

SUPPORTING INFORMATION

for

From skin sensitizer to wastewater: the unknown photo-deactivation process of low-lying excited states of Isothiazolinones, a non-adiabatic dynamics investigation

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Ground State XYZ Coordinates

ISO

C 0.00000000 0.00000000 0.00000000
C -1.35040900 -0.08992100 0.00000000
S -2.14624000 1.45056300 0.00000000
N -0.62411600 2.22000200 0.00000000
C 0.49760100 1.38218400 0.00000000
O 1.64919200 1.79930400 0.00000000
H -0.54020500 3.22819600 0.00000000
H -1.96482300 -0.98762900 0.00000000
H 0.68296300 -0.84498500 0.00000000

MIT

C 0.00000000 0.00000000 0.00000000
N 0.14745700 -1.44627900 0.00000000
C -0.95278400 -2.31701600 -0.00000000
C -0.42149500 -3.69103700 -0.00000000
C 0.94005900 -3.75641800 -0.00000000
S 1.69409400 -2.19159100 -0.00000000
H 1.57084800 -4.64809200 -0.00000000
H -1.08536000 -4.55685700 -0.00000000
O -2.12318100 -1.93618000 0.00000000
H -1.08497900 0.18279800 0.00000000
H 0.44998400 0.44803700 0.90129300
H 0.44998400 0.44803700 -0.90129300

CIT

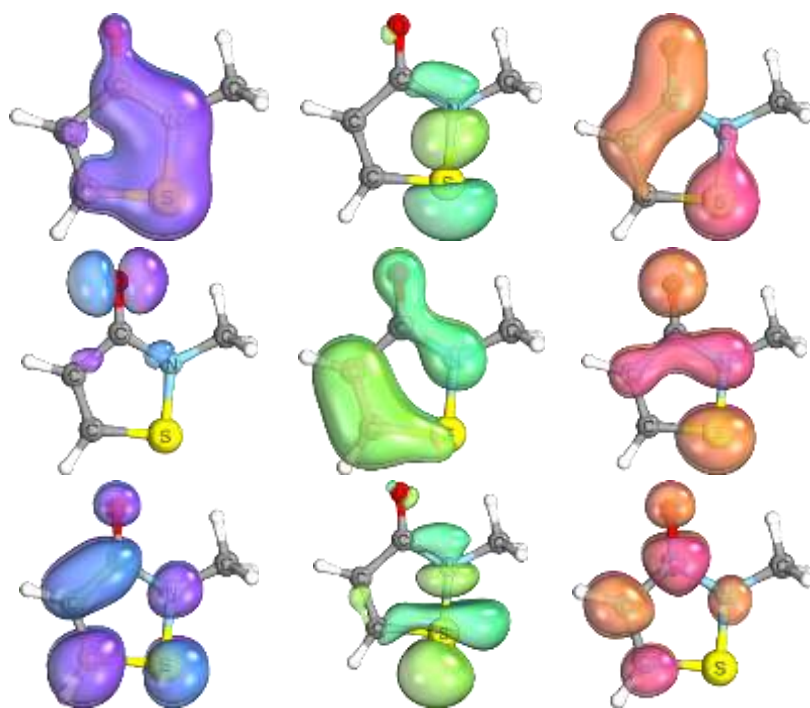
C 0.00000000 0.00000000 0.00000000
N 0.41520000 -1.39417900 0.00000000
C 1.76284600 -1.78661100 0.00000000
C 1.80203100 -3.25924300 0.00000000
C 0.56452600 -3.82689900 0.00000000
S -0.74258600 -2.66828200 0.00000000
Cl 0.17575500 -5.50477100 0.00000000
H 2.74068600 -3.81420200 0.00000000
O 2.70165000 -0.99341100 0.00000000
H 0.93309100 0.58260600 0.00000000
H -0.58614300 0.24252500 -0.90176400
H -0.58614300 0.24252500 0.90176400

BIT

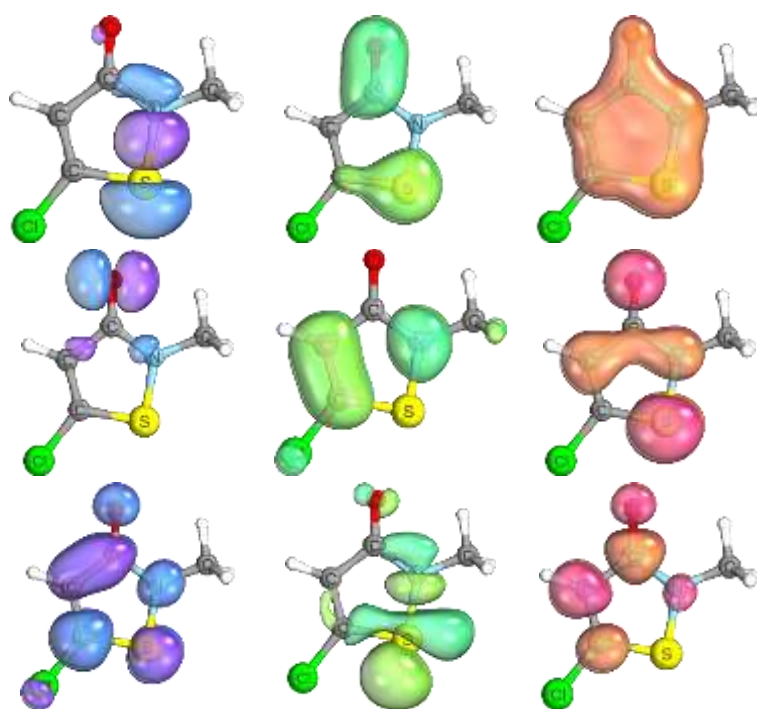
C 0.000000 0.000000 0.000000

C	1.345753	-0.323777	0.000000
C	1.748344	-1.664684	0.000000
C	0.821610	-2.695550	0.000000
C	-0.529422	-2.357215	0.000000
C	-0.942320	-1.025076	0.000000
C	-2.406891	-0.855221	0.000000
N	-2.964848	-2.120917	0.000000
S	-1.892813	-3.464466	0.000000
O	-3.052347	0.175351	0.000000
H	-3.962073	-2.259198	0.000000
H	1.142801	-3.727992	0.000000
H	2.803214	-1.904575	0.000000
H	2.091945	0.458434	0.000000
H	-0.341526	1.026187	0.000000

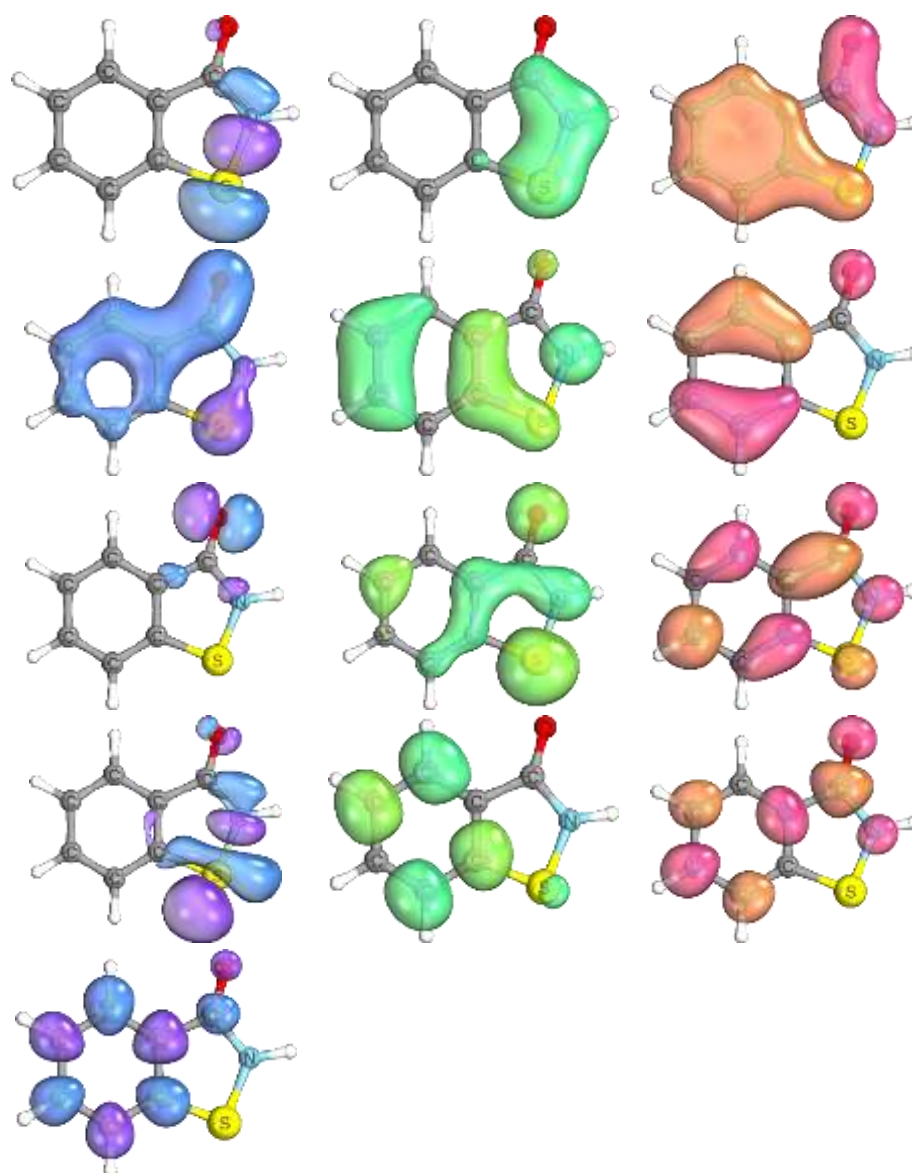
MIT (12,9) Active Space



CIT (12,9) Active Space



BIT (16,13) Active Space



S-N Dissociation Path XYZ Coordinates

P1

C	0.00000000	0.00000000	0.00000000
C	-1.35040900	-0.08992100	0.00000000
S	-2.14624000	1.45056300	0.00000000
N	-0.62411600	2.22000200	0.00000000
C	0.49760100	1.38218400	0.00000000
O	1.64919200	1.79930400	0.00000000
H	-0.54020500	3.22819600	0.00000000
H	-1.96482300	-0.98762900	0.00000000
H	0.68296300	-0.84498500	0.00000000

P2

C	0.0070235	-0.0020548	-0.0131961
C	-1.3530250	-0.0978126	-0.0043806
S	-2.1309400	1.4669226	0.0414893
N	-0.6319210	2.2172979	-0.0398177
C	0.5013577	1.3626221	-0.0007117
O	1.6398061	1.8235033	0.0361971
H	-0.5392393	3.2246739	-0.0134954
H	-1.9771864	-0.9868145	0.0022489
H	0.6880873	-0.8506238	-0.0083339

P3

C	0.0380126	-0.0019987	0.0064602
C	-1.3471072	-0.0647993	-0.0264407
S	-2.2231983	1.4371098	0.0507291
N	-0.5331744	2.2529534	-0.0519738
C	0.5074915	1.3903720	-0.0066124
O	1.6909907	1.8025751	0.0310705
H	-0.3831759	3.2683026	0.0128743
H	-1.9493908	-0.9793677	-0.0483350
H	0.7341795	-0.8433562	0.0719035

P4

C	0.0232445	0.0533178	-0.0030557
C	-1.3597250	-0.0357182	-0.0050718
S	-2.3050182	1.3765983	0.0500778
N	-0.4494557	2.3373712	-0.0646852
C	0.5497905	1.4364583	-0.0068271
O	1.7560448	1.7474133	0.0370442
H	-0.1795979	3.3206057	0.0270746
H	-1.8856390	-0.9956087	-0.0160540
H	0.6892519	-0.8108833	-0.0106824

P5

C	0.0180173	0.1235577	-0.0183113
C	-1.3565856	-0.0314682	0.0046861

S	-2.3708950	1.3193354	0.0594614
N	-0.3747164	2.4510487	-0.0971041
C	0.5495573	1.4846413	-0.0190707
O	1.8102559	1.6604917	0.0599132
H	-0.0519371	3.4152919	0.0305181
H	-1.8169665	-1.0265990	-0.0046367
H	0.7115920	-0.7185901	-0.0244909

P6

C	0.0138849	0.1332411	-0.0283518
C	-1.3386545	-0.0254631	0.0063797
S	-2.4437013	1.2878263	0.0660523
N	-0.2899638	2.5152539	-0.1011579
C	0.5716490	1.4830009	-0.0313397
O	1.8361484	1.6565243	0.0723154
H	0.2189973	3.4107401	-0.0818431
H	-1.7869021	-1.0268352	0.0154687
H	0.7044332	-0.7106065	-0.0363585

P7

C	0.0126494	0.1510474	-0.0312823
C	-1.3433080	-0.0020814	0.0161527
S	-2.5261362	1.2519024	0.0639382
N	-0.2180753	2.5669873	-0.0972961
C	0.6440070	1.4817259	-0.0264031
O	1.8778313	1.6533941	0.0634549
H	0.3934840	3.4001461	-0.0820890
H	-1.7703318	-1.0151918	0.0334536
H	0.6767116	-0.7163724	-0.0403168

P8 – Conical Intersection

C	-0.03743163	0.17229585	-0.01284994
C	-1.38516801	-0.03356561	0.00113684
S	-2.66365892	1.12424828	0.03647354
N	-0.29736956	2.57802237	-0.02357434
C	0.58056098	1.50801306	0.00499038
O	1.81732500	1.67626333	0.05533206
H	0.28707774	3.43089611	-0.02990963
H	-1.75655108	-1.06866111	-0.00684236
H	0.64257958	-0.68247838	-0.02475546

S-C Dissociation Path XYZ Coordinates

P1

C	0.000000	0.000000	0.000000
C	-1.350408	-0.089921	0.000000
S	-2.146239	1.450562	0.000000
N	-0.624116	2.220001	0.000000
C	0.497601	1.382183	0.000000
O	1.649191	1.799303	0.000000
H	-0.540205	3.228195	0.000000
H	-1.964822	-0.987629	0.000000
H	0.682963	-0.844985	0.000000

P2

C	-0.004222	-0.002453	-0.000841
C	-1.348178	-0.137386	0.000940
S	-2.178298	1.559421	0.000019
N	-0.624496	2.244796	-0.000719
C	0.483232	1.386251	0.001043
O	1.637319	1.794768	0.002815
H	-0.494632	3.249850	-0.001407
H	-1.949008	-1.044789	-0.000275
H	0.703316	-0.829432	-0.003306

P3

C	-0.009678	-0.004773	-0.001651
C	-1.345537	-0.185469	0.001966
S	-2.205784	1.668751	-0.000032
N	-0.625236	2.269713	-0.001383
C	0.467810	1.390289	0.002020
O	1.624433	1.789879	0.005491
H	-0.449622	3.269546	-0.002689
H	-1.931684	-1.102966	-0.000552
H	0.722211	-0.812796	-0.006681

P4

C	-0.016286	-0.007029	-0.002425
C	-1.342311	-0.234138	0.003070
S	-2.228804	1.778394	-0.000151
N	-0.626283	2.294696	-0.001996
C	0.451358	1.394253	0.002934
O	1.610545	1.784610	0.008034
H	-0.405154	3.287230	-0.003849
H	-1.912717	-1.162037	-0.000845
H	0.739699	-0.795130	-0.010121

P5

C	-0.023990	-0.009288	-0.003159
C	-1.338360	-0.283355	0.004240

S	-2.247447	1.888235	-0.000335
N	-0.627590	2.319705	-0.002564
C	0.433883	1.398098	0.003785
O	1.595651	1.778921	0.010446
H	-0.361202	3.302853	-0.004893
H	-1.892002	-1.221877	-0.001167
H	0.755802	-0.776481	-0.013622

P6

C	-0.032755	-0.011610	-0.003849
C	-1.333564	-0.333082	0.005465
S	-2.261778	1.998194	-0.000580
N	-0.629111	2.344707	-0.003089
C	0.415375	1.401781	0.004574
O	1.579736	1.772767	0.012729
H	-0.317742	3.316364	-0.005824
H	-1.869454	-1.282367	-0.001534
H	0.770517	-0.756892	-0.017183

P7

C	-0.042563	-0.014052	-0.004490
C	-1.327824	-0.383275	0.006734
S	-2.271836	2.108218	-0.000881
N	-0.630804	2.369677	-0.003573
C	0.395812	1.405261	0.005302
O	1.562773	1.766095	0.014885
H	-0.274745	3.327707	-0.006645
H	-1.845003	-1.343389	-0.001959
H	0.783827	-0.736402	-0.020798

P8

C	-0.06623171	-0.06677969	-0.02821659
C	-1.32749176	-0.50310323	-0.02381444
S	-2.32358203	2.13400233	0.02745615
N	-0.68139677	2.33491659	0.02771068
C	0.34101100	1.36402051	0.01481518
O	1.50522303	1.73148410	0.03300819
H	-0.29507412	3.28285612	0.04545056
H	-1.81048180	-1.48088374	-0.05598025
H	0.79319615	-0.75176410	-0.06388147