

SUPPORTING INFORMATION

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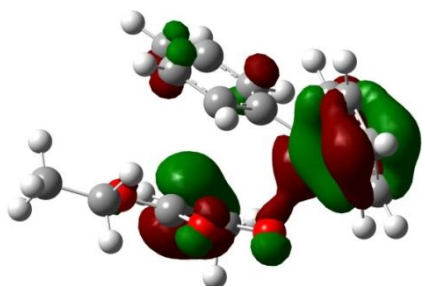
Title: Mechanism of Ylide Transfer to Carbonyl Compounds: Density Functional Calculations

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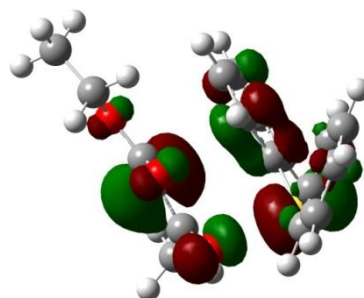
Content

Figure S1	Frontier molecular orbitals of transition states for sigmatropic rearrangements	S2
Table S1	Relative energies of intermediates and transition states computed at the B3LYP-I, B3LYP-II, and M06-2X levels	S3
Table S2	Optimized geometries and single-point energies of reactants, intermediates and transition states	S4

A

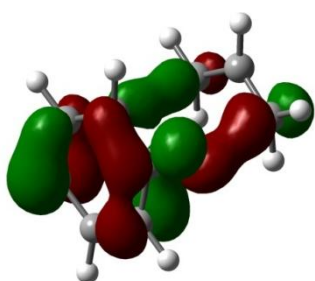


TS (6→9) HOMO

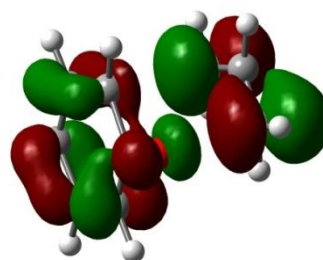


TS (6→9) LUMO

B

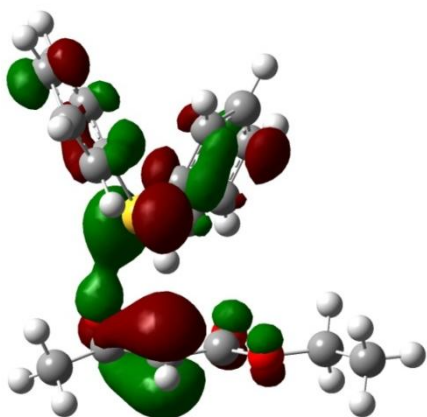


HOMO

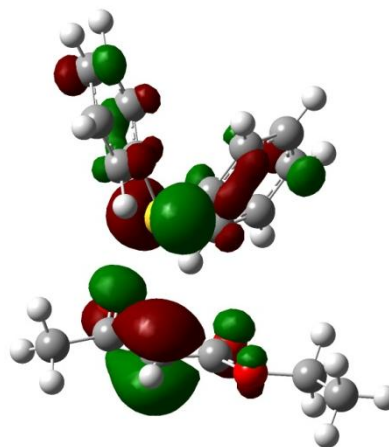


LUMO

C



TS (6→8) HOMO



TS (6→8) LUMO

Figure S1. Frontier molecular orbitals of transition states (TS): (A) TS (6→9), (B) TS for the ortho-Claisen rearrangement of an allyl phenyl ether, and (C) TS (6→8).

Table S1. Relative energies (in kcal/mol) of intermediates and transition states computed at the B3LYP-I, B3LYP-II, and M06-2X levels for the conversions on the pathways shown in Scheme 1 of the main paper.

	Sulfur reagents					
	Ra			Rb		
	B3LYP-I	B3LYP-II	M06-2X	B3LYP-I	B3LYP-II	M06-2X
A : Deprotonation of carbonyl compound						
1 + Ra or Rb	0.0	0.0	0.0	0.0	0.0	0.0
1 + \cdotOX + 2	13.7	30.0	27.5	-10.1	-11.0	-9.8
(1 + \cdotOX) + 2	13.7	27.4	25.6	-11.9	-13.8	-11.9
TS(1\rightarrow3) + 2	19.2	28.5	27.9	25.0	20.9	22.4
(3 + HOX) + 2	12.5	22.2	20.8	-11.9	-12.1	-11.3
(1 + 2) + \cdotOX	49.4	26.7	26.1	-4.7	-12.1	0.9
TS(1\rightarrow6) + \cdotOX	52.8	60.4	71.7	3.6	-3.6	0.7
(6 + HOX) + \cdotOX	52.4	30.1	26.7	-9.2	-13.5	-14.9
B : Nucleophilic addition of enolate to the sulfonium ion						
(2 + 3) + HOX	4.4	8.6	5.6	— ^a	— ^a	— ^a
TS(3\rightarrow4) + HOX	13.2	20.0	18.0	— ^a	— ^a	— ^a
(4 + \cdotOX) + HOX	-12.4	-5.6	-9.1	-34.0	-42.9	-44.7
TS(4\rightarrow5) + HOX	-9.0	-4.8	-8.8	-13.3	-24.8	-28.7
(5 + HOX) + HOX	-32.0	-20.9	-28.6	-13.9	-24.7	-28.6
5 + HOX + HOX	-24.4	-9.3	-18.6	-10.7	-14.3	-20.1
C : Nucleophilic displacement at central carbon atom of enolate						
(6 + \cdotOX) + HOX	11.6	25.9	21.4	-11.8	-15.6	-18.2
TS(6\rightarrow7) + HOX	23.5	34.6	41.9	5.9	-0.04	13.8
(7 + Ph₂S) + HOX	-41.7	-29.6	-38.0	-32.9	-36.6	-41.7
TS(7\rightarrow8) + HOX	24.9	29.0	38.1	9.4	-1.7	9.3
(8 + \cdotOX)^b + HOX	-12.4	-5.6	-9.1	-33.0	-42.5	-44.1
D : [1,3] Sigmatropic shift						
6 + \cdotOX + HOX	15.4	33.5	27.8	-9.1	-10.8	-14.0

TS(6→8) + ·OX+ HOX	38.5	57.3	70.7	14.0	13.0	28.9
8^b + ·OX+ HOX	-4.7	9.6	4.7	-29.3	-34.6	-37.2
E : [3,3] Sigmatropic rearrangement						
6 + ·OX+ HOX	15.9	34.8	30.0	-9.1	-10.8	-14.0
TS(6→9) + ·OX+ HOX	32.4	46.3	56.5	7.9	2.1	14.6
9 + ·OX + HOX	4.9	17.1	16.0	-19.7	-27.1	-25.8
(9 + ·OX) + HOX	— ^a	— ^a	— ^a	-27.9	-36.2	-34.9
TS(9→10) + HOX	— ^a	— ^a	— ^a	-22.8	-34.8	-35.9
(10 + HOX) + HOX	— ^a	— ^a	— ^a	-53.0	-60.0	-66.0
10 + HOX + HOX	-57.7	-42.7	-52.5	-43.9	-47.7	-53.1

^aThe transition state could not be located.

Table S2. Optimized geometries (B3LYP, Cartesian coordinates in Å) and single-point energies of reactants, intermediates and transition states (B3LYP-D, in a.u.). Notation: E = total electronic energy, Tc = thermal correction at 298K to obtain the Gibbs free energy, Nimag = number of imaginary frequencies.

1				·OC(CF₃)₂Ph			
E = -460.3907561 (-460.406968)				E = -1020.4393113 (-1020.467863)			
Tc = 0.117416		Nimag = 0		Tc = 0.086435		Nimag = 0	
6	1.094034	0.497672	-0.797980	8	-0.795009	0.000466	-1.869297
6	1.985042	-0.266845	0.184630	6	-1.195949	-1.281213	0.091291
6	3.298344	-0.764737	-0.366258	9	-1.119148	-1.371611	1.454964
1	3.813743	0.024062	-0.923502	9	-0.600395	-2.403976	-0.389852
1	3.931906	-1.130563	0.443037	9	-2.516134	-1.393416	-0.205925
8	1.643023	-0.459592	1.341648	6	-0.540307	0.000125	-0.562553
6	-0.256603	0.841623	-0.210399	6	-1.195270	1.281450	0.092040
8	-1.132319	-0.160308	-0.366976	6	0.986971	-0.000170	-0.193631
8	-0.516579	1.895229	0.345857	6	1.502473	-0.001054	1.113065
6	-2.467371	0.025871	0.189629	6	1.886206	0.000632	-1.265996
1	-2.906634	0.916200	-0.268251	6	2.884129	-0.001217	1.333633
1	-2.367217	0.201287	1.264085	1	0.838483	-0.001654	1.969200
6	-3.267581	-1.225010	-0.112381	6	3.267463	0.000528	-1.049240
1	-4.277713	-1.113345	0.293942	1	1.470126	0.001277	-2.267568
1	-3.348336	-1.390471	-1.190927	6	3.773052	-0.000415	0.254285
1	-2.809286	-2.106501	0.345882	1	3.263363	-0.001957	2.352002
1	1.609029	1.424923	-1.070294	1	3.947126	0.001165	-1.897376
1	0.981608	-0.097797	-1.709831	1	4.845541	-0.000519	0.428027
1	3.104713	-1.581879	-1.071829	9	-1.116345	1.372053	1.455576
				9	-2.515945	1.393394	-0.203172
				9	-0.600608	2.404218	-0.390177

2 E = -1881.5821275 (-1881.6475001) Tc = 0.257009 Nimag = 0				Ra E = -2902.0432356 (-2902.1631825) Tc = 0.368413 Nimag = 0			
8	0.100403	0.050943	0.137004	8	1.771568	-0.448495	-0.127931
6	1.676702	0.676132	-1.676579	6	2.469241	1.401461	1.273925
9	2.962295	0.599769	-2.053345	9	3.138034	2.578280	1.339615
9	1.395686	1.960041	-1.389493	9	2.967420	0.606210	2.243435
9	0.917330	0.321729	-2.737712	9	1.184748	1.676233	1.608404
16	-1.356822	0.004368	-0.740644	16	-0.223401	-0.525445	0.192062
6	-2.197679	-1.319943	0.123307	6	-0.205762	-1.979911	-0.907272
6	-1.889763	-1.660599	1.444560	6	0.316097	-1.827535	-2.193580
6	-3.175195	-1.990252	-0.621283	6	-0.765566	-3.187629	-0.484324
6	-2.603170	-2.703238	2.036221	6	0.284151	-2.916581	-3.067838
1	-1.106014	-1.148295	1.989685	1	0.749010	-0.888140	-2.510207
6	-3.884839	-3.020905	-0.002201	6	-0.783004	-4.269429	-1.366625
1	-3.380202	-1.722924	-1.652849	1	-1.187351	-3.288416	0.508102
6	-3.599484	-3.375317	1.319387	6	-0.258641	-4.136811	-2.655984
1	-2.376341	-2.988791	3.057927	1	0.689393	-2.806132	-4.068646
1	-4.648022	-3.552021	-0.560766	1	-1.210489	-5.212964	-1.042498
1	-4.148193	-4.184362	1.790477	1	-0.275366	-4.981318	-3.337953
6	-2.094881	1.522373	-0.194530	6	0.055939	-1.290148	1.838408
6	-2.119338	2.546562	-1.155756	6	-0.756354	-0.930653	2.915762
6	-2.633711	1.692727	1.089422	6	1.108624	-2.196990	1.999061
6	-2.682490	3.773876	-0.808165	6	-0.501656	-1.484996	4.174128
1	-1.718310	2.389388	-2.151339	1	-1.591162	-0.258691	2.785178
6	-3.187347	2.927495	1.415548	6	1.342241	-2.751116	3.257959
1	-2.630345	0.887492	1.813900	1	1.742750	-2.458407	1.163200
6	-3.210294	3.963408	0.472247	6	0.542844	-2.394238	4.348449
1	-2.712126	4.574900	-1.538717	1	-1.132490	-1.204656	5.011630
1	-3.607382	3.079386	2.403959	1	2.154566	-3.460309	3.381683
1	-3.650350	4.919516	0.736704	1	0.732259	-2.825220	5.326618
6	1.407911	-0.220726	-0.418570	6	2.566227	0.684705	-0.117727
6	1.468834	-1.739573	-0.789051	6	2.112130	1.657922	-1.263111
6	2.386717	0.168660	0.699116	6	4.040178	0.264090	-0.379339
6	3.628648	-0.467632	0.846400	6	5.104213	1.180065	-0.355389
6	2.047149	1.226877	1.556402	6	4.310964	-1.081549	-0.658548
6	4.510059	-0.054105	1.846960	6	6.411270	0.750449	-0.601062
1	3.930425	-1.274340	0.191115	1	4.931500	2.228080	-0.147674
6	2.933557	1.631603	2.555530	6	5.618787	-1.507319	-0.905640
1	1.095335	1.732022	1.452655	1	3.492528	-1.789300	-0.681780
6	4.166405	0.992683	2.705396	6	6.674970	-0.593593	-0.877105
1	5.466625	-0.556171	1.950175	1	7.221559	1.472975	-0.576075
1	2.655692	2.448419	3.213918	1	5.807979	-2.554964	-1.120497
1	4.854607	1.308495	3.483222	1	7.691700	-0.923936	-1.068122
9	2.583155	-2.055981	-1.472898	9	2.839602	2.796845	-1.343451
9	0.413151	-2.084595	-1.562336	9	0.818952	2.033690	-1.134257
9	1.416580	-2.497716	0.316678	9	2.222240	1.035408	-2.459792
				8	-2.113714	-0.681784	0.504716
				6	-3.029387	0.170300	-0.130164
				6	-2.663488	1.672659	-0.135034
				6	-2.940361	2.530717	-1.211063
				6	-2.088915	2.219541	1.022291
				6	-2.635627	3.892389	-1.131532
				1	-3.395960	2.163597	-2.120848
				6	-1.788301	3.579472	1.102780
				1	-1.873505	1.587146	1.873037
				6	-2.059690	4.423791	0.023723
				1	-2.853811	4.534445	-1.979394
				1	-1.340573	3.973956	2.009643
				1	-1.825073	5.482251	0.082677
				6	-4.339951	-0.009012	0.726368
				6	-3.309553	-0.382270	-1.574078

	9	-4.823874	-1.269246	0.676156
	9	-5.331039	0.815541	0.319985
	9	-4.098802	0.268107	2.024842
	9	-3.445737	-1.720633	-1.579134
	9	-2.281090	-0.086394	-2.402967
	9	-4.435521	0.125144	-2.135056

(1 + \cdotOC(CF₃)₂Ph) E = -1480.8300702 (-1480.8789143) Tc = 0.218943 Nimag = 0				TS(1→3)-Ra E = -1480.8212153 (-1480.8772223) Tc = 0.221548 Nimag = 1 (-1248.85 cm ⁻¹)			
6	-2.838811	1.169842	0.549669	6	-2.299078	0.970355	1.008100
6	-3.139188	2.653248	0.366802	6	-2.362118	2.433493	0.904706
6	-4.420455	3.176485	0.970178	6	-2.781153	3.108113	-0.387089
1	-4.352386	3.119570	2.063664	1	-2.669709	4.189131	-0.280028
1	-4.591285	4.211661	0.670848	1	-2.179700	2.750253	-1.227018
8	-2.357868	3.383341	-0.227490	8	-2.016799	3.140520	1.869411
6	-3.626679	0.315610	-0.422772	6	-3.146738	0.101359	0.184283
8	-3.644081	-0.968630	-0.038088	8	-3.354821	-1.098406	0.805553
8	-4.159309	0.726324	-1.442052	8	-3.613252	0.329250	-0.930933
6	-4.312042	-1.921641	-0.916881	6	-4.101917	-2.098004	0.073642
1	-3.826035	-1.884291	-1.895505	1	-3.587932	-2.303742	-0.870378
1	-5.353249	-1.609185	-1.033839	1	-5.094457	-1.700437	-0.160348
6	-4.196947	-3.290290	-0.276133	6	-4.189828	-3.337899	0.944556
1	-4.690621	-4.029807	-0.914495	1	-4.751525	-4.115926	0.417257
1	-3.149466	-3.583186	-0.158394	1	-3.194021	-3.729889	1.173782
1	-4.679896	-3.307729	0.705532	1	-4.704880	-3.122375	1.886035
1	-1.767935	0.974112	0.378301	1	-0.987513	0.667711	0.719000
8	0.302196	0.599330	0.115625	8	0.250709	0.444449	0.846091
6	1.113534	-1.464475	-0.739808	6	1.084427	1.034858	-1.317005
9	2.069738	-2.442426	-0.696665	9	1.831759	0.673606	-2.394102
9	1.038028	-1.074878	-2.039263	9	1.565702	2.226462	-0.891998
9	-0.058650	-2.090107	-0.460221	9	-0.166355	1.263361	-1.784873
6	1.359966	-0.208482	0.187053	6	1.090885	0.001553	-0.136322
1	-3.080931	0.851531	1.569317	1	-2.280719	0.652919	2.052077
1	-5.270374	2.553749	0.671415	1	-3.820150	2.860336	-0.624911
6	1.523992	-0.712298	1.676346	6	0.584015	-1.393056	-0.646716
6	2.714439	0.454650	-0.250387	6	2.543822	-0.150490	0.394702
6	2.646127	1.787285	-0.673081	6	2.782649	0.169859	1.736704
6	3.965534	-0.184056	-0.245536	6	3.617609	-0.587281	-0.398189
6	3.793672	2.474061	-1.080448	6	4.065448	0.057918	2.280360
1	1.672077	2.264318	-0.672135	1	1.950533	0.507180	2.342150
6	5.115870	0.500856	-0.652146	6	4.900296	-0.698933	0.146599
1	4.058632	-1.215365	0.073683	1	3.469598	-0.843046	-1.439935
6	5.035858	1.832597	-1.070860	6	5.130400	-0.377276	1.487200
1	3.717006	3.508580	-1.404690	1	4.229752	0.311684	3.323765
1	6.074961	-0.009934	-0.640232	1	5.718723	-1.038230	-0.481799
1	5.930650	2.362350	-1.385746	1	6.128103	-0.464973	1.907521
9	2.502229	-1.643899	1.895280	9	1.300363	-1.918414	-1.676377
9	0.382995	-1.264699	2.162918	9	-0.701779	-1.342132	-1.068502
9	1.818119	0.334940	2.490878	9	0.629743	-2.297828	0.359036

(3 + HOC(CF₃)₂Ph) E = -1480.831974 (-1480.8872175) Tc = 0.222754 Nimag = 0				(2 +3) E = -2341.5143652 (-2341.6127089) Tc = 0.387050 Nimag = 0			
6	2.699411	-0.642704	1.143555	6	-3.763834	-1.589123	-0.827945
6	2.703619	-2.064692	1.105738	6	-2.413832	-1.362658	-0.777528
6	3.268032	-2.813259	-0.096456	6	-1.446974	-2.496372	-1.013303
1	4.359829	-2.719889	-0.124122	1	-0.857013	-2.706529	-0.114795
1	3.003761	-3.870132	-0.010680	1	-1.981456	-3.407214	-1.286780
8	2.238929	-2.754381	2.059423	8	-1.934035	-0.139014	-0.570603
6	3.330193	0.234067	0.206427	6	-4.812314	-0.611098	-0.578900
8	3.245973	1.553727	0.628648	8	-6.040859	-1.178162	-0.772184

8	3.895907	-0.033976	-0.865180	8	-4.694326	0.562331	-0.231261
6	3.832476	2.551384	-0.227936	6	-7.195340	-0.335217	-0.544062
1	3.355543	2.511400	-1.213137	1	-7.128198	0.540466	-1.196931
1	4.897372	2.333396	-0.364170	1	-7.178656	0.013768	0.493249
6	3.626895	3.905593	0.429058	6	-8.434502	-1.159978	-0.838052
1	4.061997	4.690158	-0.199060	1	-9.327156	-0.547753	-0.674102
1	2.561693	4.122474	0.558775	1	-8.441319	-1.503978	-1.877045
1	4.110992	3.944976	1.410230	1	-8.492574	-2.033069	-0.180603
1	0.682470	-0.348287	0.693164	1	-4.096443	-2.587236	-1.085649
8	-0.237127	-0.054765	0.922648	1	-0.742398	-2.243008	-1.812329
6	-1.258700	-1.687395	-0.508698	16	-0.108285	0.119858	0.051050
9	-2.054852	-1.922688	-1.575800	6	-0.289902	1.827986	-0.555606
9	-1.750063	-2.397028	0.527516	6	-0.618585	2.009468	-1.900214
9	-0.042654	-2.201441	-0.803185	6	-0.058959	2.908392	0.296216
6	-1.159909	-0.174405	-0.119453	6	-0.720672	3.310765	-2.397940
1	2.370446	-0.190383	2.075772	1	-0.801976	1.159890	-2.546748
1	2.899266	-2.407181	-1.041166	6	-0.169593	4.203523	-0.214763
6	-0.650397	0.682614	-1.325746	1	0.207572	2.751339	1.334490
6	-2.524933	0.345925	0.364167	6	-0.499372	4.406165	-1.558368
6	-2.635786	0.850359	1.666620	1	-0.977633	3.462408	-3.441488
6	-3.658635	0.331348	-0.463309	1	0.003479	5.050851	0.441111
6	-3.861193	1.332140	2.134652	1	-0.583684	5.415228	-1.949750
1	-1.765742	0.864920	2.310261	6	-0.672843	0.244893	1.806512
6	-4.881273	0.813667	0.009677	6	0.203962	-0.065514	2.850162
1	-3.603451	-0.051074	-1.474686	6	-1.996912	0.623677	2.063720
6	-4.987905	1.315773	1.309251	6	-0.259123	-0.006321	4.168643
1	-3.930440	1.719408	3.146723	1	1.234697	-0.315275	2.652246
1	-5.748921	0.794920	-0.642707	6	-2.435597	0.688801	3.387893
1	-5.939696	1.690107	1.674126	1	-2.680709	0.845811	1.253965
9	-1.433195	0.591107	-2.423986	6	-1.574664	0.370138	4.441910
9	0.598023	0.318010	-1.697491	1	0.422843	-0.250132	4.977130
9	-0.596808	1.984027	-0.974712	1	-3.460016	0.987102	3.588134
				1	-1.926785	0.417693	5.467751
				8	1.718676	0.487282	0.632335
				6	2.796775	-0.050943	-0.074097
				6	4.015907	0.140320	0.904409
				6	3.049406	0.832239	-1.349031
				6	2.689195	-1.557121	-0.413932
				6	3.174602	-2.119418	-1.604931
				6	2.134422	-2.413648	0.549893
				6	3.091580	-3.497228	-1.826733
				1	3.623738	-1.506103	-2.374978
				6	2.056545	-3.789537	0.329932
				1	1.761913	-2.012453	1.483296
				6	2.534067	-4.338698	-0.862506
				1	3.468471	-3.907568	-2.758609
				1	1.621922	-4.428108	1.092913
				1	2.472882	-5.408533	-1.037282
				9	4.272677	0.646905	-1.905654
				9	2.130008	0.555777	-2.304693
				9	2.945523	2.145310	-1.074144
				9	5.154597	-0.407116	0.421882
				9	3.764578	-0.449514	2.092879
				9	4.276478	1.441328	1.158780

TS(3→4)-Ra				4 + ¹OC(CF₃)₂Ph			
E = -2341.500302 (-2341.5945057)				E = -2341.5410652 (-2341.6352825)			
Tc = 0.382572 Nimag = 1 (-27.70 cm ⁻¹)				Tc = 0.379269 Nimag = 0			
6	-2.979513	-1.369628	-1.761106	6	-1.333775	0.719686	-0.727984
6	-1.984751	-2.371818	-1.782788	6	-1.561088	0.791968	-2.254641
6	-1.047072	-2.382420	-2.992411	6	-1.015156	-0.329855	-3.095655
1	-1.131261	-3.348568	-3.503995	1	-0.983051	-0.013037	-4.139006

1	-1.257828	-1.585756	-3.711655	1	-0.020729	-0.626232	-2.750817
8	-1.784241	-3.259641	-0.899984	8	-2.118139	1.769450	-2.720814
6	-4.021457	-1.224631	-0.792403	6	-1.919040	1.930463	-0.007185
8	-4.852071	-0.157588	-1.120180	8	-1.036017	2.923995	-0.038295
8	-4.257296	-1.894438	0.223418	8	-3.019893	1.989720	0.507149
6	-5.961269	0.100146	-0.240573	6	-1.452386	4.204916	0.537301
1	-5.586072	0.321087	0.764908	1	-1.690536	4.035618	1.590259
1	-6.587805	-0.795762	-0.171431	1	-2.358669	4.527043	0.018558
6	-6.740772	1.274592	-0.807207	6	-0.307771	5.179052	0.355126
1	-7.593260	1.500077	-0.157698	1	-0.592867	6.146449	0.780165
1	-6.113465	2.169494	-0.871585	1	0.592859	4.830079	0.868245
1	-7.123623	1.047052	-1.807404	1	-0.077876	5.323746	-0.704421
1	-3.008518	-0.669609	-2.588307	1	-0.226849	0.653526	-0.559398
1	-0.009602	-2.288569	-2.651751	1	-1.669410	-1.207012	-3.021848
16	-0.043761	0.177363	0.316461	16	-1.834504	-0.940336	-0.049343
6	-1.012161	1.668242	0.192232	6	-1.904305	-0.700694	1.748390
6	-1.390643	2.020837	-1.112166	6	-0.671761	-0.484731	2.374325
6	-1.371520	2.442449	1.304295	6	-3.100122	-0.813035	2.458415
6	-2.127106	3.189286	-1.302407	6	-0.657162	-0.351771	3.765176
1	-1.128356	1.392356	-1.955286	1	0.241477	-0.411007	1.783043
6	-2.107890	3.605560	1.092060	6	-3.056271	-0.689889	3.849621
1	-1.097734	2.149731	2.310159	1	-4.042905	-0.990524	1.955852
6	-2.481233	3.979414	-0.205000	6	-1.841717	-0.456002	4.500961
1	-2.429130	3.473648	-2.304610	1	0.286993	-0.175297	4.270677
1	-2.394948	4.216815	1.941004	1	-3.976511	-0.774683	4.418522
1	-3.058761	4.885546	-0.357537	1	-1.818322	-0.359481	5.581900
6	-0.413740	-0.558252	1.906696	6	-3.490221	-1.358341	-0.615023
6	0.107389	-0.040065	3.099755	6	-3.630478	-2.696725	-1.010142
6	-1.238299	-1.687312	1.862030	6	-4.553724	-0.451201	-0.693677
6	-0.231484	-0.675938	4.292848	6	-4.869540	-3.134674	-1.481046
1	0.776291	0.812379	3.100360	1	-2.791302	-3.382368	-0.953818
6	-1.571320	-2.295338	3.076605	6	-5.780623	-0.906790	-1.179435
1	-1.603377	-2.102844	0.922483	1	-4.424528	0.576171	-0.377249
6	-1.074242	-1.794704	4.281893	6	-5.940462	-2.240914	-1.568072
1	0.166093	-0.297603	5.228789	1	-4.989718	-4.168600	-1.786861
1	-2.211316	-3.171497	3.069469	1	-6.612955	-0.214063	-1.249246
1	-1.332239	-2.282025	5.216841	1	-6.900183	-2.582781	-1.942501
8	1.480515	0.838780	0.681334	8	1.322268	-0.153475	-0.067422
6	2.623473	0.568894	-0.168060	6	2.644039	0.014534	-0.222627
6	3.812779	1.020567	0.760598	6	3.148376	1.064852	0.839904
6	2.512933	1.546019	-1.388066	6	2.917006	0.583226	-1.666681
6	2.782441	-0.901981	-0.551671	6	3.473131	-1.300239	-0.045805
6	3.195668	-1.311157	-1.829508	6	4.869219	-1.385405	-0.171384
6	2.555882	-1.876354	0.436463	6	2.754543	-2.462695	0.256528
6	3.364073	-2.668142	-2.111327	6	5.524638	-2.608548	0.004519
1	3.394843	-0.595360	-2.615638	1	5.457678	-0.506475	-0.405460
6	2.720012	-3.230369	0.146059	6	3.407716	-3.685954	0.433232
1	2.255778	-1.587297	1.436323	1	1.677224	-2.381732	0.347070
6	3.125407	-3.631180	-1.129053	6	4.797804	-3.763739	0.308052
1	3.680237	-2.966883	-3.105527	1	6.605463	-2.655079	-0.095960
1	2.532633	-3.967507	0.919952	1	2.830779	-4.576400	0.667984
1	3.253884	-4.684978	-1.355193	1	5.309577	-4.712194	0.444704
9	3.664237	1.638986	-2.078095	9	4.207286	0.943759	-1.926637
9	1.549771	1.116504	-2.234932	9	2.588043	-0.345836	-2.601788
9	2.169139	2.784025	-0.997597	9	2.163652	1.678917	-1.936008
9	4.989925	0.801629	0.147563	9	4.471884	1.391719	0.770738
9	3.806192	0.325566	1.910812	9	2.943295	0.585987	2.093747
9	3.747285	2.326742	1.078975	9	2.474222	2.239590	0.761170

TS(4→5)-Ra E = -2341.5356879 (-2341.6339353)	(5 + HOC(CF₃)₂Ph) E = -2341.5723308 (-2341.6596874)
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Tc = 0.379642 NImag = 1 (-1096.69 cm ⁻¹)				Tc = 0.385163 NImag = 0			
6	-1.142101	0.768297	-0.473265	6	-1.969602	-0.211518	0.124196
6	-1.177886	1.300945	-1.891936	6	-0.630041	-0.203407	-0.403824
6	-0.866325	0.343432	-3.023472	6	-0.387482	-0.003324	-1.897981
1	-0.534550	0.923101	-3.886638	1	0.688204	-0.004847	-2.074861
1	-0.103012	-0.384855	-2.740961	1	-0.840350	-0.802821	-2.491500
8	-1.405198	2.484610	-2.109644	8	0.370069	-0.344738	0.339693
6	-1.589892	1.725081	0.600901	6	-2.385042	-0.386653	1.513671
8	-0.749208	2.755513	0.692086	8	-1.392675	-0.703456	2.369748
8	-2.565128	1.577782	1.324543	8	-3.554190	-0.264725	1.887678
6	-1.069992	3.789126	1.669573	6	-1.773107	-0.882935	3.760148
1	-1.060615	3.333110	2.663260	1	-2.513052	-1.686257	3.821488
1	-2.079930	4.154034	1.464418	1	-2.239555	0.038709	4.119927
6	-0.030316	4.883376	1.535240	6	-0.513782	-1.217295	4.536663
1	-0.245343	5.673749	2.261351	1	-0.767634	-1.366132	5.591182
1	0.974364	4.499092	1.733165	1	-0.052043	-2.135926	4.162075
1	-0.048342	5.323141	0.533717	1	0.217834	-0.406307	4.471108
1	0.125627	0.400560	-0.316361	1	1.928062	-0.415039	-0.120054
1	-1.772551	-0.201930	-3.313119	1	-0.799777	0.945305	-2.255217
16	-1.904734	-0.898215	-0.401443	16	-3.245594	-0.005538	-1.057172
6	-1.931652	-1.408534	1.340995	6	-4.469983	-1.336285	-0.919723
6	-0.700572	-1.777064	1.892781	6	-4.260267	-2.420687	-1.779276
6	-3.126808	-1.525341	2.051806	6	-5.563770	-1.293208	-0.051168
6	-0.675207	-2.253332	3.206017	6	-5.154997	-3.493331	-1.750904
1	0.213275	-1.671365	1.316507	1	-3.416766	-2.431640	-2.462121
6	-3.081279	-2.017684	3.358308	6	-6.457138	-2.366697	-0.044802
1	-4.073486	-1.239707	1.610687	1	-5.709581	-0.449500	0.610076
6	-1.860526	-2.377764	3.936628	6	-6.252697	-3.465518	-0.886313
1	0.274172	-2.535080	3.650277	1	-4.997799	-4.338955	-2.412742
1	-4.004069	-2.112778	3.921660	1	-7.310788	-2.344146	0.625403
1	-1.834059	-2.757309	4.953302	1	-6.951757	-4.295987	-0.871411
6	-3.622724	-0.863354	-0.956270	6	-4.169612	1.525690	-0.729331
6	-4.001738	-1.972088	-1.725244	6	-5.323663	1.770344	-1.480595
6	-4.507928	0.190740	-0.703486	6	-3.646122	2.484912	0.136333
6	-5.300342	-2.030660	-2.235339	6	-5.978548	2.995094	-1.332525
1	-3.297436	-2.773150	-1.926056	1	-5.714782	1.024948	-2.165469
6	-5.798270	0.120416	-1.233129	6	-4.309447	3.708263	0.269953
1	-4.200434	1.033224	-0.097326	1	-2.739920	2.285936	0.696793
6	-6.195389	-0.984932	-1.992550	6	-5.474455	3.963479	-0.458225
1	-5.603318	-2.886653	-2.829395	1	-6.879111	3.190158	-1.906190
1	-6.493855	0.931960	-1.044932	1	-3.911797	4.457415	0.947344
1	-7.201450	-1.028928	-2.397728	1	-5.985996	4.914622	-0.348991
8	1.204491	-0.339826	-0.280025	8	2.827714	-0.676003	-0.489953
6	2.511197	0.048058	-0.196524	6	3.901898	0.102694	-0.071422
6	2.775114	0.588375	1.254148	6	4.017657	-0.016120	1.485825
6	2.772017	1.180559	-1.249204	6	3.631323	1.584315	-0.499847
6	3.477287	-1.136424	-0.476217	6	5.191303	-0.415929	-0.737651
6	4.875908	-1.013721	-0.455647	6	6.441986	0.180796	-0.512475
6	2.913408	-2.386532	-0.759142	6	5.108648	-1.522713	-1.592892
6	5.687471	-2.122369	-0.714159	6	7.586013	-0.324661	-1.135006
1	5.346011	-0.062032	-0.240490	1	6.540194	1.036853	0.143197
6	3.725700	-3.494323	-1.017356	6	6.255800	-2.025159	-2.212831
1	1.834167	-2.477129	-0.774444	1	4.147512	-1.987930	-1.769676
6	5.117018	-3.366883	-0.995763	6	7.498461	-1.428600	-1.987145
1	6.767469	-2.008753	-0.694178	1	8.545462	0.148780	-0.950024
1	3.268809	-4.455644	-1.234611	1	6.173489	-2.884217	-2.871985
1	5.750154	-4.226422	-1.195794	1	8.389677	-1.819250	-2.469172
9	4.009081	1.739184	-1.193013	9	4.581154	2.454667	-0.087766
9	2.623383	0.689768	-2.503199	9	3.566428	1.667387	-1.846004
9	1.887758	2.197549	-1.122034	9	2.450560	2.035595	-0.017569
9	4.016210	1.107452	1.454086	9	4.989514	0.759005	2.020452
9	2.626705	-0.416356	2.151673	9	4.288113	-1.293701	1.828554

9	1.896582	1.554867	1.601923	9	2.862282	0.323369	2.100236
(1 + 2)-Ra				TS(1→6)-Ra			
E = -2341.9159608 (-2342.0597001)				E = -2341.9104633 (-2342.0059871)			
Tc = 0.390635 NIMag = 0				Tc = 0.392635 NImag = 0			
C	4.12814400	-0.60206900	-1.71846300	C	0.07282200	1.58900300	1.77215700
C	4.16251100	0.92102600	-1.91643400	C	1.05545200	0.72810500	2.46507400
C	5.49340100	1.54097900	-2.26306400	C	1.06535000	0.67320000	3.95956100
H	6.28659800	1.15523700	-1.61389100	H	1.25036900	1.68157200	4.34639000
H	5.76396000	1.25957500	-3.28887200	H	0.06316300	0.37880400	4.29465200
O	3.14159600	1.57823200	-1.79836600	O	1.88817800	-0.02208900	1.89002000
C	4.50611200	-0.95559600	-0.28482100	C	0.69602700	2.61696300	0.84680400
O	5.78308700	-1.35011200	-0.19790000	O	0.05811900	3.78149600	0.93657100
O	3.73972600	-0.85922800	0.65604300	O	1.65010500	2.39485500	0.11892100
C	6.29990300	-1.73191800	1.11599900	C	0.51808000	4.88929700	0.09223900
H	5.83332600	-1.09406500	1.86939600	H	1.60269000	4.81877700	-0.00269900
H	7.36505200	-1.50369500	1.05039500	H	0.25890200	5.77458200	0.67410900
C	6.05523600	-3.20602900	1.38929300	C	-0.17701300	4.87973400	-1.25727600
H	6.51659000	-3.47806700	2.34446700	H	0.13713000	5.76345600	-1.82258500
H	4.98587800	-3.42463800	1.45386700	H	0.08592900	3.99123700	-1.83708900
H	6.50047400	-3.82780800	0.60733500	H	-1.26341200	4.91666200	-1.13855800
H	3.10649000	-0.94400800	-1.89089500	H	-0.56016900	0.87656000	1.12610000
O	-1.43022200	0.03054600	0.05335300	O	-1.19778900	-0.43280400	0.28692900
C	-3.84903000	-0.40950300	-0.33670900	C	-2.33076700	-1.70970900	-1.36042700
F	-4.72371300	-1.38731200	-0.58420100	F	-3.33924400	-1.77988100	-2.27199300
F	-3.69873500	0.32982400	-1.45502800	F	-2.48049700	-2.77927900	-0.54003800
F	-4.38631100	0.40257800	0.60349700	F	-1.18354600	-1.91170900	-2.05473200
S	-1.59223300	1.55457700	0.77940500	S	2.01947700	-0.43582600	-0.15871000
C	-0.25974100	1.51470500	1.96627200	C	3.66811900	0.08276000	-0.37716900
C	0.92475500	0.79897300	1.76130100	C	4.73389400	-0.33751100	0.44932400
C	-0.50313500	2.24957500	3.13457700	C	3.86513600	1.00942400	-1.42562000
C	1.89781000	0.84190100	2.75956500	C	6.00645000	0.15092700	0.18919100
H	1.09019600	0.20113200	0.87287200	H	4.55924100	-0.99727400	1.29084700
C	0.49099000	2.28996900	4.11277300	C	5.15515100	1.45336800	-1.69002500
H	-1.44384200	2.77102000	3.28403300	C	3.02728300	1.35392000	-2.02012800
C	1.68472500	1.58790800	3.92435600	C	6.21949300	1.03051200	-0.88433500
H	2.81490000	0.28353000	2.60950000	H	6.83460500	-0.14584900	0.82319700
H	0.32220700	2.85426600	5.02393000	H	5.32815500	2.14154100	-2.50985400
H	2.44918600	1.61274900	4.69464000	H	7.22049700	1.40069200	-1.08068500
C	-1.09872500	2.60267400	-0.56445200	C	2.05993600	-2.15462000	0.09411200
C	0.20067300	2.62775300	-1.09015200	C	0.82810000	-2.72335900	0.51108400
C	-2.12490200	3.42023300	-1.06819200	C	3.18855800	-2.96638800	-0.18718000
C	0.46553500	3.49017900	-2.15100600	C	0.75572700	-4.09771000	0.68728000
H	0.99571400	1.99976800	-0.70742600	H	-0.03612400	-2.07709100	0.66851800
C	-1.83375900	4.28430500	-2.12297900	C	3.07885400	-4.33767700	-0.02039400
H	-3.12439500	3.38240500	-0.64635300	H	4.10337300	-2.54029200	-0.57613800
C	-0.54395400	4.31653900	-2.66152700	C	1.87460600	-4.90232600	0.42969600
H	1.46671500	3.50856100	-2.56726300	H	-0.17397100	-4.54744800	1.01784900
H	-2.61204300	4.92701600	-2.52073500	H	3.92590900	-4.97347800	-0.25285400
H	-0.32210500	4.99088500	-3.48289100	H	1.80553300	-5.97732400	0.56164700
C	-2.45932400	-0.99631900	0.09894500	C	-2.28931900	-0.38640000	-0.51096500
H	4.81999000	-1.09112300	-2.40816400	H	-0.57261800	2.07852700	2.49932600
H	5.43624600	2.62793700	-2.19297400	H	1.81081900	-0.02783600	4.33172500
C	-2.51921800	-1.53958300	1.56354800	C	-2.13905000	0.84128500	-1.48143900
C	-2.00063300	-2.03877400	-0.92537100	C	-3.63635000	-0.26183100	0.26831100
C	-2.18585700	-3.41414800	-0.71968900	C	-4.89362600	-0.12696500	-0.34315100
C	-1.43397000	-1.59287000	-2.13027100	C	-3.57055300	-0.29767300	1.66621400
C	-1.80334000	-4.32506600	-1.70519600	C	-6.05234900	-0.02423800	0.43299300
H	-2.63433100	-3.79271200	0.18948400	H	-4.98613200	-0.10012600	-1.42212300
C	-1.05286400	-2.51051600	-3.10870200	C	-4.72847600	-0.19743900	2.44282100
H	-1.28756300	-0.53445400	-2.30611400	H	-2.59822100	-0.40868300	2.13161900
C	-1.23584200	-3.87917500	-2.89996700	C	-5.97588000	-0.05869300	1.82838000
H	-1.95481200	-5.38589100	-1.53363900	H	-7.01555500	0.08208700	-0.05793800

H	-0.61890800	-2.15162100	-4.03670000	H	-4.65406200	-0.22768300	3.52632900
H	-0.94263900	-4.59250200	-3.66387300	H	-6.87790100	0.02100700	2.42824500
F	-3.55743600	-2.36966100	1.75095100	F	-3.08878800	0.94474500	-2.45147400
F	-2.65274900	-0.51812100	2.44372700	F	-0.94674800	0.83920000	-2.12523200
F	-1.38590600	-2.18321300	1.87733500	F	-2.19075700	1.99503300	-0.76804300

(6 + HOC(CF₃)₂Ph)				(6 + ⁻OC(CF₃)₂Ph)			
E = -2341.9111296 (-2342.0543457)				E = -2341.5028233 (-2341.5850017)			
Tc = 0.392346 NImag = 0				Tc = 0.37837 NImag = 0			
C	-2.27434800	2.21327400	-2.17100600	C	-2.03128500	2.25184800	-1.74433100
C	-2.81875400	1.00768200	-2.40212300	C	-2.35967500	1.04086300	-2.22819200
C	-3.13503100	0.43657300	-3.74593900	C	-2.25846100	0.62516400	-3.65805500
H	-4.20558100	0.21375400	-3.81757800	H	-3.23838100	0.29531200	-4.02056600
H	-2.87003900	1.13966600	-4.53740700	H	-1.91013500	1.45226300	-4.27817500
O	-3.27713700	0.14194300	-1.38466500	O	-2.93747600	0.01388200	-1.46112100
C	-2.05844700	2.82965000	-0.84746500	C	-2.21452200	2.72167500	-0.36285400
O	-1.70712600	4.11139900	-0.97538700	O	-1.87669100	4.01489900	-0.24991500
O	-2.20207000	2.25241800	0.22501600	O	-2.63468300	2.04813400	0.57314500
C	-1.48574600	4.89340300	0.24053400	C	-2.01903300	4.62848000	1.06482800
H	-2.15237900	4.51700400	1.01856700	H	-1.39334000	4.07389500	1.76933900
H	-1.78584700	5.90273200	-0.04554400	H	-3.06258700	4.53177400	1.37635700
C	-0.02786200	4.83731800	0.66375500	C	-1.59292400	6.07718100	0.94018600
H	0.11921600	5.48944700	1.53117100	H	-1.68915000	6.56495700	1.91522300
H	0.26519600	3.82293500	0.94692800	H	-0.55003700	6.15523700	0.61904900
H	0.62701300	5.18596700	-0.13991200	H	-2.22352600	6.61328300	0.22466700
H	3.17309400	-1.67418200	-1.54911600	H	-1.62543300	2.96856900	-2.44796500
O	2.52218600	-1.51706200	-0.84891100	H	-1.56937100	-0.22039900	-3.75840800
C	2.25404500	-0.57760800	1.29626200	S	-2.13335500	-0.58078100	-0.11006900
F	2.53964700	0.44022000	2.12546300	C	-3.54808600	-0.86370900	0.96381100
F	2.65023800	-1.71959500	1.87735200	C	-4.85863300	-0.84264500	0.48492400
F	0.89861900	-0.63908100	1.18537600	C	-3.24377500	-1.09710700	2.30792800
S	-2.21443600	-0.40308800	-0.20788100	C	-5.89566100	-1.07781000	1.39145300
C	-3.28075800	-0.34184700	1.23804400	H	-5.07011800	-0.63564300	-0.55688700
C	-4.65873300	-0.15203500	1.13384400	C	-4.29488800	-1.33735800	3.19501500
C	-2.63107000	-0.48947600	2.46608600	H	-2.21792600	-1.08872300	2.66274000
C	-5.40999100	-0.12881000	2.31132600	C	-5.61643300	-1.32753300	2.73837700
H	-5.13079000	-0.00402600	0.17009100	H	-6.92176100	-1.06276000	1.03876200
C	-3.40295900	-0.47027900	3.62899400	H	-4.07681600	-1.51996800	4.24200700
H	-1.55304100	-0.60605600	2.52314300	H	-6.42956700	-1.50815300	3.43413600
C	-4.78708100	-0.29172500	3.55191700	C	-1.67004100	-2.20658800	-0.67010500
H	-6.48304200	0.02332100	2.25417300	C	-0.28877100	-2.39105300	-0.83297200
H	-2.91721500	-0.58183800	4.59282000	C	-2.60528200	-3.21791900	-0.93978500
H	-5.37999300	-0.27003300	4.46069700	C	0.15541400	-3.63797000	-1.28466800
C	-2.13784200	-2.13837700	-0.61988400	H	0.41770600	-1.58662400	-0.59862700
C	-0.88874600	-2.58706600	-1.07445100	C	-2.13610400	-4.44622000	-1.39510200
C	-3.23995300	-2.99951200	-0.51137900	H	-3.66755500	-3.05480200	-0.79743700
C	-0.75122000	-3.93015400	-1.43233100	C	-0.75923300	-4.65515200	-1.56581000
H	-0.03590100	-1.91727300	-1.12867800	H	1.21932900	-3.80915900	-1.41320600
C	-3.08408000	-4.33171300	-0.88231400	H	-2.84019000	-5.24294900	-1.61132200
H	-4.19375400	-2.63909000	-0.14262700	H	-0.40365700	-5.61949400	-1.91561800
C	-1.84311100	-4.79561600	-1.34076300	O	1.48696500	-0.00312600	0.03813600
H	0.21098400	-4.29589100	-1.77500300	C	2.79135000	0.26531100	-0.04591700
H	-3.92600700	-5.01222800	-0.80690900	C	3.02638900	1.78289300	0.32390300
H	-1.72988900	-5.83862300	-1.61961700	C	3.26843400	0.03306700	-1.53443700
C	2.94813700	-0.39856900	-0.09069700	C	3.69638300	-0.60856100	0.89227000
H	-2.00984000	2.81330300	-3.03380300	C	5.09168500	-0.49068500	1.00254100
H	-2.59495100	-0.50369300	-3.90368400	C	3.04356200	-1.57078400	1.67122700
C	2.38391800	0.85831500	-0.83426200	C	5.80926800	-1.31660800	1.87447200
C	4.47269400	-0.36119100	0.09025200	H	5.63141800	0.24245600	0.41534900
C	5.19120100	0.82955500	0.27452800	C	3.75791900	-2.39838000	2.54267800
C	5.16390300	-1.58366400	0.10199400	H	1.96635100	-1.64889500	1.57556300
C	6.57617500	0.79382200	0.44447400	C	5.14638000	-2.27395200	2.64846000

H	4.68927200	1.78848400	0.28879400	H	6.88814200	-1.20912700	1.94674700
C	6.54903800	-1.61262100	0.27152400	H	3.23021400	-3.13852600	3.13840300
H	4.62256400	-2.51858500	0.00347500	H	5.70567000	-2.91395400	3.32515200
C	7.26010600	-0.42342200	0.44000500	F	4.57409000	0.33743600	-1.80337000
H	7.11877200	1.72412100	0.57958000	F	3.11289700	-1.27456300	-1.87004300
H	7.06712900	-2.56642600	0.27910800	F	2.53668800	0.74624800	-2.42919000
H	8.33741100	-0.44476400	0.57139800	F	4.30179400	2.25051400	0.15923900
F	2.47393600	2.00132700	-0.12513600	F	2.71504600	1.99647900	1.62935300
F	1.07709500	0.69516000	-1.14804400	F	2.23677200	2.61776400	-0.39767800
F	3.04723000	1.03045600	-1.99589400				

TS(6→7)-Ra				(7 + Ph₂S)-Ra			
E = -2341.4838809 (-2341.5712901)				E = -2341.5877827 (-2341.6735269)			
Tc = 0.379745		Nimag = 1(-210.86)		Tc = 0.378152			
C	0.02520600	1.18577200	-1.75001200	C	1.62706600	1.28570300	0.15985000
C	-1.10845200	0.41148000	-1.88022900	C	0.67587900	2.00575800	-0.84082100
C	-1.15394100	-0.78414200	-2.79388300	C	0.89186300	3.48321000	-1.03331600
H	-2.08579800	-0.78504300	-3.36696900	H	0.07698900	3.89916400	-1.62667100
H	-0.30409300	-0.79823800	-3.47870800	H	0.97201400	4.00673600	-0.07683800
O	-2.21535500	0.72573500	-1.23177300	O	-0.17164100	1.36936400	-1.43535500
C	0.16109000	2.34991100	-0.84732200	C	1.24353500	1.69443900	1.59761300
O	1.09402000	3.19732500	-1.32296900	O	1.93320500	2.77060700	1.97897700
O	-0.47586300	2.55733600	0.17481600	O	0.40326200	1.12282300	2.26021400
C	1.36385000	4.39067600	-0.53795000	C	1.62594300	3.33014700	3.29775900
H	1.69633000	4.07855700	0.45632300	H	1.78746200	2.54475000	4.03986000
H	0.43143300	4.95204800	-0.42857600	H	0.56937600	3.60992400	3.30569500
C	2.42534000	5.19012300	-1.26741100	C	2.53865300	4.51923300	3.51110400
H	2.64945500	6.09747900	-0.69769800	H	2.33005200	4.95756200	4.49194200
H	3.34947400	4.61409600	-1.37262300	H	3.59008200	4.21833800	3.48658200
H	2.08062400	5.48681400	-2.26266600	H	2.37208400	5.28701700	2.74996800
H	0.83544600	1.03487200	-2.44965100	H	2.64833600	1.61919400	-0.03949800
H	-1.12237200	-1.70852500	-2.20564700	H	1.84139500	3.63711700	-1.56060400
S	-2.63318600	-0.21381400	0.55220900	S	-4.14097400	-1.12616300	-1.41046800
C	-3.95446900	0.89286200	0.97495200	C	-4.24807100	-1.76428200	0.26623500
C	-3.59612200	2.24544800	1.11716200	C	-3.08167500	-1.87424500	1.03500700
C	-5.25743700	0.45081800	1.25561200	C	-5.47091600	-2.22246300	0.78011500
C	-4.56743700	3.16064500	1.51911600	C	-3.13956700	-2.43859300	2.31413100
H	-2.58190600	2.56333200	0.90159800	H	-2.13696100	-1.51910700	0.63628400
C	-6.21087800	1.38281600	1.66422600	C	-5.52468700	-2.77170200	2.06295800
H	-5.52348100	-0.59585700	1.17732300	H	-6.37180700	-2.14951100	0.17888800
C	-5.87217800	2.73415900	1.79130500	C	-4.35926300	-2.88365900	2.83058300
H	-4.30237800	4.20803800	1.62147500	H	-2.23221800	-2.52262800	2.90474700
H	-7.21873000	1.04803200	1.88731100	H	-6.47386800	-3.12156000	2.45812600
H	-6.62196000	3.45185600	2.10891000	H	-4.40320200	-3.31809500	3.82485100
C	-3.39600200	-1.72605100	0.03324600	C	-4.94523800	0.47904300	-1.31764500
C	-2.88000200	-2.90561000	0.59526800	C	-5.43797600	1.01303100	-2.51890100
C	-4.39926100	-1.76367100	-0.94955300	C	-5.04837700	1.22299000	-0.13403100
C	-3.40089900	-4.13387100	0.18715600	C	-6.02276200	2.28180600	-2.53312700
H	-2.09422600	-2.86119800	1.34226700	H	-5.37038500	0.43754400	-3.43786800
C	-4.90275100	-2.99922900	-1.34902800	C	-5.64896900	2.48541300	-0.15597500
H	-4.76486600	-0.84815500	-1.40053800	H	-4.66578400	0.82399200	0.79931700
C	-4.40869800	-4.18096700	-0.78091800	C	-6.13536200	3.02256300	-1.35193800
H	-3.01673200	-5.04978700	0.62374000	H	-6.40055000	2.68416100	-3.46869800
H	-5.67640700	-3.04108200	-2.10874700	H	-5.72824300	3.05126200	0.76799000
H	-4.80718000	-5.13903900	-1.09932300	H	-6.59798200	4.00472800	-1.36304400
O	1.61588500	0.22605300	0.00560900	O	1.48035800	-0.12048000	0.00635300
C	2.72377600	-0.53133300	-0.07501300	C	2.63121100	-0.93828100	-0.13695200
C	3.73922300	0.12261100	-1.08814800	C	2.01081700	-2.33235100	-0.50928500
C	2.33350300	-1.96599400	-0.59638200	C	3.33849900	-1.05167900	1.26074800
C	3.44645700	-0.68830100	1.30726700	C	3.57349900	-0.48575400	-1.26534800
C	4.62633100	-1.42314800	1.50641900	C	4.97098400	-0.58516500	-1.19074800
C	2.86300100	-0.04270000	2.40396100	C	2.98985300	0.00948200	-2.44379400

C	5.20250600	-1.50804700	2.77825300	C	5.76456800	-0.18558400	-2.26936400
H	5.10772300	-1.93277200	0.68096600	H	5.46162700	-0.97239700	-0.30756000
C	3.43817800	-0.12738800	3.67522100	C	3.78643900	0.40740200	-3.51775300
H	1.95434100	0.52395200	2.23629000	H	1.91201100	0.08306900	-2.52484400
C	4.61152900	-0.86208000	3.86805500	C	5.17808500	0.31221200	-3.43431300
H	6.11541900	-2.08143700	2.91313500	H	6.84423300	-0.26601300	-2.19160100
H	2.96904400	0.38114200	4.51310000	H	3.31587300	0.78967900	-4.41817300
H	5.06122500	-0.93033200	4.85456200	H	5.79875400	0.62252400	-4.26924400
F	3.37157500	-2.83585100	-0.76479800	F	4.25236900	-2.04458700	1.31222500
F	1.48079800	-2.55933600	0.27580000	F	3.97593400	0.10660500	1.55755900
F	1.69457100	-1.92015900	-1.79147700	F	2.45426900	-1.27309800	2.24820100
F	4.86735900	-0.60396500	-1.33762600	F	2.97745400	-3.24218400	-0.75142400
F	4.15648800	1.32390100	-0.61916500	F	1.25522000	-2.23675700	-1.61843600
F	3.17835700	0.35673600	-2.30216400	F	1.22371400	-2.82546600	0.46849800

TS(7→8)-Ra				(8 + ·OC(CF₃)₂Ph)			
E = (-2341.4816466) -2341.5801725				E = -2341.5410793 (-2341.635336)			
Tc = 0.379404 NImag = 1 (-143.31)				Tc = 0.380719 NImag = 0			
C	0.35856200	-0.06225900	-1.77005400	C	-1.32414700	0.69945600	-0.72669800
C	1.30092400	0.96044000	-2.27622400	C	-1.52906100	0.75645400	-2.25744200
C	0.85382400	2.39999500	-2.25545200	C	-0.96457000	-0.37147100	-3.07795300
H	1.72506600	3.05723400	-2.24820500	H	-0.91965300	-0.06638700	-4.12431100
H	0.28761600	2.59279900	-3.17572700	H	0.02641600	-0.65737400	-2.71482800
O	2.35103000	0.60843900	-2.81492000	O	-2.08463000	1.72563900	-2.74226300
C	0.73600200	-1.50806200	-1.77577600	C	-1.90687200	1.92250900	-0.02557100
O	-0.21730400	-2.21344100	-2.39952700	O	-1.02558500	2.91661400	-0.08228300
O	1.76262000	-1.98030800	-1.32248700	C	-3.00349400	1.98986900	0.49684200
C	0.01381500	-3.64664500	-2.55132700	O	-1.43994200	4.20752900	0.47203400
H	0.10009000	-4.07901300	-1.55060600	H	-1.67206600	4.05770100	1.52928900
H	0.96480100	-3.78577500	-3.07260300	H	-2.34947200	4.51911600	-0.04751200
C	-1.15409700	-4.22054000	-3.32654400	C	-0.29752900	5.17939000	0.26548800
H	-1.00563800	-5.29769500	-3.45147500	H	-0.58125800	6.15394100	0.67484300
H	-2.09607100	-4.06208800	-2.79413500	H	0.60657300	4.84068400	0.77939100
H	-1.22864100	-3.76760900	-4.31965900	H	-0.07412900	5.30534900	-0.79782100
H	-0.69031800	0.15012100	-1.90927400	H	-0.21957400	0.62472500	-0.54190000
H	0.19650700	2.62081300	-1.41264800	H	-1.61358000	-1.25242600	-3.00343700
S	1.73043300	0.66855600	0.72275800	S	-1.84985700	-0.95022900	-0.04365900
C	2.08483000	-0.82030600	1.64908500	C	-1.92164700	-0.70781200	1.75315300
C	1.04591100	-1.75177100	1.81697600	C	-0.68643400	-0.52067600	2.38313400
C	3.32126000	-1.01245000	2.29312500	C	-3.12196600	-0.79272600	2.45935300
C	1.25008600	-2.86817800	2.62909800	C	-0.67305500	-0.38867500	3.77408200
H	0.10023700	-1.58643300	1.31152100	H	0.22994700	-0.46611100	1.79476700
C	3.50929400	-2.13719200	3.09468400	C	-3.07965300	-0.67143500	3.85073800
H	4.11850900	-0.28634500	2.19217700	H	-4.06689000	-0.94855400	1.95366700
C	2.47888400	-3.06970300	3.26437400	C	-1.86202500	-0.46610100	4.50602500
H	0.44650100	-3.58756400	2.75445600	H	0.27326500	-0.23407600	4.28266600
H	4.46194700	-2.27786500	3.59611200	H	-4.00333900	-0.73544700	4.41676300
H	2.63471600	-3.94466900	3.88791200	H	-1.83981300	-0.37097500	5.58711700
C	3.33857400	1.23951700	0.21157600	C	-3.50780200	-1.35185700	-0.61506500
C	3.63782600	2.59642700	0.42180800	C	-3.66050700	-2.69022400	-1.00572100
C	4.25702600	0.40085700	-0.44596400	C	-4.56184400	-0.43432000	-0.70102200
C	4.87095200	3.10121000	0.00748200	C	-4.90229300	-3.11747300	-1.47918600
H	2.92274800	3.24055600	0.92369900	H	-2.82870400	-3.38435000	-0.94364100
C	5.48880000	0.91684500	-0.84770000	C	-5.79164500	-0.87939800	-1.18918200
H	3.99885800	-0.63334500	-0.64243500	H	-4.42363300	0.59293600	-0.38829400
C	5.79846200	2.26235300	-0.62106400	C	-5.96382300	-2.21331200	-1.57319700
H	5.10959000	4.14531600	0.18363800	H	-5.03183300	-4.15132500	-1.78142100
H	6.20186400	0.26942000	-1.34850100	H	-6.61666100	-0.17852800	-1.26440000
H	6.75822000	2.65828600	-0.93850500	H	-6.92576700	-2.54687900	-1.94940200
O	-1.03565700	-0.13244200	0.28179400	O	1.32227800	-0.18585200	-0.04970300
C	-2.36945900	0.10903300	0.40683700	C	2.64123500	0.01056200	-0.19691600
C	-2.78256200	-0.31534000	1.87134700	C	3.12703900	1.02676800	0.90659200

C	-3.14673900	-0.81058400	-0.60636600	C	2.90448900	0.63815200	-1.61832400
C	-2.76337400	1.60483400	0.23555600	C	3.49330900	-1.29504800	-0.06898700
C	-4.03444000	2.05541100	-0.15274200	C	4.88922000	-1.35187800	-0.21109500
C	-1.77872900	2.55506300	0.53790900	C	2.79754800	-2.47858100	0.20328800
C	-4.30124000	3.42448400	-0.25722900	C	5.56702100	-2.56860600	-0.08209700
H	-4.82964600	1.35499400	-0.37612200	H	5.46012100	-0.45569000	-0.42226000
C	-2.04824500	3.92280000	0.44635400	C	3.47326500	-3.69541100	0.33376700
H	-0.80055200	2.20873000	0.84888200	H	1.72002900	-2.41913600	0.30742000
C	-3.31140000	4.36392200	0.04188800	C	4.86298300	-3.74523900	0.19133500
H	-5.28842300	3.75240400	-0.56980500	H	6.64728500	-2.59335200	-0.19544700
H	-1.27043000	4.64132200	0.68890000	H	2.91415200	-4.60274300	0.54584400
H	-3.52286000	5.42636700	-0.03618800	H	5.39207700	-4.68870700	0.29166600
F	-4.49433200	-0.87211700	-0.41963500	F	4.18243400	1.05424600	-1.85496000
F	-2.95262600	-0.36409200	-1.87596100	F	2.61580000	-0.26871500	-2.58812300
F	-2.70734300	-2.08426700	-0.56811300	F	2.11338600	1.71428800	-1.85573000
F	-4.09082700	-0.08458300	2.15699000	F	4.44655900	1.37210800	0.85768100
F	-2.05983800	0.37819800	2.77923200	F	2.92124100	0.49830900	2.14018000
F	-2.56121400	-1.62934000	2.11478000	F	2.43812600	2.19505900	0.86826800

TS(6→8)-Ra				TS(6→9)-Ra			
E = -1321.0206033(-1321.0672567)				E = -1321.0303925 (-1321.0846864)			
Tc = 0.271484 NImag = 1(-73.81)				Tc = 0.273464 NImag = 1 (-111.34)			
C	2.14547100	-1.95599000	-0.54823100	C	1.74242100	0.23583100	1.17515100
C	1.25666100	-2.12222500	-1.65898000	C	0.83868800	0.91649600	2.04077900
C	0.84059600	-3.52186100	-2.04661100	C	1.28571900	2.19908400	2.70485200
H	0.73424700	-3.57903900	-3.13255000	H	0.46748800	2.92401000	2.70948900
H	1.54940900	-4.27909000	-1.70440000	H	1.53070300	1.97709500	3.75038400
O	0.75541800	-1.13188500	-2.25117900	O	-0.32862400	0.47682700	2.25015800
C	2.78693100	-0.70047300	-0.13937500	S	-1.75241100	1.43672800	0.45526600
O	3.40920300	-0.86607100	1.04629400	C	-2.47653700	-0.09777900	-0.05298900
O	2.80500200	0.34529800	-0.77803000	C	-2.62061600	-0.43813500	-1.41080000
C	4.13097700	0.28175100	1.57658800	C	-3.03568000	-0.89474300	0.96041700
H	3.42601700	1.11182700	1.67957300	C	-3.30203900	-1.60764500	-1.74252600
H	4.89548100	0.56858800	0.84848000	H	-2.23617700	0.20722500	-2.19203100
C	4.73157400	-0.12652600	2.90611000	C	-3.71225300	-2.05980300	0.60754100
H	5.28442700	0.72001700	3.32493500	H	-2.92083900	-0.61903800	2.00278000
H	3.95314200	-0.41420100	3.61901600	C	-3.84201400	-2.42005200	-0.73959600
H	5.42575400	-0.96334100	2.78483700	H	-3.42037800	-1.87598700	-2.78714400
H	2.41443400	-2.83372500	0.03037400	H	-4.13388400	-2.68884400	1.38441400
H	-0.13888900	-3.73987000	-1.60305100	H	-4.37293200	-3.32783600	-1.00743700
S	-0.74287700	-0.25244100	-0.23722100	C	-0.40170100	1.74746700	-0.57601200
C	-2.36240000	-0.57310400	0.34832900	C	-0.01901700	3.10623500	-0.71723200
C	-2.51416800	-1.75018600	1.11905400	C	0.37722100	0.72182400	-1.19647200
C	-3.48991900	0.19966000	-0.01647800	C	1.04968000	3.42844700	-1.53355800
C	-3.78014600	-2.12111000	1.55298400	H	-0.58854700	3.88463900	-0.22044200
H	-1.64496300	-2.34277900	1.38498700	C	1.43670500	1.08076100	-2.04132800
C	-4.74823000	-0.19375900	0.41903700	H	0.07635000	-0.31384500	-1.11026600
H	-3.37957700	1.06861900	-0.65420900	C	1.76863300	2.41871800	-2.21069200
C	-4.89624000	-1.34505500	1.20721500	H	1.32673000	4.46869500	-1.66609800
H	-3.90161400	-3.01113500	2.16076500	H	1.99485900	0.30302300	-2.55017300
H	-5.61913800	0.38706500	0.13493600	H	2.59087800	2.69420400	-2.86264000
H	-5.88427700	-1.64412400	1.54181800	C	1.67700800	-1.20318000	0.81560500
C	-0.60771500	1.49012600	-0.35589600	O	2.80303900	-1.54187400	0.15947100
C	0.28378400	1.98454100	-1.33966500	O	0.77927300	-1.98551100	1.07994600
C	-1.26995100	2.37302000	0.53226400	C	2.93921200	-2.93737500	-0.24032200
C	0.47944600	3.35690900	-1.44606700	H	2.11564800	-3.17718700	-0.91910200
H	0.78712000	1.29041400	-2.00047600	H	2.84066100	-3.55766400	0.65468900
C	-1.04635300	3.73634400	0.41538300	C	4.29271800	-3.09562100	-0.90169200
H	-1.91205400	1.99017000	1.31625700	H	4.41922300	-4.13715000	-1.21286300
C	-0.18228300	4.23195900	-0.57655800	H	4.37626000	-2.46021100	-1.78820500
H	1.14616300	3.74525700	-2.20841900	H	5.10124300	-2.84402700	-0.20905900
H	-1.53311600	4.41968400	1.10298700	H	2.68507700	0.71979300	0.94259000

H	-0.02170600	5.30185300	-0.66163300	H	2.16780500	2.63673500	2.23349800
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2 (Ph₂S-OSO₂CF₃) E = -1822.7187725 (-1822.7541709) Tc = 0.160287 Nimag = 0				Diphenyl Sulfide E = -936.7077149 (-936.7322283) Tc = 0.144835 Nimag = 0			
16	0.596570	0.071336	-0.772511	16	-0.002373	1.292310	-0.890218
6	1.998715	-0.902220	-0.263990	6	-1.390891	0.306176	-0.236678
6	2.850962	-1.283611	-1.309051	6	-2.138011	-0.458741	-1.134786
6	2.221162	-1.274182	1.068045	6	-1.720531	0.367619	1.119776
6	3.986945	-2.030688	-0.993451	6	-3.221067	-1.204438	-0.655514
1	2.640970	-1.008504	-2.337451	1	-1.886001	-0.473661	-2.191342
6	3.353270	-2.035397	1.353272	6	-2.808322	-0.372839	1.586020
1	1.525067	-1.004774	1.853619	1	-1.140951	0.990268	1.794170
6	4.235574	-2.403787	0.330043	6	-3.554451	-1.161687	0.700917
1	4.663413	-2.331512	-1.785983	1	-3.807112	-1.805290	-1.344111
1	3.542987	-2.342830	2.376021	1	-3.074095	-0.335039	2.638130
1	5.114078	-2.995327	0.566211	1	-4.399462	-1.735598	1.068969
6	0.844342	1.738862	-0.246410	6	1.380816	0.240811	-0.314180
6	0.165896	2.695023	-1.023710	6	2.152789	0.673439	0.762855
6	1.664134	2.097870	0.834955	6	1.682319	-0.937161	-1.003481
6	0.302976	4.040472	-0.690771	6	3.237506	-0.107449	1.176835
1	-0.446282	2.393181	-1.867027	1	1.905618	1.606465	1.258906
6	1.784792	3.448130	1.148098	6	2.766166	-1.710459	-0.580110
1	2.200119	1.353237	1.409739	1	1.086568	-1.254084	-1.854889
6	1.106250	4.413462	0.391806	6	3.542303	-1.297509	0.509380
1	-0.210499	4.792867	-1.279096	1	3.843871	0.217896	2.016867
1	2.413280	3.748600	1.979275	1	3.007480	-2.629629	-1.105223
1	1.212938	5.463399	0.644474	1	4.386851	-1.899260	0.831146
8	-0.568922	-0.425972	0.400841	8	0.067932	2.576800	-0.056918
16	-1.832432	-1.454348	-0.027111				
8	-1.930049	-2.423525	1.045375				
8	-1.718766	-1.805755	-1.431675				
6	-3.255864	-0.211228	0.190242				
9	-3.203493	0.308497	1.410499				
9	-4.391972	-0.881896	0.023628				
9	-3.148456	0.745138	-0.724864				

OSO₂CF₃ E = -961.6368 (-961.6421666) Tc = -0.006209 Nimag = 0				Triflic anhydride E = -1847.630344 (-1847.6464949) Tc = 0.005983 Nimag = 0			
8	1.255094	-1.084855	-0.955413	8	-0.051209	-0.394209	0.623383
16	0.919619	0.000006	-0.000022	16	-1.350213	-0.738250	-0.418950
8	1.255035	1.369845	-0.461771	8	-1.939848	-1.996473	-0.006904
8	1.255247	-0.285070	1.417022	8	-0.982191	-0.443961	-1.790338
6	-0.961636	-0.000048	0.000040	6	-2.403230	0.693440	0.268686
9	-1.447029	0.248835	-1.233604	9	-1.790443	1.843521	0.021327
9	-1.446724	0.944141	0.832333	9	-2.577180	0.526222	1.572673
9	-1.447035	-1.192884	0.401428	9	-3.572406	0.647507	-0.362846
				16	1.557149	-0.818777	0.380213
				8	2.082983	-1.049038	1.709287
				8	1.658892	-1.773331	-0.706502
				6	2.191758	0.872594	-0.216266
				9	1.899796	1.793113	0.694586
				9	3.509550	0.770696	-0.363426
				9	1.620554	1.171422	-1.376328

(1 + OSO₂CF₃) E = -1422.0290125 (-1422.0535337) Tc = 0.121988 Nimag = 0				TS(1→3)-Rb E = -1421.9701897 (-1421.9982094) Tc = 0.128873 Nimag = 1(-173.3)			
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C	-1.85980300	0.38060000	0.17823200	C	1.60559200	1.41207100	-0.46148700
C	-1.97564100	1.85267200	-0.21910300	C	0.81220700	2.46722500	0.04894400
C	-0.88986400	2.75565900	0.30971000	C	0.24940400	3.46239800	-0.96575800
H	-0.98460500	3.75340500	-0.12159300	H	-0.83835700	3.52827900	-0.85274900
H	-0.96998600	2.82097900	1.40156600	H	0.65734900	4.45676800	-0.74838600
O	-2.88788100	2.26042200	-0.92414200	O	0.50268700	2.64903300	1.26540000
C	-3.00300000	-0.45617800	-0.34647100	C	2.39089700	0.48407700	0.29905900
O	-4.03689800	-0.47662500	0.50824400	O	3.12884100	-0.33576000	-0.53906100
O	-2.99736900	-1.03661600	-1.41930500	O	2.47281000	0.34552600	1.52808500
C	-5.22232500	-1.22204600	0.10430100	C	3.95069800	-1.33962200	0.08787300
H	-4.93225900	-2.26373600	-0.05788100	H	3.32080800	-1.99126700	0.70293600
H	-5.57945400	-0.81021400	-0.84343600	H	4.67539900	-0.85386200	0.75002000
C	-6.25005500	-1.08241600	1.20936700	C	4.64636000	-2.12223000	-1.01243400
H	-7.15433400	-1.63361600	0.93276400	H	5.28227000	-2.89553000	-0.56878100
H	-5.87400200	-1.49176500	2.15182800	H	3.91876100	-2.61185200	-1.66771400
H	-6.52160300	-0.03390700	1.36446100	H	5.27794000	-1.46811600	-1.62221600
H	-0.91148900	0.00230800	-0.21959700	H	-0.13103100	0.53788000	0.79385300
O	1.44249100	0.26790700	-0.65406800	O	-0.82650400	0.00206800	1.26024400
S	2.71118900	-0.49368500	-0.77364000	S	-1.45418800	-1.16433100	0.37230600
O	2.56230400	-1.96905100	-0.73457300	O	-0.55674500	-1.58317200	-0.69681600
O	3.65501300	0.01790400	-1.79735700	O	-2.05453800	-2.11817800	1.29297900
C	3.58933100	-0.11041100	0.84549100	C	-2.88415600	-0.24732800	-0.44604800
F	4.78388100	-0.73320400	0.90763400	F	-3.54510300	-1.10434400	-1.23075900
F	2.85672300	-0.51576900	1.90298800	F	-2.41619400	0.76144900	-1.18642800
F	3.80681700	1.21412500	0.97789100	F	-3.71280800	0.23120400	0.48468700
H	-1.80492500	0.31976800	1.27034800	H	1.72558700	1.34991000	-1.53699400
H	0.09370300	2.33056700	0.08360300	H	0.48679300	3.20663400	-2.00190200

(3 + HOSO₂CF₃)				(4 + ⁻OSO₂CF₃)			
E = -1422.0289731 (-1422.0507977)				E = -2282.7339243(-2282.7985396)			
Tc = 0.126979 NImag = 0				Tc = 0.283781 NImag = 0			
C	-3.52262800	1.52192300	0.06017500	C	-0.54164800	-0.68061800	0.49018200
C	-2.40141200	2.30381900	0.08195400	C	-0.46016500	-1.71542900	1.63737600
C	-2.42456800	3.79406000	0.19412800	C	0.66326500	-2.70693200	1.53543900
H	-1.87702700	4.10839200	1.08950000	H	1.61596800	-2.16551600	1.55790700
H	-1.92051300	4.24008300	-0.67024600	H	0.60600100	-3.41392800	2.36361100
O	-1.16406900	1.79486600	0.00396200	O	-1.25395200	-1.67436100	2.55974400
C	-3.41817100	0.08366300	-0.05095900	C	-1.10042400	-1.26499900	-0.81787300
O	-4.60558900	-0.54635500	-0.05769300	O	-1.76532800	-2.39134500	-0.59421500
O	-2.34018800	-0.53407500	-0.13398400	O	-0.94076700	-0.74033500	-1.90165600
C	-4.59422000	-1.99731300	-0.16680200	C	-2.34098700	-3.07969000	-1.75810000
H	-4.01648600	-2.40329400	0.66807200	H	-1.52231100	-3.30566800	-2.44517200
H	-4.09208700	-2.27046700	-1.09906300	H	-3.03039900	-2.38499300	-2.24271000
C	-6.03524200	-2.46718400	-0.14039700	C	-3.03279900	-4.32614100	-1.25051600
H	-6.06100700	-3.55838600	-0.22196300	H	-3.47035300	-4.85800900	-2.10086200
H	-6.52557900	-2.18160600	0.79518700	H	-2.32546600	-4.99632400	-0.75394000
H	-6.60219900	-2.04731400	-0.97682400	H	-3.83610900	-4.07550400	-0.55207300
H	-1.25036900	0.80687400	-0.06577500	H	0.45766900	-0.26690800	0.29422700
O	1.41929100	-0.54410300	-0.39164700	H	0.62310700	-3.24506700	0.58313100
S	2.62964300	-0.92987600	0.37413800	S	-1.54650000	0.76173500	1.12811100
O	2.61278100	-0.55309600	1.80934800	C	-0.86055900	2.23411800	0.35188600
O	3.14659500	-2.29163400	0.08925300	C	-0.88772000	3.36898300	1.17353600
C	3.96213800	0.18809600	-0.34262900	C	-0.32897700	2.26868200	-0.94163700
F	5.15240000	-0.03212500	0.25296600	C	-0.38645300	4.57205300	0.67384800
F	3.64954000	1.48881300	-0.17054500	H	-1.28665600	3.31741400	2.18136100
F	4.11730100	-0.02693200	-1.66535900	C	0.17792000	3.48001300	-1.41684700
H	-4.50192800	1.97633000	0.12674200	H	-0.30517700	1.38136300	-1.56340200
H	-3.44621300	4.17239900	0.24786700	C	0.14574900	4.62672900	-0.61734400
				H	-0.40288100	5.45782800	1.30001900
				H	0.59776400	3.52184600	-2.41649300
				H	0.54295600	5.56193800	-0.99892500
				C	-3.22239500	0.55512200	0.48177800

	C	-3.62246100	1.08167300	-0.74940000
	C	-4.10819200	-0.13046800	1.32161900
	C	-4.94770300	0.90027300	-1.15033000
	H	-2.93241000	1.62765900	-1.38119400
	C	-5.42686900	-0.30687800	0.89896200
	H	-3.77525100	-0.52109100	2.27700500
	C	-5.84515100	0.20690600	-0.33227100
	H	-5.27433800	1.30517700	-2.10251700
	H	-6.12478900	-0.83785200	1.53780500
	H	-6.87347900	0.07255700	-0.65239200
	O	2.49789400	0.10047300	0.52802200
	S	3.56502200	0.22382500	-0.50197600
	O	3.26929300	-0.45536000	-1.78533500
	O	4.16356700	1.57418100	-0.61855800
	C	4.96119500	-0.80646700	0.22402400
	F	4.57585900	-2.08573200	0.40584200
	F	6.03230500	-0.80863200	-0.59433100
	F	5.35188000	-0.31802200	1.41809500

TS(4→5)-Rb E = -2282.7009906 (-2282.7697582) Tc = 0.28362 NImag = 1 (-501.28)	(5 + HOSO₂CF₃) E = -2282.7018917 (-2282.7695155) Tc = 0.28619 NIMag = 0						
C	-0.44002400	-0.85938400	0.66446900	C	0.56136800	-0.96804300	-0.58330300
C	-0.17802700	-1.73359900	1.85409300	C	0.27227400	-1.90291300	-1.69903700
C	-0.47301400	-1.19527800	3.24787500	C	0.58846000	-1.47727300	-3.13437900
H	-1.54763100	-1.22805400	3.45953200	H	1.66850500	-1.48161100	-3.32284700
H	0.03878900	-1.83626600	3.96702900	H	0.11972800	-2.20545400	-3.79767000
O	0.32212700	-2.84893900	1.73221700	O	-0.23348400	-3.00228300	-1.49995400
C	-0.38264100	-1.37881900	-0.73354800	C	0.42139300	-1.32352300	0.84552100
O	0.60402100	-2.26154500	-0.92206200	O	-0.64449700	-2.09747700	1.08728200
O	-1.11777300	-0.99536700	-1.63703200	O	1.16781000	-0.91372000	1.73047300
C	0.77721100	-2.76801300	-2.27758300	C	-0.87935700	-2.46091200	2.47168200
H	0.96595600	-1.91907200	-2.93999700	H	-1.07328500	-1.54608500	3.03964900
H	-0.15398500	-3.24950600	-2.58807000	H	0.02823400	-2.92389800	2.87042100
C	1.93865000	-3.74156400	-2.25430800	C	-2.06123700	-3.41123700	2.49516600
H	2.09599100	-4.13738500	-3.26268800	H	-2.26529300	-3.71441600	3.52777300
H	2.85982300	-3.24796300	-1.93145100	H	-2.95781500	-2.93149200	2.09318400
H	1.73652700	-4.58193000	-1.58349500	H	-1.85402100	-4.30727400	1.90299900
H	0.86970500	0.00600100	0.78026200	H	-1.07806500	-0.01623500	-0.84306500
H	-0.14408800	-0.16074100	3.37801600	H	0.21460600	-0.47569200	-3.36791400
S	-1.72605100	0.35317200	0.98125200	S	1.74650900	0.27594000	-0.95700700
C	-1.39340700	1.88025900	0.07826300	C	1.39853900	1.79057600	-0.02910100
C	-1.04606500	2.96867100	0.88806900	C	0.76248000	2.80171100	-0.75872200
C	-1.49376200	2.00051200	-1.31229700	C	1.74423300	1.96347100	1.31459600
C	-0.77473000	4.20027600	0.28699600	C	0.44737600	4.00377000	-0.12203200
H	-0.98797900	2.85950600	1.96594800	H	0.50438000	2.65103100	-1.80205100
C	-1.22502300	3.24018100	-1.89430600	C	1.43392400	3.17660500	1.93114200
H	-1.76449300	1.14531900	-1.91678800	H	2.21601600	1.16007600	1.86480900
C	-0.86416300	4.33500500	-1.10065700	C	0.78509900	4.19095500	1.22008600
H	-0.50119100	5.04887900	0.90542200	H	-0.06145300	4.78594400	-0.67608600
H	-1.29652200	3.34775300	-2.97195100	H	1.68888800	3.32066100	2.97650900
H	-0.65644500	5.29380700	-1.56542900	H	0.53880400	5.12602800	1.71397900
C	-3.32712900	-0.25381500	0.36505400	C	3.42018100	-0.20991400	-0.41898500
C	-4.32422100	0.67245600	0.05018800	C	4.43769200	0.74729100	-0.46943600
C	-3.57881500	-1.62680500	0.36600200	C	3.69038000	-1.54202100	-0.11107300
C	-5.59432800	0.20281400	-0.29652300	C	5.74733100	0.36002700	-0.17857200
H	-4.12603300	1.73815700	0.06496800	H	4.21751800	1.78046200	-0.71921800
C	-4.85450800	-2.07912200	0.02043900	C	5.00651700	-1.91680200	0.17158400
H	-2.80383500	-2.34093700	0.62008100	H	2.89153800	-2.27376000	-0.07776900
C	-5.86107100	-1.16861100	-0.31364400	C	6.03304200	-0.97022900	0.14233700
H	-6.37149100	0.91620500	-0.55152300	H	6.54165200	1.09969200	-0.20659500

H	-5.05411700	-3.14582300	0.00986700	H	5.22242500	-2.95059100	0.42287200
H	-6.84928100	-1.52655400	-0.58443400	H	7.05277900	-1.26732200	0.36722000
O	1.76289000	0.62218700	1.04439500	O	-1.84168100	0.54117600	-1.21499200
S	2.76670700	1.01895700	-0.08401700	S	-2.87141500	1.05014400	-0.10234200
O	2.29099000	0.62591100	-1.41070700	O	-2.34955600	0.80469100	1.23590900
O	3.26762600	2.37305200	0.14502200	O	-3.37914000	2.34751700	-0.51507800
C	4.21163300	-0.11889900	0.31795700	C	-4.27328300	-0.17657200	-0.38058700
F	3.83213800	-1.39982500	0.25544800	F	-3.84087600	-1.42520300	-0.18940700
F	5.18899300	0.09141500	-0.57459800	F	-5.25029700	0.09123300	0.49530500
F	4.67901900	0.14002700	1.54526500	F	-4.75224300	-0.05896800	-1.62224000

(1 + 2)-Rb				TS(1→6)-Rb			
E = -2283.099574 (-2283.1628138)				E = -2283.0862753 (-2283.1493221)			
Tc = 0.296658				Tc = 0.294337 NImag = 0			
C	-0.63913700	1.59240700	0.74673800	C	-0.73111000	1.16449200	1.09686000
C	0.10376400	0.70282100	1.70895300	C	0.17120100	0.32578200	1.79283500
C	-0.31611900	0.69710900	3.14397000	C	-0.15490900	-0.19155700	3.15091000
H	-1.36006100	0.35977400	3.16900000	H	-1.13365700	-0.68562200	3.09365700
H	0.31447400	0.03950800	3.74052200	H	0.59768100	-0.89537100	3.50336700
O	1.03138000	-0.05564800	1.37644500	O	1.31016500	-0.16722000	1.35053100
C	0.23932700	2.61180900	0.03017400	C	-0.25001000	2.26301300	0.19857400
O	-0.45614700	3.70860700	-0.24543400	O	-1.23940500	3.11451500	-0.05672200
O	1.40709200	2.43040300	-0.26953900	O	0.88919500	2.37559600	-0.23148200
C	0.22453200	4.76718900	-0.99822200	C	-0.93307100	4.26297800	-0.91293700
H	0.56326100	4.33986600	-1.94509600	H	-0.57278400	3.88077600	-1.87121700
H	1.09666100	5.08057500	-0.41961500	H	-0.13160900	4.83264000	-0.43654600
C	-0.77063400	5.89082500	-1.19600800	C	-2.20539000	5.07093400	-1.05724000
H	-0.28985500	6.69786900	-1.75738400	H	-2.00618200	5.93753600	-1.69514900
H	-1.64213200	5.55040600	-1.76253600	H	-2.99870600	4.47806600	-1.52149700
H	-1.10677700	6.29343400	-0.23614700	H	-2.55534900	5.43282700	-0.08612600
H	-1.10228400	0.94247800	-0.01408500	H	-1.40889900	0.32478000	0.30612400
O	-2.30103300	-0.73462600	-0.82418800	O	-2.08491100	-0.40663900	-0.51745600
S	-3.29731100	-1.14186800	0.20687600	S	-3.16406000	-1.31276400	0.10056000
O	-3.80188700	-2.52664200	0.07300100	O	-3.33433600	-2.55143000	-0.66497500
O	-2.94884400	-0.71621300	1.58477600	O	-3.04905600	-1.39196900	1.56479100
C	-4.79484700	-0.08464100	-0.21169500	C	-4.72629200	-0.31732700	-0.22128600
F	-5.80440400	-0.32635500	0.64662500	F	-5.78688400	-0.97881700	0.26447100
F	-5.23519100	-0.34401700	-1.45795200	F	-4.89962600	-0.12903800	-1.53680600
F	-4.49262100	1.22653400	-0.14050500	F	-4.64957900	0.87849100	0.38063000
S	1.91833300	-0.41374700	-0.65909300	S	1.86217100	-0.15819300	-0.35940000
C	3.52605400	-0.00084300	-0.18170700	C	3.43738200	0.62379200	-0.13060600
C	4.21907700	-0.63649900	0.87970100	C	4.23637100	0.40318100	0.99998400
C	4.09383000	1.09149800	-0.88767800	C	3.81964900	1.48344300	-1.16976800
C	5.49756300	-0.20343600	1.18750000	C	5.46326900	1.05948400	1.07238300
H	3.74329100	-1.40758600	1.47289400	H	3.90581200	-0.23646500	1.80961200
C	5.38940600	1.48028500	-0.58249000	C	5.06409000	2.10791500	-1.08459700
H	3.52885200	1.59655600	-1.66197300	H	3.16744000	1.66345700	-2.01716500
C	6.08802400	0.83801600	0.44999000	C	5.87937600	1.89873500	0.03124400
H	6.03631500	-0.66202800	2.00893300	H	6.09351900	0.91354600	1.94300700
H	5.85148300	2.29169100	-1.13312200	H	5.38342100	2.76978100	-1.88219000
H	7.09223600	1.16441500	0.70007700	H	6.83953200	2.39995800	0.09741000
C	1.74218200	-2.12600600	-0.62406700	C	2.12826700	-1.89353200	-0.50199500
C	0.40435000	-2.57557300	-0.82755600	C	1.00258400	-2.59902200	-0.97592200
C	2.81923200	-3.05142800	-0.52855800	C	3.34720500	-2.54053400	-0.23214700
C	0.15798400	-3.93592200	-0.88611100	C	1.10036300	-3.97557200	-1.15167900
H	-0.41813400	-1.86901200	-0.91514900	H	0.07477400	-2.08125600	-1.19832600
C	2.54293800	-4.40383300	-0.60660500	C	3.42281000	-3.91619700	-0.42326300
H	3.84351200	-2.71165700	-0.46019600	H	4.21820900	-1.98903700	0.09660300
C	1.21884600	-4.84884900	-0.77001700	C	2.30539200	-4.63117600	-0.87450300
H	-0.85607300	-4.29228500	-1.02635700	H	0.24259300	-4.53245100	-1.51205700
H	3.35548500	-5.12004600	-0.56131600	H	4.35688600	-4.43094900	-0.22660400
H	1.01784200	-5.91356900	-0.82856800	H	2.37956200	-5.70376000	-1.02164200

H	-0.28899800	1.72295600	3.52805800	H	-0.24926300	0.65066100	3.84423900
H	-1.44823800	2.10442200	1.26567000	H	-1.54425100	1.49464600	1.74270100
(6 + HOSO₂CF₃) E = -2283.1067466 (-2283.1649893) Tc = 0.299199 NImag = 0				(6 + OSO₂CF₃) E = -2282.6985767 (-2282.75504) Tc = 0.283799 NImag = 0			
C	-0.36439000	1.55060600	1.35348100	C	0.16708300	1.84896300	2.19208100
C	0.26624600	0.46165200	1.83937500	C	1.10718400	0.92597800	2.46220700
C	-0.21891100	-0.37598100	2.97517800	C	1.30360600	0.25086600	3.77835600
H	-1.14395900	0.02759800	3.38842300	O	2.10499600	0.52779100	1.55236100
H	-0.38186900	-1.40731900	2.64607600	C	0.01324800	2.60214100	0.93761000
O	1.52199500	0.00511600	1.42062700	O	-0.97546100	3.50149100	1.03934000
C	0.16828700	2.51189600	0.37248500	O	0.69638700	2.45868800	-0.07230000
O	-0.68009000	3.53266800	0.19902300	C	-1.23607200	4.34084300	-0.12424700
O	1.25109900	2.42165200	-0.19765800	H	-1.47953400	3.68857800	-0.96716000
C	-0.27213600	4.59347000	-0.71704000	H	-0.32031500	4.88883200	-0.36197000
H	-0.08780400	4.14462300	-1.69657900	C	-2.38048700	5.26835900	0.23027800
H	0.66406800	5.01982500	-0.34710900	H	-2.59934600	5.91240800	-0.62710500
C	-1.38981100	5.61520100	-0.75594200	H	-3.28474400	4.70316400	0.47449600
H	-1.11066000	6.42584800	-1.43602700	H	-2.12207200	5.90585800	1.08104600
H	-2.32024600	5.16832800	-1.11841000	S	1.65157000	-0.11797100	0.06644500
H	-1.56647400	6.04418500	0.23479600	C	3.04871200	0.46534800	-0.91371400
H	-1.93077300	0.04684300	-0.10691900	C	3.74266700	1.61784400	-0.54178100
O	-2.46238100	-0.34436700	-0.83137400	C	3.32879000	-0.22676600	-2.09719700
S	-3.61917400	-1.31187600	-0.25806700	C	4.76854700	2.07021900	-1.37540600
O	-3.94102600	-2.24855900	-1.32040400	H	3.49801200	2.14375200	0.37135600
O	-3.30946900	-1.73514300	1.10072500	C	4.34827400	0.25169400	-2.92184500
C	-5.05751500	-0.09375400	-0.14968400	H	2.77794000	-1.11835300	-2.37657000
F	-6.13410800	-0.75914600	0.27330100	C	5.06888900	1.39412700	-2.56117800
F	-5.29814100	0.43341900	-1.34978000	H	5.32776900	2.95626500	-1.09330100
F	-4.76112900	0.87655000	0.71692600	H	4.57836400	-0.27611300	-3.84136900
S	1.86228000	-0.24112900	-0.20801900	H	5.86420000	1.75688300	-3.20437900
C	3.54839900	0.37846200	-0.25322700	C	2.00151400	-1.84715900	0.28712300
C	4.27615300	0.61926600	0.91305500	C	0.88565600	-2.69298800	0.20477200
C	4.07009500	0.60901800	-1.52934700	C	3.29096300	-2.32936800	0.56245500
C	5.58177100	1.09940000	0.78469900	C	1.07897400	-4.06421900	0.39119900
H	3.84000700	0.45546800	1.89069300	H	-0.10255300	-2.29088200	-0.00492500
C	5.38032500	1.07992400	-1.63299200	C	3.45696600	-3.69716400	0.75547900
H	3.47786900	0.43233900	-2.42163700	H	4.13807500	-1.65520700	0.62495400
C	6.13294700	1.32457900	-0.48021600	C	2.35505800	-4.56097200	0.66649300
H	6.16379300	1.29712500	1.67881100	H	0.23159800	-4.73813500	0.32298700
H	5.80329200	1.26480900	-2.61470700	H	4.44376400	-4.09282300	0.97166000
H	7.14824100	1.69774200	-0.56753200	H	2.49758200	-5.62699300	0.81314700
C	2.02336900	-2.01306400	-0.24796000	O	-2.01982100	-1.22389700	-0.46534600
C	0.98889800	-2.67999700	-0.92224600	S	-3.39802800	-1.55730000	-0.02371600
C	3.09179500	-2.70381800	0.34270000	O	-3.85537200	-2.92223800	-0.38128200
C	1.02831500	-4.07268900	-1.00030300	O	-3.73743000	-1.11764100	1.35143400
H	0.17668000	-2.12439800	-1.37974800	C	-4.46748000	-0.45007500	-1.10483300
C	3.10969200	-4.09326000	0.25862600	F	-4.27371300	-0.71640300	-2.41255900
H	3.88949800	-2.17397700	0.85033400	F	-5.77632000	-0.63142500	-0.83573000
C	2.08324500	-4.77422200	-0.41060800	F	-4.17999300	0.85147700	-0.90093100
H	0.23929200	-4.60348900	-1.52198100	H	1.15861200	-0.83010600	3.67581500
H	3.92715100	-4.64610700	0.70910800	H	0.60611100	0.64050400	4.52117400
H	2.11203800	-5.85720500	-0.47522900	H	-0.52694500	2.09133300	2.98769900
H	0.54255900	-0.39841100	3.76264400	H	2.32810500	0.41295200	4.13097800
H	-1.31366600	1.80577900	1.81062600				

TS(6→7)-Rb E = -2282.670396 (-2282.7302316) Tc = 0.280895 NImag = 1 (-155.37)				(7 + Ph₂S)-Rb E = -2282.7322262 (-2282.7884838) Tc = 0.279956			
C	-1.17156100	0.39505700	1.46817500	C	-2.08930300	1.36689500	0.45232500
C	0.11898100	-0.18506900	1.64928100	C	-1.64306300	1.81756800	1.87111800

C	0.23769800	-1.54822800	2.27834000	C	-0.89948000	0.83853300	2.73184100
O	1.15057300	0.45870000	1.30283600	H	-1.54543000	-0.01373500	2.96871900
C	-1.42434100	1.67111300	0.74766300	H	-0.02914900	0.43716800	2.20080200
O	-2.54180200	2.23939000	1.22428700	O	-1.91825300	2.95259200	2.20798200
O	-0.74384400	2.13178600	-0.15267500	C	-1.18406800	1.95521000	-0.64761100
C	-2.95281000	3.50140700	0.61839900	O	-1.40892100	3.25381800	-0.78379600
H	-3.11874000	3.32324000	-0.44768400	O	-0.39066500	1.28989600	-1.28139800
H	-2.13052400	4.21402800	0.72710000	C	-0.60463600	3.97343300	-1.77790900
C	-4.20968100	3.96241900	1.32668800	H	-0.77027000	3.49727300	-2.74712600
H	-4.54133900	4.90821600	0.88712400	H	0.44636800	3.85932900	-1.50224200
H	-5.01545200	3.23102300	1.21590300	C	-1.05149400	5.41940700	-1.76135100
H	-4.02438000	4.12572000	2.39238700	H	-0.46626100	5.98050500	-2.49642000
S	2.30010900	-0.15585400	-0.76354300	H	-2.10935900	5.50828400	-2.02482700
C	3.27401000	1.32484300	-0.76062400	H	-0.89162700	5.87092900	-0.77806100
C	2.55558700	2.53460300	-0.71790000	H	-3.11322600	1.71302500	0.29936200
C	4.67312100	1.32381800	-0.90379300	H	-0.58843300	1.33505200	3.65136000
C	3.24936200	3.74068500	-0.80353600	S	2.81979100	-1.03719100	1.52226300
H	1.47687400	2.52002300	-0.60426400	C	2.75591400	-2.25878700	0.20472400
C	5.34804800	2.54029400	-0.98881600	C	1.75498000	-3.23871100	0.29846600
H	5.22431500	0.39317900	-0.96607000	C	3.67372500	-2.30346600	-0.85369300
C	4.64262700	3.74837700	-0.93595800	C	1.67985600	-4.25572200	-0.65616400
H	2.69994600	4.67597200	-0.76376300	H	1.03350700	-3.20382000	1.10995200
H	6.42721200	2.54274100	-1.10487800	C	3.58172700	-3.31810900	-1.81141600
H	5.17663600	4.69095000	-1.00392600	H	4.45354800	-1.55395500	-0.93511300
C	3.36690000	-1.45471100	-0.20194800	C	2.58999800	-4.29928400	-1.71744900
C	3.26653400	-2.68687400	-0.87163600	H	0.90014400	-5.00744700	-0.57371000
C	4.20124300	-1.31457700	0.92136000	H	4.29515800	-3.34061300	-2.63037200
C	4.02379600	-3.77095200	-0.42797400	H	2.52519200	-5.08585200	-2.46300600
H	2.61365300	-2.78970300	-1.73252100	C	3.74159300	0.32973800	0.80751000
C	4.95222200	-2.40644600	1.35136900	C	5.02913400	0.61137200	1.28330400
H	4.25103200	-0.37229300	1.45512900	C	3.15640900	1.15615800	-0.16429900
C	4.86729400	-3.63260600	0.67938500	C	5.73158500	1.71451800	0.78580300
H	3.95599800	-4.72043100	-0.94901400	H	5.47844100	-0.02975800	2.03511000
H	5.59683400	-2.30321200	2.21840500	C	3.86963500	2.24653300	-0.66755800
H	5.45357100	-4.47904200	1.02282000	H	2.15260100	0.94852300	-0.52208100
O	-1.95887200	-0.86163700	-0.29381800	C	5.15550000	2.52981200	-0.19201000
S	-3.16291200	-1.75093800	-0.10880800	H	6.72848800	1.92926600	1.15912000
O	-3.01845800	-3.07414400	-0.74677200	H	3.41642400	2.88077200	-1.42379900
O	-3.71937300	-1.72792000	1.25938900	H	5.70296000	3.38323500	-0.58080400
C	-4.47168100	-0.88918100	-1.15054600	O	-2.01921400	-0.07842100	0.40646700
F	-4.08751800	-0.81685500	-2.43726500	S	-2.87127700	-0.90142500	-0.70590700
F	-5.63222200	-1.56728700	-1.09381300	O	-2.05928500	-2.02601800	-1.13367400
F	-4.69099400	0.35984000	-0.70406900	O	-3.51546700	0.01468900	-1.63808900
H	0.26163900	-2.30427600	1.48368800	C	-4.21864800	-1.59627400	0.42258300
H	-0.61052300	-1.77799300	2.92695700	F	-3.66946400	-2.36228100	1.36387900
H	-1.99541600	0.01374100	2.06049100	F	-4.88484900	-0.58940200	0.99230000
H	1.17022000	-1.61772400	2.84251000	F	-5.05424700	-2.32339700	-0.32037500

TS(7→8)-Rb E = -2282.6647832 (-2282.7328431) Tc = 0.284484 NImag = 1 (-149.24)				(8 + iOX)-Rb E = -2282.7323771 (-2282.797961) Tc = 0.285914 NImag = 0			
C	-2.08930300	1.36689500	0.45232500	C	-0.51432100	0.52932400	-0.90167800
C	-1.64306300	1.81756800	1.87111800	C	-0.52721400	-0.05906400	-2.34608900
C	-0.89948000	0.83853300	2.73184100	C	0.44468300	-1.16197200	-2.64406000
H	-1.54543000	-0.01373500	2.96871900	H	1.46635300	-0.78780700	-2.49717800
H	-0.02914900	0.43716800	2.20080200	H	0.31842700	-2.00493300	-1.95590100
O	-1.91825300	2.95259200	2.20798200	O	-1.26906100	0.43861800	-3.17039000
C	-1.18406800	1.95521000	-0.64761100	C	-1.29689200	1.84005300	-0.83234000
O	-1.40892100	3.25381800	-0.78379600	O	-0.49658900	2.83385400	-1.20219300
O	-0.39066500	1.28989600	-1.28139800	O	-2.46320800	1.95203500	-0.51173100
C	-0.60463600	3.97343300	-1.77790900	C	-1.08709400	4.17359900	-1.29142600
H	-0.77027000	3.49727300	-2.74712600	H	-1.46393700	4.43712300	-0.30037600

H	0.44636800	3.85932900	-1.50224200	H	-1.92774400	4.12134500	-1.98748300
C	-1.05149400	5.41940700	-1.76135100	C	-0.00173500	5.11583800	-1.76608200
H	-0.46626100	5.98050500	-2.49642000	H	-0.41584800	6.12613300	-1.83986900
H	-2.10935900	5.50828400	-2.02482700	H	0.83618700	5.13861700	-1.06348800
H	-0.89162700	5.87092900	-0.77806100	H	0.37016800	4.82404000	-2.75238600
H	-3.11322600	1.71302500	0.29936200	H	0.53200100	0.70053600	-0.61198000
H	-0.58843300	1.33505200	3.65136000	H	0.30765100	-1.50302600	-3.67052900
S	2.81979100	-1.03719100	1.52226300	S	-1.00004600	-0.77160700	0.34667400
C	2.75591400	-2.25878700	0.20472400	C	-1.40697700	0.14318100	1.85631200
C	1.75498000	-3.23871100	0.29846600	C	-0.30967300	0.62771400	2.57800700
C	3.67372500	-2.30346600	-0.85369300	C	-2.72010200	0.28686800	2.30620100
C	1.67985600	-4.25572200	-0.65616400	C	-0.55171800	1.30080300	3.77743100
H	1.03350700	-3.20382000	1.10995200	H	0.70415500	0.49360700	2.21347500
C	3.58172700	-3.31810900	-1.81141600	C	-2.93680700	0.95049800	3.51574800
H	4.45354800	-1.55395500	-0.93511300	H	-3.55676300	-0.10327900	1.74062700
C	2.58999800	-4.29928400	-1.71744900	C	-1.85919100	1.45972700	4.24636700
H	0.90014400	-5.00744700	-0.57371000	H	0.28641800	1.68953400	4.34643500
H	4.29515800	-3.34061300	-2.63037200	H	-3.95184000	1.06901800	3.88049400
H	2.52519200	-5.08585200	-2.46300600	H	-2.03831300	1.97618600	5.18399500
C	3.74159300	0.32973800	0.80751000	C	-2.48170400	-1.61458100	-0.22209200
C	5.02913400	0.61137200	1.28330400	C	-2.44274800	-3.00526900	-0.04388100
C	3.15640900	1.15615800	-0.16429900	C	-3.58164500	-0.97380800	-0.80593800
C	5.73158500	1.71451800	0.78580300	C	-3.54048200	-3.76581600	-0.44957600
H	5.47844100	-0.02975800	2.03511000	H	-1.57645000	-3.48487900	0.39959200
C	3.86963500	2.24653300	-0.66755800	C	-4.66269700	-1.75571100	-1.21565600
H	2.15260100	0.94852300	-0.52208100	H	-3.59339600	0.10153100	-0.93190200
C	5.15550000	2.52981200	-0.19201000	C	-4.64540100	-3.14281100	-1.03621100
H	6.72848800	1.92926600	1.15912000	H	-3.52331800	-4.84203700	-0.31440900
H	3.41642400	2.88077200	-1.42379900	H	-5.52066700	-1.27428200	-1.67333100
H	5.70296000	3.38323500	-0.58080400	H	-5.49365200	-3.73880200	-1.35758600
O	-2.01921400	-0.07842100	0.40646700	O	2.30789600	0.36119600	0.51761600
S	-2.87127700	-0.90142500	-0.70590700	S	3.62347300	0.18063100	-0.15621600
O	-2.05928500	-2.02601800	-1.13367400	O	4.70800200	1.05020800	0.35262900
O	-3.51546700	0.01468900	-1.63808900	O	3.54278200	0.05447400	-1.63153900
C	-4.21848800	-1.59627400	0.42258300	C	4.14421400	-1.53945100	0.39841500
F	-3.66946400	-2.36228100	1.36387900	F	4.26772400	-1.59876700	1.73903600
F	-4.88484900	-0.58940200	0.99230000	F	3.23527100	-2.46170500	0.02387700
F	-5.05424700	-2.32339700	-0.32037500	F	5.32946900	-1.87961900	-0.14417800

(9 + \cdotOX)-Rb				TS(9\rightarrow10)-Rb			
E = -2282.7241804 (-2282.7878425)				E = -2282.7160306 (-2282.7856902)			
Tc = 0.283104 NImag = 0				Tc = 0.283871 NImag = 0			
C	0.25182800	-2.44527400	-0.39841100	C	-0.18721300	2.06525000	-0.22248100
C	0.64802300	-1.95842500	-1.81426600	C	-0.46537400	1.64522300	-1.68521800
C	0.59909300	-2.98168800	-2.91692800	C	-0.57161700	2.76917700	-2.68722000
H	1.02048900	-3.94175800	-2.60500900	H	-1.14821700	3.61544700	-2.30240500
H	-0.45304000	-3.16093100	-3.17223100	H	0.43818900	3.14022700	-2.90259400
O	0.95222000	-0.79407400	-2.00251000	O	-0.55843700	0.47450700	-2.00166700
S	-2.24167500	-0.66068700	-0.90979600	S	2.53071800	0.78013800	-0.83461200
C	-3.88752100	-0.05568200	-0.51906900	C	4.15337800	0.05964300	-0.56257500
C	-4.14332300	1.32037900	-0.57352100	C	4.40214600	-1.25644300	-0.97380000
C	-4.91396600	-0.97466000	-0.26674900	C	5.18082600	0.85081500	-0.03161600
C	-5.44426800	1.77874900	-0.35122100	C	5.68746200	-1.78674500	-0.83463300
H	-3.34138900	2.02015300	-0.78382800	H	3.60259400	-1.85674300	-1.39532200
C	-6.21010300	-0.50231900	-0.04621800	C	6.46234200	0.31032200	0.10324000
H	-4.70380200	-2.03881000	-0.24179400	H	4.98056200	1.87319200	0.27202900
C	-6.47434800	0.87039500	-0.08758800	C	6.71525900	-1.00583400	-0.29628400
H	-5.64982300	2.84382800	-0.38754200	H	5.88336400	-2.80693800	-1.14958500
H	-7.01027500	-1.20783000	0.15379400	H	7.26033100	0.91917200	0.51665300
H	-7.48399400	1.23195600	0.08087700	H	7.71304200	-1.42099700	-0.19253300
C	-1.41646000	-0.75478100	0.60736600	C	1.64652700	0.47356600	0.65095800
C	-1.99946900	-0.37598500	1.82152800	C	2.21531500	-0.20806900	1.73574200

C	0.00979900	-1.23295300	0.57291000	C	0.25601800	0.92543200	0.73473000
C	-1.28891600	-0.48857200	3.00695800	C	1.52814800	-0.32435800	2.93753700
H	-3.01676700	-0.00632700	1.84342400	H	3.21741800	-0.60964900	1.65482000
C	0.65785800	-1.35010200	1.90510400	C	-0.35048800	0.87403500	2.05464800
H	0.55942100	-0.37535200	0.10516300	H	-0.28391300	-0.21613700	0.38730600
C	0.04741700	-0.97140200	3.05804000	C	0.24410700	0.22772500	3.11039500
H	-1.77665400	-0.19249500	3.93109500	H	2.00425800	-0.84396900	3.76358500
H	1.68810100	-1.68807600	1.91952200	H	-1.35617700	1.26025400	2.17028300
H	0.56426600	-1.03015700	4.00876000	H	-0.26693700	0.14511800	4.06264800
C	1.30723300	-3.44394800	0.10801200	C	-1.39418300	2.85750600	0.30672200
O	2.54549800	-2.98750800	-0.09127400	O	-2.54646800	2.24434900	0.02641600
O	1.03027200	-4.51422700	0.61269900	O	-1.29769800	3.91605900	0.89804300
C	3.65940000	-3.84749700	0.32217800	C	-3.78365700	2.90737400	0.44729200
H	3.57337900	-4.78839400	-0.22666100	H	-3.79794900	3.90304400	-0.00276200
H	3.54763700	-4.05155600	1.38987300	H	-3.75538300	3.01460300	1.53451300
C	4.94335200	-3.10987400	0.00719100	C	-4.94136800	2.04851500	-0.01567700
H	5.79278600	-3.73177500	0.30602200	H	-5.87979000	2.52367600	0.28654100
H	5.02814600	-2.90448400	-1.06375600	H	-4.94447900	1.94464900	-1.10456700
H	4.99995800	-2.16489900	0.55486300	H	-4.89877700	1.05310900	0.43486000
O	0.75529000	1.83977200	0.52297400	O	-0.63584100	-1.56330200	0.18057000
S	1.85141400	2.80160400	0.80254200	S	-1.93167100	-2.19371000	0.65799500
O	1.45502400	3.98003500	1.61123200	O	-1.74007500	-3.57526800	1.13051100
O	3.14502600	2.18265100	1.17996600	O	-2.75904300	-1.29866600	1.48507000
C	2.20717800	3.54226600	-0.88954200	C	-2.90118400	-2.39072600	-0.94136200
F	1.11151600	4.14532900	-1.39418300	F	-2.19585800	-3.09620000	-1.84143100
F	2.59556900	2.59210300	-1.76354000	F	-3.20225800	-1.19732700	-1.47307400
F	3.18921200	4.46358100	-0.81618700	F	-4.05017600	-3.04669000	-0.69477900
H	1.12172700	-2.60835200	-3.79802000	H	-1.01799800	2.40072800	-3.61160200
H	-0.66613700	-3.03347200	-0.47264000	H	0.62156900	2.80442200	-0.24638700

(10 + HOSO₂CF₃)			
E = -2282.7641425 (-2282.8267532)			
Tc = 0.288005 NImag = 0			
C	0.59179900	1.81275600	-0.58300900
C	-0.48057900	1.36435700	-1.58678200
C	-0.48775500	2.04457400	-2.92533900
H	-0.22550100	3.10245700	-2.85398900
H	0.27866300	1.56075100	-3.54543900
O	-1.27258900	0.45323400	-1.35385500
S	2.54926200	-0.55169000	-1.07305200
C	4.22458900	-0.98299600	-0.58314900
C	4.74710300	-2.21342200	-1.00174900
C	5.03063100	-0.08324700	0.13043400
C	6.07507600	-2.54218900	-0.70723500
H	4.11996300	-2.91027500	-1.54891500
C	6.34821900	-0.42737200	0.43762800
H	4.63087700	0.87607000	0.44366400
C	6.87505000	-1.65443600	0.01636400
H	6.47559900	-3.49688100	-1.03498700
H	6.96700500	0.26913500	0.99567100
H	7.90293400	-1.91413700	0.25082100
C	1.73226000	-0.20391900	0.49350300
C	1.94789700	-1.04008500	1.59981800
C	0.81999800	0.86996200	0.59127000
C	1.28215600	-0.81376600	2.80260000
H	2.64219700	-1.86935100	1.51520500
C	0.14002100	1.06266900	1.80484300
H	-1.56079100	-0.59417000	-0.27289600
C	0.36860500	0.23891200	2.90535400
H	1.46724600	-1.46661300	3.65019600
H	-0.57579200	1.87390200	1.89354200
H	-0.16479000	0.41683100	3.83368700

C	0.32108800	3.25104800	-0.11074300
O	-0.98569000	3.53355900	-0.10180200
O	1.19932300	4.02080000	0.22514500
C	-1.38537200	4.87269700	0.33684600
H	-0.89865800	5.59873700	-0.31897400
H	-1.01557300	5.01526900	1.35513700
C	-2.89574300	4.94600400	0.25726300
H	-3.22173100	5.93967700	0.57980600
H	-3.24547300	4.78602000	-0.76676800
H	-3.36201100	4.20299500	0.91067900
O	-1.79393300	-1.40843600	0.31014300
S	-3.30994300	-1.48875700	0.73889600
O	-3.40439400	-2.34678500	1.91290700
O	-3.95624200	-0.17971200	0.70040300
C	-4.03311300	-2.47851500	-0.69148000
F	-3.43293600	-3.66905900	-0.77928200
F	-3.86336800	-1.81294800	-1.83917300
F	-5.34078100	-2.65840300	-0.47469700
H	-1.45751200	1.92040400	-3.40855600
H	1.52462700	1.88055900	-1.15516800