

Supporting Information

MECHANISTIC INSIGHTS INTO SMILES REARRANGEMENT. FOCUS ON π - π STACKING INTERACTIONS ALONG THE RADICAL CASCADE

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1. Conformational exploration

In the Smiles rearrangement, the radical intermediate species **2** exhibits an asymmetric carbon, and in the course of the reaction a second asymmetric carbon arises. Moreover, even up to three asymmetric carbons may appear in an alternative route. Thereby, a minimum of four stereoisomers should be considered. All the conformational possibilities have been carefully examined (Figure S1) and the most favourable pathway (labels in red) is reported in the article.

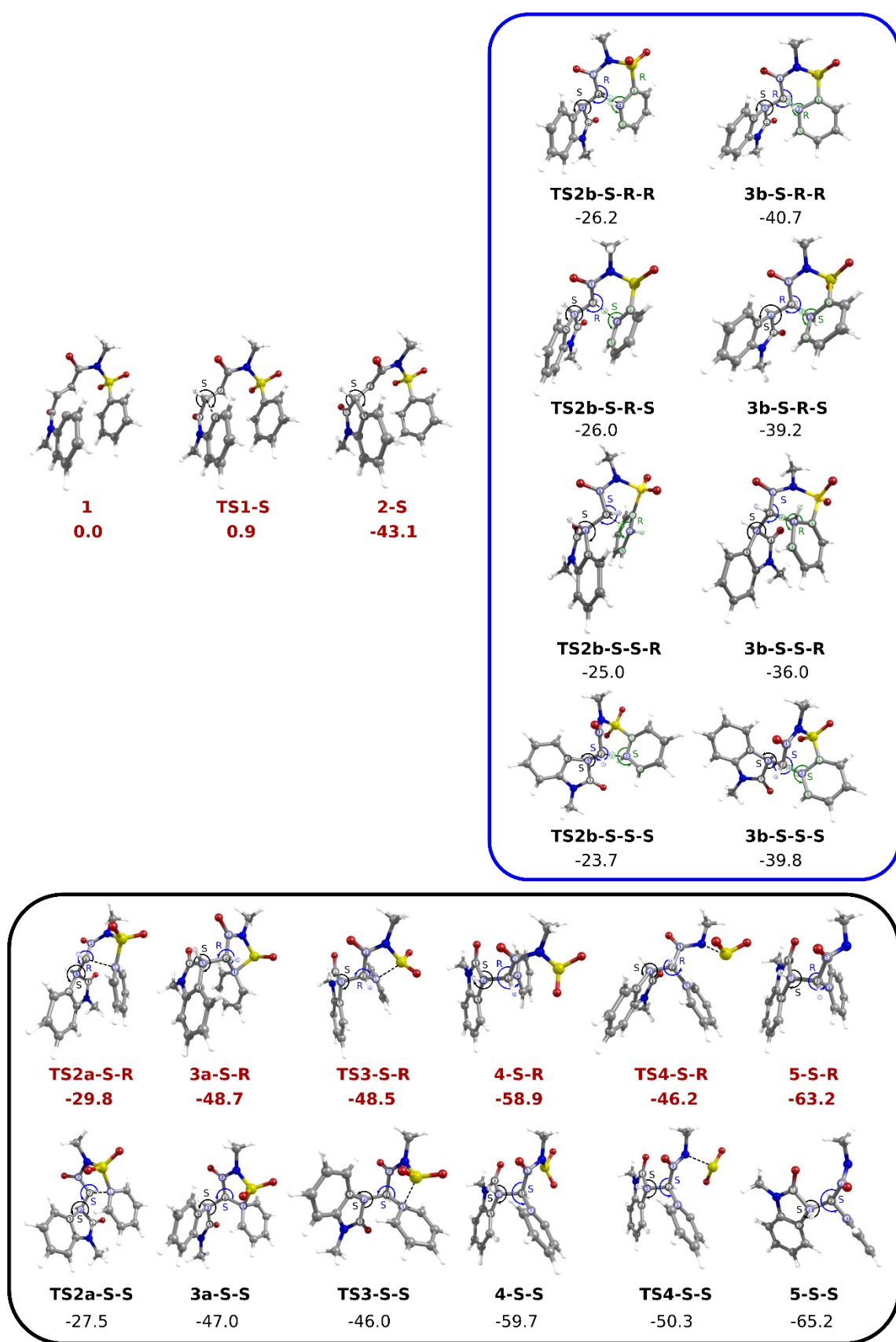


Figure S1. Standard Gibbs (kcal) free energy profile calculated at 447 K for the radical cascade reaction. DFT(M06-2X)/6-311++G** considering n-decane as solvent (PCM).

2. Spin density distribution analysis

The results of the spin density analysis are presented in Figure 5 (spin density isosurfaces) as they provide insights into the localization of the unpaired electron in the intermediate species involved in the radical cascade. For the studied doublet state, Mulliken atomic spin populations (the difference between α and β electrons) are given in the following as well. It was already pointed out the strong dependence between the chosen exchange-correlation functional and the reliability of the spin density calculations. [1,2,3] In this particular case, the spin density profiles obtained at the U-M062X/6-311++G** theory level are consistent with the proposed reaction mechanism and the experimental data behind. For the initial radical **1**, the spin density is mostly concentrated at the *ortho* position of the phenyl ring (1.02 e) where the hydrogen atom is missing. This state corresponds to the starting prior to the 5-*exo-trig* cyclisation. In addition, a small but significant radical character also appears on the α -carbon of **TS1** (0.22 e). This prefigures the formation of the oxindole group that shifts the radical center to this α -carbon bearing most of the spin density (0.91 e) in **2**. This intermediate **2** can undergo an attack on the *ortho* position of the phenyl moiety yielding the fused bicyclic radical **3b**. In this species, the unpaired electron density is actually delocalized over the *ipso* (0.38 e) and *meta* positions (0.47 e and 0.59 e) of the cyclohexadienyl fragment. However, as discussed previously, the high energy of the intermediate **3b** with respect to **3a**, as well as its inability to regenerate the phenyl ring through a subsequent S-C cleavage enable us to discard the **2** $\rightarrow$ **3b** route. As can be seen from Figure 5, the spin density of intermediate **2** is mostly localized on its α -carbon (0.91 e) and points towards the *ipso* position of the adjacent phenyl group. This configuration promotes the formation of the strained spirocyclic compound **3a** with the spin density distribution now delocalized over the *ortho* (0.41 e) and *para* (0.61 e) positions of the cyclohexadienyl fragment. Interestingly, it can be noticed in Figure 5 that the intermediate **TS3** has a significant radical character on the sulphur atom (0.23 e), prefiguring the next step: the S-C cleavage. This bond cleavage regenerates the phenyl ring aromaticity in the resulting sulfonamide radical **4** shifting the spin density to the sulphur (0.43 e). A small but significant radical character is also present on the nitrogen atom. Finally, the N-S cleavage leading to the SO₂ release, shifts the excess of electron spin density to the nitrogen atom (0.90 e) of the produced *N*-amino radical **5**.

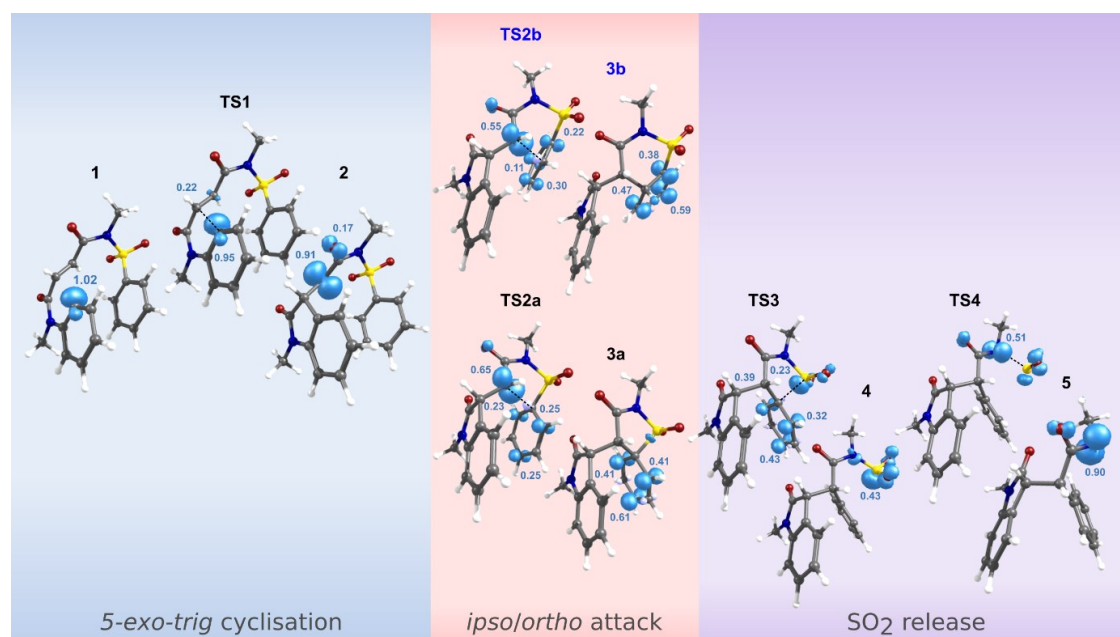


Figure S2. Spin density profiles (DFT M06-2X/6-311++G**) for the doublet state species involved in the Smiles reaction. Isosurfaces of 0.01 a.u. have been considered. The blue surface (positive spin density) corresponds to an excess of α -electron density.

Atomic coordinates, Energies (Hartrees), and Number of Imaginary Frequencies

1

scf done: -1504.441638

Number of imaginary frequencies: 0

C	-2.347700	-1.792771	-2.995281
C	-2.027839	-1.730709	-1.629869
C	-0.677852	-1.799356	-1.334469
C	0.340631	-1.955176	-2.231798
C	-0.001666	-2.021391	-3.587432
C	-1.340175	-1.932548	-3.949312
N	-3.024403	-1.587610	-0.642573
C	-4.407356	-1.415941	-1.074661
C	-2.759340	-1.512155	0.713285
O	-3.622169	-1.255458	1.528261
C	-1.342024	-1.731722	1.138848
C	-0.715206	-0.769590	1.813663
C	0.735743	-0.930051	2.090412
O	1.264412	-2.015155	2.188340
N	1.518002	0.228238	2.179387
C	2.962436	0.010674	2.358708
S	0.971009	1.774102	1.705759
O	2.152218	2.609638	1.734919
C	0.444871	1.592819	0.012682
C	1.418237	1.413763	-0.965368
C	1.016899	1.312886	-2.290834
C	-0.334468	1.392954	-2.620274
C	-1.291846	1.578216	-1.628896
C	-0.906906	1.683678	-0.295920
O	-0.187742	2.114084	2.502874
H	1.373512	-2.010630	-1.906183
H	0.767981	-2.139884	-4.340551
H	-1.619146	-1.981457	-4.995067
H	-3.377185	-1.738900	-3.323397
H	-5.023301	-1.289982	-0.190472
H	-4.740974	-2.295370	-1.628239
H	-4.498660	-0.531744	-1.709530
H	-0.842304	-2.664880	0.901776
H	-1.222525	0.145229	2.086715
H	3.096311	-0.650250	3.212270
H	3.443135	0.964137	2.548754
H	3.390248	-0.463481	1.473457
H	-1.635031	1.849196	0.488906
H	-2.341716	1.641463	-1.889100
H	-0.641820	1.301622	-3.655238
H	1.758457	1.171202	-3.067467
H	2.466903	1.374087	-0.693097

TS1

scf done: -1504.441158

Number of imaginary frequencies: 1

C	0.095489	0.112056	0.099800
C	0.025874	0.025858	1.487221
C	1.162628	-0.042346	2.282243
C	2.409167	-0.006881	1.664281
C	2.499270	0.086321	0.280246
C	1.346475	0.143076	-0.501019
S	-1.582441	-0.051927	2.249422
O	-1.399353	-0.300293	3.663206
N	-2.244590	1.507602	2.054286
C	-3.316067	1.696656	1.063196
C	-1.596981	2.677957	2.477067
O	-1.958104	3.747369	2.034797
C	-0.456366	2.550434	3.413767
C	0.452800	3.535666	3.445813
C	1.655096	3.395462	4.335580
O	1.541776	3.329553	5.541777
N	2.875056	3.323348	3.695342
C	4.087383	3.203091	4.492563
C	2.967578	3.330863	2.293091
C	1.828234	3.380628	1.512226
C	1.791520	3.426860	0.147878
C	3.021782	3.390935	-0.523094
C	4.197895	3.314757	0.212805
C	4.187900	3.287044	1.608536
O	-2.429327	-0.917371	1.456676
H	0.852914	3.478146	-0.392929
H	3.051385	3.420534	-1.605812
H	5.151260	3.285725	-0.301177
H	5.124780	3.242280	2.149468
H	3.800964	3.188808	5.539740
H	4.747875	4.052433	4.306888
H	4.610614	2.276805	4.245069
H	0.265244	4.482405	2.948538
H	-0.326005	1.650693	3.997531
H	-3.998459	2.448586	1.452832
H	-3.839434	0.757003	0.924273
H	-2.905359	2.049756	0.115139
H	1.069657	-0.136613	3.357258
H	3.307695	-0.053456	2.267690
H	3.472391	0.120900	-0.194561
H	1.422974	0.210540	-1.579358
H	-0.811640	0.135034	-0.493496

2

scf done: -1504.516859

Number of imaginary frequencies: 0

C	-1.021606	-1.790178	-3.215063
C	-1.245071	-1.812452	-1.849133
C	-0.196171	-1.796673	-0.921419
C	1.112147	-1.755745	-1.360867
C	1.358104	-1.729438	-2.739670
C	0.307177	-1.748337	-3.648012
N	-2.477314	-1.849214	-1.185481
C	-3.763876	-1.848143	-1.846085
C	-2.314410	-1.854060	0.177944
O	-3.201300	-1.834762	0.999462
C	-0.806734	-1.862062	0.466379
C	-0.450385	-0.756186	1.398727
C	0.929943	-0.623221	1.828013
O	1.721066	-1.549086	1.747410
N	1.351902	0.607186	2.367990
C	2.749362	0.656866	2.823252
S	0.629076	2.061956	1.855425
O	1.557278	3.103189	2.241907
C	0.602550	1.919289	0.081397
C	1.811402	1.989978	-0.604177
C	1.802267	1.824391	-1.982531
C	0.600809	1.593586	-2.650089
C	-0.598657	1.539613	-1.948812
C	-0.606997	1.703578	-0.566983
O	-0.739727	2.085885	2.324969
H	1.930091	-1.753695	-0.651061
H	2.379410	-1.698095	-3.099161
H	0.515952	-1.733542	-4.711390
H	-1.842139	-1.808903	-3.922256
H	-4.532441	-1.855587	-1.075630
H	-3.869518	-2.734127	-2.475799
H	-3.874731	-0.952873	-2.462505
H	-0.557616	-2.823508	0.937551
H	-1.223030	-0.123243	1.813258
H	2.905109	-0.188687	3.489188
H	2.911430	1.585940	3.359435
H	3.442718	0.576204	1.982868
H	-1.528563	1.673564	0.002068
H	-1.529649	1.364419	-2.474071
H	0.601503	1.452412	-3.724090
H	2.731871	1.874418	-2.535895
H	2.733886	2.183418	-0.068637

TS2a

scf done: -1504.494126

Number of imaginary frequencies: 1

C	-0.179432	0.027495	0.023414
C	-0.017869	0.020143	1.434268
C	1.293745	0.039397	1.983723
C	2.380185	-0.144019	1.154164
C	2.204482	-0.254206	-0.228792
C	0.924910	-0.150600	-0.784084
C	-0.863036	-1.793701	2.209641
C	-2.315278	-1.494563	2.065323
N	-2.586102	-0.135139	2.120040
S	-1.279419	0.896409	2.377922
C	-0.340922	-3.025269	1.535305
C	1.110881	-3.327377	1.790647
C	1.739981	-3.523695	0.558087
N	0.814072	-3.373462	-0.480056
C	-0.418541	-2.989964	-0.004567
C	3.096962	-3.779723	0.459040
C	3.829733	-3.830509	1.648890
C	3.218114	-3.635077	2.882240
C	1.843239	-3.382218	2.958508
C	1.154930	-3.417155	-1.883868
O	-1.372920	-2.686826	-0.679872
O	-3.175908	-2.328522	1.909343
C	-3.950089	0.390754	2.113605
O	-0.883475	0.881395	3.774851
O	-1.632227	2.158533	1.761558
H	3.065463	-0.389546	-0.872289
H	3.374661	-0.192926	1.580830
H	1.412886	0.149872	3.054947
H	-1.171126	0.121428	-0.402906
H	0.792048	-0.195382	-1.858766
H	-4.569920	-0.346111	1.606865
H	-3.963905	1.331298	1.566471
H	-4.315536	0.541994	3.130174
H	-0.486374	-1.622087	3.215820
H	-0.983611	-3.866127	1.839242
H	0.256710	-3.182412	-2.452323
H	1.931712	-2.680050	-2.107081
H	1.512263	-4.411413	-2.159677
H	1.367790	-3.225101	3.920917
H	3.807866	-3.680655	3.789200
H	4.894427	-4.026776	1.604912
H	3.576762	-3.927887	-0.500845

3a

scf done: -1504.524935

Number of imaginary frequencies: 0

C	-0.137452	0.059997	-0.038204
C	-0.022065	0.141661	1.442471
C	1.378910	0.223502	1.938929
C	2.437768	0.237855	1.083854
C	2.260249	0.181523	-0.316392
C	0.955576	0.081428	-0.847928
S	-0.765603	-1.435735	2.180004
N	-1.172639	-0.662376	3.627965
C	-1.417015	0.686903	3.480524
C	-1.021434	1.158666	2.081008
C	-0.575823	2.625542	2.062978
C	-0.301672	3.150763	0.678992
C	1.020197	3.603447	0.636770
N	1.609605	3.474250	1.899035
C	0.757470	2.867576	2.790969
C	1.593956	4.085268	-0.528231
C	0.792779	4.117177	-1.672941
C	-0.531137	3.691213	-1.641084
C	-1.087692	3.202125	-0.454829
C	3.002112	3.741356	2.176385
O	1.023885	2.573459	3.933801
O	-1.917310	1.380063	4.327478
C	-1.588674	-1.419718	4.804075
O	0.199739	-2.471549	2.483824
O	-1.968256	-1.789596	1.443118
H	3.117366	0.201854	-0.975904
H	0.817784	0.037019	-1.921700
H	-1.137627	-0.012836	-0.449465
H	1.530484	0.260838	3.011110
H	3.440233	0.294577	1.492608
H	-1.457142	-0.772116	5.668979
H	-0.947474	-2.295290	4.896584
H	-2.634392	-1.720696	4.725962
H	-1.947773	1.092995	1.496201
H	-1.343668	3.200409	2.590024
H	3.182089	3.514949	3.225679
H	3.637860	3.107887	1.550432
H	3.236083	4.790275	1.984387
H	-2.116458	2.857908	-0.433707
H	-1.133136	3.735930	-2.540005
H	1.212650	4.488439	-2.600242
H	2.622178	4.424878	-0.554496

TS2b

scf done: -1504.485619

Number of imaginary frequencies: 1

C	1.722722	1.952112	1.724603
C	0.934772	0.370099	2.864736
C	0.818830	0.660909	4.335882
N	1.803711	1.420090	4.958921
S	2.980056	2.262821	4.071987
C	1.985675	2.886373	2.765229
C	0.838574	2.401826	0.697887
C	0.175654	3.605898	0.820744
C	0.389927	4.444811	1.922036
C	1.308060	4.076965	2.907728
C	-0.368219	-0.062896	2.256198
C	-0.341269	-0.622367	0.862000
C	-1.371434	-0.015645	0.131281
N	-2.021014	0.936975	0.922406
C	-1.401163	1.072717	2.149105
C	-1.613535	-0.332874	-1.194495
C	-0.783218	-1.288441	-1.790218
C	0.245750	-1.894652	-1.079625
C	0.471021	-1.562751	0.262504
C	-3.020474	1.856835	0.427910
O	-1.639098	1.924176	2.969924
O	-0.089789	0.205287	4.997104
C	1.654824	1.665401	6.399567
O	3.910188	1.299641	3.516101
O	3.450133	3.327951	4.931878
H	2.516924	1.270350	1.444477
H	0.706871	1.788726	-0.186135
H	-0.502923	3.923504	0.037342
H	-0.140655	5.384342	2.003752
H	1.500905	4.710354	3.765689
H	1.613782	0.705826	6.911780
H	2.508973	2.238049	6.748307
H	0.732212	2.214533	6.588426
H	1.779002	-0.284520	2.658416
H	-0.826204	-0.791758	2.941410
H	1.272181	-2.038454	0.817835
H	-3.923524	1.318818	0.132803
H	-2.636457	2.411276	-0.433420
H	-3.257729	2.552403	1.231020
H	-2.411303	0.140959	-1.753479
H	-0.947576	-1.556404	-2.827058
H	0.876598	-2.628496	-1.565192

3b

scf done: -1504.18718307

Number of imaginary frequencies: 0

C	1.838808	1.903157	2.010193
C	1.110257	0.705525	2.752219
C	0.651121	0.915540	4.210877
N	1.486012	1.652337	5.043116
S	2.938325	2.294102	4.455761
C	2.321807	2.950314	2.963966
C	1.108630	2.548405	0.866597
C	1.006684	3.895168	0.714294
C	1.541048	4.800722	1.662870
C	2.185249	4.293676	2.809498
C	-0.039275	0.073302	1.970718
C	0.270466	-0.549277	0.636908
C	-0.735242	-0.165157	-0.260719
N	-1.619263	0.719650	0.364344
C	-1.200208	1.023698	1.646488
C	-0.752847	-0.605541	-1.573529
C	0.280125	-1.455901	-1.980953
C	1.287380	-1.840796	-1.103834
C	1.285501	-1.386953	0.221029
C	-2.684362	1.419814	-0.318365
O	-1.679403	1.870275	2.361037
O	-0.335085	0.372422	4.644314
C	1.198641	1.817113	6.472935
O	3.845233	1.200797	4.155381
O	3.332179	3.326946	5.389924
H	2.727159	1.425721	1.563092
H	0.742431	1.895678	0.083469
H	0.504722	4.288534	-0.161951
H	1.440805	5.868154	1.523982
H	2.559709	4.958221	3.580016
H	1.997228	1.387270	7.080020
H	1.095188	2.875500	6.705042
H	0.267510	1.293177	6.661792
H	1.878975	-0.067243	2.871698
H	-0.485309	-0.687458	2.621471
H	2.071141	-1.690171	0.905081
H	-3.427358	0.712162	-0.691209
H	-2.286759	1.999167	-1.156613
H	-3.150042	2.093161	0.398681
H	-1.533044	-0.302508	-2.261288
H	0.293843	-1.816860	-3.002385
H	2.078549	-2.495827	-1.446271

TS3

scf done: -1504.522359

Number of imaginary frequencies: 1

C	-0.339853	0.793765	0.252660
C	-0.006509	0.362599	1.596191
C	1.364704	0.577893	2.018535
C	2.312470	1.014745	1.127900
C	1.965902	1.333569	-0.194610
C	0.629353	1.229293	-0.613220
S	-0.122549	-1.771820	1.542930
N	-0.456470	-1.785532	3.211652
C	-1.084493	-0.655302	3.682923
C	-1.132324	0.466844	2.641661
C	-1.236764	1.855221	3.300686
C	-1.472912	2.947115	2.291894
C	-0.386907	3.826801	2.334036
N	0.501929	3.435558	3.341561
C	0.080468	2.285800	3.966405
C	-0.277644	4.900299	1.466309
C	-1.308570	5.084761	0.540519
C	-2.403349	4.228098	0.496832
C	-2.489350	3.145571	1.379117
C	1.772482	4.072783	3.602455
O	0.667894	1.712829	4.855521
O	-1.588237	-0.580416	4.775371
C	-0.430613	-3.031698	3.973782
O	1.127059	-2.495031	1.357118
O	-1.302252	-2.205943	0.799310
H	2.725083	1.675290	-0.886502
H	0.356490	1.514010	-1.621967
H	-1.373562	0.722154	-0.065017
H	1.638095	0.332305	3.038028
H	3.339339	1.122995	1.455943
H	-1.376413	-3.567028	3.877593
H	-0.259640	-2.775048	5.017662
H	0.391304	-3.643046	3.603772
H	-2.076343	0.299391	2.107115
H	-2.008587	1.796982	4.072440
H	2.244785	3.545336	4.429059
H	2.411170	4.012418	2.716615
H	1.627171	5.120096	3.874638
H	-3.338433	2.470968	1.338425
H	-3.192637	4.399104	-0.224405
H	-1.252681	5.916313	-0.151823
H	0.571125	5.572318	1.500966

4

scf done: -1504.536592

Number of imaginary frequencies: 0

C	0.453859	0.327735	-0.035808
C	0.421056	0.306128	1.359990
C	1.580365	-0.034731	2.064402
C	2.746917	-0.358367	1.380552
C	2.770578	-0.335389	-0.010964
C	1.622872	0.010460	-0.718087
S	-0.842125	-2.324648	1.794337
N	-1.028482	-1.503166	3.273114
C	-1.140881	-0.104454	3.346625
C	-0.852903	0.708143	2.083845
C	-0.869658	2.222089	2.404672
C	-0.974545	3.059687	1.158186
C	0.177071	3.845436	1.054429
N	1.007858	3.615374	2.155213
C	0.464695	2.685990	3.012571
C	0.390696	4.699461	-0.014654
C	-0.597978	4.753281	-1.001231
C	-1.750988	3.981128	-0.911309
C	-1.943986	3.122683	0.177403
C	2.297456	4.238283	2.351731
O	0.977350	2.298076	4.037227
O	-1.480199	0.393244	4.388648
C	-1.123506	-2.263988	4.529589
O	-0.719462	-3.739082	2.138454
O	-1.888651	-1.876692	0.874172
H	3.679175	-0.592142	-0.542560
H	1.633978	0.025125	-1.801272
H	-0.445578	0.582340	-0.586051
H	1.569249	-0.042549	3.149393
H	3.637198	-0.627658	1.936068
H	-0.590161	-1.710562	5.298964
H	-0.672796	-3.241345	4.386848
H	-2.169319	-2.375135	4.818190
H	-1.696469	0.513831	1.413136
H	-1.667184	2.423479	3.123231
H	2.708117	3.861401	3.286408
H	2.969762	3.984259	1.528747
H	2.192136	5.323794	2.411927
H	-2.841487	2.516421	0.244464
H	-2.503595	4.043981	-1.687230
H	-0.460155	5.411729	-1.850600
H	1.287990	5.301688	-0.087846

TS4

scf done: -1504.512894

Number of imaginary frequencies: 1

C	0.506159	0.246523	-0.094462
C	0.515874	0.414422	1.292704
C	1.634896	0.000866	2.021410
C	2.711474	-0.593620	1.372204
C	2.690081	-0.765448	-0.008888
C	1.587269	-0.338791	-0.742927
S	-1.054833	-2.088526	1.827630
N	-0.905244	-0.885838	3.513947
C	-1.063973	0.501506	3.320562
C	-0.669151	1.079271	1.964579
C	-0.483163	2.611951	2.075025
C	-0.427725	3.290547	0.733814
C	0.829122	3.886697	0.592958
N	1.585578	3.678035	1.751260
C	0.887844	2.945546	2.682320
C	1.196215	4.564550	-0.557453
C	0.255113	4.636308	-1.588453
C	-1.000957	4.053081	-1.462262
C	-1.349527	3.371395	-0.290394
C	2.950913	4.119344	1.928211
O	1.306898	2.601342	3.764344
O	-1.488714	1.180300	4.224238
C	-1.689228	-1.456737	4.591326
O	-1.039654	-3.405533	2.440512
O	-2.352020	-1.603698	1.351749
H	3.529615	-1.231374	-0.511056
H	1.564618	-0.468087	-1.818325
H	-0.359733	0.566917	-0.664472
H	1.661732	0.142973	3.095572
H	3.569284	-0.920825	1.947443
H	-1.307335	-1.009728	5.514729
H	-1.530501	-2.532898	4.612429
H	-2.751977	-1.213350	4.518765
H	-1.551237	0.909651	1.333531
H	-1.261943	3.016960	2.724832
H	3.280856	3.788704	2.911196
H	3.592219	3.679518	1.160752
H	3.011439	5.208364	1.870882
H	-2.328143	2.912554	-0.193342
H	-1.713481	4.127200	-2.274211
H	0.512511	5.159651	-2.501584
H	2.173186	5.021299	-0.658063

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scf done: -955.940998

Number of imaginary frequencies: 0

C	-0.264953	-0.106982	-0.180503
C	-0.137680	0.025012	1.202219
C	1.132509	-0.105685	1.772128
C	2.241661	-0.365161	0.974173
C	2.101713	-0.493862	-0.404456
C	0.843458	-0.364100	-0.981011
N	-0.764831	-1.512308	3.534769
C	-1.624762	-0.459856	3.279326
C	-1.362661	0.374105	2.020519
C	-1.379715	1.865744	2.442873
C	-1.221582	2.832486	1.303487
C	-0.053134	3.571090	1.513973
N	0.546625	3.177226	2.719712
C	-0.163753	2.174012	3.321478
C	0.383798	4.530652	0.617424
C	-0.394627	4.742408	-0.524295
C	-1.560855	4.019047	-0.747312
C	-1.981835	3.052271	0.172894
C	1.808219	3.685955	3.209998
O	0.143636	1.598865	4.346906
O	-2.616448	-0.266299	3.951083
C	-0.300277	-1.623999	4.891922
H	2.967411	-0.696623	-1.023741
H	0.721758	-0.463366	-2.053108
H	-1.243781	-0.003118	-0.637144
H	1.261411	-0.007257	2.844053
H	3.217662	-0.471113	1.433197
H	0.422485	-0.825029	5.100466
H	0.151512	-2.599214	5.056543
H	-1.144993	-1.465273	5.573307
H	-2.250776	0.218794	1.399357
H	-2.286540	2.042309	3.027587
H	2.028027	3.180616	4.148533
H	2.602960	3.480694	2.488630
H	1.744031	4.762315	3.382111
H	-2.889517	2.484664	-0.002729
H	-2.146598	4.204558	-1.638957
H	-0.079800	5.485920	-1.246724
H	1.292055	5.095361	0.788705

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