

## Supporting Information

### A Detailed Density Functional Theory Exploration of the Photodissociation Mechanism of Ruthenium Complexes for Photoactivated Chemotherapy

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**Figure S1.** Optimized geometry of the **Ru** complex together with selected bond lengths (in Å). Atoms coordinated to ruthenium are labelled. S2

**Figure S2.** Simulated absorption spectra of the **Ru** complex compared with the corresponding experimental one. The experimental spectrum is reported in ref 1 S3

**Table S1.** TD-DFT benchmark for the reproduction of the experimental spectrum of the **Ru** complex on the structure optimized at B3LYP-D3/6-31G\* level in CH<sub>3</sub>CN implicit solvent. S4

**Table S2.** Excitation energies  $\Delta E$ (eV), MO contribution % and theoretical assignment for the the most important singlet states of **Ru** complex calculated by M05 functional. S6

**Figure S3.** Natural Transition Orbitals (NTOs) for the most important transitions of Ru complex. S7

**Table S3.** Excitation energies  $\Delta E$ (eV), MO contribution % and theoretical assignment for the triplet states below the bright state (486 nm) of Ru complex calculated by M05 functional. S8

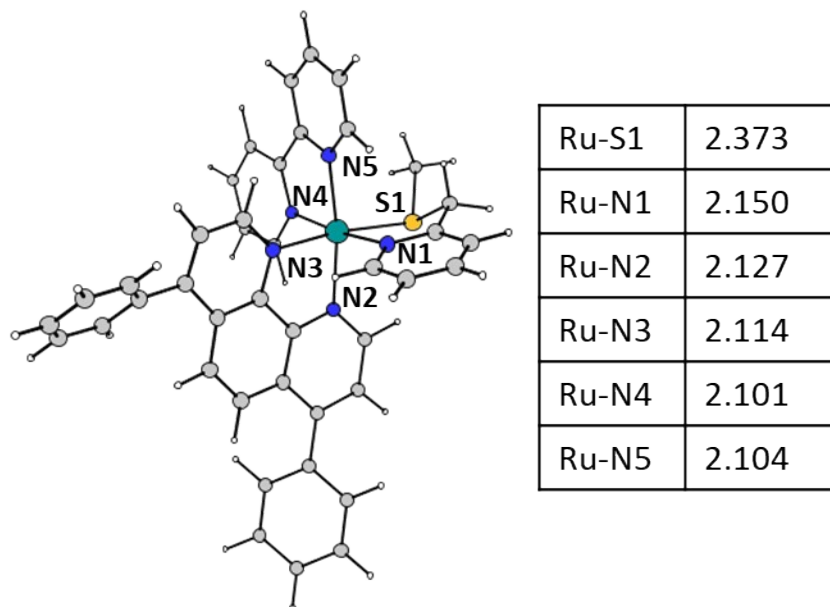
**Figure S4.** Natural Transition Orbitals (NTOs) for the triplet states T1-T6 of Ru complex below the bright state (486 nm). S9

**Table S4.** Selected bond distances (Å) for the ground state and the triplet states Ta, Tb, c and Td of the Ru complex. S10

**Table S5.** Cartesian coordinates of GS and Ta, Tb, Tc and Td triplet states. S11

**Table S6.** Cartesian coordinates of all the stationary points intercepted along the light-induced substitution pathways . S18

**References** S36



**Figure S1**

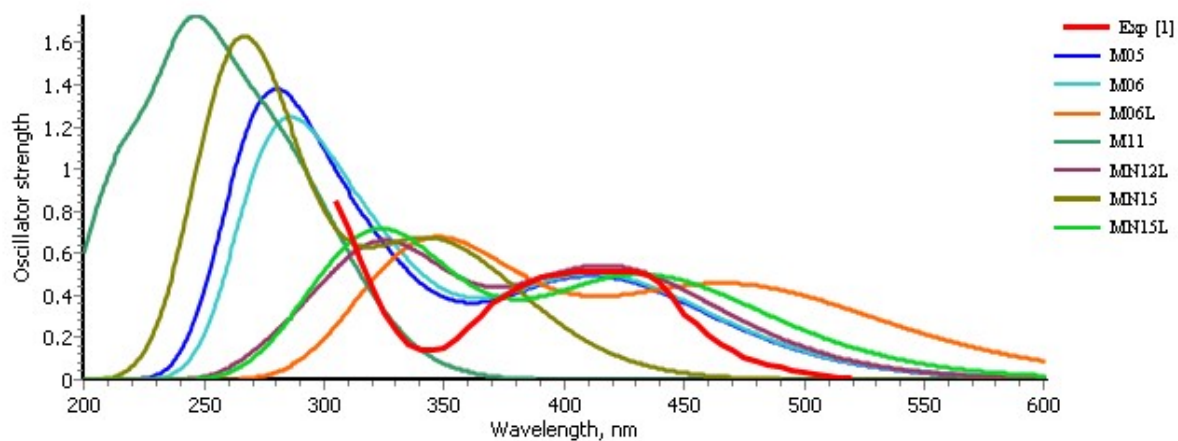
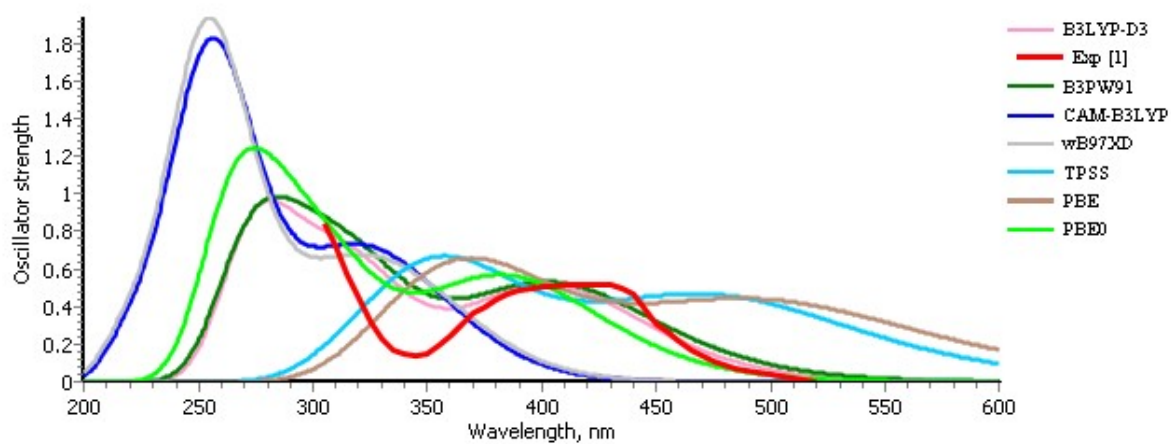


Figure S2

Table S1.

	$\lambda$	eV	$f$	MO contribution <sup>a</sup>
<b>exp<sup>b</sup></b>	430			
<b>B3LYP-D3</b>	467	2.65	0.002	H $\rightarrow$ L (69%) H $\rightarrow$ L+1 (21%)
	438	2.83	0.048	H -1 $\rightarrow$ L+1 (33%) H -2 $\rightarrow$ L+1 (22%)
<b>B3PW91</b>	468	2.65	0.003	H $\rightarrow$ L (72%) H $\rightarrow$ L+1 (22%)
	441	2.81	0.042	H -1 $\rightarrow$ L+1 (33%) H -1 $\rightarrow$ L (24%)
	408	3.04	0.106	H-1 $\rightarrow$ L+2 (72%)
<b>camB3LYP</b>	365	3.39	0.001	H-1 $\rightarrow$ L+1 (71%)
	315		0.266	H $\rightarrow$ L+2 (83%)
<b>B97D</b>	618	2.01	0.003	H $\rightarrow$ L (95%)
	551	3.53	0.165	H $\rightarrow$ L (57%)
<b><math>\omega</math>B97XD</b>	371	3.34	0.001	H-1 $\rightarrow$ L+1 (63%)
	355	3.49	0.158	H $\rightarrow$ L (55%)
<b>TPSS</b>	581	2.13	0.003	H $\rightarrow$ L (96%)
	528	2.34	0.015	H-1 $\rightarrow$ L+1 (50%) H-1 $\rightarrow$ L+2 (21%)
<b>PBE</b>	626	1.98	0.003	H $\rightarrow$ L (95%)
	565	2.19	0.011	H-1 $\rightarrow$ L+1 (61%) H-1 $\rightarrow$ L+2 (25%)
<b>PBE0</b>	439	2.82	0.002	H $\rightarrow$ L+1 (32%) H $\rightarrow$ L (30%) H-1 $\rightarrow$ L (18%) H-1 $\rightarrow$ L+1 (17%)
	416	2.98	0.063	H $\rightarrow$ L (25%) H-2 $\rightarrow$ L+1 (20%)
<b>M05</b>	486	2.55	0.002	H $\rightarrow$ L+1 (55%) H $\rightarrow$ L (40%)
	434	2.86	0.143	H-2 $\rightarrow$ L (87%)
<b>M06</b>	485	2.56	0.002	H $\rightarrow$ L+1 (49%) H $\rightarrow$ L (44%)
	453	2.74	0.045	H-1 $\rightarrow$ L (32%) H-1 $\rightarrow$ L+1 (20%)
<b>M06L</b>	576	2.15	0.004	H $\rightarrow$ L (97%)
	524	2.36	0.016	H-1 $\rightarrow$ L+1 (47%) H-1 $\rightarrow$ L+2 (24%)
<b>M11</b>	378	3.28	0.000(1)	H-2 $\rightarrow$ L+17 (27%) H-1 $\rightarrow$ L+17 (26%)
	310	4.00	0.013	H $\rightarrow$ L (28%) H-1 $\rightarrow$ L+1 (19%)
<b>MN12L</b>	479	2.58	0.003	H $\rightarrow$ L (99%)
	455	2.72	0.025	H-1 $\rightarrow$ L+1 (67%)

				H → L+ (15%)
<b>MN15</b>	419	2.96	0.000(1)	H-1 → L+9 (47%) H-2 → L+9 (16%)
	373	3.32	0.147	H → L+ (57%) H-2 → L+1 (20%)
<b>MN15L</b>	514	2.41	0.004	H → L (98%)
	472	2.63	0.013	H → L+2 (64%)

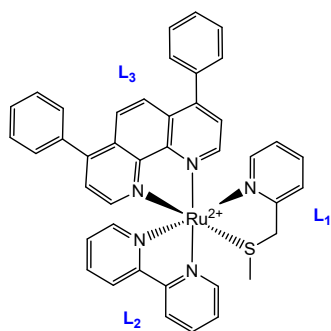
<sup>a</sup>Only contributions larger than 15% are reported; <sup>b</sup> data in CH<sub>3</sub>CN from ref 2.

**Table S2**

Band	State	$\Delta E$	$\lambda$	$f$	MO contribution <sup>a</sup>	Theoretical Assignment <sup>b</sup>
I	Tr1	2.55	486	0.002	H $\rightarrow$ L+1 61% H $\rightarrow$ L 33%	ML <sub>2</sub> CT (78%)
	Tr2	2.86	434	0.140	H-2 $\rightarrow$ L 86%	ML <sub>2/3</sub> CT (70%)
	Tr3	3.07	403	0.123	H-2 $\rightarrow$ L+1 34% H $\rightarrow$ L+2 32%	ML <sub>2/3</sub> CT (71%)
II	Tr4	3.93	316	0.256	H-3 $\rightarrow$ L+2 71%	L <sub>3</sub> C (80%)
	Tr5	4.24	292	0.151	H-4 $\rightarrow$ L+2 33% H-4 $\rightarrow$ L+1 13% H $\rightarrow$ L+7 13%	L <sub>3</sub> C (69%)/ ML <sub>3</sub> CT (23%)
	Tr6	4.43	280	0.233	H-7 $\rightarrow$ L 41% H-7 $\rightarrow$ L+1 13%	L <sub>2</sub> C (63%) /ML <sub>2</sub> CT (20%)
	Tr7	4.48	277	0.406	H-9 $\rightarrow$ L 24% H-4 $\rightarrow$ L 22% H-8 $\rightarrow$ L+2 15%	L <sub>2</sub> C (66%) / L <sub>3</sub> L <sub>2</sub> CT (26%)
	Tr8	4.75	261	0.127	H-8 $\rightarrow$ L+2 24% H-9 $\rightarrow$ L 16% H-10 $\rightarrow$ L 15% H-1 $\rightarrow$ L+8 12%	L <sub>3</sub> C (51%) / L <sub>3</sub> L <sub>2</sub> CT (25%) / ML <sub>2</sub> CT (20%)

<sup>a</sup>Only contributions larger than 11% are reported.

<sup>b</sup>Only contributions larger than 18% are reported. TheoDORÉ software together with NTO plots were used for assigning states character.



Ru	Tr1 (486 nm)	Tr2 (434 nm)	Tr3 (403 nm)	Tr4 (316 nm)
Particle				
Hole				
	Tr5 (292 nm)	Tr6 (280 nm)	Tr7 (277 nm)	Tr8 (261 nm)
Particle				
Hole				

Figure S3

**Table S3.**

State	$\Delta E$	$\lambda$	MO contribution <sup>a</sup>	Theoretical Assignment <sup>b</sup>
T1	1.9 9	622	H-3 $\rightarrow$ L+2 18% H-1 $\rightarrow$ L+2 16%	L <sub>3</sub> C (77%) / ML <sub>3</sub> CT (18%)
T2	2.2 2	558	H-1 $\rightarrow$ L+1 19% H $\rightarrow$ L+1 15% H $\rightarrow$ L 15% H-1 $\rightarrow$ L 12%	L <sub>2</sub> C (47%) / ML <sub>2</sub> CT (43%)
T3	2.2 9	542	H-1 $\rightarrow$ L 27% H-1 $\rightarrow$ L+1 26% H-2 $\rightarrow$ L+1 15%	ML <sub>3</sub> CT (46%) / L <sub>3</sub> C (42%)
T4	2.4 8	501	H-2 $\rightarrow$ L+1 39% H-2 $\rightarrow$ L 35%	ML <sub>2</sub> CT (63%) / L <sub>2</sub> C (23%)
T5	2.4 9	497	H $\rightarrow$ L+1 35% H $\rightarrow$ L+9 33% H-1 $\rightarrow$ L 17%	ML <sub>1/2/3</sub> CT (54%) / MC (25%)
T6	2.5 5	486	H $\rightarrow$ L 33% H $\rightarrow$ L+9 23% H-1 $\rightarrow$ L+1 13%	ML <sub>2</sub> CT (60%) / MC (19%)



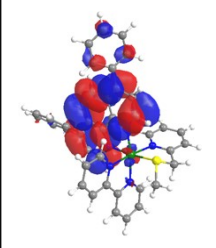
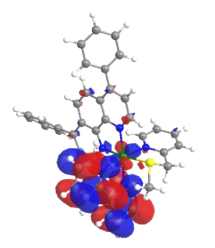
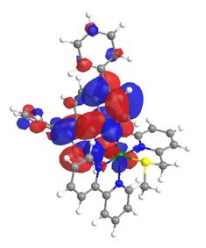
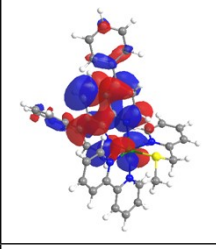
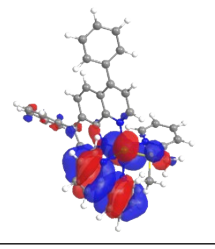
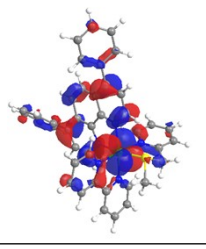
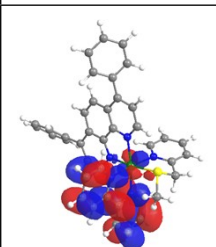
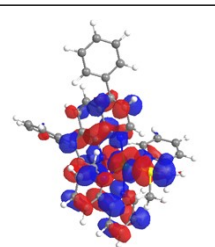
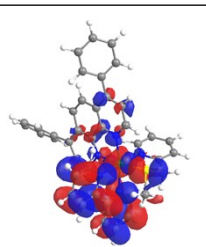
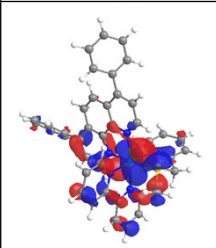
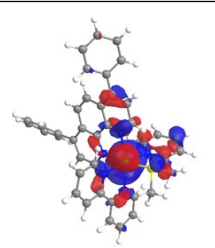
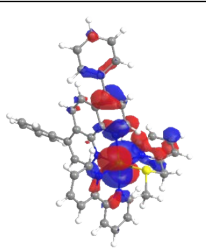
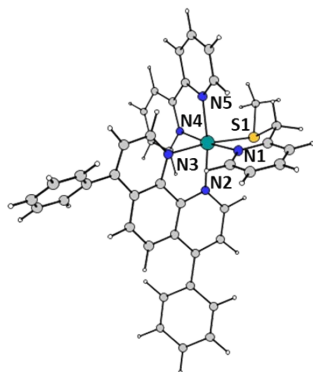
Ru	T1 (622 nm)	T2 (558 nm)	T3 (542 nm)
Particle			
Hole			
	T4 (501 nm)	T5 (497 nm)	T6 (486 nm)
Particle			
Hole			

Figure S4

**Table S4**

State	Ru-S	Ru-N1	Ru-N2	Ru-N3	Ru-N4	Ru-N5
S0	2.373	2.150	2.105	2.090	2.080	2.083
Ta	2.395	2.137	2.028	2.120	2.123	2.146
Tb	2.400	2.176	2.151	2.122	2.071	2.067
Tc	2.449	2.805	2.140	2.133	2.387	2.172
Td	2.949	2.188	2.193	2.422	2.126	2.115

**Table S5**

<b>GS</b> E=-2347.527007 Hartree			
Ru	0.74933500	-0.74904900	-0.31288000
C	3.42371300	-0.38942300	0.89070500
C	3.56656600	-0.23072800	-1.42748500
C	4.93863200	-0.02744300	-1.37916800
C	5.56567200	-0.01186500	-0.13786900
C	4.80007100	-0.19489200	1.00700400
C	2.52606700	-0.58246400	2.04403300
C	0.33016900	-0.93347900	2.73431700
C	0.69302500	-0.91023300	4.07325000
C	2.03295700	-0.72080800	4.39583200
C	2.95521000	-0.55012300	3.37104700
H	3.03779200	-0.25776300	-2.37271700
H	5.49348700	0.11255400	-2.29917100
H	6.63611000	0.14035600	-0.05800000
H	5.27587000	-0.18578100	1.97910800
H	-0.70415700	-1.06558200	2.43831100
H	-0.06469500	-1.03701000	4.83711400
H	2.35774800	-0.69795900	5.42988300
H	3.99863600	-0.38839300	3.60880500
N	1.21842600	-0.78659200	1.73763200
N	2.82271400	-0.41062100	-0.32607100
C	0.11255800	-0.95318300	-4.70025800
C	-0.01788400	0.37668400	-5.07175500
C	0.02186500	1.35144700	-4.03310900
C	0.24308000	0.90771500	-2.71028500
C	0.32138000	-1.30363400	-3.36504700
C	-0.20228700	2.74949200	-4.24539300
C	0.29409000	1.85397200	-1.63202900
C	0.13312100	3.23497100	-1.88061700
C	-0.14686800	3.64627700	-3.22259500
C	0.20153100	4.12892700	-0.77249200
C	0.36664100	3.57292900	0.48811300
C	0.49543800	2.19187000	0.64539400
H	-0.44336700	3.09484000	-5.24309600
H	0.08665700	-1.73821000	-5.44714900
H	0.44560300	-2.34455700	-3.08991000
H	-0.34459300	4.69255700	-3.42013600
H	0.42356900	4.20659100	1.36548700
H	0.63095400	1.76181400	1.63080600
N	0.47265600	1.34554200	-0.38024700
N	0.40554800	-0.40835400	-2.38371600
C	0.10313000	5.59669600	-0.91961100
C	-0.80595100	6.31871000	-0.13342800
C	0.94114400	6.29329000	-1.80284400
C	-0.88607300	7.70444800	-0.24021900
H	-1.46450200	5.78915500	0.54874400
C	0.86628200	7.68025600	-1.89870400
H	1.66903000	5.74978100	-2.39795900
C	-0.05003800	8.38851400	-1.12193200
H	-1.60313400	8.24925800	0.36603400
H	1.52800200	8.20730500	-2.57899300
H	-0.11059600	9.46953400	-1.20185400
C	-0.18789400	0.72903800	-6.49759000
C	-1.18100000	0.09888500	-7.26051800
C	0.66293400	1.65434300	-7.12004800

C	-1.32998700	0.39996200	-8.61163600
H	-1.84915500	-0.61480900	-6.78754600
C	0.51856600	1.94444500	-8.47410700
H	1.45418200	2.12968700	-6.54790700
C	-0.48060400	1.32227300	-9.22179300
H	-2.11130300	-0.08667700	-9.18720600
H	1.19064100	2.65519600	-8.94490100
H	-0.59530500	1.55351000	-10.27634500
C	-4.03193200	-1.96165600	-0.08872300
C	-3.03770500	-2.90779500	0.12890400
C	-1.70081600	-2.51699700	0.11427600
C	-2.30931100	-0.32659200	-0.34359400
C	-3.65885300	-0.64282500	-0.32559200
H	-5.07699800	-2.25112000	-0.07636800
H	-3.28847400	-3.94573700	0.31576100
H	-1.98547300	0.68861000	-0.53554400
H	-4.39301600	0.13417300	-0.50275600
N	-1.33727600	-1.23325900	-0.12820600
C	-0.62189300	-3.50891400	0.42543100
S	0.90273600	-3.10886900	-0.50637900
C	2.14927300	-3.85113100	0.58099400
H	3.12321500	-3.60207100	0.15655000
H	2.07161800	-3.45781700	1.59561100
H	2.01821600	-4.93417400	0.57894100
H	-0.37012000	-3.46486000	1.49007700
H	-0.93627200	-4.52764600	0.19338800
<b>Ta</b>	E=-2347.448237 Hartree		
Ru	0.87461100	-0.70729100	-0.38206800
C	3.50997800	-0.43905400	0.99961100
C	3.77559600	-0.27516500	-1.31130600
C	5.14912600	-0.11701600	-1.18810000
C	5.71043900	-0.12633900	0.08289800
C	4.88194800	-0.28739100	1.18703600
C	2.54962900	-0.60802600	2.10357700
C	0.30161800	-0.86791400	2.66787000
C	0.59316100	-0.88734200	4.02400500
C	1.92095900	-0.76385800	4.41860600
C	2.90709200	-0.61632800	3.45069400
H	3.29105400	-0.27297000	-2.27900300
H	5.75369900	0.01028900	-2.07774200
H	6.77925500	-0.00804600	0.21879600
H	5.30584400	-0.29377700	2.18240000
H	-0.72057700	-0.94415200	2.31475100
H	-0.20891500	-0.99370200	4.74391500
H	2.18951300	-0.77370400	5.46869500
H	3.94118400	-0.50659200	3.74923600
N	1.25451800	-0.74675900	1.72993300
N	2.97583500	-0.43625300	-0.24703000
C	0.67973900	-0.89751400	-4.70732400
C	0.20585400	0.40423200	-5.07152600
C	0.16400300	1.38358800	-4.02152000
C	0.45666500	0.97754900	-2.70105400
C	0.96916300	-1.22236100	-3.41822000
C	-0.09900700	2.77233800	-4.22620100
C	0.40483300	1.90503800	-1.64152000
C	0.14203800	3.28862400	-1.86357700
C	-0.10832000	3.68578400	-3.20222600

C	0.11787700	4.15406000	-0.73552000
C	0.29998600	3.59068200	0.52348300
C	0.52744200	2.21704600	0.66011400
H	-0.28539900	3.12223900	-5.23412500
H	0.78446100	-1.66418100	-5.46672300
H	1.32098400	-2.21164900	-3.15432600
H	-0.32359000	4.72478300	-3.41997500
H	0.29110800	4.20937000	1.41284900
H	0.66718000	1.78324900	1.64360200
N	0.58645800	1.39351100	-0.37688400
N	0.82428200	-0.32481100	-2.37266000
C	-0.09097400	5.61318800	-0.85545900
C	-1.08033300	6.24503600	-0.08886800
C	0.72010100	6.39325300	-1.69286700
C	-1.26638000	7.62237200	-0.17231800
H	-1.71675600	5.65060400	0.56012200
C	0.53976800	7.77205400	-1.76462700
H	1.50899500	5.92104100	-2.27051000
C	-0.45670400	8.38940000	-1.00936200
H	-2.04495400	8.09591200	0.41783900
H	1.18208000	8.36399900	-2.40938100
H	-0.59952900	9.46396900	-1.07050700
C	-0.19662200	0.67034600	-6.45493700
C	-1.36897900	1.38943000	-6.76362000
C	0.55946900	0.15883200	-7.52862300
C	-1.75547400	1.60046400	-8.08339900
H	-2.00079500	1.75511600	-5.95985200
C	0.17384700	0.37585600	-8.84722200
H	1.47295800	-0.39209000	-7.32423000
C	-0.98462200	1.10003900	-9.13346500
H	-2.66961400	2.14878600	-8.29157600
H	0.78356100	-0.01789800	-9.65526600
H	-1.28599900	1.26765700	-10.16304200
C	-3.90528300	-1.82750200	-0.46350200
C	-2.94460400	-2.79924800	-0.20873900
C	-1.60567900	-2.43372700	-0.11868500
C	-2.15284200	-0.20796100	-0.53977200
C	-3.50206700	-0.50632700	-0.62629200
H	-4.95222100	-2.10038000	-0.53425400
H	-3.22483000	-3.83698600	-0.07305400
H	-1.80095400	0.80600700	-0.67224300
H	-4.21254800	0.28655600	-0.82540300
N	-1.21490600	-1.14486300	-0.29589100
C	-0.57055300	-3.45162300	0.24889700
S	1.02057000	-3.09011800	-0.57848600
C	2.19781200	-3.81885000	0.58915600
H	3.19492700	-3.57461400	0.21954400
H	2.05916900	-3.42357500	1.59582700
H	2.06211300	-4.90101900	0.57975800
H	-0.39379500	-3.42975400	1.32922800
H	-0.89034600	-4.45905300	-0.02030700
<b>Tb</b> E=-2347.453275 Hartree			
Ru	0.77100700	-0.73547100	-0.29058400
C	3.37549300	-0.29861500	0.97877000
C	3.54205600	-0.04070600	-1.37458700
C	4.88439600	0.25817000	-1.30714900
C	5.50059200	0.27876600	-0.03141700

C	4.75859200	0.00764700	1.08966700
C	2.50583900	-0.57457400	2.06414600
C	0.26722600	-1.05002500	2.71636400
C	0.60823200	-1.13268200	4.04408700
C	1.97221400	-0.94604900	4.39958800
C	2.89735000	-0.67284200	3.42664300
H	3.02450800	-0.07470000	-2.32715400
H	5.43877400	0.46507800	-2.21424400
H	6.55555600	0.51479700	0.06112000
H	5.22209900	0.03646500	2.06863700
H	-0.76205700	-1.17423000	2.39587400
H	-0.15436500	-1.33019300	4.78725200
H	2.28093000	-1.02121500	5.43682100
H	3.93928100	-0.53667100	3.69121300
N	1.16546400	-0.78391200	1.73817300
N	2.80073100	-0.32579000	-0.28461500
C	0.04240900	-0.96459900	-4.67529600
C	-0.08287000	0.36455400	-5.05528300
C	-0.00703900	1.35292000	-4.02940000
C	0.24108700	0.91871500	-2.71041600
C	0.27638600	-1.30589600	-3.34277100
C	-0.21869800	2.75180800	-4.24562700
C	0.32930700	1.86884700	-1.64159400
C	0.18866900	3.24932000	-1.89381400
C	-0.12236800	3.65483800	-3.23044400
C	0.30872900	4.14564100	-0.79026100
C	0.50402300	3.59417900	0.46900600
C	0.61311000	2.21297100	0.63410200
H	-0.48242100	3.09396100	-5.23844000
H	-0.00677600	-1.75541100	-5.41422900
H	0.39898300	-2.34446300	-3.05733600
H	-0.31006100	4.70236500	-3.43000600
H	0.60204900	4.23203700	1.33924600
H	0.77534300	1.77793100	1.61314300
N	0.53414900	1.37054500	-0.39144200
N	0.39069300	-0.39552000	-2.38003800
C	0.23333600	5.61281800	-0.94237100
C	-0.63194000	6.35477800	-0.12564200
C	1.05006800	6.28737000	-1.86208600
C	-0.69204200	7.74056600	-0.24016900
H	-1.27370500	5.84161800	0.58433200
C	0.99689100	7.67470300	-1.96313500
H	1.74654600	5.72776100	-2.47925900
C	0.12248300	8.40342400	-1.15752200
H	-1.37624400	8.30203000	0.38820600
H	1.64231000	8.18574200	-2.67056100
H	0.07797600	9.48475400	-1.24261600
C	-0.28628300	0.70298600	-6.47854500
C	-1.29829500	0.06383500	-7.20892400
C	0.54951500	1.62215900	-7.13000100
C	-1.48167200	0.35233200	-8.55811900
H	-1.95508400	-0.64404400	-6.71209800
C	0.37156800	1.89673500	-8.48305800
H	1.35633000	2.10175900	-6.58386300
C	-0.64688300	1.26761100	-9.19825600
H	-2.27773100	-0.13895600	-9.10874200
H	1.03232200	2.60110700	-8.97847600

H	-0.78773300	1.48812200	-10.25184200
C	-4.00239000	-2.05601100	-0.28570300
C	-3.00448400	-2.99201100	-0.03676600
C	-1.67659600	-2.57990300	0.00773800
C	-2.30187400	-0.39073000	-0.45735300
C	-3.64536900	-0.72840200	-0.49375800
H	-5.04186000	-2.36256400	-0.31950200
H	-3.24791800	-4.03493000	0.12921800
H	-1.98499800	0.63053800	-0.62860000
H	-4.38521500	0.03748600	-0.69169400
N	-1.33140100	-1.28967700	-0.21127400
C	-0.60005100	-3.55694200	0.37502500
S	0.99180700	-3.12251500	-0.40842600
C	2.18059800	-3.76681500	0.79384900
H	3.16699700	-3.45001200	0.45268700
H	1.98073700	-3.37408500	1.79050400
H	2.11810400	-4.85560000	0.78078900
H	-0.44345300	-3.54793900	1.45861000
H	-0.86465400	-4.57258100	0.07774800
<b>Tc</b> E=-2347.471403 Hartree			
Ru	1.17541200	-0.58404700	-0.27411700
C	3.80212400	-0.39101000	1.53015800
C	4.46336400	-0.18037000	-0.68059700
C	5.81101800	-0.16249400	-0.33533200
C	6.14352100	-0.27333500	1.01090300
C	5.13163400	-0.38781200	1.95862000
C	2.64671700	-0.48871900	2.45391800
C	0.33120100	-0.67089100	2.66159300
C	0.39741800	-0.63923800	4.04730300
C	1.64822000	-0.53183800	4.64594700
C	2.77936500	-0.45343000	3.84283500
H	4.14370400	-0.10114500	-1.71605000
H	6.57095700	-0.06672000	-1.10204700
H	7.18136700	-0.27078900	1.32580300
H	5.38639200	-0.47853500	3.00695800
H	-0.61783500	-0.75758100	2.14133500
H	-0.51233000	-0.69937400	4.63238200
H	1.74589100	-0.50447200	5.72542900
H	3.75551500	-0.35648700	4.29978000
N	1.42368100	-0.60235400	1.88346200
N	3.49190000	-0.29609100	0.22567600
C	-0.10131800	-1.00481100	-4.50222800
C	-0.42107400	0.29232000	-4.87760100
C	-0.20684300	1.32696300	-3.92121800
C	0.32171500	0.96754700	-2.66277500
C	0.41104200	-1.27146800	-3.23263800
C	-0.54802100	2.70050600	-4.13847000
C	0.55704400	1.96839800	-1.66533500
C	0.29301700	3.32809000	-1.93791300
C	-0.30435500	3.65405600	-3.19752700
C	0.58432300	4.28293600	-0.92054100
C	1.06514800	3.80375200	0.29042900
C	1.26998400	2.43686400	0.48319800
H	-1.02602600	2.98051100	-5.06887900
H	-0.23309300	-1.82656400	-5.19614400
H	0.66617000	-2.28634600	-2.94954800
H	-0.59000400	4.68036700	-3.39221700

H	1.30676900	4.48789500	1.09533600
H	1.64622800	2.06519900	1.42937000
N	1.03175500	1.53511400	-0.46434800
N	0.61257600	-0.32193100	-2.32212900
C	0.39547100	5.73649700	-1.11091200
C	-0.33535400	6.47538200	-0.16981400
C	0.97608200	6.40469600	-2.19903800
C	-0.49618400	7.84959000	-0.32348500
H	-0.79487300	5.96689200	0.67263300
C	0.82390000	7.78111100	-2.34229800
H	1.56832500	5.84935000	-2.92026800
C	0.08360600	8.50565600	-1.40878000
H	-1.07569800	8.40727900	0.40564900
H	1.28784600	8.28729800	-3.18307900
H	-0.03889500	9.57804800	-1.52532300
C	-0.97221700	0.54706700	-6.22489700
C	-2.08746700	-0.18058000	-6.66343500
C	-0.37825200	1.47495700	-7.09247100
C	-2.60774300	0.02828700	-7.93762000
H	-2.55774700	-0.89558100	-5.99432600
C	-0.89399600	1.67166400	-8.37066700
H	0.50240100	2.02514500	-6.77454400
C	-2.01188300	0.95348200	-8.79404900
H	-3.47934200	-0.53250500	-8.26055400
H	-0.41894900	2.38526400	-9.03662900
H	-2.41587400	1.11269100	-9.78906800
C	-3.22889000	-2.16924000	-2.31263400
C	-2.39968100	-3.05052700	-1.62045900
C	-1.57882500	-2.54524300	-0.61366200
C	-2.36247900	-0.40910000	-0.95056900
C	-3.21715700	-0.82086800	-1.97102800
H	-3.87123400	-2.53335900	-3.10778100
H	-2.38653500	-4.10816900	-1.86072100
H	-2.31262300	0.63810400	-0.65950300
H	-3.84645100	-0.10099900	-2.48223000
N	-1.55188500	-1.24092700	-0.29073200
C	-0.64054800	-3.42834000	0.15695300
S	1.10204600	-3.03170100	-0.28651000
C	1.98058700	-3.76281000	1.11840800
H	3.03595200	-3.51464700	0.99511700
H	1.60936700	-3.36510900	2.06380000
H	1.85515300	-4.84585500	1.08384100
H	-0.74613000	-3.25449900	1.23081700
H	-0.79976800	-4.48654300	-0.05486200
<b>Td</b>	E=-2347.474251 Hartree		
Ru	0.76758600	-0.69887500	-0.16950800
C	3.45811000	-0.48992400	1.09142000
C	3.59734400	0.03059600	-1.17573700
C	4.97492700	0.18348500	-1.10726300
C	5.60472500	-0.01922200	0.11641100
C	4.83973100	-0.35687200	1.22634200
C	2.55401400	-0.81335500	2.20675500
C	0.34186100	-1.18900000	2.84330400
C	0.69240300	-1.30534700	4.18013500
C	2.03443300	-1.18521200	4.52640100
C	2.97111400	-0.93093200	3.53224100
H	3.06212700	0.17417500	-2.10726200



H	5.53209200	0.45272400	-1.99647300
H	6.67980000	0.08502800	0.20991700
H	5.32035300	-0.51665600	2.18288700
H	-0.69178700	-1.27218900	2.52647100
H	-0.07410800	-1.48803700	4.92337700
H	2.35056400	-1.27696500	5.55931400
H	4.01453500	-0.81341200	3.79421400
N	1.24471500	-0.96621300	1.87344800
N	2.85529100	-0.30263000	-0.10977200
C	0.05261800	-0.82811000	-4.55663800
C	-0.09737400	0.48605300	-4.97029000
C	-0.03713400	1.50011600	-3.97108000
C	0.21734700	1.11519600	-2.63258300
C	0.29055000	-1.12063500	-3.21382900
C	-0.27193000	2.88454800	-4.25159100
C	0.29732000	2.12727900	-1.60307100
C	0.13391700	3.49430300	-1.93187000
C	-0.18848800	3.83604100	-3.28286100
C	0.24651200	4.45006800	-0.87897900
C	0.46262100	3.97498600	0.40646100
C	0.59185800	2.60021300	0.63089600
H	-0.54186900	3.17346900	-5.25973200
H	0.01710400	-1.64088800	-5.27261500
H	0.42901200	-2.14899400	-2.90168600
H	-0.39262800	4.87019500	-3.53191800
H	0.55751600	4.66358900	1.23833900
H	0.77128100	2.21754400	1.63266800
N	0.51988700	1.70500800	-0.33994200
N	0.38473200	-0.18900500	-2.26817700
C	0.14328600	5.90803000	-1.11094000
C	-0.74821600	6.67540200	-0.34835300
C	0.95960900	6.55126200	-2.05262800
C	-0.83247600	8.05265900	-0.53468000
H	-1.38908000	6.18696600	0.37985700
C	0.88083400	7.93024400	-2.22888500
H	1.67296500	5.97283500	-2.63230200
C	-0.01808300	8.68347900	-1.47437500
H	-1.53582400	8.63243800	0.05508700
H	1.52565000	8.41589400	-2.95479600
H	-0.08188600	9.75792200	-1.61677700
C	-0.30896000	0.78077500	-6.40414100
C	-1.33115900	0.12707900	-7.10624800
C	0.52959900	1.66913100	-7.09308000
C	-1.52106300	0.36965200	-8.46398700
H	-1.98934800	-0.55869700	-6.58087700
C	0.34457800	1.89980200	-8.45363200
H	1.34180400	2.16239600	-6.56728500
C	-0.68342100	1.25518800	-9.14096600
H	-2.32461000	-0.13410400	-8.99230200
H	1.00733900	2.58203000	-8.97688000
H	-0.82945800	1.44079700	-10.20063100
C	-3.94114100	-2.25551300	-0.41737400
C	-2.93222900	-3.16530900	-0.12132300
C	-1.61789900	-2.72340500	0.01848700
C	-2.28039200	-0.54426400	-0.44083900
C	-3.61038300	-0.91419500	-0.57133500
H	-4.96676500	-2.59125800	-0.52489800

H	-3.15757500	-4.21715500	0.01127900
H	-1.97918400	0.48945900	-0.56838300
H	-4.35755300	-0.16321700	-0.79848000
N	-1.29842800	-1.41960000	-0.15884600
C	-0.54569900	-3.69117400	0.43428900
S	0.94556700	-3.60749000	-0.61993400
C	2.17342900	-4.28675000	0.52365200
H	3.13131400	-4.26125000	0.00134200
H	2.23909900	-3.67909700	1.42896200
H	1.92899700	-5.31920000	0.77939800
H	-0.23096800	-3.46992400	1.45902700
H	-0.93661900	-4.70946300	0.42372700

**Table S6**

PATH TRIPLET Tc			
Tc E=-2423.873867 Hartree			
Ru	0.52122000	-1.04899300	1.09505900
N	-2.85300300	-2.32441400	0.38355100
O	-2.55646600	-0.40336900	2.52163700
C	5.07144700	-0.96471300	0.23360500
C	5.62064100	-1.15017400	1.49815300
C	4.78290900	-1.20439700	2.60729300
C	2.42492000	-1.09709400	3.53289900
C	0.17584600	-1.07685900	4.14999800
C	0.49403700	-1.09348300	5.50157500
C	1.83472600	-1.11783000	5.86811800
C	2.80635900	-1.11304900	4.87501300
H	3.20308800	-0.71007200	-0.83073700
H	5.69174600	-0.91200400	-0.65341000
H	6.69282500	-1.25233500	1.62514800
H	5.20648700	-1.35397900	3.59219000
H	-0.85527600	-1.03486200	3.80713400
H	-0.29889300	-1.08549400	6.23992900
H	2.12564400	-1.13132300	6.91264100
H	3.85306700	-1.11112900	5.14970700
N	1.11434500	-1.08858800	3.18796000
N	2.88359600	-0.90851300	1.19302300
C	-0.81063800	-1.45327800	-3.11003700
C	-1.09819500	-0.15009300	-3.49079900
C	-0.87836800	0.87915300	-2.52978600
C	-0.37531200	0.50916800	-1.26390600
C	-0.33308000	-1.73130100	-1.83015700
C	-1.16912500	2.26294700	-2.75669300
C	-0.07512000	1.51111800	-0.28527600
C	-0.27298100	2.87796800	-0.57474400
C	-0.87778000	3.21520100	-1.82798500
C	0.10221900	3.83196100	0.41604600
C	0.58897900	3.34780200	1.62315000
C	0.73301500	1.97560700	1.83225000
H	-1.64083400	2.55284500	-3.68735000
H	-0.94201200	-2.27253700	-3.80705400
H	-0.10397200	-2.75133100	-1.54566400
H	-1.12180400	4.25063900	-2.03085800
H	0.89172900	4.03153200	2.40744900
H	1.12470000	1.59711100	2.76968000
N	0.42060800	1.07365300	0.90589000
N	-0.13183700	-0.78770500	-0.91288700
C	0.00501300	5.29036100	0.19750500
C	-0.64089800	6.09921200	1.14312300
C	0.59779600	5.89218700	-0.92250100
C	-0.70739700	7.47797300	0.96277900
H	-1.10830500	5.64287200	2.01069300
C	0.54057300	7.27270200	-1.09244800
H	1.12681300	5.28099600	-1.64763100
C	-0.11612500	8.06785800	-0.15384600
H	-1.22164700	8.09131900	1.69609200
H	1.01358200	7.72644500	-1.95775300
H	-0.16444900	9.14373500	-0.29094900
C	-1.60408800	0.11502000	-4.85373200

C	-2.71085100	-0.60042100	-5.33240700
C	-0.96830900	1.03439000	-5.70078700
C	-3.18244500	-0.38742900	-6.62459700
H	-3.21257400	-1.31124100	-4.68202300
C	-1.43494600	1.23480200	-6.99716100
H	-0.09188500	1.57325000	-5.35334600
C	-2.54507500	0.52918000	-7.46008700
H	-4.04793600	-0.93906300	-6.97821000
H	-0.92662400	1.94065700	-7.64658200
H	-2.91008300	0.69078500	-8.46969000
C	-3.36322800	-4.00485100	-1.77596100
C	-2.53225800	-4.41791900	-0.73797200
C	-2.30275900	-3.54569400	0.32826500
C	-3.64880600	-1.93659300	-0.61654800
C	-3.93608500	-2.73782400	-1.71861400
H	-3.55950400	-4.66411100	-2.61507500
H	-2.06996200	-5.39941100	-0.75155700
H	-4.07334900	-0.93926500	-0.53010000
H	-4.59136900	-2.37633300	-2.50347900
C	3.68891200	-0.85074400	0.13093600
C	-1.40433600	-3.93301700	1.46670900
S	0.35260800	-3.49958200	1.10900300
C	1.14358200	-4.22857100	2.56702300
H	2.20257000	-3.97174500	2.51806800
H	0.70461700	-3.84173700	3.48746400
H	1.02957700	-5.31226900	2.51471800
H	-1.69705200	-3.42153900	2.38561400
H	-1.41225300	-5.01274700	1.63040800
C	3.40482400	-1.07329600	2.42177100
H	-2.61646400	-1.04814400	1.78390300
H	-2.22063200	0.39766700	2.10139500
<b>TS<sub>1c</sub></b> E=-2423.870206 Hartree			
Ru	-0.86441200	0.92746300	0.32175400
N	-4.23359200	-0.42305600	-0.46463700
O	-3.96914900	2.18674600	0.71550500
C	3.69923100	1.07721000	-0.49533800
C	4.24228800	0.99668300	0.78281900
C	3.39538800	0.94972600	1.88516000
C	1.02260000	0.94501500	2.78013300
C	-1.22226400	0.84555700	3.38174700
C	-0.92294900	0.86978000	4.73597200
C	0.41389100	0.93475300	5.11248300
C	1.39104300	0.97223000	4.12646100
H	1.83233700	1.16050500	-1.58931300
H	4.32652300	1.11958400	-1.37796800
H	5.31696200	0.97048400	0.92587100
H	3.81617400	0.88216700	2.88008000
H	-2.25228300	0.78414400	3.04740600
H	-1.72270700	0.83601000	5.46575700
H	0.69597200	0.95644800	6.15911500
H	2.43365900	1.02855600	4.41017400
N	-0.28382400	0.88409000	2.42242700
N	1.50069200	1.04900900	0.43890600
C	-2.19559500	0.51694600	-3.88369000
C	-2.43392600	1.82539000	-4.28035500
C	-2.17267300	2.85760800	-3.33303700
C	-1.68000200	2.48502700	-2.06393500

C	-1.72607200	0.23755900	-2.60116700
C	-2.41491700	4.24828200	-3.57554100
C	-1.34481300	3.48589500	-1.09601300
C	-1.49848500	4.85500800	-1.39952600
C	-2.09068200	5.19954700	-2.65699200
C	-1.09794700	5.80650700	-0.41650000
C	-0.63077300	5.31920900	0.79665900
C	-0.52969500	3.94476800	1.01787400
H	-2.87723100	4.54428000	-4.50897800
H	-2.36026500	-0.30561300	-4.56966300
H	-1.53757800	-0.78709000	-2.30348400
H	-2.29907100	6.24058400	-2.87085100
H	-0.31075800	6.00044700	1.57631700
H	-0.15362400	3.56507300	1.96119700
N	-0.86505200	3.04537900	0.09869600
N	-1.48471400	1.18485800	-1.69786100
C	-1.15105000	7.26528800	-0.64854000
C	-1.77890200	8.10100400	0.28570500
C	-0.53469100	7.83966100	-1.77012900
C	-1.80445600	9.47947200	0.09287600
H	-2.26435100	7.66602000	1.15434000
C	-0.55119900	9.21967900	-1.95284200
H	-0.01979700	7.20673700	-2.48673100
C	-1.19001700	10.04198500	-1.02535100
H	-2.30505800	10.11390100	0.81767100
H	-0.06051600	9.65171500	-2.81944300
H	-1.20655200	11.11749600	-1.17247400
C	-2.93384700	2.09192400	-5.64533100
C	-4.06592400	1.40973500	-6.11334700
C	-2.26917000	2.97893400	-6.50462500
C	-4.53363500	1.62424500	-7.40670200
H	-4.59008700	0.72400500	-5.45380000
C	-2.73237600	3.18081100	-7.80201800
H	-1.37379000	3.49122100	-6.16543100
C	-3.86757600	2.50891500	-8.25415100
H	-5.41860800	1.09878700	-7.75187100
H	-2.20188200	3.86132600	-8.46069500
H	-4.22988400	2.67184600	-9.26452400
C	-4.73694900	-2.21221600	-2.53998500
C	-3.91137200	-2.57152700	-1.47821100
C	-3.68669600	-1.64671200	-0.45572500
C	-5.02518800	-0.08866800	-1.48776900
C	-5.31055300	-0.94451800	-2.54830900
H	-4.92896100	-2.91314800	-3.34562200
H	-3.44908700	-3.55229600	-1.43973200
H	-5.44567100	0.91402000	-1.45758100
H	-5.96275800	-0.62247000	-3.35267200
C	2.31379900	1.10029800	-0.61712300
C	-2.79293100	-1.98227100	0.70195200
S	-1.04352400	-1.52286900	0.34360100
C	-0.23237100	-2.24692800	1.79272300
H	0.81939600	-1.96170600	1.74467800
H	-0.67850400	-1.88248200	2.71873100
H	-0.31867000	-3.33251900	1.72866800
H	-3.10651700	-1.45296300	1.60339200
H	-2.77955300	-3.05702300	0.89490600
C	2.01410100	0.98195600	1.67917100

H	-3.97451500	1.23327300	0.49443600
H	-3.51662400	2.23767700	1.56434600
<b>Tc-H<sub>2</sub>O</b> E=-2500.264234 Hartree			
Ru	0.47589400	-0.74647800	1.38439900
N	-3.03763500	-2.36996100	0.04216800
O	-1.68824000	-0.71049700	1.70658200
C	4.56441200	-0.23471700	-0.06231300
C	5.32105100	-0.41471000	1.09193700
C	4.67761100	-0.71378100	2.28588200
C	2.51238500	-1.17423900	3.50401200
C	0.38114200	-1.51158300	4.37612700
C	0.88632100	-1.82990500	5.62790200
C	2.26577700	-1.81316300	5.80931100
C	3.08482300	-1.48263500	4.73740300
H	2.55316000	-0.21232700	-0.84326800
H	5.02512100	-0.00296000	-1.01494200
H	6.40100000	-0.32317000	1.06535700
H	5.25616300	-0.85225100	3.19004000
H	-0.68665100	-1.52047100	4.19365300
H	0.20807000	-2.08587900	6.43279500
H	2.70161200	-2.05776000	6.77135300
H	4.15972100	-1.47437600	4.86291500
N	1.16461200	-1.18916100	3.33561000
N	2.55923700	-0.64424000	1.17697600
C	-0.73713900	-1.20255300	-2.83164400
C	-0.99626100	0.07476800	-3.30599500
C	-0.80429400	1.16428400	-2.40662500
C	-0.32565200	0.88367600	-1.10547700
C	-0.30164800	-1.39169600	-1.52021500
C	-1.10884000	2.52447400	-2.73747700
C	-0.04514500	1.96731800	-0.19244000
C	-0.27098700	3.30605700	-0.58874000
C	-0.85772700	3.54461400	-1.87228400
C	0.06323300	4.33798300	0.33772800
C	0.54688700	3.95929600	1.58186300
C	0.72455000	2.60360200	1.88129500
H	-1.56523400	2.73944100	-3.69576500
H	-0.85967700	-2.06667000	-3.47411100
H	-0.10846700	-2.38978300	-1.14186700
H	-1.11814300	4.55790500	-2.15294000
H	0.81962100	4.70842600	2.31644800
H	1.11972600	2.29515900	2.84590400
N	0.44806200	1.63842700	1.02098900
N	-0.09853000	-0.38695200	-0.67258300
C	-0.07553500	5.77550200	0.01451700
C	-0.77842400	6.62384400	0.88126200
C	0.53137600	6.32124100	-1.12605200
C	-0.88498200	7.98441200	0.60504900
H	-1.25674900	6.21129300	1.76476000
C	0.43253000	7.68414300	-1.39357700
H	1.10131700	5.68058700	-1.79250300
C	-0.27927900	8.51803000	-0.53188300
H	-1.44200300	8.62738000	1.27955800
H	0.91615300	8.09414200	-2.27483400
H	-0.35938000	9.57974200	-0.74435000
C	-1.44844500	0.25449400	-4.70241300

C	-2.53307000	-0.49239300	-5.18313800
C	-0.78032200	1.12335200	-5.57754800
C	-2.95267800	-0.35889700	-6.50366900
H	-3.05764500	-1.16726100	-4.51318400
C	-1.19448100	1.24509100	-6.90122700
H	0.07960300	1.68644600	-5.22726300
C	-2.28425300	0.50946400	-7.36592100
H	-3.80226100	-0.93438400	-6.85801400
H	-0.66147900	1.91338500	-7.57038300
H	-2.60908400	0.61020200	-8.39693400
C	-4.06682200	-3.98287200	-1.96757700
C	-3.40193500	-4.54377900	-0.88119700
C	-2.90542100	-3.70398000	0.11723700
C	-3.67828700	-1.83572500	-1.00203600
C	-4.21848600	-2.60039000	-2.03025800
H	-4.46619200	-4.61826300	-2.75126700
H	-3.27375600	-5.61794800	-0.80102000
H	-3.75311400	-0.75083800	-1.01399000
H	-4.74146100	-2.12377100	-2.85198100
C	3.18563700	-0.35186400	0.02520600
C	-2.19299400	-4.25409700	1.31821100
S	-0.38590100	-4.33443200	1.02639900
C	0.14310200	-4.91498600	2.65814100
H	1.23049800	-4.99404300	2.61346100
H	-0.13650800	-4.19854000	3.43486100
H	-0.28902700	-5.89334400	2.88009500
H	-2.37485700	-3.61939300	2.18919600
H	-2.54497800	-5.26343900	1.54442900
C	3.28933800	-0.83443900	2.30534600
H	-2.22195500	-1.33090800	1.11401300
H	-2.04264100	-0.81095700	2.60004100
O	2.92025400	-3.83251300	1.21383400
H	3.59195300	-3.81675200	0.52029700
H	2.19444300	-3.31920400	0.83930000
<b>TS<sub>2c</sub></b> E=-2500.259707 Hartree			
Ru	0.65857600	-1.25464700	1.20053300
N	-3.07916500	-1.73116500	0.07007200
O	-1.51150900	-0.45145100	1.96896400
C	4.80015500	-0.57103800	-0.27264400
C	5.55521800	-0.69873400	0.88903200
C	4.91543800	-0.96812200	2.09346800
C	2.74744600	-1.38932700	3.33122400
C	0.63053100	-1.70377000	4.23932100
C	1.14076000	-1.84898200	5.52065600
C	2.51743400	-1.76690000	5.69828000
C	3.32477600	-1.53339200	4.59278200
H	2.78673000	-0.62661500	-1.05519000
H	5.26013200	-0.35797400	-1.23008900
H	6.63332600	-0.58653400	0.86248600
H	5.49769800	-1.06065000	3.00105500
H	-0.43449500	-1.77213700	4.05825400
H	0.46670100	-2.02564400	6.35009000
H	2.95942400	-1.87926100	6.68174100
H	4.39735200	-1.46180000	4.71738300
N	1.40178400	-1.48456200	3.16366100
N	2.80503100	-0.99098700	0.97532700
C	-0.48172600	-1.66065500	-3.03033300

C	-0.81306000	-0.38237400	-3.45588900
C	-0.69886200	0.67411400	-2.50573000
C	-0.20185500	0.37059000	-1.21586500
C	-0.06541700	-1.88300800	-1.71982800
C	-1.10486500	2.02207900	-2.77153300
C	0.04412600	1.43301900	-0.27159500
C	-0.28859800	2.76740200	-0.60243000
C	-0.92159900	3.01701000	-1.86143500
C	-0.00916100	3.78049300	0.36105000
C	0.54636600	3.38677900	1.56973400
C	0.84201900	2.03801600	1.79913000
H	-1.58989600	2.24498000	-3.71372800
H	-0.53589400	-2.50219600	-3.71082700
H	0.17150800	-2.88793700	-1.38928800
H	-1.26594000	4.01831500	-2.08957700
H	0.78167300	4.12160000	2.33126400
H	1.29188700	1.72367200	2.73743500
N	0.60736600	1.09079700	0.90812000
N	0.07311700	-0.90737300	-0.82253000
C	-0.28408400	5.21346900	0.11221400
C	-1.04471400	5.94940400	1.03115800
C	0.24182000	5.86670900	-1.01184800
C	-1.28750300	7.30448400	0.82186900
H	-1.46122900	5.45206800	1.90219900
C	0.00666700	7.22437200	-1.21259000
H	0.85401400	5.31469400	-1.71896500
C	-0.76223700	7.94532200	-0.29960300
H	-1.88874600	7.85897000	1.53584700
H	0.42784300	7.71886700	-2.08247000
H	-0.94955500	9.00256800	-0.46053500
C	-1.25054400	-0.17239400	-4.85217900
C	-2.23299400	-1.00564900	-5.40724300
C	-0.66016700	0.81035100	-5.66097700
C	-2.63189000	-0.84478400	-6.73091300
H	-2.69517900	-1.77339000	-4.79406200
C	-1.05237100	0.96048900	-6.98826500
H	0.12640000	1.44085800	-5.25771200
C	-2.04301800	0.13868500	-7.52476800
H	-3.40241200	-1.48986800	-7.14154200
H	-0.57869500	1.71829600	-7.60451100
H	-2.35109500	0.26116800	-8.55854200
C	-3.88699400	-3.20750200	-2.14146300
C	-3.30386600	-3.83728400	-1.04531900
C	-2.92062600	-3.06383100	0.05167500
C	-3.63333400	-1.13269000	-0.98735200
C	-4.06312600	-1.82713300	-2.11451900
H	-4.20060100	-3.78870100	-3.00273200
H	-3.15491800	-4.91179800	-1.03434100
H	-3.73400100	-0.05159000	-0.92843600
H	-4.51558300	-1.29597300	-2.94462800
C	3.42299800	-0.72069300	-0.18194900
C	-2.31349900	-3.69381900	1.27290200
S	-0.47763100	-3.72712400	1.18818600
C	-0.12368700	-4.64674300	2.70428800
H	0.96322000	-4.67995600	2.78584600
H	-0.55852100	-4.15643500	3.57678100
H	-0.51943000	-5.65957900	2.60998800



H	-2.60880600	-3.15309500	2.17442300
H	-2.63058300	-4.73456000	1.36777300
C	3.52792600	-1.11380800	2.11262800
H	-2.19018600	-0.82369000	1.34676500
H	-1.86333200	-0.59929700	2.85673400
O	2.77455300	-4.27821000	1.08584600
H	3.69752000	-4.10044000	1.30759600
H	2.60994600	-3.70265900	0.32871600
<b><sup>3</sup>Ru-H<sub>2</sub>O</b> E=-2500.265379 Hartree			
Ru	0.44066900	-0.95795500	1.07116400
N	-3.08461500	-1.95723200	0.16823500
O	-2.10336500	0.12917100	1.84327700
C	4.99277300	-0.93391200	0.21578500
C	5.52661300	-1.25222500	1.46205700
C	4.68701000	-1.32202900	2.56987000
C	2.34213100	-1.08503200	3.50865300
C	0.10549500	-0.96742000	4.13439100
C	0.42112100	-1.01326700	5.48484200
C	1.76043400	-1.10407000	5.84671400
C	2.72671200	-1.13362100	4.84928000
H	3.14427600	-0.47941000	-0.81897900
H	5.61647800	-0.86221700	-0.66757600
H	6.58786000	-1.44527100	1.57463600
H	5.09719500	-1.57636000	3.53908600
H	-0.92155600	-0.89247000	3.79893600
H	-0.36983200	-0.97816600	6.22430100
H	2.05351700	-1.14172100	6.88993500
H	3.77400900	-1.17856000	5.11816300
N	1.03306400	-1.01071100	3.16501100
N	2.81503800	-0.79342200	1.18806900
C	-0.78320000	-1.37198900	-3.16362800
C	-1.08882800	-0.07138300	-3.54197700
C	-0.88908700	0.95831200	-2.57697500
C	-0.37504400	0.59302000	-1.31436800
C	-0.31953000	-1.64891900	-1.87812800
C	-1.21685900	2.33654600	-2.79076100
C	-0.07043100	1.59698300	-0.33836700
C	-0.31630600	2.95934500	-0.61187900
C	-0.94894800	3.28798400	-1.85410100
C	0.03686600	3.91327600	0.38643100
C	0.57903800	3.43328100	1.57107400
C	0.77970800	2.06398300	1.75694500
H	-1.70442800	2.62147300	-3.71476700
H	-0.89902500	-2.19057500	-3.86422100
H	-0.09347600	-2.66812000	-1.58590400
H	-1.22931000	4.31663600	-2.04437100
H	0.87338400	4.11850300	2.35743100
H	1.20994000	1.68890600	2.67898000
N	0.46789500	1.16478500	0.83221800
N	-0.13047000	-0.70241800	-0.96092200
C	-0.15140900	5.36855900	0.20432700
C	-0.83734500	6.10900500	1.17736000
C	0.38273800	6.03604100	-0.90754400
C	-1.00021900	7.48399800	1.03257600
H	-1.26026100	5.60069800	2.03888900
C	0.22843400	7.41317800	-1.04286000
H	0.94039600	5.47952800	-1.65499700

C	-0.46726100	8.13931400	-0.07688000
H	-1.54459800	8.04274100	1.78757500
H	0.65579600	7.91869400	-1.90322300
H	-0.59151700	9.21219600	-0.18706700
C	-1.59659900	0.19167900	-4.90473400
C	-2.67561200	-0.55564600	-5.39813200
C	-0.99299400	1.14570100	-5.73721300
C	-3.15344000	-0.33938600	-6.68738700
H	-3.15150000	-1.29525200	-4.76101600
C	-1.46546500	1.35043500	-7.03076800
H	-0.13654300	1.70994800	-5.38054400
C	-2.54958400	0.61371700	-7.50672300
H	-3.99814900	-0.91627000	-7.05085600
H	-0.98237500	2.08473600	-7.66781400
H	-2.92006500	0.77938900	-8.51367300
C	-3.59606000	-3.70791300	-1.93472000
C	-2.84279500	-4.11817300	-0.83849500
C	-2.61269900	-3.21234600	0.19952800
C	-3.80404800	-1.57118100	-0.88917600
C	-4.09331900	-2.40840100	-1.96323100
H	-3.79323900	-4.39474500	-2.75125600
H	-2.44307600	-5.12531600	-0.78320800
H	-4.16302300	-0.54490200	-0.87425000
H	-4.69119400	-2.04820600	-2.79323300
C	3.62080700	-0.71556200	0.12901500
C	-1.81746100	-3.61274600	1.40902900
S	-0.00541500	-3.39430200	1.14573800
C	0.61920800	-4.16776400	2.65843000
H	1.70530400	-4.09772900	2.59889400
H	0.23999000	-3.66506900	3.54852800
H	0.31846700	-5.21683800	2.65545800
H	-2.11458900	-3.02746000	2.28054800
H	-1.94912100	-4.67502000	1.62690200
C	3.32293800	-1.07396100	2.39865000
H	-2.55084000	-0.58200800	1.33088000
H	-2.59525700	0.17728000	2.67284900
O	3.13598300	-4.02368500	0.56948100
H	3.99003700	-3.57418700	0.56562700
H	2.72955500	-3.74101100	-0.25907600
<b>PATH_TRIPLET Td</b>			
<b>Td E=-2423.869255 Hartree</b>			
Ru	0.29186200	-1.08847500	1.15763100
C	2.95023200	-0.59964400	2.41381700
C	2.98225700	0.10433200	0.19475900
C	4.32361500	0.45190300	0.27001400
C	4.99260200	0.25247600	1.47333600
C	4.29975700	-0.27571200	2.55555300
C	2.11861600	-1.13277000	3.50489200
C	-0.00971700	-1.84678600	4.13133000
C	0.38466400	-2.03706700	5.44713500
C	1.70700700	-1.77227600	5.78757200
C	2.57880200	-1.31131700	4.80893000
H	2.42128900	0.23509900	-0.72360400
H	4.82341100	0.86411400	-0.59823500
H	6.04217000	0.50558800	1.57231100
H	4.81140900	-0.43340900	3.49611800
H	-1.03059000	-2.03951000	3.82331800

H	-0.33400800	-2.38603900	6.17865300
H	2.05692600	-1.91334300	6.80397600
H	3.60521900	-1.08570900	5.06728900
N	0.83123900	-1.41831500	3.17572400
N	2.31121000	-0.41241000	1.23346000
C	-0.49655800	-1.39673800	-3.20661500
C	-0.64645400	-0.10005400	-3.67329300
C	-0.60170100	0.95234500	-2.71348500
C	-0.35553200	0.61837500	-1.36058100
C	-0.25484300	-1.63509300	-1.85340200
C	-0.84239300	2.32478700	-3.04424900
C	-0.31615600	1.66242100	-0.36324600
C	-0.47949400	3.01648300	-0.73947800
C	-0.77657700	3.30991800	-2.10775000
C	-0.39251000	4.00531500	0.28472700
C	-0.21382800	3.57056900	1.59052500
C	-0.09141000	2.20378800	1.86287000
H	-1.10050500	2.57736300	-4.06520100
H	-0.52986100	-2.23745600	-3.88970800
H	-0.11854100	-2.65005900	-1.49920900
H	-0.98049400	4.33393300	-2.39592700
H	-0.14070200	4.28513500	2.40251500
H	0.05941000	1.85222600	2.88055600
N	-0.13189600	1.27869200	0.91797800
N	-0.16039000	-0.66606100	-0.94682100
C	-0.47598100	5.45499300	0.00093800
C	-1.37141000	6.26056000	0.71803200
C	0.36783800	6.05367400	-0.94618200
C	-1.43223900	7.63139000	0.48174800
H	-2.03327700	5.80686400	1.44990300
C	0.31247500	7.42639700	-1.17210700
H	1.08469300	5.44570700	-1.49023500
C	-0.59032600	8.21769300	-0.46264500
H	-2.13873000	8.24114400	1.03645200
H	0.97860200	7.87738900	-1.90112500
H	-0.63584400	9.28726600	-0.64346400
C	-0.84630300	0.13950700	-5.11894100
C	-1.85925200	-0.54347800	-5.80630400
C	-0.00526600	1.00658300	-5.83161400
C	-2.03771000	-0.35014100	-7.17348700
H	-2.51980500	-1.21261400	-5.26277300
C	-0.17877600	1.18794200	-7.20109500
H	0.80001000	1.52191300	-5.31641400
C	-1.19777400	0.51464100	-7.87411100
H	-2.83445600	-0.87577600	-7.69066200
H	0.48581300	1.85420300	-7.74228400
H	-1.33522600	0.66190200	-8.94091300
C	-4.44418200	-2.61530300	1.30833700
C	-3.44165200	-3.55883900	1.48348700
C	-2.10128700	-3.17018000	1.45107700
C	-2.73410900	-0.96874800	1.07149200
C	-4.08159800	-1.28824800	1.10087900
H	-5.48756700	-2.90983500	1.33614600
H	-3.68374400	-4.60290000	1.64780200
H	-2.41467600	0.05425500	0.91186700
H	-4.82096300	-0.50855000	0.96187500
N	-1.75323900	-1.87917900	1.24020500

C	-1.03216000	-4.20281600	1.64990400
S	-0.72979700	-5.13928600	0.10120200
C	0.34731300	-6.43275000	0.77797400
H	0.62588600	-7.07762200	-0.05714100
H	1.25099200	-5.99998100	1.21417700
H	-0.18618700	-7.02226000	1.52665300
H	-0.09240500	-3.75521500	1.97959500
H	-1.35404700	-4.92003200	2.40939300
O	1.85552500	-3.18005700	0.41177400
H	2.54990600	-2.92687000	-0.21194800
H	1.31038700	-3.82737300	-0.06826300
<b>TS<sub>d</sub></b> E=-2423.858677 Hartree			
Ru	1.12525400	-0.57638700	-0.28040600
C	3.90587400	-0.04438800	1.02486300
C	4.09517100	0.49414700	-1.22527400
C	5.42986100	0.85766800	-1.08615700
C	6.00633800	0.75737900	0.17588600
C	5.24034600	0.30516100	1.24477100
C	2.99842000	-0.50624800	2.09905400
C	0.82361400	-1.09480900	2.69739900
C	1.17687000	-1.27600000	4.02636700
C	2.50399000	-1.07590100	4.38900800
C	3.41699700	-0.68363100	3.41846700
H	3.59282500	0.55344900	-2.18695900
H	5.99320300	1.20832500	-1.94286200
H	7.04358400	1.03246500	0.33273100
H	5.68513100	0.23686000	2.22918900
H	-0.19903800	-1.23466300	2.36579300
H	0.42436700	-1.56991300	4.74813300
H	2.82718200	-1.21582900	5.41446900
H	4.45010600	-0.51736800	3.69394000
N	1.70541200	-0.73284700	1.75079700
N	3.35899300	0.05390700	-0.20252600
C	0.26837500	-0.95793400	-4.58540300
C	0.06349900	0.34407100	-5.01942900
C	0.08776200	1.37466500	-4.03514900
C	0.38629500	1.01610300	-2.70238700
C	0.54270200	-1.22558800	-3.24352400
C	-0.22731600	2.74490900	-4.30834400
C	0.42487500	2.02031200	-1.67736500
C	0.16269800	3.37312200	-1.98644200
C	-0.19275700	3.69638300	-3.33471700
C	0.21002900	4.32003400	-0.92118100
C	0.47397300	3.84330100	0.35611900
C	0.71411400	2.48370400	0.56771700
H	-0.52544800	3.02198700	-5.31193600
H	0.25195700	-1.78186700	-5.28919100
H	0.71493900	-2.24291300	-2.91192600
H	-0.46415200	4.71644200	-3.57696600
H	0.52086300	4.52488400	1.19742600
H	0.93555700	2.10654200	1.56122000
N	0.69656900	1.59386000	-0.41688900
N	0.62678800	-0.27216500	-2.31900300
C	-0.01405300	5.76658600	-1.12970900
C	-0.95939500	6.44590200	-0.34846300
C	0.73637100	6.48705500	-2.07037700
C	-1.16176700	7.81289500	-0.51723500

H	-1.55054400	5.89619500	0.37808400
C	0.54036200	7.85651700	-2.22709200
H	1.49104100	5.97859400	-2.66309100
C	-0.41211200	8.52136100	-1.45555800
H	-1.90642200	8.32377700	0.08526500
H	1.13554300	8.40409000	-2.95119000
H	-0.56805500	9.58809600	-1.58350600
C	-0.16481700	0.61248400	-6.45492500
C	-1.13903100	-0.11100200	-7.15704200
C	0.61632400	1.55037100	-7.14642400
C	-1.33840900	0.11078900	-8.51684500
H	-1.75425100	-0.83464600	-6.63041100
C	0.42209600	1.76092400	-8.50879900
H	1.39382600	2.09767200	-6.62164200
C	-0.55824200	1.04595300	-9.19597500
H	-2.10476300	-0.44769500	-9.04529400
H	1.04094600	2.48220200	-9.03343600
H	-0.71181200	1.21539500	-10.25725500
C	-4.08361800	-1.72342800	-0.36500800
C	-3.22569300	-2.76929200	-0.05053000
C	-1.85861100	-2.52015400	0.10076100
C	-2.18158400	-0.28431600	-0.35958300
C	-3.55156000	-0.44694400	-0.51641800
H	-5.14728000	-1.90134700	-0.48320300
H	-3.60409500	-3.77709200	0.08274100
H	-1.73667100	0.69865900	-0.47155000
H	-4.17580700	0.40731200	-0.75206400
N	-1.34032100	-1.28773300	-0.06535300
C	-0.94256600	-3.65420300	0.45764900
S	-0.35094300	-4.51800000	-1.05065300
C	0.45310700	-5.94089700	-0.26240800
H	0.88116300	-6.54464400	-1.06440500
H	1.25225300	-5.61673500	0.40868500
H	-0.27876100	-6.53706000	0.28652700
H	-0.08120900	-3.30770100	1.03314400
H	-1.48093400	-4.38992000	1.05981600
O	2.25363700	-2.70352000	-0.55867300
H	3.00829700	-2.64922900	-1.16325800
H	1.63672800	-3.35308900	-0.95601800
<b><sup>3</sup>Ru-H<sub>2</sub>O+H<sub>2</sub>O E=-2500.278104 Hartree</b>			
Ru	1.39048000	-0.86987300	1.65734900
N	-2.74464700	-1.09148600	0.87337600
O	-0.45696100	-1.78551700	2.35843800
C	4.96748600	0.96348400	-0.09937500
C	5.84770100	0.99821300	0.97739000
C	5.43770400	0.49615700	2.20631300
C	3.62049500	-0.58372500	3.59294300
C	1.75014300	-1.52328100	4.62748300
C	2.41887100	-1.63698800	5.83802700
C	3.73974200	-1.20585200	5.91137300
C	4.34595300	-0.67320300	4.77962700
H	2.98157000	0.38611400	-0.71032100
H	5.24520000	1.34428200	-1.07475700
H	6.84296100	1.41344700	0.86592100
H	6.11267900	0.52345000	3.05188400
H	0.71942000	-1.83821400	4.51054200
H	1.90877000	-2.05504900	6.69749900

H	4.29560700	-1.28084000	6.83923000
H	5.37314400	-0.33525400	4.82714200
N	2.33440200	-1.01431400	3.53172600
N	3.30174900	-0.05929600	1.28094100
C	0.05149300	-2.11041400	-2.35855300
C	-0.50158600	-0.98993000	-2.95919700
C	-0.48706400	0.23036000	-2.22396100
C	0.07939300	0.22225500	-0.92897100
C	0.59025500	-2.02797500	-1.07379300
C	-1.07202800	1.44681600	-2.70165200
C	0.08469400	1.42819800	-0.13755700
C	-0.45452300	2.62612300	-0.66208400
C	-1.04991100	2.58995900	-1.96296200
C	-0.43793900	3.78160900	0.17368000
C	0.07455600	3.64543000	1.45607200
C	0.58259400	2.41230200	1.88127900
H	-1.56538500	1.44625200	-3.66556200
H	0.06868900	-3.06196900	-2.87626600
H	1.01977400	-2.90359000	-0.59785200
H	-1.52404300	3.48348500	-2.35040000
H	0.10736500	4.49601800	2.12738500
H	1.00209200	2.29853500	2.87734600
N	0.59372100	1.33766100	1.10989900
N	0.60486000	-0.90116300	-0.36736900
C	-0.94972500	5.09530700	-0.27541700
C	-1.90557400	5.77340900	0.49351200
C	-0.46242100	5.70016700	-1.44291700
C	-2.37424700	7.02273800	0.09523100
H	-2.29392600	5.31091800	1.39621500
C	-0.92459600	6.95461100	-1.83221200
H	0.29598700	5.19650800	-2.03509100
C	-1.88436700	7.61667400	-1.06730000
H	-3.12314100	7.53135500	0.69451900
H	-0.53109600	7.41550300	-2.73294000
H	-2.24760000	8.59249000	-1.37492000
C	-1.10475700	-1.10506000	-4.30464400
C	-2.10349600	-2.06281600	-4.52990300
C	-0.67988100	-0.29734500	-5.36869700
C	-2.67624900	-2.19771000	-5.79197400
H	-2.44003800	-2.68990200	-3.70860200
C	-1.24664700	-0.44415100	-6.63208300
H	0.10931600	0.43197600	-5.21101700
C	-2.24907800	-1.39004400	-6.84530700
H	-3.45705600	-2.93503100	-5.95124300
H	-0.90235500	0.18051800	-7.45049200
H	-2.69381200	-1.49846500	-7.82978200
C	-4.23262200	-0.10288000	-1.26086100
C	-4.09529500	-1.47206000	-1.06662900
C	-3.35805500	-1.93365800	0.02833100
C	-2.90095900	0.22612000	0.69002400
C	-3.64319800	0.77114800	-0.35022100
H	-4.80282300	0.27640300	-2.10267900
H	-4.56134100	-2.18107500	-1.74302500
H	-2.40318700	0.86993100	1.41196700
H	-3.73799400	1.84630600	-0.45143900
C	3.70293900	0.42851600	0.09692400
C	-3.28143800	-3.40197200	0.34173800

S	-2.23879000	-4.33077300	-0.84672700
C	-2.80651400	-6.01095700	-0.46560100
H	-2.22417800	-6.68956800	-1.09123500
H	-2.63341100	-6.25554100	0.58498900
H	-3.86654700	-6.12012200	-0.70464400
H	-2.89241000	-3.54952300	1.35173700
H	-4.28355300	-3.83657500	0.29022300
C	4.15536100	-0.03470400	2.33767700
H	-1.28187700	-1.52723600	1.86436300
H	-0.35010000	-2.75698600	2.18315200
O	0.03069200	-4.31761300	1.55918800
H	-0.21540900	-5.05438800	2.13442100
H	-0.49980000	-4.44423200	0.74780400
PATH SINGLET			
<sup>1</sup> Ru-H <sub>2</sub> O+H <sub>2</sub> O E=-2500.296350 Hartree			
Ru	1.37622500	-0.92345500	1.50779400
N	-2.78373700	-1.11473800	0.78907200
O	-0.47426500	-1.79913700	2.28256000
C	5.02524800	0.50140500	-0.40409200
C	5.81960500	0.84278000	0.68495900
C	5.31912700	0.66130400	1.96871400
C	3.41854900	-0.08390500	3.46202700
C	1.50299000	-0.81836100	4.57361700
C	2.07627700	-0.58180500	5.81583100
C	3.37175200	-0.07669800	5.86534800
C	4.05023700	0.17368300	4.67775800
H	3.10445600	-0.28949900	-0.98535900
H	5.37177400	0.62447700	-1.42319900
H	6.81581700	1.24567500	0.54152900
H	5.92649600	0.92437400	2.82514900
H	0.49777200	-1.21097900	4.46725800
H	1.51374900	-0.79155800	6.71780500
H	3.85323400	0.12129700	6.81648000
H	5.05949100	0.56405700	4.70658600
N	2.15406500	-0.57424100	3.42687900
N	3.26746000	-0.18630600	1.07027700
C	0.08542300	-2.21454900	-2.49980800
C	-0.46402300	-1.06002000	-3.04068800
C	-0.43082900	0.12120900	-2.24438700
C	0.13368200	0.02459300	-0.95749100
C	0.64573600	-2.21007800	-1.21925200
C	-0.98380500	1.38353000	-2.63275800
C	0.14100200	1.14823000	-0.07591500
C	-0.36859300	2.39400500	-0.49486700
C	-0.93946900	2.46708400	-1.80709100
C	-0.35539200	3.47107200	0.43796300
C	0.10337400	3.19659400	1.71998100
C	0.58132800	1.93036600	2.06027000
H	-1.46819000	1.47032100	-3.59750600
H	0.08875500	-3.13677500	-3.06865400
H	1.08526200	-3.10677500	-0.79482800
H	-1.38741800	3.39896600	-2.12956100
H	0.12659800	3.97563900	2.47302800
H	0.95430400	1.72835900	3.05642800
N	0.61986700	0.92370900	1.18602700
N	0.66702800	-1.12271500	-0.45556100
C	-0.81067600	4.83373800	0.09385000

C	-1.74031800	5.49019700	0.91273200
C	-0.29187700	5.50710500	-1.02215300
C	-2.15251000	6.78576000	0.61336300
H	-2.15426800	4.97515400	1.77457700
C	-0.69780300	6.80683500	-1.31183800
H	0.44974100	5.02104800	-1.64914300
C	-1.63182000	7.44739000	-0.49826000
H	-2.88188800	7.27769800	1.24936400
H	-0.27978900	7.32002400	-2.17225400
H	-1.95080200	8.45927700	-0.72844200
C	-1.08588600	-1.09989200	-4.38141500
C	-2.09686500	-2.03578100	-4.64217000
C	-0.67217600	-0.23783800	-5.40650500
C	-2.69157400	-2.09660700	-5.89974200
H	-2.42567700	-2.70401800	-3.85069600
C	-1.26157300	-0.30987600	-6.66609000
H	0.12708000	0.47441400	-5.22310700
C	-2.27534300	-1.23492000	-6.91406700
H	-3.48126900	-2.81800300	-6.08598500
H	-0.92546400	0.35627000	-7.45466200
H	-2.73746200	-1.28562400	-7.89520200
C	-4.21787900	-0.16942500	-1.40197100
C	-4.06549800	-1.53413500	-1.18995900
C	-3.35608400	-1.97366100	-0.06761100
C	-2.95600300	0.19814300	0.58793600
C	-3.67201300	0.72218500	-0.48108900
H	-4.76657400	0.19294200	-2.26528100
H	-4.49855700	-2.25675100	-1.87378700
H	-2.49455000	0.85702000	1.32070000
H	-3.78127000	1.79468400	-0.59483900
C	3.75656000	-0.00843300	-0.16727900
C	-3.27089700	-3.43718700	0.26612900
S	-2.25765300	-4.38602800	-0.93085400
C	-2.81961000	-6.05816300	-0.50884100
H	-2.25502900	-6.74891900	-1.13738500
H	-2.61992300	-6.28490800	0.54091100
H	-3.88572900	-6.16846900	-0.71874900
H	-2.86045600	-3.56884300	1.26972900
H	-4.27469700	-3.87119400	0.24490300
C	4.03641400	0.14464900	2.14283600
H	-1.30381900	-1.53169400	1.80844200
H	-0.37081400	-2.76159700	2.07543000
O	0.06242500	-4.32070200	1.43209100
H	-0.14562600	-5.06838900	2.00830200
H	-0.48125400	-4.46218200	0.63240400
<b>TS<sub>50</sub> E=-2500.293708 Hartree</b>			
Ru	1.24669300	-0.72161800	1.42987000
N	-2.78482700	-1.42495500	0.26245000
O	-0.76127900	-1.14924000	2.19840600
C	5.10048900	-0.00143800	-0.46202300
C	5.95064000	0.12015200	0.63169200
C	5.42365900	-0.00000800	1.91186900
C	3.40701200	-0.36118800	3.39408700
C	1.37339200	-0.62680200	4.50430900
C	1.98863500	-0.56316800	5.74698800
C	3.36922600	-0.39886500	5.79772200
C	4.08481200	-0.29524300	4.61059700



H	3.05590900	-0.34665600	-1.05590600
H	5.46386500	0.08828800	-1.47875700
H	7.00924600	0.30952300	0.49469900
H	6.07275500	0.09987400	2.77216000
H	0.30050900	-0.74977000	4.40548000
H	1.39196900	-0.64309700	6.64778400
H	3.88665000	-0.34920900	6.74923700
H	5.15907600	-0.16571800	4.64014000
N	2.06097100	-0.53389600	3.35640800
N	3.23882600	-0.36473900	1.00075400
C	-0.08350500	-1.77857600	-2.63602300
C	-0.56036500	-0.57256100	-3.13521700
C	-0.48031800	0.56835400	-2.28322000
C	0.09444800	0.39428000	-1.00846700
C	0.46410700	-1.85723700	-1.35314600
C	-1.02093000	1.85841600	-2.59174800
C	0.19610800	1.48788100	-0.09383700
C	-0.28087500	2.76674800	-0.44585600
C	-0.92669900	2.90115200	-1.71854000
C	-0.14513700	3.81862700	0.50607700
C	0.41520900	3.49607500	1.73514100
C	0.84484500	2.19832400	2.01468300
H	-1.54238100	1.99905000	-3.53048100
H	-0.11661600	-2.67476000	-3.24462400
H	0.84127700	-2.79587500	-0.96251900
H	-1.37221100	3.85329000	-1.97912400
H	0.54699100	4.25776900	2.49467600
H	1.28440200	1.95325600	2.97343800
N	0.74584100	1.20855800	1.12722500
N	0.55170100	-0.80231500	-0.54971200
C	-0.57586600	5.20635400	0.23707700
C	-1.40416400	5.86868700	1.15451000
C	-0.13564000	5.89562400	-0.90253400
C	-1.79625000	7.18511800	0.92878900
H	-1.75689900	5.34198700	2.03635500
C	-0.52088900	7.21590900	-1.11938000
H	0.52994300	5.40534000	-1.60673300
C	-1.35530200	7.86198700	-0.20781500
H	-2.44742500	7.68123300	1.64178900
H	-0.16430600	7.74077100	-2.00015800
H	-1.65857100	8.88988400	-0.38133700
C	-1.13909900	-0.51810100	-4.49362700
C	-2.10931400	-1.45738800	-4.87287600
C	-0.71298700	0.43403800	-5.43135600
C	-2.65669200	-1.43017700	-6.15234400
H	-2.44855800	-2.19754100	-4.15434700
C	-1.25410400	0.45095700	-6.71404700
H	0.06170500	1.14657000	-5.16416500
C	-2.23143600	-0.47568500	-7.07564800
H	-3.41682500	-2.15514900	-6.42652800
H	-0.90770500	1.18765400	-7.43218400
H	-2.65707200	-0.45601200	-8.07419600
C	-4.36587200	-1.50502400	-2.02727000
C	-4.01313400	-2.67702000	-1.36688500
C	-3.22666400	-2.59949400	-0.21420500
C	-3.13850900	-0.30245000	-0.37395000
C	-3.92737500	-0.28566000	-1.51839500

H	-4.97744400	-1.54318000	-2.92307000
H	-4.34603700	-3.64321500	-1.73129400
H	-2.76821600	0.62686900	0.05383200
H	-4.17940400	0.65442400	-1.99630900
C	3.75343100	-0.24309200	-0.23379400
C	-2.86816800	-3.84135300	0.55119300
S	-1.41277800	-4.69247500	-0.17544900
C	-1.56329600	-6.28816200	0.67488600
H	-0.72681000	-6.90399900	0.33987900
H	-1.50408700	-6.16158200	1.75844000
H	-2.50183400	-6.77784400	0.40641700
H	-2.65606100	-3.59811800	1.59499200
H	-3.69937000	-4.55023100	0.52153000
C	4.06079900	-0.24043900	2.07816800
H	-1.48429700	-1.21181000	1.51617300
H	-0.61913200	-2.07710000	2.48642600
O	0.45156500	-3.52034000	2.33349500
H	0.68055900	-4.20267100	2.97797300
H	0.12718500	-3.99392700	1.54423500
<b><sup>1</sup>Ru-2H<sub>2</sub>O</b> E=-2500.306057 Hartree			
Ru	0.90476600	-0.81446200	1.41052000
N	-3.01963000	-1.77550200	0.18405300
O	-1.25061400	-1.10229400	2.21180900
C	4.77102700	-0.38024300	-0.56342400
C	5.65076900	-0.28086900	0.50881900
C	5.14460200	-0.33014700	1.80150600
C	3.14405400	-0.52343000	3.33547200
C	1.13209200	-0.66049300	4.49996700
C	1.77855800	-0.58308600	5.72595200
C	3.16545700	-0.47819100	5.73984500
C	3.85380400	-0.44585500	4.53312300
H	2.69773000	-0.61274400	-1.10724400
H	5.11666500	-0.34579700	-1.58966100
H	6.71614800	-0.16532000	0.34506700
H	5.81695700	-0.25109000	2.64598800
H	0.05213600	-0.73345200	4.43886600
H	1.19982000	-0.60561100	6.64153500
H	3.70802400	-0.41865400	6.67661700
H	4.93275400	-0.35990800	4.53181000
N	1.79051800	-0.63705200	3.33149800
N	2.91909200	-0.57744500	0.94587800
C	-0.43544700	-1.68196900	-2.74867900
C	-0.82911800	-0.43910400	-3.22644700
C	-0.74028700	0.66516800	-2.32870400
C	-0.21123400	0.43107400	-1.04134800
C	0.05143600	-1.82471100	-1.44809200
C	-1.21174600	1.98491200	-2.62365600
C	-0.05448700	1.51059800	-0.11019700
C	-0.45281900	2.81843300	-0.45785100
C	-1.07854400	3.00674800	-1.73273300
C	-0.25374100	3.85782700	0.49661100
C	0.28056000	3.50000000	1.72650300
C	0.63427800	2.17701900	1.99632500
H	-1.70721000	2.16579300	-3.56950900
H	-0.47924900	-2.55597900	-3.38796500
H	0.36619100	-2.79523500	-1.08385300
H	-1.46971400	3.98496700	-1.98359800

H	0.45670700	4.25044900	2.48824900
H	1.06157100	1.90381600	2.95384400
N	0.48349100	1.19659900	1.10709500
N	0.17100200	-0.80289000	-0.60461400
C	-0.58544800	5.27217600	0.22287200
C	-1.37592000	5.99333700	1.12888300
C	-0.08177100	5.92688100	-0.91093100
C	-1.66915000	7.33445300	0.89744400
H	-1.77685800	5.49469700	2.00641400
C	-0.36759800	7.27120800	-1.13330100
H	0.55499000	5.38856700	-1.60669700
C	-1.16533400	7.97673200	-0.23311300
H	-2.29259900	7.87703900	1.60133700
H	0.03743900	7.76774400	-2.00957200
H	-1.39145400	9.02364500	-0.41074200
C	-1.31506200	-0.30574300	-4.61573400
C	-2.29032600	-1.18736100	-5.10416200
C	-0.78237500	0.66264000	-5.48002000
C	-2.73810800	-1.08778100	-6.41835100
H	-2.70992100	-1.94170100	-4.44564600
C	-1.22359300	0.75162600	-6.79735400
H	-0.00238200	1.33067800	-5.12725600
C	-2.20670000	-0.11814000	-7.26798800
H	-3.50310400	-1.76909000	-6.77768300
H	-0.79485700	1.49960600	-7.45702000
H	-2.55419800	-0.04332300	-8.29379300
C	-4.43302500	-2.32513400	-2.14532100
C	-4.01031000	-3.35674100	-1.31338300
C	-3.30963800	-3.04335100	-0.14659400
C	-3.43589100	-0.78884500	-0.61660800
C	-4.14572500	-1.00942000	-1.79179800
H	-4.98484900	-2.54565600	-3.05364700
H	-4.22540400	-4.39211400	-1.55538000
H	-3.18738400	0.22187300	-0.30085200
H	-4.45534700	-0.17440100	-2.41043700
C	3.41673300	-0.52788400	-0.30204200
C	-2.86548200	-4.12121800	0.79976300
S	-1.26196600	-4.84931800	0.28738200
C	-1.12377000	-6.14317700	1.55049600
H	-0.18232500	-6.66428400	1.36834900
H	-1.10726500	-5.70755500	2.55215300
H	-1.95020300	-6.85141000	1.46175600
H	-2.76691600	-3.72237700	1.81152700
H	-3.59526900	-4.93441600	0.81731400
C	3.77311700	-0.47701600	2.00289800
H	-1.90078000	-1.33818400	1.48911300
H	-1.27148700	-1.86017800	2.81316500
O	1.18169100	-3.11837100	1.69380600
H	2.00082200	-3.43179000	1.28183300
H	0.46045000	-3.61027500	1.24255200

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