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Supporting Information: Mechanistic Insights into Light-Driven Hydrogen Evolution Reaction from Formic Acid by an Iridium Photocatalyst

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Table of Contents

1、Additional Figures and Tables

2、<u>Cartesian coordinates of all optimized structures</u>

1、Additional Figures and Tables

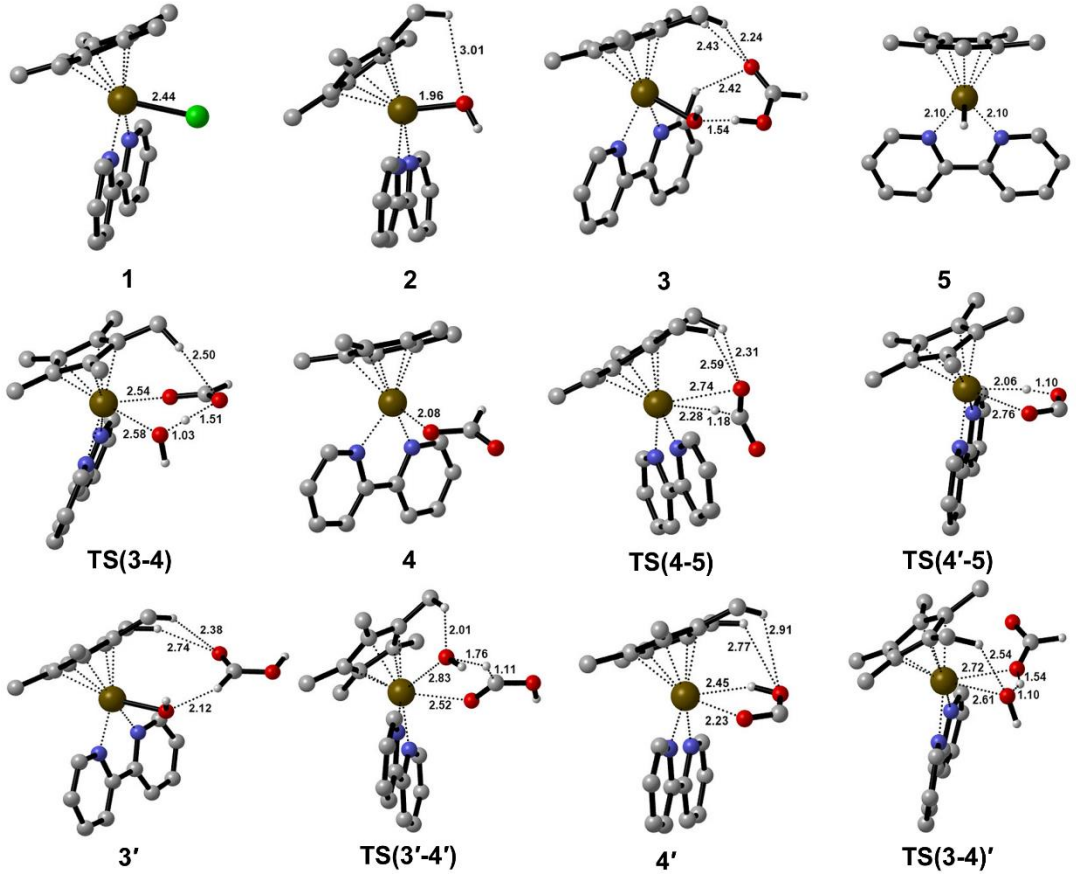
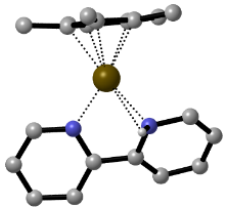
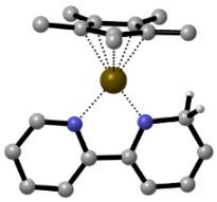
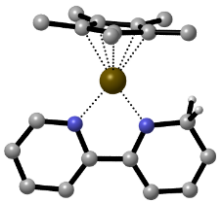
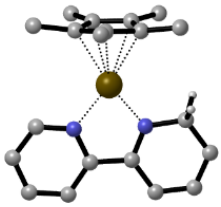


Figure S1. Optimized structures of intermediates and transition states for the formation of metal hydride **5** from catalyst $[Cp^*Ir(bpy)(Cl)]^+$ (**1**) (distances are in Å).

Table S1. S_0 and T_1 minima and T_1/S_0 conical intersections of isomers of metal hydride **5** (energy values in parentheses are in kcal/mol). Absolute values of SOC matrix elements are caculated at B3LYP-D3/TZP with scalar-relativistic ZORA level (unit: cm^{-1}).

Isomers	S_0	T_1	T_1/S_0	$\lvert\langle T_1\lvert SOC\rvert S_0\rangle\rvert$	
				X, *Y*	*Z*
5_7		 (11.3)			
5_6	 (-18.0)	 (0.6)	 (20.2/29.9)	159.0	38.5

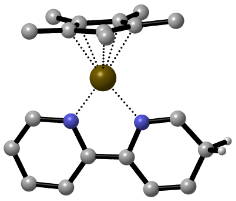
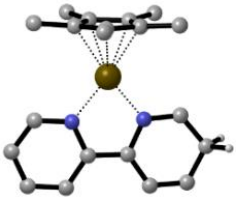
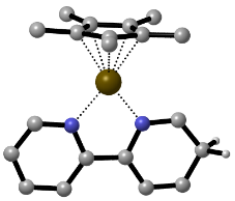
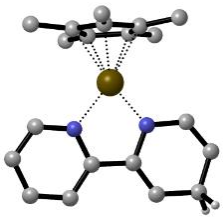
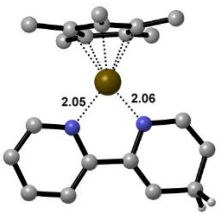
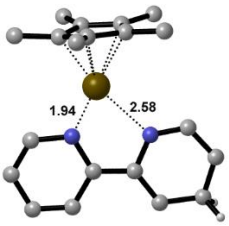
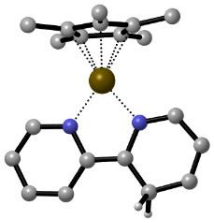
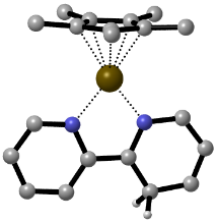
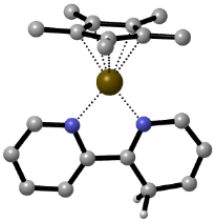
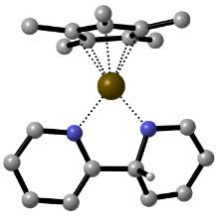
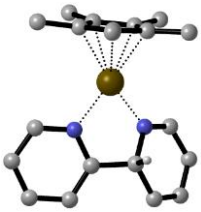
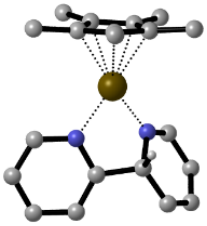
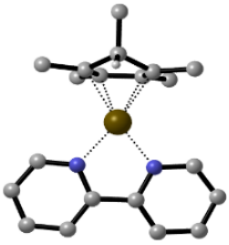
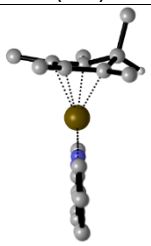
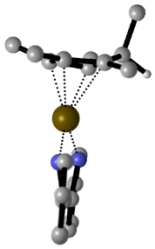
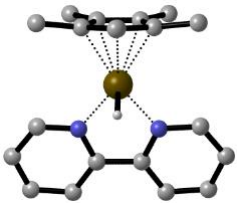
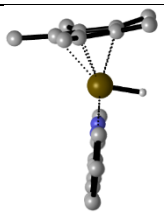
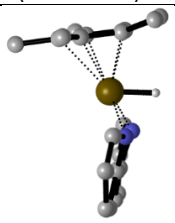
5_5	 (-6.8)	 (-1.4)	 (-0.9/-1.9)	8.7	34.6
5_4	 (-19.8)	 (4.0)	 (35.0/36.9)	52.1	83.7
5_3	 (-5.5)	 (-3.4)	 (-3.2/-0.5)	6.5	38.8
5_2	 (-12.0)	 (9.8)	 (18.0/21.9)	42.2	67.8
5_1	 (-30.1)	 (1.8)	 (52.5/53.5)	471	45.5
5	 (-39.4)	 (2.0)	 (40.2/49.3)	117	0.2

Table S2. Vertical electronic transitions of metal hydride **5** computed at TD-B3LYP-D3/BSII/PCM level (H: HOMO, L: LUMO).

Electron State	Electronic Configuration	Character	E (eV)/λ (nm)	f
$S_0 \longrightarrow S_1$	H ⟶ L (98%)	dπ ⟶ π*	2.79 (444)	0.1099
$S_0 \longrightarrow S_2$	H-1 ⟶ L (99%)	dπn ⟶ π*	2.96 (419)	0.0001
$S_0 \longrightarrow T_1$	H ⟶ L (96%)	dπ ⟶ π*	2.44 (508)	0.0000
$S_0 \longrightarrow T_2$	H-1 ⟶ L (77%)	dπn ⟶ π*	2.72 (456)	0.0000

Table S3. Frontier molecular orbital composition (%) for **5** in its ground state at the B3LYP-D3/TZP calculation level.

Orbital	Energy (eV)	% of composition			Main bond type
		Ir–H	bpy	Cp*	
LUMO+2	-4.577	3.4	91.6	2.6	π^*_{bpy}
LUMO+1	-4.762		97.1		π^*_{bpy}
LUMO	-5.594	2.8	93.4	1.6	π^*_{bpy}
HOMO	-8.906	34.4	7.7	50.6	6s,d_{z^2},d_{yz},H_{1s} + π_{Cp^*}
HOMO-1	-9.571	45.9	17.7	30.3	$d_{xy,xz}$ + n_{bpy} + π_{Cp^*}

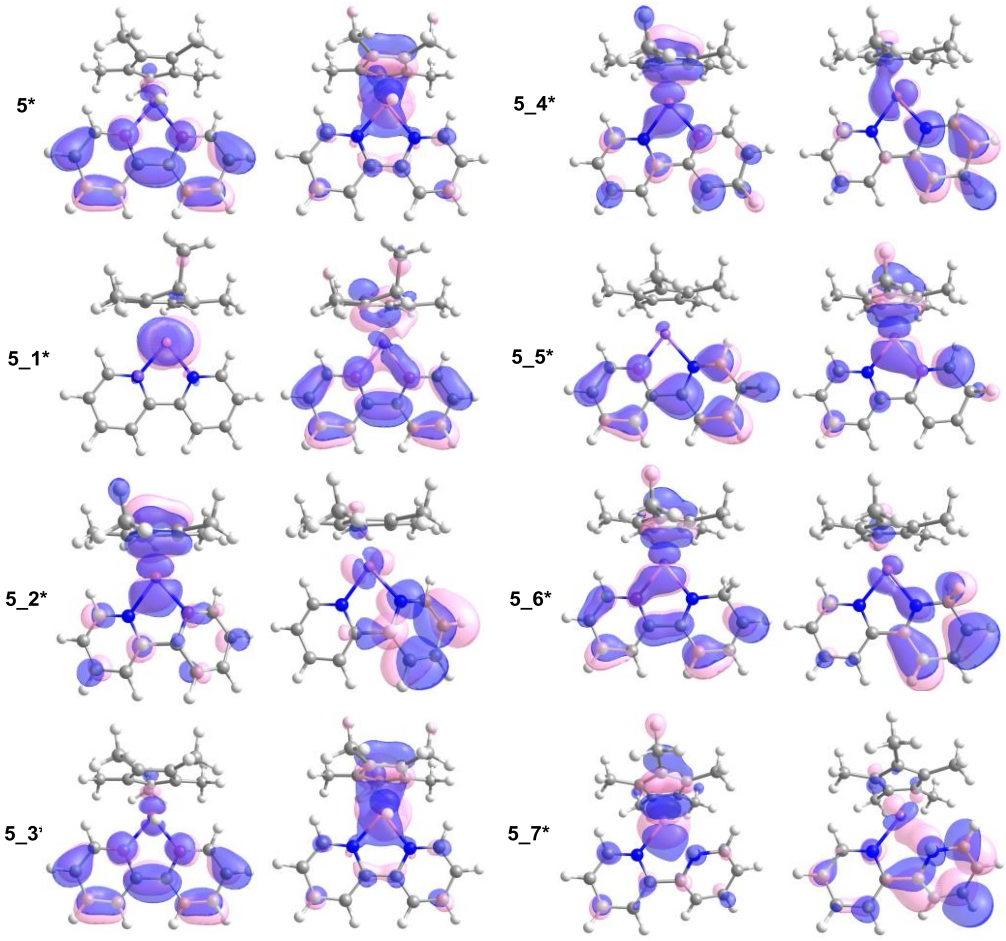


Figure S2. Singly occupied molecular orbitals (SOMOs) of isomers **5***, **5_1***, **5_2***, **5_3***, **5_4***, **5_5***, **5_6***, and **5_7*** obtained through biorthogonalizing unrestricted molecular orbitals to ensure their maximum alignment. The suffix * stands for structures in triplet state.

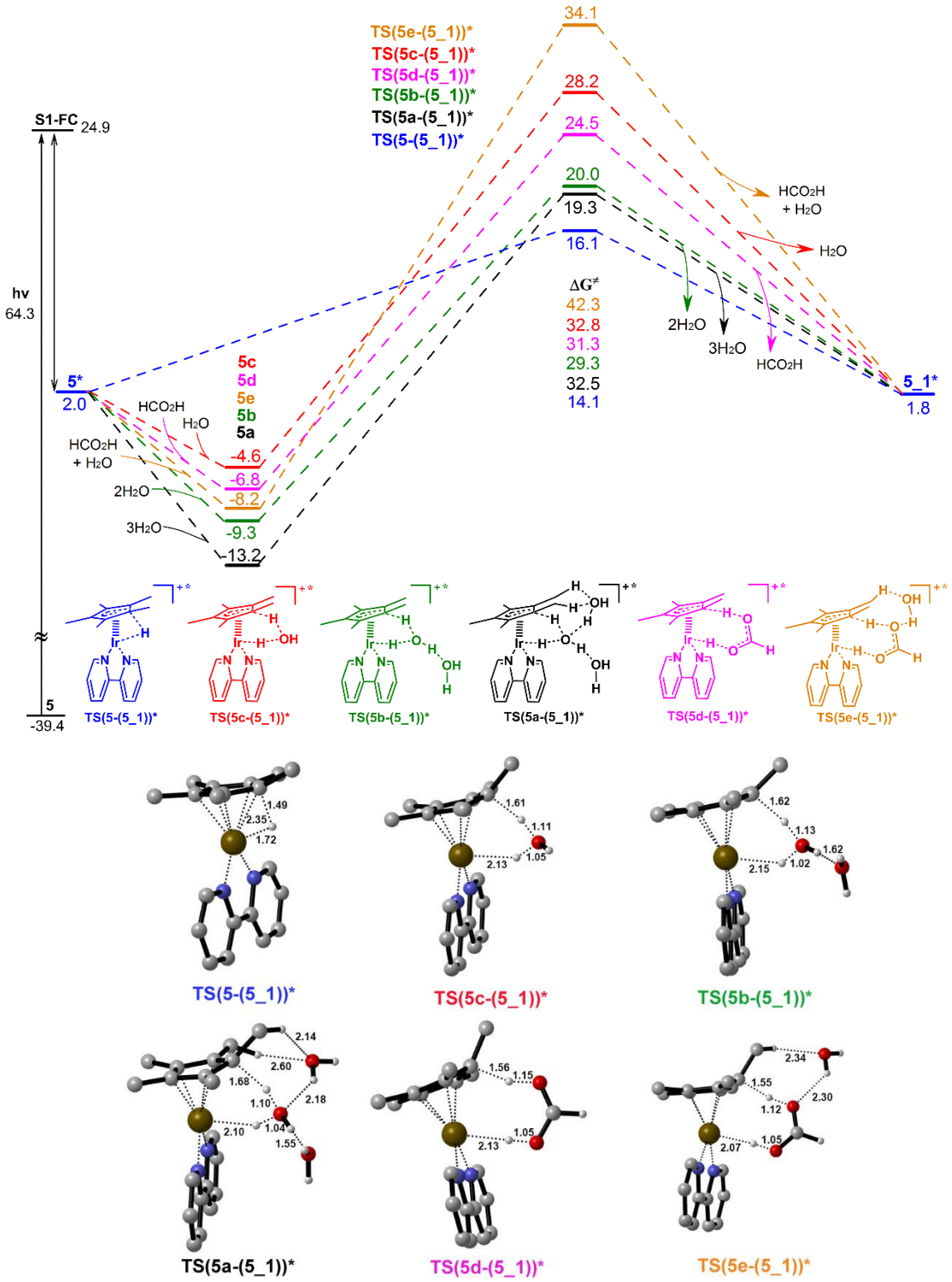


Figure S3. B3LYP-D3/BSII/PCM computed triplet free-energy (in kcal/mol) profiles for conversion from **5*** to **5_1***. Also shown are optimized structures of transition states with selected distances in Å. Six different pathways (unassisted, 1~3 water assisted, 1 formic acid assisted, and 1 water and 1 formic acid co-assisted) are investigated.

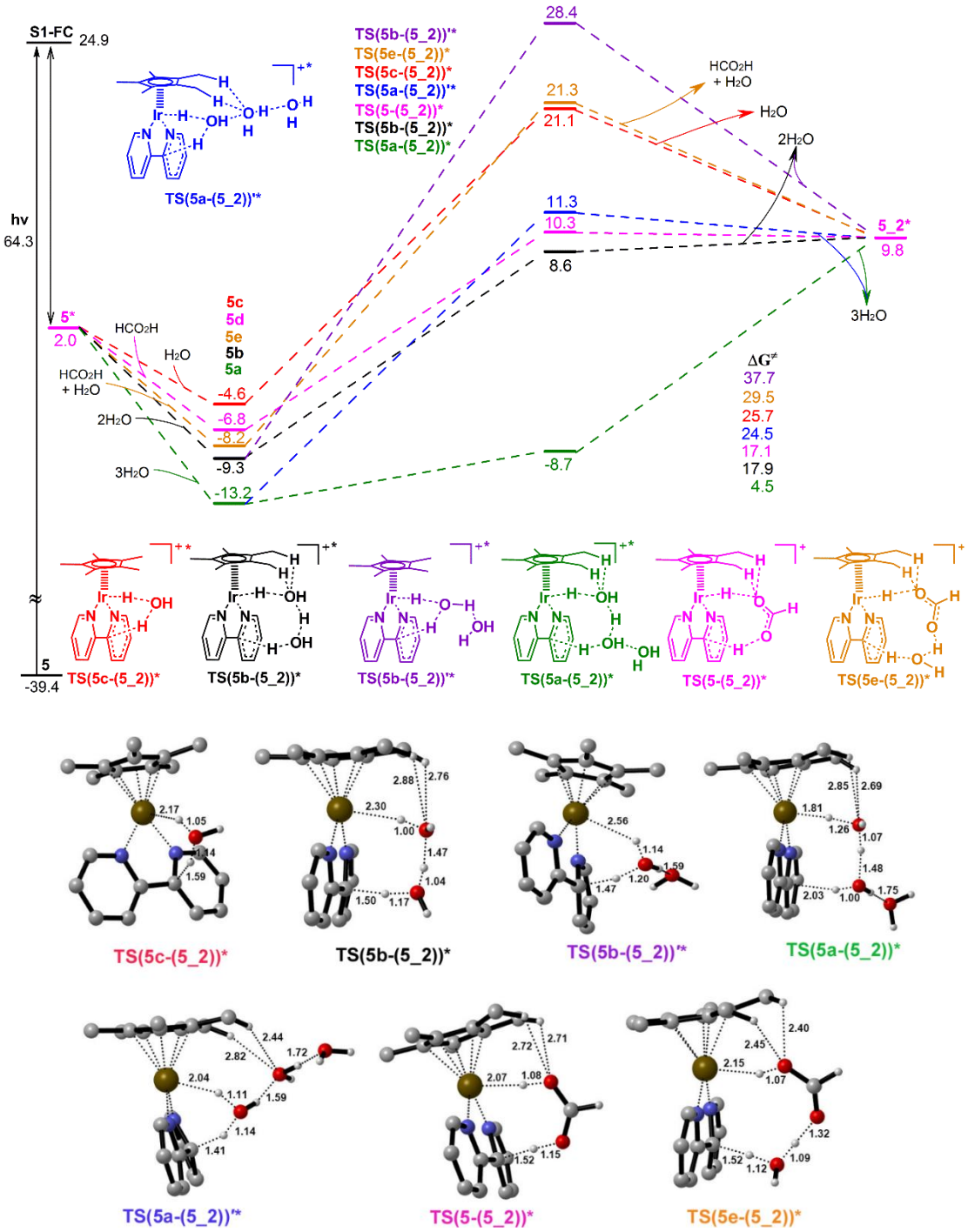


Figure S4. B3LYP-D3/BSII/PCM computed triplet free-energy (in kcal/mol) profiles for conversion from **5*** to **5_2***. Also shown are optimized structures of transition states with selected distances in Å. Seven different pathways (1~3 water assisted, 1 formic acid assisted, and 1 water and 1 formic acid co-assisted) are investigated.

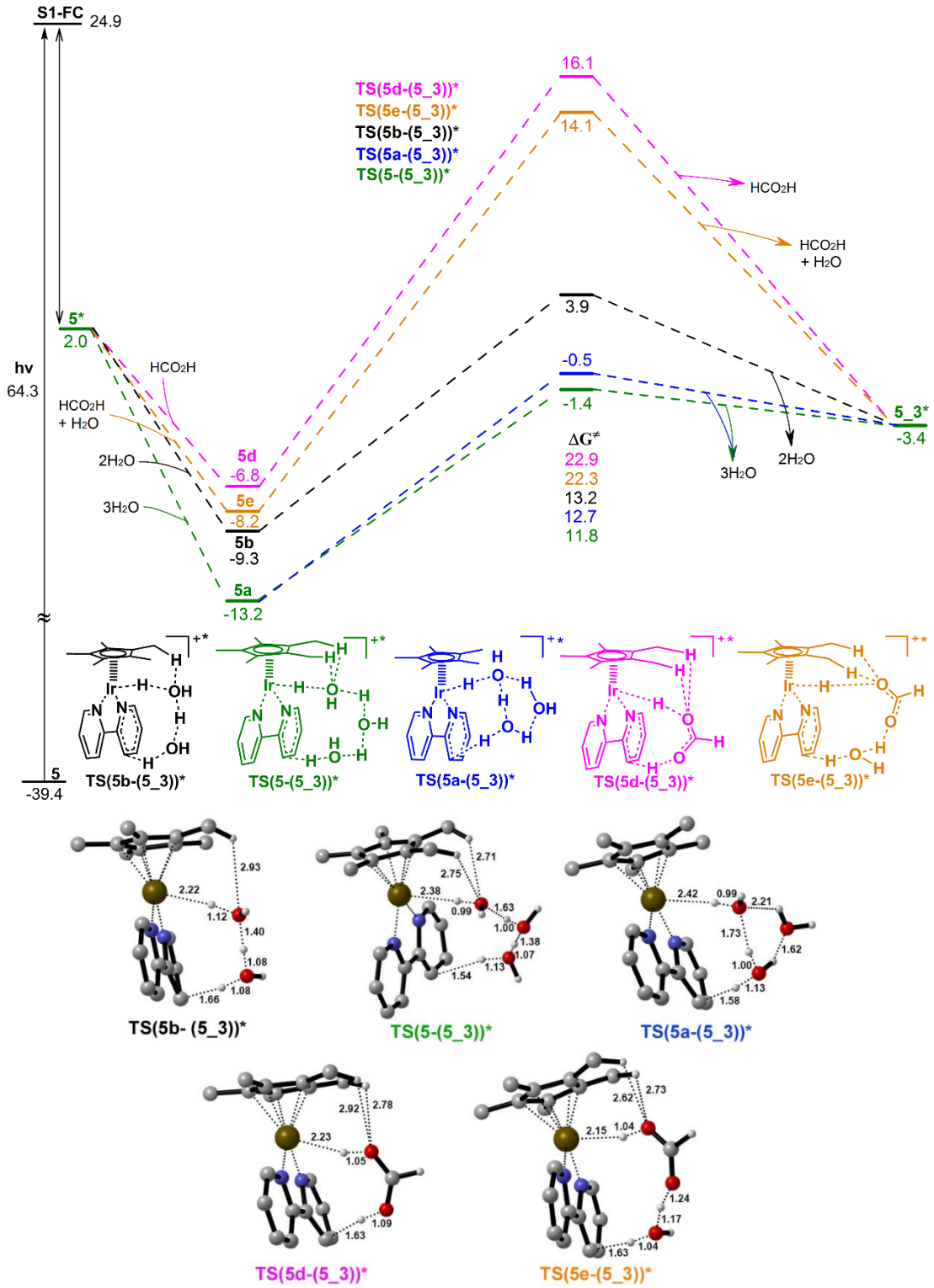


Figure S5. B3LYP-D3/BSII/PCM computed triplet free-energy (in kcal/mol) profiles for conversion from **5*** to **5_3***. Also shown are optimized structures of transition states with selected distances in Å. Five different pathways (2~3 water assisted, 1 formic acid assisted, and 1 water and 1 formic acid co-assisted) are investigated.

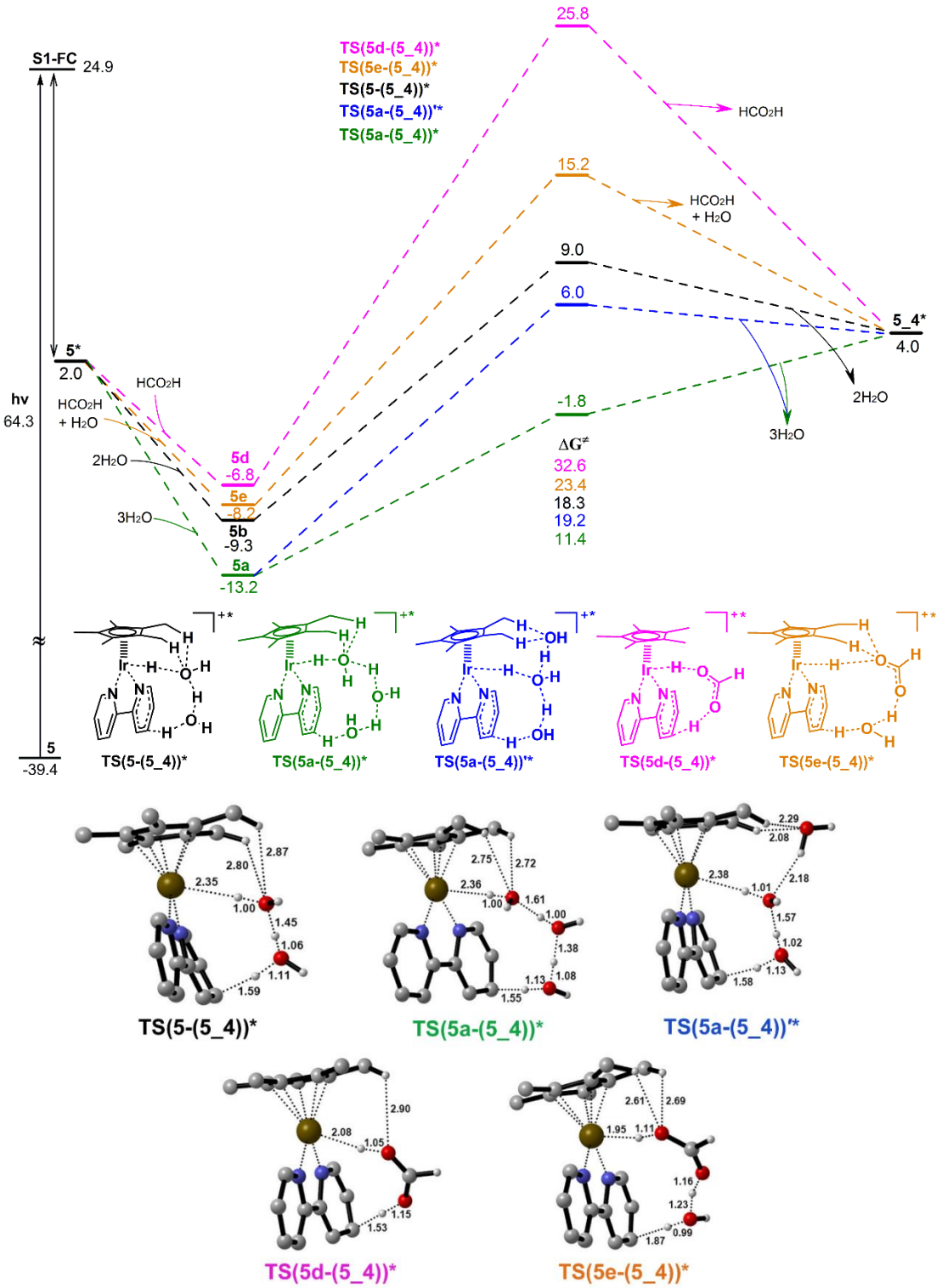


Figure S6. B3LYP-D3/BSII/PCM computed triplet free-energy (in kcal/mol) profiles for conversion from **5*** to **5_4***. Also shown are optimized structures of transition states with selected distances in Å. Five different pathways (2~3 water assisted, 1 formic acid assisted, and 1 water and 1 formic acid co-assisted) are investigated.

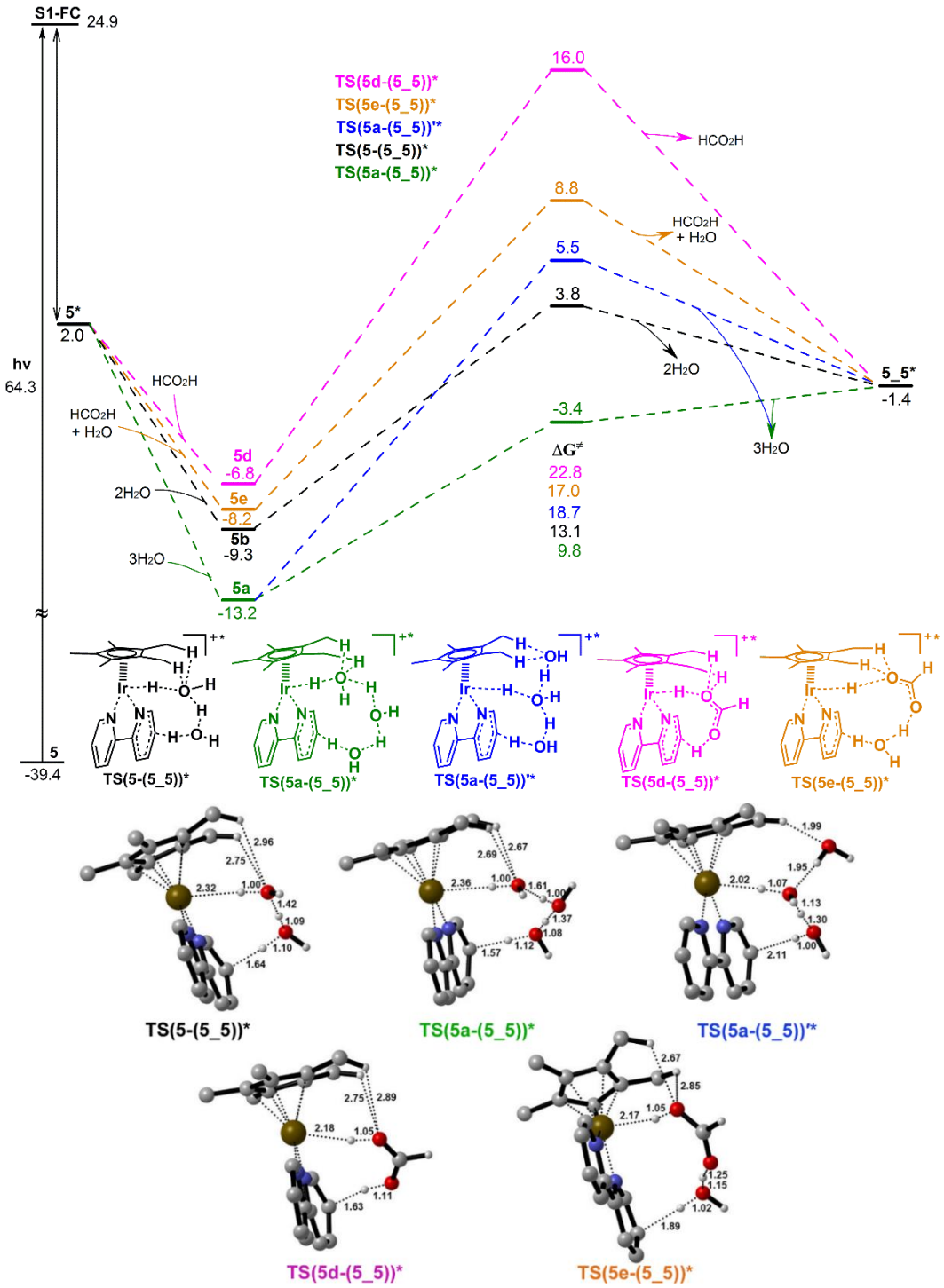


Figure S7. B3LYP-D3/BSII/PCM computed triplet free-energy (in kcal/mol) profiles for conversion from **5*** to **5_5***. Also shown are optimized structures of transition states with selected distances in Å. Five different pathways (2~3 water assisted, 1 formic acid assisted, and 1 water and 1 formic acid co-assisted) are investigated.

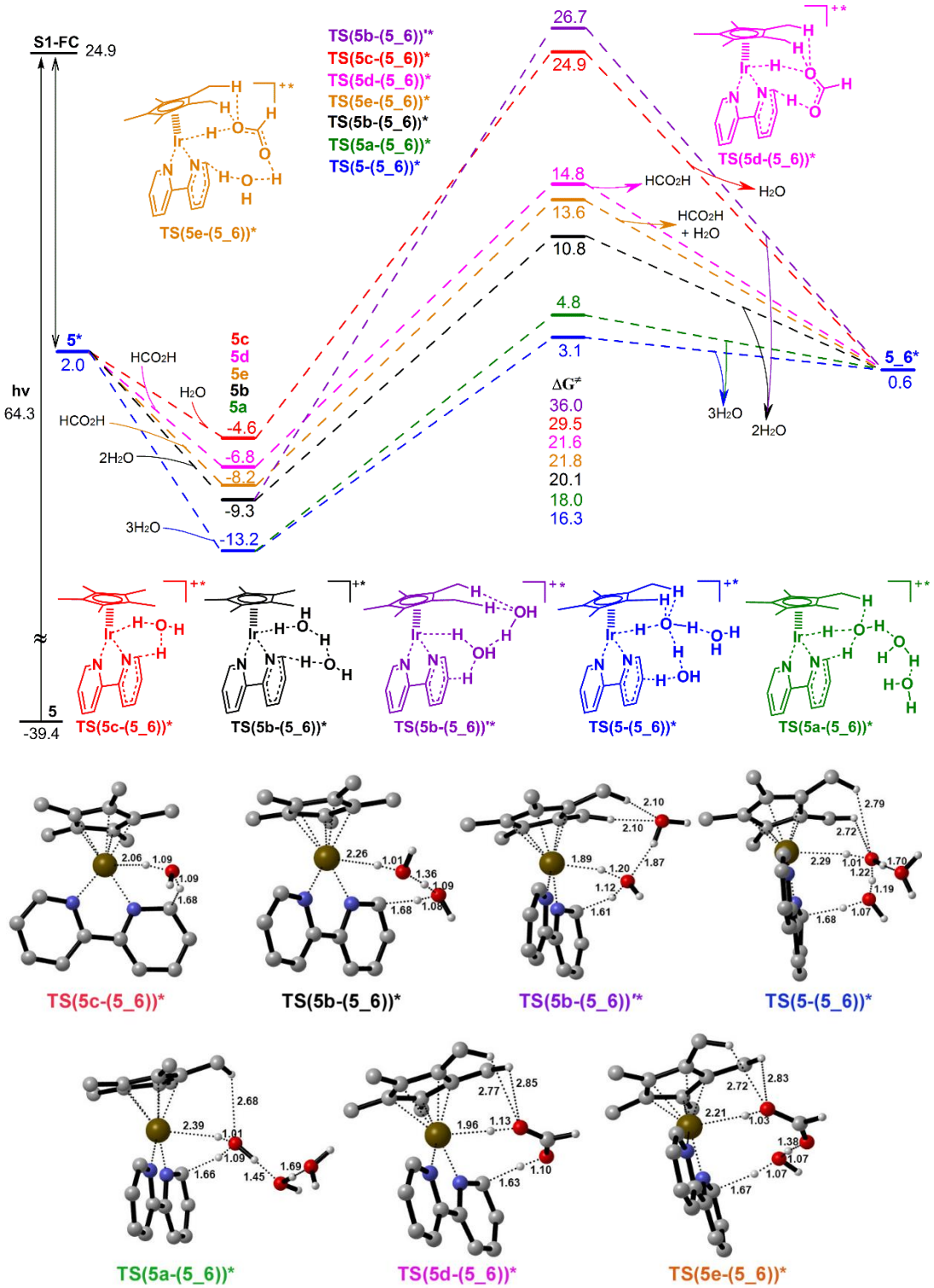


Figure S8. B3LYP-D3/BSII/PCM computed triplet free-energy (in kcal/mol) profiles for conversion from **5*** to **5_6***. Also shown are optimized structures of transition states with selected distances in Å. Seven different pathways (1~3 water assisted, 1 formic acid assisted, and 1 water and 1 formic acid co-assisted) are investigated.

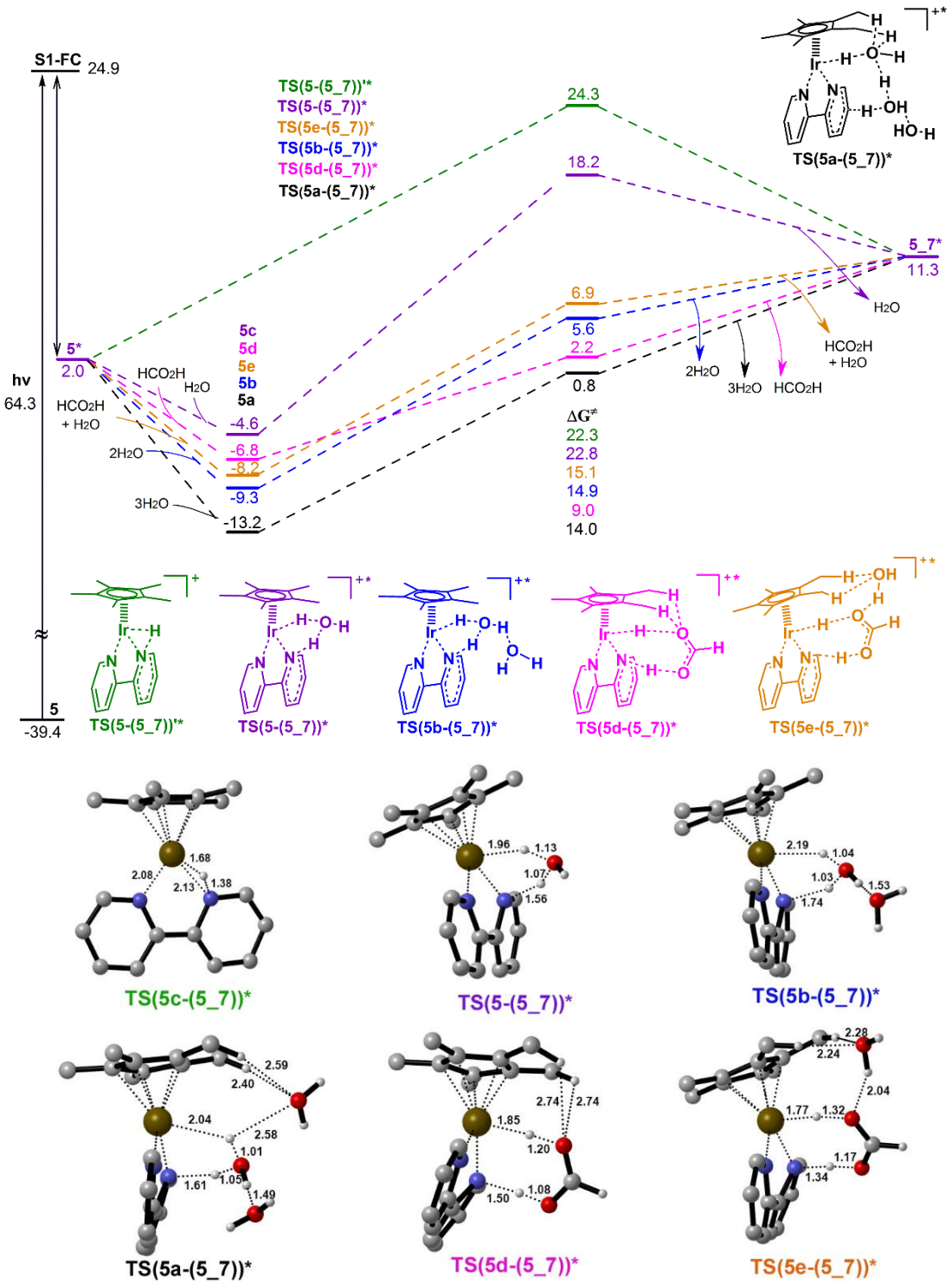


Figure S9. B3LYP-D3/BSII/PCM computed triplet free-energy (in kcal/mol) profiles for conversion from **5*** to **5_7***. Also shown are optimized structures of transition states with selected distances in Å. Six different pathways (unassisted, 1~3 water assisted, 1 formic acid assisted, and 1 water and 1 formic acid co-assisted) are investigated.

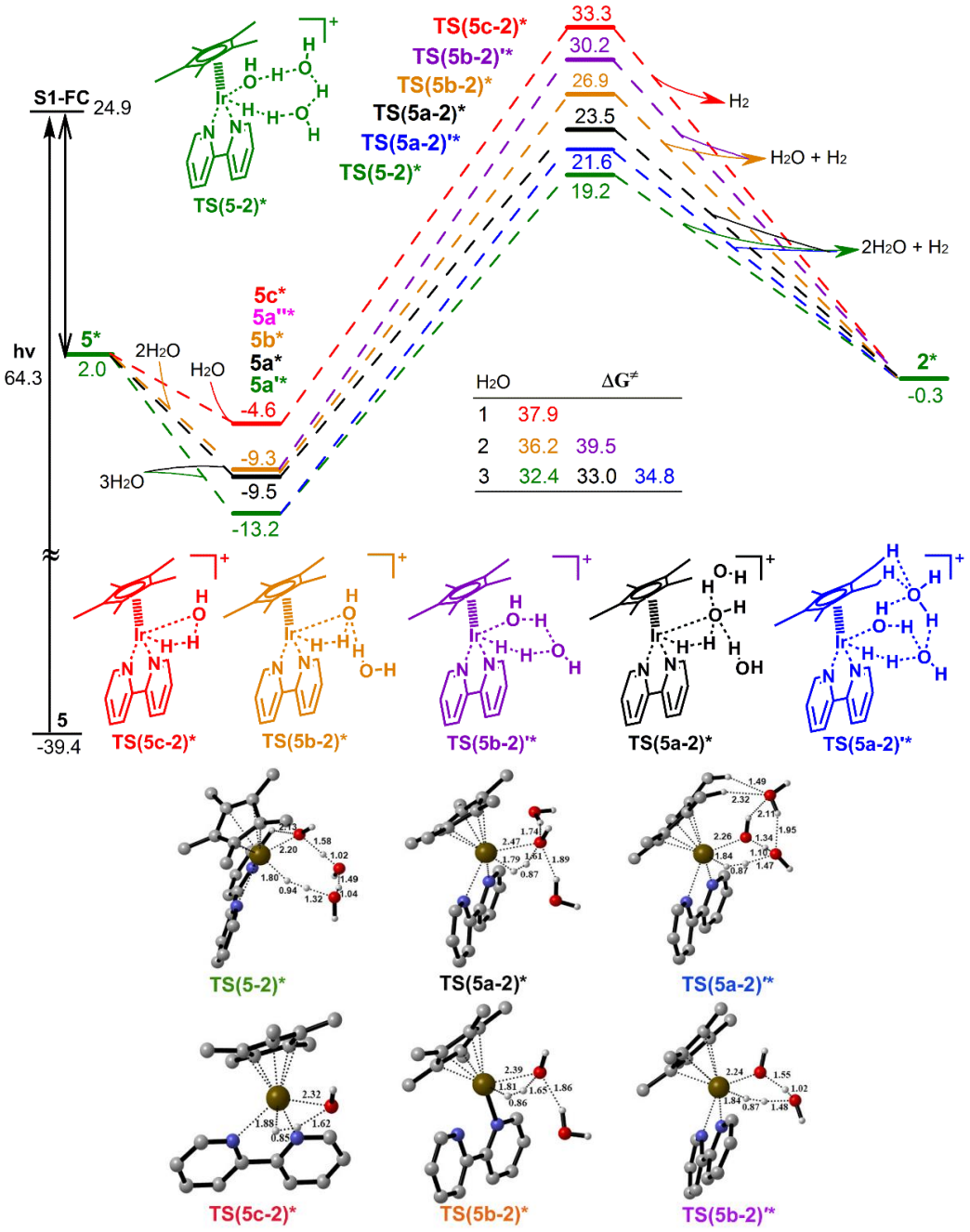


Figure S10. B3LYP-D3/BSII/PCM computed triplet free-energy (in kcal/mol) profile for H_2 evolution from **5***. Also shown are optimized transition states with some selected distances in Å. Six different pathways asissted with 1~3 water are investigated.

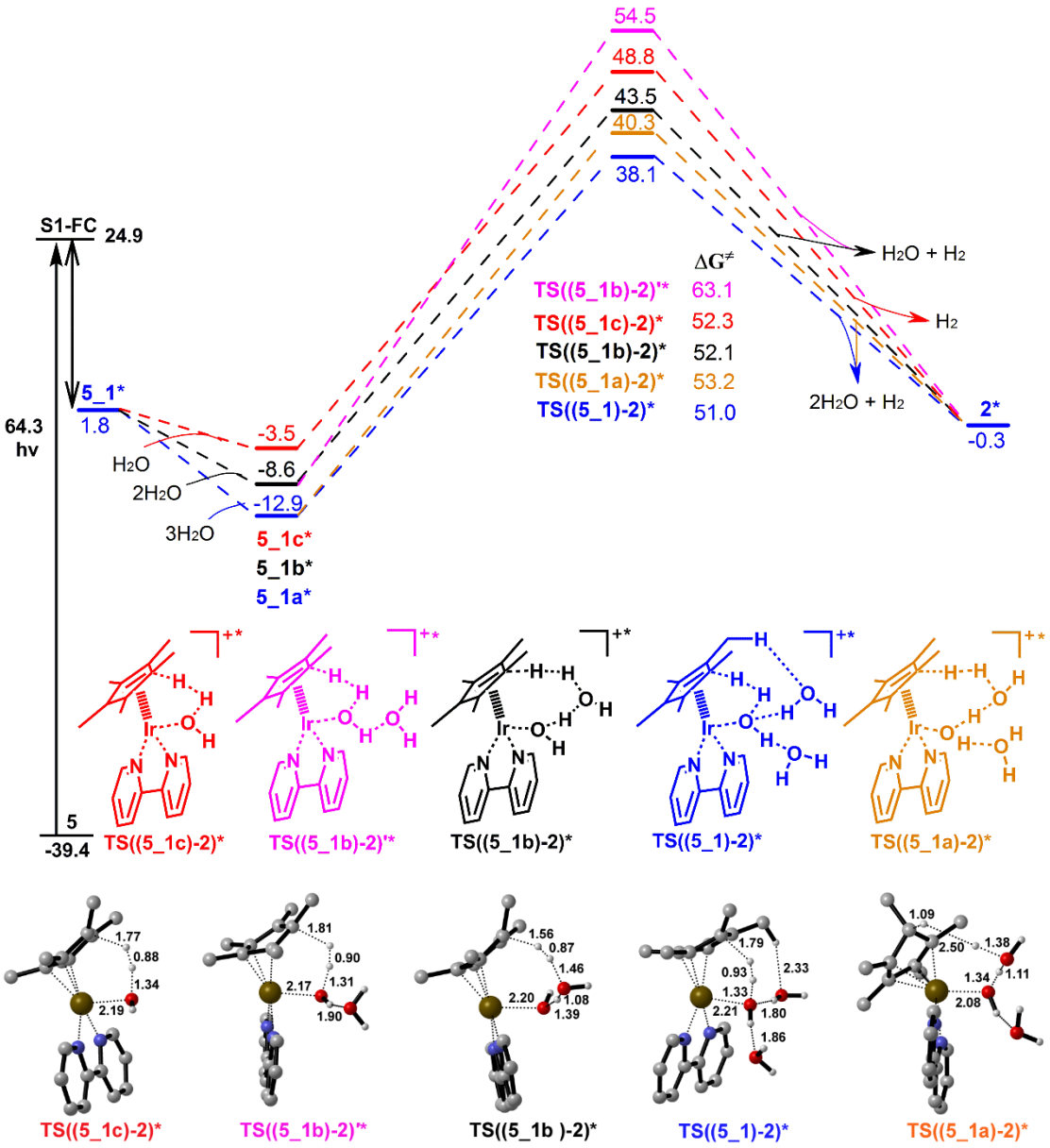


Figure S11. B3LYP-D3/BSII/PCM computed triplet free-energy (in kcal/mol) profile for H_2 evolution from **5_1***. Also shown are optimized transition states with some selected distances in Å. Five different pathways asissted with 1~3 water are investigated.

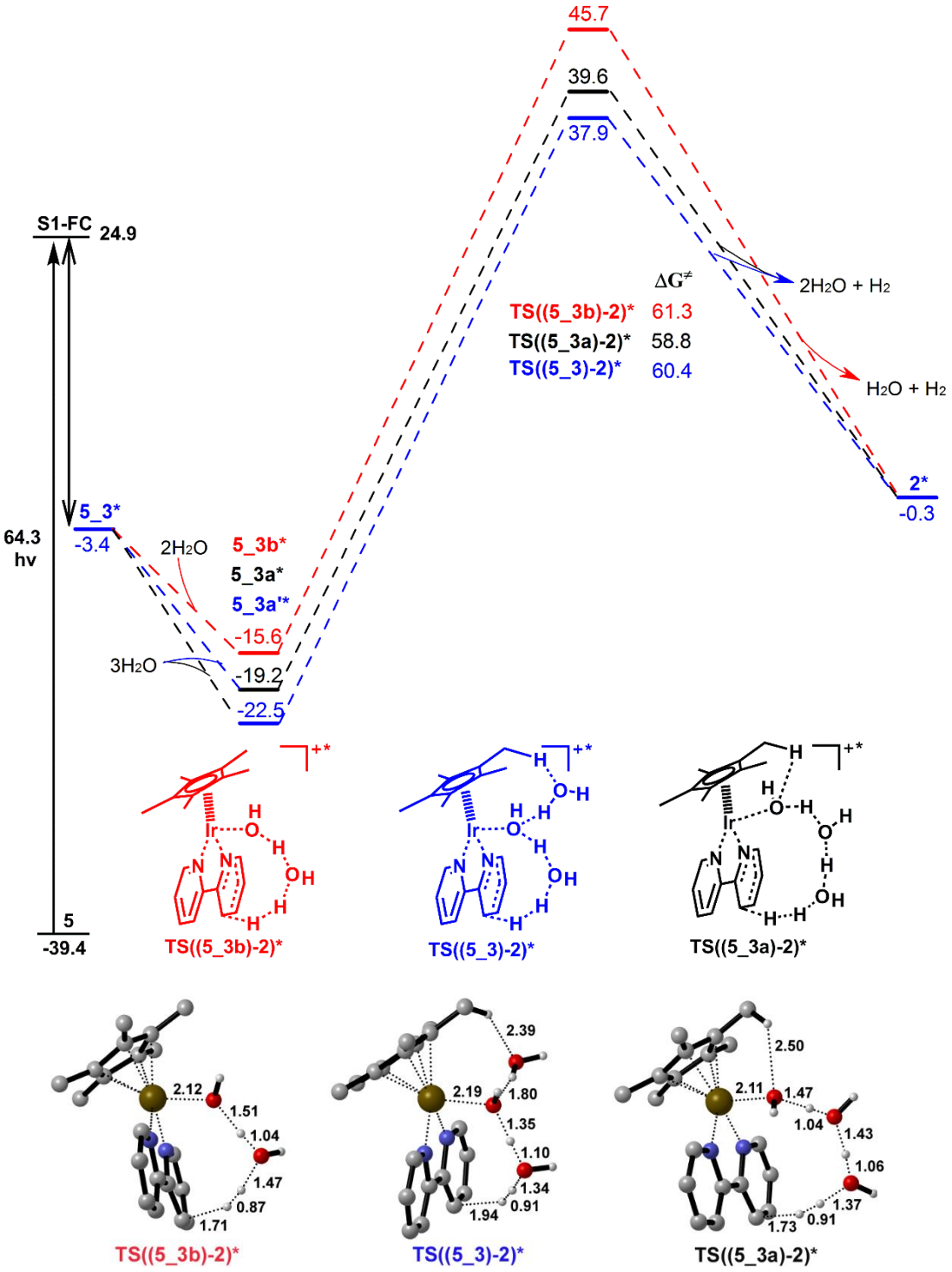


Figure S12. B3LYP-D3/BSII/PCM computed triplet free-energy (in kcal/mol) profile for H_2 evolution from **5_3***. Also shown are optimized transition states with some selected distances in Å. Three different pathways asissted with 2~3 water are investigated.

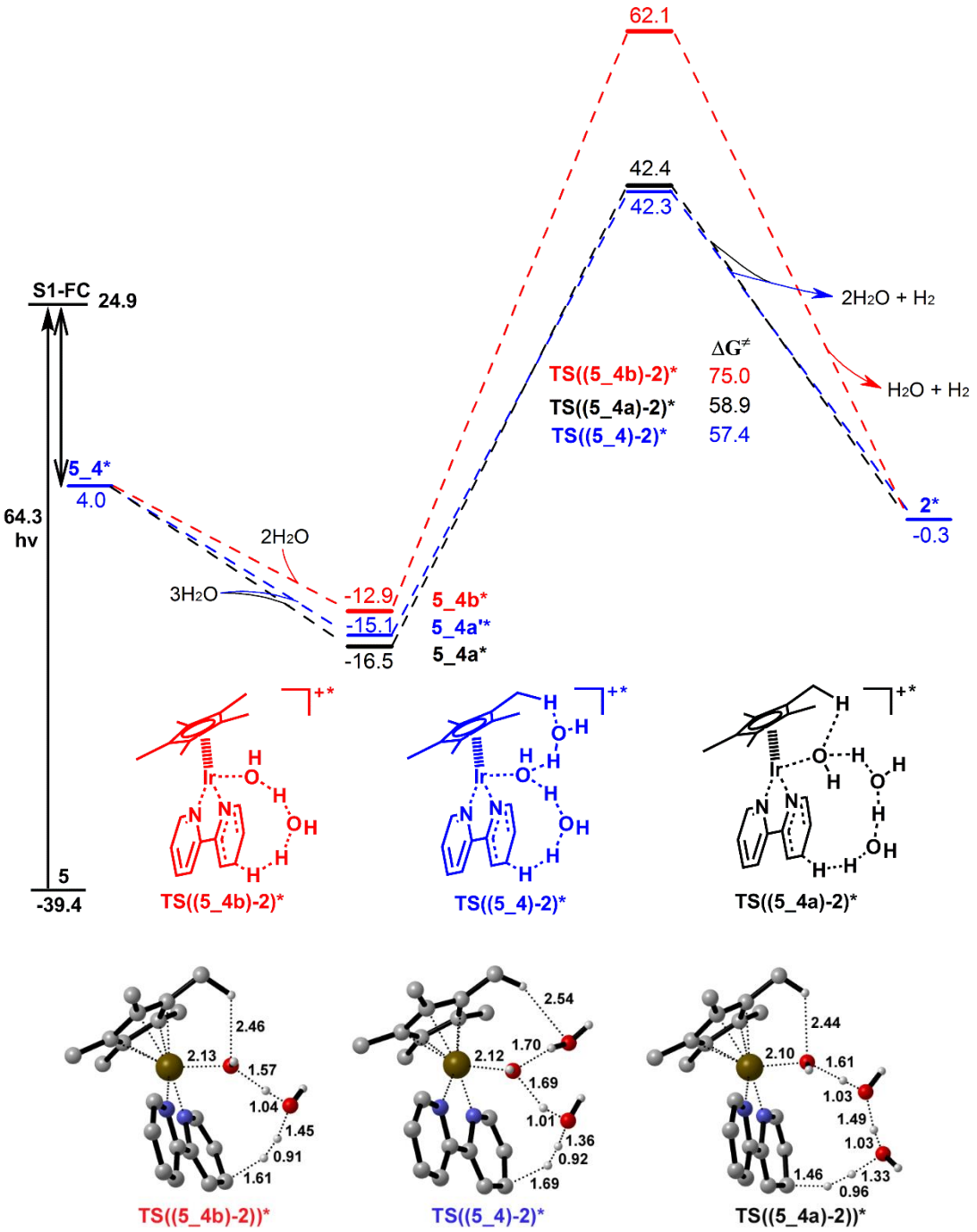


Figure S13. B3LYP-D3/BSII/PCM computed triplet free-energy (in kcal/mol) profile for H_2 evolution from **5_4***. Also shown are optimized transition states with some selected distances in Å. Three different pathways asissted with 2~3 water are investigated.

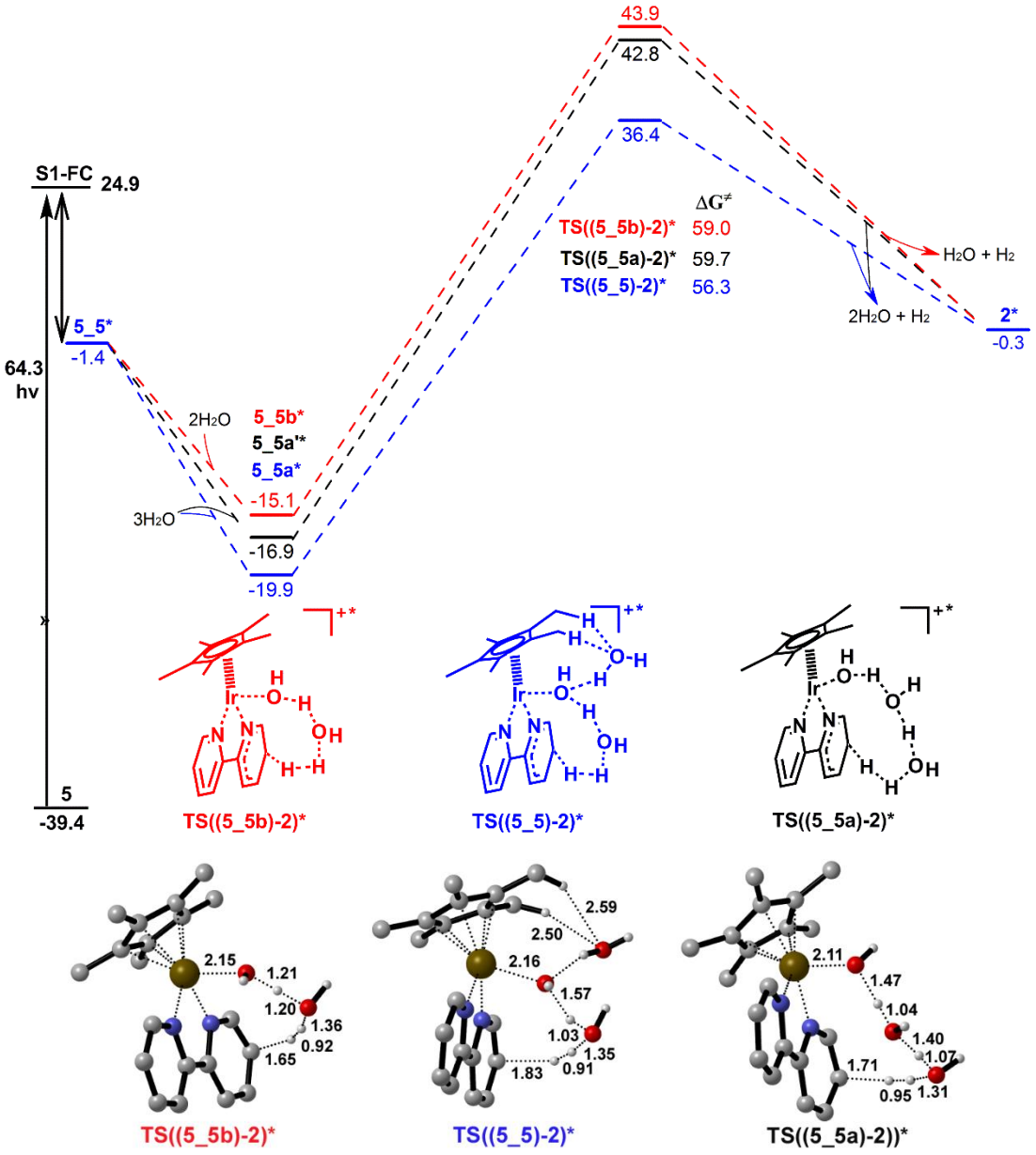


Figure S14. B3LYP-D3/BSII/PCM computed triplet free-energy (in kcal/mol) profile for H_2 evolution from **5_5***. Also shown are optimized transition states with some selected distances in Å. Three different pathways asissted with 2~3 water are investigated.

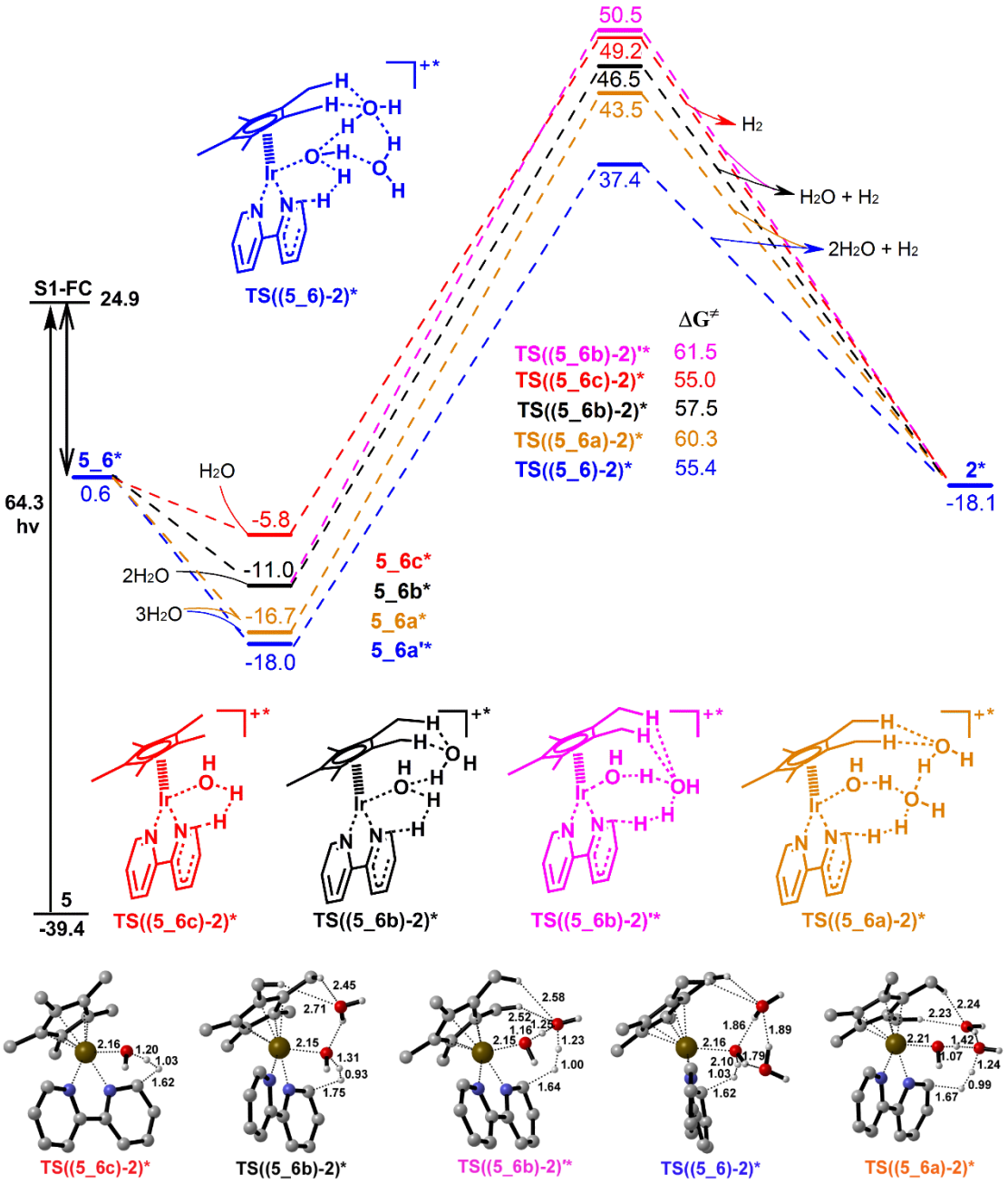


Figure S15. B3LYP-D3/BSII/PCM computed triplet free-energy (in kcal/mol) profile for H_2 evolution from **5_6***. Also shown are optimized transition states with some selected distances in Å. Five different pathways asissted with 1~3 water are investigated.

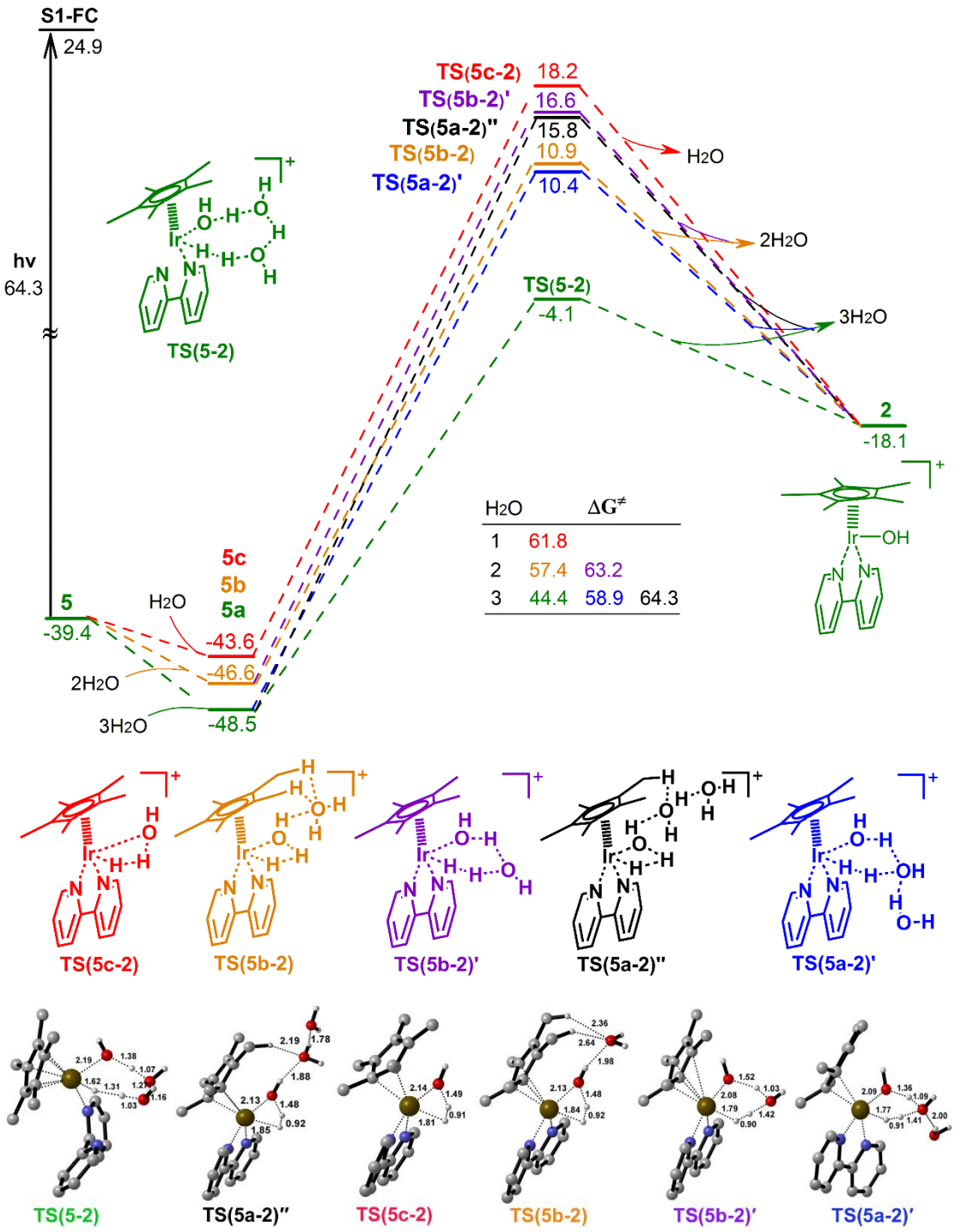


Figure S16. B3LYP-D3/BSII/PCM computed ground-state free-energy (in kcal/mol) profile for H_2 evolution from **5**. Also shown are optimized transition states with some selected distances in Å. Six different pathways asissted with 1~3 water are investigated.

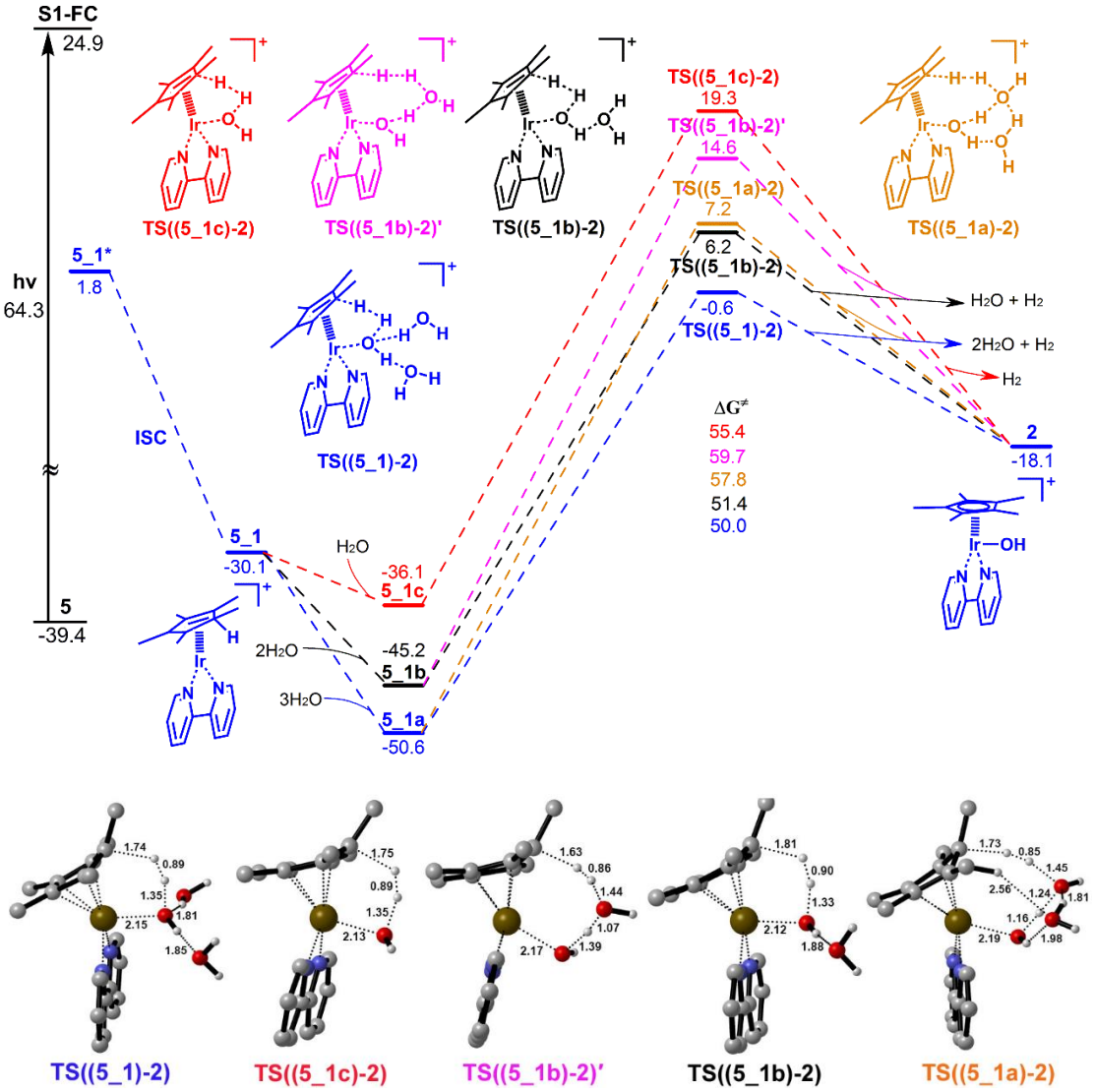


Figure S17. B3LYP-D3/BSII/PCM computed ground-state free-energy (in kcal/mol) profile for H_2 evolution from **5_1**. Also shown are optimized transition states with some selected distances in Å. Six different pathways asissted with 1~3 water are investigated.

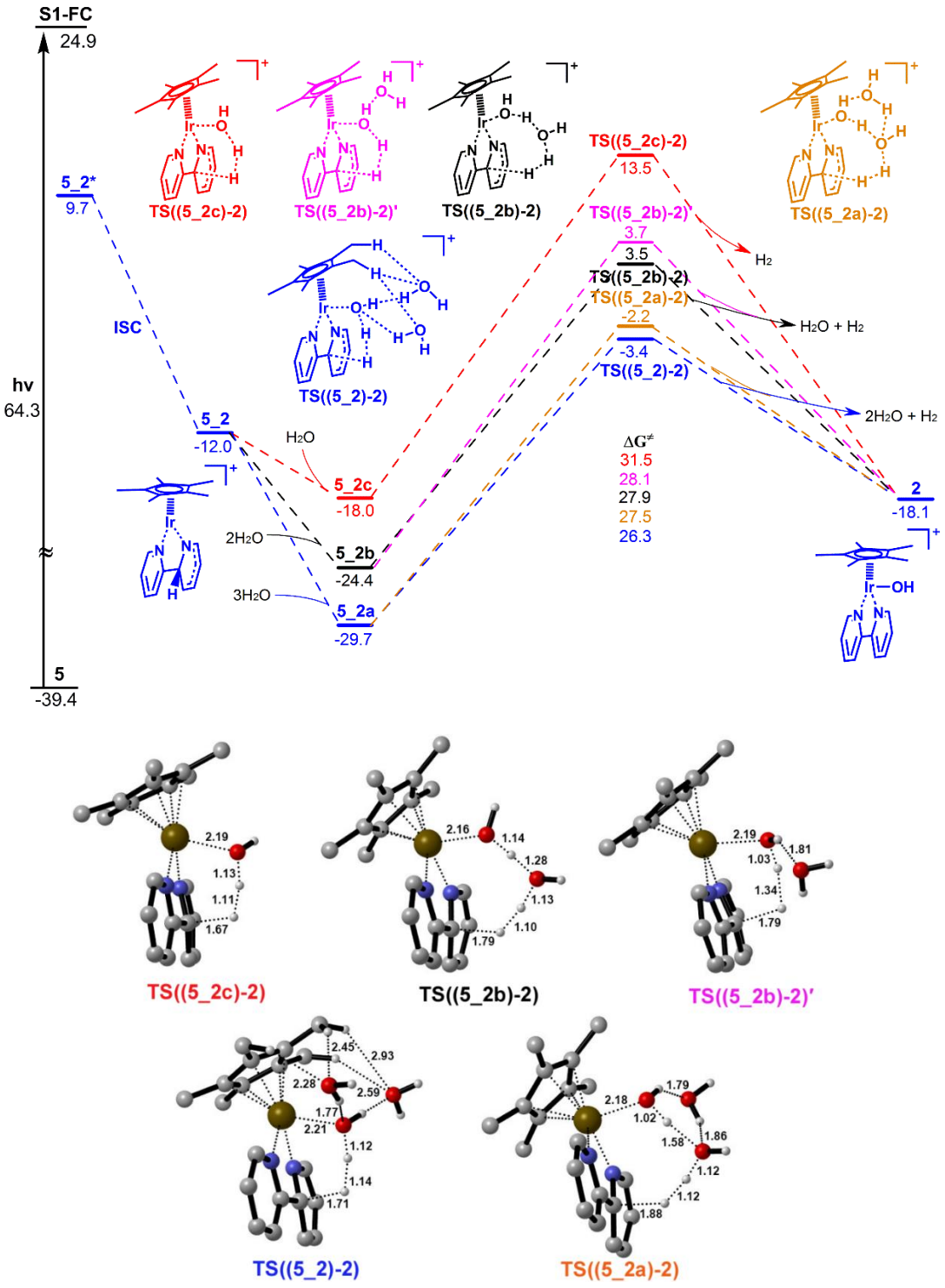


Figure S18. B3LYP-D3/BSII/PCM computed ground-state free-energy (in kcal/mol) profile for H_2 evolution from **5_2**. Also shown are optimized transition states with some selected distances in Å. Five different pathways asissted with 1~3 water are investigated.

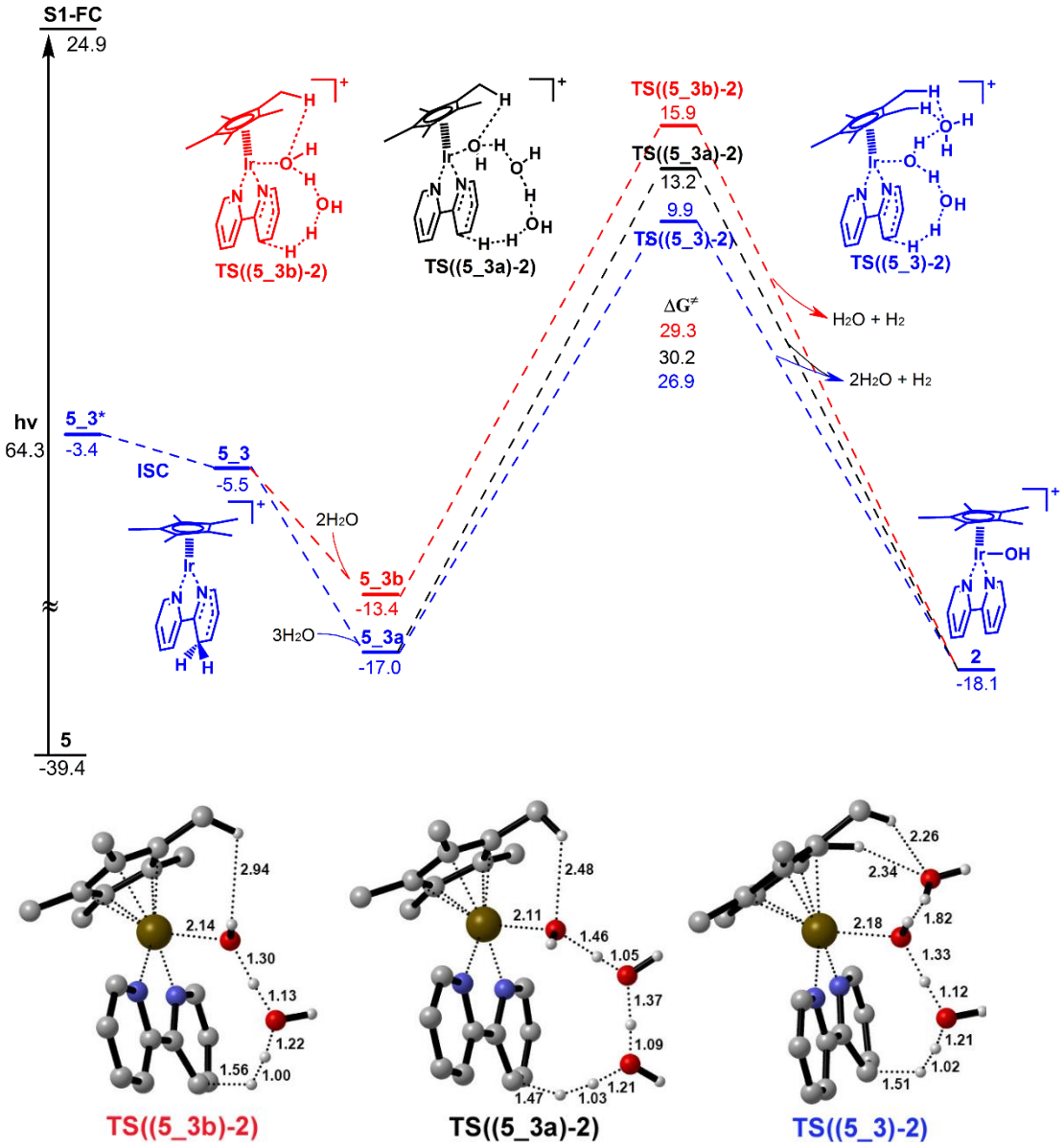


Figure S19. B3LYP-D3/BSII/PCM computed ground-state free-energy (in kcal/mol) profile for H_2 evolution from **5_3**. Also shown are optimized transition states with some selected distances in Å. Six different pathways asissted with 2~3 water are investigated.

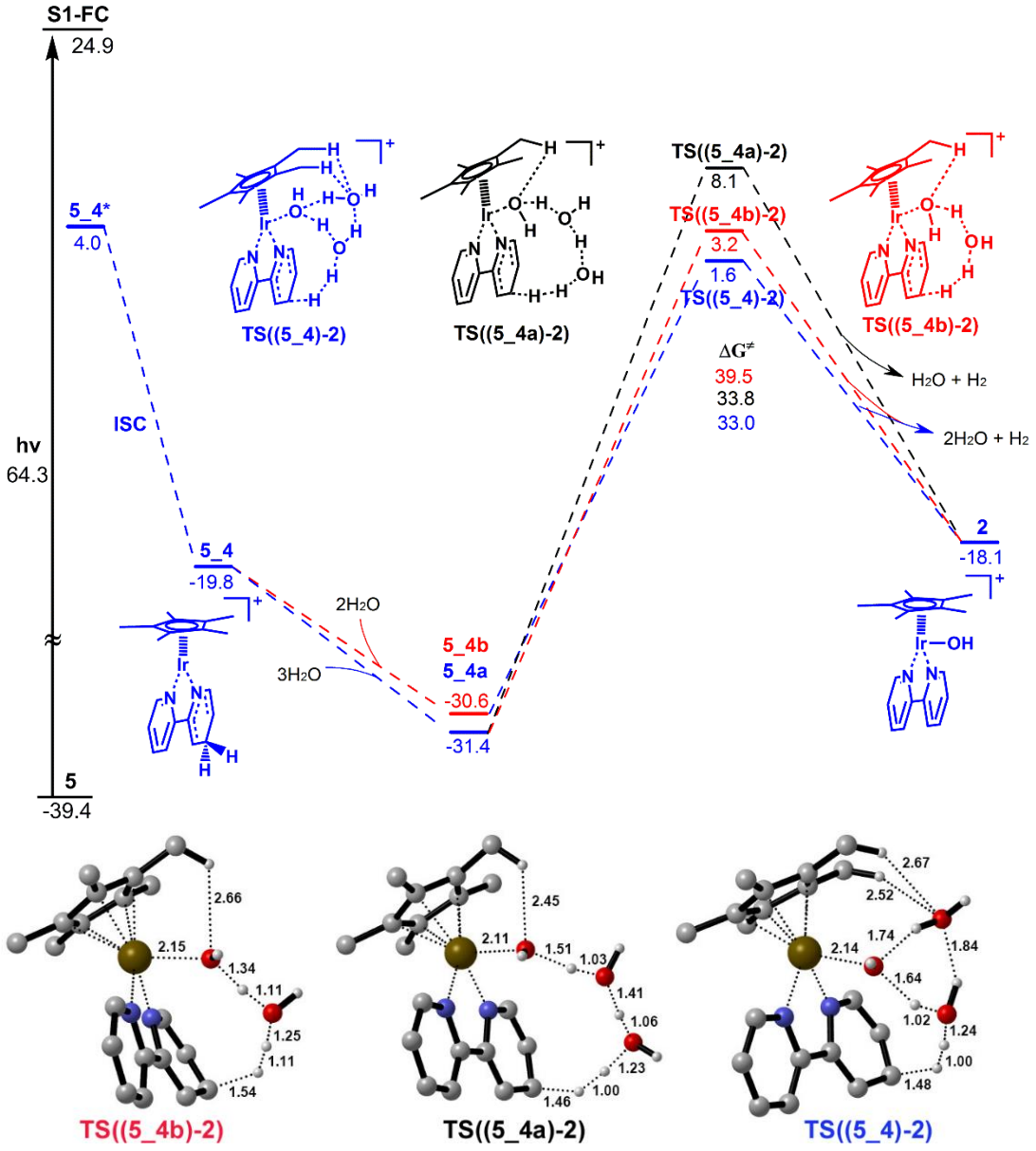


Figure S20. B3LYP-D3/BSII/PCM computed ground-state free-energy (in kcal/mol) profile for H_2 evolution from **5_4**. Also shown are optimized transition states with some selected distances in Å. Three different pathways asissted with 2~3 water are investigated.

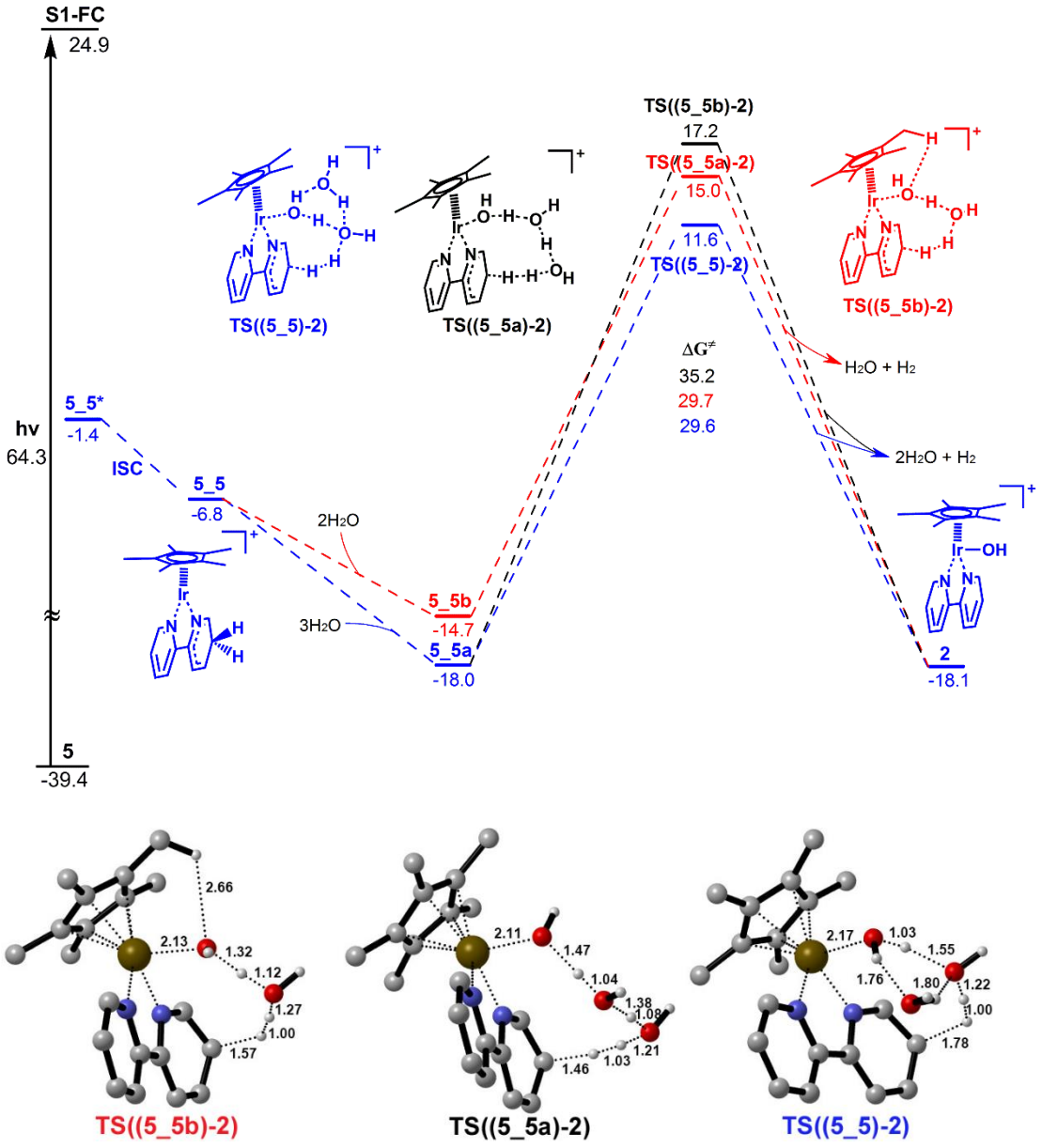


Figure S21. B3LYP-D3/BSII/PCM computed ground-state free-energy (in kcal/mol) profile for H_2 evolution from **5_5**. Also shown are optimized transition states with some selected distances in Å. Three different pathways asissted with 2~3 water are investigated.

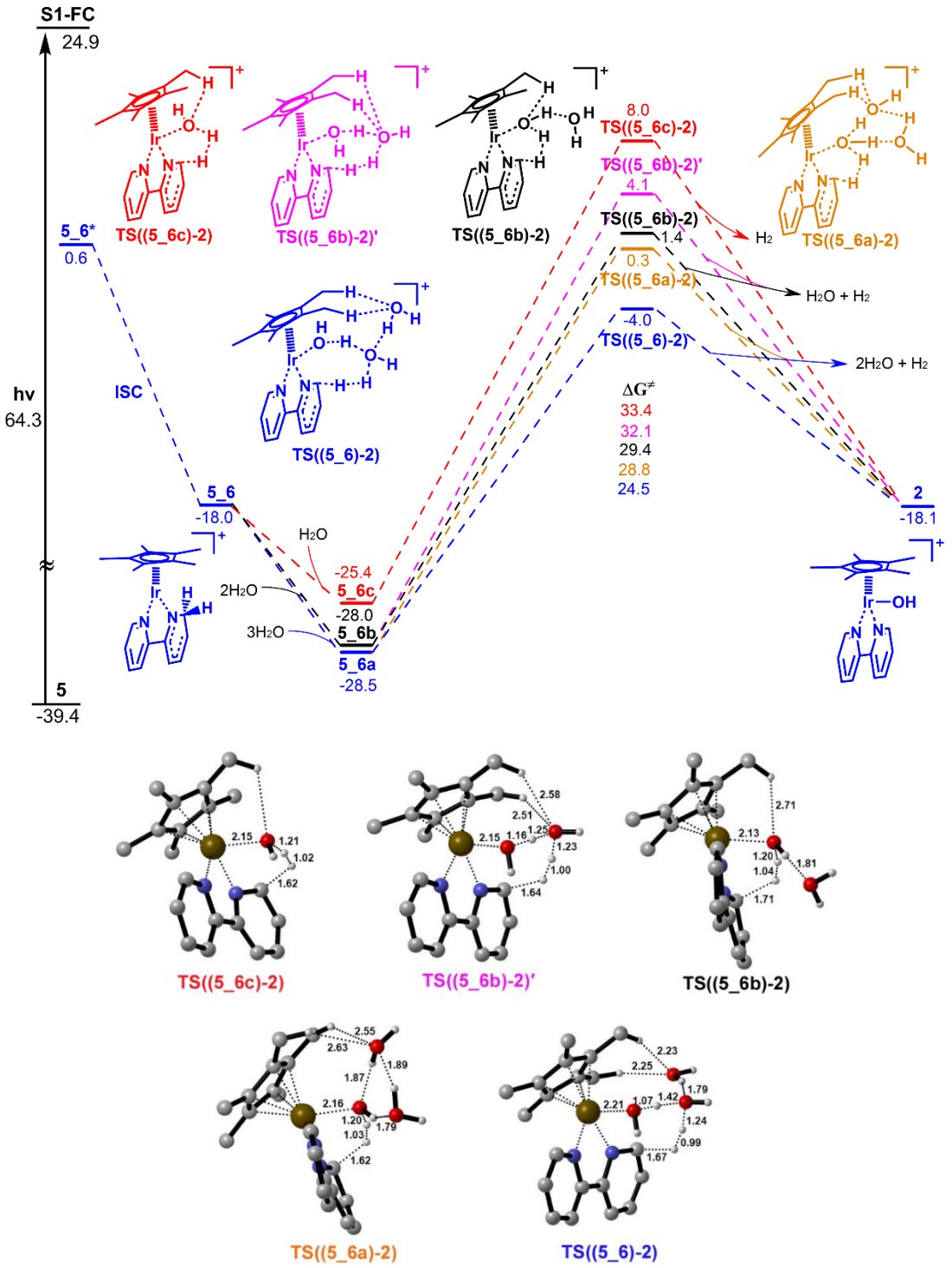
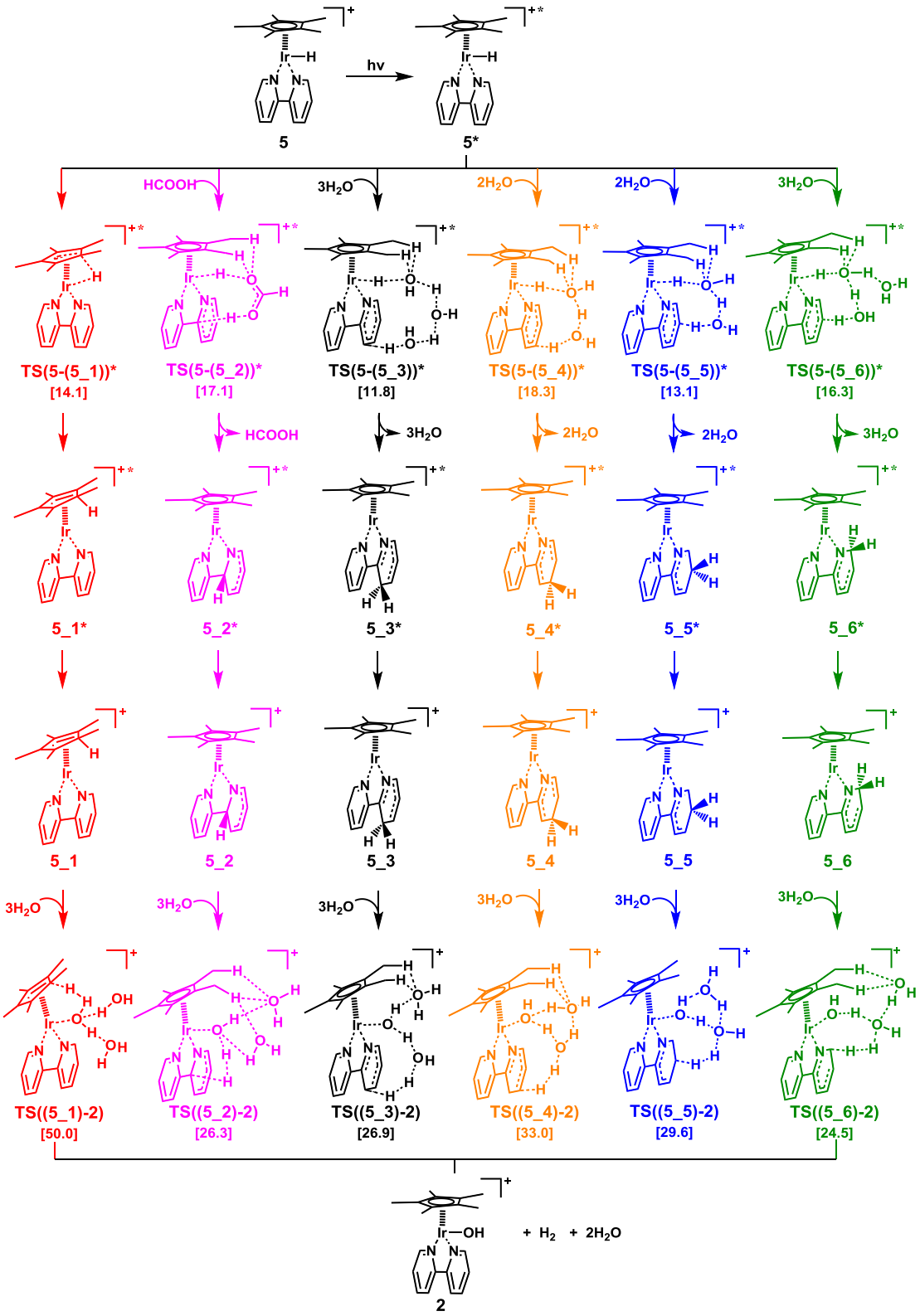


Figure S22. B3LYP-D3/BSII/PCM computed ground-state free-energy (in kcal/mol) profile for H_2 evolution from **5_6**. Also shown are optimized transition states with some selected distances in Å. Five different pathways asissted with 1~3 water are investigated.



Scheme S1. Optimal reaction paths for H_2 release in ground state starting from each isomer of metal hydride 5. Key intermediates and transition states are shown with free energy barriers in brackets (in kcal/mol).

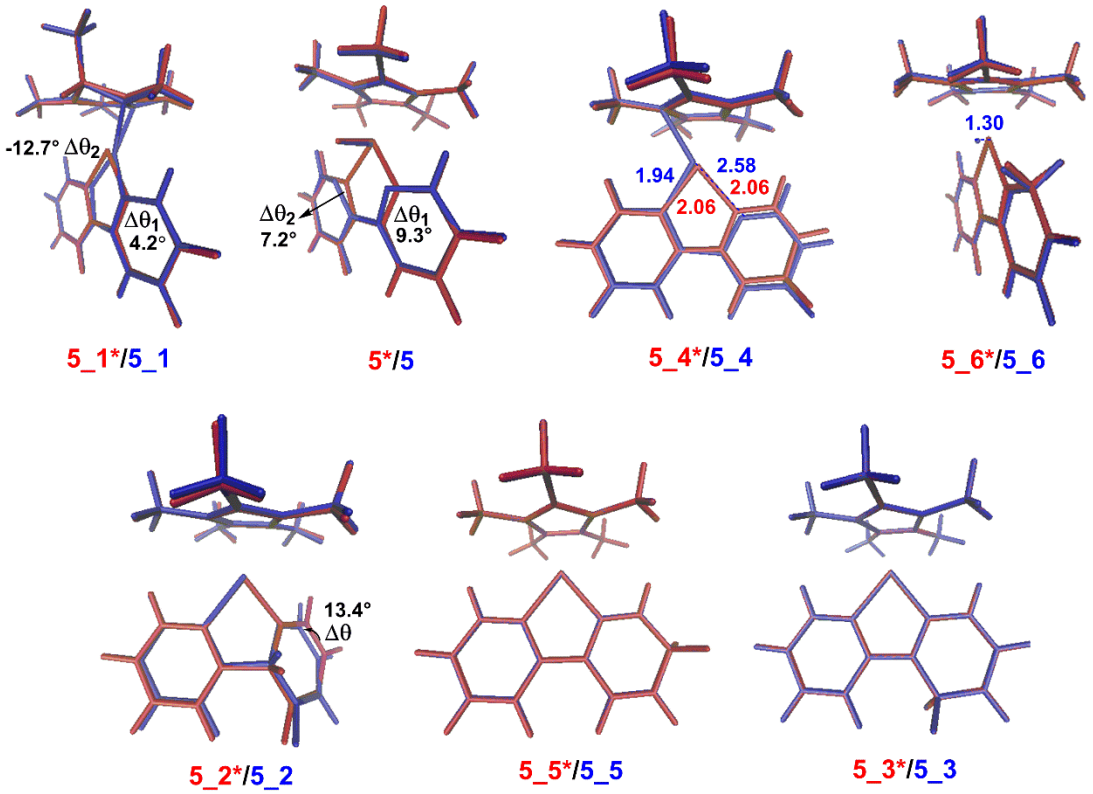


Figure S23. Overlays of B3LYP-D3/BSI optimized T_1 (in red) and T_1/S_0 conical intersection (in blue) structures of **5***, **5_1***, **5_2***, **5_3***, **5_4***, **5_5***, and **5_6***. Also shown are the differences of key dihedral angles (Δθ, in °) and bond lengths (in Å).

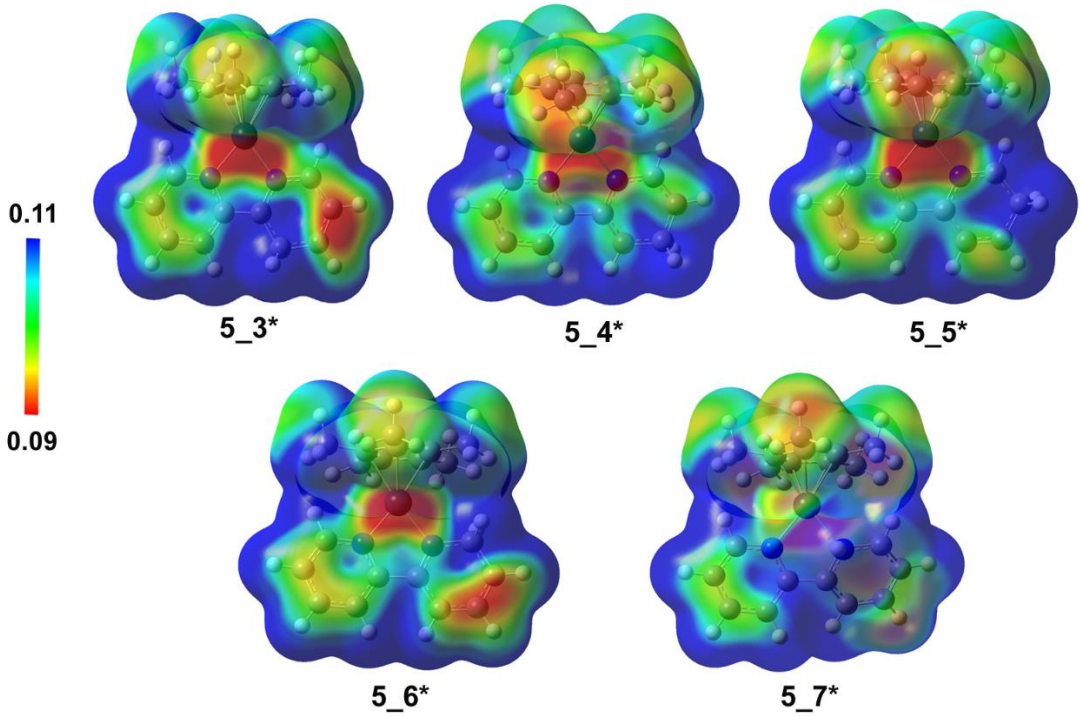


Figure S24. The B3LYP-D3/BSII/PCM computed electrostatic potentials of triplet **5_3***, **5_4***, **5_5***, **5_6*** and **5_7***.

Table S4. Numbers and Intensities of Imaginary Frequencies (IF, cm^{-1}) of Transition States Optimized at the B3LYP/BSI Level.

TS	IF	n	TS	IF	n
TS(3-4)	-153.5	1	**TS(3-4)′**	-148.1	1
TS(3′-4′)	-171.0	1	**TS(4-5)**	-539.3	1
TS(4′-5)	-234.0	1	**TS(5-(5_1))***	-971.4	1
TS(5-(5_2))*	-1044.3	1	**TS(5-(5_3))***	-717.2	1
TS(5-(5_4))*	-582.4	1	**TS(5-(5_5))***	-328.0	1
TS(5-(5_6))*	-956.9	1	**TS(5-(5_7))***	-823.5	1
TS(5-2)*	-548.1	1	**TS(5_1)-2)***	-1019.5	1
TS(5_3)-2)*	-958.8	1	**TS(5_4)-2)***	-543.93	1
TS(5_5)-2)*	-543.54	1	**TS(5_6)-2)***	-1513.4	1
TS((5_1)-2)	-1096.5	1	**TS((5_2)-2)**	-1210.6	1
TS((5_3)-2)	-1596.1	1	**TS((5_4)-2)**	-1350.1	1
TS((5_5)-2)	-1283.0	1	**TS((5_6)-2)**	-1512.9	1

2、Cartesian coordinates and energies of calculated species

Optimized structures and Free Energies using B3LYP/BSI (LANL2DZ & 6-31G**) in Gas Phase.

a) the formation of **5**

1

G-gas = -1449.986199 Hartree

Symbol	X	Y	Z
C	2.4665510	0.7384770	0.1916490
N	1.2447820	1.3109410	0.0357830
C	1.1544430	2.6463960	-0.0904750
C	2.2652410	3.4776190	-0.0173090
C	3.5210360	2.9054280	0.1817510
C	3.6207470	1.5217080	0.2784790
H	0.1632490	3.0427820	-0.2630440
H	2.1401340	4.5492100	-0.1225670
H	4.4098560	3.5241050	0.2455490
H	4.5894420	1.0550780	0.4072560
C	2.2425580	-3.4715640	0.0175370
C	3.5016400	-2.9052680	0.2134040
C	3.6102180	-1.5213730	0.2962930
C	2.4617500	-0.7308810	0.2006280
N	1.2362650	-1.2979380	0.0513100
C	1.1373400	-2.6342200	-0.0645290
H	2.1110140	-4.5431620	-0.0793110
H	4.3864370	-3.5289390	0.2840020
H	4.5818540	-1.0597310	0.4206620
H	0.1439620	-3.0239200	-0.2397360
C	-2.4426310	-0.8493880	-0.2909240

C	-2.5345650	0.6029670	-0.4497290
C	-2.0899970	1.2068970	0.7674970
C	-1.6921560	0.1537180	1.6908520
C	-1.9732540	-1.1092000	1.0427420
C	-2.9150770	-1.8463110	-1.3051060
H	-2.5500410	-2.8525690	-1.0876820
H	-4.0107870	-1.8866550	-1.3153000
H	-2.5719980	-1.5748370	-2.3058980
C	-3.0775830	1.2908620	-1.6630230
H	-2.8831450	2.3646460	-1.6434370
H	-2.6288240	0.8854650	-2.5725840
H	-4.1631420	1.1462120	-1.7161190
C	-2.1212720	2.6669010	1.1006120
H	-1.2826660	2.9616360	1.7362310
H	-2.1223900	3.2936650	0.2063390
H	-3.0415520	2.8903440	1.6536660
C	-1.3061310	0.3429770	3.1274870
H	-0.6919510	-0.4840980	3.4906020
H	-0.7431530	1.2676120	3.2744270
H	-2.2002270	0.3959220	3.7611030
C	-1.8510260	-2.4508970	1.6967120
H	-0.9659280	-2.5208340	2.3335490
H	-2.7277060	-2.6180080	2.3340460
H	-1.8250010	-3.2640880	0.9690180
Ir	-0.4086440	0.0025270	-0.1218590
Cl	0.1243400	-0.0302680	-2.5026220

2

G-gas = -1065.507691 Hartree

Symbol	X	Y	Z
C	-2.5770990	-0.5223470	0.0774000
N	-1.4612770	-1.2319010	-0.2254020
C	-1.5200940	-2.5762180	-0.2576680
C	-2.6843140	-3.2795840	0.0278200
C	-3.8297970	-2.5624200	0.3746490
C	-3.7736890	-1.1726320	0.3991110
H	-0.5994070	-3.0835700	-0.5212520
H	-2.6848690	-4.3626800	-0.0190330
H	-4.7531720	-3.0766720	0.6199200
H	-4.6519500	-0.5995680	0.6704050
C	-1.9746150	3.6532710	-0.2381410
C	-3.2832380	3.2008610	-0.0652670
C	-3.5176870	1.8340430	0.0558790
C	-2.4358390	0.9470390	0.0121230
N	-1.1717870	1.3995570	-0.1422600

C	-0.9475860	2.7154690	-0.2745550
H	-1.7497980	4.7083480	-0.3469970
H	-4.1118750	3.9008450	-0.0381170
H	-4.5307990	1.4655470	0.1618400
H	0.0867570	3.0095700	-0.4123790
C	1.8354480	1.0182510	1.4095400
C	2.5283010	1.0217840	0.1782630
C	2.6615660	-0.3598890	-0.2830660
C	2.0528010	-1.2201400	0.7140970
C	1.4132650	-0.3486030	1.6723470
C	1.4873610	2.1913880	2.2700390
H	0.4118650	2.2413740	2.4743280
H	1.9891590	2.1178830	3.2428880
H	1.7918740	3.1377260	1.8180390
C	3.1341100	2.1953970	-0.5302160
H	2.9607760	2.1428200	-1.6085660
H	2.7400520	3.1468590	-0.1657660
H	4.2206530	2.2120590	-0.3788850
C	3.5268430	-0.7925080	-1.4307730
H	3.3049050	-1.8170560	-1.7356250
H	3.3795790	-0.1516400	-2.3031720
H	4.5858440	-0.7463100	-1.1489570
C	2.1980260	-2.7101850	0.8235910
H	1.3300660	-3.1677380	1.3061880
H	2.3325460	-3.1778730	-0.1548720
H	3.0763490	-2.9610270	1.4314490
C	0.7038080	-0.7945890	2.9197470
H	0.2031620	-1.7554690	2.7778950
H	1.4118320	-0.9127410	3.7495380
H	-0.0494490	-0.0676900	3.2354530
Ir	0.4600220	-0.2012550	-0.4563320
O	0.3586040	-0.2590620	-2.4167660
H	-0.5386320	-0.4377520	-2.7385290

3

G-gas = -1255.319839 Hartree

Symbol	X	Y	Z
C	2.6938930	0.0340150	-0.0501910
N	1.7421100	0.9454500	-0.3742410
C	2.1059420	2.1014420	-0.9559750
C	3.4328280	2.4232450	-1.2119730
C	4.4231640	1.5067750	-0.8602280
C	4.0471640	0.3004720	-0.2795130
H	1.3012380	2.7727590	-1.2254160
H	3.6753540	3.3696840	-1.6816180

H	5.4702950	1.7228020	-1.0440590
H	4.8004450	-0.4312050	-0.0155060
C	1.0243410	-3.5360810	1.4625540
C	2.4135320	-3.4564390	1.3962700
C	2.9986100	-2.2914860	0.9086170
C	2.1857340	-1.2248050	0.5185590
N	0.8344450	-1.3037760	0.6219460
C	0.2667700	-2.4415610	1.0572670
H	0.5229800	-4.4322230	1.8099450
H	3.0339220	-4.2916360	1.7039980
H	4.0759170	-2.2195290	0.8260250
H	-0.8136600	-2.4764340	1.0352620
C	-2.2564660	0.2273040	1.0038550
C	-2.4522300	0.7943510	-0.2943420
C	-1.6875290	2.0295950	-0.3769520
C	-1.0647370	2.2359180	0.9216650
C	-1.3745810	1.1141000	1.7582890
C	-2.9677460	-0.9709970	1.5520110
H	-2.4410050	-1.3964250	2.4095410
H	-3.9608470	-0.6671240	1.9058430
H	-3.0947730	-1.7469970	0.7961670
C	-3.3192450	0.2171850	-1.3694270
H	-3.0128050	0.5558700	-2.3618190
H	-3.2908660	-0.8739340	-1.3495600
H	-4.3560140	0.5423930	-1.2188450
C	-1.7627210	3.0302590	-1.4931340
H	-0.8839030	3.6795410	-1.5232970
H	-1.8549210	2.5452910	-2.4678320
H	-2.6382460	3.6782190	-1.3651100
C	-0.2895590	3.4477590	1.3393930
H	0.4646630	3.2091990	2.0920740
H	0.2079410	3.9322060	0.4965760
H	-0.9746270	4.1842760	1.7762350
C	-1.0028740	0.9490570	3.2017490
H	-0.0712180	1.4665520	3.4402410
H	-1.7889120	1.3603300	3.8464240
H	-0.8790200	-0.1033020	3.4673130
Ir	-0.2700690	0.3858340	-0.0459970
O	0.0414790	-0.5970630	-1.8673230
H	-0.3788660	-0.0744540	-2.5623790
C	-1.6401020	-3.5178120	-1.7861090
O	-2.2418070	-3.0049790	-0.8512540
O	-0.6359440	-2.9954930	-2.4485260
H	-1.8955350	-4.5185800	-2.1703810

H	-0.4130880	-2.0417240	-2.1294710

3′

G-gas = -1255.304918 Hartree

Symbol	X	Y	Z
C	-1.9726380	1.8947450	-0.1557950
N	-1.9231700	0.5839350	-0.5042800
C	-2.9521460	0.0424280	-1.1796220
C	-4.0932750	0.7635840	-1.5063730
C	-4.1698660	2.1036280	-1.1273030
C	-3.0964280	2.6726080	-0.4513780
H	-2.8377860	-0.9945010	-1.4669500
H	-4.8969300	0.2804070	-2.0502610
H	-5.0461920	2.6983230	-1.3625010
H	-3.1296670	3.7155100	-0.1618010
C	1.6195860	3.1860600	1.6425230
C	0.6030820	4.1278730	1.4957040
C	-0.5986040	3.7348840	0.9147080
C	-0.7678140	2.4067930	0.5149760
N	0.2155660	1.4911210	0.7022890
C	1.3910530	1.8788470	1.2252470
H	2.5830750	3.4506480	2.0629940
H	0.7470850	5.1557840	1.8116180
H	-1.3900950	4.4584300	0.7638010
H	2.1685900	1.1290330	1.2725430
C	1.2732390	-1.7909830	1.0747800
C	1.1137720	-2.2842340	-0.2584640
C	-0.2874780	-2.6111590	-0.4613560
C	-0.9706930	-2.3744060	0.8039080
C	-0.0272550	-1.8447870	1.7388070
C	2.5757370	-1.4496350	1.7338450
H	2.4278540	-0.8249240	2.6180690
H	3.0644960	-2.3716360	2.0720040
H	3.2568850	-0.9342670	1.0531610
C	2.2100650	-2.4493200	-1.2642530
H	1.8496450	-2.3008470	-2.2848050
H	3.0223110	-1.7441860	-1.0821990
H	2.6175310	-3.4658460	-1.2030830
C	-0.8550520	-3.3234880	-1.6545560
H	-1.9278780	-3.1450490	-1.7670090
H	-0.3655640	-3.0138100	-2.5810150
H	-0.7173890	-4.4072130	-1.5562420
C	-2.4012870	-2.7096570	1.0973510
H	-2.8189590	-2.0685740	1.8762400
H	-3.0355980	-2.6283360	0.2119220

H	-2.4689540	-3.7468000	1.4471460
C	-0.2762570	-1.5359020	3.1851730
H	-1.3293600	-1.3204470	3.3773470
H	0.0077810	-2.3911030	3.8103540
H	0.3081080	-0.6762980	3.5222360
Ir	-0.1526310	-0.4618250	-0.0421020
O	0.5352270	0.5014170	-1.7386050
H	0.4416480	-0.1190100	-2.4733350
C	3.6198790	1.1509800	-1.5338900
O	4.0221780	0.7344270	-0.4625760
O	4.4011600	1.7531160	-2.4373010
H	2.5751690	1.0774410	-1.8750240
H	5.3057860	1.7775530	-2.0757180

TS(3-4)

G-gas = -1255.286845 Hartree

Symbol	X	Y	Z
C	-2.6264330	0.5415770	0.1926260
N	-1.4486140	1.1903990	0.3582880
C	-1.4502090	2.5007540	0.6661870
C	-2.6254440	3.2337330	0.7823610
C	-3.8441010	2.5851430	0.5802950
C	-3.8435100	1.2240790	0.2927060
H	-0.4800830	2.9433990	0.8505280
H	-2.5789030	4.2877690	1.0319220
H	-4.7808720	3.1270410	0.6580190
H	-4.7801260	0.6986570	0.1530660
C	-2.0629410	-3.6085010	-0.3356550
C	-3.3746390	-3.1407930	-0.2951990
C	-3.5978910	-1.7762120	-0.1350160
C	-2.5060100	-0.9092640	-0.0410250
N	-1.2348430	-1.3743460	-0.1073180
C	-1.0185870	-2.6948160	-0.2304510
H	-1.8414870	-4.6648080	-0.4378950
H	-4.2122240	-3.8261700	-0.3726920
H	-4.6097480	-1.3953590	-0.0729780
H	0.0147080	-3.0081180	-0.2032140
C	2.0774130	-0.7660010	-1.1956580
C	2.6066320	0.2328910	-0.3074450
C	1.9727290	1.4990610	-0.5902300
C	1.0659510	1.2964110	-1.7102210
C	1.1152820	-0.1125920	-2.0745650
C	2.5171030	-2.1968570	-1.2476560
H	1.8519440	-2.7997680	-1.8697490
H	3.5225840	-2.2711540	-1.6775390

H	2.5346780	-2.6276350	-0.2435850
C	3.6589240	0.0205750	0.7326560
H	3.3259230	0.3318650	1.7249350
H	3.9550420	-1.0265680	0.7945550
H	4.5433060	0.6116650	0.4659120
C	2.3165260	2.7937750	0.0812620
H	1.6217480	3.5898220	-0.1961410
H	2.2955640	2.6842930	1.1681310
H	3.3197760	3.1215680	-0.2154460
C	0.3183600	2.3628480	-2.4471380
H	-0.5950110	1.9757750	-2.9039570
H	0.0477050	3.1956550	-1.7953230
H	0.9494540	2.7641170	-3.2493040
C	0.4256890	-0.7405420	-3.2458990
H	-0.5099440	-0.2304990	-3.4847520
H	1.0724940	-0.6846830	-4.1297820
H	0.2015310	-1.7942020	-3.0669080
Ir	0.3818740	0.0825620	-0.0597090
O	0.5205830	1.0809530	2.3142750
H	-0.3191560	1.0069270	2.7874500
C	1.5183640	-1.7871330	2.6927730
O	0.9008180	-1.7898290	1.5805860
O	1.8346920	-0.7951120	3.3892390
H	1.8092070	-2.7863130	3.0766710
H	1.1138100	0.3902040	2.7878140

TS(3-4)′

G-gas = -1255.282810 Hartree

Symbol	X	Y	Z
C	-2.6932430	0.0102200	-0.0876580
N	-1.7179980	-0.8915070	-0.3718160
C	-2.0545700	-2.1255790	-0.7937010
C	-3.3768100	-2.5343730	-0.9104630
C	-4.3890870	-1.6317240	-0.5814240
C	-4.0424690	-0.3469420	-0.1763510
H	-1.2310460	-2.7791920	-1.0514850
H	-3.6010510	-3.5379190	-1.2538140
H	-5.4328470	-1.9192000	-0.6528290
H	-4.8144840	0.3755680	0.0575540
C	-1.1032950	3.8529050	0.5989830
C	-2.4836140	3.7071930	0.7082030
C	-3.0454390	2.4482990	0.5073440
C	-2.2094780	1.3637550	0.2368320
N	-0.8609090	1.5130330	0.1815490
C	-0.3181020	2.7346740	0.3241340

H	-0.6243970	4.8191130	0.7109010
H	-3.1187670	4.5599770	0.9244920
H	-4.1198870	2.3184770	0.5504860
H	0.7535370	2.8136420	0.1550790
C	2.0964040	0.1107580	1.2519230
C	2.5079230	-0.6521960	0.1195630
C	1.7737080	-1.9176060	0.1064310
C	0.9221900	-1.9347990	1.2627640
C	1.0574140	-0.6496210	1.9436320
C	2.6753920	1.4185220	1.6919040
H	2.0075780	1.9430140	2.3789670
H	3.6154770	1.2335910	2.2260720
H	2.8758500	2.0676130	0.8354060
C	3.5631690	-0.2764630	-0.8676030
H	3.3037370	-0.6140240	-1.8732090
H	3.7257250	0.8006480	-0.8901190
H	4.5022530	-0.7688380	-0.5832030
C	1.9998910	-3.0210680	-0.8809870
H	1.2771690	-3.8305310	-0.7548100
H	1.9119140	-2.6467040	-1.9034410
H	3.0000380	-3.4496710	-0.7492500
C	0.0976150	-3.0832560	1.7532840
H	-0.8176650	-2.7501570	2.2474410
H	-0.1717000	-3.7717130	0.9506040
H	0.6808740	-3.6518820	2.4877420
C	0.4334220	-0.2843620	3.2545990
H	-0.5436700	-0.7557150	3.3821480
H	1.0758640	-0.6167360	4.0791890
H	0.3064970	0.7957560	3.3494880
Ir	0.2939000	-0.2838760	-0.0341410
O	0.2336790	-0.8662140	-2.5773030
H	-0.6164970	-0.8232550	-3.0349220
C	1.8801120	2.3385210	-2.0980420
O	2.4041400	2.9234710	-1.1389320
O	0.9774310	1.4248800	-2.0357280
H	2.1902380	2.6174240	-3.1278470
H	0.6184970	0.0602660	-2.6643680

TS(3′-4′)

G-gas = -1255.234469 Hartree

Symbol	X	Y	Z
C	-2.4943670	0.8694770	0.0182870
N	-1.2389560	1.3480380	0.2029790
C	-1.0506030	2.6485960	0.4879090
C	-2.1158910	3.5442870	0.5373100

C	-3.4094180	3.0752530	0.3143570
C	-3.6029070	1.7182840	0.0684180
H	-0.0252950	2.8926860	0.7543790
H	-1.9252110	4.5885420	0.7585830
H	-4.2589810	3.7496350	0.3478030
H	-4.6028200	1.3272800	-0.0743230
C	-2.4948080	-3.3417950	-0.2982830
C	-3.7290000	-2.6947550	-0.3675090
C	-3.7667840	-1.3065780	-0.2894360
C	-2.5729290	-0.5898080	-0.1623970
N	-1.3763340	-1.2293510	-0.1377210
C	-1.3435610	-2.5731740	-0.1810740
H	-2.4187900	-4.4227450	-0.3314400
H	-4.6482550	-3.2623190	-0.4674990
H	-4.7160390	-0.7858690	-0.3167860
H	-0.3642070	-3.0274230	-0.1052130
C	2.1948080	-1.0929680	-0.7511680
C	2.6454380	0.1735380	-0.1900020
C	2.0520080	1.2417540	-0.9297010
C	1.2174180	0.6559660	-1.9719560
C	1.3607890	-0.7926610	-1.8909350
C	2.6805990	-2.4465810	-0.3278450
H	2.0312670	-3.2449930	-0.6952130
H	3.6843640	-2.6336250	-0.7274050
H	2.7326730	-2.5281110	0.7597130
C	3.5424270	0.3661600	0.9830450
H	3.0265860	1.0288600	1.6984320
H	3.8022750	-0.5797750	1.4616740
H	4.4712030	0.8504880	0.6583250
C	2.3165870	2.6919680	-0.6817720
H	1.5999040	3.3316490	-1.2017180
H	2.2543770	2.8775770	0.3956720
H	3.3179690	2.9548260	-1.0437970
C	0.5216440	1.4107410	-3.0625640
H	-0.3242150	0.8504570	-3.4669320
H	0.1522110	2.3747250	-2.7070630
H	1.2194220	1.6065470	-3.8858090
C	0.8138330	-1.7757190	-2.8777660
H	-0.1224990	-1.4305500	-3.3214780
H	1.5370610	-1.9105800	-3.6913530
H	0.6413980	-2.7563140	-2.4300290
Ir	0.3867800	-0.0178400	-0.1011650
O	1.1643530	1.7294820	1.9911340
H	0.7088190	2.2330130	2.6830950

C	0.7471040	-0.7608410	3.0619750
O	0.2716200	-1.2997170	2.0595970
O	0.8276280	-1.3893620	4.2265780
H	1.1145100	0.2941090	3.0001080
H	0.4541170	-2.2852970	4.1293560

4

G-gas = -1178.892407 Hartree

Symbol	X	Y	Z
C	-2.4302300	0.8589150	-0.2124550
N	-1.1943220	1.3973520	-0.0585890
C	-1.0719010	2.7143280	0.1773000
C	-2.1694230	3.5646190	0.2393490
C	-3.4438800	3.0274710	0.0660900
C	-3.5732050	1.6608180	-0.1580500
H	-0.0658700	3.0805690	0.3315580
H	-2.0196120	4.6210240	0.4305270
H	-4.3242970	3.6593860	0.1143130
H	-4.5559570	1.2225430	-0.2778530
C	-2.2865520	-3.3270280	-0.7732980
C	-3.5395690	-2.7162290	-0.8049110
C	-3.6211370	-1.3396830	-0.6253990
C	-2.4543670	-0.5972470	-0.4225770
N	-1.2382190	-1.2024740	-0.4049090
C	-1.1632850	-2.5366220	-0.5655190
H	-2.1734700	-4.3980120	-0.8966230
H	-4.4393220	-3.3020730	-0.9598860
H	-4.5860490	-0.8486520	-0.6378870
H	-0.1736380	-2.9702590	-0.5085100
C	2.2915940	-1.1160480	-0.3222160
C	2.5843950	-0.0580750	0.6110280
C	2.3085690	1.2028580	-0.0245510
C	1.9034340	0.9246820	-1.4017130
C	1.8902000	-0.4938850	-1.5829720
C	2.5890010	-2.5720730	-0.1148540
H	2.0301160	-3.2061340	-0.8075900
H	3.6529360	-2.7671920	-0.2955240
H	2.3627040	-2.8958560	0.9041290
C	3.0878770	-0.2277640	2.0097270
H	2.6651120	0.5207250	2.6827440
H	2.8521910	-1.2144350	2.4111060
H	4.1787660	-0.1136570	2.0184890
C	2.6177040	2.5519260	0.5551100
H	2.1014480	3.3543250	0.0224980
H	2.3497940	2.6112030	1.6128030

H	3.6915760	2.7585240	0.4727430
C	1.6313200	1.9595480	-2.4505790
H	1.0031630	1.5674490	-3.2526260
H	1.1352080	2.8401180	-2.0346770
H	2.5745880	2.2959720	-2.8970860
C	1.6128860	-1.2252800	-2.8611640
H	0.9902200	-0.6374520	-3.5381220
H	2.5549770	-1.4449020	-3.3774330
H	1.1095170	-2.1785280	-2.6838810
Ir	0.4239600	0.0329440	0.0248900
C	-0.2249430	-1.1725670	2.6893990
O	-0.6792300	-1.2973100	3.8037990
O	-0.3321280	-0.0718210	1.9640260
H	0.3287100	-1.9984080	2.1856710

4′

G-gas = -1178.836126 Hartree

Symbol	X	Y	Z
C	-2.5102930	0.7363680	-0.1022330
N	-1.2920440	1.3274420	0.0116710
C	-1.2224050	2.6574880	0.2027830
C	-2.3521770	3.4634020	0.2526300
C	-3.6077930	2.8716530	0.1153510
C	-3.6840330	1.4944380	-0.0579200
H	-0.2315040	3.0711310	0.3294660
H	-2.2419210	4.5308620	0.4059280
H	-4.5118260	3.4699510	0.1534560
H	-4.6494650	1.0122830	-0.1471800
C	-2.1946500	-3.4498800	-0.5458430
C	-3.4758120	-2.8957160	-0.5678090
C	-3.6125000	-1.5211930	-0.4214220
C	-2.4759890	-0.7224950	-0.2557520
N	-1.2315930	-1.2736590	-0.2285120
C	-1.1056630	-2.6096180	-0.3698000
H	-2.0355890	-4.5168280	-0.6519730
H	-4.3511120	-3.5236880	-0.6947420
H	-4.5967390	-1.0700060	-0.4362050
H	-0.0976020	-3.0006760	-0.3251300
C	2.3315650	-0.9854570	-0.2957750
C	2.5830850	0.1849400	0.5174450
C	2.1756380	1.3443460	-0.2260550
C	1.7420800	0.8994880	-1.5492520
C	1.8435130	-0.5256520	-1.5900970
C	2.8012950	-2.3801940	0.0076410
H	2.1983450	-3.1381940	-0.4992840

H	3.8324180	-2.5082310	-0.3438880
H	2.7925020	-2.5965820	1.0779850
C	3.2134120	0.2038720	1.8764280
H	2.8409420	1.0347180	2.4781980
H	3.0305270	-0.7183270	2.4289810
H	4.2986430	0.3265940	1.7683120
C	2.4033380	2.7668870	0.1959870
H	1.8108660	3.4686260	-0.3960600
H	2.1701900	2.9202090	1.2526550
H	3.4555620	3.0377590	0.0477190
C	1.3472500	1.8041930	-2.6765140
H	0.7590000	1.2796450	-3.4317100
H	0.7601080	2.6563050	-2.3245020
H	2.2426970	2.2035060	-3.1682890
C	1.5752820	-1.4034130	-2.7742150
H	0.8842710	-0.9373490	-3.4792290
H	2.5114900	-1.6058230	-3.3084650
H	1.1571590	-2.3692040	-2.4797630
Ir	0.3840840	0.0493680	0.0516390
C	-0.1356540	-0.6959550	3.0499210
O	-0.3104380	0.1889600	2.1706260
O	0.4977350	-1.8041770	2.6858390
H	0.7267440	-1.7077420	1.7206920

TS(4-5)

G-gas = -1178.846641 Hartree

Symbol	X	Y	Z
C	-2.4024240	0.6312970	-0.4339650
N	-1.1800030	1.2186840	-0.3822810
C	-1.0837410	2.5585120	-0.4551060
C	-2.1945950	3.3719540	-0.6274020
C	-3.4546110	2.7792400	-0.7062310
C	-3.5578990	1.3968150	-0.6040790
H	-0.0919230	2.9739950	-0.3457960
H	-2.0685330	4.4470140	-0.6817060
H	-4.3453150	3.3855600	-0.8323090
H	-4.5297730	0.9214140	-0.6382610
C	-2.1712640	-3.5627030	0.0251130
C	-3.4370030	-3.0010130	-0.1510680
C	-3.5469190	-1.6250640	-0.3062790
C	-2.3961660	-0.8316960	-0.2834440
N	-1.1689430	-1.3902080	-0.1194980
C	-1.0664280	-2.7245280	0.0392030
H	-2.0372950	-4.6300920	0.1579010
H	-4.3242940	-3.6250940	-0.1607970

H	-4.5206000	-1.1689530	-0.4309290
H	-0.0679150	-3.1116390	0.1927730
C	2.3506490	-1.2317170	-0.0119830
C	2.5829050	-0.0551940	0.7822740
C	2.3562900	1.1174480	-0.0372250
C	2.0135520	0.6621010	-1.3655950
C	1.9835040	-0.7942550	-1.3509420
C	2.6090250	-2.6435960	0.4235090
H	2.1103790	-3.3686940	-0.2238490
H	3.6830830	-2.8576890	0.3729660
H	2.2854840	-2.8173450	1.4523610
C	2.9542650	-0.0041010	2.2271760
H	2.2158500	0.5970850	2.7685860
H	3.0041500	-0.9984130	2.6730390
H	3.9366030	0.4705290	2.3359240
C	2.5843840	2.5256930	0.4217500
H	2.2028570	3.2551090	-0.2965920
H	2.1018680	2.6975010	1.3866230
H	3.6587500	2.7157120	0.5305120
C	1.8176470	1.5190020	-2.5761690
H	1.1181050	1.0705170	-3.2843920
H	1.4536790	2.5149850	-2.3177920
H	2.7786950	1.6449240	-3.0899600
C	1.7839110	-1.6783490	-2.5419210
H	1.1323460	-1.2148570	-3.2851020
H	2.7509320	-1.8771990	-3.0202230
H	1.3501480	-2.6411600	-2.2639770
Ir	0.4708840	-0.0490330	0.0255980
C	-0.7614330	0.4329360	2.3807200
O	-1.9701380	0.3928600	2.5868580
O	0.0806460	1.3744170	2.3317920
H	-0.2787120	-0.6019390	2.1031640

TS(4′-5)

G-gas = -1178.830370 Hartree

Symbol	X	Y	Z
C	-2.4813310	0.7080220	-0.2672980
N	-1.2400700	1.2647800	-0.1929830
C	-1.1195660	2.6077310	-0.2633800
C	-2.2119200	3.4440830	-0.4325870
C	-3.4891110	2.8837830	-0.5173570
C	-3.6208880	1.5044700	-0.4268290
H	-0.1177780	2.9987580	-0.1539130
H	-2.0601930	4.5162090	-0.4844950
H	-4.3645880	3.5118090	-0.6425930

H	-4.6017020	1.0477070	-0.4759440
C	-2.3090370	-3.4854900	0.1334030
C	-3.5698570	-2.9110460	-0.0494670
C	-3.6602880	-1.5325230	-0.1840020
C	-2.5005040	-0.7499100	-0.1428050
N	-1.2741360	-1.3200650	0.0359150
C	-1.1949990	-2.6628650	0.1751270
H	-2.1861300	-4.5562820	0.2499270
H	-4.4624570	-3.5264030	-0.0814790
H	-4.6261050	-1.0622300	-0.3215020
H	-0.2039170	-3.0641400	0.3388200
C	2.2189390	-1.2688940	-0.2013530
C	2.5751540	-0.0564680	0.4900520
C	2.2841720	1.0613570	-0.3781930
C	1.8335720	0.5285560	-1.6513340
C	1.7758820	-0.9020220	-1.5402680
C	2.5127380	-2.6618800	0.2760100
H	1.9149690	-3.4095930	-0.2514410
H	3.5648260	-2.9100080	0.0905800
H	2.3326010	-2.7714510	1.3481150
C	3.2356950	0.0264090	1.8320080
H	3.0121960	0.9680380	2.3347420
H	2.9332100	-0.7925850	2.4869780
H	4.3237930	-0.0358880	1.7005670
C	2.6231010	2.4933190	-0.0825730
H	2.1155380	3.1785640	-0.7660280
H	2.3519580	2.7648820	0.9401850
H	3.6998570	2.6615630	-0.2041300
C	1.5299320	1.3368470	-2.8747170
H	0.8543070	0.8125650	-3.5533830
H	1.0787100	2.3001390	-2.6245960
H	2.4567590	1.5461520	-3.4234220
C	1.4198430	-1.8686930	-2.6278290
H	0.8059430	-1.4029470	-3.4011730
H	2.3297830	-2.2495190	-3.1077330
H	0.8721490	-2.7304940	-2.2372170
Ir	0.3815090	-0.0386210	0.0329980
C	0.0116010	0.8766280	3.1504060
O	0.2554260	1.6248880	2.2318380
O	-0.1314620	-0.3851320	3.0568250
H	0.0290340	-0.5805730	1.9863660

5

G-gas = -990.352037 Hartree

Symbol	X	Y	Z

C	-2.4976220	-0.7337300	-0.0134970
N	-1.2673240	-1.3015340	-0.1423610
C	-1.1680270	-2.6451810	-0.1832560
C	-2.2736060	-3.4784040	-0.0784300
C	-3.5390990	-2.9073920	0.0619930
C	-3.6480650	-1.5221520	0.0897120
H	-0.1703990	-3.0422070	-0.3149080
H	-2.1380420	-4.5534210	-0.1139260
H	-4.4243750	-3.5291370	0.1419020
H	-4.6207680	-1.0561450	0.1882660
C	-2.2719080	3.4787870	-0.0783820
C	-3.5376250	2.9083890	0.0625550
C	-3.6472790	1.5232010	0.0902350
C	-2.4972840	0.7341890	-0.0134900
N	-1.2667630	1.3013990	-0.1427650
C	-1.1667980	2.6450090	-0.1836860
H	-2.1358150	4.5537380	-0.1138910
H	-4.4225460	3.5305800	0.1429110
H	-4.6201710	1.0576880	0.1892540
H	-0.1690020	3.0414690	-0.3157570
C	2.2424240	1.1631850	-0.0096470
C	2.5313160	-0.0018590	-0.8066090
C	2.2419250	-1.1642280	-0.0060900
C	1.9092520	-0.7047020	1.3466100
C	1.9095580	0.7078560	1.3444120
C	2.5498650	2.5814980	-0.3964740
H	1.9833820	3.2996470	0.2027260
H	3.6118220	2.8012300	-0.2313510
H	2.3332770	2.7688170	-1.4508780
C	3.1090920	-0.0040170	-2.1908800
H	2.8037210	-0.8872710	-2.7547970
H	2.8044460	0.8779700	-2.7571550
H	4.2044390	-0.0043760	-2.1313290
C	2.5485030	-2.5838750	-0.3885620
H	1.9805030	-3.2998300	0.2118220
H	2.3332930	-2.7738820	-1.4427630
H	3.6100260	-2.8041360	-0.2213570
C	1.6486260	-1.6107010	2.5124750
H	1.1413680	-1.0909800	3.3275410
H	1.0339610	-2.4705670	2.2297670
H	2.5930030	-2.0058660	2.9062700
C	1.6484960	1.6176420	2.5072250
H	1.1430440	1.0999210	3.3246740
H	2.5925110	2.0160750	2.8985530

H	1.0318160	2.4752690	2.2219610
H	0.0063980	-0.0007550	-1.8599410
Ir	0.3724970	-0.0003120	-0.3153120

b) Different isomers of **5**

^{1}5 (S_1)

G-gas = -990.265739 Hartree

Symbol	X	Y	Z
C	-2.4077540	-0.7165360	0.0523640
N	-1.2589050	-1.3333180	-0.4288910
C	-1.2194730	-2.6549020	-0.6348920
C	-2.2944830	-3.4860840	-0.3565380
C	-3.4421010	-2.9021930	0.2252800
C	-3.4981550	-1.5414060	0.4373770
H	-0.2898630	-3.0454580	-1.0346910
H	-2.2352940	-4.5456360	-0.5691100
H	-4.2868130	-3.5249130	0.5026010
H	-4.3795680	-1.0943230	0.8810970
C	-2.2954050	3.4857160	-0.3565150
C	-3.4428980	2.9015270	0.2252830
C	-3.4985630	1.5407220	0.4373480
C	-2.4079120	0.7161600	0.0523390
N	-1.2592390	1.3332230	-0.4289380
C	-1.2201930	2.6548390	-0.6349040
H	-2.2364890	4.5452810	-0.5690910
H	-4.2877790	3.5240120	0.5026030
H	-4.3798700	1.0933540	0.8809980
H	-0.2907440	3.0456910	-1.0347940
C	2.4512450	0.7321630	-0.4916900
C	2.4511520	-0.7318720	-0.4917890
C	1.9989790	-1.1658910	0.8033250
C	1.8145660	-0.0000380	1.6408360
C	1.9989510	1.1659110	0.8033770
C	2.9975610	1.6032930	-1.5809240
H	2.5409330	2.5950570	-1.5774640
H	4.0778000	1.7371270	-1.4422260
H	2.8413210	1.1626920	-2.5673270
C	2.9972380	-1.6027280	-1.5814090
H	2.5400590	-2.5942390	-1.5786640
H	2.8412770	-1.1614540	-2.5675600
H	4.0773930	-1.7371640	-1.4426980
C	1.9277210	-2.5859550	1.2811450
H	1.1053910	-2.7377840	1.9840410
H	1.7999730	-3.2858950	0.4538420

H	2.8587350	-2.8530370	1.7950940
C	1.4978970	0.0000050	3.0976040
H	0.9303280	0.8857040	3.3921400
H	0.9372880	-0.8895620	3.3936250
H	2.4286230	0.0042910	3.6834390
C	1.9272300	2.5858460	1.2814710
H	1.1060780	2.7366670	1.9859400
H	2.8589240	2.8538910	1.7937110
H	1.7971950	3.2857760	0.4545100
H	0.2172460	0.0003790	-1.8782030
Ir	0.3511850	0.0001140	-0.3206690

5_1 (S_0)

G-gas = -990.340108 Hartree

Symbol	X	Y	Z
Ir	-0.2726340	0.0000040	0.0539890
N	1.3715420	-1.3077410	-0.0313990
N	1.3714490	1.3078770	-0.0312790
H	-2.0653310	0.0009240	-2.2929160
C	1.2770040	-2.6505920	-0.0073130
H	0.2745610	-3.0508980	0.0533810
C	2.3890360	-3.4831590	-0.0611170
H	2.2558570	-4.5586700	-0.0372610
C	3.6544070	-2.9066570	-0.1495930
H	4.5452530	-3.5239890	-0.1973890
C	3.7601480	-1.5183080	-0.1758640
H	4.7351120	-1.0516500	-0.2425130
C	2.6054650	-0.7371150	-0.1131710
C	2.6054130	0.7373390	-0.1132110
C	3.7600200	1.5186150	-0.1761770
H	4.7350030	1.0520230	-0.2430190
C	3.6541800	2.9069590	-0.1499790
H	4.5449730	3.5243530	-0.1979760
C	2.3887830	3.4833700	-0.0613240
H	2.2555190	4.5588720	-0.0375180
C	1.2768220	2.6507220	-0.0072830
H	0.2743600	3.0509630	0.0535280
C	-2.1146570	-0.7374880	0.9103140
C	-2.1980130	-1.5968920	2.1361380
H	-1.8235440	-2.6060780	1.9500730
H	-3.2432960	-1.6902180	2.4571120
H	-1.6300390	-1.1730760	2.9676010
C	-2.1168540	-1.1522570	-0.4522760
C	-2.1907070	-2.5715100	-0.9371780
H	-1.6024880	-2.7113240	-1.8498850

H	-3.2286470	-2.8314540	-1.1802300
H	-1.8538960	-3.2951820	-0.1901550
C	-2.5965490	0.0004520	-1.3326390
C	-4.1165690	0.0004270	-1.6113210
H	-4.4050030	0.8819180	-2.1915270
H	-4.6870330	-0.0000380	-0.6770520
H	-4.4048460	-0.8806020	-2.1923070
C	-2.1170840	1.1524880	-0.4512530
C	-2.1914160	2.5721830	-0.9347770
H	-1.8541970	3.2951820	-0.1872820
H	-3.2295520	2.8322520	-1.1768680
H	-1.6038240	2.7129280	-1.8477440
C	-2.1148250	0.7364790	0.9109390
C	-2.1980050	1.5949020	2.1374600
H	-1.6316910	1.1692850	2.9691220
H	-3.2434650	1.6898530	2.4573950
H	-1.8215000	2.6035850	1.9527430

5_2 (S_0)

G-gas = -990.305271 Hartree

Symbol	X	Y	Z
Ir	0.3357540	0.0157620	-0.0680390
N	-1.0840620	1.3019120	-0.3642880
N	-1.3431120	-1.2394750	-0.0366990
C	-0.9445010	2.6836280	-0.4204280
H	0.0366420	3.0451180	-0.7054820
C	-1.9418720	3.5284470	-0.0503890
H	-1.7832690	4.5998050	-0.0922610
C	-3.1498470	2.9822990	0.5386160
H	-3.8090220	3.6342090	1.1036500
C	-3.4005690	1.6652560	0.4332120
H	-4.2545840	1.1886350	0.9021610
C	-2.4809800	0.8470660	-0.4570170
C	-2.5370790	-0.6350670	-0.2471570
C	-3.7247950	-1.3653270	-0.2897030
H	-4.6609090	-0.8505130	-0.4769340
C	-3.6907480	-2.7407410	-0.0930900
H	-4.6056120	-3.3236400	-0.1173040
C	-2.4568730	-3.3578270	0.1329070
H	-2.3800250	-4.4277410	0.2897330
C	-1.3116090	-2.5808140	0.1488870
H	-0.3357790	-3.0168150	0.3089940
C	2.0258960	-0.4470290	1.3006340
C	1.9286060	-0.8159940	2.7491210
H	1.3454690	-0.0825450	3.3101060

H	2.9301690	-0.8588600	3.1953330
H	1.4620520	-1.7933820	2.8890740
C	2.1614380	0.9174850	0.7878040
C	2.2280440	2.1526470	1.6325030
H	1.9395850	3.0451700	1.0739530
H	3.2535740	2.3019670	1.9918230
H	1.5774380	2.0774720	2.5066420
C	2.3111430	0.8358490	-0.6332390
C	2.5910480	1.9644120	-1.5788070
H	2.0741290	1.8318190	-2.5323390
H	3.6663130	2.0153720	-1.7884730
H	2.2969610	2.9297880	-1.1616940
C	2.2834550	-0.5775870	-1.0054200
C	2.4889190	-1.1090330	-2.3892870
H	2.0238680	-2.0882660	-2.5209440
H	3.5618650	-1.2200950	-2.5927450
H	2.0773520	-0.4347250	-3.1432280
C	2.1612240	-1.3527690	0.1944370
C	2.2393440	-2.8480340	0.2796000
H	1.7446290	-3.2362050	1.1732310
H	3.2896110	-3.1582190	0.3367400
H	1.8082240	-3.3351860	-0.5988070
H	-2.8030160	1.0249330	-1.5044510

5_3 (S_0)

G-gas = -990.297146 Hartree

Symbol	X	Y	Z
C	2.4440010	0.7835960	-0.0062510
N	1.1474650	1.3200560	0.0032050
C	1.0012880	2.6859690	0.0124870
C	2.0578170	3.5513910	0.0121040
C	3.3805840	3.0235270	0.0009870
C	3.5660070	1.6689710	-0.0083530
H	-0.0207530	3.0405090	0.0186700
H	1.8802620	4.6201630	0.0192930
H	4.2332830	3.6946750	-0.0004540
H	4.5637340	1.2460590	-0.0178530
C	2.3858580	-3.4047260	0.0204750
C	3.6206050	-2.8571190	0.0112370
C	3.8413350	-1.3730030	-0.0243870
C	2.5350350	-0.6030810	-0.0126870
N	1.3159170	-1.2397030	-0.0094510
C	1.2271870	-2.5616490	0.0027770
H	2.2428930	-4.4796100	0.0415710
H	4.5015440	-3.4931390	0.0257630

H	4.4808890	-1.0880910	0.8280720
H	0.2343320	-2.9881700	0.0016270
C	-2.2086020	-1.3111290	-0.1087960
C	-2.2005090	-0.3635200	-1.1914250
C	-2.2574490	0.9820840	-0.6232170
C	-2.2495680	0.8537190	0.8008500
C	-2.1970970	-0.5748770	1.1226680
C	-2.3188240	-2.7998750	-0.2507360
H	-1.9052310	-3.3270770	0.6124890
H	-3.3745840	-3.0864690	-0.3252240
H	-1.8207140	-3.1644310	-1.1525350
C	-2.2554920	-0.6850970	-2.6507370
H	-1.7637270	0.0843200	-3.2496070
H	-1.7815170	-1.6434880	-2.8717730
H	-3.3012380	-0.7452060	-2.9799240
C	-2.4229580	2.2403590	-1.4204340
H	-2.2057420	3.1310630	-0.8276990
H	-1.7770300	2.2523090	-2.3019340
H	-3.4598660	2.3264510	-1.7668700
C	-2.3836990	1.9540360	1.8080730
H	-1.7999270	1.7492860	2.7084870
H	-2.0593990	2.9165820	1.4076490
H	-3.4335900	2.0593930	2.1078490
C	-2.2532250	-1.1473950	2.5040020
H	-1.7467430	-0.5033470	3.2259920
H	-3.2983220	-1.2482830	2.8242940
H	-1.7936150	-2.1364600	2.5522980
H	4.4465860	-1.1259620	-0.9138500
Ir	-0.3657010	0.0126410	0.0011110

5_4 (S_0)

G-gas = -990.322833 Hartree

Symbol	X	Y	Z
C	2.4688320	0.8395960	-0.0108980
N	1.2103460	1.3629790	-0.0112800
C	1.0540710	2.7075770	-0.0089400
C	2.1274890	3.5795070	-0.0050230
C	3.4242790	3.0530830	-0.0044740
C	3.5908150	1.6764300	-0.0080170
H	0.0352930	3.0678710	-0.0117740
H	1.9503320	4.6488760	-0.0026750
H	4.2881530	3.7093830	-0.0012510
H	4.5850440	1.2470360	-0.0076140
C	2.2474280	-3.3997700	-0.0014740
C	3.6428280	-2.8518620	-0.0041060

C	3.6352370	-1.3566370	-0.0076080
C	2.4985180	-0.6237120	-0.0108380
N	1.2129680	-1.2018160	-0.0113900
C	1.1670200	-2.6046020	-0.0049360
H	2.1098270	-4.4759000	0.0023650
H	4.2128840	-3.2201950	0.8653340
H	4.5951970	-0.8516460	-0.0070150
H	0.1667850	-3.0166830	-0.0053250
C	-2.1874060	-1.1104870	-0.5983460
C	-2.2256700	0.2281100	-1.1807570
C	-2.2833080	1.1807640	-0.1077470
C	-2.2024420	0.4636450	1.1327270
C	-2.1714330	-0.9658020	0.8258790
C	-2.2887180	-2.3852260	-1.3804590
H	-1.9963870	-3.2541780	-0.7877110
H	-3.3260070	-2.5435290	-1.6992150
H	-1.6665890	-2.3611270	-2.2786140
C	-2.3333410	0.5287700	-2.6431350
H	-1.9408490	1.5188760	-2.8842510
H	-1.7924900	-0.2055020	-3.2440700
H	-3.3857910	0.5029680	-2.9539040
C	-2.4904490	2.6577960	-0.2647920
H	-2.1339200	3.2177600	0.6030300
H	-2.0016760	3.0501180	-1.1602170
H	-3.5617030	2.8701510	-0.3633930
C	-2.2809760	1.0509400	2.5080640
H	-1.7443280	0.4387550	3.2360070
H	-1.8610620	2.0586060	2.5420970
H	-3.3271650	1.1149670	2.8331330
C	-2.2203820	-2.0631230	1.8442420
H	-1.6334610	-1.8143730	2.7313480
H	-3.2563630	-2.2280620	2.1645350
H	-1.8454410	-3.0078150	1.4457660
H	4.2111740	-3.2244870	-0.8728810
Ir	-0.3464810	-0.0259740	-0.0052100

5_5 (S_0)

G-gas = -990.296924 Hartree

Symbol	X	Y	Z
C	2.4468450	0.8339910	-0.0026380
N	1.1319740	1.3350950	0.0028070
C	0.9489230	2.7023550	0.0069620
C	1.9782140	3.5939780	0.0050230
C	3.3189180	3.1026660	-0.0015210
C	3.5417520	1.7578590	-0.0049560

H	-0.0824690	3.0271190	0.0103360
H	1.7712230	4.6575440	0.0079750
H	4.1522120	3.7974420	-0.0037130
H	4.5518560	1.3669500	-0.0096060
C	2.4835060	-3.4271980	0.0084310
C	3.7798360	-2.6694840	-0.0027320
C	3.7918470	-1.3247050	-0.0082440
C	2.5756700	-0.5498860	-0.0048340
N	1.3440410	-1.2252350	-0.0025300
C	1.2924920	-2.5248950	0.0020770
H	2.4019570	-4.0976470	0.8829830
H	4.7029410	-3.2383430	-0.0054880
H	4.7377890	-0.7946990	-0.0156230
H	0.3053630	-2.9732920	0.0008570
C	-2.1840600	-1.3391250	-0.0973900
C	-2.1900750	-0.4042230	-1.1897050
C	-2.2655060	0.9463420	-0.6343390
C	-2.2587020	0.8318570	0.7913550
C	-2.1857140	-0.5922480	1.1275450
C	-2.2637720	-2.8313770	-0.2236260
H	-1.8325250	-3.3416070	0.6413500
H	-3.3136780	-3.1413510	-0.2858980
H	-1.7673350	-3.1948140	-1.1270060
C	-2.2422950	-0.7406950	-2.6459020
H	-1.7617610	0.0294400	-3.2529080
H	-1.7552490	-1.6944660	-2.8586430
H	-3.2871500	-0.8189690	-2.9740320
C	-2.4511930	2.1939410	-1.4436360
H	-2.2503850	3.0939580	-0.8593420
H	-1.8044020	2.2086550	-2.3244670
H	-3.4890360	2.2582920	-1.7920210
C	-2.4134780	1.9393450	1.7876030
H	-1.8334850	1.7502770	2.6938550
H	-2.0996970	2.9027880	1.3811970
H	-3.4668080	2.0328440	2.0791370
C	-2.2389320	-1.1525140	2.5141630
H	-1.7430920	-0.4955910	3.2319350
H	-3.2834290	-1.2645300	2.8326250
H	-1.7672060	-2.1353910	2.5737010
H	2.3972700	-4.1162660	-0.8507460
Ir	-0.3584500	0.0173600	0.0015560

5_6 (S_0)

G-gas = -990.318671 Hartree

Symbol	X	Y	Z

C	2.4932330	0.7777320	-0.0173990
N	1.2474860	1.3350260	-0.0125880
C	1.1266260	2.6840430	-0.0061080
C	2.2222330	3.5264240	-0.0039870
C	3.5064980	2.9657420	-0.0097080
C	3.6377850	1.5864940	-0.0165660
H	0.1172920	3.0705820	-0.0042250
H	2.0737690	4.6001380	0.0014890
H	4.3867390	3.5998430	-0.0089010
H	4.6208740	1.1322260	-0.0216640
C	2.3342930	-3.4780400	0.0112660
C	3.5384200	-2.8810170	0.0329290
C	3.6142280	-1.4424410	0.0042390
C	2.4793490	-0.6799720	-0.0191990
N	1.1984570	-1.2240160	-0.0274240
C	1.0550260	-2.6941230	-0.0593290
H	2.2371190	-4.5597810	0.0337500
H	4.4540840	-3.4608880	0.0749660
H	4.5859660	-0.9648430	0.0134420
H	0.4005610	-2.9981080	0.7700290
C	-2.1986570	-1.0606280	-0.5931300
C	-2.2137520	0.2771130	-1.1764350
C	-2.2495600	1.2318510	-0.1039930
C	-2.1812680	0.5141710	1.1367910
C	-2.1776050	-0.9144470	0.8314220
C	-2.3269430	-2.3364610	-1.3686290
H	-2.0001760	-3.2017080	-0.7886650
H	-3.3757620	-2.5031360	-1.6424810
H	-1.7480120	-2.3079550	-2.2955470
C	-2.3169210	0.5818000	-2.6384310
H	-1.9010310	1.5626410	-2.8781640
H	-1.7941490	-0.1633780	-3.2419050
H	-3.3700040	0.5815690	-2.9479700
C	-2.4274970	2.7126700	-0.2613470
H	-2.0529070	3.2662650	0.6029820
H	-1.9367990	3.0938540	-1.1604730
H	-3.4947550	2.9474530	-0.3524230
C	-2.2438450	1.1060210	2.5113160
H	-1.7246960	0.4808510	3.2409370
H	-1.7955270	2.1014500	2.5437320
H	-3.2878220	1.2001890	2.8359040
C	-2.2499430	-2.0123390	1.8468200
H	-1.6866360	-1.7648210	2.7496230
H	-3.2928850	-2.1812670	2.1416230

H	-1.8666220	-2.9565000	1.4534750
H	0.5167930	-2.9746770	-0.9775360
Ir	-0.3339900	-0.0151250	-0.0060400

5* (T_1)

G-gas = -990.275809 Hartree

Symbol	X	Y	Z
C	-2.5264090	-0.7098760	0.0179990
N	-1.2700470	-1.3102170	-0.0877890
C	-1.1677970	-2.6644580	-0.1419280
C	-2.2571780	-3.4963530	-0.0569780
C	-3.5445230	-2.9109900	0.0901930
C	-3.6683910	-1.5419020	0.1263980
H	-0.1648630	-3.0554340	-0.2577030
H	-2.1239880	-4.5700240	-0.1050390
H	-4.4249740	-3.5399030	0.1675860
H	-4.6460290	-1.0866570	0.2333060
C	-2.2572170	3.4963580	-0.0571070
C	-3.5444640	2.9109910	0.0907500
C	-3.6683510	1.5419080	0.1270530
C	-2.5264380	0.7098520	0.0179930
N	-1.2701720	1.3102110	-0.0884240
C	-1.1678790	2.6644340	-0.1425360
H	-2.1240450	4.5700210	-0.1053470
H	-4.4248710	3.5399040	0.1686820
H	-4.6459250	1.0867020	0.2347210
H	-0.1649730	3.0553340	-0.2588360
C	2.1781940	1.1680070	0.5713660
C	2.3569320	0.7337350	-0.7824360
C	2.3568800	-0.7336350	-0.7824830
C	2.1781820	-1.1680380	0.5713180
C	2.1317250	-0.0000720	1.4252200
C	2.2406030	2.5830960	1.0655760
H	1.5165630	2.7739490	1.8616440
H	3.2386020	2.7857570	1.4721470
H	2.0681560	3.3034660	0.2639980
C	2.6728340	1.6040380	-1.9612760
H	2.3347430	1.1556270	-2.8972540
H	2.2098830	2.5890510	-1.8752290
H	3.7573440	1.7518570	-2.0344570
C	2.6725290	-1.6040170	-1.9613270
H	2.2073780	-2.5880810	-1.8763670
H	2.3366220	-1.1544290	-2.8975210
H	3.7568200	-1.7541030	-2.0331700
C	2.2405930	-2.5832060	1.0653230

H	1.5158270	-2.7745140	1.8606210
H	2.0692750	-3.3034490	0.2633930
H	3.2382510	-2.7855760	1.4728740
C	2.0533630	-0.0001030	2.9161370
H	1.5434170	-0.8874080	3.2985690
H	3.0662050	0.0006830	3.3434200
H	1.5420790	0.8864440	3.2985570
H	0.0427950	0.0000990	-1.7206140
Ir	0.3056900	0.0000280	-0.1797400

5_1* (T_1)

G-gas = -990.278458 Hartree

Symbol	X	Y	Z
C	-2.6066800	0.7594300	-0.0930680
N	-1.3412620	1.3244050	-0.0732000
C	-1.2360960	2.6844430	-0.1171500
C	-2.3291580	3.5162350	-0.1806590
C	-3.6230860	2.9524070	-0.1959950
C	-3.7494370	1.5790530	-0.1509340
H	-0.2299590	3.0784630	-0.1024040
H	-2.1816610	4.5893600	-0.2177340
H	-4.5023180	3.5856050	-0.2394570
H	-4.7321310	1.1228060	-0.1544380
C	-2.3982740	-3.4436120	0.0048720
C	-3.6768830	-2.8536480	-0.1096980
C	-3.7794020	-1.4773440	-0.1414070
C	-2.6248350	-0.6765350	-0.0581950
N	-1.3777050	-1.2665640	0.0545040
C	-1.2946570	-2.6279080	0.0782990
H	-2.2753820	-4.5197380	0.0417210
H	-4.5653670	-3.4721020	-0.1750470
H	-4.7506240	-1.0070250	-0.2379780
H	-0.2963330	-3.0345130	0.1718530
C	2.1327220	-0.9991400	0.6512890
C	2.2164000	0.4049010	1.0512590
C	2.1440920	1.1911830	-0.1427530
C	2.5574710	0.3070950	-1.3290570
C	2.0898630	-1.0386050	-0.7774950
C	2.2353710	-2.1688090	1.5881250
H	1.8451790	-3.0853840	1.1407290
H	3.2887010	-2.3542580	1.8312440
H	1.7052560	-1.9939200	2.5273770
C	2.3853110	0.9023030	2.4543080
H	1.9669110	1.9030340	2.5815330
H	1.9168910	0.2404020	3.1859030

H	3.4547320	0.9601500	2.6960770
C	2.3161340	2.6829940	-0.1944310
H	1.8641680	3.1054270	-1.0970790
H	1.8890050	3.1843070	0.6777750
H	3.3824860	2.9400910	-0.2214770
C	4.0684170	0.3551500	-1.6592140
H	4.3086760	-0.3448890	-2.4645380
H	4.3571120	1.3548820	-1.9957810
H	4.6703360	0.0965620	-0.7823480
C	2.0598060	-2.2696940	-1.6300210
H	1.5258260	-2.0869850	-2.5670310
H	3.0836740	-2.5687810	-1.8921000
H	1.5943110	-3.1223570	-1.1313520
H	2.0039050	0.5734900	-2.2386060
Ir	0.2387910	0.0230010	0.0844880

5_2* (T_1)

G-gas = -990.274543 Hartree

Symbol	X	Y	Z
Ir	0.3614220	-0.0043330	0.0083210
N	-1.2368610	1.2888520	0.0068950
N	-1.2495550	-1.3088970	0.0357720
C	-1.3301520	2.4819100	0.5584770
H	-0.4241770	2.8683440	1.0138700
C	-2.5206000	3.2426860	0.6079270
H	-2.5015300	4.2194690	1.0760270
C	-3.7124360	2.7009100	0.0805610
H	-4.6375450	3.2652510	0.1400590
C	-3.6957140	1.4661660	-0.5049890
H	-4.5912530	1.0528390	-0.9563440
C	-2.4196530	0.6929370	-0.6533870
C	-2.4747800	-0.7715960	-0.2242460
C	-3.6334450	-1.5327650	-0.1536940
H	-4.5961660	-1.0792350	-0.3547600
C	-3.5482330	-2.8868630	0.1763700
H	-4.4447640	-3.4951020	0.2315670
C	-2.2927590	-3.4378120	0.4306920
H	-2.1759880	-4.4839480	0.6902300
C	-1.1726060	-2.6240160	0.3544250
H	-0.1790710	-3.0035690	0.5516300
C	2.3637800	-0.2190020	1.1264030
C	2.5622340	-0.5462150	2.5735320
H	2.0792890	0.1868380	3.2238530
H	3.6329670	-0.5491170	2.8177240
H	2.1678790	-1.5328950	2.8272730

C	2.2406240	1.1022790	0.5655780
C	2.3576410	2.3850550	1.3356610
H	1.9110040	3.2254430	0.7984710
H	3.4133190	2.6361640	1.4964830
H	1.8860800	2.3146870	2.3196450
C	2.1881000	0.9800400	-0.8763180
C	2.1881560	2.1155810	-1.8559980
H	1.6788810	1.8460640	-2.7841750
H	3.2161730	2.4014260	-2.1108980
H	1.6950900	3.0018140	-1.4493960
C	2.2593180	-0.4191320	-1.2077850
C	2.3302530	-1.0026350	-2.5847810
H	1.8516940	-1.9836070	-2.6342980
H	3.3774540	-1.1330300	-2.8879160
H	1.8523130	-0.3557130	-3.3237510
C	2.2939060	-1.1615130	0.0336100
C	2.4918090	-2.6457070	0.1473800
H	2.1297540	-3.0320210	1.1041190
H	3.5575270	-2.8964200	0.0831980
H	1.9845310	-3.1859220	-0.6564550
H	-2.1607370	0.6643550	-1.7320640

5_3* (T_1)

G-gas = -990.297075 Hartree

Symbol	X	Y	Z
C	2.4660230	0.7982410	-0.0111900
N	1.2051680	1.3534250	-0.0136880
C	1.0927700	2.6989240	-0.0143520
C	2.1929400	3.5448630	-0.0096620
C	3.4784850	2.9915880	-0.0053620
C	3.6109080	1.6091350	-0.0070750
H	0.0841620	3.0896790	-0.0206990
H	2.0398390	4.6179750	-0.0096820
H	4.3566460	3.6281740	-0.0011480
H	4.5932540	1.1520080	-0.0046540
C	2.3252700	-3.4306130	-0.0050780
C	3.5815800	-2.8958150	-0.0045190
C	3.7754850	-1.4133350	-0.0084960
C	2.4858700	-0.6370590	-0.0115550
N	1.2672040	-1.2317300	-0.0128850
C	1.1872600	-2.6019430	-0.0097310
H	2.1771850	-4.5053930	-0.0027210
H	4.4646350	-3.5255860	-0.0015350
H	4.3837620	-1.1094060	0.8614170
H	0.1877680	-3.0104300	-0.0132600

C	-2.2004970	-1.1265720	-0.5830320
C	-2.2780110	0.1898160	-1.1839460
C	-2.2844910	1.1617750	-0.1191080
C	-2.2406520	0.4567300	1.1372480
C	-2.1820180	-0.9644880	0.8469950
C	-2.2907480	-2.4194040	-1.3383750
H	-1.9484120	-3.2684880	-0.7426240
H	-3.3333040	-2.6211220	-1.6125930
H	-1.7060700	-2.3934790	-2.2615260
C	-2.4145660	0.4749450	-2.6466530
H	-2.0152880	1.4573070	-2.9081870
H	-1.8983640	-0.2729480	-3.2527290
H	-3.4740100	0.4612090	-2.9350210
C	-2.4951920	2.6372290	-0.2931840
H	-2.1313210	3.2060580	0.5661320
H	-2.0060440	3.0176790	-1.1938610
H	-3.5657280	2.8539270	-0.3898440
C	-2.3289500	1.0674080	2.5013740
H	-1.8162040	0.4577640	3.2485870
H	-1.8909320	2.0677690	2.5258630
H	-3.3787140	1.1579680	2.8091010
C	-2.2193160	-2.0588970	1.8701430
H	-1.6761750	-1.7815570	2.7764880
H	-3.2564230	-2.2745630	2.1552310
H	-1.7873220	-2.9877110	1.4911060
H	4.3857180	-1.1141120	-0.8786810
Ir	-0.3593270	0.0045490	-0.0083870

5_4* (T_1)

G-gas = -990.287229 Hartree

Symbol	X	Y	Z
C	2.4831450	0.8521670	-0.0015510
N	1.2151050	1.3732250	-0.0051770
C	1.0629130	2.7220260	-0.0069070
C	2.1370700	3.5948130	-0.0049690
C	3.4334550	3.0714590	-0.0009960
C	3.5985580	1.6898330	0.0005430
H	0.0415330	3.0774600	-0.0101770
H	1.9580990	4.6639810	-0.0065160
H	4.2977470	3.7268310	0.0007490
H	4.5944120	1.2638790	0.0033220
C	2.3196170	-3.3957230	-0.0050480
C	3.7034860	-2.8404870	0.0028080
C	3.7034780	-1.3483770	0.0033340
C	2.5445390	-0.6183120	-0.0007600

N	1.2927150	-1.2157270	-0.0055250
C	1.2268900	-2.5865080	-0.0086750
H	2.1818850	-4.4719150	-0.0078830
H	4.2678980	-3.2260440	0.8716780
H	4.6627000	-0.8439860	0.0071130
H	0.2258710	-2.9955060	-0.0145480
C	-2.1753850	-1.1020490	-0.7093320
C	-2.3234350	0.2556280	-1.1611490
C	-2.3166610	1.1100970	0.0061440
C	-2.3006040	0.2656190	1.1814710
C	-2.1627050	-1.0957700	0.7383510
C	-2.2060540	-2.3139250	-1.5938270
H	-1.7637780	-3.1878550	-1.1101330
H	-3.2416660	-2.5765240	-1.8422290
H	-1.6723820	-2.1431150	-2.5320280
C	-2.4820800	0.7023620	-2.5803560
H	-2.0691620	1.7011200	-2.7411110
H	-1.9940350	0.0181370	-3.2779250
H	-3.5468050	0.7416140	-2.8468600
C	-2.5862330	2.5876840	0.0029290
H	-2.1663040	3.0798310	0.8845010
H	-2.1807270	3.0738070	-0.8886980
H	-3.6658610	2.7800060	0.0112490
C	-2.4327360	0.7261970	2.5989280
H	-1.9500640	0.0377080	3.2959630
H	-1.9972730	1.7174900	2.7463850
H	-3.4929630	0.7896150	2.8783410
C	-2.1731470	-2.3002170	1.6332440
H	-1.6190650	-2.1213770	2.5579890
H	-3.2029390	-2.5612250	1.9062140
H	-1.7406940	-3.1776590	1.1471570
H	4.2775480	-3.2253290	-0.8599610
Ir	-0.3387460	0.0376290	-0.0086070

5_5* (T_1)

G-gas = -990.294756 Hartree

Symbol	X	Y	Z
C	2.4721310	0.8430600	-0.0125680
N	1.2027990	1.3705380	-0.0157060
C	1.0566830	2.7118710	-0.0164460
C	2.1347450	3.5867410	-0.0111110
C	3.4303060	3.0628830	-0.0060130
C	3.5954300	1.6837120	-0.0076320
H	0.0384350	3.0756510	-0.0235950
H	1.9553190	4.6557130	-0.0112130

H	4.2947800	3.7180260	-0.0011840
H	4.5908430	1.2575960	-0.0043020
C	2.4254710	-3.4631800	-0.0054130
C	3.7164050	-2.7137940	-0.0062900
C	3.7337150	-1.3566940	-0.0100500
C	2.5275080	-0.5981970	-0.0130090
N	1.2868670	-1.2345920	-0.0147130
C	1.2332670	-2.5625680	-0.0114720
H	2.3718820	-4.1426370	0.8641870
H	4.6430370	-3.2785870	-0.0035350
H	4.6819920	-0.8324980	-0.0103040
H	0.2437020	-3.0008230	-0.0159080
C	-2.1903280	-1.1481450	-0.5623250
C	-2.2905580	0.1523990	-1.1858840
C	-2.2860380	1.1412530	-0.1363240
C	-2.2458210	0.4585460	1.1347300
C	-2.1733090	-0.9618840	0.8680780
C	-2.2716830	-2.4569290	-1.2915620
H	-1.9028370	-3.2889550	-0.6867890
H	-3.3148120	-2.6848210	-1.5421210
H	-1.7056210	-2.4374050	-2.2266250
C	-2.4445860	0.4135090	-2.6517540
H	-2.0542100	1.3941840	-2.9327550
H	-1.9290160	-0.3395720	-3.2521970
H	-3.5063570	0.3889530	-2.9310320
C	-2.5110540	2.6119390	-0.3348770
H	-2.1593700	3.1981770	0.5179220
H	-2.0195930	2.9838590	-1.2380220
H	-3.5830230	2.8165650	-0.4417460
C	-2.3419890	1.0951620	2.4869710
H	-1.8321890	0.5010890	3.2487780
H	-1.9040880	2.0960360	2.4949260
H	-3.3928480	1.1923740	2.7889900
C	-2.1984020	-2.0430810	1.9058290
H	-1.6761640	-1.7395040	2.8161010
H	-3.2330620	-2.2841480	2.1793240
H	-1.7365320	-2.9655270	1.5457980
H	2.3746210	-4.1496730	-0.8695530
Ir	-0.3494010	0.0022690	-0.0110320

5_6* (T_1)

G-gas = -990.289902 Hartree

Symbol	X	Y	Z
C	2.4870810	0.7962830	-0.0111930
N	1.2245530	1.3448840	-0.0149270

C	1.1078840	2.6969740	-0.0155440
C	2.2023920	3.5428180	-0.0095780
C	3.4908280	2.9920280	-0.0038880
C	3.6243500	1.6090790	-0.0056880
H	0.0973900	3.0820790	-0.0233110
H	2.0473000	4.6157540	-0.0097820
H	4.3681820	3.6294630	0.0013650
H	4.6096280	1.1595340	-0.0022650
C	2.4150140	-3.4587620	-0.0052620
C	3.6413920	-2.8325570	-0.0037240
C	3.7132360	-1.4387620	-0.0086040
C	2.5010400	-0.6612530	-0.0117090
N	1.2923740	-1.2158050	-0.0131970
C	1.1472830	-2.6736190	-0.0147550
H	2.3297100	-4.5404980	-0.0024000
H	4.5551450	-3.4182030	0.0012410
H	4.6714140	-0.9371750	-0.0080780
H	0.5236670	-2.9439490	0.8525840
C	-2.1899010	-1.1295640	-0.5594560
C	-2.2712090	0.1726950	-1.1848330
C	-2.2697240	1.1683210	-0.1391620
C	-2.2276310	0.4857870	1.1295230
C	-2.1678250	-0.9397360	0.8673830
C	-2.2980990	-2.4391230	-1.2834240
H	-1.8999840	-3.2675600	-0.6939080
H	-3.3510640	-2.6675760	-1.4890860
H	-1.7750590	-2.4186430	-2.2429840
C	-2.4117230	0.4328540	-2.6514620
H	-2.0045640	1.4067110	-2.9319320
H	-1.9064570	-0.3303520	-3.2474600
H	-3.4729080	0.4246120	-2.9339750
C	-2.4854070	2.6395660	-0.3422970
H	-2.1305300	3.2252150	0.5094850
H	-1.9886910	3.0057320	-1.2448050
H	-3.5556550	2.8513230	-0.4520510
C	-2.3100020	1.1215930	2.4821950
H	-1.7920200	0.5274070	3.2382310
H	-1.8755520	2.1237920	2.4857570
H	-3.3587520	1.2144470	2.7929730
C	-2.2238500	-2.0136550	1.9115240
H	-1.6673330	-1.7353340	2.8095810
H	-3.2639550	-2.1962020	2.2094210
H	-1.8233930	-2.9607190	1.5431750
H	0.5384470	-2.9430470	-0.8923550

Ir	-0.3421330	0.0229070	-0.0118550

5_7* (T_1)

G-gas = -990.267462 Hartree

Symbol	X	Y	Z
C	2.5771530	0.5773360	-0.1234250
N	1.3803120	1.2486490	-0.1672410
C	1.3973530	2.6003320	-0.1658690
C	2.5727500	3.3342720	-0.0970230
C	3.7942520	2.6565750	-0.0361870
C	3.7936780	1.2667150	-0.0609190
H	0.4306610	3.0836100	-0.2151140
H	2.5267390	4.4172400	-0.0951420
H	4.7298470	3.2037030	0.0114000
H	4.7231020	0.7088340	-0.0532930
C	1.8246670	-3.6015580	-0.1060530
C	3.0172500	-3.1377440	0.5162610
C	3.2994780	-1.7677920	0.4862550
C	2.4611570	-0.8695160	-0.1432590
N	1.2491150	-1.3314080	-0.8002060
C	0.9879140	-2.7459530	-0.7463370
H	1.5694490	-4.6557720	-0.0845950
H	3.6798370	-3.8274880	1.0240060
H	4.1670040	-1.3790390	1.0096050
H	0.0902790	-3.0478270	-1.2678870
C	-2.3518330	-0.9328750	-0.3451170
C	-2.4697420	0.3808990	-0.9188160
C	-2.1355970	1.3294380	0.1213220
C	-1.9422700	0.6015100	1.3638150
C	-2.0689110	-0.8001280	1.0694700
C	-2.6763280	-2.2181660	-1.0492290
H	-2.1872280	-3.0741250	-0.5780560
H	-3.7562170	-2.4068990	-1.0148980
H	-2.3853840	-2.1903690	-2.1030880
C	-2.8897780	0.7105880	-2.3172560
H	-2.4219410	1.6306280	-2.6757420
H	-2.6352060	-0.0899840	-3.0156910
H	-3.9775050	0.8545360	-2.3655750
C	-2.2425590	2.8205170	-0.0062080
H	-1.6553440	3.3385100	0.7563380
H	-1.9183270	3.1688890	-0.9907050
H	-3.2849650	3.1364680	0.1229900
C	-1.7348170	1.2096710	2.7172630
H	-1.1784100	0.5414140	3.3781420
H	-1.1870200	2.1530430	2.6571290

H	-2.7007720	1.4208360	3.1937050
C	-2.0051110	-1.9216920	2.0618480
H	-1.3891370	-1.6612490	2.9255340
H	-3.0101070	-2.1625300	2.4314570
H	-1.5923470	-2.8314300	1.6194340
H	1.2447480	-1.0257160	-1.7798010
Ir	-0.3316880	0.0560970	-0.1226140

5/**5*** (S_0/T_1)

E-gas = -990.531527770 Hartree

Symbol	X	Y	Z
C	-2.4629790	-0.6961430	-0.1723790
N	-1.2743270	-1.3674900	-0.6039100
C	-1.1409720	-2.7145910	-0.2966110
C	-2.2128820	-3.4984120	-0.0159290
C	-3.5087370	-2.8704060	0.1181020
C	-3.6125280	-1.5184980	0.1352820
H	-0.1486040	-3.1379920	-0.4206520
H	-2.0889700	-4.5650200	0.1220330
H	-4.3933440	-3.4872830	0.2249800
H	-4.5611370	-1.0347770	0.3601070
C	-2.2081900	3.4928590	-0.0105870
C	-3.5119330	2.8686680	0.1180980
C	-3.6081620	1.5175020	0.1391910
C	-2.4590960	0.6939560	-0.1679100
N	-1.2701010	1.3672160	-0.6540010
C	-1.1362240	2.7186190	-0.2967780
H	-2.0853450	4.5597180	0.1308200
H	-4.3948020	3.4866510	0.2233470
H	-4.5565760	1.0323370	0.3640940
H	-0.1457320	3.1440880	-0.4220870
C	2.1573810	1.1807400	0.6279040
C	2.2233130	0.7382470	-0.7358910
C	2.2210580	-0.7363230	-0.7350510
C	2.1700870	-1.1797720	0.6329240
C	2.1408550	-0.0039980	1.4583960
C	2.2610040	2.6035490	1.1054440
H	1.5468270	2.8265150	1.9017390
H	3.2638070	2.8108520	1.4949990
H	2.0868150	3.2991770	0.2833750
C	2.5685940	1.5828180	-1.9210010
H	2.2624270	1.1376270	-2.8695780
H	2.1497790	2.5890400	-1.8662360
H	3.6628010	1.6715870	-1.9318320
C	2.5671810	-1.5817830	-1.9200620

H	2.1472110	-2.5876650	-1.8670110
H	2.2640300	-1.1359830	-2.8694510
H	3.6614490	-1.6731210	-1.9296330
C	2.2632180	-2.6041150	1.1059870
H	1.5468950	-2.8257390	1.9008740
H	2.0882530	-3.2979560	0.2824530
H	3.2642340	-2.8156180	1.4969550
C	2.0640750	-0.0009710	2.9469460
H	1.5561920	-0.8929060	3.3247940
H	3.0787160	0.0009380	3.3682720
H	1.5544690	0.8910600	3.3228340
H	0.0430400	-0.0012390	-1.6532670
Ir	0.2098830	0.0131400	-0.1088100

5_1/**5_1*** (S_0/T_1)

E-gas = -990.533994954 Hartree

Symbol	X	Y	Z
C	-2.6459560	0.7020510	-0.1898630
N	-1.2881130	1.3190770	-0.2723490
C	-1.1960190	2.7526610	-0.2340600
C	-2.2629610	3.5387650	-0.1961120
C	-3.6111030	2.9367410	-0.2332170
C	-3.7836450	1.6111740	-0.2207010
H	-0.1954660	3.1607180	-0.2091780
H	-2.1677440	4.6187730	-0.1436830
H	-4.4712510	3.5913980	-0.1931980
H	-4.7816750	1.1889410	-0.1915580
C	-2.3028540	-3.4098270	-0.0226870
C	-3.6536670	-2.8227110	-0.0797760
C	-3.8197040	-1.4915290	-0.0374000
C	-2.6547150	-0.6046480	0.0212150
N	-1.3410300	-1.2048980	0.3265240
C	-1.2333570	-2.6039640	0.0784610
H	-2.1922840	-4.4838360	-0.0469980
H	-4.5048110	-3.4823660	-0.2096860
H	-4.7997880	-1.0468190	-0.1642310
H	-0.2562790	-3.0466900	0.1302220
C	2.1469770	-1.0241880	0.6165840
C	2.0016290	0.3506970	1.1362060
C	1.9535070	1.1541500	-0.1969590
C	2.5461800	0.2892150	-1.3262610
C	2.2290340	-1.0786400	-0.7820750
C	2.2290550	-2.1937440	1.5539340
H	1.8696560	-3.1298960	1.1156550
H	3.2840450	-2.3480250	1.8244650

H	1.6837520	-1.9916140	2.4821200
C	2.3996250	0.8720220	2.4903730
H	1.9935740	1.8798700	2.6323570
H	1.9756600	0.2483670	3.2869680
H	3.4897270	0.9207730	2.6249370
C	2.2181240	2.6357000	-0.2055710
H	1.8458910	3.1199500	-1.1092730
H	1.8360810	3.1651430	0.6695840
H	3.3084750	2.7520740	-0.2103640
C	4.0569610	0.3905620	-1.6380910
H	4.2918160	-0.3126070	-2.4406460
H	4.3460940	1.3839450	-1.9906110
H	4.6771750	0.1294650	-0.7747780
C	2.1144270	-2.2894180	-1.6440700
H	1.5500760	-2.0572640	-2.5547690
H	3.1042560	-2.6413130	-1.9650670
H	1.6229540	-3.1196860	-1.1335320
H	1.9964810	0.5198620	-2.2459050
Ir	0.1214950	0.1569560	0.3237720

5_2/**5_2*** (S_0/T_1)

E-gas = -990.586930563 Hartree

Symbol	X	Y	Z
Ir	0.3830000	-0.0463280	-0.1445760
N	-1.2889370	1.2939400	0.2005620
N	-1.2330890	-1.3108730	0.0487190
C	-1.5237860	2.3502770	0.8961230
H	-0.7311360	2.6937450	1.5578300
C	-2.7605320	3.0951170	0.8013900
H	-2.8932830	3.9821470	1.4107170
C	-3.7355730	2.6606940	-0.0889190
H	-4.6537930	3.2284960	-0.2084800
C	-3.5451190	1.4966070	-0.8186350
H	-4.2850860	1.1635370	-1.5400510
C	-2.2997520	0.7101840	-0.6779840
C	-2.4503960	-0.7336530	-0.1882940
C	-3.6421730	-1.4155020	0.0062260
H	-4.5896480	-0.9193690	-0.1732580
C	-3.6018040	-2.7519400	0.4098130
H	-4.5203360	-3.3161660	0.5311240
C	-2.3594280	-3.3497650	0.6334480
H	-2.2793600	-4.3845760	0.9489000
C	-1.2048940	-2.6059730	0.4494520
H	-0.2204050	-3.0240390	0.6158080
C	2.3971360	-0.2301650	1.0641940

C	2.5787520	-0.5981810	2.5044130
H	2.2257610	0.1938170	3.1705300
H	3.6394750	-0.7713590	2.7342790
H	2.0385240	-1.5145820	2.7620530
C	2.2766000	1.0799610	0.5156940
C	2.3108380	2.3639990	1.2923190
H	1.7698840	3.1623210	0.7762520
H	3.3456640	2.7084410	1.4172640
H	1.8835690	2.2473730	2.2934670
C	2.2143130	0.9863120	-0.9345090
C	2.2707380	2.1387260	-1.8949870
H	1.8067980	1.8835190	-2.8519440
H	3.3103990	2.4299780	-2.0971490
H	1.7574460	3.0211700	-1.5020200
C	2.2947570	-0.4090800	-1.2854570
C	2.4093880	-0.9703030	-2.6711580
H	1.9958120	-1.9802610	-2.7358890
H	3.4656530	-1.0262960	-2.9687350
H	1.8919570	-0.3471150	-3.4054740
C	2.3001240	-1.1631040	-0.0552650
C	2.4706580	-2.6507850	0.0548650
H	2.0444040	-3.0390340	0.9855710
H	3.5362210	-2.9151120	0.0571410
H	2.0046450	-3.1773940	-0.7831580
H	-1.7308100	0.6086390	-1.6477160

5_3/**5_3*** (S_0/T_1)

E-gas = -990.621099188 Hartree

Symbol	X	Y	Z
C	2.4665890	0.8041580	-0.0111780
N	1.2075660	1.3551020	-0.0136700
C	1.0920510	2.6964630	-0.0143710
C	2.1956580	3.5447460	-0.0096560
C	3.4772450	2.9938730	-0.0053690
C	3.6096000	1.6068990	-0.0070820
H	0.0841200	3.0895360	-0.0207000
H	2.0399120	4.6180240	-0.0096790
H	4.3566560	3.6282250	-0.0011500
H	4.5933260	1.1519950	-0.0046540
C	2.3237150	-3.4300680	-0.0050680
C	3.5831120	-2.8958940	-0.0045180
C	3.7740410	-1.4144740	-0.0084920
C	2.4872510	-0.6393560	-0.0115620
N	1.2626440	-1.2292950	-0.0129270
C	1.1891280	-2.6049400	-0.0096970

H	2.1771740	-4.5053920	-0.0027210
H	4.4647790	-3.5254490	-0.0015400
H	4.3834040	-1.1089680	0.8614280
H	0.1878410	-3.0103720	-0.0132710
C	-2.2005700	-1.1258310	-0.5835080
C	-2.2785330	0.1898200	-1.1841450
C	-2.2843060	1.1611630	-0.1194190
C	-2.2409520	0.4561130	1.1377310
C	-2.1824590	-0.9634430	0.8475940
C	-2.2906640	-2.4192710	-1.3382530
H	-1.9483730	-3.2686110	-0.7425690
H	-3.3333690	-2.6211410	-1.6126320
H	-1.7060050	-2.3934920	-2.2616540
C	-2.4149240	0.4748880	-2.6466580
H	-2.0152370	1.4573920	-2.9082610
H	-1.8982950	-0.2729810	-3.2528340
H	-3.4740990	0.4612550	-2.9352320
C	-2.4951110	2.6370760	-0.2931690
H	-2.1313080	3.2061450	0.5662570
H	-2.0060290	3.0177370	-1.1939970
H	-3.5657990	2.8539800	-0.3898520
C	-2.3292920	1.0673540	2.5013860
H	-1.8161420	0.4577440	3.2486930
H	-1.8908760	2.0678780	2.5259160
H	-3.3787910	1.1580740	2.8092900
C	-2.2192620	-2.0587580	1.8700330
H	-1.6761350	-1.7815270	2.7766100
H	-3.2564770	-2.2746260	2.1552530
H	-1.7872440	-2.9878660	1.4910710
H	4.3853620	-1.1136760	-0.8786980
Ir	-0.3570700	0.0012840	-0.0084330

5_4/5_4* (S_0/T_1)

E-gas = -990.560489050 Hartree

Symbol	X	Y	Z
C	2.4666520	0.7255140	-0.0010180
N	1.1367310	1.2668390	0.0117800
C	1.0423820	2.6679240	0.0461940
C	2.1053480	3.5112750	0.0238800
C	3.4309790	2.9753620	-0.0409320
C	3.5811330	1.6201260	-0.0569110
H	0.0289460	3.0403730	0.0919920
H	1.9408060	4.5837240	0.0527860
H	4.2945540	3.6311480	-0.0695810
H	4.5741410	1.1892900	-0.1047580

C	2.6750220	-3.4961250	-0.0276760
C	4.0129730	-2.8739250	0.0207860
C	3.9647860	-1.3734850	0.0273150
C	2.7069980	-0.6747800	0.0383710
N	1.5451850	-1.3994000	0.0681540
C	1.4950650	-2.7045910	0.0163380
H	2.5770960	-4.5779290	-0.0710730
H	4.5260760	-3.2962800	0.9097880
H	4.9046290	-0.8459290	0.0906530
H	0.5157320	-3.1720200	0.0216510
C	-2.3170620	-1.0194060	-0.7235610
C	-2.4632980	0.3167870	-1.1828310
C	-2.3756040	1.1863120	-0.0135940
C	-2.3946780	0.3167400	1.1809850
C	-2.3089950	-1.0212610	0.7363680
C	-2.3193870	-2.2473700	-1.5845340
H	-1.8076980	-3.0820050	-1.0970700
H	-3.3481390	-2.5767130	-1.7799890
H	-1.8384900	-2.0701690	-2.5503200
C	-2.6355790	0.7658710	-2.6006610
H	-2.1570840	1.7323560	-2.7838680
H	-2.2232270	0.0428480	-3.3094570
H	-3.7034600	0.8781140	-2.8328460
C	-2.6598380	2.6605110	-0.0040470
H	-2.2267880	3.1493140	0.8745330
H	-2.2660830	3.1531440	-0.8987170
H	-3.7426820	2.8454440	0.0223040
C	-2.5214610	0.7901350	2.5942320
H	-2.1187200	0.0644680	3.3054760
H	-2.0107200	1.7443090	2.7510200
H	-3.5817700	0.9392330	2.8432880
C	-2.2941990	-2.2422330	1.6089860
H	-1.7780800	-2.0607180	2.5561010
H	-3.3185160	-2.5597470	1.8442670
H	-1.8089110	-3.0891390	1.1154850
H	4.6042140	-3.2928030	-0.8170930
Ir	-0.4818200	0.1914550	-0.0547320

5_5/5_5* (S_0/T_1)

E-gas = -990.618464288 Hartree

Symbol	X	Y	Z
C	2.4721640	0.8447730	-0.0125640
N	1.2036280	1.3712340	-0.0156960
C	1.0565080	2.7110280	-0.0164540
C	2.1356190	3.5867770	-0.0111090

C	3.4298010	3.0635790	-0.0060160
C	3.5950400	1.6829330	-0.0076350
H	0.0384190	3.0756150	-0.0235950
H	1.9553370	4.6557410	-0.0112120
H	4.2947900	3.7180460	-0.0011850
H	4.5908760	1.2575930	-0.0043030
C	2.4253820	-3.4631730	-0.0054090
C	3.7161130	-2.7143660	-0.0062900
C	3.7335450	-1.3558820	-0.0100550
C	2.5274910	-0.5993710	-0.0130120
N	1.2860590	-1.2334970	-0.0147270
C	1.2332270	-2.5633810	-0.0114630
H	2.3720430	-4.1426440	0.8642100
H	4.6430970	-3.2785810	-0.0035340
H	4.6820230	-0.8324710	-0.0103040
H	0.2437550	-3.0008310	-0.0159110
C	-2.1903540	-1.1479890	-0.5623940
C	-2.2906440	0.1524690	-1.1858930
C	-2.2860380	1.1410960	-0.1364230
C	-2.2458400	0.4584170	1.1348310
C	-2.1734450	-0.9616280	0.8681790
C	-2.2716620	-2.4568880	-1.2915210
H	-1.9028140	-3.2889970	-0.6867670
H	-3.3148560	-2.6848260	-1.5421380
H	-1.7055930	-2.4374110	-2.2266730
C	-2.4446750	0.4134890	-2.6517350
H	-2.0541900	1.3942280	-2.9327820
H	-1.9289880	-0.3395970	-3.2522400
H	-3.5064010	0.3889620	-2.9310900
C	-2.5110390	2.6118860	-0.3348700
H	-2.1593570	3.1982140	0.5179690
H	-2.0195780	2.9838840	-1.2380740
H	-3.5830660	2.8165870	-0.4417510
C	-2.3420810	1.0951400	2.4869580
H	-1.8321620	0.5010730	3.2488240
H	-1.9040650	2.0960880	2.4949420
H	-3.3928880	1.1924040	2.7890460
C	-2.1983800	-2.0430410	1.9057860
H	-1.6761440	-1.7394910	2.8161520
H	-3.2331010	-2.2841630	2.1793370
H	-1.7364980	-2.9655810	1.5457840
H	2.3747800	-4.1496790	-0.8695760
Ir	-0.3487940	0.0011240	-0.0110430

5_6/5_6* (S_0/T_1)

E-gas = -990.584088326 Hartree

Symbol	X	Y	Z
C	2.5829910	0.8101550	0.0274940
N	1.3312570	1.3439900	-0.0232710
C	1.1766340	2.6775900	-0.0061720
C	2.2522340	3.5530590	0.0009540
C	3.5374490	3.0277270	-0.0108710
C	3.7063590	1.6381510	0.0100970
H	0.1492630	3.0218180	-0.0119270
H	2.0641100	4.6235600	0.0001920
H	4.3903840	3.6938900	-0.0244820
H	4.7140560	1.2465390	0.0072760
C	2.4751900	-3.4830690	0.0097780
C	3.7108650	-2.8721320	-0.0073730
C	3.8035180	-1.4820890	0.0196270
C	2.5912950	-0.6799050	0.0789710
N	1.4132050	-1.2188990	0.1710960
C	1.2419220	-2.6554640	0.0362950
H	2.3512430	-4.5645410	-0.0568880
H	4.6030860	-3.4937830	-0.0414290
H	4.7800420	-1.0088720	0.0338660
H	0.5157470	-3.0014820	0.7758160
C	-2.1760950	-1.1183730	-0.5648000
C	-2.3325550	0.1715280	-1.1936290
C	-2.2429550	1.1582330	-0.1619350
C	-2.2857040	0.4513870	1.1485750
C	-2.2704800	-0.9135010	0.8970210
C	-2.3558150	-2.4393930	-1.2686150
H	-1.9053760	-3.2532640	-0.6913960
H	-3.4182900	-2.6864020	-1.4122910
H	-1.8821240	-2.4244870	-2.2554450
C	-2.5200190	0.4289620	-2.6649820
H	-2.0961370	1.3943790	-2.9554970
H	-2.0257560	-0.3450640	-3.2568940
H	-3.5822570	0.4318400	-2.9558010
C	-2.5235000	2.6285930	-0.3423030
H	-2.1756420	3.2253300	0.5068870
H	-2.0723480	3.0296130	-1.2552530
H	-3.6045700	2.8046230	-0.4213350
C	-2.3574430	1.1159270	2.4873880
H	-1.8485840	0.5240470	3.2543040
H	-1.9078940	2.1145760	2.4866600
H	-3.4012580	1.2323560	2.8087020
C	-2.3014990	-2.0032900	1.9255000

H	-1.6996030	-1.7517830	2.8062560
H	-3.3334000	-2.1719720	2.2614130
H	-1.9321760	-2.9494370	1.5175480
H	0.6643820	-2.7570910	-0.9129880
Ir	-0.2788640	0.0561860	-0.4066530

2* (T_1)

G-gas = -1065.507690 Hartree

Symbol	X	Y	Z
C	2.5770990	0.5223470	0.0774000
N	1.4612770	1.2319010	-0.2254020
C	1.5200940	2.5762180	-0.2576680
C	2.6843140	3.2795840	0.0278200
C	3.8297970	2.5624200	0.3746490
C	3.7736890	1.1726320	0.3991110
H	0.5994070	3.0835700	-0.5212520
H	2.6848690	4.3626800	-0.0190330
H	4.7531720	3.0766720	0.6199200
H	4.6519500	0.5995680	0.6704050
C	1.9746150	-3.6532710	-0.2381410
C	3.2832380	-3.2008610	-0.0652670
C	3.5176870	-1.8340430	0.0558790
C	2.4358390	-0.9470390	0.0121230
N	1.1717870	-1.3995570	-0.1422600
C	0.9475860	-2.7154690	-0.2745550
H	1.7497980	-4.7083480	-0.3469970
H	4.1118750	-3.9008450	-0.0381170
H	4.5307990	-1.4655470	0.1618400
H	-0.0867570	-3.0095700	-0.4123790
C	-1.8354480	-1.0182510	1.4095400
C	-2.5283010	-1.0217840	0.1782630
C	-2.6615660	0.3598890	-0.2830660
C	-2.0528010	1.2201400	0.7140970
C	-1.4132650	0.3486030	1.6723470
C	-1.4873610	-2.1913880	2.2700390
H	-0.4118650	-2.2413740	2.4743280
H	-1.9891590	-2.1178830	3.2428880
H	-1.7918740	-3.1377260	1.8180390
C	-3.1341100	-2.1953970	-0.5302160
H	-2.9607760	-2.1428200	-1.6085660
H	-2.7400520	-3.1468590	-0.1657660
H	-4.2206530	-2.2120590	-0.3788850
C	-3.5268430	0.7925080	-1.4307730
H	-3.3049050	1.8170560	-1.7356250
H	-3.3795790	0.1516400	-2.3031720

H	-4.5858440	0.7463090	-1.1489570
C	-2.1980260	2.7101850	0.8235910
H	-1.3300660	3.1677380	1.3061880
H	-2.3325460	3.1778730	-0.1548720
H	-3.0763490	2.9610270	1.4314490
C	-0.7038080	0.7945890	2.9197470
H	-0.2031620	1.7554690	2.7778950
H	-1.4118320	0.9127410	3.7495380
H	0.0494490	0.0676900	3.2354530
Ir	-0.4600220	0.2012550	-0.4563320
O	-0.3586040	0.2590620	-2.4167660
H	0.5386320	0.4377520	-2.7385290

2/**2*** (S_0/T_1)

E-gas = -1065.83029340 Hartree

Symbol	X	Y	Z
C	2.5923740	0.5458390	0.0762310
N	1.4900310	1.2672790	-0.2450040
C	1.5655330	2.6103810	-0.2764340
C	2.7328930	3.3007620	0.0272630
C	3.8653520	2.5703280	0.3890890
C	3.7923840	1.1813040	0.4127270
H	0.6535130	3.1277300	-0.5517610
H	2.7443890	4.3843660	-0.0156250
H	4.7920180	3.0732100	0.6466390
H	4.6603910	0.5973490	0.6955220
C	1.9421550	-3.6231870	-0.2264930
C	3.2560840	-3.1834170	-0.0645630
C	3.5037580	-1.8195050	0.0604520
C	2.4318300	-0.9214610	0.0174750
N	1.1619170	-1.3609490	-0.1311820
C	0.9239460	-2.6756260	-0.2545460
H	1.7059580	-4.6763750	-0.3341350
H	4.0790880	-3.8908750	-0.0477280
H	4.5212020	-1.4609170	0.1651380
H	-0.1146690	-2.9605540	-0.3775510
C	-1.8364740	-1.0458880	1.4000920
C	-2.5405900	-1.0533560	0.1830100
C	-2.6457430	0.3242140	-0.3008830
C	-2.0336640	1.1918920	0.6937560
C	-1.3891050	0.3219340	1.6461160
C	-1.5034510	-2.2083130	2.2801900
H	-0.4275740	-2.2652700	2.4871170
H	-2.0057180	-2.1103270	3.2519170
H	-1.8196560	-3.1606640	1.8464910

C	-3.1615010	-2.2240620	-0.5163920
H	-2.9826330	-2.1848140	-1.5959310
H	-2.7869170	-3.1797370	-0.1396420
H	-4.2500370	-2.2209880	-0.3713510
C	-3.5305820	0.7621400	-1.4332480
H	-3.3090400	1.7870660	-1.7415780
H	-3.4097340	0.1221750	-2.3115470
H	-4.5844620	0.7228460	-1.1281280
C	-2.2036910	2.6792320	0.8198080
H	-1.3432060	3.1436310	1.3110160
H	-2.3413460	3.1564520	-0.1544540
H	-3.0882090	2.9113080	1.4284020
C	-0.6905930	0.7715330	2.8992110
H	-0.1975550	1.7387620	2.7650920
H	-1.4083360	0.8803970	3.7232410
H	0.0673100	0.0509810	3.2217980
Ir	-0.4397980	0.2467370	-0.4904280
O	-0.3346330	0.3107330	-2.4459920
H	0.5581900	0.5347260	-2.7632420

c) Hydride transfer in triplet state

TS(5-(5_1))*

G-gas = -990.252131 Hartree

Symbol	X	Y	Z
C	-2.5542160	0.7101260	-0.0503640
N	-1.2917400	1.3062510	-0.0400190
C	-1.1885120	2.6620130	-0.0351140
C	-2.2810440	3.4940940	-0.0421920
C	-3.5766500	2.9097520	-0.0556500
C	-3.7017200	1.5405390	-0.0579300
H	-0.1805770	3.0569910	-0.0253560
H	-2.1433790	4.5683620	-0.0384080
H	-4.4604350	3.5386680	-0.0631090
H	-4.6844800	1.0837760	-0.0646990
C	-2.2811420	-3.4940400	-0.0422070
C	-3.5767320	-2.9096630	-0.0555640
C	-3.7017690	-1.5404490	-0.0578150
C	-2.5542410	-0.7100700	-0.0503610
N	-1.2917890	-1.3062290	-0.0401320
C	-1.1885870	-2.6619830	-0.0351940
H	-2.1435030	-4.5683110	-0.0384540
H	-4.4605300	-3.5385600	-0.0629430
H	-4.6845170	-1.0836610	-0.0644530
H	-0.1806570	-3.0569700	-0.0254570

C	2.2032480	-0.7329830	1.0235460
C	2.2033210	0.7329070	1.0235660
C	2.2331110	1.1787430	-0.3251420
C	2.2712290	-0.0000220	-1.2241480
C	2.2330380	-1.1787940	-0.3251760
C	2.2892090	-1.5940820	2.2481410
H	1.8794080	-2.5903630	2.0731730
H	3.3382430	-1.7129020	2.5456680
H	1.7535990	-1.1535300	3.0913340
C	2.2893320	1.5939580	2.2481860
H	1.8797210	2.5903160	2.0732100
H	1.7535790	1.1534810	3.0913260
H	3.3383630	1.7125880	2.5458000
C	2.3772500	2.5883130	-0.8124780
H	1.7456030	2.7841000	-1.6835950
H	2.1322760	3.3168370	-0.0374810
H	3.4163730	2.7722750	-1.1120940
C	2.8928030	-0.0000090	-2.6023360
H	2.6072180	-0.8853260	-3.1737360
H	2.6071780	0.8852910	-3.1737430
H	3.9851230	0.0000180	-2.4977870
C	2.3771230	-2.5883530	-0.8125490
H	1.7454340	-2.7841020	-1.6836430
H	3.4162270	-2.7723350	-1.1122170
H	2.1321770	-3.3168900	-0.0375570
H	0.8298860	0.0000300	-1.6052770
Ir	0.2840530	0.0000010	0.0244840

TS(5-(5_2))*

G-gas = -1179.995006 Hartree

Symbol	X	Y	Z
C	-2.2851950	0.9440490	-0.5095650
N	-1.0208730	1.4396720	-0.3158820
C	-0.8275180	2.7774430	-0.2831730
C	-1.8583110	3.6886160	-0.4374030
C	-3.1541480	3.1968300	-0.6442820
C	-3.3667770	1.8278620	-0.6798530
H	0.1939460	3.1004720	-0.1330720
H	-1.6503870	4.7512610	-0.4017480
H	-3.9867530	3.8792450	-0.7825210
H	-4.3619370	1.4351360	-0.8486890
C	-2.2695050	-3.2454080	-1.0750860
C	-3.5165850	-2.5755170	-1.1437940
C	-3.5828470	-1.2326250	-0.8747060
C	-2.4012520	-0.5108070	-0.4440230

N	-1.1467180	-1.1888000	-0.5218580
C	-1.1293390	-2.5002130	-0.7843590
H	-2.1807100	-4.3050470	-1.2791220
H	-4.4130940	-3.1187270	-1.4244710
H	-4.5314840	-0.7107140	-0.9272470
H	-0.1523630	-2.9685930	-0.7774340
C	2.3816580	-1.2085500	-0.5247820
C	2.2613370	-0.9247130	0.8843020
C	2.3479460	0.5147860	1.0502880
C	2.5069070	1.0951960	-0.2587760
C	2.6127900	0.0280910	-1.2248300
C	2.4820310	-2.5734700	-1.1417200
H	1.9738160	-2.6256710	-2.1085240
H	3.5342880	-2.8312150	-1.3114120
H	2.0662210	-3.3467080	-0.4916440
C	2.2470580	-1.9388510	1.9899000
H	1.7595910	-1.5537270	2.8878620
H	1.7294170	-2.8545430	1.6943010
H	3.2730340	-2.2157170	2.2633890
C	2.4268390	1.2479000	2.3565130
H	2.0344700	2.2643690	2.2757550
H	1.8706250	0.7371510	3.1450360
H	3.4714510	1.3242070	2.6841190
C	2.7740620	2.5437270	-0.5507220
H	2.3149370	2.8654610	-1.4896120
H	2.4150820	3.1947010	0.2500110
H	3.8533600	2.7159400	-0.6402460
C	2.8731810	0.1814960	-2.6892050
H	2.5144400	1.1419310	-3.0672480
H	3.9516460	0.1337260	-2.8933070
H	2.3972750	-0.6113270	-3.2716710
H	-0.3005520	-0.1917280	1.7641460
Ir	0.4872390	0.0203210	-0.1356140
C	-1.8606780	-0.5014200	3.0197610
O	-0.6248980	-0.2756020	2.7875540
O	-2.7965330	-0.6518990	2.1927220
H	-2.1231360	-0.5682010	4.0800470
H	-2.5959170	-0.5490160	1.0606240

TS(5-(5_3))*

G-gas = -1219.511167 Hartree

Symbol	X	Y	Z
Ir	0.7025430	0.0126490	-0.1275190
N	-1.2227510	-0.3323070	-0.8361080
N	-0.1656590	1.8883800	0.0563310

H	-0.6175770	-0.6225490	1.7501380
C	-1.6802560	-1.4992260	-1.3852470
H	-0.9509030	-2.2964710	-1.4517100
C	-2.9612110	-1.6682010	-1.8366170
H	-3.2542980	-2.6175540	-2.2709920
C	-3.9290640	-0.5971810	-1.6780530
H	-4.8123890	-0.5926850	-2.3177330
C	-3.3763820	0.6664900	-1.2882170
H	-4.0085030	1.5481890	-1.3107680
C	-2.0779310	0.7709980	-0.8424870
C	-1.4677870	2.0076840	-0.3544630
C	-2.1153940	3.2484450	-0.2887010
H	-3.1426630	3.3382190	-0.6203160
C	-1.4419730	4.3643570	0.1907390
H	-1.9425480	5.3259680	0.2371540
C	-0.1146020	4.2289170	0.6081270
H	0.4515190	5.0709770	0.9889940
C	0.4811590	2.9803730	0.5233060
H	1.5060180	2.8209260	0.8300850
C	2.8344470	-0.4373790	-1.0227770
C	3.4101080	0.1018780	-2.2945590
H	2.8268450	-0.2073880	-3.1651790
H	4.4353900	-0.2652430	-2.4390020
H	3.4542230	1.1938890	-2.2898110
C	2.0711480	-1.6468700	-0.8810110
C	1.7942650	-2.6196260	-1.9902730
H	1.0157370	-3.3367570	-1.7207950
H	2.6968740	-3.1996000	-2.2180650
H	1.4868060	-2.1130310	-2.9090540
C	1.7875170	-1.8500840	0.5225280
C	1.1854830	-3.0799170	1.1377130
H	0.6232190	-2.8427910	2.0439360
H	1.9696860	-3.7990840	1.4066590
H	0.5057230	-3.5852060	0.4468110
C	2.3470750	-0.7321200	1.2490590
C	2.4115190	-0.6002580	2.7415770
H	2.4843220	0.4447800	3.0537460
H	3.2961440	-1.1190440	3.1334790
H	1.5337110	-1.0385840	3.2223560
C	2.9335090	0.1666090	0.2847340
C	3.7422080	1.3908760	0.6057820
H	3.6615330	2.1495830	-0.1778510
H	4.8041490	1.1331500	0.6990300
H	3.4402170	1.8433810	1.5542400

O	-1.1306930	-0.8396620	2.5688290
H	-2.6698450	-1.3504950	2.4570820
H	-0.9713380	-0.1048880	3.1753890
O	-3.5978110	-1.7274190	2.4626600
H	-3.5318540	-2.6299380	2.7994950
H	-4.4227090	-1.5926460	1.3602480
O	-5.1134690	-1.5027840	0.5415290
H	-4.6365900	-1.0692990	-0.3924040
H	-5.8750840	-0.9679880	0.8111390

TS(5-(5_4))*

G-gas = -1143.084022 Hartree

Symbol	X	Y	Z
Ir	0.5215310	0.0630350	-0.1258020
N	-1.3230480	-0.6350880	-0.7778090
N	-0.6520100	1.7798290	-0.0196370
H	-0.7291560	-0.9141050	1.6123710
C	-1.6023640	-1.8940150	-1.2386060
H	-0.7416110	-2.4888200	-1.5188370
C	-2.8765960	-2.3851290	-1.3322160
H	-3.0439430	-3.3905690	-1.7009160
C	-3.9811010	-1.5733120	-0.8570410
H	-5.0013960	-1.8727450	-1.0840920
C	-3.6945830	-0.1879610	-0.6663680
H	-4.5097150	0.5098420	-0.5019240
C	-2.3897760	0.2522240	-0.5979400
C	-1.9853460	1.6214490	-0.2955590
C	-2.8460640	2.7274260	-0.2785410
H	-3.8928550	2.5979890	-0.5265430
C	-2.3518710	3.9885860	0.0287910
H	-3.0153020	4.8472830	0.0377520
C	-0.9901970	4.1364050	0.3111220
H	-0.5600040	5.1020020	0.5499210
C	-0.1800540	3.0114880	0.2717230
H	0.8806010	3.0694300	0.4770900
C	2.7282520	0.0676470	-0.9269390
C	3.2494570	0.8073980	-2.1194330
H	2.7823070	0.4632390	-3.0451310
H	4.3324010	0.6548730	-2.2208910
H	3.0804080	1.8841420	-2.0377340
C	2.2009510	-1.2674210	-0.9219990
C	2.1383640	-2.1767480	-2.1138920
H	1.4474130	-3.0082780	-1.9577140
H	3.1251310	-2.6142890	-2.3098560
H	1.8277450	-1.6436370	-3.0161870

C	1.8870860	-1.6276250	0.4449490
C	1.4880760	-2.9934870	0.9252770
H	0.8877190	-2.9437470	1.8367960
H	2.3765590	-3.5992950	1.1425430
H	0.9044890	-3.5313440	0.1741630
C	2.2251350	-0.5028220	1.2875960
C	2.2107070	-0.4852040	2.7865770
H	2.0372140	0.5207580	3.1777060
H	3.1761610	-0.8265870	3.1826690
H	1.4420600	-1.1476450	3.1926030
C	2.6694220	0.5661430	0.4295560
C	3.2336580	1.8774620	0.8961150
H	3.1350610	2.6574240	0.1358800
H	4.3038390	1.7786090	1.1151910
H	2.7480940	2.2273850	1.8112940
O	-1.2979650	-1.2674490	2.3544270
H	-1.2625300	-0.6021690	3.0548440
H	-2.5803650	-1.8315710	1.9891140
O	-3.4887270	-2.2883310	1.7049500
H	-4.1916210	-2.1041700	2.3462460
H	-3.7965700	-1.9896690	0.6784490

TS(5-(5_5))*

G-gas = -1143.092629 Hartree

Symbol	X	Y	Z
Ir	0.4858830	0.0651160	-0.1195130
N	-1.3749700	-0.6705730	-0.6426580
N	-0.6913570	1.7662680	0.0689890
H	-0.5733880	-0.7895010	1.7612170
C	-1.6553150	-1.9443880	-0.8956210
H	-0.8058700	-2.6165780	-0.9486480
C	-2.9777340	-2.4527320	-0.9692510
H	-3.1183410	-3.4614720	-1.3480700
C	-4.0250410	-1.4664710	-1.1268030
H	-5.0323330	-1.7812870	-1.3807520
C	-3.7409250	-0.1428320	-0.9315740
H	-4.5233030	0.6013970	-1.0251420
C	-2.4157540	0.2724870	-0.6034730
C	-2.0274790	1.5983820	-0.2449910
C	-2.9015250	2.7089100	-0.1842190
H	-3.9476540	2.5828680	-0.4354170
C	-2.4224520	3.9510380	0.1879250
H	-3.0944940	4.8022480	0.2300290
C	-1.0629620	4.1007480	0.5083430
H	-0.6483370	5.0562200	0.8060100

C	-0.2439870	2.9843170	0.4321000
H	0.8107390	3.0442650	0.6660790
C	2.5953840	0.0319330	-1.1425900
C	2.9660770	0.6444690	-2.4567910
H	2.3620420	0.2437970	-3.2744680
H	4.0183310	0.4359870	-2.6929740
H	2.8435700	1.7300910	-2.4480550
C	2.1003200	-1.3054330	-0.9387030
C	1.9432140	-2.3356820	-2.0186170
H	1.3054080	-3.1653570	-1.7050350
H	2.9188700	-2.7640490	-2.2784880
H	1.5175940	-1.9070300	-2.9296180
C	1.9564380	-1.5281050	0.4811050
C	1.6687270	-2.8427450	1.1467450
H	1.1405970	-2.7132710	2.0945070
H	2.6040260	-3.3763670	1.3569620
H	1.0635340	-3.4960360	0.5128450
C	2.3230940	-0.3026000	1.1591720
C	2.4540270	-0.1226930	2.6419210
H	2.2923700	0.9162370	2.9396460
H	3.4619660	-0.4042900	2.9735280
H	1.7433570	-0.7464570	3.1896330
C	2.6643490	0.6698140	0.1493470
C	3.2369830	2.0332840	0.4085100
H	2.9754090	2.7439480	-0.3801930
H	4.3317170	1.9814250	0.4486020
H	2.9016730	2.4427170	1.3650030
O	-1.1081600	-1.1892230	2.5112860
H	-1.3165030	-0.4623800	3.1144700
H	-2.1558660	-2.0489090	2.0993450
O	-2.8811430	-2.7503810	1.7461930
H	-3.7416920	-2.6276750	2.1753150
H	-2.9803560	-2.6976940	0.6567910

TS(5-(5_6))*

G-gas = -1219.504587 Hartree

Symbol	X	Y	Z
C	-2.2411410	1.0049030	-0.7586480
N	-1.0214390	1.4817390	-0.3580560
C	-0.8713780	2.8125010	-0.1543380
C	-1.9001480	3.7195990	-0.3410100
C	-3.1472220	3.2453360	-0.7611580
C	-3.3108290	1.8817050	-0.9681560
H	0.1127490	3.1297070	0.1625220
H	-1.7233190	4.7747760	-0.1661550

H	-3.9738960	3.9282680	-0.9268240
H	-4.2651870	1.4919570	-1.2998480
C	-2.2040780	-3.1915960	-1.3099280
C	-3.3796710	-2.5354950	-1.5768860
C	-3.4436370	-1.1244350	-1.3424630
C	-2.3025410	-0.4516470	-0.9368650
N	-1.1192690	-1.0871980	-0.6841050
C	-1.0936800	-2.5094660	-0.7244250
H	-2.1092770	-4.2585470	-1.4941540
H	-4.2409800	-3.0609360	-1.9737710
H	-4.3615170	-0.5847940	-1.5370470
H	-0.0998740	-2.9302650	-0.8472600
C	2.2666940	-0.9573020	0.7388510
C	2.3325580	0.4437200	1.1072860
C	2.4942090	1.2080280	-0.1028510
C	2.6036460	0.2913990	-1.2113540
C	2.4073350	-1.0385170	-0.6949790
C	2.2630680	-2.1170470	1.6924290
H	1.7707650	-2.9944850	1.2667310
H	3.2921870	-2.4071140	1.9405710
H	1.7546760	-1.8735210	2.6278860
C	2.3757490	0.9813190	2.5072390
H	3.4077620	0.9895780	2.8812470
H	2.0027090	2.0074100	2.5574610
H	1.7813980	0.3730470	3.1929690
C	2.7377150	2.6873950	-0.1845950
H	2.2838740	3.1287830	-1.0764450
H	2.3518390	3.2129640	0.6927370
H	3.8138150	2.8932910	-0.2317840
C	2.8761170	0.6502460	-2.6384400
H	3.9546080	0.6128660	-2.8440000
H	2.3878850	-0.0422120	-3.3285280
H	2.5342870	1.6605120	-2.8759370
C	2.5383540	-2.2976100	-1.5013630
H	2.0425680	-2.2152230	-2.4721620
H	3.5974020	-2.5143760	-1.6882220
H	2.1227700	-3.1615700	-0.9787540
H	-0.3152350	-0.3576220	1.9033830
Ir	0.5043700	0.0995790	-0.1910110
O	-0.7243180	-0.7683430	2.7254710
H	-1.0749600	-1.8897720	2.3971490
H	-1.4337850	-0.1574400	3.0633280
O	-1.2871270	-2.9816900	1.9673980
H	-2.1462150	-3.3506140	2.2206010

H	-1.2491120	-2.9155180	0.9007330
O	-2.5271140	0.9607420	3.6479830
H	-2.2923440	1.3916340	4.4802570
H	-3.4753790	0.7859380	3.6994130

TS(5-(5_7))*

G-gas = -1066.659987 Hartree

Symbol	X	Y	Z
C	-2.5012270	0.7514940	-0.0811190
N	-1.2585480	1.3433560	0.0530750
C	-1.1639290	2.6918440	0.0899400
C	-2.2609320	3.5259910	-0.0174090
C	-3.5336070	2.9417350	-0.1667260
C	-3.6510790	1.5662510	-0.1919870
H	-0.1616070	3.0857540	0.2018000
H	-2.1285650	4.6007750	0.0133340
H	-4.4179680	3.5652540	-0.2489390
H	-4.6261800	1.1018180	-0.2793590
C	-2.2064810	-3.4549610	-0.2678410
C	-3.4408680	-2.8502970	-0.6539450
C	-3.5636630	-1.4774410	-0.5707210
C	-2.5058020	-0.6827740	-0.0971970
N	-1.3053420	-1.2914790	0.3636090
C	-1.1921360	-2.6742750	0.1969420
H	-2.0673420	-4.5280890	-0.3353590
H	-4.2551670	-3.4554620	-1.0352250
H	-4.4692010	-0.9933590	-0.9200740
H	-0.2462400	-3.0928390	0.5194340
C	2.3973320	-0.7223860	0.6622300
C	2.4235400	0.7305990	0.6584480
C	2.2049530	1.1686960	-0.7012710
C	2.1179310	0.0090730	-1.5472920
C	2.1539490	-1.1536410	-0.6912760
C	2.7420360	-1.6055040	1.8255340
H	2.2581850	-2.5822020	1.7520170
H	3.8248240	-1.7787420	1.8627240
H	2.4476960	-1.1600760	2.7786600
C	2.8007150	1.6080110	1.8148910
H	3.8827550	1.7914460	1.8134010
H	2.3047680	2.5805730	1.7682660
H	2.5491530	1.1477780	2.7732290
C	2.2688860	2.5877580	-1.1862110
H	1.5578200	2.7767160	-1.9949090
H	2.0718280	3.3025590	-0.3838480
H	3.2714300	2.8086950	-1.5718080

C	1.9777840	0.0028490	-3.0362410
H	1.4083610	-0.8613530	-3.3869420
H	1.4861060	0.9070720	-3.4030410
H	2.9671920	-0.0450980	-3.5113230
C	2.1437410	-2.5723770	-1.1804380
H	1.9879820	-3.2830460	-0.3664930
H	1.3653650	-2.7390340	-1.9298370
H	3.1075100	-2.8162550	-1.6430670
H	-1.1620270	-1.0451950	1.8971310
Ir	0.3663880	0.0392240	0.0836150
O	-0.6597290	-0.6192400	2.7414080
H	0.0272160	-0.0900800	2.0127190
H	-1.2375270	0.0290940	3.1812750

d) H_2 generation in triplet state

5* + $H_2O \rightarrow$ **2* +** H_2

TS(5-2)*

G-gas = -1219.469782 Hartree

Symbol	X	Y	Z
C	2.7413680	-0.4188590	-0.3271570
N	1.7569570	-1.2708740	0.0113400
C	2.0610010	-2.5325120	0.3351000
C	3.3637190	-3.0260290	0.3101970
C	4.3910560	-2.1557660	-0.0526620
C	4.0806920	-0.8356610	-0.3653270
H	1.2289330	-3.1634930	0.6278990
H	3.5616450	-4.0591620	0.5739940
H	5.4218860	-2.4942250	-0.0783040
H	4.8744410	-0.1418060	-0.6132170
C	1.4964310	3.5868610	-0.9638840
C	2.7874660	3.2315090	-1.3511270
C	3.2025960	1.9181210	-1.1632290
C	2.3288590	0.9778760	-0.6020180
N	1.0612840	1.3290570	-0.2636250
C	0.6645230	2.6092900	-0.4317680
H	1.1272950	4.6001250	-1.0768150
H	3.4599930	3.9612600	-1.7901180
H	4.1995100	1.6210840	-1.4634880
H	-0.3456560	2.8214890	-0.1000670
C	-2.0929320	0.2203800	-1.7967520
C	-2.9689020	0.1618650	-0.7174780
C	-2.5620580	-0.9928880	0.1140590
C	-1.6188080	-1.7816790	-0.6417270
C	-1.1928790	-0.9462610	-1.7390330

C	-2.0352240	1.2596300	-2.8733190
H	-1.0291690	1.6815110	-2.9707310
H	-2.2916360	0.8247270	-3.8469450
H	-2.7253100	2.0828590	-2.6808840
C	-3.9846690	1.1787680	-0.3137750
H	-4.8461820	0.7157730	0.1763510
H	-3.5378410	1.8940860	0.3897970
H	-4.3526280	1.7443280	-1.1729050
C	-3.3443330	-1.4792690	1.3012180
H	-2.7810440	-2.2109450	1.8833920
H	-3.6183090	-0.6594410	1.9709250
H	-4.2774750	-1.9544650	0.9730000
C	-1.3288450	-3.2401600	-0.4434350
H	-0.4022470	-3.5428990	-0.9349160
H	-1.2675580	-3.5058190	0.6150630
H	-2.1377810	-3.8375470	-0.8827900
C	-0.2920890	-1.3567960	-2.8679500
H	0.4657470	-2.0717120	-2.5418460
H	-0.8745320	-1.8295320	-3.6692310
H	0.2214680	-0.4958240	-3.3043280
H	-0.0535730	-0.7651720	1.8412860
Ir	-0.5069780	-0.0928830	0.2398310
O	-1.2347370	1.6176820	1.4087830
H	0.1409190	-0.4929110	2.7181240
H	-1.9774700	1.2992740	1.9395930
O	0.2032250	2.3421760	3.4261500
H	0.9630590	2.8922360	3.2037910
H	-0.3262410	2.1767890	2.5744390
O	0.3664070	-0.1017700	3.9595280
H	1.2317950	-0.4111290	4.2633970
H	0.3965840	0.9300790	3.8592970

TS(5a-2)*

G-gas = -1219.463438 Hartree

Symbol	X	Y	Z
C	-2.8052400	-0.3343000	0.1465630
N	-1.8737970	-1.2959760	0.0063880
C	-2.2525610	-2.5345460	-0.3339420
C	-3.5843210	-2.8891610	-0.5306020
C	-4.5577830	-1.9013440	-0.3880250
C	-4.1654160	-0.6093370	-0.0529920
H	-1.4598980	-3.2637720	-0.4551470
H	-3.8428790	-3.9073830	-0.7993730
H	-5.6065040	-2.1281420	-0.5504850
H	-4.9052080	0.1777580	0.0206000

C	-1.3347090	3.5470710	0.9853550
C	-2.6798840	3.2886510	1.2247130
C	-3.1666090	2.0127370	0.9644150
C	-2.3108910	1.0196840	0.4790830
N	-0.9896760	1.2746460	0.2917580
C	-0.5229420	2.5184760	0.5203270
H	-0.9014830	4.5264060	1.1536210
H	-3.3408200	4.0612150	1.6038980
H	-4.2079820	1.7832950	1.1507720
H	0.5240530	2.7022500	0.3108180
C	2.2007380	0.0739390	1.2880670
C	2.9194430	-0.3062130	0.1216470
C	2.3278340	-1.5475310	-0.3542490
C	1.4457370	-2.0551240	0.6685340
C	1.2784580	-1.0048740	1.6432170
C	2.4620310	1.3022650	2.1034960
H	1.6218050	1.5428110	2.7583830
H	3.3343440	1.1303340	2.7474310
H	2.6762460	2.1658900	1.4683560
C	4.0149370	0.4681580	-0.5358810
H	4.1856860	0.1344730	-1.5624660
H	3.8074020	1.5423790	-0.5408170
H	4.9568630	0.3137560	0.0078880
C	2.8093170	-2.3289090	-1.5432290
H	2.0484580	-3.0236280	-1.9051770
H	3.0847570	-1.6739980	-2.3730830
H	3.6987120	-2.9136730	-1.2786040
C	0.9388420	-3.4602480	0.7753560
H	0.0099420	-3.5204950	1.3457070
H	0.7808620	-3.9163860	-0.2051420
H	1.6813700	-4.0764860	1.2988270
C	0.5358430	-1.1173870	2.9422970
H	-0.3320980	-1.7741930	2.8514340
H	1.1890850	-1.5301400	3.7207970
H	0.1842100	-0.1435420	3.2905730
H	-0.3104840	-0.5929190	-1.8812280
Ir	0.4053170	-0.2546910	-0.2770990
O	1.0500580	1.4420980	-1.9502240
H	0.0371820	0.1941410	-2.0332950
H	1.7391500	1.0347010	-2.4972800
O	-1.5954950	2.0660660	-2.6288580
H	-1.7966580	2.4556900	-3.4877430
H	-0.6218060	2.0515500	-2.5733530
O	2.3974260	3.3245930	-0.5355930

H	1.9307670	2.7314340	-1.1720970
H	2.5369830	4.1630940	-0.9917440

TS(5a-2)'*

G-gas = -1219.469161 Hartree

Symbol	X	Y	Z
C	2.9126060	-0.3083670	0.2340140
N	1.9189860	-1.2157280	0.2354350
C	2.1987280	-2.4970370	0.5007300
C	3.4918280	-2.9523630	0.7476770
C	4.5316170	-2.0240020	0.7332250
C	4.2401750	-0.6862790	0.4836640
H	1.3549470	-3.1775370	0.5212030
H	3.6703430	-4.0018500	0.9541790
H	5.5533150	-2.3317840	0.9310730
H	5.0327580	0.0511220	0.5114550
C	1.6921210	3.7295010	-0.2015900
C	3.0434510	3.4315260	-0.3604500
C	3.4525770	2.1078300	-0.2414840
C	2.5137540	1.1026560	0.0201860
N	1.1926020	1.4023690	0.1237910
C	0.7994070	2.6903450	0.0334170
H	1.3227110	4.7470050	-0.2630020
H	3.7679980	4.2124330	-0.5673030
H	4.4980840	1.8539160	-0.3622750
H	-0.2599370	2.8498670	0.1965860
C	-1.6303250	0.4758610	-1.9300330
C	-2.6831560	0.0895430	-1.0830510
C	-2.2997970	-1.1920050	-0.4783590
C	-1.1614040	-1.7077960	-1.1975740
C	-0.6575860	-0.6237620	-2.0079030
C	-1.5231400	1.7474670	-2.7137810
H	-0.4975720	2.1269970	-2.7276130
H	-1.8177380	1.5790020	-3.7572520
H	-2.1697750	2.5291410	-2.3099960
C	-3.9183780	0.8573220	-0.7446510
H	-4.1743460	0.7589680	0.3141270
H	-3.8226590	1.9184360	-0.9860830
H	-4.7723380	0.4681760	-1.3157960
C	-3.1799830	-1.9854240	0.4434660
H	-2.6364860	-2.8170190	0.8968460
H	-3.5854720	-1.3640950	1.2460940
H	-4.0220880	-2.4067160	-0.1208580
C	-0.7299930	-3.1423360	-1.2485550
H	0.3089240	-3.2481330	-1.5664400

H	-0.8560550	-3.6434790	-0.2854950
H	-1.3491390	-3.6825440	-1.9761470
C	0.4353850	-0.7161500	-3.0326650
H	1.2073550	-1.4287510	-2.7352520
H	0.0270540	-1.0491140	-3.9952300
H	0.9151040	0.2517170	-3.1990170
H	-0.0841400	-0.8905170	1.7777460
Ir	-0.3727240	-0.1006050	0.1395870
O	-1.3833510	1.5085890	1.3628230
H	-0.3501590	-0.4316990	2.4691640
H	-2.3409690	1.3437460	1.4001870
O	-0.9802710	0.4306440	3.4834990
H	-0.3659390	0.8145470	4.1235020
H	-1.1093850	1.0921570	2.6107720
O	-3.6881420	0.4151340	2.7310880
H	-2.9119430	0.2865560	3.3076550
H	-4.3670560	0.8154020	3.2874300

TS(5b-2)*

G-gas = -1143.046934 Hartree

Symbol	X	Y	Z
C	2.6353750	-0.6982770	-0.1599410
N	1.5531990	-1.4524000	0.1094450
C	1.7066630	-2.7439760	0.4238150
C	2.9514360	-3.3668390	0.4609090
C	4.0795450	-2.6007380	0.1713760
C	3.9231110	-1.2523470	-0.1348970
H	0.8006640	-3.2916040	0.6586980
H	3.0285760	-4.4172560	0.7188010
H	5.0708170	-3.0415120	0.1983900
H	4.7956470	-0.6404690	-0.3256660
C	1.8560480	3.4283270	-0.7522010
C	3.1234090	2.9483070	-1.0672260
C	3.3877700	1.5942030	-0.8928980
C	2.3859480	0.7376510	-0.4255930
N	1.1402970	1.2129170	-0.1725010
C	0.8950170	2.5309220	-0.3039980
H	1.6056580	4.4791080	-0.8425020
H	3.8986190	3.6143240	-1.4316920
H	4.3703330	1.2041930	-1.1253040
H	-0.0943370	2.8508270	-0.0031810
C	-2.0356800	0.4796870	-1.4409010
C	-2.9329230	0.4615140	-0.3410780
C	-2.7061200	-0.7950320	0.3563440
C	-1.8955290	-1.6493780	-0.4813560

C	-1.4071870	-0.8331820	-1.5664590
C	-1.8739580	1.6084700	-2.4130340
H	-0.8804460	1.6182560	-2.8664360
H	-2.6020750	1.5064250	-3.2276360
H	-2.0454250	2.5771630	-1.9379440
C	-3.7819860	1.6013500	0.1225760
H	-4.5711280	1.2623770	0.7981330
H	-3.1769360	2.3479410	0.6517380
H	-4.2623030	2.1008540	-0.7241290
C	-3.4589800	-1.2434210	1.5758270
H	-2.9427770	-2.0533590	2.0949010
H	-3.6027860	-0.4260390	2.2865080
H	-4.4534240	-1.6093810	1.2919570
C	-1.7618500	-3.1364820	-0.3454640
H	-0.8840710	-3.5174300	-0.8712150
H	-1.7059850	-3.4504320	0.7001310
H	-2.6397640	-3.6276040	-0.7842040
C	-0.6362890	-1.3117070	-2.7613390
H	0.0280220	-2.1401570	-2.5067120
H	-1.3228580	-1.6607980	-3.5425110
H	-0.0266070	-0.5147170	-3.1935040
H	0.0495340	-0.4365480	2.0084380
Ir	-0.5176960	-0.0519270	0.3343800
O	-0.9599510	1.8039730	1.7688610
H	-0.1749150	0.3924970	2.1060790
H	-1.7427810	1.5930180	2.2996750
O	1.6251810	2.1421560	2.7308570
H	1.7765740	2.6066040	3.5622460
H	0.6674990	2.2251290	2.5565280

TS(5b-2)'*

G-gas = -1143.051117 Hartree

Symbol	X	Y	Z
C	2.7528610	-0.3854310	-0.1059060
N	1.7446650	-1.2519950	0.1017510
C	2.0185210	-2.5460990	0.3008970
C	3.3139890	-3.0575430	0.2690020
C	4.3653960	-2.1730900	0.0335540
C	4.0855080	-0.8216130	-0.1457600
H	1.1692060	-3.1902090	0.4995950
H	3.4874150	-4.1153870	0.4326510
H	5.3915280	-2.5252560	0.0064450
H	4.8982100	-0.1208940	-0.2911380
C	1.6135070	3.6985240	-0.2730880
C	2.9139360	3.3640980	-0.6426040

C	3.2933380	2.0265350	-0.6119450
C	2.3747170	1.0427010	-0.2265930
N	1.0962830	1.3804040	0.0874620
C	0.7344810	2.6811140	0.0787290
H	1.2720910	4.7275110	-0.2598170
H	3.6238670	4.1276690	-0.9434840
H	4.3003300	1.7475760	-0.8945260
H	-0.2838240	2.8680530	0.4014920
C	-1.8903420	0.4357850	-1.6325920
C	-2.8950470	0.2738130	-0.6562490
C	-2.5851510	-0.9662450	0.0560000
C	-1.6030370	-1.7009470	-0.7101280
C	-1.0913090	-0.7895490	-1.7055630
C	-1.7361720	1.6129540	-2.5459150
H	-0.6928400	1.7732270	-2.8280150
H	-2.3006060	1.4501850	-3.4729590
H	-2.1132630	2.5299170	-2.0872130
C	-3.9271570	1.2879490	-0.2790940
H	-4.6842060	0.8652220	0.3856610
H	-3.4728620	2.1500490	0.2261590
H	-4.4440870	1.6677840	-1.1663100
C	-3.4127090	-1.5355480	1.1723230
H	-2.8825300	-2.3280720	1.7037770
H	-3.6851470	-0.7709550	1.9047060
H	-4.3439770	-1.9594470	0.7765860
C	-1.3465930	-3.1755670	-0.6117860
H	-0.4103390	-3.4600000	-1.0952030
H	-1.3225770	-3.5193730	0.4257790
H	-2.1512830	-3.7237200	-1.1177180
C	-0.1448690	-1.1226980	-2.8211490
H	0.5448620	-1.9214840	-2.5419440
H	-0.7019540	-1.4554780	-3.7058910
H	0.4496460	-0.2543700	-3.1166420
H	-0.0326690	-0.8472020	1.9317540
Ir	-0.5014310	-0.0670580	0.3374630
O	-1.3206420	1.5729210	1.6297670
H	0.0191140	-0.2871780	2.5955140
H	-2.2396980	1.3638340	1.8432740
O	-0.1460710	0.6989610	3.6887840
H	0.6844230	1.1463110	3.9022100
H	-0.6248110	1.2563940	2.9749240

TS(5c-2)*

G-gas = -1066.633954 Hartree

Symbol	X	Y	Z

C	-2.6932900	-0.4209400	-0.0364360
N	-1.6748840	-1.2265240	-0.3885450
C	-1.8889390	-2.5380460	-0.5416240
C	-3.1315640	-3.1280890	-0.3205660
C	-4.1859270	-2.3101730	0.0822150
C	-3.9687690	-0.9422830	0.2215940
H	-1.0356780	-3.1303170	-0.8536340
H	-3.2627300	-4.1951720	-0.4621050
H	-5.1685670	-2.7277550	0.2765010
H	-4.7861780	-0.2985120	0.5212390
C	-1.7232640	3.7087330	-0.0782350
C	-3.0313700	3.3467480	0.2296490
C	-3.3622560	1.9956600	0.2622380
C	-2.3853360	1.0276430	0.0074350
N	-1.1052370	1.3977460	-0.2588030
C	-0.7896610	2.7072900	-0.3193390
H	-1.4197480	4.7475990	-0.1409590
H	-3.7877180	4.0994250	0.4267510
H	-4.3816440	1.6989830	0.4728310
H	0.2333310	2.9161310	-0.6054990
C	1.7901790	0.4959000	1.5036780
C	2.8431230	0.3744880	0.5626370
C	2.6286800	-0.8841630	-0.1389990
C	1.6429800	-1.6552880	0.5808930
C	1.0511560	-0.7674230	1.5571630
C	1.5558410	1.6719910	2.4026800
H	0.5405360	1.6837890	2.8037030
H	2.2437600	1.6307880	3.2564000
H	1.7321390	2.6185890	1.8857730
C	3.8263560	1.4379810	0.1954370
H	4.7356730	1.0098450	-0.2351960
H	3.3914490	2.1268330	-0.5400960
H	4.1160080	2.0268410	1.0700470
C	3.5222410	-1.4100670	-1.2247220
H	3.0790350	-2.2658990	-1.7373210
H	3.7446730	-0.6448160	-1.9733480
H	4.4793900	-1.7345740	-0.7980880
C	1.4297170	-3.1354620	0.4608650
H	0.5026030	-3.4528750	0.9417430
H	1.4088500	-3.4637270	-0.5811970
H	2.2509630	-3.6700390	0.9543310
C	0.0941410	-1.1575470	2.6457010
H	-0.5887500	-1.9462250	2.3223130
H	0.6433990	-1.5302880	3.5190170

H	-0.5088800	-0.3083880	2.9762350
H	0.0775630	-0.3939750	-2.2514370
Ir	0.5032630	-0.0172070	-0.4610440
O	1.3168090	1.6413330	-1.8702110
H	0.4306030	0.3751630	-2.3440440
H	2.1608120	1.3225440	-2.2239990

TS((5_1)-2)*

G-gas = -1219.449626 Hartree

Symbol	X	Y	Z
Ir	-0.2246920	-0.0552550	-0.2739850
N	1.3367060	1.3738490	-0.2270840
N	1.5434420	-1.2465710	-0.1640580
H	-1.3963080	-0.6275520	2.1651500
C	1.1323100	2.7027580	-0.1856420
H	0.1078840	3.0228980	-0.0623110
C	2.1816300	3.6142760	-0.2570670
H	1.9681970	4.6763590	-0.2214110
C	3.4844530	3.1354630	-0.3671080
H	4.3245950	3.8190220	-0.4326250
C	3.6991850	1.7588180	-0.3781190
H	4.7070600	1.3683760	-0.4461420
C	2.6084470	0.8918120	-0.2979730
C	2.7244310	-0.5785640	-0.2576800
C	3.9385930	-1.2694010	-0.2883100
H	4.8741330	-0.7303390	-0.3734340
C	3.9420860	-2.6586670	-0.2045870
H	4.8790800	-3.2051770	-0.2277260
C	2.7262700	-3.3305140	-0.0859240
H	2.6808380	-4.4109160	-0.0079620
C	1.5517860	-2.5880170	-0.0697320
H	0.5819320	-3.0614220	0.0149480
C	-1.8974140	-0.3164950	-1.5036350
C	-1.6780570	-0.4576730	-2.9855810
H	-1.1757430	0.4168070	-3.4071250
H	-2.6474900	-0.5581460	-3.4922640
H	-1.0849030	-1.3430710	-3.2279830
C	-2.2285330	0.9112700	-0.7841720
C	-2.2993800	2.2898830	-1.3860020
H	-2.1582260	3.0557790	-0.6180600
H	-3.2807410	2.4671690	-1.8450840
H	-1.5433910	2.4383950	-2.1613820
C	-3.0253400	0.5310750	0.3727270
C	-3.7050850	1.4966020	1.2784400
H	-2.9479450	2.1458240	1.7406330

H	-4.2667510	0.9937840	2.0681030
H	-4.3943980	2.1471890	0.7260600
C	-2.9804900	-0.8855150	0.5153460
C	-4.0906440	-1.7310790	1.0869510
H	-3.7321550	-2.7099050	1.4126540
H	-4.8502380	-1.8970100	0.3103970
H	-4.5776190	-1.2469300	1.9353530
C	-2.0686040	-1.3889780	-0.5452850
C	-1.9715440	-2.8559170	-0.8709700
H	-1.2088280	-3.0528680	-1.6289500
H	-2.9227770	-3.2445630	-1.2568260
H	-1.7264520	-3.4459310	0.0190980
O	-0.2978960	0.0773070	1.9346380
H	-2.1596260	-1.0815280	2.0915660
H	0.4048430	-0.4846280	2.3265540
O	1.6204960	-1.5490880	3.2546310
H	2.1257500	-1.0240000	3.8893640
H	1.1288290	-2.1799670	3.7972470
O	-0.7445460	2.7904500	2.1535900
H	-0.9042530	3.1091750	3.0498500
H	-0.5540750	1.8307080	2.2402310

TS((5_3)-2)*

G-gas = -1219.441143 Hartree

Symbol	X	Y	Z
Ir	0.6118420	-0.0348500	0.1109670
N	-1.1956220	-0.7883230	-0.6797800
N	-0.6305460	1.6546310	0.0928150
H	-4.1315690	-0.4666980	0.1987590
C	-1.4137270	-2.0436390	-1.0729850
H	-0.6107510	-2.7428420	-0.8705310
C	-2.5789810	-2.4858000	-1.7209910
H	-2.6526890	-3.5186480	-2.0370900
C	-3.6174760	-1.5733920	-1.9163500
H	-4.5388810	-1.8704350	-2.4059710
C	-3.4955600	-0.2796200	-1.4029570
H	-4.2382600	0.4699900	-1.6507520
C	-2.2084900	0.1643120	-0.8503540
C	-1.9044110	1.4730130	-0.4485410
C	-2.7839370	2.5928990	-0.5500260
H	-3.7667350	2.4608660	-0.9867180
C	-2.3915020	3.8280570	-0.0938400
H	-3.0613490	4.6780150	-0.1700630
C	-1.1084090	3.9782350	0.4807770
H	-0.7672490	4.9301560	0.8692650

C	-0.2762950	2.8688470	0.5451090
H	0.7136980	2.9389250	0.9805510
C	2.0987710	-0.4932550	-1.4855690
C	1.8401050	-0.7591730	-2.9380900
H	1.0984750	-1.5497180	-3.0776180
H	2.7626340	-1.0803880	-3.4367050
H	1.4763810	0.1325820	-3.4523520
C	2.1902120	-1.5136530	-0.4397650
C	2.0876880	-2.9959550	-0.6509140
H	1.6505650	-3.5034880	0.2125330
H	3.0846680	-3.4218770	-0.8164130
H	1.4890390	-3.2395130	-1.5317290
C	2.5839610	-0.8635200	0.7752160
C	2.7835050	-1.5064660	2.1130480
H	3.7635160	-1.2387900	2.5208470
H	2.7306510	-2.5946220	2.0475980
H	2.0096000	-1.1652440	2.8088570
C	2.6985480	0.5569980	0.5231970
C	3.2302380	1.5631280	1.5010520
H	2.9499020	2.5847410	1.2321420
H	4.3263530	1.5295650	1.5278310
H	2.8667750	1.3651240	2.5122710
C	2.4340650	0.7690690	-0.8927580
C	2.5554200	2.0766890	-1.6137210
H	1.9294270	2.1068420	-2.5075670
H	3.5951820	2.2313770	-1.9257710
H	2.2763910	2.9207140	-0.9788920
O	-1.9132320	-2.2540280	2.3152080
H	-1.6742180	-2.7059480	3.1349340
H	-3.1875490	-1.6050380	2.4007960
O	-0.2324610	-0.4086510	2.0059200
H	-1.2015050	-1.5070710	2.1762480
H	-0.6334850	0.4134080	2.3202720
O	-4.0961940	-1.0548810	2.3943210
H	-4.8257830	-1.6878850	2.4879130
H	-4.1691730	-0.6450080	1.0888350

TS((5_4)-2)*

G-gas = -1219.430590 Hartree

Symbol	X	Y	Z
Ir	-0.5819000	-0.1094910	-0.1043810
N	1.2654440	-0.3522640	0.6965230
N	0.2010180	1.8228480	-0.2751930
H	4.7223520	-0.9073830	0.4822380
C	1.7734000	-1.5421930	1.1146560

H	1.1321480	-2.4021090	0.9659960
C	3.0218750	-1.6783070	1.6558020
H	3.4043160	-2.6559870	1.9215490
C	3.9428540	-0.5243630	1.6558130
H	4.7525050	-0.5284550	2.3984060
C	3.3075940	0.7505950	1.4396670
H	3.8845890	1.6544190	1.5977480
C	2.0496240	0.8298470	0.8261710
C	1.4494650	2.0011530	0.2913460
C	2.0360120	3.2946510	0.2732780
H	3.0143640	3.4422290	0.7153760
C	1.3729230	4.3506060	-0.3078780
H	1.8250940	5.3369650	-0.3216120
C	0.1053010	4.1389240	-0.8961760
H	-0.4405720	4.9416010	-1.3769390
C	-0.4312730	2.8673460	-0.8537510
H	-1.3967230	2.6493650	-1.2941590
C	-2.4494500	0.2330020	1.0767480
C	-2.7492940	1.4261780	1.9334740
H	-2.1141740	1.4568390	2.8207150
H	-3.7930690	1.3975200	2.2685840
H	-2.6030420	2.3608780	1.3869010
C	-1.8721560	-1.0095180	1.5089730
C	-1.4437860	-1.3493380	2.9040650
H	-0.5585680	-1.9897770	2.9150280
H	-2.2481110	-1.8915690	3.4157620
H	-1.2200540	-0.4552530	3.4884750
C	-1.8404680	-1.9146790	0.3712780
C	-1.4688270	-3.3683750	0.3918470
H	-1.0333120	-3.6840800	-0.5593010
H	-2.3577940	-3.9859620	0.5708660
H	-0.7568880	-3.5981290	1.1883510
C	-2.4665330	-1.2359820	-0.7382340
C	-2.6303680	-1.8109710	-2.1110700
H	-3.3541010	-1.2418490	-2.6974780
H	-2.9748700	-2.8476720	-2.0589490
H	-1.6686870	-1.7824580	-2.6364220
C	-2.8199180	0.0916680	-0.3288650
C	-3.6231440	1.0751700	-1.1298590
H	-3.5212060	2.0918540	-0.7435950
H	-4.6886680	0.8204200	-1.0799330
H	-3.3338970	1.0785830	-2.1836340
O	2.4626740	-1.7813250	-2.4759990
H	3.8325280	-1.7969900	-1.8848350

H	2.2323720	-2.5418520	-3.0214700
O	0.2524530	-0.4227140	-2.0032180
H	1.6015480	-1.2519950	-2.2917980
H	0.3240900	0.4365670	-2.4429520
O	4.8016700	-1.9258590	-1.5722240
H	4.8260350	-1.3411600	-0.3725810
H	5.3355190	-1.3411470	-2.1345200

TS((5_5)-2)*

G-gas = -1219.442717 Hartree

Symbol	X	Y	Z
Ir	0.6376880	-0.0967220	0.1541870
N	-1.1879690	-0.8016390	-0.6047160
N	-0.5194540	1.6512450	0.0093970
H	-3.6230300	-2.6963430	0.1831030
C	-1.5113080	-2.0770820	-0.7909900
H	-0.7681220	-2.8077960	-0.4904200
C	-2.7625040	-2.5011080	-1.2787280
H	-2.8918610	-3.5396630	-1.5619770
C	-3.6701260	-1.4735540	-1.7827940
H	-4.6018900	-1.7633770	-2.2547990
C	-3.3398680	-0.1640430	-1.6143560
H	-4.0114750	0.6137660	-1.9584070
C	-2.1196920	0.2076510	-0.9715680
C	-1.7465490	1.5248540	-0.6203450
C	-2.5425890	2.6840760	-0.8297940
H	-3.4969890	2.5931690	-1.3339940
C	-2.1109820	3.9119840	-0.3800830
H	-2.7208170	4.7958160	-0.5358090
C	-0.8778410	4.0056100	0.2975540
H	-0.5135490	4.9480470	0.6886780
C	-0.1263420	2.8514350	0.4657430
H	0.8220850	2.8705960	0.9885620
C	2.0469560	-0.8369830	-1.3948620
C	1.7002240	-1.3432210	-2.7624700
H	0.9487340	-2.1357410	-2.7222410
H	2.5917810	-1.7588450	-3.2471120
H	1.3123750	-0.5484370	-3.4024940
C	2.1729520	-1.6648440	-0.1968970
C	2.0641300	-3.1610130	-0.1509240
H	1.7317880	-3.5196140	0.8266630
H	3.0389330	-3.6204210	-0.3553540
H	1.3694900	-3.5399780	-0.9047020
C	2.6336760	-0.8118430	0.8685530
C	2.9353300	-1.2372720	2.2729750

H	4.0167780	-1.3673220	2.3987010
H	2.4610820	-2.1897610	2.5202250
H	2.6029810	-0.4880500	2.9955900
C	2.7601900	0.5323550	0.3698910
C	3.3511800	1.6898880	1.1194370
H	3.0779790	2.6470210	0.6690570
H	4.4464590	1.6323630	1.1081200
H	3.0312350	1.7013270	2.1645410
C	2.4109540	0.5055720	-1.0477480
C	2.4963640	1.6742100	-1.9821650
H	1.8556560	1.5394780	-2.8556090
H	3.5267680	1.7970310	-2.3364730
H	2.2023650	2.6057910	-1.4925120
O	-2.7922560	0.0623580	2.3063280
H	-2.9373400	0.6951080	3.0192940
H	-3.6703670	-1.0248810	2.2576110
O	-0.3096530	-0.2039170	2.0389720
H	-1.7664900	-0.0692240	2.1973630
H	0.0208410	-0.9947290	2.4825910
O	-4.3512720	-1.8429640	2.1391720
H	-4.1649350	-2.5037300	2.8242780
H	-3.9999750	-2.3950950	1.0040220

TS((5_6)-2)*

G-gas = -1219.506661 Hartree

Symbol	X	Y	Z
Ir	-0.4509660	0.1243550	-0.0215410
N	1.1693300	1.4843350	0.0278590
N	1.2242010	-1.0806290	-0.5081250
H	0.7883880	2.0805430	2.2901340
C	1.0550810	2.6234740	0.7881360
H	0.0735940	3.0804090	0.7751160
C	2.1997620	3.4923140	0.8879540
H	2.0644310	4.4871600	1.2973040
C	3.4326240	3.0195190	0.5330420
H	4.3136380	3.6461660	0.6297320
C	3.5624740	1.6955130	0.0437060
H	4.5410520	1.2778730	-0.1546830
C	2.4142410	0.9621240	-0.1898200
C	2.4174210	-0.4394040	-0.6310420
C	3.5470930	-1.1249840	-1.0909250
H	4.4829660	-0.5950940	-1.2177620
C	3.4588540	-2.4792670	-1.3868920
H	4.3294950	-3.0184280	-1.7457280
C	2.2395130	-3.1349260	-1.2065470

H	2.1307440	-4.1959890	-1.3994050
C	1.1483080	-2.4001580	-0.7666260
H	0.1843700	-2.8635350	-0.6003460
C	-2.2970690	1.3305080	-0.2341860
C	-2.6010520	2.7108240	0.2679040
H	-2.4687350	2.7903590	1.3497960
H	-3.6410820	2.9745050	0.0407010
H	-1.9674480	3.4617460	-0.2099090
C	-2.6531200	0.0960660	0.4159590
C	-3.2790130	-0.0311110	1.7690180
H	-2.9577310	-0.9453500	2.2710460
H	-4.3697100	-0.0726100	1.6585740
H	-3.0422830	0.8222000	2.4076820
C	-2.3241030	-1.0055300	-0.4521660
C	-2.6447560	-2.4477890	-0.1843570
H	-3.7204250	-2.6274150	-0.2999240
H	-2.3566700	-2.7392800	0.8294120
H	-2.1357030	-3.1101970	-0.8887960
C	-1.7972970	-0.4356390	-1.6865460
C	-1.4375480	-1.2055490	-2.9202140
H	-0.6935720	-0.6809050	-3.5228030
H	-2.3320920	-1.3457640	-3.5385770
H	-1.0447560	-2.1968920	-2.6853630
C	-1.7750720	0.9972480	-1.5556220
C	-1.3911400	1.9891080	-2.6105050
H	-0.8685220	2.8465720	-2.1804140
H	-2.2882550	2.3627460	-3.1185520
H	-0.7398840	1.5458980	-3.3660120
O	0.1549970	-0.0287070	2.0460290
H	0.4942220	1.0935670	2.3206630
H	0.9433720	-0.6211460	2.1390880
O	1.7458640	-2.1845850	2.4722900
H	2.3390330	-2.2381200	3.2322790
H	0.8956510	-2.5727170	2.7678090
O	-0.9675460	-2.3495980	3.0304440
H	-1.2942400	-2.4230010	3.9364320
H	-0.8079330	-1.3954950	2.8713000

e) H_2 generation in the Ground state

TS(5-2)

G-gas = -1219.527418 Hartree

Symbol	X	Y	Z
C	2.6216370	-0.6035550	-0.1841740
N	2.4454450	-0.9069080	1.1101190

C	2.9208460	-2.0763760	1.5509520
C	3.5863260	-2.9980710	0.7391840
C	3.7662840	-2.6811430	-0.6056640
C	3.2826600	-1.4603320	-1.0766150
H	2.7720850	-2.2839230	2.6085770
H	3.9565680	-3.9291490	1.1552280
H	4.2784340	-3.3649360	-1.2756720
H	3.4098950	-1.1763640	-2.1162480
C	1.6510200	3.3416970	-1.4601870
C	2.9466190	2.8610910	-1.6218010
C	3.2194680	1.5615630	-1.2095530
C	2.2154390	0.7638990	-0.6429110
N	0.9491990	1.2365120	-0.5010740
C	0.6966620	2.5009640	-0.9059110
H	1.3717260	4.3460580	-1.7583980
H	3.7282460	3.4815530	-2.0484990
H	4.2206040	1.1544790	-1.2921170
H	-0.3203810	2.8345550	-0.7632030
C	-2.1090820	-0.3793120	-1.6177970
C	-2.9289520	-0.3898770	-0.4421910
C	-2.3957500	-1.3535000	0.5074940
C	-1.2546050	-1.9963520	-0.1350300
C	-1.0666830	-1.3763600	-1.4159990
C	-2.3689730	0.3696870	-2.8917980
H	-1.4400940	0.6140210	-3.4131070
H	-2.9818920	-0.2281780	-3.5782070
H	-2.9033770	1.3058540	-2.7115120
C	-4.1574810	0.4445250	-0.2411610
H	-4.3892660	0.5825410	0.8167190
H	-4.0653100	1.4288960	-0.7090460
H	-5.0182060	-0.0491630	-0.7084670
C	-3.0318740	-1.7834350	1.7969300
H	-2.2796880	-2.0893750	2.5272960
H	-3.6201180	-0.9788890	2.2435600
H	-3.7032300	-2.6354330	1.6316100
C	-0.5043440	-3.1754610	0.4068130
H	0.5118640	-3.2267350	0.0127120
H	-0.4392050	-3.1413960	1.4961220
H	-1.0193660	-4.1042260	0.1315970
C	-0.0683050	-1.7742560	-2.4597780
H	0.8016960	-2.2670070	-2.0252500
H	-0.5331720	-2.4742930	-3.1649480
H	0.2780430	-0.9114820	-3.0345150
H	0.0300100	-0.1525110	1.5478170

Ir	-0.8471750	0.1450140	0.2206080
O	1.2576450	1.1341320	3.0588750
H	0.7172160	0.5643610	2.3959740
H	0.9100200	0.9895180	3.9519630
O	0.7036010	3.2657930	2.0823420
H	0.4078330	4.0284590	2.6001650
H	1.0447160	2.2218000	2.7163810
O	-1.2343600	2.0852000	1.1767030
H	-0.2037040	2.8526700	1.6910280
H	-1.9925150	2.4816300	0.7341440

TS(5a-2)'

G-gas = -1219.504482 Hartree

Symbol	X	Y	Z
C	-2.5643650	-1.0329950	0.1779610
N	-1.3935400	-1.4943870	-0.3552060
C	-1.3747760	-2.7255300	-0.9044160
C	-2.4697950	-3.5795670	-0.8758020
C	-3.6462600	-3.1456130	-0.2669600
C	-3.6931690	-1.8547520	0.2467650
H	-0.4492450	-3.0157320	-1.3788580
H	-2.3925290	-4.5615740	-1.3284200
H	-4.5186520	-3.7884870	-0.2167740
H	-4.6109080	-1.4760830	0.6790100
C	-2.4152670	3.0973580	1.0369590
C	-3.5702020	2.4113620	1.4045990
C	-3.6470140	1.0398170	1.1691440
C	-2.5689050	0.3845950	0.5716340
N	-1.4351650	1.0669630	0.2534730
C	-1.3557550	2.3896750	0.4768870
H	-2.3188840	4.1694070	1.1583590
H	-4.4071080	2.9332430	1.8567420
H	-4.5405690	0.4910870	1.4410720
H	-0.4372950	2.8772770	0.1756840
C	2.1460040	0.0492750	1.7263070
C	3.2784430	0.1605610	0.8973520
C	3.1207340	-0.7644440	-0.1577890
C	1.8977220	-1.5256660	0.0165170
C	1.2690230	-1.0151350	1.2438390
C	1.8684570	0.9475730	2.8829210
H	0.9836990	0.6473490	3.4462660
H	2.7252550	0.9709380	3.5665240
H	1.7206520	1.9773860	2.5321410
C	4.3932040	1.1555610	1.0890150
H	4.0174590	2.1793440	1.2006090

H	4.9703860	0.9301860	1.9934360
H	5.0964730	1.1487740	0.2530490
C	4.0810840	-0.9874010	-1.2805100
H	3.5752260	-1.3511170	-2.1778320
H	4.6497200	-0.0891700	-1.5351980
H	4.8131310	-1.7544520	-0.9902870
C	1.8885750	-2.9801860	-0.4192640
H	1.0274010	-3.5183590	-0.0222270
H	1.8946780	-3.0958390	-1.5080980
H	2.7765490	-3.4986750	-0.0358210
C	0.4990670	-1.8700410	2.2320650
H	-0.1528660	-2.5864030	1.7298310
H	1.1867740	-2.4410410	2.8682830
H	-0.1293240	-1.2619240	2.8893170
H	-0.4075710	0.0823750	-2.0849780
Ir	0.1586510	-0.1025930	-0.4182760
O	0.2575810	2.2249880	-2.6854760
H	-0.2001100	0.9453060	-2.3060130
H	0.7870360	2.1508220	-3.4923250
O	1.3108120	1.6374190	-0.5965520
H	2.2555370	1.4659020	-0.5032360
H	0.8996760	2.1082780	-1.8107850
O	-0.7247320	4.6293540	-1.3854710
H	-0.2880010	5.4340580	-1.6885580
H	-0.5119320	3.9580100	-2.0548830

TS(5a-2)''

G-gas = -1219.496936 Hartree

Symbol	X	Y	Z
C	-3.0479090	0.0282590	-0.2364290
N	-2.0579750	-0.8865750	-0.4718270
C	-2.4095000	-2.1308440	-0.8537850
C	-3.7329810	-2.5445920	-0.9430570
C	-4.7469730	-1.6382410	-0.6374130
C	-4.3949660	-0.3364910	-0.2969620
H	-1.5934370	-2.7966580	-1.0936890
H	-3.9536050	-3.5604160	-1.2508310
H	-5.7905310	-1.9300210	-0.6878210
H	-5.1637520	0.4014410	-0.1026240
C	-1.4873290	3.9308220	0.1937600
C	-2.8546650	3.7626080	0.4197520
C	-3.4108440	2.4908890	0.3101070
C	-2.5891890	1.4094770	-0.0191660
N	-1.2575470	1.5930940	-0.2126820
C	-0.7124070	2.8198040	-0.1187740

H	-1.0211170	4.9075050	0.2596290
H	-3.4816550	4.6103340	0.6753700
H	-4.4703140	2.3431540	0.4814220
H	0.3566680	2.8553580	-0.3090480
C	1.4523820	-0.0661910	2.0025040
C	2.6216590	-0.4851600	1.3880390
C	2.2861250	-1.5749020	0.5213830
C	0.8851090	-1.8798830	0.6176550
C	0.3122890	-0.8899210	1.5423520
C	1.2911780	1.0869330	2.9364450
H	0.5820550	1.8166380	2.5277480
H	0.8806060	0.7572420	3.8989980
H	2.2327640	1.6037900	3.1273080
C	4.0005560	0.0950100	1.5256870
H	4.3370810	0.5901710	0.6090610
H	4.0475570	0.8299550	2.3322440
H	4.7331640	-0.6866970	1.7580500
C	3.2750890	-2.3164650	-0.3081670
H	2.8251180	-3.1572130	-0.8386330
H	3.7412310	-1.6447130	-1.0395510
H	4.0804780	-2.6992490	0.3324440
C	0.4006510	-3.3071520	0.4582970
H	-0.6534960	-3.4086360	0.7195950
H	0.5397080	-3.6912790	-0.5570990
H	0.9512890	-3.9730660	1.1345100
C	-0.8173540	-1.1868740	2.5081950
H	-1.5983490	-1.7990950	2.0533150
H	-0.4471760	-1.7295290	3.3877550
H	-1.2891680	-0.2670510	2.8680160
H	-0.1072370	0.2215120	-2.2506860
Ir	-0.1228640	-0.1308320	-0.4343150
O	1.5512910	1.1078410	-0.8693780
H	0.6034790	0.7051450	-1.9356790
H	2.3453570	0.6504300	-1.2136050
O	3.8822880	0.2138590	-2.2039640
H	4.6184730	0.8127100	-1.9602790
H	3.7668480	0.3050070	-3.1570770
O	5.9274750	1.8194360	-1.2893360
H	5.9322200	2.7829800	-1.3404110
H	6.8510100	1.5470800	-1.3557530

TS(5b-2)

G-gas = -1143.078886 Hartree

Symbol	X	Y	Z
C	2.8022360	-0.3860040	0.0513230

N	1.6935450	-1.1481440	0.2996160
C	1.8573660	-2.4633300	0.5459950
C	3.0949100	-3.0917470	0.4798480
C	4.2206270	-2.3357080	0.1573610
C	4.0688320	-0.9675060	-0.0416050
H	0.9615140	-3.0081810	0.8055820
H	3.1640600	-4.1544250	0.6828120
H	5.2006120	-2.7955720	0.0878510
H	4.9341190	-0.3481940	-0.2438250
C	1.8959810	3.7405520	0.0841440
C	3.1919750	3.3751550	-0.2835110
C	3.5315630	2.0254610	-0.3276920
C	2.5674270	1.0655850	-0.0092620
N	1.3054680	1.4429180	0.3230090
C	0.9713050	2.7451050	0.3797090
H	1.5979410	4.7815230	0.1397360
H	3.9307570	4.1303450	-0.5304320
H	4.5333660	1.7249930	-0.6102290
H	-0.0570000	2.9394510	0.6697220
C	-1.7804310	0.4602130	-1.7902540
C	-2.9531450	0.1841660	-1.1001110
C	-2.7428160	-1.0234680	-0.3642310
C	-1.4288310	-1.5471510	-0.6207720
C	-0.7694650	-0.5798320	-1.5093630
C	-1.5074520	1.6448430	-2.6561360
H	-1.4574090	1.3435630	-3.7111340
H	-2.2768330	2.4138530	-2.5673500
H	-0.5383230	2.0941820	-2.4146040
C	-4.2149300	0.9985340	-1.0531800
H	-5.0084460	0.5377630	-1.6544550
H	-4.5947440	1.0855330	-0.0311100
H	-4.0614440	2.0084950	-1.4398350
C	-3.7754380	-1.6812600	0.4863090
H	-3.3627780	-2.4986840	1.0801560
H	-4.2630950	-0.9619270	1.1508300
H	-4.5616680	-2.0972890	-0.1596540
C	-1.1868260	-3.0429050	-0.6271190
H	-0.1846840	-3.2900290	-0.9796160
H	-1.3257450	-3.4997080	0.3578460
H	-1.8860630	-3.5363640	-1.3138490
C	0.2324730	-0.9533780	-2.5824750
H	0.9286240	-1.7237190	-2.2445310
H	-0.2765080	-1.3400420	-3.4747490
H	0.8256030	-0.0881170	-2.8945580

H	0.0823730	0.0656640	2.3203830
Ir	-0.0838380	-0.0931220	0.4911110
O	-1.4971390	1.3459170	1.1806740
H	-0.5652280	0.6823290	2.1174440
H	-2.3435670	0.9816000	1.4953630
O	-4.0182830	0.9323760	2.5422660
H	-4.0036310	0.5681600	3.4367500
H	-4.2581490	1.8614790	2.6541270

TS(5b-2)′

G-gas = -1143.090362 Hartree

Symbol	X	Y	Z
C	2.6517300	0.6247760	0.2335650
N	1.5152900	1.2849720	-0.1433970
C	1.5973920	2.6028920	-0.4126390
C	2.7644720	3.3369140	-0.2396100
C	3.9089840	2.6854250	0.2162840
C	3.8507000	1.3135140	0.4360540
H	0.6949690	3.0647960	-0.7843950
H	2.7665300	4.3969180	-0.4667600
H	4.8357960	3.2275160	0.3710470
H	4.7397800	0.7752860	0.7403880
C	2.1159500	-3.5659840	0.2855400
C	3.3413680	-3.0724640	0.7348630
C	3.5504880	-1.6965940	0.7537600
C	2.5356650	-0.8395230	0.3195060
N	1.3444920	-1.3408980	-0.1022270
C	1.1334310	-2.6706890	-0.1200070
H	1.9146770	-4.6307670	0.2500130
H	4.1231810	-3.7473150	1.0669780
H	4.4929520	-1.2953810	1.1057810
H	0.1460730	-2.9656410	-0.4610490
C	-2.2148540	-0.5593050	1.5616880
C	-3.2959120	-0.2727480	0.7343880
C	-2.9721760	0.9161130	0.0028140
C	-1.7108590	1.4404790	0.4340360
C	-1.1640480	0.4699310	1.3950730
C	-2.0530910	-1.7405870	2.4574470
H	-1.1355940	-2.2860100	2.2088970
H	-1.9548950	-1.4202570	3.5023250
H	-2.8921690	-2.4354490	2.3966070
C	-4.5734950	-1.0525420	0.5637220
H	-4.5473210	-2.0032970	1.0999790
H	-5.4329260	-0.4883620	0.9447390
H	-4.7882150	-1.2753340	-0.4882620

C	-3.8729230	1.5491590	-1.0041420
H	-3.3659660	2.3184400	-1.5886620
H	-4.2991740	0.8087590	-1.6893430
H	-4.7245560	2.0191040	-0.4923010
C	-1.5002470	2.9399600	0.4953770
H	-0.5474480	3.2003360	0.9560720
H	-1.5493410	3.4167820	-0.4889440
H	-2.2802990	3.4001490	1.1148940
C	-0.3138300	0.8499620	2.5924260
H	0.4266960	1.6119420	2.3403620
H	-0.9333640	1.2496490	3.4058230
H	0.2271990	-0.0150970	2.9882880
H	0.4387680	0.2422880	-2.1728500
Ir	-0.1416470	0.0465700	-0.4903230
O	-0.3949870	-1.5874850	-3.3365590
H	0.1446390	-0.4825700	-2.6171500
H	-0.9472840	-1.2688800	-4.0642300
O	-1.3625660	-1.5390760	-1.0462930
H	-2.2795240	-1.4285850	-0.7695510
H	-0.9968580	-1.7231110	-2.5125550

TS(5c-2)

G-gas = -1066.665637 Hartree

Symbol	X	Y	Z
C	-2.6183390	-0.5494310	0.1727790
N	-1.4692220	-1.2319450	-0.1189070
C	-1.5248200	-2.5743570	-0.2269420
C	-2.6851840	-3.3008660	0.0104010
C	-3.8465990	-2.6188350	0.3688080
C	-3.8095940	-1.2301690	0.4356950
H	-0.6044270	-3.0596310	-0.5169640
H	-2.6677620	-4.3802350	-0.0887660
H	-4.7685180	-3.1539050	0.5700210
H	-4.7091180	-0.6737450	0.6685960
C	-2.1236750	3.6255680	-0.2489200
C	-3.3458620	3.1754700	0.2522330
C	-3.5483890	1.8086080	0.4261680
C	-2.5220770	0.9181220	0.1001110
N	-1.3333460	1.3784220	-0.3647490
C	-1.1334470	2.6956200	-0.5462680
H	-1.9330830	4.6809310	-0.4081210
H	-4.1339330	3.8781960	0.5016220
H	-4.4923800	1.4437120	0.8125550
H	-0.1574140	2.9646460	-0.9383730
C	1.9800900	0.5848900	1.5092320

C	3.1264920	0.6071320	0.6822490
C	3.0792570	-0.5354300	-0.1289620
C	1.8851750	-1.3291320	0.1754810
C	1.2114950	-0.6262440	1.2748650
C	1.6139520	1.6796470	2.4539700
H	0.6718500	1.4910930	2.9710840
H	2.4000250	1.8023230	3.2100040
H	1.5410350	2.6400860	1.9291030
C	4.1159860	1.7367580	0.6344060
H	3.6488720	2.6598410	0.2723640
H	4.5255800	1.9471780	1.6284190
H	4.9611190	1.5145760	-0.0205120
C	4.0755580	-0.9376530	-1.1670850
H	3.5823980	-1.3064840	-2.0722800
H	4.7575970	-0.1299250	-1.4396990
H	4.6866570	-1.7692760	-0.7895790
C	1.9522690	-2.8365380	0.0165800
H	1.0999210	-3.3361280	0.4800680
H	1.9967340	-3.1440130	-1.0327250
H	2.8453100	-3.2386430	0.5123030
C	0.4547550	-1.3011220	2.3984410
H	-0.1301910	-2.1530060	2.0490230
H	1.1554940	-1.6764030	3.1544000
H	-0.2332240	-0.6142440	2.8997510
H	-0.2149160	-0.0573490	-2.3412180
Ir	0.1815990	-0.0572540	-0.5711620
O	1.3892270	1.4269780	-1.5195890
H	0.4129190	0.6047420	-2.2867190
H	2.2582510	1.0808340	-1.7620770

TS((5_1)-2)

G-gas = -1219.494074 Hartree

Symbol	X	Y	Z
Ir	-0.3499090	-0.0570320	-0.0400240
N	1.1669470	1.3960300	-0.1799190
N	1.4061230	-1.2140360	-0.1738630
H	-1.4903460	-0.1419640	2.2787090
C	0.9554510	2.7226330	-0.0895210
H	-0.0566330	3.0321120	0.1272080
C	1.9863540	3.6474160	-0.2135910
H	1.7634960	4.7050500	-0.1328900
C	3.2853830	3.1892330	-0.4216790
H	4.1116910	3.8847900	-0.5239170
C	3.5121270	1.8174280	-0.4761130
H	4.5177700	1.4393740	-0.6129220

C	2.4375450	0.9340260	-0.3461960
C	2.5711630	-0.5297460	-0.3451410
C	3.7868880	-1.2076320	-0.4842230
H	4.7062880	-0.6533560	-0.6268750
C	3.8125410	-2.5968510	-0.4393710
H	4.7499270	-3.1312990	-0.5520110
C	2.6160020	-3.2856130	-0.2383800
H	2.5870790	-4.3678510	-0.1817240
C	1.4404900	-2.5593630	-0.1041700
H	0.4906200	-3.0476030	0.0686760
C	-1.6390040	-0.8921300	-1.5428130
C	-1.2378380	-1.7671530	-2.6928240
H	-0.6256310	-1.2229270	-3.4150710
H	-2.1269360	-2.1386300	-3.2164740
H	-0.6669310	-2.6378180	-2.3593080
C	-1.7680880	0.5428710	-1.5447760
C	-1.5195930	1.4680980	-2.6980200
H	-1.1225520	2.4314080	-2.3691470
H	-2.4568010	1.6649210	-3.2325010
H	-0.8105510	1.0388100	-3.4091560
C	-2.3431940	0.9270260	-0.2520470
C	-2.7398460	2.3202410	0.1524490
H	-2.3477070	2.5622500	1.1461930
H	-3.8308310	2.4286580	0.1667130
H	-2.3566740	3.0660890	-0.5485570
C	-2.8808100	-0.2759900	0.3908180
C	-4.2640870	-0.3911020	0.9799800
H	-4.3840090	-1.3008160	1.5707910
H	-4.9770350	-0.4297110	0.1421090
H	-4.5174610	0.4674900	1.6036050
C	-2.1499380	-1.3671400	-0.2538650
C	-2.3514970	-2.8091610	0.1192740
H	-1.6493980	-3.4696170	-0.3956860
H	-3.3593230	-3.1490420	-0.1509280
H	-2.2339000	-2.9566430	1.1974710
O	-0.1751570	0.0768100	2.0961010
H	-2.3443570	-0.2607620	2.0495770
H	0.3221410	-0.6584300	2.5166890
O	1.1380250	-2.1059180	3.3318100
H	1.9091660	-1.8501370	3.8548610
H	0.5388910	-2.5221760	3.9656750
O	-0.3948170	2.8006740	2.5306490
H	-0.7739900	3.0066100	3.3932100
H	-0.2392220	1.8336920	2.5367920

TS((5_2)-2)

G-gas = -1219.501190 Hartree

Symbol	X	Y	Z
Ir	-0.3753510	0.0158700	-0.0760500
N	1.2911960	1.2955660	-0.2569540
N	1.2866170	-1.3310030	-0.0224960
H	-0.2585480	0.9569820	2.4522280
C	1.2046150	2.6398960	-0.3765380
H	0.2075050	3.0342680	-0.5314200
C	2.3052750	3.4689070	-0.3548660
H	2.1861930	4.5376870	-0.4844890
C	3.5825360	2.8683820	-0.2581680
H	4.4784110	3.4756720	-0.3433610
C	3.6875490	1.5151950	-0.0693150
H	4.6584290	1.0475680	0.0369420
C	2.4991110	0.7320440	0.1091120
C	2.5122210	-0.7548570	0.0085490
C	3.6685710	-1.5353180	-0.0198640
H	4.6431610	-1.0642040	-0.0162690
C	3.5570230	-2.9219640	-0.0371560
H	4.4486810	-3.5403270	-0.0585150
C	2.2894050	-3.5034610	-0.0148130
H	2.1566700	-4.5790760	-0.0020080
C	1.1768950	-2.6727840	-0.0065170
H	0.1734190	-3.0723080	0.0354830
C	-1.5621830	-0.7204480	-1.7723180
C	-1.0738930	-1.5449700	-2.9242050
H	-0.3528090	-0.9973860	-3.5340180
H	-1.9159300	-1.8258380	-3.5681330
H	-0.5952740	-2.4667110	-2.5854670
C	-1.6517100	0.7179780	-1.7355460
C	-1.2686710	1.6439480	-2.8481320
H	-0.9618250	2.6251250	-2.4812300
H	-2.1318510	1.7960260	-3.5074950
H	-0.4540710	1.2398470	-3.4519820
C	-2.2501040	1.1019840	-0.4691330
C	-2.6628030	2.4845230	-0.0550450
H	-2.4822820	2.6581100	1.0086090
H	-3.7317210	2.6347020	-0.2487380
H	-2.1252420	3.2504450	-0.6193900
C	-2.5838060	-0.1238740	0.2368280
C	-3.2502960	-0.2130550	1.5743450
H	-2.8350160	-1.0371740	2.1603440
H	-4.3238580	-0.3919250	1.4369180

H	-3.1366640	0.7157890	2.1368050
C	-2.1730670	-1.2435070	-0.5535170
C	-2.4482010	-2.6820420	-0.2300200
H	-1.9188470	-3.3545840	-0.9091860
H	-3.5187590	-2.8887370	-0.3475170
H	-2.1599410	-2.9152780	0.7986800
O	0.1634600	0.1551180	2.0629980
H	1.2625450	0.3547950	2.0649100
H	2.3450470	0.5721840	1.8012260
O	-0.8489880	-2.4104150	2.5944810
H	-0.7634780	-2.7349130	3.4987010
H	-0.4326020	-1.5274180	2.5839630
O	-0.9801200	2.4320920	3.1126030
H	-1.2595120	2.3880510	4.0370230
H	-0.3701360	3.1809020	3.0666170

TS((5_3)-2)

G-gas = -1219.497163 Hartree

Symbol	X	Y	Z
Ir	-0.4910940	0.1154500	-0.0575940
N	1.0963280	-1.1167040	0.5675020
N	1.1460470	1.4331360	-0.0682340
H	3.9252660	-1.5762250	-0.7640010
C	0.9606910	-2.4165370	0.8339920
H	-0.0290580	-2.8394110	0.7435130
C	2.0670370	-3.1867940	1.2618000
H	1.8952900	-4.1990690	1.6123030
C	3.3213940	-2.6410660	1.2466230
H	4.1844870	-3.2044420	1.5846920
C	3.5105190	-1.3323660	0.6629560
H	4.4473280	-0.8315960	0.8857820
C	2.3238440	-0.5187850	0.6077150
C	2.3456430	0.8853360	0.2953950
C	3.5051290	1.6876160	0.2977330
H	4.4555370	1.2571840	0.5872200
C	3.4253680	3.0229030	-0.0572790
H	4.3162770	3.6425530	-0.0492720
C	2.1876090	3.5625990	-0.4323140
H	2.0839130	4.5994200	-0.7296580
C	1.0806360	2.7312610	-0.4262880
H	0.1047420	3.0906200	-0.7273150
C	-1.9335550	1.2811090	1.1375690
C	-1.6503310	2.5045800	1.9542290
H	-0.9651060	2.2945370	2.7774830
H	-2.5856660	2.8813660	2.3853480

H	-1.2202350	3.3092180	1.3538980
C	-1.9133390	-0.0781530	1.6135290
C	-1.5841910	-0.5299600	3.0033850
H	-1.0564220	-1.4864830	2.9980800
H	-2.5059850	-0.6600680	3.5827890
H	-0.9581840	0.1953210	3.5264000
C	-2.3802780	-0.9423050	0.5352510
C	-2.6793490	-2.4090290	0.6292510
H	-2.3377480	-2.9399960	-0.2632010
H	-3.7612160	-2.5586590	0.7318440
H	-2.2109570	-2.8574400	1.5084450
C	-2.6706580	-0.1037740	-0.5930350
C	-3.1998340	-0.5939800	-1.9045110
H	-3.0569930	0.1402930	-2.7005950
H	-4.2781670	-0.7747370	-1.8149310
H	-2.7178300	-1.5334540	-2.1878710
C	-2.3803870	1.2701220	-0.2480160
C	-2.7193270	2.4735980	-1.0784330
H	-2.1335950	3.3496870	-0.7895200
H	-3.7755040	2.7390720	-0.9481920
H	-2.5559730	2.2942720	-2.1438100
O	2.6995910	-0.7704910	-2.4359850
H	3.4164150	-1.2535390	-1.5888730
H	2.8124540	-1.3238540	-3.2224080
O	0.3062550	-0.5304540	-1.9857110
H	1.6145780	-0.6756930	-2.1936620
H	-0.0273470	0.0866710	-2.6509810
O	-0.9214660	-3.0270300	-2.0263030
H	-0.8885890	-3.4691000	-2.8828060
H	-0.4488880	-2.1755920	-2.1341590

TS((5_4)-2)

G-gas = -1219.498027 Hartree

Symbol	X	Y	Z
Ir	0.4990650	0.0709060	0.0236030
N	-1.2884130	-0.5788800	-0.8276360
N	-0.7928380	1.7413270	0.2629610
H	-4.1151730	-2.3260210	0.2944440
C	-1.4856760	-1.7965170	-1.4075490
H	-0.5905980	-2.3208650	-1.7167780
C	-2.7233360	-2.3410130	-1.6014740
H	-2.8188410	-3.3066640	-2.0841660
C	-3.8744770	-1.6879910	-1.0233190
H	-4.8593980	-1.9956550	-1.3657870
C	-3.6738080	-0.2824580	-0.7634580

H	-4.5313920	0.3521990	-0.5768370
C	-2.3964180	0.1932310	-0.5869470
C	-2.0873030	1.5457270	-0.0982340
C	-3.0206240	2.5835290	0.0085560
H	-4.0458770	2.4190570	-0.2987950
C	-2.6227940	3.8219070	0.4949060
H	-3.3380120	4.6340040	0.5746150
C	-1.2922040	4.0036640	0.8797810
H	-0.9387150	4.9497580	1.2735020
C	-0.4127860	2.9391300	0.7504100
H	0.6254950	3.0261310	1.0439460
C	2.2563070	0.9448870	-1.0106500
C	2.3264700	2.2511230	-1.7422250
H	1.6932070	2.2510130	-2.6313530
H	3.3566720	2.4449840	-2.0641150
H	2.0184130	3.0886540	-1.1116390
C	1.9647480	-0.3367100	-1.5905150
C	1.6714070	-0.6013450	-3.0354210
H	1.0050020	-1.4558830	-3.1687430
H	2.6048810	-0.8273550	-3.5648810
H	1.2113120	0.2614680	-3.5204630
C	2.0945930	-1.3467770	-0.5469100
C	2.0197030	-2.8366960	-0.7189230
H	1.4694190	-3.3096050	0.0991540
H	3.0289350	-3.2647470	-0.7502980
H	1.5310010	-3.1076370	-1.6575590
C	2.5170490	-0.6667430	0.6558590
C	2.8316950	-1.3403140	1.9548270
H	2.6773120	-0.6747090	2.8068710
H	3.8846540	-1.6476250	1.9605270
H	2.2226590	-2.2351090	2.0932800
C	2.6050270	0.7413110	0.3920020
C	3.1552260	1.7786550	1.3262730
H	2.8248620	2.7860440	1.0613270
H	4.2511100	1.7838850	1.2817390
H	2.8704690	1.5885420	2.3640030
O	-2.6470190	-2.1720990	1.9592500
H	-3.5101230	-2.3018940	1.0751350
H	-2.0150170	-2.9338390	1.9443420
O	-0.5243090	-0.6730800	1.7613170
H	-2.0089440	-1.3980470	1.8190750
H	-0.3304790	-0.0871310	2.5047670
O	-0.2138780	-3.3268940	1.9756120
H	0.0419900	-3.6713070	2.8410720

H	-0.1092310	-2.3415320	2.0175280

TS((5_5)-2)

G-gas = -1219.499785 Hartree

Symbol	X	Y	Z
Ir	0.5724080	-0.0091500	0.0865590
N	-1.1374530	-0.9940650	-0.6240840
N	-0.8559210	1.5500420	-0.0512060
H	-2.8954630	-3.4471420	0.6787610
C	-1.2114960	-2.3146130	-0.7452180
H	-0.3111570	-2.8753590	-0.5314740
C	-2.4419140	-2.9813950	-0.9850980
H	-2.4154960	-4.0418580	-1.2000470
C	-3.4950670	-2.1728720	-1.4952510
H	-4.3914860	-2.6342690	-1.8941270
C	-3.4003690	-0.8040630	-1.3907640
H	-4.2262160	-0.1780610	-1.7088320
C	-2.2316780	-0.2083530	-0.8758370
C	-2.0662660	1.1982680	-0.5754890
C	-3.0614100	2.1745210	-0.7578790
H	-4.0210780	1.8927130	-1.1726020
C	-2.8178670	3.4871580	-0.3917330
H	-3.5837850	4.2429680	-0.5323470
C	-1.5819540	3.8235700	0.1747590
H	-1.3575720	4.8344650	0.4942580
C	-0.6351010	2.8247830	0.3286940
H	0.3309120	3.0298840	0.7717160
C	2.1623920	0.6592780	-1.2789210
C	2.0431660	1.6073350	-2.4337040
H	1.4071120	1.2024330	-3.2231350
H	3.0321190	1.8016130	-2.8659470
H	1.6222910	2.5669750	-2.1249320
C	2.0866440	-0.7787010	-1.3418170
C	1.8189300	-1.5902730	-2.5707090
H	1.2816700	-2.5129890	-2.3424080
H	2.7722520	-1.8693250	-3.0354540
H	1.2378910	-1.0332080	-3.3076660
C	2.3565890	-1.3082720	-0.0200470
C	2.5164920	-2.7524690	0.3541290
H	2.2229050	-2.9328660	1.3907840
H	3.5641790	-3.0589210	0.2468560
H	1.9226420	-3.4097380	-0.2854530
C	2.6787310	-0.1812510	0.8398240
C	3.0437130	-0.2972010	2.2864040
H	3.0838790	0.6780340	2.7734660

H	4.0290120	-0.7669860	2.3848890
H	2.3165410	-0.9122900	2.8227270
C	2.5635920	1.0241810	0.0809680
C	2.9404800	2.4002820	0.5421640
H	2.4504250	3.1763820	-0.0494710
H	4.0215130	2.5458800	0.4287500
H	2.6963530	2.5611930	1.5949590
O	-2.0307390	-2.2258150	2.3209540
H	-2.5431020	-2.9260490	1.4598810
H	-1.9938740	-2.7899120	3.1060990
O	-0.2724100	-0.4172930	2.0395190
H	-0.8083420	-1.2949210	2.0911300
H	-1.0094580	0.2066060	2.2738230
O	-2.7363250	0.3752890	2.5609040
H	-2.7887370	-0.6131590	2.5524650
H	-3.0575990	0.6537030	3.4274370

TS((5_6)-2)

G-gas = -1219.506650 Hartree

Symbol	X	Y	Z
Ir	-0.4510150	0.1245200	-0.0217760
N	1.1697070	1.4842220	0.0287670
N	1.2241050	-1.0805680	-0.5084200
H	0.7900900	2.0784880	2.2919320
C	1.0559070	2.6227990	0.7899580
H	0.0744340	3.0797670	0.7777000
C	2.2006770	3.4914440	0.8901280
H	2.0655340	4.4860350	1.3001440
C	3.4334120	3.0187060	0.5347220
H	4.3145420	3.6451510	0.6316520
C	3.5629630	1.6949580	0.0446270
H	4.5414530	1.2772230	-0.1540520
C	2.4145540	0.9618960	-0.1892800
C	2.4174700	-0.4394900	-0.6311410
C	3.5470480	-1.1251420	-1.0912690
H	4.4830170	-0.5953530	-1.2179480
C	3.4585590	-2.4793300	-1.3876390
H	4.3291040	-3.0185170	-1.7466550
C	2.2391350	-3.1348330	-1.2074320
H	2.1301960	-4.1958130	-1.4005650
C	1.1480600	-2.4000310	-0.7672870
H	0.1840630	-2.8632920	-0.6011180
C	-2.2966570	1.3311960	-0.2352520
C	-2.6003530	2.7117380	0.2663620
H	-2.4690710	2.7913330	1.3483680

H	-3.6400310	2.9759370	0.0381260
H	-1.9658870	3.4622430	-0.2109810
C	-2.6530580	0.0970030	0.4151300
C	-3.2789490	-0.0300810	1.7681560
H	-2.9588130	-0.9453390	2.2690580
H	-4.3697320	-0.0698880	1.6579750
H	-3.0407450	0.8223420	2.4074470
C	-2.3240900	-1.0049390	-0.4526570
C	-2.6442550	-2.4471610	-0.1838100
H	-3.7202000	-2.6268120	-0.2965950
H	-2.3536140	-2.7382430	0.8293790
H	-2.1369010	-3.1097540	-0.8892820
C	-1.7970900	-0.4354800	-1.6871310
C	-1.4371860	-1.2057530	-2.9205390
H	-0.6928660	-0.6814480	-3.5230150
H	-2.3315920	-1.3458120	-3.5391470
H	-1.0447680	-2.1971690	-2.6853780
C	-1.7744100	0.9974920	-1.5565230
C	-1.3900100	1.9891990	-2.6114140
H	-0.8651470	2.8454050	-2.1815110
H	-2.2870590	2.3648690	-3.1180890
H	-0.7405890	1.5451250	-3.3680060
O	0.1539020	-0.0296830	2.0456470
H	0.4946240	1.0919840	2.3213430
H	0.9414520	-0.6232600	2.1387220
O	1.7430740	-2.1865800	2.4717190
H	2.3370070	-2.2396120	3.2311490
H	0.8928980	-2.5737620	2.7686550
O	-0.9688140	-2.3491050	3.0343160
H	-1.2955580	-2.4226640	3.9402640
H	-0.8100360	-1.3950060	2.8750420