8.179793	2.282107	0.049019

P(S₀)4-nitro benzyne + I₂

C	-6.394127	1.931388	0.061269
C	-5.018228	1.985929	0.051576
C	-4.339099	3.016491	0.005952
C	-4.738910	4.333160	-0.042524
C	-6.132759	4.396786	-0.037790
C	-6.910158	3.230689	0.013078
H	-7.031469	1.060331	0.099788
H	-4.112906	5.213228	-0.080473
H	-6.634986	5.353803	-0.074267
I	-0.798824	2.339904	-0.040039
I	-1.719482	-0.146424	0.060962
N	-8.378152	3.379739	0.017288
O	-8.839148	4.499141	-0.006997
O	-9.044553	2.368938	0.045176

Min1(S₀)

1,2,4-di-iodo methoxy benzene

C	-5.269772	1.821754	0.022632
C	-3.875850	1.853838	-0.023137
C	-3.199564	3.064403	-0.046524
C	-3.942038	4.246881	-0.021650
C	-5.316399	4.225650	0.023771
C	-5.991943	3.006371	0.044406
H	-5.773318	0.866161	0.041025
H	-3.427528	5.199238	-0.039294
H	-5.888200	5.144799	0.042988
I	-1.124063	3.241850	-0.117229
I	-2.913461	0.001773	-0.053011
O	-7.339698	3.073308	0.085262
C	-8.069453	1.859090	0.092056
H	-9.119704	2.138606	0.114106
H	-7.866296	1.273384	-0.808660
H	-7.832311	1.262392	0.977259

Min2(S₁)

1,2,4-di-iodo methoxy benzene

C	-5.344124	1.831322	0.064244
C	-3.956591	1.883375	0.041465
C	-3.258242	3.021402	-0.015414
C	-3.906209	4.244625	-0.055021
C	-5.290017	4.253443	-0.034478
C	-6.010155	3.052716	0.024272
H	-5.872410	0.888094	0.111101
H	-3.359552	5.181002	-0.102210
H	-5.846491	5.183172	-0.064402
I	-0.780165	2.477994	-0.041198
I	-2.821259	0.035358	0.091742
O	-7.359651	3.174279	0.038286
C	-8.126587	1.985544	0.064270
H	-9.168892	2.294612	0.062677
H	-7.927494	1.370157	-0.818011
H	-7.921675	1.402503	0.966893

Min3(T₁)

1,2,4-di-iodo methoxy benzene

C	-5.361249	1.882068	0.081763
C	-3.967237	1.933304	0.045970
C	-3.345673	3.135813	-0.020235
C	-4.005204	4.341716	-0.058055
C	-5.388834	4.305381	-0.028489
C	-6.064845	3.082080	0.037646
H	-5.868489	0.928498	0.137204
H	-3.474901	5.284779	-0.111156
H	-5.973666	5.216726	-0.058482
I	0.004839	1.918776	-0.069251
I	-2.849288	0.168378	0.103859
O	-7.415729	3.162220	0.053956
C	-8.155033	1.955024	0.055287
H	-9.203503	2.242053	0.041284
H	-7.929300	1.355866	-0.831658
H	-7.951399	1.366915	0.954572

P(S₀)

4-methoxy benzyne + I₂

C	-6.255597	1.864709	0.072297
C	-4.882097	2.012907	0.044074
C	-4.232926	3.058969	-0.003815
C	-4.734758	4.349622	-0.047159
C	-6.121985	4.330547	-0.026354
C	-6.868690	3.127226	0.031463
H	-6.807429	0.937585	0.116374
H	-4.166166	5.268767	-0.090246
H	-6.680421	5.258784	-0.054273
I	-0.620068	2.398243	-0.157103
I	-1.484231	-0.098590	0.078441
O	-8.214038	3.299060	0.043895
C	-9.027695	2.141636	0.084939
H	-10.056153	2.493705	0.082856
H	-8.856235	1.509534	-0.791111
H	-8.842812	1.562093	0.993921

Min1(S₀)

1,2,4-di-iodo hydroxy benzene

C	-5.253255	1.819077	0.050923
C	-3.865711	1.834225	0.041158
C	-3.178040	3.045543	-0.011793
C	-3.908362	4.227988	-0.056090
C	-5.290301	4.219670	-0.047434
C	-5.966371	3.008353	0.006964
H	-5.799225	0.885566	0.092225
H	-3.386720	5.175708	-0.097997
H	-5.840669	5.153337	-0.082388
I	-1.099314	3.203160	-0.027576
I	-2.913929	-0.020969	0.108077
O	-7.318459	2.922706	0.018932
H	-7.706344	3.802136	-0.017301

Min2(S₁)

1,2,4-di-iodo hydroxy benzene

C	-5.402043	1.860530	0.051387
C	-4.027633	1.824096	0.032020
C	-3.283481	2.948178	-0.018416
C	-3.865674	4.203956	-0.054580
C	-5.249992	4.277843	-0.038215
C	-6.016345	3.112845	0.015328
H	-6.017895	0.967889	0.091935
H	-3.268863	5.109059	-0.095089
H	-5.740740	5.244764	-0.067738
I	-1.148454	2.726605	-0.045807
I	-2.449577	-0.199384	0.065851
O	-7.373475	3.144972	0.034047
H	-7.682611	4.055248	0.006948

Min3(T₁)

1,2,4-di-iodo hydroxy benzene

C	-5.520307	1.905082	0.049206
C	-4.156253	1.860096	0.029449
C	-3.319077	2.933714	-0.019638
C	-3.901402	4.196522	-0.054704
C	-5.282476	4.312670	-0.039077
C	-6.092757	3.178745	0.013357
H	-6.147120	1.022411	0.089284
H	-3.284979	5.087340	-0.093955
H	-5.737739	5.296415	-0.068385
I	-1.246405	2.688454	-0.041777
I	-1.666894	-0.629877	0.074759
O	-7.444045	3.252966	0.031658
H	-7.727329	4.172061	0.007490

P(S₀)4-hydroxy benzyne + I₂

C	-6.476646	1.879410	0.058598
C	-5.099962	1.838592	0.050173
C	-4.322121	2.796622	0.008478
C	-4.643072	4.137043	-0.038784
C	-6.027910	4.304085	-0.034442

C	-6.918911	3.209944	0.012825
H	-7.175656	1.054604	0.093976
H	-3.956122	4.972360	-0.074704
H	-6.441810	5.307008	-0.069361
I	-0.711844	2.784489	-0.054729
I	-1.191953	0.178873	0.055573
O	-8.266853	3.400515	0.015954
H	-8.470441	4.339255	-0.012657

MECI-1 (S₂/S₁)

1,2-di-iodo benzene

C	-5.258854	1.829036	0.039833
C	-3.886785	1.897517	0.024933
C	-3.201488	3.053304	-0.018941
C	-3.878278	4.252593	-0.049135
C	-5.262349	4.219279	-0.030856
C	-5.958132	3.014800	0.011691
H	-5.758638	0.868233	0.069118
H	-3.345081	5.189065	-0.086107
H	-5.798590	5.153856	-0.052298
H	-7.036478	2.999916	0.024090
I	-1.040619	3.082465	-0.037363
I	-2.817416	-0.232536	0.078609

MECI-1 (S₂/S₁)

1,2,4-di-iodo methyl benzene

C	-5.316885	1.869897	0.004612
C	-3.927001	1.882735	-0.006913
C	-3.272084	3.069702	-0.011843
C	-3.930762	4.290090	-0.010801
C	-5.314818	4.288669	-0.000640
C	-6.018100	3.075254	0.010323
H	-5.866933	0.935515	0.013397
H	-3.382406	5.232569	-0.013910
H	-5.837744	5.240693	0.003962
I	-0.856604	3.118294	-0.028085
I	-2.871492	0.010898	-0.008363
C	-7.524290	3.052757	0.022058
H	-7.926412	3.794351	0.714406
H	-7.929185	3.277506	-0.967941
H	-7.905599	2.072908	0.314205

MECI-1 (S₂/S₁)

1,2,4-di-iodo formyl benzene

C	-5.356833	1.825084	0.036530
C	-3.815777	1.823657	0.017688
C	-3.130760	3.003932	-0.021140
C	-3.913679	4.334176	-0.046010
C	-5.267811	4.331836	-0.029332
C	-6.035584	2.995851	0.014610
H	-5.887814	0.897354	0.066999
H	-3.380005	5.260232	-0.076504
H	-5.805335	5.256928	-0.046614
I	-1.041019	3.005720	-0.047013
I	-2.762580	0.011081	0.051501

C	-7.576073	2.994161	0.033594
O	-8.206821	4.082453	0.013188
H	-8.108385	2.066999	0.064083

MECI-1 (S₂/S₁)

1,2,4-di-iodo cyano benzene

C	-5.324103	2.462978	0.941796
C	-3.969830	2.227896	0.821340
C	-3.244056	2.742642	-0.224535
C	-3.872767	3.519743	-1.191968
C	-5.231583	3.769027	-1.090068
C	-5.962381	3.242550	-0.023800
H	-5.898484	2.054742	1.768281
H	-3.309135	3.929339	-2.021297
H	-5.721723	4.373706	-1.842423
I	-1.180672	2.394634	-0.425386
I	-2.910272	0.782889	2.664582
C	-7.374202	3.491061	0.098552
N	-8.502104	3.668756	0.228294

MECI-1 (S₂/S₁)

1,2,4-di-iodo nitro benzene

C	-5.293150	1.865386	0.081244
C	-3.914913	1.906410	0.052927
C	-3.236392	3.096149	-0.048634
C	-3.934003	4.296990	-0.132816
C	-5.318258	4.284150	-0.083305
C	-5.975619	3.069612	0.022596
H	-5.843381	0.933925	0.145600
H	-3.405039	5.235491	-0.242232
H	-5.879962	5.206604	-0.127613
I	-1.136448	3.165267	-0.075227
I	-2.728924	-0.387546	0.048861
N	-7.449816	3.052895	0.049172
O	-8.029682	4.115323	0.021648
O	-7.999469	1.974628	0.092903

MECI-1 (S₂/S₁)

1,2,4- di-iodo methoxy benzene

C	-5.347520	1.854440	-0.228024
C	-3.973981	1.881156	-0.125770
C	-3.309226	3.053115	0.016798
C	-3.976540	4.277876	0.052936
C	-5.348206	4.291152	-0.059663
C	-6.049451	3.063594	-0.188552
H	-5.899719	0.931967	-0.328002
H	-3.426180	5.212285	0.179393
H	-5.859107	5.245536	-0.015480
I	-0.992919	3.023899	0.198688
I	-2.855603	-0.031294	-0.186825
O	-7.401307	3.058628	-0.232867
C	-8.002463	1.825006	0.195208
H	-9.076013	1.955620	0.322512
H	-7.825458	1.026970	-0.527985
H	-7.555089	1.549762	1.152034

MECI-1 (S₂/S₁)

1,2,4-di-iodo hydroxy benzene

C	-5.317039	1.766893	0.097556
C	-3.933806	1.812737	0.047797
C	-3.276659	3.009971	-0.017973
C	-3.958241	4.220300	-0.034508
C	-5.334515	4.209745	0.012469
C	-6.017299	2.982071	0.069126
H	-5.872464	0.834015	0.136155
H	-3.421571	5.169165	-0.081701
H	-5.865818	5.154353	0.008530
I	-0.879023	3.054488	-0.106246
I	-2.779749	-0.005984	0.060162
O	-7.370806	2.912029	0.111577
H	-7.784763	3.664761	-0.325953

MECI-2(S₀/S₁)

1,2-di-chloro benzene

C	-5.502419	1.765481	0.043999
C	-4.133222	1.718933	0.031556
C	-3.338687	2.771703	-0.006144
C	-3.857297	4.043302	-0.037042
C	-5.237573	4.175587	-0.027721
C	-6.055839	3.049488	0.012912
H	-6.132954	0.885902	0.075255
H	-3.170189	4.888509	-0.067813
H	-5.677972	5.164648	-0.052924
H	-7.134131	3.163955	0.020656
Cl	-1.374041	2.822017	-0.028126
Cl	-1.839090	0.513210	0.035223

MECI-2(S₀/S₁)

1,2-di-bromo benzene

C	-5.222965	1.820970	0.022767
C	-3.870099	2.064801	-0.044476
C	-3.294286	3.216449	-0.104028
C	-4.014592	4.396243	-0.084065
C	-5.398974	4.244007	-0.013140
C	-5.992430	2.979106	0.037416
H	-5.651548	0.825161	0.067758
H	-3.563226	5.380204	-0.128739
H	-6.029958	5.126058	-0.000321
H	-7.071203	2.896987	0.093439
Br	-0.695815	1.774772	0.209067
Br	-2.648318	0.237979	-0.055844

MECI-2(S₀/S₁)

1,2-di-iodo benzene

C	-5.531826	1.815724	0.084046
C	-4.155788	1.789900	0.050328
C	-3.370220	2.819143	-0.020192
C	-3.874011	4.106385	-0.071474
C	-5.255040	4.229881	-0.044712
C	-6.074106	3.101573	0.033264
H	-6.166779	0.941309	0.144764

H	-3.211412	4.968130	-0.130819
H	-5.700462	5.216914	-0.085737
H	-7.151525	3.224167	0.055039
I	-1.003114	2.756273	-0.076179
I	-1.959130	-0.006665	0.061503

MECI-2(S₀/S₁)

1,2,4-di-iodo methyl benzene

C	-5.325409	1.806224	0.079676
C	-3.950925	1.874325	0.066071
C	-3.253178	2.950056	-0.009586
C	-3.809744	4.211551	-0.086698
C	-5.201033	4.222656	-0.077684
C	-5.966729	3.046312	0.005243
H	-5.895233	0.885630	0.139780
H	-3.229930	5.126001	-0.153271
H	-5.718450	5.174581	-0.140737
I	-0.780997	2.541641	-0.026314
I	-2.074628	-0.021303	0.142620
C	-7.470335	3.120827	0.029111
H	-7.912941	2.136546	-0.125291
H	-7.823697	3.499984	0.990482
H	-7.844898	3.790134	-0.746727

MECI-2(S₀/S₁)

1,2,4-di-iodo formyl benzene

C	-5.524174	1.850540	0.038899
C	-4.148230	1.817509	0.030593
C	-3.389269	2.866457	-0.000660
C	-3.873754	4.161825	-0.030762
C	-5.254357	4.274982	-0.028396
C	-6.072867	3.136994	0.007083
H	-6.163643	0.974463	0.066697
H	-3.221291	5.029768	-0.056067
H	-5.726426	5.249939	-0.053989
I	-0.985467	2.610768	-0.013624
I	-2.145712	-0.026914	0.038734
C	-7.549224	3.281570	0.010271
O	-8.131941	4.336192	-0.035300
H	-8.109558	2.328252	0.058085

MECI-2(S₀/S₁)

1,2,4-di-iodo cyano benzene

C	-5.517543	1.826709	0.049784
C	-4.144309	1.808971	0.032911
C	-3.391449	2.865686	-0.011488
C	-3.885781	4.153526	-0.049658
C	-5.268410	4.262066	-0.038444
C	-6.072335	3.114017	0.012319
H	-6.152500	0.950362	0.088822
H	-3.241869	5.027481	-0.087266
H	-5.738454	5.237241	-0.069190
I	-0.992820	2.636905	-0.032520
I	-2.134060	-0.005815	0.051893
C	-7.504382	3.260935	0.028022

N	-8.647019	3.373909	0.043451
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MECI-2(S₀/S₁)

1,2,4-di-iodo nitro benzene

C	-5.536218	1.819134	0.049826
C	-4.161220	1.776343	0.035062
C	-3.385057	2.822363	-0.010286
C	-3.874749	4.113527	-0.052568
C	-5.251059	4.253950	-0.043774
C	-6.048510	3.113882	0.009014
H	-6.196480	0.963761	0.089340
H	-3.208744	4.972650	-0.090923
H	-5.712522	5.230516	-0.076981
I	-1.022272	2.729858	-0.028262
I	-2.038881	0.020947	0.064677
N	-7.514003	3.292577	0.024763
O	-7.946646	4.422884	-0.011261
O	-8.202902	2.298518	0.073987

MECI-2(S₀/S₁)

1,2,4-di-iodo methoxy benzene

C	-5.291834	1.927894	0.060158
C	-3.911057	2.043035	0.030023
C	-3.337593	3.197446	-0.025493
C	-3.970504	4.424703	-0.063935
C	-5.356619	4.353399	-0.036925
C	-6.017305	3.112250	0.023896
H	-5.756134	0.946201	0.109492
H	-3.465484	5.380774	-0.114221
H	-5.959725	5.254122	-0.064264
I	-0.728986	1.857460	0.000971
I	-2.961598	-0.109415	0.082007
O	-7.370668	3.155198	0.042357
C	-8.061058	1.917154	0.067958
H	-9.121267	2.156428	0.065489
H	-7.820901	1.315166	-0.813472
H	-7.818781	1.347781	0.970176

MECI-2(S₀/S₁)

1,2,4-di-iodo hydroxy benzene

C	-5.475956	1.842470	0.051394
C	-4.104944	1.874905	0.029526
C	-3.361783	2.926215	-0.016898
C	-3.878718	4.205133	-0.054094
C	-5.267073	4.276022	-0.037273
C	-6.055490	3.114516	0.015477
H	-6.095387	0.954850	0.090667
H	-3.265448	5.100111	-0.093440
H	-5.758853	5.242977	-0.065516
I	-0.925021	2.521617	-0.046582
I	-2.218376	-0.043898	0.063377
O	-7.412982	3.173368	0.033609
H	-7.706752	4.088313	0.007421

Vibrational frequencies for relevant energy stationary points concerning the 1,2-di-iodobenzene derivatives photolysis.

Min1(S₀)

1,2-di-chloro benzene

0:	0.00 cm** ⁻¹
1:	0.00 cm** ⁻¹
2:	0.00 cm** ⁻¹
3:	0.00 cm** ⁻¹
4:	0.00 cm** ⁻¹
5:	0.00 cm** ⁻¹
6:	131.92 cm** ⁻¹
7:	207.90 cm** ⁻¹
8:	239.90 cm** ⁻¹
9:	342.51 cm** ⁻¹
10:	438.01 cm** ⁻¹
11:	451.01 cm** ⁻¹
12:	492.00 cm** ⁻¹
13:	537.10 cm** ⁻¹
14:	682.66 cm** ⁻¹
15:	744.35 cm** ⁻¹
16:	764.33 cm** ⁻¹
17:	774.51 cm** ⁻¹
18:	896.97 cm** ⁻¹
19:	989.30 cm** ⁻¹
20:	1024.78 cm** ⁻¹
21:	1061.66 cm** ⁻¹
22:	1071.23 cm** ⁻¹
23:	1156.98 cm** ⁻¹
24:	1167.79 cm** ⁻¹
25:	1179.58 cm** ⁻¹
26:	1284.54 cm** ⁻¹
27:	1286.68 cm** ⁻¹
28:	1481.57 cm** ⁻¹
29:	1514.45 cm** ⁻¹
30:	1655.65 cm** ⁻¹
31:	1666.29 cm** ⁻¹
32:	3216.68 cm** ⁻¹
33:	3227.78 cm** ⁻¹
34:	3236.69 cm** ⁻¹
35:	3241.45 cm** ⁻¹

Min2(S₁)

0:	0.00 cm** ⁻¹
1:	0.00 cm** ⁻¹
2:	0.00 cm** ⁻¹
3:	0.00 cm** ⁻¹
4:	0.00 cm** ⁻¹
5:	0.00 cm** ⁻¹
6:	0.00 cm** ⁻¹
7:	139.80 cm** ⁻¹
8:	176.43 cm** ⁻¹
9:	177.96 cm** ⁻¹
10:	316.26 cm** ⁻¹

11: 390.31 cm**-1
12: 406.98 cm**-1
13: 494.82 cm**-1
14: 610.02 cm**-1
15: 694.74 cm**-1
16: 699.53 cm**-1
17: 757.37 cm**-1
18: 868.48 cm**-1
19: 950.80 cm**-1
20: 970.89 cm**-1
21: 1024.34 cm**-1
22: 1047.02 cm**-1
23: 1109.24 cm**-1
24: 1133.58 cm**-1
25: 1171.04 cm**-1
26: 1256.61 cm**-1
27: 1307.32 cm**-1
28: 1462.22 cm**-1
29: 1479.91 cm**-1
30: 1605.31 cm**-1
31: 1675.83 cm**-1
32: 3205.25 cm**-1
33: 3213.26 cm**-1
34: 3219.97 cm**-1
35: 3232.42 cm**-1

Min3(T_i)

0: 0.00 cm**-1
1: 0.00 cm**-1
2: 0.00 cm**-1
3: 0.00 cm**-1
4: 0.00 cm**-1
5: 0.00 cm**-1
6: 14.53 cm**-1
7: 31.85 cm**-1
8: 51.60 cm**-1
9: 184.49 cm**-1
10: 287.48 cm**-1
11: 420.10 cm**-1
12: 424.37 cm**-1
13: 503.13 cm**-1
14: 623.11 cm**-1
15: 708.70 cm**-1
16: 715.24 cm**-1
17: 766.51 cm**-1
18: 882.16 cm**-1
19: 977.64 cm**-1
20: 988.28 cm**-1
21: 1022.20 cm**-1
22: 1051.01 cm**-1
23: 1120.24 cm**-1
24: 1137.78 cm**-1
25: 1172.27 cm**-1
26: 1250.22 cm**-1

27: 1305.55 cm^{**}-1
28: 1459.68 cm^{**}-1
29: 1481.26 cm^{**}-1
30: 1613.33 cm^{**}-1
31: 1668.32 cm^{**}-1
32: 3207.47 cm^{**}-1
33: 3217.33 cm^{**}-1
34: 3226.38 cm^{**}-1
35: 3234.89 cm^{**}-1

P(S₀)

0: 0.00 cm^{**}-1
1: 0.00 cm^{**}-1
2: 0.00 cm^{**}-1
3: 0.00 cm^{**}-1
4: 0.00 cm^{**}-1
5: 0.00 cm^{**}-1
6: 12.89 cm^{**}-1
7: 27.64 cm^{**}-1
8: 32.84 cm^{**}-1
9: 47.70 cm^{**}-1
10: 61.87 cm^{**}-1
11: 387.93 cm^{**}-1
12: 400.95 cm^{**}-1
13: 460.29 cm^{**}-1
14: 594.15 cm^{**}-1
15: 626.15 cm^{**}-1
16: 626.32 cm^{**}-1
17: 778.16 cm^{**}-1
18: 848.12 cm^{**}-1
19: 901.01 cm^{**}-1
20: 971.60 cm^{**}-1
21: 1015.94 cm^{**}-1
22: 1019.32 cm^{**}-1
23: 1078.87 cm^{**}-1
24: 1127.12 cm^{**}-1
25: 1171.12 cm^{**}-1
26: 1278.72 cm^{**}-1
27: 1316.53 cm^{**}-1
28: 1449.09 cm^{**}-1
29: 1502.02 cm^{**}-1
30: 1516.19 cm^{**}-1
31: 2070.70 cm^{**}-1
32: 3201.58 cm^{**}-1
33: 3216.27 cm^{**}-1
34: 3238.41 cm^{**}-1
35: 3241.55 cm^{**}-1

MECI-2(S₀/S_i)

0: 0.00 cm^{**}-1
1: 0.00 cm^{**}-1
2: 0.00 cm^{**}-1
3: 0.00 cm^{**}-1
4: 0.00 cm^{**}-1

5: 0.00 cm**⁻¹
6: 0.00 cm**⁻¹
7: 0.00 cm**⁻¹
8: 204.70 cm**⁻¹
9: 290.19 cm**⁻¹
10: 299.19 cm**⁻¹
11: 411.95 cm**⁻¹
12: 469.53 cm**⁻¹
13: 545.03 cm**⁻¹
14: 600.48 cm**⁻¹
15: 679.74 cm**⁻¹
16: 760.36 cm**⁻¹
17: 886.81 cm**⁻¹
18: 895.79 cm**⁻¹
19: 918.86 cm**⁻¹
20: 996.35 cm**⁻¹
21: 1028.31 cm**⁻¹
22: 1052.54 cm**⁻¹
23: 1129.11 cm**⁻¹
24: 1167.50 cm**⁻¹
25: 1283.49 cm**⁻¹
26: 1315.97 cm**⁻¹
27: 1419.41 cm**⁻¹
28: 1483.50 cm**⁻¹
29: 1603.55 cm**⁻¹
30: 1669.26 cm**⁻¹
31: 2725.98 cm**⁻¹
32: 3208.68 cm**⁻¹
33: 3227.80 cm**⁻¹
34: 3231.02 cm**⁻¹
35: 3319.47 cm**⁻¹

Min1(S₀)

1,2-di-bromo benzene

0: 0.00 cm**⁻¹
1: 0.00 cm**⁻¹
2: 0.00 cm**⁻¹
3: 0.00 cm**⁻¹
4: 0.00 cm**⁻¹
5: 0.00 cm**⁻¹
6: 106.73 cm**⁻¹
7: 134.16 cm**⁻¹
8: 217.10 cm**⁻¹
9: 258.74 cm**⁻¹
10: 369.83 cm**⁻¹
11: 392.44 cm**⁻¹
12: 445.19 cm**⁻¹
13: 522.45 cm**⁻¹
14: 661.97 cm**⁻¹
15: 727.24 cm**⁻¹
16: 739.48 cm**⁻¹
17: 772.84 cm**⁻¹
18: 896.67 cm**⁻¹
19: 990.13 cm**⁻¹
20: 1026.52 cm**⁻¹
21: 1039.50 cm**⁻¹

22: 1071.55 cm**⁻¹
23: 1148.10 cm**⁻¹
24: 1152.26 cm**⁻¹
25: 1176.75 cm**⁻¹
26: 1283.53 cm**⁻¹
27: 1284.80 cm**⁻¹
28: 1475.55 cm**⁻¹
29: 1507.01 cm**⁻¹
30: 1650.64 cm**⁻¹
31: 1660.33 cm**⁻¹
32: 3216.69 cm**⁻¹
33: 3227.47 cm**⁻¹
34: 3236.05 cm**⁻¹
35: 3241.23 cm**⁻¹

Min2(S_i)

0: 0.00 cm**⁻¹
1: 0.00 cm**⁻¹
2: 0.00 cm**⁻¹
3: 0.00 cm**⁻¹
4: 0.00 cm**⁻¹
5: 0.00 cm**⁻¹
6: 0.00 cm**⁻¹
7: 118.85 cm**⁻¹
8: 150.80 cm**⁻¹
9: 162.83 cm**⁻¹
10: 274.04 cm**⁻¹
11: 316.26 cm**⁻¹
12: 404.89 cm**⁻¹
13: 483.90 cm**⁻¹
14: 612.53 cm**⁻¹
15: 660.76 cm**⁻¹
16: 707.58 cm**⁻¹
17: 761.27 cm**⁻¹
18: 881.93 cm**⁻¹
19: 951.30 cm**⁻¹
20: 976.78 cm**⁻¹
21: 1024.35 cm**⁻¹
22: 1048.32 cm**⁻¹
23: 1082.16 cm**⁻¹
24: 1133.68 cm**⁻¹
25: 1164.94 cm**⁻¹
26: 1269.63 cm**⁻¹
27: 1308.11 cm**⁻¹
28: 1465.88 cm**⁻¹
29: 1471.54 cm**⁻¹
30: 1611.84 cm**⁻¹
31: 1668.63 cm**⁻¹
32: 3199.56 cm**⁻¹
33: 3208.20 cm**⁻¹
34: 3215.34 cm**⁻¹
35: 3230.20 cm**⁻¹

Min3(T_i)

0: 0.00 cm**⁻¹
1: 0.00 cm**⁻¹
2: 0.00 cm**⁻¹
3: 0.00 cm**⁻¹
4: 0.00 cm**⁻¹
5: 0.00 cm**⁻¹
6: 0.00 cm**⁻¹
7: 12.81 cm**⁻¹
8: 49.44 cm**⁻¹
9: 169.50 cm**⁻¹
10: 240.17 cm**⁻¹
11: 325.34 cm**⁻¹
12: 417.04 cm**⁻¹
13: 491.24 cm**⁻¹
14: 621.91 cm**⁻¹
15: 683.09 cm**⁻¹
16: 708.61 cm**⁻¹
17: 762.97 cm**⁻¹
18: 877.96 cm**⁻¹
19: 978.28 cm**⁻¹
20: 984.51 cm**⁻¹
21: 1025.42 cm**⁻¹
22: 1049.49 cm**⁻¹
23: 1110.07 cm**⁻¹
24: 1132.96 cm**⁻¹
25: 1171.70 cm**⁻¹
26: 1249.49 cm**⁻¹
27: 1307.33 cm**⁻¹
28: 1458.39 cm**⁻¹
29: 1477.93 cm**⁻¹
30: 1611.38 cm**⁻¹
31: 1664.30 cm**⁻¹
32: 3207.04 cm**⁻¹
33: 3216.05 cm**⁻¹
34: 3222.50 cm**⁻¹
35: 3233.48 cm**⁻¹

P(S₀)

0: 0.00 cm**⁻¹
1: 0.00 cm**⁻¹
2: 0.00 cm**⁻¹
3: 0.00 cm**⁻¹
4: 0.00 cm**⁻¹
5: 0.00 cm**⁻¹
6: 0.00 cm**⁻¹
7: 18.00 cm**⁻¹
8: 30.18 cm**⁻¹
9: 40.41 cm**⁻¹
10: 60.50 cm**⁻¹
11: 344.62 cm**⁻¹
12: 389.76 cm**⁻¹
13: 401.44 cm**⁻¹
14: 461.27 cm**⁻¹
15: 624.69 cm**⁻¹

16: 626.60 cm^{**}-1
17: 772.03 cm^{**}-1
18: 848.02 cm^{**}-1
19: 900.44 cm^{**}-1
20: 968.76 cm^{**}-1
21: 1014.56 cm^{**}-1
22: 1016.46 cm^{**}-1
23: 1079.16 cm^{**}-1
24: 1124.00 cm^{**}-1
25: 1166.31 cm^{**}-1
26: 1277.81 cm^{**}-1
27: 1315.99 cm^{**}-1
28: 1447.40 cm^{**}-1
29: 1500.87 cm^{**}-1
30: 1515.84 cm^{**}-1
31: 2069.40 cm^{**}-1
32: 3201.54 cm^{**}-1
33: 3216.19 cm^{**}-1
34: 3238.21 cm^{**}-1
35: 3241.56 cm^{**}-1

MECI-2(S₀/S_i)

0: 0.00 cm^{**}-1
1: 0.00 cm^{**}-1
2: 0.00 cm^{**}-1
3: 0.00 cm^{**}-1
4: 0.00 cm^{**}-1
5: 0.00 cm^{**}-1
6: 0.00 cm^{**}-1
7: 0.00 cm^{**}-1
8: 0.00 cm^{**}-1
9: 164.41 cm^{**}-1
10: 174.20 cm^{**}-1
11: 406.70 cm^{**}-1
12: 428.51 cm^{**}-1
13: 464.54 cm^{**}-1
14: 552.58 cm^{**}-1
15: 673.24 cm^{**}-1
16: 742.34 cm^{**}-1
17: 753.40 cm^{**}-1
18: 881.58 cm^{**}-1
19: 893.64 cm^{**}-1
20: 994.28 cm^{**}-1
21: 1040.06 cm^{**}-1
22: 1043.99 cm^{**}-1
23: 1120.66 cm^{**}-1
24: 1166.26 cm^{**}-1
25: 1269.38 cm^{**}-1
26: 1303.02 cm^{**}-1
27: 1427.57 cm^{**}-1
28: 1432.51 cm^{**}-1
29: 1524.82 cm^{**}-1
30: 1611.26 cm^{**}-1
31: 3061.39 cm^{**}-1
32: 3207.33 cm^{**}-1

33: 3218.13 cm^{**}-1
34: 3228.42 cm^{**}-1
35: 4917.31 cm^{**}-1

Min1(S₀)

1,2-di-iodo benzene

0: 0.00 cm^{**}-1
1: 0.00 cm^{**}-1
2: 0.00 cm^{**}-1
3: 0.00 cm^{**}-1
4: 0.00 cm^{**}-1
5: 0.00 cm^{**}-1
6: 91.96 cm^{**}-1
7: 101.03 cm^{**}-1
8: 197.32 cm^{**}-1
9: 214.35 cm^{**}-1
10: 328.29 cm^{**}-1
11: 335.61 cm^{**}-1
12: 437.89 cm^{**}-1
13: 505.84 cm^{**}-1
14: 654.01 cm^{**}-1
15: 707.03 cm^{**}-1
16: 731.44 cm^{**}-1
17: 768.40 cm^{**}-1
18: 894.17 cm^{**}-1
19: 987.83 cm^{**}-1
20: 1024.95 cm^{**}-1
21: 1025.06 cm^{**}-1
22: 1070.62 cm^{**}-1
23: 1132.96 cm^{**}-1
24: 1147.85 cm^{**}-1
25: 1180.01 cm^{**}-1
26: 1274.02 cm^{**}-1
27: 1289.44 cm^{**}-1
28: 1467.76 cm^{**}-1
29: 1499.50 cm^{**}-1
30: 1642.63 cm^{**}-1
31: 1653.61 cm^{**}-1
32: 3214.82 cm^{**}-1
33: 3224.43 cm^{**}-1
34: 3232.04 cm^{**}-1
35: 3238.66 cm^{**}-1

Min2(S₁)

0: 0.00 cm^{**}-1
1: 0.00 cm^{**}-1
2: 0.00 cm^{**}-1
3: 0.00 cm^{**}-1
4: 0.00 cm^{**}-1
5: 0.00 cm^{**}-1
6: 48.65 cm^{**}-1
7: 81.28 cm^{**}-1
8: 117.64 cm^{**}-1
9: 147.62 cm^{**}-1
10: 251.91 cm^{**}-1

11: 263.20 cm**-1
12: 407.81 cm**-1
13: 479.02 cm**-1
14: 618.54 cm**-1
15: 639.46 cm**-1
16: 708.24 cm**-1
17: 761.66 cm**-1
18: 886.06 cm**-1
19: 955.16 cm**-1
20: 972.03 cm**-1
21: 1019.74 cm**-1
22: 1048.49 cm**-1
23: 1067.02 cm**-1
24: 1132.54 cm**-1
25: 1164.55 cm**-1
26: 1273.47 cm**-1
27: 1316.51 cm**-1
28: 1463.59 cm**-1
29: 1471.88 cm**-1
30: 1612.82 cm**-1
31: 1659.36 cm**-1
32: 3188.33 cm**-1
33: 3201.27 cm**-1
34: 3209.53 cm**-1
35: 3226.43 cm**-1

Min3(T_i)

0: 0.00 cm**-1
1: 0.00 cm**-1
2: 0.00 cm**-1
3: 0.00 cm**-1
4: 0.00 cm**-1
5: 0.00 cm**-1
6: 23.60 cm**-1
7: 35.11 cm**-1
8: 53.90 cm**-1
9: 157.19 cm**-1
10: 210.19 cm**-1
11: 276.74 cm**-1
12: 426.49 cm**-1
13: 482.92 cm**-1
14: 621.80 cm**-1
15: 667.80 cm**-1
16: 706.66 cm**-1
17: 772.84 cm**-1
18: 894.25 cm**-1
19: 981.58 cm**-1
20: 989.21 cm**-1
21: 1029.55 cm**-1
22: 1052.13 cm**-1
23: 1102.03 cm**-1
24: 1135.14 cm**-1
25: 1177.51 cm**-1
26: 1254.50 cm**-1

27: 1307.31 cm^{**}-1
28: 1455.59 cm^{**}-1
29: 1478.00 cm^{**}-1
30: 1607.69 cm^{**}-1
31: 1658.75 cm^{**}-1
32: 3205.39 cm^{**}-1
33: 3214.45 cm^{**}-1
34: 3222.08 cm^{**}-1
35: 3231.43 cm^{**}-1

P(S₀)

Benzynes + I₂

0: 0.00 cm^{**}-1
1: 0.00 cm^{**}-1
2: 0.00 cm^{**}-1
3: 0.00 cm^{**}-1
4: 0.00 cm^{**}-1
5: 0.00 cm^{**}-1
6: 0.00 cm^{**}-1
7: 0.00 cm^{**}-1
8: 0.00 cm^{**}-1
9: 43.48 cm^{**}-1
10: 55.85 cm^{**}-1
11: 230.38 cm^{**}-1
12: 387.90 cm^{**}-1
13: 399.08 cm^{**}-1
14: 454.09 cm^{**}-1
15: 619.81 cm^{**}-1
16: 625.82 cm^{**}-1
17: 755.79 cm^{**}-1
18: 848.98 cm^{**}-1
19: 886.95 cm^{**}-1
20: 957.13 cm^{**}-1
21: 1005.65 cm^{**}-1
22: 1014.00 cm^{**}-1
23: 1077.75 cm^{**}-1
24: 1118.43 cm^{**}-1
25: 1157.49 cm^{**}-1
26: 1275.50 cm^{**}-1
27: 1314.84 cm^{**}-1
28: 1445.12 cm^{**}-1
29: 1499.47 cm^{**}-1
30: 1515.50 cm^{**}-1
31: 2065.60 cm^{**}-1
32: 3201.97 cm^{**}-1
33: 3216.82 cm^{**}-1
34: 3239.40 cm^{**}-1
35: 3241.78 cm^{**}-1

MECI-2(S₀/S_i)

0: 0.00 cm^{**}-1
1: 0.00 cm^{**}-1
2: 0.00 cm^{**}-1
3: 0.00 cm^{**}-1
4: 0.00 cm^{**}-1

5: 0.00 cm**⁻¹
6: 0.00 cm**⁻¹
7: 46.58 cm**⁻¹
8: 119.41 cm**⁻¹
9: 143.71 cm**⁻¹
10: 174.35 cm**⁻¹
11: 401.23 cm**⁻¹
12: 418.60 cm**⁻¹
13: 470.76 cm**⁻¹
14: 565.51 cm**⁻¹
15: 651.27 cm**⁻¹
16: 678.15 cm**⁻¹
17: 767.76 cm**⁻¹
18: 881.50 cm**⁻¹
19: 936.02 cm**⁻¹
20: 981.26 cm**⁻¹
21: 1021.90 cm**⁻¹
22: 1041.07 cm**⁻¹
23: 1110.24 cm**⁻¹
24: 1164.16 cm**⁻¹
25: 1214.21 cm**⁻¹
26: 1279.48 cm**⁻¹
27: 1341.64 cm**⁻¹
28: 1474.06 cm**⁻¹
29: 1501.86 cm**⁻¹
30: 1626.01 cm**⁻¹
31: 1816.79 cm**⁻¹
32: 3171.69 cm**⁻¹
33: 3203.93 cm**⁻¹
34: 3223.15 cm**⁻¹

Min1(S₀)

1,2,4 di-iodo methyl benzene

0: 0.00 cm**⁻¹
1: 0.00 cm**⁻¹
2: 0.00 cm**⁻¹
3: 0.00 cm**⁻¹
4: 0.00 cm**⁻¹
5: 0.00 cm**⁻¹
6: 58.09 cm**⁻¹
7: 81.21 cm**⁻¹
8: 100.40 cm**⁻¹
9: 151.83 cm**⁻¹
10: 175.50 cm**⁻¹
11: 268.13 cm**⁻¹
12: 293.87 cm**⁻¹
13: 318.57 cm**⁻¹
14: 411.48 cm**⁻¹
15: 442.87 cm**⁻¹
16: 546.83 cm**⁻¹
17: 596.38 cm**⁻¹
18: 683.87 cm**⁻¹
19: 728.66 cm**⁻¹
20: 836.96 cm**⁻¹
21: 862.56 cm**⁻¹
22: 911.83 cm**⁻¹

23: 993.91 cm**⁻¹
24: 1018.34 cm**⁻¹
25: 1038.89 cm**⁻¹
26: 1075.10 cm**⁻¹
27: 1140.34 cm**⁻¹
28: 1166.90 cm**⁻¹
29: 1245.78 cm**⁻¹
30: 1276.75 cm**⁻¹
31: 1295.38 cm**⁻¹
32: 1418.36 cm**⁻¹
33: 1421.64 cm**⁻¹
34: 1484.82 cm**⁻¹
35: 1487.93 cm**⁻¹
36: 1517.90 cm**⁻¹
37: 1631.02 cm**⁻¹
38: 1672.36 cm**⁻¹
39: 3070.42 cm**⁻¹
40: 3141.96 cm**⁻¹
41: 3163.88 cm**⁻¹
42: 3205.79 cm**⁻¹
43: 3216.22 cm**⁻¹
44: 3228.75 cm**⁻¹

Min2(S_i)

0: 0.00 cm**⁻¹
1: 0.00 cm**⁻¹
2: 0.00 cm**⁻¹
3: 0.00 cm**⁻¹
4: 0.00 cm**⁻¹
5: 0.00 cm**⁻¹
6: 47.67 cm**⁻¹
7: 79.06 cm**⁻¹
8: 91.11 cm**⁻¹
9: 103.27 cm**⁻¹
10: 112.64 cm**⁻¹
11: 224.67 cm**⁻¹
12: 238.16 cm**⁻¹
13: 283.01 cm**⁻¹
14: 379.28 cm**⁻¹
15: 413.31 cm**⁻¹
16: 511.37 cm**⁻¹
17: 565.23 cm**⁻¹
18: 634.70 cm**⁻¹
19: 711.54 cm**⁻¹
20: 788.18 cm**⁻¹
21: 830.21 cm**⁻¹
22: 900.58 cm**⁻¹
23: 981.49 cm**⁻¹
24: 989.64 cm**⁻¹
25: 1022.53 cm**⁻¹
26: 1072.07 cm**⁻¹
27: 1077.06 cm**⁻¹
28: 1153.85 cm**⁻¹
29: 1229.89 cm**⁻¹
30: 1279.78 cm**⁻¹

31: 1306.06 cm**-1
32: 1417.52 cm**-1
33: 1420.26 cm**-1
34: 1486.73 cm**-1
35: 1487.71 cm**-1
36: 1493.18 cm**-1
37: 1616.71 cm**-1
38: 1663.61 cm**-1
39: 3068.21 cm**-1
40: 3139.41 cm**-1
41: 3161.13 cm**-1
42: 3177.29 cm**-1
43: 3194.01 cm**-1
44: 3209.54 cm**-1

Min3(T_i)

0: 0.00 cm**-1
1: 0.00 cm**-1
2: 0.00 cm**-1
3: 0.00 cm**-1
4: 0.00 cm**-1
5: 0.00 cm**-1
6: 17.51 cm**-1
7: 39.32 cm**-1
8: 71.76 cm**-1
9: 88.40 cm**-1
10: 122.59 cm**-1
11: 181.48 cm**-1
12: 251.48 cm**-1
13: 280.91 cm**-1
14: 365.17 cm**-1
15: 419.41 cm**-1
16: 517.18 cm**-1
17: 588.57 cm**-1
18: 640.61 cm**-1
19: 699.95 cm**-1
20: 803.01 cm**-1
21: 845.57 cm**-1
22: 884.35 cm**-1
23: 997.69 cm**-1
24: 1004.34 cm**-1
25: 1017.15 cm**-1
26: 1073.55 cm**-1
27: 1105.81 cm**-1
28: 1166.45 cm**-1
29: 1225.39 cm**-1
30: 1265.07 cm**-1
31: 1295.49 cm**-1
32: 1416.16 cm**-1
33: 1418.96 cm**-1
34: 1480.90 cm**-1
35: 1485.78 cm**-1
36: 1506.45 cm**-1
37: 1599.14 cm**-1
38: 1669.60 cm**-1

39: 3075.41 cm**⁻¹
40: 3144.90 cm**⁻¹
41: 3169.70 cm**⁻¹
42: 3203.00 cm**⁻¹
43: 3204.99 cm**⁻¹
44: 3220.92 cm**⁻¹

P(S₀)

0: 0.00 cm**⁻¹
1: 0.00 cm**⁻¹
2: 0.00 cm**⁻¹
3: 0.00 cm**⁻¹
4: 0.00 cm**⁻¹
5: 0.00 cm**⁻¹
6: 0.00 cm**⁻¹
7: 0.00 cm**⁻¹
8: 15.94 cm**⁻¹
9: 36.34 cm**⁻¹
10: 41.54 cm**⁻¹
11: 180.69 cm**⁻¹
12: 231.02 cm**⁻¹
13: 240.67 cm**⁻¹
14: 361.93 cm**⁻¹
15: 376.85 cm**⁻¹
16: 407.76 cm**⁻¹
17: 466.54 cm**⁻¹
18: 584.76 cm**⁻¹
19: 645.14 cm**⁻¹
20: 689.95 cm**⁻¹
21: 835.86 cm**⁻¹
22: 910.99 cm**⁻¹
23: 936.66 cm**⁻¹
24: 982.58 cm**⁻¹
25: 1018.61 cm**⁻¹
26: 1072.96 cm**⁻¹
27: 1075.02 cm**⁻¹
28: 1149.71 cm**⁻¹
29: 1218.85 cm**⁻¹
30: 1273.87 cm**⁻¹
31: 1327.64 cm**⁻¹
32: 1402.32 cm**⁻¹
33: 1421.87 cm**⁻¹
34: 1476.75 cm**⁻¹
35: 1487.86 cm**⁻¹
36: 1506.92 cm**⁻¹
37: 1552.56 cm**⁻¹
38: 2072.41 cm**⁻¹
39: 3070.36 cm**⁻¹
40: 3141.49 cm**⁻¹
41: 3160.80 cm**⁻¹
42: 3195.67 cm**⁻¹
43: 3224.68 cm**⁻¹
44: 3234.07 cm**⁻¹

MECI-2(S₀/S₁)

0: 0.00 cm**⁻¹
1: 0.00 cm**⁻¹
2: 0.00 cm**⁻¹
3: 0.00 cm**⁻¹
4: 0.00 cm**⁻¹
5: 0.00 cm**⁻¹
6: 0.00 cm**⁻¹
7: 38.14 cm**⁻¹
8: 50.36 cm**⁻¹
9: 81.49 cm**⁻¹
10: 119.48 cm**⁻¹
11: 163.69 cm**⁻¹
12: 260.53 cm**⁻¹
13: 312.60 cm**⁻¹
14: 394.21 cm**⁻¹
15: 417.33 cm**⁻¹
16: 474.23 cm**⁻¹
17: 495.25 cm**⁻¹
18: 523.35 cm**⁻¹
19: 679.39 cm**⁻¹
20: 744.61 cm**⁻¹
21: 828.53 cm**⁻¹
22: 885.75 cm**⁻¹
23: 965.50 cm**⁻¹
24: 986.03 cm**⁻¹
25: 1024.06 cm**⁻¹
26: 1049.61 cm**⁻¹
27: 1072.37 cm**⁻¹
28: 1148.74 cm**⁻¹
29: 1211.20 cm**⁻¹
30: 1266.99 cm**⁻¹
31: 1326.11 cm**⁻¹
32: 1393.64 cm**⁻¹
33: 1422.37 cm**⁻¹
34: 1485.90 cm**⁻¹
35: 1488.34 cm**⁻¹
36: 1518.35 cm**⁻¹
37: 1590.81 cm**⁻¹
38: 1772.85 cm**⁻¹
39: 3070.73 cm**⁻¹
40: 3140.38 cm**⁻¹
41: 3159.37 cm**⁻¹
42: 3194.88 cm**⁻¹
43: 3208.95 cm**⁻¹
44: 3210.22 cm**⁻¹

Min1(S₀)

1,2,4- di-iodo formyl benzene

0: 0.00 cm**⁻¹
1: 0.00 cm**⁻¹
2: 0.00 cm**⁻¹
3: 0.00 cm**⁻¹
4: 0.00 cm**⁻¹
5: 0.00 cm**⁻¹
6: 44.18 cm**⁻¹
7: 75.33 cm**⁻¹

8: 100.44 cm**⁻¹
9: 128.94 cm**⁻¹
10: 176.04 cm**⁻¹
11: 241.94 cm**⁻¹
12: 264.88 cm**⁻¹
13: 283.68 cm**⁻¹
14: 352.09 cm**⁻¹
15: 444.72 cm**⁻¹
16: 520.81 cm**⁻¹
17: 539.87 cm**⁻¹
18: 662.38 cm**⁻¹
19: 729.01 cm**⁻¹
20: 733.31 cm**⁻¹
21: 855.26 cm**⁻¹
22: 875.19 cm**⁻¹
23: 930.66 cm**⁻¹
24: 1015.19 cm**⁻¹
25: 1037.84 cm**⁻¹
26: 1046.21 cm**⁻¹
27: 1130.46 cm**⁻¹
28: 1157.09 cm**⁻¹
29: 1231.55 cm**⁻¹
30: 1280.91 cm**⁻¹
31: 1298.31 cm**⁻¹
32: 1396.04 cm**⁻¹
33: 1441.22 cm**⁻¹
34: 1513.39 cm**⁻¹
35: 1634.22 cm**⁻¹
36: 1665.57 cm**⁻¹
37: 1815.79 cm**⁻¹
38: 2972.22 cm**⁻¹
39: 3213.17 cm**⁻¹
40: 3227.16 cm**⁻¹
41: 3239.72 cm**⁻¹

Min2(S_i)

0: 0.00 cm**⁻¹
1: 0.00 cm**⁻¹
2: 0.00 cm**⁻¹
3: 0.00 cm**⁻¹
4: 0.00 cm**⁻¹
5: 0.00 cm**⁻¹
6: 41.30 cm**⁻¹
7: 65.14 cm**⁻¹
8: 78.34 cm**⁻¹
9: 102.97 cm**⁻¹
10: 132.05 cm**⁻¹
11: 175.59 cm**⁻¹
12: 220.25 cm**⁻¹
13: 279.31 cm**⁻¹
14: 293.50 cm**⁻¹
15: 416.63 cm**⁻¹
16: 489.03 cm**⁻¹
17: 506.14 cm**⁻¹
18: 631.69 cm**⁻¹

19: 673.89 cm**-1
20: 716.54 cm**-1
21: 826.19 cm**-1
22: 850.80 cm**-1
23: 924.84 cm**-1
24: 997.31 cm**-1
25: 1006.44 cm**-1
26: 1048.52 cm**-1
27: 1072.84 cm**-1
28: 1145.23 cm**-1
29: 1213.74 cm**-1
30: 1288.00 cm**-1
31: 1321.51 cm**-1
32: 1396.26 cm**-1
33: 1435.97 cm**-1
34: 1489.09 cm**-1
35: 1614.80 cm**-1
36: 1658.06 cm**-1
37: 1810.36 cm**-1
38: 2967.63 cm**-1
39: 3174.18 cm**-1
40: 3207.09 cm**-1
41: 3231.57 cm**-1

Min3(T_i)

0: 0.00 cm**-1
1: 0.00 cm**-1
2: 0.00 cm**-1
3: 0.00 cm**-1
4: 0.00 cm**-1
5: 0.00 cm**-1
6: 0.00 cm**-1
7: 36.53 cm**-1
8: 68.19 cm**-1
9: 73.05 cm**-1
10: 130.12 cm**-1
11: 147.34 cm**-1
12: 222.95 cm**-1
13: 276.40 cm**-1
14: 282.16 cm**-1
15: 424.69 cm**-1
16: 501.79 cm**-1
17: 509.83 cm**-1
18: 630.43 cm**-1
19: 682.15 cm**-1
20: 707.71 cm**-1
21: 835.45 cm**-1
22: 857.64 cm**-1
23: 908.49 cm**-1
24: 1009.08 cm**-1
25: 1011.84 cm**-1
26: 1049.29 cm**-1

27: 1102.38 cm**⁻¹
28: 1151.17 cm**⁻¹
29: 1204.03 cm**⁻¹
30: 1267.29 cm**⁻¹
31: 1307.73 cm**⁻¹
32: 1398.99 cm**⁻¹
33: 1431.80 cm**⁻¹
34: 1497.76 cm**⁻¹
35: 1598.97 cm**⁻¹
36: 1664.28 cm**⁻¹
37: 1815.01 cm**⁻¹
38: 2975.77 cm**⁻¹
39: 3202.73 cm**⁻¹
40: 3220.32 cm**⁻¹
41: 3235.69 cm**⁻¹

P(S₀)

0: 0.00 cm**⁻¹
1: 0.00 cm**⁻¹
2: 0.00 cm**⁻¹
3: 0.00 cm**⁻¹
4: 0.00 cm**⁻¹
5: 0.00 cm**⁻¹
6: 0.00 cm**⁻¹
7: 0.00 cm**⁻¹
8: 23.27 cm**⁻¹
9: 38.58 cm**⁻¹
10: 44.11 cm**⁻¹
11: 104.95 cm**⁻¹
12: 231.09 cm**⁻¹
13: 234.11 cm**⁻¹
14: 250.20 cm**⁻¹
15: 380.59 cm**⁻¹
16: 406.33 cm**⁻¹
17: 473.92 cm**⁻¹
18: 485.46 cm**⁻¹
19: 643.06 cm**⁻¹
20: 646.38 cm**⁻¹
21: 756.01 cm**⁻¹
22: 853.06 cm**⁻¹
23: 928.11 cm**⁻¹
24: 939.74 cm**⁻¹
25: 1005.78 cm**⁻¹
26: 1052.96 cm**⁻¹
27: 1072.51 cm**⁻¹
28: 1133.53 cm**⁻¹
29: 1214.30 cm**⁻¹
30: 1273.94 cm**⁻¹
31: 1333.50 cm**⁻¹
32: 1393.38 cm**⁻¹
33: 1445.45 cm**⁻¹
34: 1497.18 cm**⁻¹
35: 1541.13 cm**⁻¹
36: 1809.02 cm**⁻¹
37: 2069.81 cm**⁻¹

38: 2968.69 cm^{**}-1
39: 3221.65 cm^{**}-1
40: 3222.86 cm^{**}-1
41: 3247.41 cm^{**}-1

MECI-2(S₀/S₁)

0: 0.00 cm^{**}-1
1: 0.00 cm^{**}-1
2: 0.00 cm^{**}-1
3: 0.00 cm^{**}-1
4: 0.00 cm^{**}-1
5: 0.00 cm^{**}-1
6: 0.00 cm^{**}-1
7: 52.94 cm^{**}-1
8: 68.64 cm^{**}-1
9: 73.75 cm^{**}-1
10: 141.23 cm^{**}-1
11: 159.76 cm^{**}-1
12: 221.55 cm^{**}-1
13: 267.48 cm^{**}-1
14: 381.03 cm^{**}-1
15: 409.82 cm^{**}-1
16: 421.89 cm^{**}-1
17: 499.52 cm^{**}-1
18: 548.98 cm^{**}-1
19: 666.07 cm^{**}-1
20: 687.04 cm^{**}-1
21: 810.28 cm^{**}-1
22: 854.28 cm^{**}-1
23: 914.59 cm^{**}-1
24: 960.55 cm^{**}-1
25: 1002.31 cm^{**}-1
26: 1009.86 cm^{**}-1
27: 1049.55 cm^{**}-1
28: 1145.92 cm^{**}-1
29: 1202.39 cm^{**}-1
30: 1276.90 cm^{**}-1
31: 1338.75 cm^{**}-1
32: 1386.89 cm^{**}-1
33: 1431.65 cm^{**}-1
34: 1494.81 cm^{**}-1
35: 1602.95 cm^{**}-1
36: 1695.07 cm^{**}-1
37: 1809.68 cm^{**}-1
38: 2971.34 cm^{**}-1
39: 3189.64 cm^{**}-1
40: 3203.96 cm^{**}-1
41: 3229.01 cm^{**}-1

Min1(S₀)

1,2,4-di-iodo cyano benzene

0: 0.00 cm^{**}-1
1: 0.00 cm^{**}-1
2: 0.00 cm^{**}-1
3: 0.00 cm^{**}-1

4: 0.00 cm**-1
5: 0.00 cm**-1
6: 67.55 cm**-1
7: 100.41 cm**-1
8: 113.59 cm**-1
9: 131.19 cm**-1
10: 218.14 cm**-1
11: 240.33 cm**-1
12: 290.74 cm**-1
13: 337.17 cm**-1
14: 434.63 cm**-1
15: 468.31 cm**-1
16: 540.24 cm**-1
17: 592.87 cm**-1
18: 617.43 cm**-1
19: 688.36 cm**-1
20: 736.54 cm**-1
21: 844.53 cm**-1
22: 862.01 cm**-1
23: 942.87 cm**-1
24: 1009.65 cm**-1
25: 1041.06 cm**-1
26: 1142.30 cm**-1
27: 1179.05 cm**-1
28: 1232.13 cm**-1
29: 1266.46 cm**-1
30: 1305.61 cm**-1
31: 1420.29 cm**-1
32: 1512.96 cm**-1
33: 1620.50 cm**-1
34: 1666.55 cm**-1
35: 2403.50 cm**-1
36: 3228.94 cm**-1
37: 3235.49 cm**-1
38: 3242.82 cm**-1

Min2(S_i)

0: 0.00 cm**-1
1: 0.00 cm**-1
2: 0.00 cm**-1
3: 0.00 cm**-1
4: 0.00 cm**-1
5: 0.00 cm**-1
6: 49.03 cm**-1
7: 72.19 cm**-1
8: 79.21 cm**-1
9: 100.69 cm**-1
10: 156.14 cm**-1
11: 215.48 cm**-1
12: 228.39 cm**-1
13: 273.26 cm**-1
14: 403.71 cm**-1
15: 448.83 cm**-1
16: 511.65 cm**-1
17: 582.07 cm**-1
18: 589.27 cm**-1

19: 651.04 cm**⁻¹
20: 725.33 cm**⁻¹
21: 766.79 cm**⁻¹
22: 850.53 cm**⁻¹
23: 932.05 cm**⁻¹
24: 994.47 cm**⁻¹
25: 999.44 cm**⁻¹
26: 1078.61 cm**⁻¹
27: 1159.05 cm**⁻¹
28: 1211.45 cm**⁻¹
29: 1288.46 cm**⁻¹
30: 1299.34 cm**⁻¹
31: 1418.38 cm**⁻¹
32: 1486.49 cm**⁻¹
33: 1606.63 cm**⁻¹
34: 1660.33 cm**⁻¹
35: 2397.69 cm**⁻¹
36: 3201.29 cm**⁻¹
37: 3209.71 cm**⁻¹
38: 3237.18 cm**⁻¹

Min3(T₁)

0: 0.00 cm**⁻¹
1: 0.00 cm**⁻¹
2: 0.00 cm**⁻¹
3: 0.00 cm**⁻¹
4: 0.00 cm**⁻¹
5: 0.00 cm**⁻¹
6: 31.31 cm**⁻¹
7: 38.42 cm**⁻¹
8: 65.39 cm**⁻¹
9: 75.19 cm**⁻¹
10: 130.58 cm**⁻¹
11: 219.01 cm**⁻¹
12: 233.08 cm**⁻¹
13: 239.39 cm**⁻¹
14: 414.73 cm**⁻¹
15: 448.25 cm**⁻¹
16: 534.09 cm**⁻¹
17: 580.13 cm**⁻¹
18: 594.09 cm**⁻¹
19: 647.18 cm**⁻¹
20: 715.60 cm**⁻¹
21: 777.13 cm**⁻¹
22: 858.39 cm**⁻¹
23: 921.67 cm**⁻¹
24: 1002.61 cm**⁻¹
25: 1011.10 cm**⁻¹
26: 1106.67 cm**⁻¹
27: 1164.72 cm**⁻¹
28: 1207.40 cm**⁻¹
29: 1263.79 cm**⁻¹
30: 1291.86 cm**⁻¹
31: 1414.78 cm**⁻¹
32: 1498.12 cm**⁻¹

33: 1588.11 cm^{**}-1
34: 1667.37 cm^{**}-1
35: 2401.83 cm^{**}-1
36: 3222.91 cm^{**}-1
37: 3226.97 cm^{**}-1
38: 3241.21 cm^{**}-1

P(S₀)

0: 0.00 cm^{**}-1
1: 0.00 cm^{**}-1
2: 0.00 cm^{**}-1
3: 0.00 cm^{**}-1
4: 0.00 cm^{**}-1
5: 0.00 cm^{**}-1
6: 0.00 cm^{**}-1
7: 13.13 cm^{**}-1
8: 22.23 cm^{**}-1
9: 40.04 cm^{**}-1
10: 46.95 cm^{**}-1
11: 164.75 cm^{**}-1
12: 174.88 cm^{**}-1
13: 231.37 cm^{**}-1
14: 389.84 cm^{**}-1
15: 407.12 cm^{**}-1
16: 449.67 cm^{**}-1
17: 520.10 cm^{**}-1
18: 539.23 cm^{**}-1
19: 589.56 cm^{**}-1
20: 669.50 cm^{**}-1
21: 685.14 cm^{**}-1
22: 851.87 cm^{**}-1
23: 931.51 cm^{**}-1
24: 935.81 cm^{**}-1
25: 996.74 cm^{**}-1
26: 1073.41 cm^{**}-1
27: 1149.91 cm^{**}-1
28: 1203.30 cm^{**}-1
29: 1270.71 cm^{**}-1
30: 1317.19 cm^{**}-1
31: 1405.12 cm^{**}-1
32: 1485.67 cm^{**}-1
33: 1546.14 cm^{**}-1
34: 2064.51 cm^{**}-1
35: 2398.70 cm^{**}-1
36: 3223.99 cm^{**}-1
37: 3241.52 cm^{**}-1
38: 3252.58 cm^{**}-1

MECI-2(S_i/S₀)

0: 0.00 cm^{**}-1
1: 0.00 cm^{**}-1
2: 0.00 cm^{**}-1
3: 0.00 cm^{**}-1
4: 0.00 cm^{**}-1
5: 0.00 cm^{**}-1

6: 0.00 cm**⁻¹
7: 13.13 cm**⁻¹
8: 22.23 cm**⁻¹
9: 40.04 cm**⁻¹
10: 46.95 cm**⁻¹
11: 164.75 cm**⁻¹
12: 174.88 cm**⁻¹
13: 231.37 cm**⁻¹
14: 389.84 cm**⁻¹
15: 407.12 cm**⁻¹
16: 449.67 cm**⁻¹
17: 520.10 cm**⁻¹
18: 539.23 cm**⁻¹
19: 589.56 cm**⁻¹
20: 669.50 cm**⁻¹
21: 685.14 cm**⁻¹
22: 851.87 cm**⁻¹
23: 931.51 cm**⁻¹
24: 935.81 cm**⁻¹
25: 996.74 cm**⁻¹
26: 1073.41 cm**⁻¹
27: 1149.91 cm**⁻¹
28: 1203.30 cm**⁻¹
29: 1270.71 cm**⁻¹
30: 1317.19 cm**⁻¹
31: 1405.12 cm**⁻¹
32: 1485.67 cm**⁻¹
33: 1546.14 cm**⁻¹
34: 2064.51 cm**⁻¹
35: 2398.70 cm**⁻¹
36: 3223.99 cm**⁻¹
37: 3241.52 cm**⁻¹
38: 3252.58 cm**⁻¹

Min1(S₀)

1,2,4-di-iodo nitro benzene

0: 0.00 cm**⁻¹
1: 0.00 cm**⁻¹
2: 0.00 cm**⁻¹
3: 0.00 cm**⁻¹
4: 0.00 cm**⁻¹
5: 0.00 cm**⁻¹
6: 0.00 cm**⁻¹
7: 66.12 cm**⁻¹
8: 100.09 cm**⁻¹
9: 130.60 cm**⁻¹
10: 138.26 cm**⁻¹
11: 219.24 cm**⁻¹
12: 271.84 cm**⁻¹
13: 275.48 cm**⁻¹
14: 367.14 cm**⁻¹
15: 440.77 cm**⁻¹
16: 488.91 cm**⁻¹
17: 523.21 cm**⁻¹
18: 555.14 cm**⁻¹
19: 671.90 cm**⁻¹

20: 717.25 cm**⁻¹
21: 766.84 cm**⁻¹
22: 778.34 cm**⁻¹
23: 865.82 cm**⁻¹
24: 908.70 cm**⁻¹
25: 957.33 cm**⁻¹
26: 1010.17 cm**⁻¹
27: 1039.56 cm**⁻¹
28: 1127.62 cm**⁻¹
29: 1156.57 cm**⁻¹
30: 1163.86 cm**⁻¹
31: 1284.71 cm**⁻¹
32: 1285.71 cm**⁻¹
33: 1419.30 cm**⁻¹
34: 1464.28 cm**⁻¹
35: 1501.84 cm**⁻¹
36: 1637.67 cm**⁻¹
37: 1653.81 cm**⁻¹
38: 1694.74 cm**⁻¹
39: 3237.75 cm**⁻¹
40: 3259.02 cm**⁻¹
41: 3264.33 cm**⁻¹

Min2(S_i)

0: 0.00 cm**⁻¹
1: 0.00 cm**⁻¹
2: 0.00 cm**⁻¹
3: 0.00 cm**⁻¹
4: 0.00 cm**⁻¹
5: 0.00 cm**⁻¹
6: 0.00 cm**⁻¹
7: 66.12 cm**⁻¹
8: 100.09 cm**⁻¹
9: 130.60 cm**⁻¹
10: 138.26 cm**⁻¹
11: 219.24 cm**⁻¹
12: 271.84 cm**⁻¹
13: 275.48 cm**⁻¹
14: 367.14 cm**⁻¹
15: 440.77 cm**⁻¹
16: 488.91 cm**⁻¹
17: 523.21 cm**⁻¹
18: 555.14 cm**⁻¹
19: 671.90 cm**⁻¹
20: 717.25 cm**⁻¹
21: 766.84 cm**⁻¹
22: 778.34 cm**⁻¹
23: 865.82 cm**⁻¹
24: 908.70 cm**⁻¹
25: 957.33 cm**⁻¹
26: 1010.17 cm**⁻¹
27: 1039.56 cm**⁻¹
28: 1127.62 cm**⁻¹
29: 1156.57 cm**⁻¹
30: 1163.86 cm**⁻¹

31: 1284.71 cm**-1
32: 1285.71 cm**-1
33: 1419.30 cm**-1
34: 1464.28 cm**-1
35: 1501.84 cm**-1
36: 1637.67 cm**-1
37: 1653.81 cm**-1
38: 1694.74 cm**-1
39: 3237.75 cm**-1
40: 3259.02 cm**-1
41: 3264.33 cm**-1

Min3(T₁)

0: 0.00 cm**-1
1: 0.00 cm**-1
2: 0.00 cm**-1
3: 0.00 cm**-1
4: 0.00 cm**-1
5: 0.00 cm**-1
6: 25.95 cm**-1
7: 37.47 cm**-1
8: 56.58 cm**-1
9: 65.31 cm**-1
10: 78.34 cm**-1
11: 151.72 cm**-1
12: 215.33 cm**-1
13: 258.49 cm**-1
14: 299.18 cm**-1
15: 423.81 cm**-1
16: 477.30 cm**-1
17: 497.76 cm**-1
18: 540.10 cm**-1
19: 628.83 cm**-1
20: 694.33 cm**-1
21: 721.83 cm**-1
22: 777.21 cm**-1
23: 866.27 cm**-1
24: 887.41 cm**-1
25: 937.37 cm**-1
26: 1006.63 cm**-1
27: 1008.75 cm**-1
28: 1102.62 cm**-1
29: 1139.47 cm**-1
30: 1149.79 cm**-1
31: 1257.43 cm**-1
32: 1312.65 cm**-1
33: 1410.56 cm**-1
34: 1462.91 cm**-1
35: 1483.36 cm**-1
36: 1610.14 cm**-1
37: 1659.45 cm**-1
38: 1689.65 cm**-1
39: 3224.99 cm**-1
40: 3246.55 cm**-1
41: 3263.54 cm**-1

P(S₀)

0: 0.00 cm**⁻¹
1: 0.00 cm**⁻¹
2: 0.00 cm**⁻¹
3: 0.00 cm**⁻¹
4: 0.00 cm**⁻¹
5: 0.00 cm**⁻¹
6: 0.00 cm**⁻¹
7: 0.00 cm**⁻¹
8: 28.27 cm**⁻¹
9: 36.91 cm**⁻¹
10: 38.73 cm**⁻¹
11: 59.48 cm**⁻¹
12: 193.53 cm**⁻¹
13: 230.41 cm**⁻¹
14: 276.86 cm**⁻¹
15: 384.54 cm**⁻¹
16: 391.65 cm**⁻¹
17: 463.71 cm**⁻¹
18: 473.11 cm**⁻¹
19: 534.98 cm**⁻¹
20: 620.64 cm**⁻¹
21: 644.82 cm**⁻¹
22: 774.06 cm**⁻¹
23: 845.71 cm**⁻¹
24: 869.03 cm**⁻¹
25: 941.18 cm**⁻¹
26: 945.90 cm**⁻¹
27: 996.63 cm**⁻¹
28: 1070.42 cm**⁻¹
29: 1125.26 cm**⁻¹
30: 1152.13 cm**⁻¹
31: 1262.58 cm**⁻¹
32: 1334.83 cm**⁻¹
33: 1420.92 cm**⁻¹
34: 1463.52 cm**⁻¹
35: 1502.50 cm**⁻¹
36: 1533.62 cm**⁻¹
37: 1668.92 cm**⁻¹
38: 2068.32 cm**⁻¹
39: 3247.93 cm**⁻¹
40: 3259.74 cm**⁻¹
41: 3266.09 cm**⁻¹

MECI-2(S₁/S₀)

0: 0.00 cm**⁻¹
1: 0.00 cm**⁻¹
2: 0.00 cm**⁻¹
3: 0.00 cm**⁻¹
4: 0.00 cm**⁻¹
5: 0.00 cm**⁻¹
6: 0.00 cm**⁻¹
7: 32.50 cm**⁻¹

8: 57.12 cm^{**}-1
9: 92.75 cm^{**}-1
10: 93.25 cm^{**}-1
11: 162.74 cm^{**}-1
12: 241.71 cm^{**}-1
13: 244.10 cm^{**}-1
14: 362.81 cm^{**}-1
15: 416.46 cm^{**}-1
16: 445.66 cm^{**}-1
17: 489.13 cm^{**}-1
18: 543.92 cm^{**}-1
19: 599.52 cm^{**}-1
20: 674.80 cm^{**}-1
21: 677.97 cm^{**}-1
22: 778.34 cm^{**}-1
23: 869.35 cm^{**}-1
24: 878.60 cm^{**}-1
25: 940.27 cm^{**}-1
26: 971.17 cm^{**}-1
27: 1010.76 cm^{**}-1
28: 1042.65 cm^{**}-1
29: 1129.84 cm^{**}-1
30: 1165.29 cm^{**}-1
31: 1267.57 cm^{**}-1
32: 1355.62 cm^{**}-1
33: 1420.70 cm^{**}-1
34: 1463.29 cm^{**}-1
35: 1474.34 cm^{**}-1
36: 1626.03 cm^{**}-1
37: 1665.33 cm^{**}-1
38: 1716.93 cm^{**}-1
39: 3181.03 cm^{**}-1
40: 3249.49 cm^{**}-1
41: 3261.75 cm^{**}-1

Min1(S₀)

1,2,4-di-iodo methoxy benzene

0: 0.00 cm^{**}-1
1: 0.00 cm^{**}-1
2: 0.00 cm^{**}-1
3: 0.00 cm^{**}-1
4: 0.00 cm^{**}-1
5: 0.00 cm^{**}-1
6: 0.00 cm^{**}-1
7: 32.50 cm^{**}-1
8: 57.12 cm^{**}-1
9: 92.75 cm^{**}-1
10: 93.25 cm^{**}-1
11: 162.74 cm^{**}-1
12: 241.71 cm^{**}-1
13: 244.10 cm^{**}-1
14: 362.81 cm^{**}-1
15: 416.46 cm^{**}-1
16: 445.66 cm^{**}-1
17: 489.13 cm^{**}-1
18: 543.92 cm^{**}-1

19: 599.52 cm**⁻¹
20: 674.80 cm**⁻¹
21: 677.97 cm**⁻¹
22: 778.34 cm**⁻¹
23: 869.35 cm**⁻¹
24: 878.60 cm**⁻¹
25: 940.27 cm**⁻¹
26: 971.17 cm**⁻¹
27: 1010.76 cm**⁻¹
28: 1042.65 cm**⁻¹
29: 1129.84 cm**⁻¹
30: 1165.29 cm**⁻¹
31: 1267.57 cm**⁻¹
32: 1355.62 cm**⁻¹
33: 1420.70 cm**⁻¹
34: 1463.29 cm**⁻¹
35: 1474.34 cm**⁻¹
36: 1626.03 cm**⁻¹
37: 1665.33 cm**⁻¹
38: 1716.93 cm**⁻¹
39: 3181.03 cm**⁻¹
40: 3249.49 cm**⁻¹
41: 3261.75 cm**⁻¹

Min2(S_i)

0: 0.00 cm**⁻¹
1: 0.00 cm**⁻¹
2: 0.00 cm**⁻¹
3: 0.00 cm**⁻¹
4: 0.00 cm**⁻¹
5: 0.00 cm**⁻¹
6: 41.01 cm**⁻¹
7: 71.36 cm**⁻¹
8: 107.15 cm**⁻¹
9: 115.00 cm**⁻¹
10: 131.76 cm**⁻¹
11: 161.24 cm**⁻¹
12: 251.76 cm**⁻¹
13: 253.09 cm**⁻¹
14: 317.32 cm**⁻¹
15: 335.67 cm**⁻¹
16: 419.62 cm**⁻¹
17: 464.93 cm**⁻¹
18: 569.59 cm**⁻¹
19: 570.44 cm**⁻¹
20: 646.60 cm**⁻¹
21: 699.15 cm**⁻¹
22: 799.60 cm**⁻¹
23: 836.33 cm**⁻¹
24: 865.22 cm**⁻¹
25: 979.01 cm**⁻¹
26: 984.19 cm**⁻¹
27: 1077.56 cm**⁻¹
28: 1092.89 cm**⁻¹
29: 1133.94 cm**⁻¹

30: 1188.63 cm**-1
31: 1216.97 cm**-1
32: 1266.62 cm**-1
33: 1288.62 cm**-1
34: 1342.82 cm**-1
35: 1419.70 cm**-1
36: 1474.71 cm**-1
37: 1499.43 cm**-1
38: 1505.28 cm**-1
39: 1511.55 cm**-1
40: 1627.28 cm**-1
41: 1670.17 cm**-1
42: 3045.23 cm**-1
43: 3115.43 cm**-1
44: 3184.27 cm**-1
45: 3190.09 cm**-1
46: 3219.65 cm**-1
47: 3233.05 cm**-1

Min3(T_i)

0: 0.00 cm**-1
1: 0.00 cm**-1
2: 0.00 cm**-1
3: 0.00 cm**-1
4: 0.00 cm**-1
5: 0.00 cm**-1
6: 0.00 cm**-1
7: 32.61 cm**-1
8: 68.34 cm**-1
9: 121.26 cm**-1
10: 136.58 cm**-1
11: 144.52 cm**-1
12: 247.47 cm**-1
13: 262.65 cm**-1
14: 317.07 cm**-1
15: 336.10 cm**-1
16: 430.92 cm**-1
17: 463.22 cm**-1
18: 565.72 cm**-1
19: 570.08 cm**-1
20: 657.10 cm**-1
21: 693.78 cm**-1
22: 826.10 cm**-1
23: 837.06 cm**-1
24: 877.15 cm**-1
25: 982.61 cm**-1
26: 992.42 cm**-1
27: 1090.31 cm**-1
28: 1099.47 cm**-1
29: 1134.36 cm**-1
30: 1190.68 cm**-1
31: 1220.26 cm**-1
32: 1258.67 cm**-1
33: 1283.76 cm**-1
34: 1338.86 cm**-1

35: 1414.02 cm**⁻¹
36: 1474.56 cm**⁻¹
37: 1500.67 cm**⁻¹
38: 1503.85 cm**⁻¹
39: 1512.06 cm**⁻¹
40: 1630.26 cm**⁻¹
41: 1654.23 cm**⁻¹
42: 3047.86 cm**⁻¹
43: 3119.07 cm**⁻¹
44: 3186.20 cm**⁻¹
45: 3216.50 cm**⁻¹
46: 3230.92 cm**⁻¹
47: 3244.79 cm**⁻¹

P(S₀)

0: 0.00 cm**⁻¹
1: 0.00 cm**⁻¹
2: 0.00 cm**⁻¹
3: 0.00 cm**⁻¹
4: 0.00 cm**⁻¹
5: 0.00 cm**⁻¹
6: 0.00 cm**⁻¹
7: 0.00 cm**⁻¹
8: 21.54 cm**⁻¹
9: 27.02 cm**⁻¹
10: 42.42 cm**⁻¹
11: 100.66 cm**⁻¹
12: 223.95 cm**⁻¹
13: 230.12 cm**⁻¹
14: 279.87 cm**⁻¹
15: 294.96 cm**⁻¹
16: 378.39 cm**⁻¹
17: 402.41 cm**⁻¹
18: 459.43 cm**⁻¹
19: 478.83 cm**⁻¹
20: 595.55 cm**⁻¹
21: 679.73 cm**⁻¹
22: 688.86 cm**⁻¹
23: 856.21 cm**⁻¹
24: 864.95 cm**⁻¹
25: 936.13 cm**⁻¹
26: 982.70 cm**⁻¹
27: 1071.75 cm**⁻¹
28: 1092.14 cm**⁻¹
29: 1135.93 cm**⁻¹
30: 1179.72 cm**⁻¹
31: 1209.74 cm**⁻¹
32: 1260.09 cm**⁻¹
33: 1278.24 cm**⁻¹
34: 1378.40 cm**⁻¹
35: 1415.75 cm**⁻¹
36: 1474.86 cm**⁻¹
37: 1489.16 cm**⁻¹
38: 1492.68 cm**⁻¹
39: 1501.77 cm**⁻¹

40: 1568.72 cm^{**}-1
41: 2071.92 cm^{**}-1
42: 3044.98 cm^{**}-1
43: 3116.82 cm^{**}-1
44: 3184.67 cm^{**}-1
45: 3218.91 cm^{**}-1
46: 3239.78 cm^{**}-1
47: 3256.58 cm^{**}-1

MECI-2(S₁/S₀)

0: 0.00 cm^{**}-1
1: 0.00 cm^{**}-1
2: 0.00 cm^{**}-1
3: 0.00 cm^{**}-1
4: 0.00 cm^{**}-1
5: 0.00 cm^{**}-1
6: 0.00 cm^{**}-1
7: 0.00 cm^{**}-1
8: 103.12 cm^{**}-1
9: 135.24 cm^{**}-1
10: 140.64 cm^{**}-1
11: 145.46 cm^{**}-1
12: 250.95 cm^{**}-1
13: 318.13 cm^{**}-1
14: 323.99 cm^{**}-1
15: 405.50 cm^{**}-1
16: 422.63 cm^{**}-1
17: 510.44 cm^{**}-1
18: 531.23 cm^{**}-1
19: 537.52 cm^{**}-1
20: 681.98 cm^{**}-1
21: 710.19 cm^{**}-1
22: 764.62 cm^{**}-1
23: 822.45 cm^{**}-1
24: 891.17 cm^{**}-1
25: 966.82 cm^{**}-1
26: 979.04 cm^{**}-1
27: 1083.82 cm^{**}-1
28: 1131.13 cm^{**}-1
29: 1193.48 cm^{**}-1
30: 1216.29 cm^{**}-1
31: 1277.87 cm^{**}-1
32: 1282.62 cm^{**}-1
33: 1303.42 cm^{**}-1
34: 1401.49 cm^{**}-1
35: 1422.94 cm^{**}-1
36: 1492.66 cm^{**}-1
37: 1503.35 cm^{**}-1
38: 1511.26 cm^{**}-1
39: 1595.54 cm^{**}-1
40: 1616.07 cm^{**}-1
41: 2980.65 cm^{**}-1
42: 3045.10 cm^{**}-1
43: 3115.56 cm^{**}-1
44: 3187.98 cm^{**}-1

45: 3213.50 cm^{**}-1
46: 3231.79 cm^{**}-1
47: 3504.82 cm^{**}-1

Min1(S₀)

1,2,4-di-iodo hydroxy benzene

0: 0.00 cm^{**}-1
1: 0.00 cm^{**}-1
2: 0.00 cm^{**}-1
3: 0.00 cm^{**}-1
4: 0.00 cm^{**}-1
5: 0.00 cm^{**}-1
6: 76.94 cm^{**}-1
7: 100.35 cm^{**}-1
8: 152.53 cm^{**}-1
9: 178.32 cm^{**}-1
10: 273.22 cm^{**}-1
11: 310.02 cm^{**}-1
12: 318.75 cm^{**}-1
13: 330.86 cm^{**}-1
14: 446.75 cm^{**}-1
15: 459.75 cm^{**}-1
16: 586.56 cm^{**}-1
17: 606.25 cm^{**}-1
18: 686.47 cm^{**}-1
19: 716.56 cm^{**}-1
20: 830.15 cm^{**}-1
21: 893.90 cm^{**}-1
22: 899.09 cm^{**}-1
23: 970.40 cm^{**}-1
24: 1031.76 cm^{**}-1
25: 1132.06 cm^{**}-1
26: 1164.37 cm^{**}-1
27: 1199.94 cm^{**}-1
28: 1263.96 cm^{**}-1
29: 1301.56 cm^{**}-1
30: 1322.13 cm^{**}-1
31: 1462.26 cm^{**}-1
32: 1517.79 cm^{**}-1
33: 1647.91 cm^{**}-1
34: 1674.16 cm^{**}-1
35: 3207.62 cm^{**}-1
36: 3230.34 cm^{**}-1
37: 3235.95 cm^{**}-1
38: 3857.79 cm^{**}-1

Min2(S_i)

0: 0.00 cm^{**}-1
1: 0.00 cm^{**}-1
2: 0.00 cm^{**}-1
3: 0.00 cm^{**}-1
4: 0.00 cm^{**}-1
5: 0.00 cm^{**}-1
6: 46.85 cm^{**}-1
7: 85.91 cm^{**}-1

8: 100.89 cm**⁻¹
9: 108.79 cm**⁻¹
10: 230.03 cm**⁻¹
11: 239.78 cm**⁻¹
12: 297.66 cm**⁻¹
13: 344.41 cm**⁻¹
14: 423.76 cm**⁻¹
15: 437.51 cm**⁻¹
16: 539.32 cm**⁻¹
17: 577.25 cm**⁻¹
18: 637.71 cm**⁻¹
19: 707.22 cm**⁻¹
20: 815.73 cm**⁻¹
21: 823.12 cm**⁻¹
22: 893.31 cm**⁻¹
23: 958.19 cm**⁻¹
24: 994.37 cm**⁻¹
25: 1076.41 cm**⁻¹
26: 1154.50 cm**⁻¹
27: 1190.04 cm**⁻¹
28: 1254.34 cm**⁻¹
29: 1303.78 cm**⁻¹
30: 1336.97 cm**⁻¹
31: 1451.82 cm**⁻¹
32: 1498.48 cm**⁻¹
33: 1636.67 cm**⁻¹
34: 1659.29 cm**⁻¹
35: 3194.15 cm**⁻¹
36: 3195.74 cm**⁻¹
37: 3210.19 cm**⁻¹
38: 3857.63 cm**⁻¹

Min3(T_i)

0: 0.00 cm**⁻¹
1: 0.00 cm**⁻¹
2: 0.00 cm**⁻¹
3: 0.00 cm**⁻¹
4: 0.00 cm**⁻¹
5: 0.00 cm**⁻¹
6: 12.38 cm**⁻¹
7: 41.91 cm**⁻¹
8: 71.93 cm**⁻¹
9: 104.60 cm**⁻¹
10: 188.25 cm**⁻¹
11: 250.32 cm**⁻¹
12: 297.53 cm**⁻¹
13: 382.97 cm**⁻¹
14: 431.87 cm**⁻¹
15: 434.44 cm**⁻¹
16: 548.60 cm**⁻¹
17: 600.22 cm**⁻¹
18: 638.29 cm**⁻¹
19: 695.12 cm**⁻¹
20: 825.17 cm**⁻¹
21: 830.92 cm**⁻¹

22: 882.77 cm**⁻¹
23: 971.19 cm**⁻¹
24: 1003.40 cm**⁻¹
25: 1103.40 cm**⁻¹
26: 1163.15 cm**⁻¹
27: 1185.84 cm**⁻¹
28: 1235.95 cm**⁻¹
29: 1307.43 cm**⁻¹
30: 1334.58 cm**⁻¹
31: 1439.55 cm**⁻¹
32: 1515.23 cm**⁻¹
33: 1626.01 cm**⁻¹
34: 1668.18 cm**⁻¹
35: 3206.05 cm**⁻¹
36: 3221.12 cm**⁻¹
37: 3222.52 cm**⁻¹
38: 3856.04 cm**⁻¹

P(S₀)

0: 0.00 cm**⁻¹
1: 0.00 cm**⁻¹
2: 0.00 cm**⁻¹
3: 0.00 cm**⁻¹
4: 0.00 cm**⁻¹
5: 0.00 cm**⁻¹
6: 0.00 cm**⁻¹
7: 0.00 cm**⁻¹
8: 15.96 cm**⁻¹
9: 42.42 cm**⁻¹
10: 53.11 cm**⁻¹
11: 231.71 cm**⁻¹
12: 261.98 cm**⁻¹
13: 342.45 cm**⁻¹
14: 393.37 cm**⁻¹
15: 406.67 cm**⁻¹
16: 429.24 cm**⁻¹
17: 469.69 cm**⁻¹
18: 591.93 cm**⁻¹
19: 667.33 cm**⁻¹
20: 700.60 cm**⁻¹
21: 839.08 cm**⁻¹
22: 889.06 cm**⁻¹
23: 944.72 cm**⁻¹
24: 962.03 cm**⁻¹
25: 1071.77 cm**⁻¹
26: 1147.59 cm**⁻¹
27: 1192.53 cm**⁻¹
28: 1248.05 cm**⁻¹
29: 1289.72 cm**⁻¹
30: 1350.15 cm**⁻¹
31: 1450.10 cm**⁻¹
32: 1500.85 cm**⁻¹
33: 1571.10 cm**⁻¹
34: 2067.42 cm**⁻¹
35: 3198.00 cm**⁻¹

36: 3234.00 cm**-1
37: 3239.55 cm**-1
38: 3869.85 cm**-1

MECI-2(S₁/S₀)

0: 0.00 cm**-1
1: 0.00 cm**-1
2: 0.00 cm**-1
3: 0.00 cm**-1
4: 0.00 cm**-1
5: 0.00 cm**-1
6: 0.00 cm**-1
7: 52.91 cm**-1
8: 58.89 cm**-1
9: 113.39 cm**-1
10: 162.47 cm**-1
11: 276.93 cm**-1
12: 323.85 cm**-1
13: 358.14 cm**-1
14: 424.98 cm**-1
15: 441.52 cm**-1
16: 469.55 cm**-1
17: 520.65 cm**-1
18: 547.56 cm**-1
19: 680.38 cm**-1
20: 778.40 cm**-1
21: 822.98 cm**-1
22: 875.75 cm**-1
23: 960.67 cm**-1
24: 975.45 cm**-1
25: 1049.80 cm**-1
26: 1154.62 cm**-1
27: 1183.22 cm**-1
28: 1242.42 cm**-1
29: 1282.53 cm**-1
30: 1355.19 cm**-1
31: 1426.64 cm**-1
32: 1520.94 cm**-1
33: 1617.85 cm**-1
34: 1754.34 cm**-1
35: 3191.29 cm**-1
36: 3205.97 cm**-1
37: 3225.25 cm**-1
38: 3864.08 cm**-1

Table S1. Total energies calculated at the TD-DFT/def2-TZVP + CPCM(benzene) level for energy stationary points involved in the 1,2-dichoro-benzene photolysis.

	ωB97XD	CAM-B3LYP	PBE0
Min1 (S_0)	-826.56693	-826.40845	-826.28819
Min2 (S_1)	-826.42706	-826.27878	-826.16578
Min3 (T_1)	-826.46504	-826.30473	-826.17330
P (S_0)	-826.45215	-826.29987	-826.17433
MECI-1 (S_2/S_1)	-826.40494	-826.25879	-826.14983

Table S2. Total energies calculated at the TD-DFT/def2-TZVP + CPCM(benzene) level for energy stationary points involved in the 1,2-di-bromo-benzene photolysis.

	ωB97XD	CAM-B3LYP	PBE0
Min1 (S_0)	-5379.429	-5379.554	-5378.567
Min2 (S_1)	-5379.257	-5379.394	-5378.415
Min3 (T_1)	-5379.303	-5379.427	-5378.429
P (S_0)	-5379.281	-5379.413	-5378.420
MECI-1 (S_2/S_1)	-5379.229	-5379.370	-5378.391

Table S3. Total energies calculated at the TD-DFT/def2-TZVP + CPCM(benzene) level for energy stationary points involved in the 1,2-di-iodo-benzene photolysis.

	ωB97XD	CAM-B3LYP	PBE0
Min1 (S_0)	-1151.48657	-1151.45133	-1150.97990
Min2 (S_1)	-1151.28534	-1151.26282	-1150.79798
Min3 (T_1)	-1151.33148	-1151.29875	-1150.81611
P (S_0)	-1151.30775	-1151.27882	-1150.80260
MECI-1 (S_2/S_1)	-1151.25651	-1151.22823	-1150.76827

Table S4. Total energies calculated at the WB97X/def2-TZVP + CPCM(benzene) level for energy stationary points involved in the 1,2,4 substituted di-iodo-benzenes photolysis.

	CH ₃	CHO	CN
Min1 (S ₀)	-865.88866	-939.90980	-918.81844
Min2 (S ₁)	-865.74840	-939.77078	-918.68062
Min3 (T ₁)	-865.79036	-939.81111	-918.71982
P (S ₀)	-865.77234	-939.79473	-918.70461
MECI-1 (S ₂ /S ₁)	-865.73700	-939.75161	-918.67156
MECI-2 (S ₂ /S ₁)	-865.72629	-939.74887	-918.65855
	NO ₂	OCH ₃	OH
Min1 (S ₀)	-1031.10876	-941.11033	-901.80907
Min2 (S ₁)	-1030.97093	-940.96898	-901.66954
Min3 (T ₁)	-1031.01007	-941.01022	-901.71125
P (S ₀)	-1030.99349	-940.95811	-901.69107
MECI-1 (S ₂ /S ₁)	-1030.96197	-940.95189	-901.65671
MECI-2 (S ₂ /S ₁)	-1030.94760	-940.94364	-901.64656

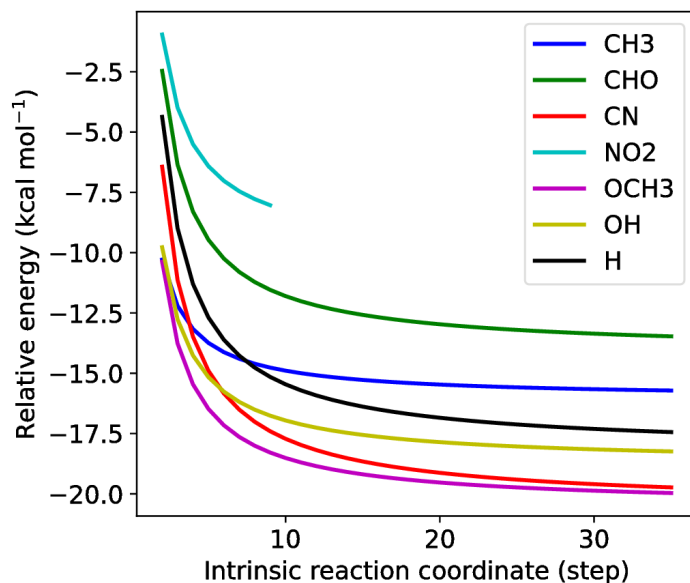


Figure S1. IRC of substituted 1,2,4-di-iodo benzenes along the FC \rightarrow MECI-1 (S_2/S_1) deactivation process.

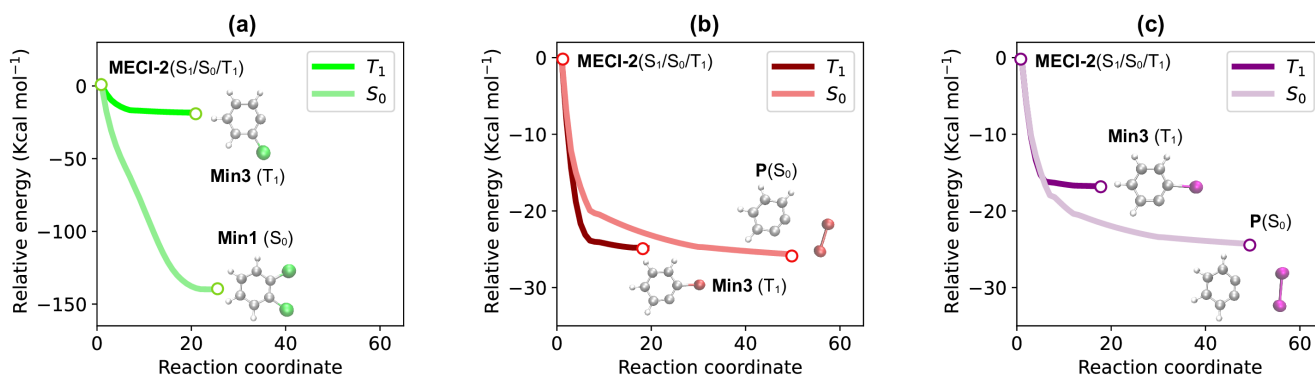


Figure S2. IRC of benzyne and phenyl radicals productions from MECI-2. Benzyne forms at S_0 for heaviest functionalized species, while the radical upon deactivation from T_1 .

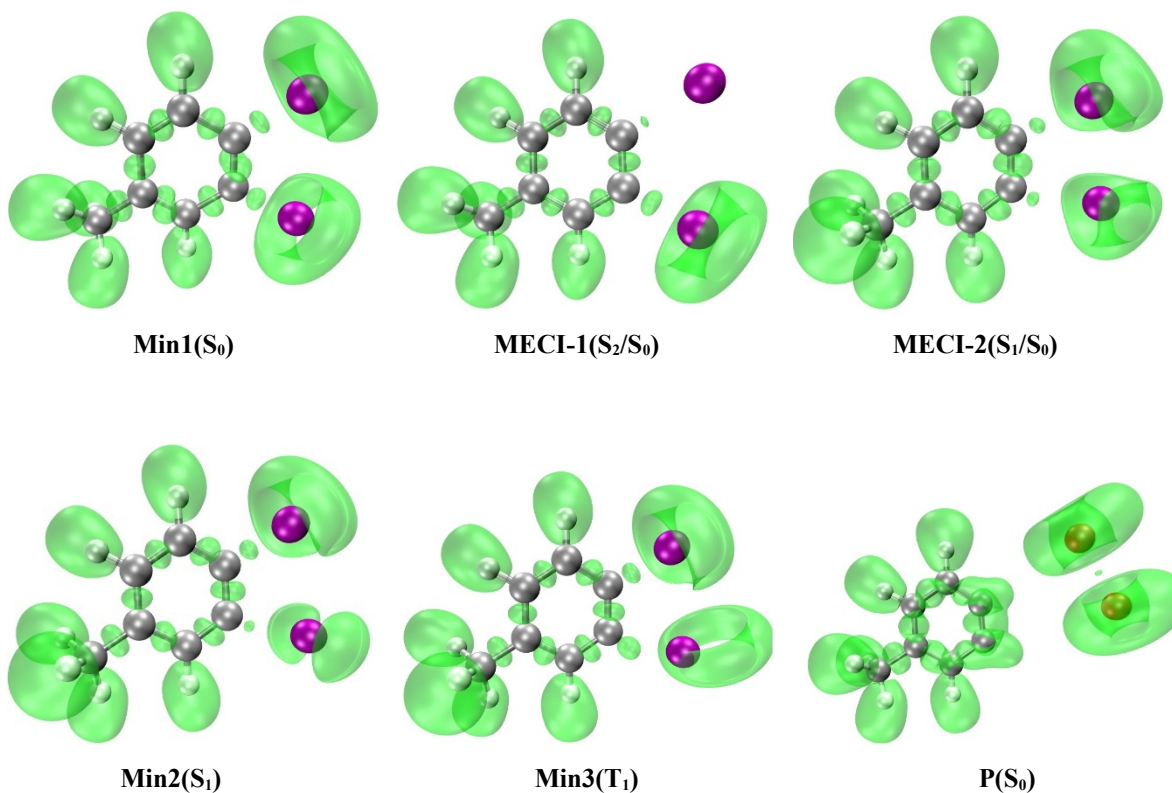


Figure S3. Relevant stationary energy points along the pathway of the 1,2-di-iodo-4-methyl benzene photolysis.

Table S5. Electronic populations, e , of monosynaptic and disynaptic basins at stationary points featuring the 1,2-di-iodo-4-methyl benzene photolysis.

Basin	Min1	MECI-1	MECI-2	Min2	Min3	P
V(C1,C2)	3.41	2.95	3.19	2.98	2.84	3.15
V(C1,I1)	1.70	1.17	-	1.58	1.65	-
V(C2,I2)	1.70	1.69	-	-	-	-
V(I1,I2)	-	-	-	-	-	0.82
V(C1)	-	-	1.26	-	-	1.14
V(C2)	-	-	0.89	1.01	1.16	-
V(I1)	-	-	-	-	-	-
V(I2)	-	-	-	-	-	-

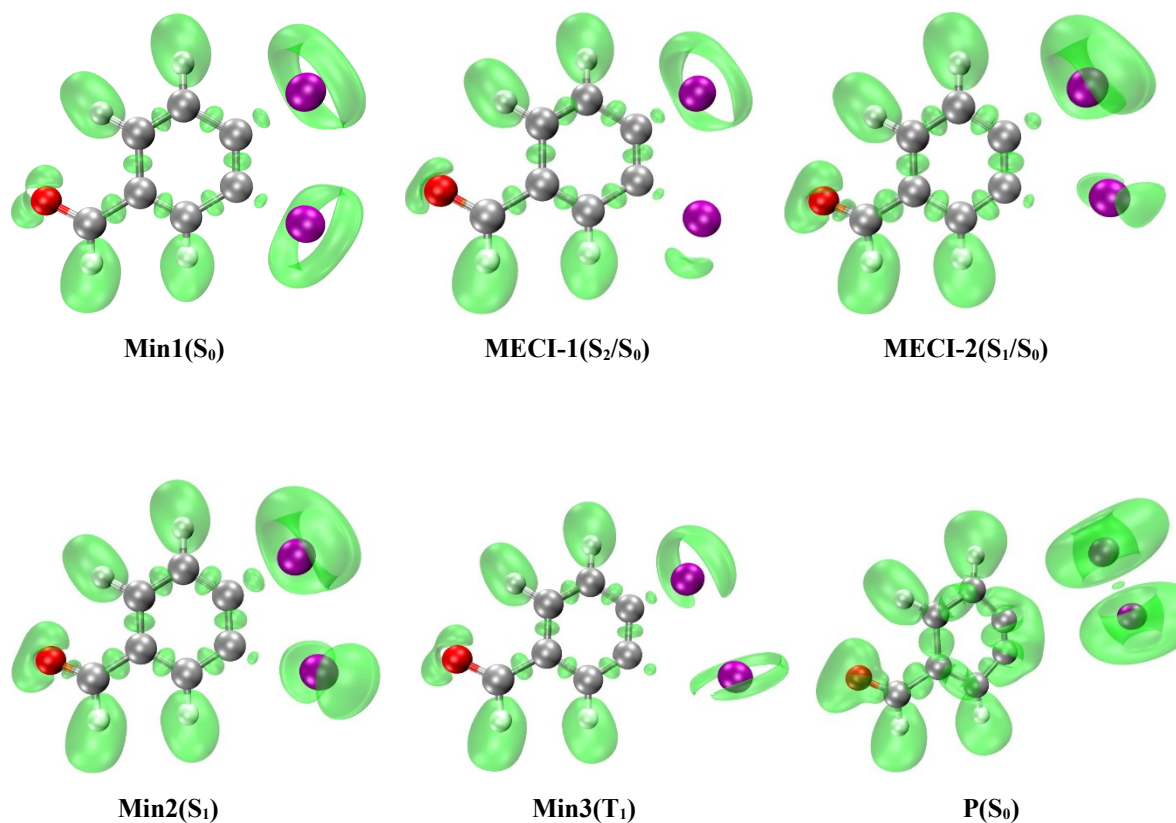


Figure S4. Relevant stationary energy points along the pathway of the 1,2-di-iodo-4-formylbenzene photolysis.

Table S6. Electronic populations, e , of monosynaptic and disynaptic basins at stationary points featuring the 1,2-di-iodo-4-formylbenzene photolysis.

Basin	Min1	MECI-1	MECI-2	Min2	Min3	P
V(C1,C2)	3.40	3.17	2.24	2.96	2.84	4.48
V(C1,I1)	2.64	2.24	1.39	1.69	1.67	-
V(C2,I2)	1.72	1.73	-	-	-	-
V(I1,I2)	-	-	-	-	-	1.00
V(C1)	-	-	-	-	-	-
V(C2)	-	-	1.00	1.05	1.18	0.42
V(I1)	-	-	-	-	-	-
V(I2)	-	-	-	-	-	-

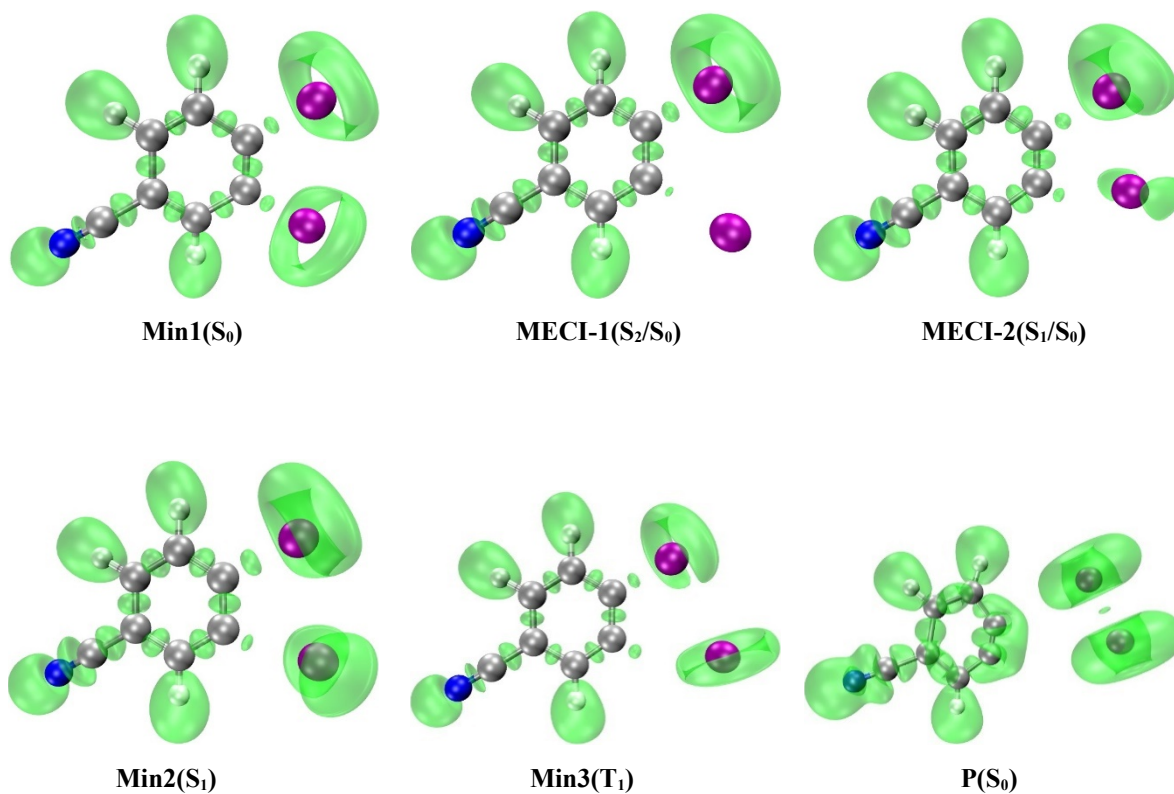


Figure S5. Relevant stationary energy points along the pathway of the 1,2-di-iodo-4-cyanobenzene photolysis.

Table S7. Electronic populations, e , of monosynaptic and disynaptic basins at stationary points featuring the 1,2-di-iodo-4-cyanobenzene photolysis.

Basin	Min1	MECI-1	MECI-2	Min2	Min3	P
V(C1,C2)	3.33	2.82	3.08	2.92	2.83	4.46
V(C1,I1)	1.72	1.67	1.40	1.70	1.68	-
V(C2,I2)	2.07	-	-	-	-	-
V(I1,I2)	-	-	-	-	-	1.00
V(C1)	-	-	-	-	-	0.39
V(C2)	-	1.15	1.01	1.06	1.14	0.46
V(I1)	-	-	-	-	-	-
V(I2)	-	-	-	-	-	-

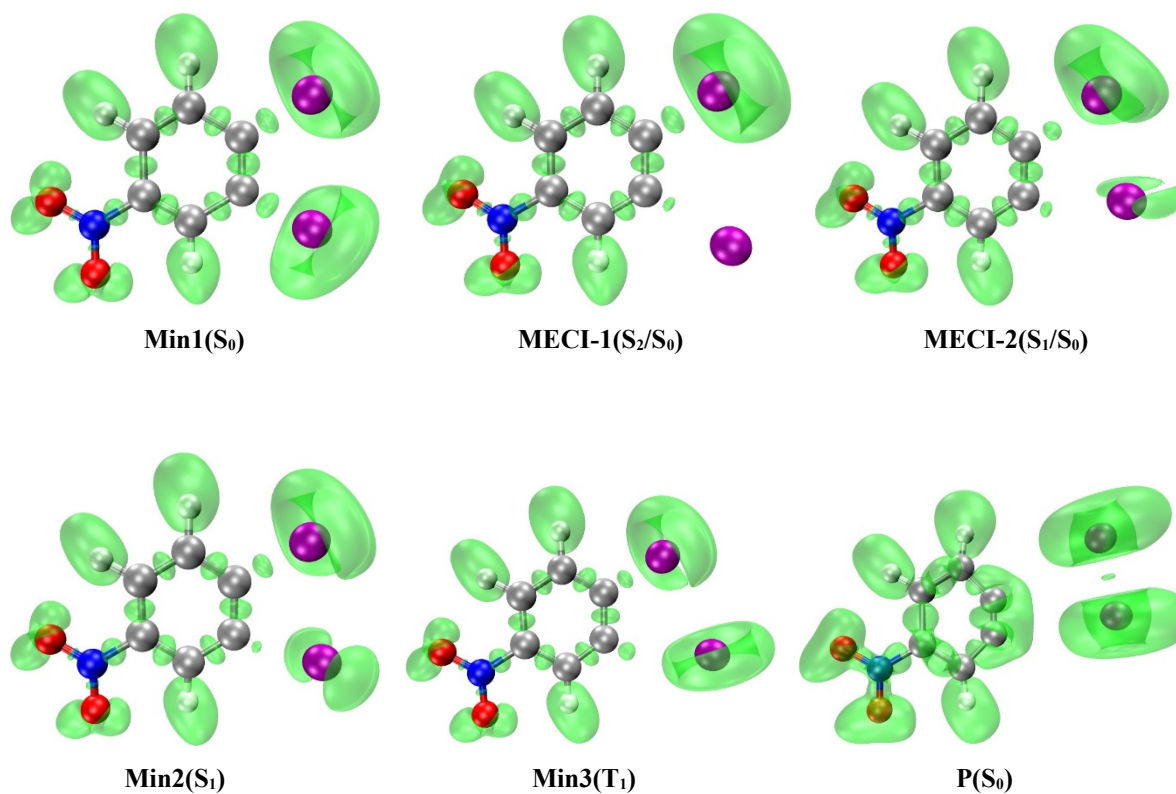


Figure S6. Relevant stationary energy points along the pathway of the 1,2-di-iodo-4-nitrobenzene photolysis.

Table S8. Electronic populations, e , of monosynaptic and disynaptic basins at stationary points featuring the 1,2-di-iodo-4-nitrobenzene photolysis.

Basin	Min1	MECI-1	MECI-2	Min2	Min3	P
V(C1,C2)	3.33	2.83	3.09	2.91	2.81	4.46
V(C1,I1)	1.92	1.75	1.46	1.70	1.69	-
V(C2,I2)	1.81	-	-	-	-	-
V(I1,I2)	-	-	-	-	-	1.00
V(C1)	-	-	-	-	-	0.39
V(C2)	-	1.16	1.02	1.11	1.14	0.48
V(I1)	-	-	-	2.11	-	-
V(I2)	-	-	-	-	-	-

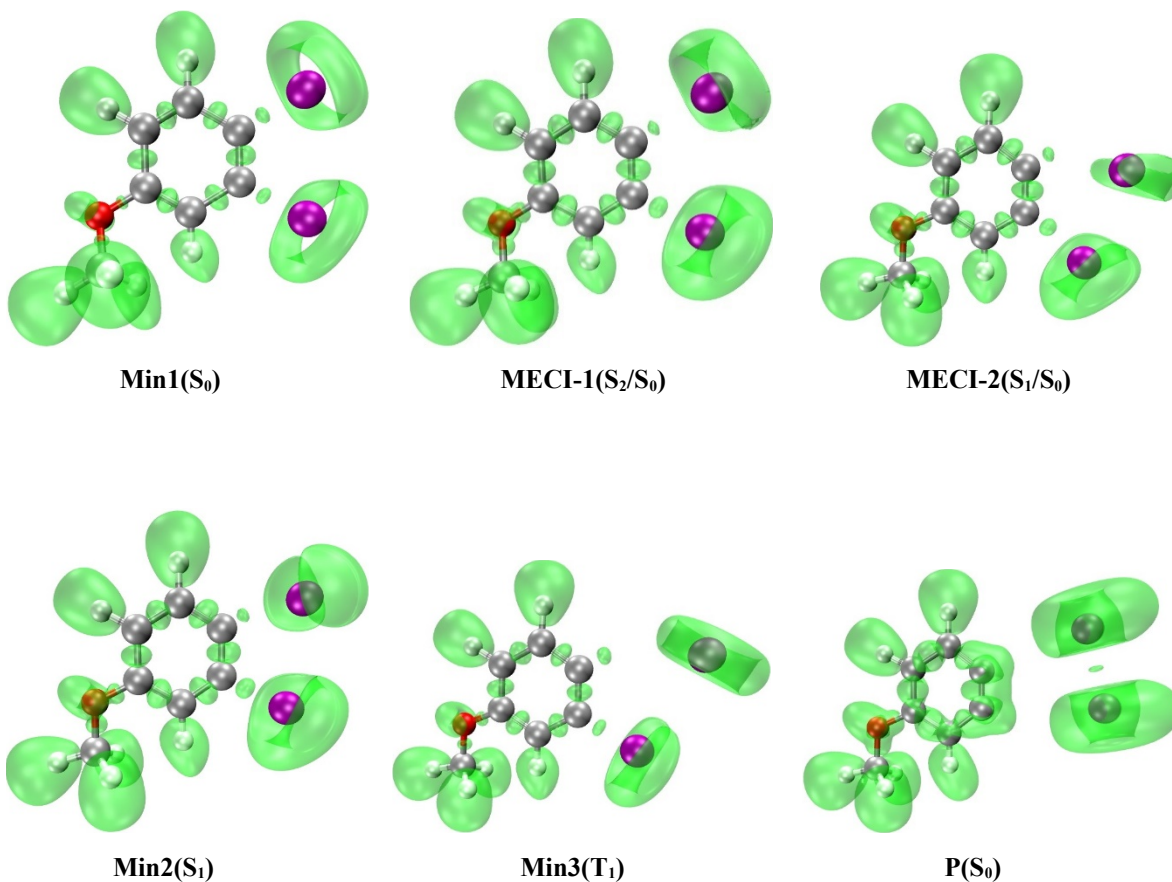


Figure S7. Relevant stationary energy points along the pathway of the 1,2-di-iodo-4-methoxybenzene photolysis.

Table S9. Electronic populations, e , of monosynaptic and disynaptic basins at stationary points featuring the 1,2-di-iodo-4-methoxybenzene photolysis.

Basin	Min1	MECI-1	MECI-2	Min2	Min3	P
V(C1,C2)	3.42	2.95	2.68	3.04	2.93	3.53
V(C1,I1)	2.47	1.33	-	-	-	-
V(C2,I2)	1.71	1.51	1.45	1.57	1.64	-
V(I1,I2)	-	-	-	-	-	1.02
V(C1)	-	-	0.98	1.59	1.20	0.75
V(C2)	-	-	-	-	-	0.83
V(I1)	-	-	-	-	-	-
V(I2)	-	-	-	-	-	-

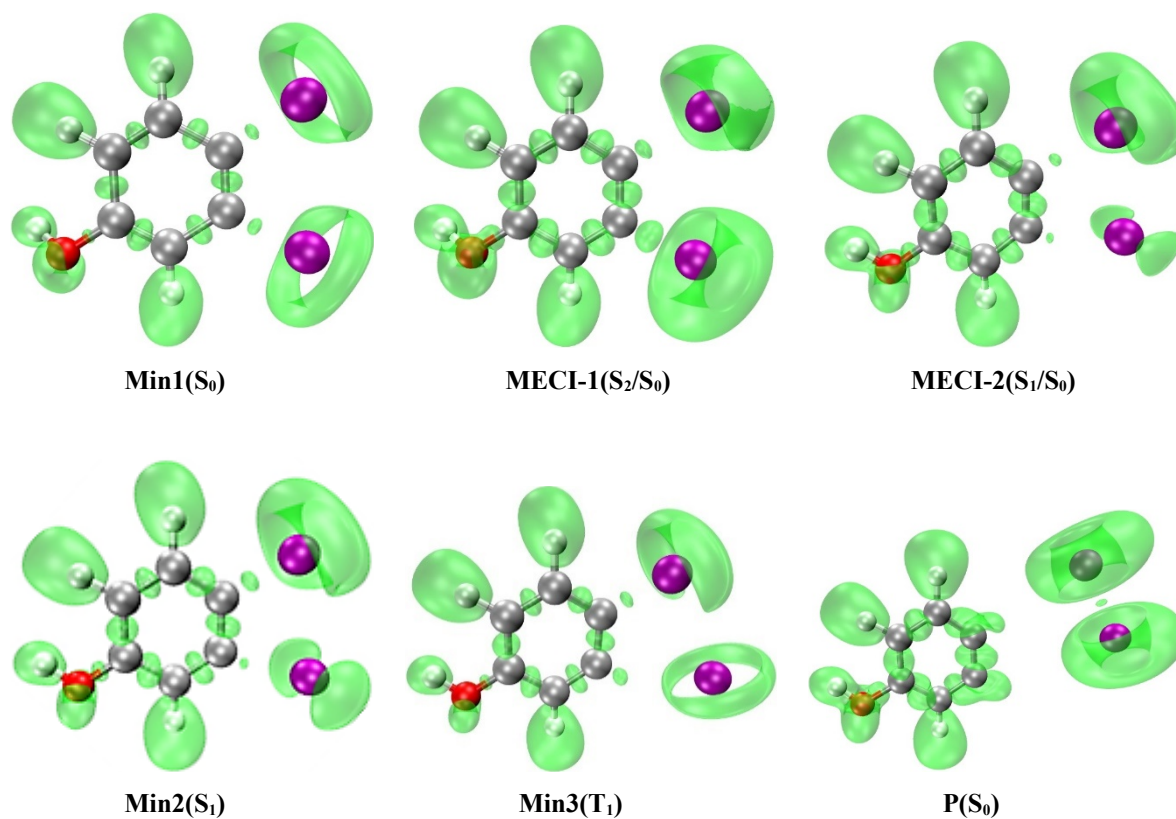


Figure S8. Relevant stationary energy points along the pathway of the 1,2-di-iodo-4-hydroxybenzene photolysis.

Table S10. Electronic populations, e , of monosynaptic and disynaptic basins at stationary points featuring the 1,2-di-iodo-4-hydroxybenzene photolysis.

Basin	Min1	MECI-1	MECI-2	Min2	Min3	P
V(C1,C2)	3.43	2.87	3.15	2.92	2.83	3.18
V(C1,I1)	1.70	1.21	1.29	1.59	1.66	-
V(C2,I2)	1.71	1.69	-	-	-	-
V(I1,I2)	-	-	-	-	-	1.06
V(C1)	-	-	-	-	-	0.77
V(C2)	-	-	0.92	1.04	1.14	1.06
V(I1)	-	-	-	-	-	-
V(I2)	-	-	-	-	-	-

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