

SUPPORTING INFORMATION

A DFT Study on the Molecular Mechanism of the [4 + 2] Cycloaddition between Thiobenzophenone and Arylalkenes *via* Radical Cations

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S6-S24. UB3LYP/6-31G* computed total energies, unique imaginary frequencies, and cartesian coordinates of the stationary points involved in the cycloadditions between **1** and **2a-c** *via* RC.

Table S1. B3LYP/6-31G* total (E, in au) and relative^a (ΔE , in kcal/mol) energies, zero point vibrational energies (ZPE, not scaled, in au) and total (E_{ZPE} , in au) and relative^a (ΔE_{ZPE} , in kcal/mol) ZPE corrected energies of the stationary points involved in the cycloadditions between **1** and **2a** and **1** and **2a-c** *via* RC.

	E	ΔE	ZPE	E_{ZPE}	ΔE_{ZPE}
1	-899.588080		0.189571	-899.398509	
2a	-348.968043		0.161956	-348.806087	
TS_{GS}	-1248.511308	28.1	0.352941	-1248.158367	29.0
3a	-1248.533389	14.3	0.356049	-1248.177340	17.1
1^{•+}	-899.314023	172.0	0.189288	-899.124735	171.8
2a^{•+}	-348.691211	173.7	0.161587	-348.529624	173.5
MCa	-1248.311592	-20.3	0.352914	-1247.958678	-19.2
TS1a	-1248.311833	-20.4	0.353172	-1247.958661	-19.2
INa	-1248.312633	-20.9	0.353723	-1247.958910	-19.3
TS2a	-1248.298269	-11.9	0.354684	-1247.943585	-9.7
3a^{•+}	-1248.314685	-22.2	0.356712	-1247.957973	-18.7
2b	-463.490844		0.194735	-463.296109	
2b^{•+}	-463.236849	159.4	0.195022	-463.041827	159.6
MCb	-1362.844635	-12.4	0.385960	-1362.458675	-11.5
TS1b	-1362.843901	-11.9	0.386268	-1362.457633	-10.9
INb	-1362.844286	-12.1	0.386827	-1362.457459	-10.7
TS2b	-1362.827950	-1.9	0.387690	-1362.440260	0.0
3b^{•+}	-1362.839802	-9.3	0.389137	-1362.450665	-6.5
2c	-482.935048		0.235118	-482.699930	
2c^{•+}	-482.705663	143.9	0.236129	-482.469534	144.6
MCc	-1382.304568	-6.8	0.426491	-1381.878077	-6.3
TS1c	-1382.300562	-4.3	0.427140	-1381.873422	-3.4
INc	-1382.301178	-4.7	0.427846	-1381.873332	-3.3
TS2c	-1382.282620	7.0	0.428684	-1381.853936	8.9
3c^{•+}	-1382.291469	1.4	0.429978	-1381.861491	4.1

^a Relative to **1**, **2a-c**, **1 + 2a** or **1 + 2a-c^{•+}**.

Table S2. B3LYP/6-311+G*//B3LYP/6-31G* total (E, in au) and relative^a (ΔE , in kcal/mol) energies of the stationary points involved in the cycloadditions between **1** and **2a** *via* RC.

	E	ΔE
1	-899.721132	
1^{•+}	-899.439683	176.6
2a	-349.043947	
2a^{•+}	-348.758101	179.4
MCa	-1248.510624	-19.7
TS1a	-1248.510078	-19.4
INa	-1248.510737	-19.8
TS2a	-1248.495702	-10.3
3a^{•+}	-1248.511612	-20.3

^a Relative to **1**, **2** or **1** + **2^{•+}**.

Table S3. Lengths of the C—S and C—C forming bonds (in Angstroms), S^2 values of RCs, imaginary frequency of TSs and lowest vibrational frequency of the molecular complexes, intermediates and cycloadducts (in cm^{-1}) of the stationary points involved in the cycloadditions between **1** and **2a** and **1** and **2a-c** via RC.

	C-S	C-C	S^2	frequency
TS_{GS}	2.11	2.28		-378.157
3a	1.78	1.54		28.328
MCa	2.82	3.85	0.7501	6.956
TS1a	2.29	3.54	0.7503	-120.207
INa	2.01	4.76	0.7504	13.669
TS2a	1.91	2.16	0.7502	-338.696
3a^{•+}	1.86	1.59	0.7502	11.425
MCb	2.92	3.88	0.7502	5.209
TS1b	2.22	4.85	0.7501	-133.091
INb	2.02	4.81	0.7502	12.473
TS2b	1.91	2.11	0.7501	-333.372
3b^{•+}	1.87	1.60	0.7659	16.976
MCc	3.21	4.07	0.7501	2.799
TS1c	2.20	4.92	0.7501	-171.421
INc	2.00	5.13	0.7502	11.343
TS2c	1.91	2.11	0.7501	-340.074
3c^{•+}	1.87	1.62	0.7602	19.990

UB3LYP/6-31G* computed total energies, unique imaginary frequencies, and cartesian coordinates of the stationary points involved in the cycloadditions between **1** and **2a-c** via RC.

1

E(UB+HF-LY) = -899.588079551 A.U.

C	0.000000000000	0.000000000000	0.000000000000
S	0.000000000000	0.000000000000	1.659252550000
C	1.272385163387	0.000000000000	-0.763971514091
C	1.383892738462	-0.708753240436	-1.976859130796
C	2.412611189539	0.659869742849	-0.267485312415
C	2.597402870662	-0.765238170831	-2.659975693552
H	0.522606699482	-1.240959588476	-2.366923994026
C	3.615743902344	0.622060660190	-0.964058291313
H	2.334070147700	1.205578274406	0.666828912868
C	3.714696467057	-0.094770443610	-2.160402041383
H	2.669097121796	-1.334351765522	-3.582799581770
H	4.480453492629	1.151364400837	-0.573324301947
H	4.657980129849	-0.129875518472	-2.698858260103
C	-1.272391847575	0.002864869547	-0.764310692893
C	-1.382132692056	0.712440012766	-1.976875988361
C	-2.413874329109	-0.655698236865	-0.268854685246
C	-2.595299251800	0.771482828604	-2.660456776723
H	-0.519788440676	1.243417022346	-2.366253226766
C	-3.616596467229	-0.615674416712	-0.965980337664
H	-2.336644141241	-1.202122473896	0.665128953169
C	-3.713950167771	0.102267665961	-2.161817276124
H	-2.665656208061	1.341515254315	-3.582825577330
H	-4.482298759005	-1.143930529491	-0.576020362843
H	-4.657005217439	0.139331981525	-2.700551810377

2a

E(UB+HF-LY) = -348.968043492 A.U.

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.394185010000
C	1.200078849180	0.000000000000	2.126723946230
C	2.408438093757	-0.000189788000	1.404281651672
C	2.410948105501	-0.000281867952	0.012677438348
C	1.207204398734	-0.000213138262	-0.698916776432
H	-0.943795083054	0.000000000000	-0.539230039379
H	-0.945737521068	0.000231726396	1.931845869441
H	3.355961115647	-0.000251925437	1.935479711061
H	3.357626331571	-0.000428471375	-0.521712365151
H	1.213187642263	-0.000214194635	-1.785525083645
C	1.132340728164	0.000147635540	3.596428524915
C	2.152929768731	0.000031404763	4.466836590367
H	0.119644553609	0.000169430480	4.002936440356
H	3.179168528800	-0.000005187929	4.099291311138
C	1.996806201241	0.000136252305	5.958931298642
H	0.941971232085	-0.000609081228	6.253590654603
H	2.476646427967	-0.879492810547	6.410115775934
H	2.475323435203	0.880610318125	6.409888444909

TS_{Gs}

E(UB+HF-LY) = -1248.51130783 A.U.

1 imaginary frequencies -378.1573 cm⁻¹

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.424398150000
C	1.179459653640	0.000000000000	2.124514995749
C	2.419938514235	-0.062259552641	1.426637373227
C	2.450668662161	-0.148362234336	0.059823291284
C	1.239993056396	-0.163778415660	-0.712626300883
H	-0.951933801731	0.027564860735	1.949229321729
H	1.175359419764	0.027925302508	3.211040490359
H	3.350421142654	-0.038382214062	1.987256617086
H	3.403194888701	-0.173694406307	-0.456602501701
C	1.237043457502	-0.163526104688	-2.129559978365
S	-0.227131974883	0.197363266287	-2.948596046484
C	-0.599363481657	2.106762094885	-0.627116338325
H	-1.384060325689	2.070840719193	0.124818671402
C	-1.034493249620	1.891802683931	-1.984909532318
H	-0.905985529298	-0.299191450941	-0.518883551669
H	-0.615020945547	2.607627664170	-2.691929379475
C	2.446093685719	-0.423217286076	-2.949276992073
C	3.278788223235	-1.520815244224	-2.657160577547
C	2.770087870662	0.372391752832	-4.064034166016
C	4.402450268044	-1.796790325564	-3.435349747866
H	3.024165197114	-2.173809576499	-1.827853663012
C	3.896675535259	0.100020189161	-4.835092302191
H	2.125478104257	1.207104493664	-4.321282453362
C	4.720765125826	-0.985196460106	-4.524847559107
H	5.023617774253	-2.655521425407	-3.194089290864
H	4.132153966102	0.737061372803	-5.683772033015
H	5.595831251303	-1.200193789642	-5.132133348759
C	0.549933514749	2.933984603761	-0.284818986672
C	0.671302092750	3.453870206631	1.022104174558
C	1.573970470567	3.236048496816	-1.208867082033
C	1.758368790068	4.242307378105	1.386548558894
H	-0.106494658309	3.236503933168	1.749835183584
C	2.662660948515	4.020767001436	-0.839157927065
H	1.520729113563	2.848410507638	-2.221559101596
C	2.762707051432	4.529516244285	0.458490750673
H	1.822541629455	4.636161872434	2.397829496332
H	3.438360635349	4.237857841980	-1.569176861144
H	3.611395959007	5.146150596294	0.741762122432
C	-2.526540136025	1.677322569959	-2.184546307777
H	-2.900333891927	0.881554563345	-1.530972732464
H	-3.072194237460	2.598533749251	-1.944200427619
H	-2.764171673525	1.403332201168	-3.217687508671

3a

E(UB+HF-LY) = -1248.53338851 A.U.

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.519942600000
C	1.178731982878	0.000000000000	2.171149944524
C	2.426434602400	0.141795408824	1.434196180845
C	2.416855896591	0.582979950894	0.151802699017
C	1.142498774317	0.876025949581	-0.508587565756
H	-0.934492810234	-0.119217362642	2.056742163122
H	1.215000928572	-0.096008434665	3.253885577398
H	3.369409910808	-0.031776944648	1.946452189520

H	3.345842834908	0.809684646715	-0.362081999496
C	1.035829144320	1.836778466273	-1.462028152795
S	-0.509093015834	2.417264219344	-2.118575252210
C	-1.370927898491	0.191036977205	-0.721691838826
H	-1.237904910956	-0.228515767035	-1.726821387487
C	-1.720496045923	1.679079896141	-0.939608824103
H	0.306594978461	-1.028725319403	-0.273344065909
H	-1.617187594959	2.230022074722	0.003788091584
C	2.195919583229	2.576839432335	-2.039142071799
C	2.475061298543	2.492906293851	-3.413022889058
C	3.004265750412	3.398745074586	-1.237480235676
C	3.541891314184	3.200408496859	-3.966841424914
H	1.856253086184	1.861574851294	-4.044768014296
C	4.071641219804	4.104653076833	-1.792754100876
H	2.785235267149	3.485727191690	-0.177646367040
C	4.344224921190	4.007666486542	-3.158442435718
H	3.747385349801	3.118292819884	-5.030913898304
H	4.687121747483	4.736096031626	-1.157251361655
H	5.174913587333	4.559428105973	-3.590349953754
C	-2.475321924576	-0.630714836801	-0.062878214447
C	-2.734334656148	-1.925217123631	-0.534031043333
C	-3.242238017029	-0.159752050405	1.014950382442
C	-3.715729844274	-2.727312944674	0.050125873107
H	-2.158023890045	-2.309685398595	-1.372957833383
C	-4.229417412059	-0.954885437314	1.598960081753
H	-3.072502218324	0.841254368384	1.403335809882
C	-4.469135736507	-2.243932340166	1.120148639978
H	-3.894619731636	-3.727379667953	-0.336207251228
H	-4.811599392876	-0.564503961817	2.429681721830
H	-5.237722297568	-2.863243827357	1.574518999112
C	-3.104717659117	1.928732079472	-1.549350637661
H	-3.230394007923	1.359971298604	-2.477240233206
H	-3.895245965952	1.625596723355	-0.858399050607
H	-3.242546730098	2.990865875703	-1.779274751320

$1^{\bullet+}$

E(UB+HF-LY) = -899.314023092 A.U.

C	0.000000000000	0.000000000000	0.000000000000
S	0.000000000000	0.000000000000	1.690592020000
C	1.308226939654	0.000000000000	-0.638968533750
C	1.519118689054	-0.786459085863	-1.798766155483
C	2.401309957706	0.705913922831	-0.067050467299
C	2.785013252892	-0.861888860310	-2.361783362049
H	0.699034406423	-1.359402753776	-2.217678669094
C	3.659421630386	0.628954875701	-0.647993726212
H	2.235749372257	1.353301788727	0.788067372407
C	3.854654745173	-0.156284442924	-1.789535892501
H	2.947709851559	-1.473323108876	-3.243592935269
H	4.485817492039	1.189313241554	-0.223082968814
H	4.840628746798	-0.216854485052	-2.240473272462
C	-1.252350958134	-0.023183394219	-0.724288582804
C	-1.337900950828	0.606309551628	-1.992318464154
C	-2.419423430118	-0.599238058313	-0.155504866028
C	-2.553112084335	0.658484454783	-2.660710310554
H	-0.462043006628	1.084976607066	-2.416545797088
C	-3.624589970481	-0.548529829885	-0.838377373164
H	-2.353667874908	-1.128180674496	0.790374586212
C	-3.694629368450	0.081778398790	-2.087844792816
H	-2.618702710461	1.153942656001	-3.624015128821
H	-4.508939099320	-1.009229281724	-0.410351691811

H	-4.641279376613	0.121061739232	-2.618507156945
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2a^{•+}

E(UB+HF-LY) = -348.691211441 A.U.

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.378019820000
C	1.232430416840	0.000000000000	2.111131483889
C	2.466602436726	0.000000000000	1.378078854432
C	2.455808906532	0.000000000000	0.001217980269
C	1.227209038225	0.000000000000	-0.694929613183
H	-0.934795215974	0.000000000000	-0.550695912001
H	-0.936441122323	0.000000000000	1.928090093041
H	3.413964055794	0.000000000000	1.905335747323
H	3.388547143790	0.000000000000	-0.553024527024
H	1.228293582606	0.000000000000	-1.781092561719
C	1.162198365069	0.000000000000	3.531268211408
C	2.233551502900	0.000000000000	4.411340524152
H	0.164339826070	0.000000000000	3.966925893876
H	3.248802460303	0.000000000000	4.018946944082
C	2.097340298649	0.000000000000	5.882328793335
H	1.058588640139	0.000333327806	6.219522072735
H	2.618356845785	-0.873074292998	6.305107738604
H	2.618991446455	0.872634704575	6.305213659565

MCa

E(UB+HF-LY) = -1248.31159163 A.U.

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.389991210000
C	1.210700690997	0.000000000000	2.092242231196
C	2.423996248684	-0.021580757004	1.398752548307
C	2.432136179373	-0.056385434080	0.007592156190
C	1.217607518946	-0.036712460885	-0.714732087509
H	-0.941891528665	-0.010885039959	1.930194125215
H	1.206769658458	0.007116951060	3.178282238116
H	3.363391214323	-0.018207592093	1.943130187415
H	3.375078023504	-0.065337333081	-0.528736684959
C	1.235308256550	-0.027636657446	-2.181018775696
S	0.097380637712	0.852240378961	-3.053204363278
C	0.394240724924	3.600738147031	-1.309953156216
H	0.437462032535	3.392803004111	-0.241346890077
C	-0.785830804290	3.298972000320	-1.955275305291
H	-0.936667613612	-0.027703989578	-0.547049220775
H	-0.888362683260	3.541942548019	-3.010566730980
C	2.233209186477	-0.808246707284	-2.913064342097
C	2.683189469921	-2.044834660349	-2.391370056370
C	2.719777646779	-0.381312851037	-4.171057662643
C	3.580652241957	-2.825181981501	-3.110544106573
H	2.291987117531	-2.404118743255	-1.446000477329
C	3.630927738446	-1.158336005819	-4.872747372989
H	2.400476402722	0.576988926956	-4.566539518682
C	4.059422550669	-2.383136656192	-4.347991667736
H	3.903637137013	-3.781444299496	-2.710990949793
H	4.013826286476	-0.811675629753	-5.827526813343
H	4.766785928809	-2.992027699989	-4.903313813489
C	1.583265307516	4.179651216783	-1.880824932893
C	2.685753188259	4.425352261861	-1.024259250207
C	1.702735656463	4.532213154140	-3.250088716365
C	3.852710782041	4.998498386111	-1.509296145377

H	2.604568470555	4.164086001565	0.027544327105
C	2.871183184252	5.101750201193	-3.730044062308
H	0.874648133246	4.364144048733	-3.930958866965
C	3.949446480264	5.338548896460	-2.863821836630
H	4.686154482212	5.186360489202	-0.839591663278
H	2.949749984441	5.372778497064	-4.778393139119
H	4.859715851216	5.791292224103	-3.245607253733
C	-2.042934015700	2.916527050044	-1.243693756905
H	-1.848046563729	2.544460354254	-0.233991534363
H	-2.687659528362	3.803903869674	-1.156851989286
H	-2.614979598042	2.169599406033	-1.802447143337

TS1a

E(UB+HF-LY) = -1248.31183325 A.U.

1 imaginary frequencies -120.2067 cm⁻¹

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.389079560000
C	1.210821109523	0.000000000000	2.091256101311
C	2.424564536181	-0.008949073378	1.397950332324
C	2.433392226464	-0.029211851637	0.007108277260
C	1.218151400981	-0.016968561934	-0.717487716183
H	-0.941474811531	-0.016259968783	1.929606991698
H	1.206886622940	0.003520867463	3.177210146271
H	3.363664510580	0.000563189884	1.942485212741
H	3.376489857708	-0.017552201265	-0.528933779156
C	1.232510030113	-0.001282734267	-2.180693335336
S	0.059826607405	0.852339654092	-3.062512977530
C	-1.079802022340	3.501924975066	-3.140963231239
H	-0.461568973891	4.147696557413	-3.762868228820
C	-0.425062154001	2.852823009092	-2.060772875154
H	-0.936834025469	-0.040799020352	-0.546824336851
H	-1.054173669285	2.439731011478	-1.276956545904
C	2.237047749979	-0.754309176867	-2.923807688682
C	2.731558695944	-1.976577372028	-2.402440293372
C	2.699414191282	-0.321041750192	-4.190535754592
C	3.646544729319	-2.731218193740	-3.125241595702
H	2.358684062946	-2.345070744599	-1.453274806894
C	3.627952447269	-1.072769017307	-4.896024743380
H	2.347840467785	0.623855204522	-4.590037045812
C	4.100969347767	-2.280350409368	-4.368970352448
H	4.002206572504	-3.675248399988	-2.724395432389
H	3.991845172735	-0.718267334337	-5.855320118270
H	4.823153635764	-2.868639558735	-4.927336081028
C	-2.437120254652	3.345759925163	-3.542256735612
C	-2.901258340847	4.077230310125	-4.671343866983
C	-3.355946735109	2.489493379652	-2.873840576366
C	-4.212178368674	3.962536649820	-5.104372810433
H	-2.210061086598	4.734202905626	-5.192457215468
C	-4.663168592823	2.376048399257	-3.317233144965
H	-3.035364142808	1.917455666516	-2.009171006181
C	-5.098025383012	3.111175928230	-4.430498314916
H	-4.551820682348	4.529869992757	-5.965228190296
H	-5.355142883877	1.718429416025	-2.800170702223
H	-6.125410420367	3.020010274124	-4.770035956293
C	0.898841860178	3.403248135827	-1.590495315637
H	1.436871376872	2.700737928224	-0.951095586682
H	1.539721280377	3.688128697350	-2.430276391444
H	0.706595016089	4.304770135014	-0.993120578853

INa

E(UB+HF-LY) = -1248.31263329A.U.

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.388835360000
C	1.211292922088	0.000000000000	2.090536689469
C	2.425402719445	-0.017024804884	1.397153268041
C	2.434288160282	-0.040561010548	0.006913463462
C	1.218374053217	-0.022971039253	-0.718129820926
H	-0.941398880356	-0.012102700835	1.929426992308
H	1.207586524262	0.007888019766	3.176421944771
H	3.364358778719	-0.010148126833	1.941891340486
H	3.377034534299	-0.033212602929	-0.529969911478
C	1.232750412379	-0.019484473061	-2.177015081805
S	0.060127199952	0.846014885978	-3.079175735019
C	-1.025309072510	3.329013217687	-3.246082124951
H	-0.403270779363	3.982427803896	-3.854511739575
C	-0.340040763469	2.597598873880	-2.180984669475
H	-0.938383405598	-0.041088098436	-0.544442810203
H	-0.986123010944	2.319351646765	-1.348429698693
C	2.203961000188	-0.796799641587	-2.927595284831
C	2.695784040746	-2.016405833206	-2.391549959291
C	2.640870920116	-0.400779970499	-4.217514368016
C	3.578991144625	-2.800912925631	-3.120288090840
H	2.341521506860	-2.358392055083	-1.425636831402
C	3.535624009039	-1.185132733030	-4.930278078113
H	2.300081543842	0.542657312942	-4.629330692983
C	4.004506942790	-2.387583832697	-4.387569532967
H	3.931302490374	-3.740818265870	-2.707058615312
H	3.878589914291	-0.858984135200	-5.907126521101
H	4.701097233667	-3.000778066188	-4.951548737200
C	-2.386406011521	3.204372356091	-3.610332667356
C	-2.879793873382	3.971813370461	-4.707029143676
C	-3.298976583043	2.340815397646	-2.936402248658
C	-4.203364097050	3.881894534606	-5.101018988823
H	-2.197414035027	4.634979450307	-5.231842275966
C	-4.620282240381	2.253888290163	-3.343578960155
H	-2.961752328584	1.745518996369	-2.093823482491
C	-5.080015560654	3.022036288506	-4.423182185227
H	-4.562653670295	4.475711779419	-5.935777821244
H	-5.304317091319	1.591358505747	-2.822006815408
H	-6.118221726991	2.952038348934	-4.733326671440
C	0.954521028406	3.249838886586	-1.712293482396
H	1.491316551568	2.632308458320	-0.990368527572
H	1.617614670232	3.468752091888	-2.554994800631
H	0.706221950462	4.197514913296	-1.220486355574

TS2a

E(UB+HF-LY) = -1248.29826868 A.U.

1 imaginary frequencies -338.6962 cm⁻¹

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.423907700000
C	1.187194802048	0.000000000000	2.123863965917
C	2.418946788678	-0.048024080531	1.427755394466
C	2.449941641723	-0.138701804352	0.047703619917
C	1.245822258994	-0.162119064106	-0.703840094110
H	-0.949864195222	0.007560654485	1.950930770524

H	1.184071840269	0.020623748661	3.209421324176
H	3.350861063945	-0.019463297755	1.983958733400
H	3.401556492588	-0.156128189230	-0.471164974854
C	1.256695580984	-0.189264625940	-2.128677132558
S	-0.106055979629	0.381624956574	-3.021974210778
C	-0.515962547208	2.004341118911	-0.608004967273
H	-1.342940812490	2.017147433794	0.098323011660
C	-0.960714314355	1.770047981158	-2.024547437790
H	-0.902700179805	-0.342905096207	-0.499218963603
H	-0.685870740871	2.644304541147	-2.622761873103
C	2.348344383821	-0.749503082720	-2.923156633410
C	3.029874304582	-1.905311837010	-2.470555332033
C	2.715628543415	-0.193552224745	-4.171087258053
C	4.045283088440	-2.469302748315	-3.233063197974
H	2.725954467310	-2.377916532336	-1.542464733938
C	3.739721872920	-0.757903126639	-4.920971173458
H	2.212756889253	0.698466643616	-4.529331244697
C	4.406579292061	-1.896473682349	-4.456869016665
H	4.547609171659	-3.365162881505	-2.881315819832
H	4.023187746392	-0.308722521437	-5.867743827053
H	5.201712156087	-2.339023623931	-5.049339970443
C	0.566937275539	2.908233503709	-0.276920492832
C	0.616886666805	3.470038263886	1.021267337099
C	1.571305254378	3.274262323648	-1.204340791326
C	1.615479443280	4.369921669912	1.371753316683
H	-0.149031858551	3.203176255343	1.744634033416
C	2.568906432490	4.173134586753	-0.848502382363
H	1.560717206714	2.866196047749	-2.210616399192
C	2.595394465722	4.723906085133	0.438339026440
H	1.629197618491	4.803172431871	2.367190180388
H	3.325468030430	4.455049091926	-1.574587995585
H	3.373233967988	5.431546794855	0.709261132347
C	-2.466353572776	1.519201266312	-2.146860429269
H	-2.780177782458	0.647706139246	-1.562608036688
H	-3.012115944080	2.395911333350	-1.781644478803
H	-2.760687797303	1.352090403528	-3.187439666749

3a^{•+}

E(UB+HF-LY) = -1248.31468537 A.U.

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.492426740000
C	1.143353492735	0.000000000000	2.233599231152
C	2.409863477292	0.021770289738	1.586543141458
C	2.517493919529	-0.027934638235	0.199113562525
C	1.377720978971	-0.086411867630	-0.622278127066
H	-0.969691845522	0.020540257358	1.981743781744
H	1.097313708998	0.007711117643	3.317957247573
H	3.314207613367	0.073059010619	2.185565425580
H	3.501265502580	-0.012039543842	-0.257618480542
C	1.472552933622	-0.288854163376	-2.023917585932
S	0.099745539289	0.088317647940	-3.010448585860
C	-0.943012168680	1.155961261015	-0.563142338511
H	-1.954167291099	0.737871325866	-0.510340817232
C	-0.652274211053	1.491326672937	-2.045498320685
H	-0.518071357715	-0.922054427188	-0.318556370013
H	0.113649939119	2.270192700022	-2.088795508692
C	2.618464205868	-0.892032167008	-2.698356329594
C	3.344611459774	-1.944676698775	-2.089044741436
C	2.993959468937	-0.473906417011	-3.997544724052
C	4.410495900319	-2.541047873653	-2.750561816990

H	3.032929844845	-2.323059567839	-1.121281573802
C	4.069505644770	-1.067370935254	-4.645578630651
H	2.459924364249	0.342595191881	-4.472028101547
C	4.779584309852	-2.101519507586	-4.026481295689
H	4.946041452095	-3.359999796132	-2.280492987586
H	4.360404236903	-0.721633583224	-5.632549853406
H	5.615264800593	-2.568014007421	-4.539483679193
C	-0.927127911380	2.433775300804	0.267556887323
C	-2.107590965117	2.875591982794	0.879257528235
C	0.239495475927	3.198023335197	0.424899348231
C	-2.125206107248	4.051964740056	1.631808939122
H	-3.022972821900	2.299224554511	0.764455615191
C	0.224199796269	4.371043334595	1.178033910595
H	1.170413460877	2.878620171624	-0.038293210328
C	-0.959239247540	4.801971884935	1.782911847823
H	-3.050596849497	4.380283172526	2.095854425651
H	1.135492426622	4.951445462149	1.290057117248
H	-0.970967007978	5.718193791346	2.365664734718
C	-1.899504862472	1.959818758061	-2.798827203670
H	-2.658106827668	1.171222662330	-2.847576176251
H	-2.331880277745	2.817700752005	-2.274447024193
H	-1.658669196453	2.275052230374	-3.818381061174

2b

E(UB+HF-LY) = -463.490843778 A.U.

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.396552990000
C	1.184627147523	0.000000000000	2.146232760655
C	2.398429116779	-0.000688297667	1.427001014135
C	2.418411532931	-0.000805295159	0.042128135331
C	1.217548989363	-0.000387133461	-0.686967642555
H	-0.944535355263	0.000103783893	-0.532053965886
H	-0.954550970632	0.000387803339	1.918450679636
H	3.344031124003	-0.001734373686	1.961478262453
H	3.355458468528	-0.001586511659	-0.506337663291
C	1.105787378689	0.000581524529	3.613477044733
C	2.117724031271	0.007378418014	4.494522555879
H	0.089316132011	-0.004419873534	4.011179955068
H	3.147717577553	0.013389514435	4.137387090376
C	1.946175540677	0.007285012303	5.985327680582
H	0.887962489880	0.000954754465	6.268297588871
H	2.424671101420	-0.869718842706	6.443431011300
H	2.414068771619	0.890457252173	6.442480641643
O	1.350000225680	-0.000429247829	-2.046143637423
C	0.170952278302	-0.002198782888	-2.833739801657
H	0.504432344667	-0.004075208157	-3.873199340982
H	-0.438666432960	-0.896536035320	-2.647361860544
H	-0.439092465852	0.892576536632	-2.650809411325

2b^{•+}

E(UB+HF-LY) = -463.236848922 A.U.

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.372841950000
C	1.214251778109	0.000000000000	2.132812390432
C	2.453733325963	0.000347059839	1.411335798046
C	2.470997391516	0.000289511839	0.045019894835
C	1.244614336955	-0.000115031473	-0.689233989802
H	-0.935506417976	-0.000057010662	-0.546067099815

H	-0.946344087545	-0.000051362686	1.905841663208
H	3.395229880973	0.001092116613	1.948875573978
H	3.398840796483	0.000811418716	-0.516862924065
C	1.121071258439	-0.000402121923	3.555683049265
C	2.169614866480	-0.001678764772	4.446121140511
H	0.114390962275	0.000113231645	3.970553272178
H	3.192116557920	-0.003352552080	4.072339171941
C	2.012119784301	-0.001232122230	5.920807919971
H	2.517103060321	-0.876617869361	6.354689722254
H	2.518984902699	0.873587377325	6.353856641936
H	0.965913757691	0.000303173911	6.235840597303
O	1.377931384423	-0.000336406798	-1.999975901799
C	0.227110738042	-0.001730996521	-2.876736993439
H	0.641585004671	-0.003379686832	-3.882986972873
H	-0.369899048878	-0.902641831770	-2.712077446760
H	-0.369710187004	0.899830337655	-2.714867678222

MCb

E(UB+HF-LY) = -1362.84464459 A.U.

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.390560500000
C	1.210119200412	0.000000000000	2.092916350343
C	2.421888478664	-0.013460332273	1.397502018231
C	2.428577330022	-0.041715475459	0.005519864612
C	1.215227077815	-0.027403990320	-0.716216565374
H	-0.942190613600	-0.015031496812	1.930455515686
H	1.207060268576	0.001356652903	3.179054305591
H	3.362313900561	-0.010093655341	1.940459149005
H	3.371630760206	-0.046862640503	-0.530886365984
C	1.227610229903	-0.017163564832	-2.187557781937
S	0.089562651132	0.864418376144	-3.047582096615
C	0.270787886716	3.696112586679	-1.152788131089
H	0.296374399091	3.471575088627	-0.087128133876
C	-0.872496824802	3.343848944067	-1.835869188732
H	-0.936603315942	-0.026589932141	-0.547117459155
H	-0.958236956926	3.590715558644	-2.891327295805
C	2.230580563537	-0.807250757063	-2.911389326620
C	2.690448741412	-2.031971620506	-2.374032542134
C	2.708979264308	-0.400298082566	-4.177445938765
C	3.588609795426	-2.820733025133	-3.084968511217
H	2.307741022498	-2.378178604532	-1.420349369632
C	3.620995144433	-1.183569307472	-4.871850569140
H	2.375036882494	0.545419565024	-4.590582636215
C	4.059592878443	-2.397425768724	-4.330807953819
H	3.917378489492	-3.768892308384	-2.670752880521
H	3.994749678267	-0.850810532282	-5.835363294416
H	4.766808447446	-3.011757730160	-4.880411226739
C	1.429174191462	4.351521637749	-1.679446725958
C	2.487700081027	4.682115659617	-0.791614298173
C	1.579550796977	4.719624570989	-3.048942254291
C	3.622675031486	5.345233276216	-1.217635317108
H	2.395367079055	4.410409203721	0.256424909086
C	2.703683961656	5.374245775528	-3.487885097981
H	0.797489589000	4.485005934767	-3.763081043645
C	3.741960722970	5.703355917686	-2.578291506447
H	4.405705532764	5.586760396914	-0.509051444106
H	2.825098610221	5.662149366106	-4.526749350699
C	-2.121009264531	2.869447478616	-1.167619945224
H	-1.933496157512	2.509108685445	-0.152360599694
H	-2.834550513749	3.704801662086	-1.104550264905

H	-2.613886361966	2.081930018036	-1.745843609486
O	4.782760026717	6.348080481354	-3.109099098642
C	5.877012486503	6.758327987009	-2.275572087807
H	6.566814019227	7.276351360080	-2.940527232382
H	5.532093776753	7.441094886590	-1.492484639938
H	6.372217061535	5.888924263604	-1.830780433008

TS1b

E(UB+HF-LY) = -1362.84390116 A.U.

1 imaginary frequencies -133.0913 cm⁻¹

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.389256020000
C	1.210995374360	0.000000000000	2.090808458317
C	2.423565909453	-0.006274014688	1.395377579501
C	2.431138691300	-0.022376733908	0.004479542236
C	1.216184447219	-0.013630533570	-0.720682392027
H	-0.941498384131	-0.016585370840	1.929855072982
H	1.208476825152	0.002277103119	3.176794560578
H	3.363429965691	0.003852503868	1.938743792285
H	3.374217563369	-0.006796589441	-0.531457058066
C	1.226502802026	0.005051454410	-2.184646664637
S	0.024889793701	0.836045933646	-3.054445178053
C	-0.998240965763	3.476330017353	-3.230420906668
H	-0.362354720386	4.070273929166	-3.885104723075
C	-0.347951241818	2.822111104951	-2.141299791364
H	-0.937597747598	-0.039627249373	-0.545552185341
H	-0.982974864573	2.493603786450	-1.322111037036
C	2.246904781546	-0.718458981873	-2.936785901640
C	2.773326324928	-1.932233134455	-2.427460616279
C	2.694623253587	-0.267417964811	-4.202093204005
C	3.703766633966	-2.660011026391	-3.158539158205
H	2.413895699881	-2.316175865745	-1.479116732775
C	3.638300783559	-0.991916754579	-4.916488833675
H	2.316183943874	0.669548706497	-4.595653146330
C	4.143352121084	-2.191019422529	-4.400575266519
H	4.082987305301	-3.597871711213	-2.764580773624
H	3.988623927243	-0.622143090147	-5.875223776338
H	4.877092479299	-2.758091412277	-4.965770282542
C	-2.359360921752	3.370941552310	-3.594582896162
C	-2.825587148500	4.074035857045	-4.743619184721
C	-3.314923550526	2.588978331708	-2.874032369974
C	-4.142131483091	4.016067901815	-5.153713087961
H	-2.119279827038	4.675040049469	-5.309987409257
C	-4.625779717962	2.519955167223	-3.277725443916
H	-3.008527201663	2.037415113025	-1.991441030496
C	-5.061812773571	3.232859291123	-4.422307915493
H	-4.457903605602	4.567514188327	-6.031008642862
H	-5.356568590071	1.928194833600	-2.736756906579
C	0.997528140878	3.358185789292	-1.706341772670
H	1.519947344692	2.669948228010	-1.039225842564
H	1.639694654495	3.579304003380	-2.564393966202
H	0.839300382683	4.293324003910	-1.153349692570
O	-6.357335413594	3.097302837382	-4.722220253588
C	-6.903854127560	3.780437432548	-5.858523120660
H	-7.958594758118	3.508639292223	-5.878725366131
H	-6.802985873609	4.865002851697	-5.745939558360
H	-6.418150201423	3.448742475978	-6.782228184667

INb

E(UB+HF-LY) = -1362.84428589 A.U.

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.389249810000
C	1.209999974052	0.000000000000	2.092167915544
C	2.423242415903	-0.010811029946	1.397313150545
C	2.431689473070	-0.028370560153	0.006955547805
C	1.217132179692	-0.017919951662	-0.720573718215
H	-0.941975724310	-0.013442863257	1.929146384330
H	1.206335665581	0.004719405406	3.178085107977
H	3.362830975588	-0.001870867208	1.941204874588
H	3.374951613013	-0.014579840460	-0.528881132041
C	1.230507654934	-0.009470444104	-2.180920292745
S	0.018757898195	0.820699992357	-3.069216759370
C	-0.939648017287	3.336235566003	-3.334548394307
H	-0.279730408303	3.935047026112	-3.959425844065
C	-0.305742602051	2.627011934930	-2.229416368350
H	-0.938551344993	-0.040054621347	-0.544192558027
H	-0.973268560786	2.404292597839	-1.396858167719
C	2.230632206845	-0.745107703025	-2.939406807155
C	2.765685730127	-1.952270718473	-2.418481592037
C	2.657611212290	-0.320216433181	-4.222557847619
C	3.681352708912	-2.694457596871	-3.152285764687
H	2.421985304640	-2.318861219246	-1.457651231406
C	3.584520038382	-1.061667310515	-4.941223708752
H	2.278243346490	0.611574845943	-4.627096150984
C	4.097757561708	-2.251534173309	-4.412246528880
H	4.066362339762	-3.625346633298	-2.747484520735
H	3.916827593120	-0.710991403097	-5.913459795678
H	4.819174178532	-2.831314417345	-4.980309019481
C	-2.287091736851	3.248464847164	-3.721827958264
C	-2.733263162630	3.972945842084	-4.869252727953
C	-3.260068227358	2.457772402458	-3.029530937880
C	-4.041498711859	3.924256815386	-5.301791030512
H	-2.015485296963	4.580580208703	-5.413579744875
C	-4.563276635237	2.398966990143	-3.458306627625
H	-2.970830633163	1.892643906117	-2.149754196180
C	-4.976508737393	3.130747001237	-4.599068937497
H	-4.341119288180	4.490413529721	-6.175431819379
H	-5.305522744636	1.801288034448	-2.939905122126
C	1.009801877301	3.236984926149	-1.765085701372
H	1.508175385968	2.618558496050	-1.017179811778
H	1.693198522202	3.395577936871	-2.605250497225
H	0.801479007082	4.211025946432	-1.307149037928
C	-6.789373724587	3.704278363513	-6.062146853499
H	-6.687956411268	4.786871687217	-5.932307033709
H	-6.287321303106	3.384298560266	-6.981241618927
H	-7.844318820143	3.436080307617	-6.105853131265
O	-6.266261041639	3.003706038248	-4.925444513415

TS2b

E(UB+HF-LY) = -1362.82795045 A.U.

1 imaginary frequencies -333.3722 cm⁻¹

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.428140990000
C	1.183553877284	0.000000000000	2.128917100875
C	2.417451283343	-0.064856482020	1.432947012544
C	2.450493656582	-0.174975618849	0.055968253223

C	1.247181666803	-0.194920745167	-0.699996155521
H	-0.951171631574	0.019861202792	1.952854803485
H	1.180222212597	0.027278968514	3.214383618347
H	3.348794128272	-0.038992895210	1.990547031375
H	3.402939013555	-0.212925240940	-0.460338513856
C	1.257198454077	-0.241297341128	-2.120604756386
S	-0.117511628976	0.313345192643	-3.013774262158
C	-0.501426759457	1.955579915966	-0.606682912306
H	-1.336719187455	1.988767271983	0.089711933663
C	-0.947474039730	1.719158049507	-2.028435118058
H	-0.899114871127	-0.365123986191	-0.491261040347
H	-0.664622773075	2.589565768885	-2.627873059259
C	2.349492944531	-0.805243670642	-2.914574661042
C	3.032794792374	-1.957052979668	-2.456889854656
C	2.714581547937	-0.256975771922	-4.165659184846
C	4.049756480380	-2.523665660704	-3.216088731719
H	2.730084542043	-2.424752472531	-1.525846397921
C	3.739284665957	-0.824261474413	-4.913471256894
H	2.207217370630	0.629914353876	-4.530517262280
C	4.409472920821	-1.958050585593	-4.443375905052
H	4.553885803373	-3.416382817286	-2.858724375488
H	4.019785409331	-0.380932535024	-5.863980361007
H	5.204735749162	-2.402838289236	-5.034046792961
C	0.562710342291	2.878520092828	-0.291745390621
C	0.599243892895	3.487552150289	0.985145395472
C	1.584286130422	3.230708634130	-1.213906550184
C	1.571407948316	4.413226165381	1.330014754342
H	-0.167795818981	3.235409500643	1.712590550059
C	2.559711650787	4.146621839467	-0.883381668493
H	1.599446630523	2.787300857479	-2.204950449811
C	2.565689616645	4.753964383432	0.392800098402
H	1.552532358082	4.870362356742	2.312042545299
H	3.333339489918	4.430046644205	-1.589245458587
C	-2.457153592407	1.489628252053	-2.145924784299
H	-2.780468598882	0.622332361477	-1.560391450043
H	-2.990532566480	2.373717803481	-1.780092079412
H	-2.756614823655	1.325049365772	-3.185519144488
O	3.552982020203	5.636445495617	0.607497116809
C	3.626957895901	6.324458921666	1.860698827271
H	4.492931844953	6.980933226840	1.780939739988
H	2.725355002466	6.922421628489	2.032779727229
H	3.773639911720	5.619754695913	2.686763875905

3b^{•+}

E(UB+HF-LY) = -1362.83980198 A.U.

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.490293610000
C	1.143978697343	0.000000000000	2.227088478463
C	2.409424027152	-0.003357538044	1.572522820466
C	2.507131782549	-0.082192402868	0.188019517680
C	1.359692693054	-0.148771935661	-0.624953387825
H	-0.970006279846	0.018367183710	1.980744294868
H	1.103894889942	0.014295244279	3.311748465429
H	3.317366436398	0.052491808021	2.165341323240
H	3.487591221397	-0.073932010129	-0.274485380946
C	1.455507879347	-0.265195216997	-2.030543756548
S	0.098285802246	0.053265632214	-3.046757438031
C	-0.760690517991	1.287867915987	-0.569937117595
H	-1.719666089132	1.292371521626	-0.037985177493
C	-1.121742525590	1.075481152803	-2.060392141762

H	-0.629120954708	-0.844441614997	-0.330959605841
H	-1.096844215414	2.045221256838	-2.565828039645
C	2.655873170549	-0.723157128415	-2.739674012212
C	3.401760979251	-1.817698506979	-2.244799437380
C	3.058616167413	-0.118733716558	-3.951476477867
C	4.517257904565	-2.278695703465	-2.934322476089
H	3.073796462855	-2.329049118130	-1.345579526383
C	4.183984693787	-0.577349370579	-4.626528689204
H	2.506086592209	0.731548828433	-4.337876717181
C	4.914583099071	-1.657586248946	-4.122580829062
H	5.070982030839	-3.131124218639	-2.553076809602
H	4.495387901285	-0.089787506641	-5.545073095063
H	5.788655256713	-2.017717848745	-4.656792380474
C	-0.070000677724	2.600947312161	-0.262680009832
C	-0.450127708142	3.326712122441	0.872762936380
C	0.943638969906	3.145881799291	-1.073022632819
C	0.146231821599	4.541789064046	1.208564743121
H	-1.242179867482	2.945433972875	1.513948630610
C	1.546926227973	4.354121176026	-0.758488525874
H	1.264535255739	2.631457423273	-1.974600890817
C	1.157141643268	5.065317659712	0.389853412458
H	-0.188584286424	5.072836990239	2.091750099363
H	2.321705009716	4.777228866186	-1.389568521377
C	-2.501360193133	0.436985763673	-2.258066958441
H	-2.585349147994	-0.518657818140	-1.729012468446
H	-3.269444488519	1.116378579052	-1.872739554047
H	-2.717266674430	0.256176924211	-3.315850506463
C	1.440539242465	7.023757839253	1.735387589481
H	2.086535478590	7.901288498829	1.700706103302
H	0.392005540343	7.339062663120	1.674250378277
H	1.609015766252	6.483004515850	2.674666083953
O	1.807378570793	6.230535973544	0.608414998290

2c

E(UB+HF-LY) = -482.935047516 A.U.

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.389863290000
C	1.184702839319	0.000000000000	2.144615355970
C	2.388693183197	-0.000356967958	1.416660193074
C	2.411869695302	-0.000362011360	0.029616601088
C	1.212923142423	-0.000091065272	-0.723984895638
H	-0.950326243491	0.000173795464	-0.520997244634
H	-0.956089775667	0.000071782434	1.909727290854
H	3.338267307834	-0.000894449254	1.945089915315
H	3.372349849315	-0.000913089904	-0.472621595467
C	1.109987772031	-0.000307462228	3.610058830542
C	2.121386376970	-0.000063434694	4.492868645322
H	0.093677573087	-0.000812086736	4.009386901006
H	3.151927215799	0.000738726011	4.136600394398
C	1.947681208471	-0.000541009919	5.983738729965
H	0.888631962286	-0.001341857099	6.264398471786
H	2.419449816490	-0.880476999343	6.443843111886
H	2.418275938793	0.879787678328	6.444290949909
C	-0.016538447346	-0.001654855639	-2.848978434660
H	0.198907513983	-0.003394585879	-3.918952749557
H	-0.625598021144	-0.889926904218	-2.625634826857
H	-0.626256859285	0.886942137464	-2.628544937965
N	1.230775049913	-0.000215064005	-2.109437391680
C	2.494424721026	0.001503900440	-2.820482272886
H	3.099238293293	0.889458335317	-2.584157443523

H	3.099627090547	-0.887408386829	-2.588543706792
H	2.302681642173	0.004188829112	-3.895069694371

2c^{•+}

E(UB+HF-LY) = -482.705663419 A.U.

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.370621880000
C	1.207945623780	0.000000000000	2.128897807525
C	2.433981528163	0.000488757757	1.396617134093
C	2.455108837002	0.001079571963	0.027581442874
C	1.234652354544	0.001099760506	-0.728289528501
H	-0.945404945493	0.000000000000	-0.526906505616
H	-0.948585017627	-0.000234571731	1.899430869283
H	3.379522506145	0.000447460427	1.927444178409
H	3.410022217101	0.000735943949	-0.481946414237
C	1.128347761719	-0.000395909151	3.561122197300
C	2.176233051398	-0.001172958495	4.436353477741
H	0.122849689940	-0.000273228032	3.979351071015
H	3.196720231329	-0.001748109101	4.055872915707
C	2.034375776375	-0.001327104564	5.917210575858
H	0.989486885853	-0.002036189213	6.238180943037
H	2.538611662034	-0.877519391841	6.348441676263
H	2.537167696964	0.875814825732	6.348296434316
C	-0.004409211755	-0.001470432866	-2.848233921352
H	0.230425880871	-0.004062419097	-3.910718686648
H	-0.594074721552	-0.894640825376	-2.619372243049
H	-0.596514537727	0.891309784047	-2.623864038437
N	1.249652596278	0.002209352968	-2.079836444979
C	2.519218590780	0.008267054951	-2.822044516208
H	3.107676527137	0.896777338860	-2.572829395392
H	3.103764841298	-0.888952485397	-2.594788696055
H	2.306316018692	0.022248539286	-3.889096618729

MCc

E(UB+HF-LY) = -1382.30456782 A.U.

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.391281970000
C	1.208855623063	0.000000000000	2.094835413709
C	2.419234685003	-0.016076234867	1.398369429565
C	2.424343779599	-0.045470287497	0.005526143908
C	1.213067524282	-0.026577520828	-0.716218385013
H	-0.942878480957	-0.013317644852	1.930590966685
H	1.205660275477	0.001816234199	3.181101195657
H	3.360628779996	-0.015392169676	1.940145510365
H	3.367411837516	-0.057453720356	-0.531155970118
C	1.225222496028	-0.001339492846	-2.194076322784
S	0.134205415018	0.943537928211	-3.034690862290
C	0.195583409542	3.966299263969	-0.893681531718
H	0.242100526251	3.731193990037	0.168823886350
C	-0.933725675969	3.588592655620	-1.570690956701
H	-0.935492081009	-0.015864034739	-0.549235290474
H	-1.028348998554	3.820165661318	-2.628999278325
C	2.208867416143	-0.831594292535	-2.910210135060
C	2.635319981969	-2.061829833385	-2.362627334007
C	2.699796527133	-0.451844451567	-4.177728646014
C	3.511962138996	-2.883723444713	-3.065208180093
H	2.246457859614	-2.387051616462	-1.404010182609
C	3.590790356230	-1.266180859135	-4.864709261862

H	2.382270878879	0.494357671786	-4.602757313595
C	3.996324610201	-2.486645056003	-4.313349642098
H	3.813184216116	-3.836626747528	-2.640579573539
H	3.971488181728	-0.953707772090	-5.832601259452
H	4.686200708942	-3.125737464915	-4.856965037489
C	1.326242918291	4.665094516900	-1.425358480691
C	2.389249689049	5.028492181120	-0.551173998128
C	1.460623429673	5.043323639078	-2.792683214196
C	3.492641438586	5.719825278047	-0.987028937153
H	2.319806650428	4.752285066762	0.497252655742
C	2.556333881554	5.731960199204	-3.247695606664
H	0.683048113800	4.782854446123	-3.502606006375
C	3.616399475894	6.102738739671	-2.359066247971
H	4.269548953240	5.973083661434	-0.277118841053
H	2.610197881106	5.995675022245	-4.296260368370
C	-2.137879350940	2.997798391173	-0.918266522421
H	-1.933452383644	2.672908541160	0.105633035092
H	-2.943659010870	3.746386181429	-0.886322558516
H	-2.522030058196	2.150545950640	-1.495334891752
C	5.772897342095	7.169939768194	-1.880404358781
H	6.531418768143	7.726289153169	-2.428603004041
H	5.388252003860	7.809608041930	-1.078882183660
H	6.244113293285	6.285603230677	-1.437804452265
N	4.699593849671	6.787490306943	-2.803678493876
C	4.815781401759	7.176503213040	-4.212843607583
H	4.819484822834	6.295151692786	-4.863186148226
H	3.990658475059	7.834057607108	-4.507212666875
H	5.751796826935	7.713467623321	-4.357170908195

TS1c

E(UB+HF-LY) = -1382.30056231 A.U.

1 imaginary frequencies -171.4214 cm⁻¹

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.389614690000
C	1.209770638015	0.000000000000	2.092459459797
C	2.421480989713	-0.009801979639	1.395888276894
C	2.428526942040	-0.026491542197	0.004844356156
C	1.214941248262	-0.016253846134	-0.722235150859
H	-0.942169360946	-0.012708605741	1.929493846530
H	1.207251920719	0.004078700374	3.178469229956
H	3.361997591412	-0.000965763770	1.938431879881
H	3.372118712477	-0.014133594164	-0.530388324457
C	1.224997037787	0.006433008841	-2.188023344082
S	0.012518650138	0.832635595025	-3.050329727818
C	-0.825131761117	3.501907323873	-3.362820054838
H	-0.125374060082	4.027668574698	-4.010801555574
C	-0.261222157572	2.851793010541	-2.222429471944
H	-0.938131506508	-0.031618563746	-0.545085869185
H	-0.947759502790	2.602319864932	-1.416652626964
C	2.255533655050	-0.702194069072	-2.944043793684
C	2.795634679892	-1.912798709513	-2.443148242545
C	2.700746760194	-0.240539657862	-4.205591582234
C	3.736131344831	-2.625821376329	-3.176721866212
H	2.440922203711	-2.306005867384	-1.496707486418
C	3.653653189119	-0.950184900319	-4.923602439666
H	2.308700028924	0.692098839195	-4.596191593781
C	4.173035244565	-2.145951506229	-4.415173519967
H	4.125386735312	-3.561275121995	-2.786413620854
H	3.999359898262	-0.570661256945	-5.880403322099
H	4.914007148297	-2.701282521354	-4.982619063217

C	-2.166717646888	3.469819858255	-3.779264755399
C	-2.552396303636	4.160118560037	-4.971061440628
C	-3.203882987599	2.776416460944	-3.080813291381
C	-3.845286010609	4.171160149664	-5.424797381312
H	-1.790512903345	4.695793831206	-5.531060599034
C	-4.500681270251	2.772946289255	-3.527939017087
H	-2.968391045286	2.232631438206	-2.171825899799
C	-4.875636440234	3.474670221672	-4.717637495326
H	-4.079705183151	4.713226955009	-6.331839662330
H	-5.247726245002	2.230604733626	-2.962646758618
C	1.093940720454	3.330367208458	-1.750184174730
H	1.547393013012	2.641241121329	-1.035604809757
H	1.782626330012	3.476077498470	-2.588298555922
H	0.969854326872	4.295906886897	-1.242881412967
C	-6.528806359548	4.214605329002	-6.368622177448
H	-7.598551840447	4.102412939246	-6.539746975627
H	-6.307871159724	5.283039855756	-6.266054050161
H	-5.998153306950	3.825503607854	-7.245101322516
N	-6.158916644992	3.480031231619	-5.156446251052
C	-7.201554038080	2.757075505481	-4.425031843725
H	-7.316675064437	3.148911967731	-3.407877992428
H	-8.150125522191	2.877903380551	-4.946355155932
H	-6.975241543460	1.686259303727	-4.369283626386

INc

E(UB+HF-LY) = -1382.30117803 A.U.

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.389752510000
C	1.208963750884	0.000000000000	2.093511102166
C	2.420726484662	-0.010739621793	1.396265466183
C	2.428252283374	-0.026843199043	0.005685099808
C	1.214916647821	-0.018804326380	-0.723910710508
H	-0.942533028964	-0.011535087132	1.929157522441
H	1.206153230557	0.004884416416	3.179455320635
H	3.361343680028	-0.001753020229	1.938733732978
H	3.371884083944	-0.013570076296	-0.529640439670
C	1.226252759518	-0.007891312933	-2.185767745716
S	-0.010109498309	0.812962368238	-3.062121740206
C	-0.875316024559	3.338918238976	-3.382436022595
H	-0.201936966898	3.885823141406	-4.040112025310
C	-0.245126517703	2.633275160997	-2.269142167374
H	-0.939152660746	-0.035488076289	-0.543577798853
H	-0.902472734877	2.468413322738	-1.414718426581
C	2.234619667406	-0.723948456839	-2.953582159358
C	2.799893670118	-1.920430712144	-2.440564286843
C	2.644868427771	-0.291393156935	-4.239212331409
C	3.728205641855	-2.641295041037	-3.180339875387
H	2.472142014187	-2.295553106056	-1.477345285102
C	3.582966964357	-1.012019035800	-4.965501474213
H	2.239039774078	0.629552166023	-4.642992923405
C	4.127808059152	-2.189949576816	-4.442503240355
H	4.136145143731	-3.563429506624	-2.777435506693
H	3.898720884779	-0.653227977726	-5.940535074480
H	4.858150314934	-2.753175663292	-5.015803149097
C	-2.224240913377	3.307533677914	-3.735153555345
C	-2.672581554564	4.016196825429	-4.898685212670
C	-3.225523706772	2.592133407124	-3.000038327314
C	-3.982716978242	4.018832241540	-5.292799090653
H	-1.941857755820	4.569122188460	-5.482815200679
C	-4.539457730668	2.581863514037	-3.389357932779

H	-2.944298749101	2.039769967748	-2.109542895347
C	-4.973936094511	3.296797029095	-4.551842658495
H	-4.263995862452	4.572632197518	-6.179217072489
H	-5.255611258445	2.024966270812	-2.798846933796
C	1.098179393132	3.215441615924	-1.847481621133
H	1.594009082477	2.595425689432	-1.099226096520
H	1.766859146685	3.332477858915	-2.706273314631
H	0.932603761465	4.205050880681	-1.405807491817
N	-6.272748142766	3.292447648339	-4.934984597855
C	-7.274488208923	2.542715459284	-4.172845654945
H	-8.244749824348	2.655194271990	-4.654472676058
H	-7.029207341882	1.475236526899	-4.141785331838
H	-7.354856118359	2.919040131593	-3.146597384476
C	-6.704648006340	4.041636987621	-6.118061822401
H	-6.489422078840	5.110417911768	-6.008868002953
H	-6.211163168175	3.670440708300	-7.023425612229
H	-7.779953462041	3.921355030927	-6.241652459176

TS2c

E(UB+HF-LY) = -1382.28262045 A.U.

1 imaginary frequencies -340.0736 cm⁻¹

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.432160460000
C	1.179626564091	0.000000000000	2.134164470343
C	2.418048364024	-0.062560424715	1.440147110426
C	2.454846471197	-0.175508526465	0.066490239248
C	1.252073565528	-0.203006512656	-0.696521198215
H	-0.952462557189	0.020232167376	1.954817877416
H	1.173860186427	0.025727389937	3.219761038096
H	3.347302358356	-0.034563772890	2.001263871124
H	3.408527501968	-0.216676163346	-0.447455702489
C	1.262857333589	-0.261001593501	-2.110996213509
S	-0.134451599035	0.243396045083	-3.005714997141
C	-0.546151416937	1.902093883145	-0.613588900291
H	-1.392357841889	1.922569186306	0.070665533038
C	-0.975119038182	1.656757955437	-2.042008815379
H	-0.889376494927	-0.399180074664	-0.484108095826
H	-0.693611213541	2.524375843784	-2.644988071839
C	2.373613681135	-0.793324027504	-2.907345750192
C	3.079396822113	-1.934226274581	-2.460788913442
C	2.732415600925	-0.223911726826	-4.149247795013
C	4.113094643884	-2.469871750268	-3.221215480987
H	2.783042059606	-2.418241727284	-1.535888281847
C	3.773043482460	-0.759848014807	-4.899402861680
H	2.202748757089	0.652189662605	-4.508816573385
C	4.466458031179	-1.883498946819	-4.440015573732
H	4.634588113614	-3.355547309447	-2.870907666190
H	4.045579528856	-0.300797042658	-5.844949951535
H	5.273083510843	-2.304830671126	-5.032567474550
C	0.475851177504	2.864585667505	-0.296864863303
C	0.492060828160	3.481846144295	0.981487637761
C	1.492915782803	3.256918846260	-1.205781566971
C	1.422739687488	4.436058640472	1.324973006172
H	-0.267202831293	3.206014144321	1.708557953378
C	2.433095500818	4.209738805542	-0.880202028302
H	1.535173369765	2.811102037662	-2.195169723764
C	2.430008194394	4.840243773244	0.399856905971
H	1.372945233368	4.885889874975	2.308362786430
H	3.176766703223	4.482712254474	-1.618197816041
C	-2.482748835370	1.419712762911	-2.170096225035

H	-2.805959663327	0.555618411552	-1.579753337394
H	-3.023239794075	2.303911518181	-1.814757583229
H	-2.773274730816	1.244512239930	-3.210590328425
C	3.318949745319	6.433153445595	2.037766886369
H	4.130411981852	7.157286117863	2.099912431818
H	2.373034912620	6.963477200376	2.200512116131
H	3.453252549743	5.699530105144	2.841481074308
N	3.349199409657	5.791382257286	0.724152747618
C	4.364808003570	6.204390269497	-0.243208412958
H	5.006624210205	5.363088407022	-0.530745007224
H	3.906827268677	6.622684431884	-1.147537173276
H	4.993157046732	6.972556058107	0.205970432315

3c^{•+}

E(UB+HF-LY) = -1382.29146907 A.U.

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.488497730000
C	1.144869230953	0.000000000000	2.216448925371
C	2.415460237346	-0.016435893931	1.556115918356
C	2.506600837626	-0.132550274851	0.183729108098
C	1.345955722267	-0.216734852782	-0.628577269282
H	-0.968371980670	0.023486985873	1.982445081943
H	1.110192005859	0.015871094188	3.301599584080
H	3.323310897934	0.048392686676	2.148194273624
H	3.482669863571	-0.148865801793	-0.288277237017
C	1.419076672945	-0.384330792697	-2.017506316496
S	0.026258456633	-0.092598330713	-3.014650270990
C	-0.708441362424	1.330114930414	-0.593592332223
H	-1.658498089388	1.379601972076	-0.048833797846
C	-1.078393686153	1.097561768522	-2.079115375667
H	-0.682160092292	-0.795250786105	-0.342203083470
H	-0.957812883609	2.038646159228	-2.623138612044
C	2.602214128276	-0.875205322790	-2.739985419499
C	3.353734844510	-1.953407461794	-2.222319404119
C	2.982520632259	-0.320473801929	-3.980860624011
C	4.455715640827	-2.443648230336	-2.915100947210
H	3.042410246522	-2.428265660755	-1.297491618833
C	4.091505058650	-0.809702195753	-4.663049827911
H	2.418469451276	0.510635992282	-4.391754194545
C	4.830770551898	-1.871356823073	-4.134014712668
H	5.014485574636	-3.282802385903	-2.511885404639
H	4.381454957481	-0.361628127888	-5.608594210723
H	5.691432300560	-2.256159286178	-4.672949065289
C	0.032817680058	2.610996716412	-0.324349459659
C	-0.289002298494	3.375994723360	0.811837510480
C	1.047924010246	3.110716284889	-1.161829859003
C	0.344107579463	4.572234150669	1.100265774720
H	-1.071105536930	3.030277603088	1.483761294576
C	1.694810849093	4.306432161266	-0.897290786710
H	1.338379229799	2.561583800846	-2.053017043986
C	1.361492123560	5.079503271228	0.247436215718
H	0.041593648916	5.124386901848	1.981241239253
H	2.459958618621	4.647704818186	-1.583347896408
C	-2.517451553042	0.599954461226	-2.254651795596
H	-2.695034655248	-0.325033134602	-1.695194002793
H	-3.211984691218	1.365416642894	-1.891211903900
H	-2.752890197455	0.407587166097	-3.306236467776
N	1.991690318474	6.265393396123	0.516916744932
C	3.020417848872	6.775877573909	-0.383479748898
H	3.392152319995	7.725773510172	-0.000646669407

H	3.867338283106	6.082189136273	-0.457460951243
H	2.620906501904	6.946317106431	-1.391075954695
C	1.633762184219	7.038398949518	1.702188537613
H	2.262391222267	7.926837321013	1.753647391805
H	0.585689409428	7.361739107548	1.668608155539
H	1.789601338756	6.456598078729	2.618934598021