

Electronic Supplementary Information

Interactions of the N3 Dye with the Iodide Redox Shuttle: Quantum Chemical Mechanistic Studies of the Dye Regeneration in Dye- Sensitized Solar Cell

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Table S1. Bond distances of I_2 , I_2^- , and I_3^- ; this work and selected previous studies (Å).

Method; <i>code</i>	Reference	I_2	I_2^-	I_3^-
All-electron scalar, PBE; <i>p6</i>	This work	2.69	3.32	2.98
Scalar SC-ECP-SDD B3LYP; <i>g03</i>	49	2.73	3.38	3.02
SC-ECP-AUG-cc-pVTZ, PW91; <i>g03</i>	66	2.69	3.28	2.98
Scalar SC-ECP B3LYP; <i>Dirac04</i>	71	2.70		
Spin-orbit SC-ECP B3LYP; <i>Dirac04</i>	71	2.72		
Scalar SC-ECP CCSD(T) TZ	Cited from ref. ⁷¹	2.70		
Scalar LC-ECP (lacvp*) B3LYP; <i>Jaguar</i>	44		3.46	3.14
Experiment	Cited from ref. ⁶⁶	2.67	3.23	

Table S2: Transition state barriers for different elementary reactions in the dye regeneration using B3LYP. The reactant, product and transition state structures corresponding to Figures 1, 2 and 3. The energy of reactants of all reactions is set to zero in order to present the barrier height and exothermicity of each reaction. The reaction scheme is followed by their corresponding energy (Kcal/mol).

Reactant	Transition State	Product
N3I _{OH} 0.00	TS-1 6.75	N3I _{Ru} -1.96
N3I _{Ru} + I ⁻ 0.00	TS-2 3.69	N3I _{Ru} -I -4.61
N3I _{OH} + I ⁻ 0.00	TS-3 12.24	N3I _{OH} -I -5.73
N3I _{Ru} -I 0.00	TS-4 4.88	N3 + I ₂ ⁻ -12.50
N3I _{OH} -I 0.00	TS-5 5.23	N3 + I ₂ ⁻ -9.83

Charge, Spin-state, Electronic energy, Free energy correction, Solvation free energy, Spin-orbit correction, Imaginary frequency (where applicable) and Cartesian coordinates (Å) for optimized structures.

The titles correspond to the figure number of manuscript.

N3				N3⁺			
Charge = 0				Charge = 0			
Spin-state = 0				Spin-state = 0			
Electronic energy = -7260.261452 au.				Electronic energy = -7260.040101			
Free energy Correction = 193.7129 Kcal				Free energy Correction = 196.0439 Kcal			
Solvation free energy = -23.59 Kcal				Solvation free energy = -47.21 Kcal			
Spin-orbit correction = 12.67 Kcal				Spin-orbit correction = 12.98 Kcal			
Ru	-0.01063264	-0.03495690	-0.70521900	Ru	-0.01432840	-0.03924546	-0.78514476
N	1.97281092	-0.50918996	-0.65253074	N	1.99519449	-0.48481751	-0.73845566
C	2.76532101	0.32863008	0.09293585	C	2.76472590	0.29894645	0.07960814
C	4.14925100	0.16267131	0.13241803	C	4.14752388	0.13252281	0.14333141
C	4.74857364	-0.86265031	-0.59712114	C	4.76630225	-0.83587421	-0.64484396
C	3.92895150	-1.70726251	-1.36311074	C	3.97268052	-1.62026894	-1.49029443
C	2.55957479	-1.49895232	-1.36679392	C	2.60011610	-1.41424056	-1.51106021
C	6.23050946	-0.99747425	-0.52730522	C	6.25634292	-0.97024716	-0.54138775
O	6.95357937	-0.28385058	0.13929253	O	6.93531571	-0.29772539	0.20394004
O	6.69291600	-2.01897224	-1.29730440	O	6.73635030	-1.92352426	-1.37144698
N	0.67021204	1.33333292	0.64135609	N	0.67315439	1.32060302	0.62299740
C	-0.08572191	2.22467502	1.32859406	C	-0.08689677	2.21895108	1.28418514
C	0.44931332	3.15063458	2.20472423	C	0.44162054	3.12337317	2.19367487
C	1.84129889	3.18227926	2.40040341	C	1.82007953	3.10417643	2.43859941
C	2.62615105	2.26525476	1.70256688	C	2.60963667	2.18066934	1.75730721
C	2.03318175	1.35140752	0.83360567	C	2.02224493	1.29822103	0.85021743
C	2.52118385	4.13862303	3.31298778	C	2.50386012	4.03140412	3.40047021
O	1.64493065	4.98733314	3.91949448	O	1.63359740	4.89126312	3.97681365
O	3.72066799	4.17035791	3.50722547	O	3.69402050	3.99941122	3.62334855
N	-0.65445874	-1.27287940	0.77836123	N	-0.66324713	-1.26320259	0.75930791
C	-2.01199384	-1.27258231	1.00661547	C	-2.00575768	-1.21724116	1.01964120
C	-2.58023603	-2.09988951	1.97330511	C	-2.56789943	-2.01014291	2.02056933
C	-1.77559331	-2.94655048	2.73463306	C	-1.75968116	-2.86764512	2.76347308
C	-0.38916440	-2.93367530	2.50093308	C	-0.38837136	-2.91244138	2.48414973
C	0.12097135	-2.09513797	1.52739705	C	0.11487554	-2.09769468	1.48045532
C	-2.42942150	-3.81150752	3.75142420	C	-2.41660379	-3.69954514	3.82596129
O	-3.62342008	-3.82457226	3.97883706	O	-3.60035748	-3.64472663	4.07677651
O	-1.53576102	-4.59858869	4.41320901	O	-1.53047382	-4.50314386	4.45674731
N	-1.99407067	0.44297249	-0.64603810	N	-2.02246004	0.41096232	-0.72748132
C	-2.60182296	1.36149749	-1.43407197	C	-2.64851225	1.26524707	-1.56708454
C	-3.97176976	1.56594200	-1.41746230	C	-4.02037234	1.47369165	-1.52984025
C	-4.76949284	0.79336735	-0.55827732	C	-4.79065724	0.77203639	-0.59484328
C	-4.14879353	-0.15872202	0.24852286	C	-4.15028088	-0.11965158	0.26344959
C	-2.76538996	-0.32410168	0.19208642	C	-2.76937043	-0.29272623	0.17950450
C	-6.25020956	0.92977607	-0.46684310	C	-6.27769399	0.91705375	-0.46552749
O	-6.73521361	1.87372168	-1.31755268	O	-6.78029409	1.78978637	-1.36770879
O	-6.95407066	0.27915652	0.27992305	O	-6.93623008	0.31734669	0.35633617
N	0.39071605	1.26148573	-2.17317086	N	0.36700383	1.30192568	-2.17316559
C	0.59249433	2.08256392	-3.01258520	C	0.71684279	2.19014211	-2.89264356

S	0.84060808	3.20596609	-4.14279312	S	1.14374654	3.38037138	-3.87765036
N	-0.45033756	-1.45679809	-2.03995357	N	-0.43018394	-1.50030151	-2.03539310
C	-0.70849102	-2.32981359	-2.80870925	C	-0.79715665	-2.44850010	-2.66405248
S	-1.03543792	-3.52373976	-3.84240138	S	-1.24744729	-3.72124845	-3.52803808
H	4.78589319	0.82472316	0.71757592	H	4.77190132	0.74754747	0.79026333
H	4.35447303	-2.51075115	-1.96046188	H	4.41622690	-2.37911887	-2.13193063
H	1.88032345	-2.11098178	-1.95758531	H	1.94084832	-1.98930197	-2.15805790
H	7.66411572	-2.01338312	-1.18551033	H	7.70697581	-1.94240438	-1.24718779
H	-1.15621540	2.18095104	1.13840622	H	-1.15103661	2.20407127	1.05660027
H	-0.20433987	3.84874023	2.72334171	H	-0.20879478	3.83403781	2.69943792
H	3.70429781	2.28385757	1.85544674	H	3.68149573	2.17529125	1.95083156
H	2.19308980	5.56740230	4.48396574	H	2.15590839	5.45820903	4.58002240
H	-3.65401013	-2.10359036	2.15523695	H	-3.63410731	-1.98449779	2.24172182
H	0.27930420	-3.57935626	3.06646928	H	0.27588372	-3.57414022	3.03623771
H	1.18614690	-2.06973104	1.30656290	H	1.17248238	-2.10608674	1.22393033
H	-2.06783546	-5.12202381	5.04447665	H	-2.03591574	-5.01016172	5.12424888
H	-1.94021708	1.91890497	-2.09468138	H	-2.00714594	1.77715507	-2.28162283
H	-4.41446645	2.31002881	-2.07611591	H	-4.48151662	2.17013701	-2.22740706
H	-4.76869044	-0.76581159	0.90669115	H	-4.75679169	-0.67138179	0.98064804
H	-7.70359980	1.87576088	-1.18346453	H	-7.74738957	1.82121521	-1.22057689

N3I_{Ru}

Charge = 0
Spin-state = 1
Electronic energy = -14377.738078 au.
Free energy Correction = 191.0360 Kcal
Solvation free energy = -19.82
Spin-orbit correction = 22.64 Kcal

Ru	0.01752721	-0.05514693	-0.85789869
N	2.01275123	-0.51379173	-0.79422573
C	2.77788112	0.26003317	0.03984271
C	4.15754653	0.07318681	0.12459962
C	4.77714889	-0.90407254	-0.65226613
C	3.98585587	-1.67884971	-1.51269122
C	2.61938103	-1.45250114	-1.55686165
C	6.25559079	-1.06428150	-0.52778005
O	6.95328635	-0.40661667	0.21692952
O	6.73805012	-2.03667775	-1.34546792
N	0.68313435	1.29933839	0.54341736
C	-0.08789644	2.16962297	1.22585090
C	0.43212898	3.04701730	2.17459332
C	1.80544834	3.03503939	2.42403144
C	2.60623086	2.11750280	1.73455287
C	2.03297756	1.25890064	0.80535155
C	2.47136633	3.93909165	3.40643307
O	1.59982427	4.80268137	3.98506759
O	3.65910602	3.90914150	3.66123741
N	-0.62226259	-1.26795032	0.68649208
C	-1.95307666	-1.19325963	0.97903555
C	-2.51240036	-1.97696288	1.99190342
C	-1.70975976	-2.86121306	2.70581799

N3IO_H

Charge = 0
Spin-state = 1
Electronic energy = -14377.732700 au.
Free energy Correction = 189.0560 Kcal
Solvation free energy = -25.65 Kcal
Spin-orbit correction = 20.56 Kcal

Ru	-0.02012739	-0.06054851	-0.78897646
C	-2.76379304	-0.30914438	0.16987433
N	-2.00921875	0.40747185	-0.72394161
C	-2.62965639	1.28989734	-1.54145706
C	-3.99734546	1.50908979	-1.49814376
C	-4.77710219	0.78911224	-0.58114430
C	-4.14368896	-0.12800581	0.25545896
N	-0.44852757	-1.52144132	-2.07034827
C	-0.73278344	-2.45322739	-2.75692910
S	-1.08648791	-3.71750623	-3.69112305
C	-6.25613353	0.94714465	-0.45611294
O	-6.94233204	0.33490029	0.33632041
C	-1.99995398	-1.23552060	1.00251809
N	-0.65216261	-1.26604242	0.74022587
C	0.13084268	-2.08385527	1.48210838
C	-0.36590992	-2.88920430	2.49250872
C	-1.74217620	-2.86609965	2.76598627
C	-2.55546711	-2.02642229	2.00705208
C	-2.38457553	-3.69253171	3.82846639
O	-1.48559301	-4.46884280	4.48845669
N	1.97652194	-0.51620782	-0.73722201
C	2.75548556	0.29032701	0.05210057
C	4.13888525	0.12449340	0.10595464

C	-0.33809820	-2.90685058	2.41748193	C	4.74978819	-0.86884876	-0.65774695
C	0.16137386	-2.09862860	1.41128781	C	3.94490469	-1.67983197	-1.47013465
C	-2.35398701	-3.70187480	3.75611222	C	2.57450088	-1.47238286	-1.48511948
O	-3.54630252	-3.72348653	3.97775415	C	2.01836053	1.30180253	0.80966074
O	-1.44887072	-4.45369768	4.43947017	N	0.66906506	1.32472569	0.57474506
N	-1.98003108	0.41714698	-0.77986981	C	-0.08796883	2.22670251	1.23675789
C	-2.60291950	1.29529727	-1.59833647	C	0.44081719	3.12056622	2.15526365
C	-3.96479932	1.53959132	-1.52379746	C	1.81699399	3.09687098	2.41234621
C	-4.73084068	0.85050316	-0.57311656	C	2.60378401	2.17747188	1.72368964
C	-4.09138655	-0.05286121	0.27202631	C	6.23436120	-1.00489842	-0.57225344
C	-2.71770114	-0.26044832	0.15035869	O	6.70636055	-1.99070595	-1.37906079
C	-6.20450181	1.03243520	-0.42012708	C	2.49232812	4.00652946	3.40868135
O	-6.69358110	1.98667083	-1.25652541	O	3.68724830	3.94022103	3.62499402
O	-6.89382952	0.40348118	0.35510397	N	0.36487566	1.23493129	-2.24730448
N	0.41333213	1.25626444	-2.28844293	C	0.63141899	2.05644179	-3.06895264
C	0.71330040	2.09760824	-3.07822277	S	0.95870166	3.17129717	-4.18390096
S	1.08371344	3.23694659	-4.15360025	O	6.94098542	-0.31784797	0.13562305
N	-0.41480544	-1.51411881	-2.13061929	O	1.61874999	4.83540669	3.98141929
C	-0.70898881	-2.45132957	-2.80626627	O	-3.57235498	-3.67617792	4.07885564
S	-1.07250315	-3.72052534	-3.72837952	O	-6.74928311	1.85937595	-1.33269232
H	4.77413556	0.68218531	0.78389446	H	4.76469749	0.76322570	0.72756074
H	4.42871679	-2.44415152	-2.14645817	H	4.38050796	-2.45856788	-2.09261659
H	1.96068643	-2.01765302	-2.21338151	H	1.90669279	-2.06362769	-2.10856104
H	7.70357962	-2.05708472	-1.19237942	H	7.67655138	-1.99380323	-1.25650525
H	-1.15112709	2.16748928	1.00261883	H	-1.15096094	2.21752824	1.00346044
H	-0.24413069	3.71040747	2.70848571	H	-0.20420810	3.83117237	2.66826744
H	3.67408718	2.10074999	1.94695557	H	3.67364196	2.16733941	1.93041047
H	2.12811712	5.33596397	4.61142154	H	2.08380335	5.42531160	4.66057542
H	-3.57080072	-1.91723791	2.23531496	H	-3.62324576	-2.00794131	2.22052531
H	0.32796582	-3.56979681	2.96531861	H	0.30672660	-3.53159421	3.05682473
H	1.21583051	-2.11367676	1.14415344	H	1.18961734	-2.08222959	1.23127920
H	-1.96965446	-4.95649892	5.09643192	H	-2.00041657	-4.96542579	5.15523660
H	-1.96432599	1.79367311	-2.32466398	H	-1.98152407	1.81121139	-2.24319486
H	-4.42458972	2.25301780	-2.20431913	H	-4.45114398	2.22712460	-2.17794685
H	-4.68140220	-0.57860463	1.01988849	H	-4.75068429	-0.69360779	0.96100853
H	-7.65420236	2.02518851	-1.07859192	H	-7.71408740	1.88742259	-1.17577983
I	-2.39496736	1.24892366	3.60111419	I	2.80127835	6.94266317	6.36607189

N3I_{Ru}-I

Charge = -1
 Spin-state = 1/2
 Electronic energy = -21495.359414 au.
 Free energy Correction = 187.0621 Kcal
 Solvation free energy = -43.62 Kcal
 Spin-orbit correction = 30.85 Kcal

Ru	0.00453178	-0.06458099	-0.75700126
N	1.98499011	-0.51088808	-0.71589398
C	2.76374432	0.30168385	0.07510790
C	4.14884157	0.15319070	0.11305550
C	4.77041604	-0.82925223	-0.65928061
C	3.96414341	-1.64927134	-1.46832432
C	2.59391459	-1.45886142	-1.47165241

N3I_{OH}-I

Charge = 0
 Spin-state = 1/2
 Electronic energy = -21495.353527 au.
 Free energy Correction = 187.8318 Kcal
 Solvation free energy = -48.65 Kcal
 Spin-orbit correction = 30.03 Kcal

Ru	0.02078042	-0.05026901	-0.76546298
N	2.00177609	-0.52504559	-0.72237677
C	2.79590953	0.29671274	0.03891254
C	4.18077538	0.13471089	0.06385494
C	4.77974102	-0.87295400	-0.69217194
C	3.95695016	-1.70439889	-1.46920053
C	2.58835550	-1.49812542	-1.46067077

C	6.24621467	-0.94853896	-0.59120777	C	6.25880280	-1.00912687	-0.63945227
O	6.97361725	-0.25932013	0.10047230	O	6.99806710	-0.31127676	0.02689220
O	6.73103956	-1.93725576	-1.40126170	O	6.71737838	-2.02218110	-1.43145476
N	0.65331196	1.25777807	0.65508336	N	0.70746741	1.28704025	0.64086924
C	-0.12312913	2.07931853	1.39805006	C	-0.04812902	2.11842320	1.39111786
C	0.39340774	2.94945412	2.34596324	C	0.50218604	3.00642985	2.30856799
C	1.78058537	2.99301892	2.54621804	C	1.89130176	3.05927143	2.46048916
C	2.58800502	2.13651512	1.79403101	C	2.67131518	2.18063416	1.70922295
C	2.01398082	1.27589133	0.86345851	C	2.06868007	1.29804581	0.81711942
C	2.44073589	3.89043295	3.52849563	C	2.60396354	3.99919573	3.40076162
O	1.55503911	4.69147030	4.18030867	O	1.75405962	4.80620000	4.03521641
O	3.64004815	3.92304853	3.74303351	O	3.81620421	3.98125253	3.52273783
N	-0.62898831	-1.35607103	0.68768046	N	-0.64666216	-1.27958593	0.72891576
C	-1.96998728	-1.32405309	0.97518929	C	-1.99068295	-1.23650370	0.97964817
C	-2.52115853	-2.16272001	1.94332976	C	-2.56778513	-2.03215795	1.97267998
C	-1.70975450	-3.06902088	2.62598695	C	-1.77048010	-2.90282192	2.71351795
C	-0.33614647	-3.08534646	2.33249676	C	-0.38750462	-2.91649385	2.46813011
C	0.15619856	-2.22442048	1.36993457	C	0.12826399	-2.09966741	1.47981649
C	-2.33494831	-3.96537128	3.62752054	C	-2.42159516	-3.76147627	3.73467240
O	-3.52682191	-4.03784674	3.85631834	O	-3.61996876	-3.83757154	3.91923109
O	-1.41512602	-4.73533007	4.28771681	O	-1.51677990	-4.48442105	4.46085350
N	-1.98187024	0.41382970	-0.64818419	N	-1.96992092	0.43727333	-0.70927278
C	-2.59080674	1.37807948	-1.37479298	C	-2.56720400	1.36110493	-1.49873513
C	-3.94232613	1.65272657	-1.25437565	C	-3.93366475	1.57859114	-1.47719668
C	-4.71671399	0.90286532	-0.35807376	C	-4.73676539	0.81581943	-0.61483225
C	-4.09474120	-0.09705913	0.38565521	C	-4.12091206	-0.11514041	0.21865830
C	-2.72973090	-0.32985934	0.22491743	C	-2.73795667	-0.29390162	0.15074495
C	-6.17221032	1.12869135	-0.15382569	C	-6.21413593	0.95840083	-0.54199714
O	-6.63850422	2.19479881	-0.86457369	O	-6.67847326	1.97313766	-1.32929455
O	-6.88891174	0.44490202	0.55034571	O	-6.94889926	0.26040361	0.12813429
N	0.39749678	1.27673832	-2.19840585	N	0.43725358	1.26702259	-2.20722934
C	0.70371306	2.03581000	-3.06188760	C	0.68501875	2.05957008	-3.05996241
S	1.09938444	3.08331426	-4.23002836	S	0.99361600	3.14338847	-4.21802811
N	-0.41467367	-1.46361933	-2.14646061	N	-0.42106645	-1.47606742	-2.10243945
C	-0.56534725	-2.36351757	-2.90888878	C	-0.64293369	-2.38364593	-2.83885469
S	-0.74429733	-3.59741525	-3.94468385	S	-0.91371288	-3.62582806	-3.84009158
H	4.76826174	0.79914157	0.73324848	H	4.81395653	0.78752963	0.66255031
H	4.40241861	-2.41911440	-2.09970379	H	4.37963349	-2.49660267	-2.08327984
H	1.92780549	-2.05309365	-2.09466486	H	1.90856241	-2.10147762	-2.05918009
H	7.69925758	-1.90977949	-1.27378966	H	7.68807599	-2.00951977	-1.31942712
H	-1.19832831	2.04615167	1.23004937	H	-1.12825069	2.05117950	1.26848503
H	-0.30161709	3.57306592	2.90646179	H	-0.15652346	3.63835175	2.90122558
H	3.66408672	2.15647181	1.95991700	H	3.75095921	2.21032404	1.85273084
H	2.09555913	5.22394616	4.79557206	H	2.25390653	5.43157432	4.65486734
H	-3.58132731	-2.12232149	2.18319768	H	-3.63397209	-1.98558574	2.18098410
H	0.33683495	-3.76809988	2.84638019	H	0.27509471	-3.56442184	3.03779980
H	1.21155578	-2.21501315	1.10579257	H	1.19120183	-2.09070390	1.24823124
H	-1.94559958	-5.26930350	4.91048277	H	-2.05751843	-4.99570250	5.09395847
H	-1.94302057	1.92660084	-2.05564071	H	-1.90265554	1.90995801	-2.16235201
H	-4.38616742	2.44989662	-1.84594598	H	-4.37120340	2.32663123	-2.13468818
H	-4.68722901	-0.66647367	1.09857179	H	-4.73213368	-0.69152977	0.90899539
H	-7.58392730	2.25830853	-0.62705089	H	-7.64636528	1.97031272	-1.19575087
I	-2.81621437	1.00283354	4.00524778	I	-3.11487247	1.20209787	3.44900882
I	-3.58318326	3.70809458	2.34636793	I	3.04070855	7.10138684	6.21397324

TS-1

Charge = 0

Spin-state = 1

Electronic energy = -14377.724707 au.

Free energy Correction = 191.0011 Kcal

Solvation free energy = -26.82 Kcal

Spin-orbit correction = 20.55 Kcal

Imaginary frequency = -10.84 cm⁻¹

Ru	-0.00783270	-0.06992856	-0.76666171
N	1.98758395	-0.51670934	-0.71102153
C	2.75526274	0.27768158	0.10208233
C	4.14003127	0.12418571	0.15701061
C	4.76445464	-0.84402301	-0.62747381
C	3.97074468	-1.64362284	-1.46265701
C	2.59873254	-1.44914075	-1.47872156
C	6.24900333	-0.96682283	-0.53773624
O	6.94629668	-0.28851644	0.18854766
O	6.73586734	-1.92984641	-1.36322974
N	0.65001063	1.25478107	0.66728229
C	-0.12133161	2.10876507	1.37882641
C	0.39323265	2.99112481	2.31714021
C	1.77788891	3.00080720	2.54024194
C	2.57862163	2.11749070	1.82036621
C	2.00318736	1.25431602	0.88871093
C	2.44184232	3.90304098	3.53460432
O	1.56810051	4.79122431	4.04775554
O	3.61748445	3.82810995	3.83249957
N	-0.65895011	-1.36224413	0.68127891
C	-2.01248884	-1.36032210	0.91380117
C	-2.58233604	-2.21823775	1.85322958
C	-1.77758112	-3.09563412	2.57765075
C	-0.39480727	-3.08651416	2.33772551
C	0.11594569	-2.21568950	1.39079118
C	-2.43515741	-3.99539092	3.56846463
O	-3.62989584	-4.01665310	3.78210080
O	-1.54119218	-4.79389945	4.20978707
N	-2.00038855	0.38909035	-0.70446504
C	-2.60929094	1.32675433	-1.46679091
C	-3.97794591	1.54236964	-1.42831768
C	-4.77011994	0.75813453	-0.57739855
C	-4.14805524	-0.21457482	0.20268018
C	-2.76657548	-0.38696559	0.12722467
C	-6.25170459	0.90328210	-0.46363244
O	-6.73377865	1.88628742	-1.26643865
O	-6.94771739	0.22303169	0.26182376
N	0.39401853	1.29413014	-2.15889568
C	0.67804689	2.14156746	-2.94742278
S	1.03010590	3.29437884	-4.01598148
N	-0.41079880	-1.46337131	-2.13085358
C	-0.67325459	-2.35793272	-2.87308009
S	-0.99712505	-3.57384922	-3.88016198
H	4.75786309	0.75255306	0.79680943

H	4.41651765	-2.40263812	-2.10204358
H	1.93935836	-2.03031734	-2.12045218
H	7.70528208	-1.92497483	-1.23516845
H	-1.18838236	2.07464939	1.16829047
H	-0.27190520	3.65395910	2.87331603
H	3.65136193	2.12173979	2.00922062
H	2.03717735	5.32232060	4.72123664
H	-3.65489663	-2.22306777	2.04167773
H	0.27176980	-3.75536089	2.87795197
H	1.18015712	-2.18783141	1.16571303
H	-2.06760633	-5.33784009	4.82882759
H	-1.95127515	1.89611721	-2.12038021
H	-4.42235736	2.30788812	-2.06083730
H	-4.76551043	-0.82665802	0.85851526
H	-7.70037758	1.90229542	-1.11921793
I	-1.92374123	5.30514879	5.53316670

TS-2

Charge = 0
Spin-state = 1/2
Electronic energy = -21495.343161 au.
Free energy Correction = 186.7384 Kcal
Solvation free energy = -43.59 Kcal
Spin-orbit correction = 33.17 Kcal
Imaginary frequency = -28.29 cm⁻¹

Ru	0.01485321	-0.06036141	-0.92241581
N	1.99895437	-0.52973254	-0.86402254
C	2.78598884	0.28472232	-0.08595737
C	4.16872760	0.11158674	-0.03579991
C	4.77352047	-0.89991701	-0.78244816
C	3.95837676	-1.72256345	-1.57726947
C	2.59152532	-1.50442111	-1.59519687
C	6.24992833	-1.04479443	-0.70645047
O	6.98550548	-0.34218570	-0.04018210
O	6.71419482	-2.07207666	-1.47730664
N	0.71146498	1.36146048	0.38611573
C	-0.04848699	2.24514944	1.06311815
C	0.45959603	3.06720613	2.05885958
C	1.82342416	2.99929994	2.36543354
C	2.62121839	2.11260638	1.64628084
C	2.05407135	1.30004506	0.66620349
C	2.42900956	3.74144571	3.52334972
O	1.54301725	4.57223164	4.08146413
O	3.57365824	3.54957114	3.89293543
N	-0.59596204	-1.16177218	0.67725324
C	-1.93522334	-1.08931354	0.97849876
C	-2.46815207	-1.76734622	2.07223570
C	-1.64129578	-2.53216318	2.89265375
C	-0.27257772	-2.58808693	2.58798191
C	0.20094056	-1.90299053	1.48401742
C	-2.25136044	-3.22873092	4.05370879

TS-3

Charge = 0
Spin-state = 1/2
Electronic energy = -21495.342701 au.
Free energy Correction = 184.9966 Kcal
Solvation free energy = -43.40 Kcal
Spin-orbit correction = 33.33 Kcal
Imaginary frequency = -19.40 cm⁻¹

Ru	0.02606229	0.02063905	-0.70231298
C	2.85198463	2.18699200	1.63804509
C	2.18977023	1.32825853	0.76068738
N	0.83079842	1.39989627	0.59129937
C	0.14304218	2.32866718	1.29170692
C	0.74740517	3.20968827	2.17561439
C	2.13470203	3.13938769	2.35718838
C	2.84404571	0.26923780	-0.00493601
N	1.98840608	-0.52850413	-0.72584371
C	2.50597947	-1.54215134	-1.46172932
C	3.86239212	-1.81459608	-1.50398358
C	4.74687824	-1.01044593	-0.76648025
C	4.21924796	0.04018666	-0.01533974
N	0.39663360	1.25664013	-2.23641722
C	0.58526209	1.97421586	-3.16726092
S	0.81803934	2.96509973	-4.42237151
C	6.21832881	-1.21570726	-0.75407048
O	7.01041352	-0.53553732	-0.13095921
C	2.87669973	4.01705967	3.33267089
O	2.06448387	4.93081837	3.85800654
N	-1.92704467	0.58208680	-0.55075140
C	-2.68122826	-0.12868316	0.35009903
C	-4.04832692	0.10615405	0.48731049
C	-4.66947504	1.07936709	-0.29395399
C	-3.88713700	1.80262038	-1.20890171
C	-2.53472859	1.52394432	-1.31071426

O	-3.44115431	-3.24628036	4.30301008	C	-1.92181206	-1.08946547	1.14331278
O	-1.32387766	-3.86642954	4.82282283	N	-0.57756280	-1.14111806	0.84298830
N	-1.96139255	0.42778687	-0.85661648	C	0.20846660	-1.96639679	1.58018785
C	-2.58806623	1.26844123	-1.71452153	C	-0.27802300	-2.76014424	2.60064441
C	-3.95117410	1.50365844	-1.66286178	C	-1.65232638	-2.72921832	2.89985111
C	-4.72593513	0.84331458	-0.69514221	C	-2.46660704	-1.87515807	2.15545505
C	-4.08537583	-0.02679653	0.18667153	C	-6.13021264	1.29329153	-0.11717457
C	-2.70868826	-0.22319276	0.09408398	O	-6.60856927	2.29415053	-0.90905590
C	-6.19622979	1.01585186	-0.56940428	C	-2.27709887	-3.55102562	3.96314258
O	-6.69324638	1.92017311	-1.46272462	O	-3.46479302	-3.56172176	4.22769942
O	-6.89956238	0.42805081	0.22950212	N	-0.52872063	-1.42823245	-1.98158796
N	0.39030612	1.14961866	-2.47795875	C	-0.77928378	-2.35013445	-2.69053931
C	0.58007240	1.89957617	-3.38192056	S	-1.09544478	-3.61395020	-3.65100936
S	0.80998910	2.92857651	-4.60913490	O	-6.83659913	0.65708448	0.64087121
N	-0.43397679	-1.57706996	-2.16194619	O	-1.36630003	-4.31708999	4.63399104
C	-0.63714630	-2.52408724	-2.85243061	O	6.60419196	-2.27084527	-1.52975988
S	-0.88820130	-3.82051910	-3.78933452	O	4.05994406	3.85749994	3.57797033
H	4.79526417	0.76224593	0.57219134	H	4.90039170	0.67529383	0.54882096
H	4.38570876	-2.51653653	-2.18573270	H	4.22828147	-2.63669954	-2.11520918
H	1.91752613	-2.10205601	-2.20592897	H	1.78051794	-2.12267476	-2.02861082
H	7.68289807	-2.06328841	-1.34941608	H	7.57753036	-2.30045396	-1.44821121
H	-1.10710160	2.25709389	0.81460032	H	-0.93330112	2.35183401	1.13289310
H	-0.20344401	3.72243121	2.61762222	H	0.13294191	3.91709810	2.73691131
H	3.67604673	2.04214729	1.91060316	H	3.92829624	2.12782935	1.79862249
H	1.80383778	4.78832966	5.02708431	H	-3.52933430	-1.83597801	2.38961380
H	-3.52646600	-1.70143230	2.31850654	H	0.40035186	-3.40446066	3.15572931
H	0.41545379	-3.15772876	3.20855709	H	1.26249209	-1.97774534	1.31105253
H	1.25349742	-1.93281755	1.21094100	H	-1.88913191	-4.80036228	5.30314236
H	-1.83118913	-4.25463692	5.56211195	H	-1.88661133	2.04096674	-2.01586660
H	-1.94491441	1.74113675	-2.45436902	H	-4.32907896	2.56910528	-1.84162427
H	-4.40774965	2.18620204	-2.37629095	H	-4.65283681	-0.45619323	1.19713984
H	-4.68141860	-0.54309698	0.93727832	H	-7.56237843	2.34834253	-0.70354021
H	-7.65372854	1.94778353	-1.28511854	H	2.50057040	5.44531768	4.60561007
I	-1.33798503	1.41261441	4.76686564	I	2.61850657	6.76107110	6.64791758
I	1.33374396	4.68983706	7.43551247	I	-2.02265387	4.59077569	4.64805567

TS-4

Charge = 0
Spin-state = 1/2
Electronic energy = -21495.350669 au.
Free energy Correction = 184.4405 Kcal
Solvation free energy = -45.66 Kcal
Spin-orbit correction = 30.58 Kcal
Imaginary frequency = --4.42 cm⁻¹

Ru	0.00775696	-0.11337982	-0.79944364
N	2.00622984	-0.50807956	-0.75285111
C	2.75045090	0.26994007	0.10659101
C	4.13246464	0.11433149	0.19991744
C	4.78885510	-0.82917831	-0.59152198
C	4.01881462	-1.60068508	-1.48454055
C	2.65042690	-1.40854675	-1.53665159

TS-5

Charge = 0
Spin-state = 1/2
Electronic energy = -21495.350212 au.
Free energy Correction = 183.4019 Kcal
Solvation free energy = -7.79 Kcal
Spin-orbit correction = 29.67 Kcal
Imaginary frequency = -8.94 cm⁻¹

Ru	0.00238373	-0.12260726	-0.88408776
C	2.65702486	2.10630459	1.57830596
C	2.06067247	1.21906726	0.68403651
N	0.70687907	1.27430724	0.42146281
C	-0.02430636	2.23311042	1.04368545
C	0.51535166	3.13544681	1.93958860
C	1.89457518	3.07721443	2.22613597

C	6.25710133	-0.95961752	-0.45634523	C	2.77737799	0.17804377	-0.03917935
O	6.95218295	-0.31522896	0.30940334	N	1.98468197	-0.59983984	-0.85435661
O	6.78019018	-1.90405921	-1.29671049	C	2.57318642	-1.56535811	-1.60304233
N	0.62272648	1.23128774	0.61275739	C	3.93069830	-1.82513353	-1.55415118
C	-0.16428474	2.09995344	1.29638866	C	4.74831548	-1.05599705	-0.70236046
C	0.31829338	2.97180034	2.25639980	C	4.15074709	-0.04532090	0.05068478
C	1.69854562	2.97072147	2.53806259	N	0.33749794	1.13760117	-2.41186369
C	2.51786718	2.09047832	1.83320166	C	0.47885391	1.91901726	-3.29770049
C	1.97435063	1.23108155	0.88003466	S	0.64767474	2.99303896	-4.49655624
C	2.32982723	3.85615687	3.55003735	C	6.21033304	-1.25624203	-0.57264800
O	1.42075107	4.64835357	4.17440973	O	6.94330290	-0.61418434	0.15801275
O	3.52211814	3.87867596	3.80443261	C	2.57600266	3.98886412	3.17731158
N	-0.55649842	-1.44511070	0.62985405	O	1.71744963	4.88418504	3.74191208
C	-1.90028764	-1.45495448	0.94555130	N	-1.97449453	0.36647714	-0.73924396
C	-2.41412285	-2.34993504	1.88039589	C	-2.68694055	-0.30139612	0.23263678
C	-1.57467995	-3.26152366	2.52330596	C	-4.04915784	-0.06356435	0.41321207
C	-0.20307071	-3.24192286	2.19461748	C	-4.71694244	0.84893791	-0.40272171
C	0.25190007	-2.33708243	1.25679205	C	-3.98194023	1.50602148	-1.40998000
C	-2.16563524	-4.19581544	3.50345315	C	-2.63229968	1.23593845	-1.54537386
O	-3.34661848	-4.25246269	3.79868401	C	-1.90223631	-1.24456052	1.01567196
O	-1.23179124	-5.02276875	4.07063595	N	-0.57136962	-1.32752118	0.65315958
N	-1.98625726	0.30397859	-0.65792480	C	0.21922378	-2.20030044	1.32839072
C	-2.64240572	1.25235002	-1.36864460	C	-0.23590054	-2.98998717	2.36469289
C	-3.99450684	1.50157877	-1.20842027	C	-1.59195514	-2.90580506	2.74980280
C	-4.72909393	0.73362214	-0.28772278	C	-2.41476717	-2.02006249	2.05310004
C	-4.06316430	-0.25986930	0.42716252	C	-6.16372966	1.06794911	-0.17091950
C	-2.69722160	-0.46393554	0.23376295	O	-6.70109127	1.97837727	-1.03716829
C	-6.18118382	0.92448443	-0.03568218	C	-2.18287909	-3.70401642	3.84300812
O	-6.69672829	1.97206368	-0.73844224	O	-3.34783157	-3.65541140	4.19961136
O	-6.85305028	0.23243864	0.70547098	N	-0.46616250	-1.58747160	-2.17952783
N	0.33472155	1.24473399	-2.24111763	C	-0.68199574	-2.51431543	-2.89301182
C	0.53183345	2.03076855	-3.11223631	S	-0.95094803	-3.78341986	-3.86208376
S	0.77686090	3.11477100	-4.28811135	O	-6.82700643	0.51467706	0.68800723
N	-0.37077444	-1.51214123	-2.19543362	O	-1.27049911	-4.53159421	4.44173409
C	-0.51435126	-2.40894063	-2.96310349	O	6.67471044	-2.26248178	-1.37346818
S	-0.68507095	-3.63646626	-4.00641789	O	3.76495588	3.95291321	3.43857526
H	4.72432247	0.72585050	0.87931917	H	4.78124389	0.56405076	0.69659104
H	4.48540295	-2.33601452	-2.13625174	H	4.35226355	-2.61220839	-2.17536517
H	2.01239189	-1.97151550	-2.21560103	H	1.89922933	-2.12589401	-2.24843162
H	7.74045354	-1.88893810	-1.11777828	H	7.63645605	-2.29113327	-1.20389368
H	-1.22291632	2.08134623	1.04704595	H	-1.08265791	2.25459856	0.79194003
H	-0.36886559	3.64370513	2.77288171	H	-0.12186435	3.87994547	2.41191136
H	3.58545514	2.09239927	2.04914117	H	3.72438761	2.06165997	1.79077558
H	1.92666708	5.18862012	4.81172961	H	-3.46333652	-1.95359990	2.33997567
H	-3.47488150	-2.35828669	2.12663353	H	0.44752899	-3.66887508	2.86981187
H	0.49384132	-3.93281325	2.66390225	H	1.25493339	-2.24780667	0.99815149
H	1.30050552	-2.30411818	0.96827139	H	-1.77754643	-4.99555528	5.13592213
H	-1.74282676	-5.58065104	4.68854705	H	-2.02115431	1.71019119	-2.31128946
H	-2.02797903	1.81147044	-2.07214642	H	-4.46102057	2.21415100	-2.08232874
H	-4.47266237	2.28537495	-1.79147345	H	-4.61700487	-0.58508452	1.18235589
H	-4.63138411	-0.85722470	1.13846679	H	-7.64406539	2.03356176	-0.78761517
H	-7.63505718	2.02086884	-0.47051837	H	2.26011630	5.42528628	4.34900009
I	-5.06675896	4.36115211	3.83389772	I	2.38101957	10.73579477	8.65967512
I	-2.47804341	5.84909724	4.25126560	I	0.98046438	8.28594267	9.46555519