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Energy & Environmental Science

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Cite this: DOI: 10.1039/c0xx00000x

www.rsc.org/ees

Supporting Information

Carbon Dioxide Reduction by Mononuclear Ruthenium Polypyridyl Complexes

Nora Planas,[a] Takashi Ono,[a] Lydia Vaquer,[a] Pere Miró,[b] Laura Gagliardi,*[,b] Christopher J. Cramer*[,b] and Antoni Llobet*[a,c]

[a] *Institute of Chemical Research of Catalonia (ICIQ), Av. Països Catalans 16, E-43007 Tarragona, Spain. Fax: 34 977 902 228; Ph: 34 977 902 200; E-mail: allobet@iciq.es*
[b] *Department of Chemistry and Supercomputing Institute, University of Minnesota, 207 Pleasant St. SE, Minneapolis, MN 55455-0431 (USA); E-mail: gagliardi@umn.edu, cramer@umn.edu*
[c] *Departament de Química, Universitat Autònoma de Barcelona, Cerdanyola del Vallès, E-08193 Barcelona, Spain.*

1. Gibbs Free Energies of the Catalytic Cycle

2. Optimized Structures

1. Gibbs Free Energies of the Catalytic Cycle

Table S1. Gibbs Free energies at the M06-L DFT level of theory of the different steps in the catalytic cycle for compounds **1**, **1d**, **1d'**, **1w**, **1w'** and **2**. Energies in kcal/mol.

	1w	**1w'**	**1**	**1d'**	**1d**	**2**
II	-8.78	-7.70	-9.39	-11.66	-9.60	-9.78
II-a	11.12	10.93	10.19	7.3	9.00	12.23
II-b	-4.32	-4.79	-5.91	-6.33	-4.93	-1.07
II-c	-15.58	-13.83	-13.67	-12.63	-13.68	-20.94
III	12.00	13.23	11.03	10.60	10.45	22.62
III-a	11.47	11.28	11.75	---	---	---
III-b	1.27	0.76	0.28	---	---	---
III-c	-0.74	1.19	-1.00	0.24	-0.72	-1.05
IV-O	3.04	0.72	4.62	7.31	5.41	-4.70
IV-a-O	4.57	5.90	7.97	8.84	9.55	2.53
IV-b-O	-1.53	-5.18	-3.35	-1.52	-4.14	-7.23
IV-N	1.80	-1.14	3.38	3.43	3.48	-5.94
IV-a-N	8.44	6.06	8.78	9.42	9.88	7.42
IV-b-N	6.64	-6.58	-5.40	-3.35	-5.71	-13.36
IV-ON	-1.81	-4.13	-0.23	2.47	0.57	-9.54
$\Delta G^{\neq}_1$	11.12	10.24	10.19	7.30	9.00	12.23
$\Delta G^{\neq}_2$	16.56	19.13	19.00	19.43	22.00	25.16

2. Optimized Structures

2.1. Tables with selected bond distances and angles.

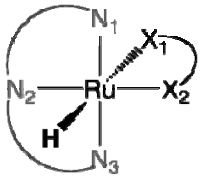

Table S3. Significant structural parameters for the corresponding **Ru-H** species.

	Ru-H	Ru-N1	Ru-N2	Ru-N3	Ru-X1	Ru-X2	N1-Ru-N3	N1-Ru-H	X1-Ru-H	N1-Ru-X2
2	1.638	2.068	1.949	2.068	2.149	2.077	158.4	90.4	168.1	100.8
1w	1.643	2.100	2.019	2.110	2.156	2.037	176.3	87.1	173.9	93.2
1w'	1.643	2.079	2.014	2.096	2.175	2.068	177.7	88.0	174.6	92.2
1	1.647	2.095	2.017	2.106	2.167	2.060	177.2	87.9	174.0	92.5
1d	1.653	2.109	2.021	2.114	2.155	2.058	176.7	87.9	174.1	92.8
1d'	1.651	2.097	2.013	2.101	2.176	2.090	177.7	88.6	174.3	92.0
3	1.650	2.065	1.985	2.065	2.178	2.119	179.0	89.5	178.1	89.9

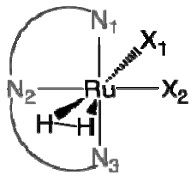

Table S4. Significant structural parameters for the corresponding **Ru-H_2** species.

	Ru-H1	Ru-H2	H1-H2	Ru-N1	Ru-N2	Ru-N3	Ru-X1	Ru-X2	N1-Ru-N3	N1-Ru-H1
2	1.755	1.756	0.835	2.097	1.980	2.099	2.070	2.070	157.4	78.8
1w	1.745	1.747	0.837	2.124	2.036	2.124	2.063	2.078	176.6	88.9
1w'	1.744	1.742	0.840	2.110	2.033	2.113	2.076	2.093	177.4	90.1
1	1.741	1.739	0.841	2.119	2.034	2.121	2.074	2.087	177.1	89.7
1d	1.739	1.737	0.842	2.127	2.035	2.122	2.069	2.086	176.7	87.9
1d'	1.734	1.737	0.845	2.116	2.031	2.117	2.083	2.103	177.5	89.8
3	1.714	1.725	0.853	2.088	2.011	2.088	2.062	2.110	179.3	89.7

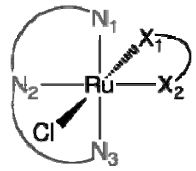

Table S5. Significant structural parameters for the corresponding **Ru-Cl** species.

	Ru-Cl	Ru-N1	Ru-N2	Ru-N3	Ru-X1	Ru-X2	N1-Ru-N3	N1-Ru-Cl	X1-Ru-Cl	N1-Ru-X2
2	2.456	2.071	1.955	2.071	2.041	2.081	159.0	89.6	172.9	100.5
1w	2.478	2.106	2.017	2.113	2.016	2.048	177.0	88.2	175.1	92.7
1w'	2.478	2.106	2.017	2.113	2.016	2.048	177.0	88.2	175.1	92.7
1	2.488	2.098	2.014	2.108	2.029	2.064	177.3	88.6	174.7	92.5
1d	2.494	2.109	2.016	2.115	2.021	2.062	177.0	88.3	174.9	92.6
1d'	2.493	2.099	2.011	2.102	2.045	2.086	177.8	88.6	174.5	91.6
3	2.490	2.069	1.990	2.069	2.059	2.098	178.7	89.3	178.5	90.0

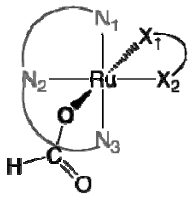

Table S6. Significant structural parameters for the corresponding **Ru-H-CO_2** species.

	Ru-H	Ru-H-C	O1-C-O2	Ru-N1	Ru-N2	Ru-N3	Ru-X1	Ru-X2	N1-Ru-N3	N1-Ru-H	X2-Ru-H
2	1.828	125.9	134.7	2.080	1.969	2.074	2.044	2.066	158.4	97.3	97.3
1w	1.846	129.4	33.5	2.110	2.021	2.113	2.029	2.057	176.9	95.4	90.4
1w'	1.872	132.2	133.8	2.098	2.017	2.110	2.034	2.073	177.3	95.04	95.8
1	1.846	129.4	133.5	2.110	2.021	2.113	2.029	2.057	176.9	95.43	90.3
1d	1.864	167.7	133.2	2.113	2.021	2.120	2.020	2.059	176.2	94.6	91.3
1d'	1.841	129.1	133.2	2.109	2.017	2.108	2.041	2.076	177.4	95.9	90.9
3	1.829	123.0	132.5	2.081	1.997	2.079	2.050	2.098	179.0	86.8	98.1

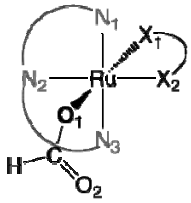

Table S7. Significant structural parameters for the corresponding **Ru-O1-CHO_2** species.

	Ru-O1	Ru-O1-C	O1-C-O2	X1-Ru-O1-O2	Ru-N1	Ru-N2	Ru-N3	Ru-X1	Ru-X2	N1-Ru-N3	N1-Ru-O
2	2.103	126.8	128.4	-165.0	2.071	1.955	2.071	2.044	2.074	158.8	86.5
1w	2.119	125.8	128.8	-139.5	2.104	2.012	2.101	2.019	2.038	176.5	84.4
1w'	2.125	126.6	128.8	-142.9	2.091	2.011	2.091	2.041	2.066	177.7	84.5
1	2.130	126.8	128.9	-139.7	2.100	2.012	2.099	2.032	2.054	177.3	84.1
1d	2.137	127.6	129.1	-145.8	2.111	2.014	2.106	2.023	2.054	176.6	84.0
1d'	2.131	127.3	129.0	-143.5	2.097	2.008	2.094	2.048	2.076	177.7	84.6
3	2.133	125.5	128.7	-166.4	2.071	1.993	2.063	2.060	2.094	176.9	86.6

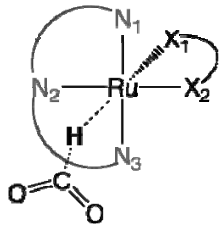

Table S8. Significant structural parameters for the corresponding transition state: **Ru-H---CO_2.**

	Ru-H	H-C	Ru-H-C	O1-C-O2	O1-C	C-O2	Ru-N1	Ru-N2	Ru-N3	Ru-X1	Ru-X2
2	1.685	1.617	129.1	151.8	1.196	1.196	2.072	1.957	2.075	2.113	2.069
1w	1.685	1.679	126.2	153.4	1.192	1.194	2.098	2.017	2.116	2.112	2.036
1w'	1.681	1.673	127.9	153.4	1.192	1.193	2.087	2.014	2.101	2.133	2.067
1	1.687	1.700	125.3	153.7	1.192	1.193	2.099	2.015	2.112	2.125	2.061
1d	1.688	1.718	125.7	154.0	1.191	1.192	2.108	2.017	2.120	2.115	2.057
1d'	1.687	1.714	124.7	153.7	1.192	1.193	2.098	2.013	2.110	2.137	2.085
3	1.672	1.732	125.3	154.8	1.191	119.092	2.073	1.989	2.082	2.145	2.106

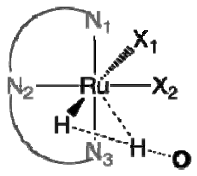

Table S8. Significant structural parameters for the corresponding transition state: **Ru-H--H-OCHO**.

	Ru-H1	Ru-H2	H1-H2	Ru-H1-H2	H2-O	H1-H2_O	Ru-N1	Ru-N2	Ru-N3	Ru-X1	Ru-X2
2	1.720	2.083	0.913	100.1	1.395	162.9	2.084	1.967	2.080	2.084	2.073
1w	1.730	2.205	0.940	107.6	1.324	166.8	2.130	2.029	2.122	2.094	2.082
1w'	1.733	2.189	0.924	107.0	1.344	168.2	2.099	2.021	2.106	2.086	2.070
1	1.731	2.197	0.938	107.0	1.325	167.6	2.118	2.023	2.112	2.085	2.070
1d	1.733	2.225	0.940	109.0	1.315	168.7	2.116	2.023	2.121	2.076	2.060
1d'	1.723	2.205	0.945	108.0	1.311	167.7	2.113	2.019	2.107	2.099	2.093
3	1.717	2.155	0.966	103.3	1.303	166.7	2.074	1.995	2.078	2.102	2.115

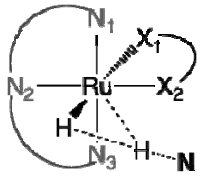

Table S9. Significant structural parameters for the corresponding transition state: **Ru-H--H-Nme**

	Ru-H1	Ru-H2	H1-H2	Ru-H1-H2	H2-N	H1-H2_N	Ru-N1	Ru-N2	Ru-N3	Ru-X1	Ru-X2
2	1.724	2.026	0.877	96.9	1.624	144.0	2.088	1.970	2.079	2.075	2.071
1w	1.722	2.063	0.893	99.2	1.535	148.0	2.111	2.024	2.109	2.069	2.047
1w'	1.718	2.070	0.900	99.7	1.516	147.0	2.096	2.070	2.102	2.088	2.070
1	1.720	2.100	0.907	101.7	1.494	149.4	2.109	2.022	2.106	2.084	2.064
1d	1.719	2.128	0.918	103.4	1.463	150.5	2.114	2.023	2.114	2.078	2.059
1d'	1.715	2.123	0.920	103.2	1.464	150.0	2.105	2.018	2.103	2.098	2.086
3	1.695	2.094	0.953	100.8	1.430	149.2	2.072	2.000	2.074	2.102	2.107

2.2 Optimized geometries for catalytic system of 2

[Ru(Trpy)(bpy)Cl]$^{1+}$

Ru	0.03543800	0.00051600	-0.43157800
Cl	-0.54405700	0.00225100	-2.81773900
N	-0.33526200	2.03621500	-0.35541300
N	-0.33427000	-2.03552000	-0.35845100
N	2.09163400	0.00143000	-0.75392700
N	0.75783000	-0.00123600	1.47700400
C	-2.53209100	-1.19532100	0.12371900
C	-2.53270000	1.19421800	0.12532600
C	-3.89745700	1.20926400	0.42270100
H	-4.42762400	2.15495300	0.53514700
C	-4.57648400	-0.00137000	0.57351000
H	-5.64186000	-0.00179400	0.80700300
C	-3.89683200	-1.21145600	0.42111400
H	-4.42651000	-2.15757100	0.53230000
C	-1.65485300	-2.35137300	-0.07899800
C	-2.07739700	-3.68126100	-0.00852300
H	-3.12286600	-3.90638800	0.20298600
C	-1.16363200	-4.71060700	-0.21450500
H	-1.48716100	-5.75109200	-0.16235300
C	0.16712400	-4.39019500	-0.49028400
H	0.91261900	-5.16772600	-0.65835900
C	0.54223000	-3.05302200	-0.55591200
H	1.56883100	-2.75869200	-0.77846900
C	-1.65606400	2.35099200	-0.07576800
C	-2.07935800	3.68055700	-0.00370500
H	-3.12498400	3.90484900	0.20793600
C	-1.16614100	4.71066200	-0.20831700
H	-1.49025700	5.75090300	-0.15495900
C	0.16483100	4.39132600	-0.48430800
H	0.90991200	5.16948000	-0.65134700
C	0.54070100	3.05444600	-0.55151000
H	1.56750900	2.76096600	-0.77424100
C	2.71787400	0.00344400	-1.96318200
H	2.05526100	0.00441700	-2.83050500
C	4.10023100	0.00420900	-2.09402200
H	4.54510300	0.00585800	-3.08953200
C	4.89685200	0.00290900	-0.94589500
H	5.98529700	0.00352800	-1.01949200
C	4.27667200	0.00086300	0.29823300
H	4.87477100	0.00002500	1.20912600
C	2.87985400	0.00015500	0.37763200
C	2.12951900	-0.00171100	1.62882300
C	2.71397700	-0.00383200	2.90007000
H	3.79910400	-0.00444500	2.99566300
C	1.91241800	-0.00532700	4.03539700
H	2.36311700	-0.00704000	5.02861400
C	0.52409800	-0.00460900	3.87886800
H	-0.14347700	-0.00565700	4.74081100
C	-0.01474500	-0.00257500	2.60000100
H	-1.09281200	-0.00201300	2.44248200
N	-1.87222600	-0.00029600	-0.00272800

[Ru(Trpy)(bpy)$^{2+}$

Ru	0.04515700	-0.00012100	-0.63895400
N	-0.33379000	2.04682100	-0.55646500
N	-0.33560900	-2.04676400	-0.55643000
N	2.08973100	-0.00091500	-0.88739800
N	0.64094500	-0.00026400	1.25152800
C	-2.55993300	-1.19304600	-0.21478400
C	-2.55888300	1.19504900	-0.21487000

C	-3.94130300	1.21255900	-0.02169400
H	-4.47703300	2.15870900	0.04768600
C	-4.63018100	0.00192600	0.07386300
H	-5.71071700	0.00240400	0.22187000
C	-3.94237800	-1.20931900	-0.02165300
H	-4.47895700	-2.15498300	0.04776400
C	-1.66850600	-2.35338000	-0.32546900
C	-2.09158100	-3.67772900	-0.20317700
H	-3.14446500	-3.89597900	-0.02294200
C	-1.16447200	-4.71236900	-0.30463500
H	-1.48756900	-5.74976600	-0.20809100
C	0.17720800	-4.40192000	-0.52723200
H	0.93283300	-5.18369400	-0.60778200
C	0.55370200	-3.06821200	-0.64622000
H	1.59071900	-2.78175300	-0.82517000
C	-1.66644900	2.35459900	-0.32566600
C	-2.08842000	3.67932500	-0.20363100
H	-3.14114300	3.89850000	-0.02357500
C	-1.16041800	4.71316400	-0.30511800
H	-1.48264800	5.75084800	-0.20877200
C	0.18102600	4.40154500	-0.52749400
H	0.93732700	5.18266300	-0.60804900
C	0.55639900	3.06750100	-0.64628000
H	1.59318900	2.78013600	-0.82508200
C	2.75208200	-0.00144100	-2.07409900
H	2.12294300	-0.00150300	-2.96633500
C	4.13887500	-0.00185700	-2.15107600
H	4.62517900	-0.00228800	-3.12673000
C	4.88788800	-0.00169300	-0.97062200
H	5.97824200	-0.00197000	-1.00333500
C	4.22409800	-0.00117500	0.25184000
H	4.78965900	-0.00104700	1.18323000
C	2.82644200	-0.00083800	0.27539000
C	2.00723600	-0.00048000	1.48080400
C	2.51046800	-0.00045400	2.78446700
H	3.58805300	-0.00063100	2.94340400
C	1.64271900	-0.00022000	3.87024800
H	2.03326900	-0.00019400	4.88840200
C	0.26706500	-0.00003800	3.63187000
H	-0.45107400	0.00012400	4.45201000
C	-0.20046800	-0.00006400	2.32554300
H	-1.26714400	0.00006400	2.10865900
N	-1.89711700	0.00070600	-0.31051900

[Ru(Trpy)(bpy)(H_2)]$^{2+}$

Ru	0.04116200	-0.00315400	-0.68583100
N	-0.33586400	2.05682200	-0.54893000
N	-0.35488200	-2.05732500	-0.54582800
N	2.10277000	-0.01209900	-0.87579300
N	0.65227800	-0.00255300	1.29181400
C	-2.56978900	-1.18295900	-0.20606900
C	-2.55876400	1.20162500	-0.20796100
C	-3.93485800	1.22585500	0.02739100
H	-4.46165900	2.17442900	0.12517100
C	-4.62755400	0.01917900	0.13608400
H	-5.70331000	0.02433800	0.31532100
C	-3.94631600	-1.19390800	0.02911600
H	-4.48192800	-2.13733000	0.12868000
C	-1.68521300	-2.34951000	-0.30290500
C	-2.11266800	-3.66935300	-0.14486600
H	-3.16473200	-3.87930400	0.04846100
C	-1.18975300	-4.70884200	-0.22652000
H	-1.51588400	-5.74238800	-0.10239400

C	0.15127300	-4.40932900	-0.46538300
H	0.90373000	-5.19526500	-0.53206700
C	0.53128800	-3.07969000	-0.61849900
H	1.56765100	-2.80003400	-0.81168300
C	-1.66384500	2.36048300	-0.30807500
C	-2.08096600	3.68433800	-0.15668700
H	-3.13150000	3.90369400	0.03445200
C	-1.14970600	4.71613400	-0.24292000
H	-1.46787600	5.75281800	-0.12446000
C	0.18895100	4.40498600	-0.47937500
H	0.94763300	5.18460200	-0.54950900
C	0.55841000	3.07146900	-0.62576500
H	1.59254300	2.78253100	-0.81716400
C	2.78348200	-0.02064500	-2.05432500
H	2.17037200	-0.02431900	-2.95613600
C	4.17063000	-0.02484000	-2.11620500
H	4.66596800	-0.03214400	-3.08727300
C	4.90649700	-0.01939100	-0.92881900
H	5.99717400	-0.02196000	-0.94803900
C	4.22659100	-0.01097000	0.28412400
H	4.78201600	-0.00706600	1.22138100
C	2.82811500	-0.00810900	0.29430500
C	2.01186100	-0.00172000	1.50668000
C	2.53053700	0.00427000	2.80531200
H	3.60808600	0.00477400	2.96102800
C	1.66841400	0.00999900	3.89610600
H	2.06790500	0.01510900	4.91108300
C	0.29112700	0.00906700	3.67195000
H	-0.41875500	0.01311600	4.49895200
C	-0.18001000	0.00248900	2.36518500
H	-1.24879000	0.00105900	2.15225300
N	-1.90935600	0.00614500	-0.34259400
H	-0.27267900	0.41749100	-2.36099700
H	-0.21809700	-0.41605200	-2.37248700

[Ru(Trpy)(bpy)(H)]$^{1+}$

Ru	-0.00871400	0.00049600	-0.65216100
N	-0.38840300	2.03154600	-0.57710000
N	-0.38792000	-2.03073200	-0.57904100
N	2.05295000	0.00106500	-0.90569700
N	0.75145500	-0.00092200	1.35767600
C	-2.59320200	-1.19582300	-0.15575100
C	-2.59349400	1.19569800	-0.15469600
C	-3.96433000	1.20838900	0.10938000
H	-4.49332000	2.15576900	0.21347100
C	-4.65195900	-0.00048700	0.23455300
H	-5.72392700	-0.00070200	0.43550600
C	-3.96402900	-1.20908900	0.10836500
H	-4.49279500	-2.15668500	0.21165200
C	-1.71089500	-2.34981500	-0.29788400
C	-2.12051200	-3.67945800	-0.15630000
H	-3.16476400	-3.90019800	0.06731200
C	-1.19647100	-4.70959700	-0.29287900
H	-1.50918800	-5.74890500	-0.18279700
C	0.13580200	-4.38914800	-0.57057800
H	0.89168100	-5.16700500	-0.68347800
C	0.49963100	-3.05587500	-0.70436200
H	1.52691900	-2.76447000	-0.92720600
C	-1.71148600	2.35004500	-0.29575800
C	-2.12146200	3.67945800	-0.15303500
H	-3.16578600	3.89973000	0.07072000
C	-1.19768000	4.70995500	-0.28867200
H	-1.51066800	5.74908600	-0.17770000

C	0.13469400	4.39009100	-0.56657000
H	0.89037700	5.16824600	-0.67874100
C	0.49888600	3.05703600	-0.70148400
H	1.52627400	2.76610000	-0.92448300
C	2.68514800	0.00254600	-2.11708600
H	2.02758400	0.00329400	-2.98619900
C	4.06547100	0.00309300	-2.25309000
H	4.50622600	0.00429900	-3.25049200
C	4.86650200	0.00212500	-1.10699700
H	5.95474400	0.00255700	-1.18314200
C	4.24681200	0.00063900	0.13645700
H	4.84595300	0.00000400	1.04670700
C	2.84959900	0.00013000	0.22374500
C	2.11755700	-0.00129400	1.48972000
C	2.72434200	-0.00296600	2.75249400
H	3.81046800	-0.00338600	2.83829800
C	1.93375000	-0.00421000	3.89616400
H	2.39693600	-0.00555800	4.88401600
C	0.54238200	-0.00373300	3.76006400
H	-0.11108600	-0.00465500	4.63290800
C	-0.00701300	-0.00208800	2.48400300
H	-1.08797100	-0.00171200	2.32950100
N	-1.92550000	0.00008600	-0.30279900
H	-0.26055000	0.00130500	-2.27085600

TS = [Ru(Trpy)(bpy)(H—H—NMe_3)]$^{2+}$

Ru	0.17760600	0.01735100	-0.27117900
N	0.59044200	1.96601800	-0.86821100
N	-0.80358800	-1.54287600	0.70990000
N	1.83695400	-0.99576900	-0.98501300
N	1.50834700	0.19118200	1.31173700
C	-2.24915100	0.29348900	1.28571700
C	-1.44959200	2.33647200	0.34486500
C	-2.52828100	3.03218200	0.89461400
H	-2.62963200	4.10563900	0.73712800
C	-3.47445900	2.33552000	1.64849700
H	-4.32222600	2.86716400	2.08201200
C	-3.33509700	0.96211000	1.85522700
H	-4.06772600	0.41865200	2.45122100
C	-1.94261900	-1.13770400	1.38701600
C	-2.72047400	-2.05411400	2.09906400
H	-3.61831700	-1.71694500	2.61762700
C	-2.34182500	-3.39328300	2.14722300
H	-2.94404500	-4.11418000	2.70188800
C	-1.18297800	-3.79484200	1.48099400
H	-0.85119800	-4.83305600	1.49958800
C	-0.44523600	-2.84963500	0.77609900
H	0.45928800	-3.12252200	0.23034400
C	-0.34469200	2.89456100	-0.43996800
C	-0.20174400	4.25116300	-0.73952900
H	-0.95022500	4.96366200	-0.39164100
C	0.89827200	4.68568500	-1.47381700
H	1.01699300	5.74373500	-1.71129200
C	1.84372500	3.74977800	-1.89626600
H	2.72023300	4.05082400	-2.47048000
C	1.65913600	2.40878200	-1.57817300
H	2.36958700	1.64319300	-1.89266200
C	1.92619700	-1.60692500	-2.19953000
H	1.04415300	-1.52398400	-2.83587100
C	3.06025100	-2.29131700	-2.61431800
H	3.07527400	-2.76101400	-3.59808100
C	4.16371500	-2.36556700	-1.75969500
H	5.06776200	-2.89723200	-2.05970600

C	4.09046600	-1.75078100	-0.51497700
H	4.93727200	-1.79761100	0.16943300
C	2.92448500	-1.07346400	-0.14187200
C	2.74045200	-0.39865600	1.14146100
C	3.71359200	-0.33289800	2.14437400
H	4.68269100	-0.80660100	1.99318000
C	3.44069000	0.33776300	3.33115200
H	4.19528800	0.39194000	4.11716700
C	2.19133600	0.93831300	3.49776900
H	1.93905500	1.47603900	4.41176900
C	1.25594800	0.84757700	2.47492100
H	0.27095900	1.30552900	2.56849100
N	-1.33785100	0.98499700	0.53417000
H	-0.55036300	-0.07054800	-1.83177900
H	-1.27603800	-0.49640900	-1.58603900
N	-2.66384500	-1.14448900	-2.12445200
C	-2.69574000	-2.59758600	-1.90035100
H	-1.72438300	-3.03225000	-2.19219600
H	-2.87707900	-2.80435300	-0.83351700
H	-3.49486000	-3.08655400	-2.49474300
C	-3.88675500	-0.50059400	-1.62039400
H	-4.05976700	-0.80069200	-0.57491500
H	-3.77132000	0.59591800	-1.66660000
H	-4.77591900	-0.78749700	-2.21897100
C	-2.48993100	-0.85343000	-3.55687600
H	-2.43216800	0.23797500	-3.70370900
H	-1.55019100	-1.30937200	-3.91146600
H	-3.32913100	-1.25191200	-4.16053200

TS = [Ru(Trpy)(bpy)(H–CO_2)]$^{1+}$

Ru	-0.04455300	0.02905600	-0.36221100
H	0.39185700	-0.11817000	-1.98323900
N	0.60968200	-1.88626000	0.09673000
N	0.03671600	2.08272800	-0.60996900
N	-2.03700500	-0.31666300	-0.79994100
N	-0.98202300	0.21510400	1.52175400
C	2.29255100	1.67132200	0.09605500
C	2.62470700	-0.65655600	0.52283100
C	3.95694700	-0.41875700	0.86611600
H	4.60471200	-1.24299700	1.16363000
C	4.45395100	0.88480900	0.81800900
H	5.49428900	1.08126200	1.07991000
C	3.62093100	1.93734400	0.43488900
H	4.00588500	2.95615800	0.39733100
C	1.27433900	2.63818600	-0.31577300
C	1.48591100	4.01644700	-0.41073400
H	2.46758600	4.43041500	-0.17950600
C	0.44422600	4.85450700	-0.79550700
H	0.60405900	5.93099000	-0.87027600
C	-0.80355100	4.29550300	-1.08136900
H	-1.64594600	4.91824400	-1.38356300
C	-0.96904100	2.91975500	-0.98009100
H	-1.92409200	2.44175800	-1.20203500
C	1.93164700	-1.94553800	0.51491600
C	2.51466500	-3.15938400	0.88864900
H	3.55493200	-3.18359500	1.21323300
C	1.76483100	-4.33076500	0.84667300
H	2.21407700	-5.28150900	1.13703300
C	0.43302600	-4.26885700	0.42921900
H	-0.18633400	-5.16490700	0.38283300
C	-0.10632400	-3.04163200	0.06448200
H	-1.13883400	-2.94846200	-0.27614900
C	-2.52441800	-0.57482200	-2.04783200

H	-1.78006600	-0.61184700	-2.84400300
C	-3.87240700	-0.78456400	-2.30155200
H	-4.20138300	-0.98676100	-3.32130000
C	-4.78457100	-0.73287700	-1.24321400
H	-5.84967400	-0.89554000	-1.41392500
C	-4.30910000	-0.46784200	0.03577200
H	-4.99940100	-0.42107000	0.87792200
C	-2.94049800	-0.26080500	0.24223800
C	-2.34429500	0.03195800	1.54441400
C	-3.06535200	0.12788800	2.74073800
H	-4.14487400	-0.01911700	2.74067300
C	-2.39906800	0.41082900	3.92756900
H	-2.95367700	0.48747100	4.86394700
C	-1.01398900	0.59437700	3.90159000
H	-0.45563300	0.81683300	4.81116600
C	-0.34374600	0.48931700	2.68929800
H	0.73679100	0.62628900	2.62243500
N	1.81416800	0.38397600	0.13736400
C	1.13831600	-1.34198700	-2.73115800
O	0.24229400	-2.04407400	-3.09709800
O	2.29735000	-1.05258000	-2.68262200

[Ru(Trpy)(bpy)(H-CO$_2$)]$^{1+}$

Ru	0.06952400	-0.00648200	-0.35316900
N	-0.06444500	2.05641600	-0.52560100
N	-0.53916300	-1.95880400	0.02886900
N	2.06780800	-0.29226200	-0.79357500
N	0.93234200	0.15601200	1.49322600
C	-2.58284100	-0.79152100	0.51232700
C	-2.31308300	1.55391000	0.16182300
C	-3.65155300	1.77443700	0.49380500
H	-4.06698000	2.78146000	0.47841600
C	-4.45480000	0.68720100	0.84005200
H	-5.50243600	0.84643600	1.09814100
C	-3.92409400	-0.60381000	0.85214000
H	-4.55306800	-1.45378400	1.11484200
C	-1.85660800	-2.06499700	0.44418800
C	-2.41309000	-3.30771100	0.75312800
H	-3.45178400	-3.37328600	1.07646800
C	-1.63795300	-4.45961600	0.64398900
H	-2.06698300	-5.43354000	0.88362000
C	-0.31153400	-4.34884300	0.22482600
H	0.32545900	-5.22783300	0.12548800
C	0.20125100	-3.09097400	-0.07329700
H	1.23076100	-2.95684900	-0.40851900
C	-1.31902300	2.56248900	-0.22216500
C	-1.57405400	3.93404900	-0.28443600
H	-2.56873200	4.31290900	-0.04934200
C	-0.55613500	4.81288700	-0.64533000
H	-0.74986900	5.88522300	-0.69515700
C	0.70860400	4.30182200	-0.93928700
H	1.53176000	4.95764900	-1.22326600
C	0.91688500	2.92868300	-0.87077200
H	1.88700300	2.48573800	-1.10043900
C	2.57205500	-0.54615200	-2.03211000
H	1.83335500	-0.63197200	-2.83197600
C	3.93162700	-0.70305100	-2.26642300
H	4.28278000	-0.90384400	-3.27889900
C	4.82614200	-0.60272900	-1.19667600
H	5.89907200	-0.72164500	-1.35374600
C	4.32610500	-0.35264600	0.07676700
H	5.00220200	-0.27682900	0.92819800
C	2.94823800	-0.20080500	0.26118600

C	2.30671200	0.05576800	1.54605400
C	2.98941000	0.18988900	2.75926000
H	4.07595900	0.11146200	2.77862300
C	2.28114400	0.42254200	3.93239900
H	2.80843400	0.52912700	4.88131500
C	0.88885200	0.51728600	3.87433800
H	0.29572500	0.69753400	4.77095900
C	0.25026600	0.38164000	2.64887400
H	-0.83381800	0.45165600	2.56264100
N	-1.80407900	0.28398600	0.17878900
C	-1.06420700	-0.77950200	-2.69876500
H	-0.39231400	0.03961200	-2.12135200
O	-2.25677600	-0.46115200	-2.74928800
O	-0.38356600	-1.68546400	-3.19370200

[Ru(Trpy)(bpy)(D-COH)]$^{1+}$

Ru	-0.08682500	0.04572400	-0.38754200
N	0.38218700	-1.97180700	-0.36937800
N	0.18379000	2.09259900	-0.22148100
N	-2.11129700	-0.02772100	-0.83357300
N	-0.90973800	-0.11204000	1.47668700
C	2.37378500	1.33163900	0.40243800
C	2.46862700	-1.05456000	0.38467600
C	3.79726000	-1.02174500	0.80799000
H	4.34892700	-1.94898900	0.96220400
C	4.41650200	0.21247900	1.01996700
H	5.45715600	0.25049200	1.34408000
C	3.70650200	1.39657700	0.81671100
H	4.18667400	2.36136800	0.98008600
C	1.46838600	2.45562000	0.15377800
C	1.82860300	3.80046100	0.27396200
H	2.84579400	4.06444600	0.56363200
C	0.88952500	4.79482000	0.01681000
H	1.16488500	5.84659000	0.10666800
C	-0.40418400	4.42633100	-0.35868300
H	-1.16699500	5.17616400	-0.56919800
C	-0.71821000	3.07670500	-0.46881900
H	-1.71391700	2.74407500	-0.76543000
C	1.66856300	-2.24044400	0.07440700
C	2.13100700	-3.55298300	0.18669800
H	3.14754500	-3.73954000	0.53338500
C	1.29388500	-4.61436400	-0.14664300
H	1.64955100	-5.64215800	-0.06184300
C	-0.00133600	-4.34220400	-0.59078800
H	-0.68632300	-5.14597200	-0.86150100
C	-0.42024400	-3.01980500	-0.68799500
H	-1.42290800	-2.76119200	-1.03147300
C	-2.65887800	0.03289700	-2.07842300
H	-1.94390400	0.10825000	-2.89890100
C	-4.02980600	0.00442100	-2.29561000
H	-4.41411400	0.05609200	-3.31469900
C	-4.89362600	-0.08641200	-1.20053200
H	-5.97509900	-0.10496000	-1.34230700
C	-4.35172000	-0.15263100	0.07816300
H	-5.00636800	-0.21935200	0.94662500
C	-2.96283000	-0.12678700	0.24564300
C	-2.28695400	-0.19442500	1.53874500
C	-2.94620000	-0.33510700	2.76470800
H	-4.03293700	-0.40839300	2.79051600
C	-2.21614800	-0.38671500	3.94625000
H	-2.72574700	-0.49840000	4.90418200
C	-0.82390200	-0.29284800	3.88231900
H	-0.21225400	-0.32469300	4.78427900

C	-0.20965000	-0.15853900	2.64515200
H	0.87407100	-0.08242200	2.55820200
N	1.77853200	0.11507700	0.19262700
C	1.39409900	-0.02936500	-3.05509100
H	1.34595900	0.23169500	-4.13527800
O	0.31122100	0.28866900	-2.43767300
O	2.40848700	-0.56189400	-2.59864900

TS = [Ru(Trpy)(bpy)(H--H-OCHO)]$^{1+}$

Ru	0.09778200	0.05137400	-0.38321000
N	0.63036400	2.02017300	-0.78925000
N	-1.08756800	-1.53835800	0.25793600
N	1.91793100	-0.87459500	-0.74255600
N	0.99848800	0.09969800	1.49548600
C	-2.63627700	0.26918800	0.55646300
C	-1.63228300	2.34911300	-0.04782300
C	-2.80479400	3.02987500	0.28655300
H	-2.86482500	4.11246000	0.17868800
C	-3.90256500	2.30801000	0.75855000
H	-4.82413100	2.82961900	1.01980500
C	-3.82166400	0.92221900	0.90047600
H	-4.67353600	0.35587900	1.27600400
C	-2.36005500	-1.16572000	0.65299500
C	-3.28797700	-2.11507100	1.08800300
H	-4.28711700	-1.79865800	1.38808900
C	-2.93472600	-3.46028600	1.12266700
H	-3.65611600	-4.20924500	1.45245600
C	-1.64782100	-3.83427500	0.72997300
H	-1.33284500	-4.87779000	0.74515400
C	-0.75625200	-2.85316800	0.31117500
H	0.25671000	-3.09954600	-0.01008700
C	-0.38079700	2.93454300	-0.53782300
C	-0.18145100	4.30184100	-0.74361200
H	-0.99097600	5.00392900	-0.54417900
C	1.05061800	4.76205300	-1.19966700
H	1.21237600	5.82849700	-1.36261200
C	2.07019200	3.84070900	-1.44297700
H	3.04968100	4.16158000	-1.79832600
C	1.82633900	2.48868400	-1.22857100
H	2.59263000	1.73466000	-1.41257400
C	2.35373400	-1.31877800	-1.95525800
H	1.65843400	-1.18933200	-2.78454200
C	3.60212300	-1.89650800	-2.14069800
H	3.89548200	-2.23274400	-3.13558300
C	4.46148600	-2.03343300	-1.04744500
H	5.44933700	-2.48092200	-1.16495300
C	4.03778600	-1.58183000	0.19714100
H	4.69534600	-1.66614100	1.06191100
C	2.76900000	-1.00901500	0.33509900
C	2.23691500	-0.49174000	1.59472800
C	2.89969600	-0.57110300	2.82493300
H	3.87254800	-1.05700200	2.89039200
C	2.30972200	-0.03645800	3.96470000
H	2.81992100	-0.09712900	4.92700600
C	1.05911700	0.57564000	3.85696500
H	0.56431600	1.00997100	4.72574200
C	0.43631300	0.62315700	2.61663900
H	-0.54236500	1.08803900	2.49268000
N	-1.56925200	0.98591700	0.08205600
H	-0.44072300	0.08046600	-2.01612600
H	-0.57431600	-0.81160700	-2.15604600
C	-2.06563200	-2.31279900	-2.68086900
H	-2.31495200	-3.35990500	-2.97390900

O	-0.81148400	-2.04525200	-2.76256800
O	-2.97620200	-1.55280600	-2.32460300

7.3 Optimized geometries for catalytic system of 1

[Ru(Bid)(bpy)(Cl)]

Ru	-0.40593600	0.15874700	-0.41870300
Cl	-0.06020000	0.60043600	-2.84299000
N	1.58879200	-0.02435500	-0.20820800
N	1.83146500	-2.45591100	-0.18673000
N	-0.50270400	-1.91716600	-0.77415100
N	2.25432300	2.32470600	-0.09973400
N	-0.21064500	2.21816300	-0.06874900
N	-2.46607200	0.27164300	-0.47073900
N	-0.86759400	-0.24000600	1.51657500
C	2.27903200	-1.21963200	-0.13223300
C	3.71207300	-0.91845000	0.04082500
C	3.83864900	0.47752200	0.03872700
C	2.47988600	1.03080400	-0.10720500
C	4.82271700	-1.74210600	0.17345000
H	4.71953100	-2.82950800	0.17304000
C	6.07862100	-1.13214300	0.30711800
H	6.97183500	-1.75148000	0.41476200
C	6.20532500	0.26497800	0.30355800
H	7.19525300	0.71470700	0.40662900
C	5.07863600	1.08938100	0.16908000
H	5.17111700	2.17767400	0.16499900
C	1.00233300	2.89953800	-0.08292700
C	1.02618400	4.31766500	-0.01784200
H	2.00677700	4.79043600	-0.05738300
C	-0.13106400	5.05560900	0.11481000
H	-0.09845600	6.14551200	0.16741300
C	-1.34666800	4.36238900	0.20041700
H	-2.29484200	4.88435700	0.33159900
C	-1.33743400	2.98240400	0.10542000
H	-2.27422800	2.43407300	0.15961400
C	0.53390000	-2.80093300	-0.49125800
C	0.31514800	-4.20294300	-0.56105500
H	1.16006100	-4.84096300	-0.30496300
C	-0.89543900	-4.72673500	-0.96132100
H	-1.04904700	-5.80621700	-1.01516200
C	-1.91297700	-3.83209600	-1.32305900
H	-2.87972200	-4.18154000	-1.68620200
C	-1.67639600	-2.47353800	-1.21640900
H	-2.45152800	-1.76877200	-1.50680000
C	-3.23600100	0.63744400	-1.53465100
H	-2.67827300	0.93820600	-2.42423500
C	-4.62344500	0.61238100	-1.50358500
H	-5.18780500	0.91105100	-2.38769500
C	-5.27323600	0.19425500	-0.33745400
H	-6.36233200	0.15442800	-0.28791400
C	-4.50623700	-0.16485800	0.76527400
H	-4.99155200	-0.48320900	1.68751200
C	-3.10965100	-0.11184100	0.68915600
C	-2.21062000	-0.40162700	1.80411200
C	-2.63483700	-0.77442000	3.08484400
H	-3.69755200	-0.90519100	3.28840700
C	-1.70210200	-0.97498200	4.09576900
H	-2.02622400	-1.26978300	5.09476200
C	-0.34688800	-0.78544800	3.80918500
H	0.41753100	-0.92253800	4.57450700
C	0.03121700	-0.42221900	2.52454400
H	1.07672900	-0.26545400	2.25927500

[Ru(Bid)(bpy)(H_2)]$^{1+}$

Ru	-0.45782700	0.03713400	-0.67020100
N	1.56588700	0.00463400	-0.46658700
N	1.97964800	-2.40375600	-0.34583800
N	-0.43558400	-2.08282300	-0.74676400
N	2.05884500	2.39585600	-0.32356600
N	-0.37991100	2.15388400	-0.62877100
N	-2.53989200	0.04532100	-0.53248800
N	-0.74917700	-0.04022100	1.38202200
C	2.33293400	-1.14147300	-0.32870300
C	3.73193700	-0.73322800	-0.10548800
C	3.75564000	0.66636300	-0.10122800
C	2.37064300	1.12287100	-0.31779700
C	4.89093200	-1.47563900	0.08092800
H	4.86650800	-2.56748700	0.07802900
C	6.09064800	-0.77572900	0.27068700
H	7.02116500	-1.32800100	0.41836500
C	6.11438800	0.62722300	0.27457400
H	7.06298400	1.14709500	0.42469800
C	4.93893800	1.36819900	0.08934900
H	4.95105300	2.46024300	0.09254200
C	0.78461800	2.89741900	-0.48400400
C	0.73265400	4.31514000	-0.48897700
H	1.68127400	4.83650700	-0.37004000
C	-0.45738900	4.99524400	-0.63857900
H	-0.48240100	6.08651800	-0.64179400
C	-1.62953400	4.24385400	-0.78856100
H	-2.60226200	4.71907500	-0.91554300
C	-1.54440100	2.86318700	-0.77877400
H	-2.44616800	2.27144000	-0.90771300
C	0.69629800	-2.86394600	-0.55104700
C	0.59912900	-4.27929800	-0.56450900
H	1.52260400	-4.83141800	-0.39674900
C	-0.60120300	-4.91998000	-0.78705700
H	-0.66143100	-6.00979400	-0.79540700
C	-1.73592000	-4.13054400	-1.01148000
H	-2.71225300	-4.57352900	-1.20837400
C	-1.60828900	-2.75350600	-0.98374600
H	-2.47944600	-2.13205900	-1.17096100
C	-3.41860400	0.10096500	-1.57387900
H	-2.97225400	0.14879200	-2.56797200
C	-4.79566600	0.09927700	-1.40070200
H	-5.44732000	0.14556900	-2.27335000
C	-5.31779800	0.03960700	-0.10649800
H	-6.39520300	0.03811800	0.06340200
C	-4.43800900	-0.01600900	0.96812200
H	-4.82233500	-0.05991900	1.98609600
C	-3.05743900	-0.01391400	0.74114400
C	-2.05746600	-0.06704300	1.80816600
C	-2.37261100	-0.13521200	3.16934000
H	-3.41399500	-0.15916900	3.48763300
C	-1.35411000	-0.17172500	4.11494600
H	-1.59217900	-0.22335800	5.17821200
C	-0.02905000	-0.13986400	3.67931200
H	0.80042800	-0.16436300	4.38609400
C	0.23571900	-0.07613300	2.31700700
H	1.25777900	-0.04881900	1.94208400
H	0.09973200	0.05891200	-2.31901200
H	-0.73253800	0.16484200	-2.38268200

[Ru(Bid)(bpy)(H)]

Ru	-0.39860400	0.20758900	-0.62877300
H	-0.19338100	0.49137900	-2.23839600
N	1.59807800	0.01354200	-0.42371600

N	1.82269500	-2.42221600	-0.37039900
N	-0.50936900	-1.86972800	-0.95467300
N	2.27784600	2.35902200	-0.29622000
N	-0.18738000	2.26863900	-0.31739500
N	-2.45599200	0.32412200	-0.60853200
N	-0.88208100	-0.22834300	1.43776900
C	2.27749000	-1.18690400	-0.31211300
C	3.70505100	-0.89617700	-0.09254500
C	3.84202400	0.49954500	-0.09298200
C	2.49408800	1.06095400	-0.28889800
C	4.80455400	-1.72742200	0.08293200
H	4.69273800	-2.81404500	0.08226400
C	6.05986300	-1.12692500	0.26028300
H	6.94382900	-1.75284800	0.40164900
C	6.19702600	0.26925900	0.25836600
H	7.18598600	0.71213000	0.39594300
C	5.08174800	1.10170000	0.08177600
H	5.18271700	2.18934200	0.07993500
C	1.03408300	2.94389200	-0.31610400
C	1.06888100	4.36437100	-0.27333400
H	2.05500300	4.82648000	-0.30545200
C	-0.08151500	5.11528100	-0.16870100
H	-0.04016200	6.20556800	-0.13175500
C	-1.30521900	4.43204400	-0.08904300
H	-2.25042900	4.96386300	0.02415600
C	-1.30833400	3.05234400	-0.16592000
H	-2.25104000	2.51395500	-0.12044400
C	0.52716000	-2.76110700	-0.67838900
C	0.30143500	-4.16375400	-0.74270600
H	1.14874900	-4.80293200	-0.49707100
C	-0.91702000	-4.68573800	-1.11712900
H	-1.07538200	-5.76485500	-1.16493400
C	-1.94044000	-3.78690700	-1.45693500
H	-2.91768200	-4.13399200	-1.79374200
C	-1.69613700	-2.42983700	-1.36491000
H	-2.47373600	-1.72326400	-1.64393900
C	-3.24101300	0.69234600	-1.66760000
H	-2.69677700	0.98565400	-2.56559600
C	-4.62687400	0.69057500	-1.62793400
H	-5.19063300	0.99100300	-2.51192300
C	-5.27570700	0.29550900	-0.45296000
H	-6.36472200	0.27528900	-0.39251100
C	-4.50175800	-0.06507700	0.64319600
H	-4.98418200	-0.36399900	1.57334000
C	-3.10376500	-0.04084800	0.56011100
C	-2.22560300	-0.36631400	1.68941300
C	-2.69075500	-0.77090600	2.94869200
H	-3.75891100	-0.88149800	3.13325600
C	-1.78091800	-1.03575500	3.96653000
H	-2.13357500	-1.35515300	4.94861100
C	-0.41470000	-0.88596600	3.71224900
H	0.32898900	-1.08158200	4.48527100
C	-0.01045000	-0.48450300	2.44475300
H	1.04544900	-0.35176200	2.19889300

TS = [Ru(Bid)(bpy)(H--CO2)]

Ru	-0.39165800	0.18761400	-0.35592500
H	-0.04068000	0.34579800	-1.99814900
N	1.59674400	0.07556900	-0.04651700
N	1.89546900	-2.33424400	0.24138800
N	-0.44755800	-1.92324400	-0.41222000
N	2.22211300	2.43127200	-0.24826400
N	-0.24005800	2.27914700	-0.26200200

N	-2.44334500	0.27698200	-0.52438200
N	-1.02458100	0.01358400	1.66516400
C	2.31274200	-1.08787000	0.16942900
C	3.73785800	-0.73945200	0.31068800
C	3.83685100	0.64806300	0.13879700
C	2.46892400	1.15042700	-0.08050700
C	4.86390000	-1.51794800	0.54761100
H	4.78233000	-2.59915600	0.67960900
C	6.10652200	-0.87046500	0.61208800
H	7.01114600	-1.45344400	0.79883700
C	6.20538600	0.51810600	0.43880600
H	7.18545400	0.99734900	0.49182200
C	5.06357900	1.29686100	0.19943400
H	5.13415300	2.37828600	0.06315900
C	0.96274800	2.98111700	-0.31596400
C	0.96187100	4.39920600	-0.39794400
H	1.93605200	4.88201300	-0.46607600
C	-0.20836600	5.12629800	-0.36290900
H	-0.19432500	6.21643700	-0.41879000
C	-1.41454100	4.42234900	-0.23106800
H	-2.37342000	4.93772000	-0.16983200
C	-1.38238800	3.04082000	-0.18708500
H	-2.31189600	2.48543300	-0.09695300
C	0.60910100	-2.74277400	-0.02120400
C	0.42229100	-4.14794300	0.08677500
H	1.28542400	-4.72896800	0.40919800
C	-0.78007600	-4.74491600	-0.22255700
H	-0.90801700	-5.82589800	-0.13934100
C	-1.82697100	-3.92357200	-0.66814700
H	-2.79389800	-4.33549900	-0.95770400
C	-1.61954400	-2.55922500	-0.74542700
H	-2.41748400	-1.91505000	-1.10591200
C	-3.13165000	0.48821200	-1.68509100
H	-2.51427600	0.64604100	-2.57028800
C	-4.51742200	0.49325900	-1.75389100
H	-5.00836600	0.66330800	-2.71271500
C	-5.25985300	0.27530700	-0.58878100
H	-6.35049300	0.26781400	-0.61246900
C	-4.58044200	0.07445200	0.60762200
H	-5.13775800	-0.08490800	1.53034000
C	-3.18126100	0.08317900	0.62928200
C	-2.38409500	-0.08328500	1.84784700
C	-2.92936400	-0.31115100	3.11821600
H	-4.00841900	-0.39364800	3.24650100
C	-2.08659500	-0.43993500	4.21696800
H	-2.50225000	-0.62092200	5.20950000
C	-0.70558100	-0.33567300	4.02951700
H	-0.01282800	-0.43162400	4.86592500
C	-0.21651700	-0.11215000	2.74801200
H	0.85346400	-0.02557000	2.54962000
C	0.26912200	-0.94152300	-3.06393600
O	1.44673200	-1.10171000	-2.97433000
O	-0.80546000	-1.15236900	-3.53657400

[Ru(Bid)(bpy)(H-CO_2)]

Ru	-0.44716500	0.08920700	-0.32607200
N	1.54498300	-0.05663100	-0.02075400
N	1.86491400	-2.47481400	-0.17800700
N	-0.48443800	-1.98075100	-0.74857400
N	2.15829600	2.29958100	0.20567400
N	-0.30045400	2.15822700	0.06025800
N	-2.49389600	0.19813900	-0.49894900
N	-1.02328200	-0.32071800	1.57570000

C	2.26855700	-1.23586000	-0.01309000
C	3.68779400	-0.91011600	0.21726800
C	3.77607900	0.48433300	0.30926900
C	2.40863400	1.01243900	0.15781400
C	4.81631400	-1.71265200	0.32468300
H	4.74311100	-2.79975900	0.24925200
C	6.05083300	-1.08054800	0.53190300
H	6.95797100	-1.68207700	0.62225800
C	6.13905400	0.31671300	0.62276800
H	7.11352800	0.78397400	0.78054900
C	4.99465700	1.11910300	0.51089100
H	5.05715200	2.20739700	0.57720700
C	0.89862100	2.85548300	0.16144700
C	0.89885000	4.27064100	0.26565000
H	1.87340700	4.75360200	0.32199400
C	-0.27430400	4.99282400	0.30952400
H	-0.26056500	6.08136400	0.38965900
C	-1.48282800	4.28501200	0.26340300
H	-2.44587100	4.79333200	0.31395200
C	-1.44772400	2.90789100	0.14283600
H	-2.38012100	2.35284000	0.10204200
C	0.58494600	-2.84178600	-0.52636600
C	0.42286400	-4.24193700	-0.70062200
H	1.29602000	-4.86034700	-0.49738100
C	-0.77075500	-4.78563200	-1.12297900
H	-0.88015300	-5.86359500	-1.25562000
C	-1.83201900	-3.91128000	-1.39554300
H	-2.79362300	-4.27379800	-1.75910500
C	-1.64763800	-2.55506400	-1.19937900
H	-2.45922500	-1.86728500	-1.42056000
C	-3.18560400	0.55643300	-1.61724900
H	-2.57329800	0.84067100	-2.47546700
C	-4.57283000	0.56022600	-1.67055400
H	-5.07630000	0.85289200	-2.59235800
C	-5.29983300	0.18216600	-0.53735600
H	-6.39050300	0.16782800	-0.55347900
C	-4.61073300	-0.16876000	0.61899400
H	-5.15810600	-0.45406900	1.51714600
C	-3.21227500	-0.14801300	0.62579700
C	-2.38142300	-0.44538300	1.79125700
C	-2.87814200	-0.80239000	3.04929800
H	-3.95296300	-0.90079000	3.19958800
C	-2.00051500	-1.02909000	4.10374900
H	-2.38179100	-1.31055800	5.08615500
C	-0.62821600	-0.88683000	3.88344000
H	0.09325700	-1.04937200	4.68428000
C	-0.17608800	-0.53549800	2.61862700
H	0.88509200	-0.41401600	2.40192600
C	0.53115700	0.84142200	-2.79031100
H	-0.27290500	0.24081300	-2.15807100
O	0.15269700	1.98495000	-3.08942200
O	1.51651500	0.15899200	-3.10623700

[Ru(Bid)(bpy)(O-COH)]

Ru	-0.42608800	0.07089000	-0.28802600
N	1.55704700	0.03214200	0.09315400
N	1.99038000	-2.37641700	0.11400600
N	-0.40799500	-2.05477200	-0.37227500
N	2.07073900	2.42335800	0.11774900
N	-0.37230800	2.17217000	-0.13921600
N	-2.43418400	0.10841300	-0.67706600
N	-1.16563300	-0.10951800	1.54105100
C	2.33696700	-1.11243300	0.16964700

C	3.74444400	-0.70558800	0.33241000
C	3.76900300	0.69417200	0.32226800
C	2.37620500	1.14788300	0.16387000
C	4.91240000	-1.44642900	0.46255100
H	4.88826600	-2.53835500	0.46488300
C	6.12048500	-0.74575300	0.58824800
H	7.05724100	-1.29748500	0.69344300
C	6.14472900	0.65716100	0.57879500
H	7.09976400	1.17797700	0.67686100
C	4.96129500	1.39671300	0.44356400
H	4.97363500	2.48878800	0.43208300
C	0.79259400	2.92069900	0.00827900
C	0.73205200	4.33797400	0.07239200
H	1.68304800	4.85882700	0.17528300
C	-0.46645600	5.01575400	0.02319400
H	-0.49834600	6.10542000	0.07869800
C	-1.64148100	4.26073800	-0.09246900
H	-2.62360500	4.73242800	-0.13004800
C	-1.54862100	2.88351900	-0.16749600
H	-2.45694400	2.29711100	-0.26730900
C	0.71319500	-2.83625000	-0.11485900
C	0.61322600	-4.25258700	-0.10523800
H	1.53042600	-4.80234800	0.10118000
C	-0.57949700	-4.89621800	-0.35457200
H	-0.64126600	-5.98604600	-0.34794300
C	-1.70541100	-4.10803400	-0.62753800
H	-2.67562600	-4.55292100	-0.84957600
C	-1.57544000	-2.73114900	-0.62484500
H	-2.44054000	-2.11666300	-0.85628800
C	-2.99620500	0.25091500	-1.90749200
H	-2.28969200	0.34507000	-2.73487300
C	-4.37210400	0.27069900	-2.09836900
H	-4.77509900	0.38677200	-3.10473000
C	-5.21759400	0.13917000	-0.99172600
H	-6.30125800	0.15087000	-1.11552500
C	-4.65762400	-0.00699700	0.27420900
H	-5.29613000	-0.10878100	1.15169200
C	-3.26746700	-0.01929300	0.41378600
C	-2.54399800	-0.15802000	1.67196600
C	-3.14077300	-0.33071500	2.92424800
H	-4.22757500	-0.36946600	2.99995300
C	-2.35002900	-0.45801500	4.06045200
H	-2.80962900	-0.59615300	5.03985600
C	-0.95962000	-0.40918800	3.92277000
H	-0.30249700	-0.50782500	4.78689500
C	-0.40198900	-0.23702300	2.66410900
H	0.67584600	-0.19603700	2.51110300
C	1.04755300	-0.00151400	-3.50834800
H	1.52529100	0.17584800	-4.50749900
O	0.45101000	0.99413000	-3.01060200
O	1.16739400	-1.15099800	-3.02560500

TS = [Ru(Bid)(bpy)(O--COH)]

Ru	-0.42608800	0.07089000	-0.28802600
N	1.55704700	0.03214200	0.09315400
N	1.99038000	-2.37641700	0.11400600
N	-0.40799500	-2.05477200	-0.37227500
N	2.07073900	2.42335800	0.11774900
N	-0.37230800	2.17217000	-0.13921600
N	-2.43418400	0.10841300	-0.67706600
N	-1.16563300	-0.10951800	1.54105100
C	2.33696700	-1.11243300	0.16964700
C	3.74444400	-0.70558800	0.33241000

C	3.76900300	0.69417200	0.32226800
C	2.37620500	1.14788300	0.16387000
C	4.91240000	-1.44642900	0.46255100
H	4.88826600	-2.53835500	0.46488300
C	6.12048500	-0.74575300	0.58824800
H	7.05724100	-1.29748500	0.69344300
C	6.14472900	0.65716100	0.57879500
H	7.09976400	1.17797700	0.67686100
C	4.96129500	1.39671300	0.44356400
H	4.97363500	2.48878800	0.43208300
C	0.79259400	2.92069900	0.00827900
C	0.73205200	4.33797400	0.07239200
H	1.68304800	4.85882700	0.17528300
C	-0.46645600	5.01575400	0.02319400
H	-0.49834600	6.10542000	0.07869800
C	-1.64148100	4.26073800	-0.09246900
H	-2.62360500	4.73242800	-0.13004800
C	-1.54862100	2.88351900	-0.16749600
H	-2.45694400	2.29711100	-0.26730900
C	0.71319500	-2.83625000	-0.11485900
C	0.61322600	-4.25258700	-0.10523800
H	1.53042600	-4.80234800	0.10118000
C	-0.57949700	-4.89621800	-0.35457200
H	-0.64126600	-5.98604600	-0.34794300
C	-1.70541100	-4.10803400	-0.62753800
H	-2.67562600	-4.55292100	-0.84957600
C	-1.57544000	-2.73114900	-0.62484500
H	-2.44054000	-2.11666300	-0.85628800
C	-2.99620500	0.25091500	-1.90749200
H	-2.28969200	0.34507000	-2.73487300
C	-4.37210400	0.27069900	-2.09836900
H	-4.77509900	0.38677200	-3.10473000
C	-5.21759400	0.13917000	-0.99172600
H	-6.30125800	0.15087000	-1.11552500
C	-4.65762400	-0.00699700	0.27420900
H	-5.29613000	-0.10878100	1.15169200
C	-3.26746700	-0.01929300	0.41378600
C	-2.54399800	-0.15802000	1.67196600
C	-3.14077300	-0.33071500	2.92424800
H	-4.22757500	-0.36946600	2.99995300
C	-2.35002900	-0.45801500	4.06045200
H	-2.80962900	-0.59615300	5.03985600
C	-0.95962000	-0.40918800	3.92277000
H	-0.30249700	-0.50782500	4.78689500
C	-0.40198900	-0.23702300	2.66410900
H	0.67584600	-0.19603700	2.51110300
C	1.04755300	-0.00151400	-3.50834800
H	1.52529100	0.17584800	-4.50749900
O	0.45101000	0.99413000	-3.01060200
O	1.16739400	-1.15099800	-3.02560500

TS = [Ru(Bid)(bpy)(H--H--OCOH)]

Ru	0.42327000	0.14980400	-0.38167200
N	-1.59014800	0.09249900	-0.19180400
N	-2.16952000	2.41747400	-0.68747400
N	0.28993500	2.22695900	-0.73751500
N	-1.93705000	-2.22945000	0.49725900
N	0.45636700	-1.93786900	-0.02566100
N	2.49217300	0.21833100	-0.34944700
N	0.81476200	0.43883200	1.64560700
C	-2.43714400	1.17632000	-0.34905100
C	-3.81091500	0.74562600	-0.03231700
C	-3.74066100	-0.60445400	0.33309900

C	-2.32635000	-1.00622400	0.22086900
C	-5.01942300	1.43023700	-0.03603900
H	-5.06759700	2.48329500	-0.32182400
C	-6.17230100	0.72507000	0.33873400
H	-7.13867500	1.23395900	0.34662500
C	-6.10217100	-0.62761300	0.70426500
H	-7.01492200	-1.15387000	0.99234800
C	-4.87749200	-1.31124100	0.70405800
H	-4.81732300	-2.36466900	0.98616400
C	-0.64928300	-2.69235800	0.35045200
C	-0.52049500	-4.08633800	0.58909900
H	-1.42708100	-4.61473900	0.88075700
C	0.68398000	-4.73822500	0.43713000
H	0.76676400	-5.81253900	0.61264500
C	1.79492200	-3.98029300	0.04285200
H	2.77499700	-4.43434400	-0.10446600
C	1.63741600	-2.62212200	-0.16682000
H	2.48946100	-2.03145900	-0.48956200
C	-0.90590900	2.92511800	-0.88192300
C	-0.89480800	4.30547000	-1.21840700
H	-1.86629700	4.78449400	-1.33339000
C	0.28265900	5.00445400	-1.37198700
H	0.27657400	6.06591500	-1.62684900
C	1.48633300	4.31207100	-1.17781600
H	2.45297700	4.80804900	-1.26824400
C	1.44124700	2.96436200	-0.87163500
H	2.36935300	2.41775900	-0.73255100
C	3.31393400	0.16046300	-1.43763100
H	2.80815900	0.11547600	-2.40237000
C	4.69828100	0.15651200	-1.34064000
H	5.30085200	0.10452000	-2.24797000
C	5.29317800	0.21782100	-0.07672700
H	6.37855800	0.21077000	0.03184000
C	4.47487900	0.29715900	1.04455800
H	4.91651900	0.36099800	2.03874400
C	3.08334700	0.30169800	0.89521900
C	2.14239600	0.42185700	2.01008600
C	2.52522000	0.53566200	3.35186200
H	3.58011800	0.51081800	3.62294600
C	1.55529200	0.67969200	4.33771600
H	1.84525200	0.76562200	5.38590700
C	0.20997800	0.71604000	3.96305200
H	-0.58082700	0.83360600	4.70429500
C	-0.11975100	0.59330800	2.61920600
H	-1.15691900	0.61374500	2.28262200
H	0.55236400	-0.73737600	-2.38774400
H	0.11196700	0.03130900	-2.08024400
C	0.23001000	-2.71053400	-3.12527500
H	0.66215000	-3.64596800	-3.54994800
O	1.07710200	-1.73994500	-3.07782700
O	-0.95137400	-2.69273000	-2.76452800

7.4 Optimized geometries for catalytic system of 1d

[Ru(Bid)(4,4'-DMe_2Bpy)(Cl)]

Ru	-0.02289800	-0.50503000	-0.50550900
N	-2.01832600	-0.29373800	-0.37272600
N	-2.35413400	1.76272900	-1.65274200
N	0.01510700	1.10488400	-1.85705200
N	-2.59637200	-2.22233300	1.01484400

N	-0.13808500	-2.12577100	0.82338200
N	2.06146200	-0.57452500	-0.50309100
N	0.42786700	0.81540800	0.98963600
C	-2.75124900	0.74289200	-0.92184900
C	-4.16505000	0.56478000	-0.54552700
C	-4.23858400	-0.60844700	0.21822400
C	-2.86615900	-1.13515900	0.32658200
C	-5.30088800	1.31408800	-0.82594300
H	-5.23868200	2.22706100	-1.42238600
C	-6.52743500	0.86044300	-0.31900300
H	-7.43891900	1.42754800	-0.52068300
C	-6.60130300	-0.31477200	0.44381500
H	-7.56944600	-0.64760200	0.82459600
C	-5.44987300	-1.06579700	0.72206600
H	-5.50177300	-1.98189900	1.31473900
C	-1.33052200	-2.70897800	1.24569100
C	-1.31247100	-3.89521600	2.02828400
H	-2.28163400	-4.30483500	2.31049500
C	-0.13163600	-4.48537500	2.42289400
C	1.06896600	-3.87061900	2.03768400
H	2.03823300	-4.27501000	2.33059700
C	1.01668600	-2.72735800	1.26185200
H	1.94133600	-2.25062700	0.95007200
C	-1.06974100	1.93989800	-2.11200600
C	-0.91563700	3.08143400	-2.94522700
H	-1.80107600	3.69924900	-3.09034500
C	0.28456800	3.37702400	-3.55386000
C	1.36196500	2.50427500	-3.33964600
H	2.33011000	2.66344500	-3.81523700
C	1.18368700	1.41314900	-2.50929500
H	2.00680900	0.72211200	-2.34883900
C	2.85706600	-1.35582100	-1.28145200
H	2.32181300	-2.02873100	-1.95559100
C	4.24258900	-1.31920000	-1.25187100
H	4.80845900	-1.97612000	-1.90859800
C	4.87505400	-0.42453400	-0.36911900
C	4.07214500	0.38383200	0.44932100
H	4.56054900	1.07193900	1.13799500
C	2.68783300	0.29079600	0.37103000
C	1.76970000	1.07281700	1.20608000
C	2.19085700	1.99687800	2.15388600
H	3.24875300	2.19429200	2.31756600
C	1.25017600	2.69998900	2.92006600
C	-0.11450800	2.43605600	2.70529300
H	-0.89536500	2.94288800	3.26742300
C	-0.47049300	1.50098700	1.74631700
H	-1.51984900	1.27192600	1.55914000
H	0.38813600	4.25437200	-4.19513500
H	-0.13212600	-5.39621500	3.02473000
O	6.21828300	-0.26579200	-0.22618500
O	1.75501200	3.58776500	3.81732600
C	7.04231500	-1.11019800	-1.08048600
H	8.07461900	-0.84052300	-0.82279900
H	6.86709700	-2.17781800	-0.86539600
H	6.85160400	-0.89706200	-2.14584200
C	0.76424500	4.33008700	4.58502100
H	0.14945800	3.64993000	5.19818100
H	1.35527400	4.98840200	5.23454800
H	0.12335100	4.93317300	3.91992000
Cl	-0.34011700	-2.10697700	-2.38909300

[Ru(Bid)(4,4'-DMe_2Bpy)]$^+$

Ru	0.04510600	0.35636100	-0.73709400

N	2.05194600	0.25310400	-0.60537800
N	2.45285300	-2.07299000	-1.25258300
N	0.04074700	-1.61580000	-1.50680100
N	2.58498300	2.50594800	0.18701000
N	0.13079400	2.33180100	-0.02370100
N	-2.03793200	0.43672200	-0.82796800
N	-0.46140300	-0.39240200	1.03567200
C	2.81952000	-0.87825600	-0.85252700
C	4.22910300	-0.55358300	-0.57502100
C	4.26816600	0.78450500	-0.16289300
C	2.88208700	1.28081200	-0.17661900
C	5.38805600	-1.31526000	-0.66250400
H	5.35267300	-2.35797000	-0.98543400
C	6.60116200	-0.70144500	-0.32110600
H	7.53054500	-1.27249700	-0.37578400
C	6.64004400	0.63948400	0.09155200
H	7.59889700	1.09284200	0.35218200
C	5.46648600	1.40136100	0.17491700
H	5.48990800	2.44493500	0.49604000
C	1.31120700	3.01836700	0.26037900
C	1.27144700	4.36922100	0.69859400
H	2.23262300	4.84630100	0.88544100
C	0.08072300	5.03203800	0.89676900
C	-1.10831300	4.32782300	0.65752300
H	-2.08512100	4.78749200	0.81019800
C	-1.03763100	3.02162000	0.21410200
H	-1.95515900	2.47537700	0.02019500
C	1.16527600	-2.43466600	-1.57454100
C	1.05232000	-3.77466300	-2.03215700
H	1.97199300	-4.35745100	-2.05792100
C	-0.15542200	-4.30477200	-2.42910400
C	-1.28605500	-3.47708000	-2.37213400
H	-2.26963900	-3.83033200	-2.68259500
C	-1.14534800	-2.18086400	-1.91496900
H	-2.01349600	-1.52972900	-1.87973300
C	-2.78750000	0.92246100	-1.85067100
H	-2.22526800	1.31685200	-2.69939300
C	-4.17388000	0.93080100	-1.84906700
H	-4.70676500	1.33570100	-2.70607500
C	-4.85101800	0.40918900	-0.73047000
C	-4.09040500	-0.09224100	0.33850700
H	-4.60985000	-0.49353300	1.20727700
C	-2.70533900	-0.06680700	0.26708100
C	-1.80942200	-0.55843600	1.31377900
C	-2.23773100	-1.15598200	2.48973100
H	-3.29821300	-1.28943700	2.69925300
C	-1.30286400	-1.61537500	3.42928900
C	0.06457900	-1.43731400	3.15073100
H	0.83936000	-1.76461800	3.83960000
C	0.43561000	-0.83171000	1.96235200
H	1.48658600	-0.68112700	1.71899900
H	-0.22747900	-5.33504800	-2.78223600
H	0.06429600	6.06783900	1.24047900
O	-6.19829800	0.34304500	-0.58137400
O	-1.81482100	-2.20490000	4.53821200
C	-6.98083900	0.84317600	-1.70525500
H	-8.02486600	0.70075700	-1.39886200
H	-6.78107500	1.91387700	-1.87830200
H	-6.77175900	0.25974600	-2.61742500
C	-0.83222600	-2.71718500	5.48636300
H	-0.21230000	-1.89935900	5.88940600
H	-1.43204900	-3.16548400	6.28835500
H	-0.19820900	-3.48618700	5.01422500

[Ru(Bid)(4,4'-DMe_2Bpy)(H_2)]$^+$

Ru	-0.02019200	0.07708000	-0.96118000
N	1.99783300	0.05687700	-0.73526200
N	2.44306200	-2.34815300	-0.76306700
N	0.02106900	-2.03338000	-1.12799200
N	2.45496100	2.44231200	-0.44727200
N	0.02758500	2.18768800	-0.82384800
N	-2.11901100	0.06944800	-0.82692000
N	-0.32985200	-0.08284000	1.09229400
C	2.77919300	-1.08457300	-0.66048000
C	4.16997100	-0.67254600	-0.39708700
C	4.17331100	0.72459700	-0.30309300
C	2.78452800	1.17455700	-0.50940900
C	5.33794100	-1.40915100	-0.24566300
H	5.32931000	-2.49874700	-0.31919000
C	6.52535100	-0.70676200	0.00258500
H	7.46223100	-1.25455800	0.12482800
C	6.52873000	0.69333500	0.09688800
H	7.46808100	1.21564400	0.29053000
C	5.34469000	1.42842900	-0.05443700
H	5.34145400	2.51812300	0.01816900
C	1.17853200	2.93683000	-0.61056300
C	1.10926500	4.35290300	-0.54494200
H	2.04786800	4.87817800	-0.37438700
C	-0.08420000	5.02681200	-0.69425300
C	-1.24216200	4.27059700	-0.91623900
H	-2.21653700	4.74121200	-1.04829300
C	-1.14043400	2.89234300	-0.97244500
H	-2.02953400	2.29664500	-1.15799100
C	1.16518500	-2.81080700	-0.99416300
C	1.08673900	-4.22412700	-1.09893700
H	2.01990200	-4.77284900	-0.97990600
C	-0.10843300	-4.86623600	-1.34280700
C	-1.25830400	-4.08018100	-1.49220400
H	-2.23295900	-4.52423000	-1.69535300
C	-1.14792600	-2.70594200	-1.38063200
H	-2.03041500	-2.08532100	-1.50709500
C	-3.00460100	0.14513000	-1.85803100
H	-2.56481300	0.21672400	-2.85387800
C	-4.38045300	0.13597200	-1.69959000
H	-5.01728500	0.19907100	-2.57858900
C	-4.90852600	0.04441500	-0.39889500
C	-4.01102500	-0.03231600	0.67706900
H	-4.41632000	-0.10355400	1.68454300
C	-2.64233800	-0.02048700	0.44482100
C	-1.64154500	-0.10644100	1.51655300
C	-1.96933800	-0.20923500	2.86090100
H	-3.00523900	-0.22693300	3.19413300
C	-0.95564000	-0.29880400	3.82743500
C	0.38140900	-0.28125100	3.39425200
H	1.21326900	-0.34885300	4.09115500
C	0.64031400	-0.17199600	2.03734000
H	1.66762200	-0.15102800	1.67435800
H	0.55931500	0.17605400	-2.59279900
H	-0.27836100	0.25122800	-2.67011000
H	-0.12273500	6.11652000	-0.64410800
H	-0.15451800	-5.95395400	-1.42145400
O	-6.22593100	0.02227100	-0.07818900
O	-1.37044400	-0.39832300	5.11401200
C	-0.31011700	-0.52953200	6.10702700
H	0.32882800	0.36929400	6.11851800
H	-0.83968100	-0.62675900	7.06321200

H	0.29510800	-1.43100500	5.91565000
C	-7.14551700	0.09268700	-1.20859500
H	-8.14382100	0.04582100	-0.75570500
H	-7.02117100	1.04212500	-1.75535000
H	-6.99725700	-0.76492700	-1.88553300

[Ru(Bid)(4,4'-DMe_2Bpy)(H)]

Ru	0.04412800	0.50226800	-0.80631500
H	0.21795700	1.23853500	-2.27408200
N	2.04167100	0.30950600	-0.65166100
N	2.34298100	-1.99509600	-1.42292400
N	-0.02353600	-1.37671500	-1.74442100
N	2.64421800	2.47105300	0.32484600
N	0.18874000	2.38771000	0.09899400
N	-2.04329500	0.53847700	-0.71754500
N	-0.39267500	-0.50387600	1.07277200
C	2.75574800	-0.84273800	-0.93410600
C	4.16610700	-0.61897100	-0.57435600
C	4.25714600	0.68887800	-0.07586800
C	2.89906500	1.25706200	-0.11766600
C	5.28650900	-1.43676700	-0.65941200
H	5.21018100	-2.45469900	-1.04847400
C	6.51581000	-0.91342500	-0.23163600
H	7.41536900	-1.53071800	-0.28678300
C	6.60697100	0.39487400	0.26686400
H	7.57625400	0.77880100	0.59301400
C	5.47084700	1.21345500	0.35186200
H	5.53600500	2.23245700	0.74006300
C	1.39092900	3.02291400	0.41965800
C	1.39001500	4.34999400	0.93279700
H	2.36546200	4.78765500	1.14313600
C	0.22052400	5.03789800	1.16576400
C	-0.99046200	4.38312400	0.88739900
H	-1.95334600	4.86426500	1.06241400
C	-0.95652200	3.10162900	0.37250600
H	-1.88765500	2.59311600	0.13941000
C	1.05673000	-2.25746700	-1.82419700
C	0.88593600	-3.55580900	-2.38123200
H	1.76900700	-4.19364800	-2.40087700
C	-0.32479700	-3.97710800	-2.88335700
C	-1.40088100	-3.07554900	-2.84240900
H	-2.38031300	-3.33608100	-3.24472500
C	-1.20734800	-1.82731600	-2.28302200
H	-2.02690900	-1.11383200	-2.26576100
C	-2.87373400	1.12364500	-1.62794300
H	-2.37151700	1.64896500	-2.44109700
C	-4.25729400	1.07691600	-1.57009000
H	-4.84081300	1.57103000	-2.34356600
C	-4.86292200	0.38362600	-0.50697200
C	-4.03188200	-0.21514400	0.44928300
H	-4.50008000	-0.74235800	1.27843600
C	-2.64838000	-0.12708700	0.33411600
C	-1.72855000	-0.71890200	1.32132600
C	-2.16051600	-1.43466100	2.43362300
H	-3.21601600	-1.61172800	2.63250700
C	-1.22201800	-1.95487300	3.33724100
C	0.14377800	-1.73056200	3.09035700
H	0.91775200	-2.10625300	3.75550900
C	0.49823100	-1.01045100	1.95854400
H	1.54964000	-0.81591200	1.73504600
H	-0.43998200	-4.97470400	-3.31166500
H	0.23490900	6.05519700	1.56172700
O	-6.20278600	0.23856000	-0.31157300

O	-1.73348900	-2.64321300	4.39371700
C	-7.04848300	0.87578300	-1.31099000
H	-8.07392300	0.65073500	-0.99081400
H	-6.88853800	1.96717400	-1.32385700
H	-6.86568300	0.45043400	-2.31230700
C	-0.74994900	-3.16704600	5.33166900
H	-0.16035400	-2.35043200	5.78122700
H	-1.34572900	-3.66890600	6.10488600
H	-0.08347100	-3.89461200	4.83839600

TS = [Ru(Bid)(4,4'-DMe_2Bpy)(H—H—NMe_3)]$^+$

N	1.86522300	-0.01762000	0.11519300
N	2.43937900	0.12527500	2.48678700
N	0.01991100	-0.32829300	2.31459200
N	2.13251600	0.23235700	-2.30386800
N	-0.09767700	-0.73160400	-1.87092700
N	-2.16205400	-0.73699200	0.25111400
N	-0.75253100	1.46757600	-0.01212500
C	2.68971600	0.22609200	1.20097100
C	3.99993500	0.67656000	0.69683800
C	3.90289600	0.72744000	-0.70093700
C	2.54092000	0.28555600	-1.05322100
C	5.17331100	1.02972500	1.35163000
H	5.24300200	0.99009000	2.44088100
C	6.26290300	1.43782800	0.56868700
H	7.20042200	1.72074100	1.05238900
C	6.16604300	1.48860600	-0.82997400
H	7.02943100	1.81088700	-1.41621600
C	4.97761800	1.13141300	-1.48337900
H	4.89764800	1.16963100	-2.57203000
C	0.91674400	-0.27532500	-2.70675900
C	0.77665500	-0.36625300	-4.11737400
H	1.59913600	0.02489300	-4.71487500
C	-0.33029600	-0.94682800	-4.69829900
H	-0.42115800	-1.01884400	-5.78373500
C	-1.32470400	-1.46045900	-3.85267700
H	-2.21144800	-1.95643500	-4.24788700
C	-1.17003800	-1.33115000	-2.48463200
H	-1.92781000	-1.73384300	-1.81697500
C	1.20282000	-0.15129200	3.02727300
C	1.19807500	-0.19621900	4.44692900
H	2.16008300	-0.06786700	4.94157900
C	0.03210600	-0.36945700	5.16135900
H	0.04152200	-0.39655200	6.25264600
C	-1.16653700	-0.49178000	4.44362900
H	-2.12561900	-0.60939200	4.94859900
C	-1.12460700	-0.46772300	3.06157300
H	-2.04478800	-0.57276900	2.49305400
C	-2.85026400	-1.89662100	0.43882500
H	-2.23680200	-2.77522200	0.64730500
C	-4.23021200	-2.00002600	0.37183100
H	-4.70177800	-2.96657600	0.53249900
C	-4.97944500	-0.84305400	0.08975600
C	-4.29115300	0.36623400	-0.08877400
H	-4.87007000	1.26532200	-0.29314500
C	-2.90479800	0.39923500	-0.00107900
C	-2.11590400	1.63272000	-0.13951700
C	-2.68133800	2.88297900	-0.35497600
H	-3.75703600	3.01242900	-0.46049000
C	-1.86207100	4.01976400	-0.43513800
C	-0.47405400	3.85529100	-0.28398100
H	0.21421400	4.69613800	-0.32494400
C	0.02444400	2.57757300	-0.08130300

H	1.09684800	2.41729200	0.03833600
H	0.89793500	-2.37801200	0.02949800
H	0.14355000	-2.18169700	0.51819000
N	1.88352400	-3.35110900	-0.44471300
Ru	-0.08889100	-0.50872400	0.22209200
C	1.21318600	-4.60956500	-0.07346300
H	0.98893100	-4.59467200	1.00601600
H	0.26613400	-4.69197200	-0.63290400
H	1.84522600	-5.48890700	-0.29848500
C	3.12399000	-3.17511300	0.32962700
H	3.63714000	-2.26156200	-0.00730600
H	2.87370100	-3.07632900	1.39933700
H	3.80601000	-4.03764300	0.19899500
C	2.14858500	-3.30943900	-1.89303300
H	1.19502900	-3.36826600	-2.44249300
H	2.65861000	-2.36733900	-2.14503300
H	2.79207000	-4.15585100	-2.20458000
O	-2.50127600	5.19831400	-0.65050100
O	-6.33203800	-0.78310300	-0.02694800
C	-7.03066300	-2.04915200	0.15706000
H	-6.87312900	-2.44046800	1.17620800
H	-8.09010800	-1.80445800	0.00850700
H	-6.70535300	-2.78900200	-0.59341800
C	-1.64302700	6.37595200	-0.68890900
H	-2.33028600	7.21280200	-0.86709400
H	-1.12323400	6.51195800	0.27411100
H	-0.91336600	6.30544300	-1.51276900

TS = [Ru(Bid)(4,4'-OMe_2Bpy)(H—CO_2)]

Ru	0.06194200	-0.62268600	0.19134800
H	0.39963400	-2.05480400	1.01558900
N	2.04648200	-0.30197900	0.08870100
N	2.36500100	1.28087500	1.92728300
N	0.00759800	0.55246200	1.94269600
N	2.64729900	-1.72485900	-1.80888300
N	0.19150500	-1.75262700	-1.57175500
N	-2.01608300	-0.78815400	0.21771300
N	-0.56876500	1.12586800	-0.86270200
C	2.77036500	0.53124600	0.92341900
C	4.18608500	0.48415000	0.51837200
C	4.27132700	-0.40667600	-0.56071300
C	2.90467900	-0.88921600	-0.82531700
C	5.31484600	1.12457800	1.01445100
H	5.24265700	1.81726200	1.85594700
C	6.54643600	0.85328900	0.40028100
H	7.45258400	1.34105700	0.76650200
C	6.63168500	-0.03838000	-0.67954200
H	7.60301800	-0.23335200	-1.13963500
C	5.48719400	-0.68109200	-1.17436600
H	5.54816600	-1.37676900	-2.01431900
C	1.38806800	-2.13027600	-2.18128700
C	1.37769600	-2.98033100	-3.32078000
H	2.34971300	-3.25229900	-3.73064400
C	0.20188600	-3.41734400	-3.88977500
C	-1.00346100	-2.99215700	-3.31005500
H	-1.97004400	-3.28667800	-3.71981400
C	-0.95978700	-2.18784900	-2.18694700
H	-1.88709800	-1.86507700	-1.72303600
C	1.08078900	1.30851600	2.41412400
C	0.91112000	2.18326000	3.52289000
H	1.78901800	2.75003300	3.83088600
C	-0.29314800	2.29445800	4.18172700
C	-1.36118900	1.50090700	3.73421000

H	-2.33357200	1.52070200	4.22690200
C	-1.16808200	0.67028700	2.64682500
H	-1.98266500	0.03718200	2.30625500
C	-2.72653300	-1.82401700	0.74409600
H	-2.12769300	-2.64721600	1.13619900
C	-4.11048900	-1.86421100	0.80694800
H	-4.59959800	-2.72910000	1.24896900
C	-4.84030500	-0.77559900	0.29685100
C	-4.13025900	0.29121200	-0.27294900
H	-4.69457600	1.12828800	-0.68090500
C	-2.74093100	0.26586000	-0.30774600
C	-1.92871700	1.33746000	-0.90625200
C	-2.47136800	2.47978500	-1.48376500
H	-3.54621900	2.64911900	-1.51709700
C	-1.62569100	3.45343700	-2.03701300
C	-0.23634200	3.23924000	-1.99299800
H	0.47009900	3.95651300	-2.40399200
C	0.23342500	2.07515400	-1.40240700
H	1.30488400	1.87098700	-1.35109700
C	0.66796400	-2.16794400	2.70431200
O	1.84347900	-2.00482000	2.81053900
O	-0.41765300	-2.42871600	3.12317200
H	-0.40824500	2.96779900	5.03323500
H	0.20876400	-4.06428300	-4.76922400
O	-6.19598900	-0.65708300	0.30085200
O	-2.24300200	4.53845500	-2.57641200
C	-6.91437800	-1.76242000	0.91993600
H	-7.97208900	-1.47639900	0.85449800
H	-6.74377500	-2.70193100	0.36774300
H	-6.62056000	-1.88029200	1.97670000
C	-1.35307000	5.55204100	-3.12694600
H	-0.75343900	5.14061300	-3.95607700
H	-2.02474400	6.33457300	-3.50293200
H	-0.69450100	5.96427700	-2.34406800

[Ru(Bid)(4,4'-OMe$_2$Bpy)(H-OCO)]

Ru	-0.01202500	-0.44316000	-0.36954700
N	-1.99632400	-0.14196100	-0.17059500
N	-2.35446600	1.66928400	-1.77326700
N	0.00213700	0.95642400	-1.94631700
N	-2.56867900	-1.85839300	1.47402700
N	-0.11725200	-1.86091600	1.18830700
N	2.05123400	-0.64540100	-0.47984100
N	0.61172200	1.03189700	0.89497500
C	-2.73711700	0.79142800	-0.87340300
C	-4.14698500	0.67490200	-0.45941400
C	-4.21286200	-0.36699100	0.47431000
C	-2.84018900	-0.87444300	0.64839200
C	-5.28491300	1.37392900	-0.84183600
H	-5.22826100	2.18351200	-1.57279500
C	-6.50622900	1.00400100	-0.26042000
H	-7.41998300	1.53405600	-0.53816100
C	-6.57227600	-0.04014600	0.67431700
H	-7.53665500	-0.30974000	1.11039500
C	-5.41852700	-0.74107800	1.05380600
H	-5.46449900	-1.55563700	1.78001200
C	-1.30402600	-2.33187100	1.74234700
C	-1.28463500	-3.38063100	2.69335500
H	-2.25138500	-3.71024000	3.07752300
C	-0.10381200	-3.94125400	3.13508700
H	-0.10245200	-4.74603600	3.87268900
C	1.09391200	-3.43576700	2.61102900
H	2.06373100	-3.82288400	2.92439300

C	1.03934800	-2.42579800	1.66825700
H	1.96287200	-2.03482200	1.25262300
C	-1.08205600	1.75894200	-2.28916800
C	-0.94357000	2.76178400	-3.28599000
H	-1.82857600	3.36002500	-3.49864200
C	0.24266600	2.95512900	-3.95931000
H	0.33327800	3.72752600	-4.72546900
C	1.32242900	2.11880900	-3.64177900
H	2.28170600	2.20355500	-4.15276800
C	1.16031000	1.16286900	-2.65632800
H	1.98686700	0.50254800	-2.40943600
C	2.73514000	-1.59179300	-1.17680500
H	2.11751600	-2.31763700	-1.71040200
C	4.11876600	-1.66112800	-1.22435700
H	4.59498700	-2.44898800	-1.80317300
C	4.86695700	-0.70246200	-0.51626900
C	4.17755700	0.27564800	0.21759200
H	4.75525500	1.01013400	0.77679900
C	2.78951800	0.28230700	0.22528500
C	1.97562100	1.23754400	0.98513300
C	2.50310600	2.26704700	1.75204600
H	3.57751300	2.43149100	1.81600900
C	1.64896300	3.12386600	2.46317800
C	0.26190000	2.90770100	2.37755800
H	-0.45212600	3.53474500	2.90570200
C	-0.20375100	1.86682900	1.59023200
H	-1.27238000	1.67174500	1.49743600
C	-1.00830500	-2.54104400	-1.83545600
H	-0.23266300	-1.65088600	-1.74138000
O	-0.57578700	-3.61529700	-1.38723700
O	-2.03062200	-2.23525500	-2.46728400
O	6.22278500	-0.63420800	-0.46802300
O	2.25438600	4.10266600	3.18241300
C	6.92740600	-1.66545600	-1.21877100
H	6.69248500	-1.59836200	-2.29425800
H	7.99060000	-1.45028900	-1.05200900
H	6.68003000	-2.66895800	-0.83397900
C	1.35775700	4.97783200	3.92769600
H	2.02379500	5.68976800	4.43137800
H	0.67791900	5.51509100	3.24557500
H	0.78220100	4.40532300	4.67412500

[Ru(Bid)(4,4'-DMe_2Bpy)(O-COH)]

Ru	-0.00745500	-0.55284500	-0.32797300
N	-1.99001500	-0.26679700	-0.18384100
N	-2.26549800	1.69727100	-1.61197200
N	0.05050500	0.87827100	-1.85575100
N	-2.60926100	-2.07520600	1.33823400
N	-0.14741300	-1.99527400	1.18812000
N	2.06244100	-0.69980600	-0.38081800
N	0.54032100	0.94074500	0.96122000
C	-2.69319800	0.75283100	-0.80186600
C	-4.10945900	0.64121900	-0.41097500
C	-4.21447200	-0.47877900	0.42697400
C	-2.85688500	-1.03411900	0.57176000
C	-5.22481300	1.40154300	-0.73980300
H	-5.13779400	2.27140600	-1.39452700
C	-6.46272400	1.01597300	-0.20491800
H	-7.35849100	1.59401900	-0.44275800
C	-6.56799400	-0.10517600	0.63175000
H	-7.54444200	-0.38633600	1.03237700
C	-5.43738900	-0.86847500	0.95836900
H	-5.51458800	-1.74294800	1.60834600

C	-1.34913500	-2.54133000	1.63535900
C	-1.34336600	-3.64588400	2.52939300
H	-2.31606400	-4.03886700	2.82303600
C	-0.16908700	-4.17321500	3.02123600
C	1.03748800	-3.57728200	2.62380100
H	1.99934900	-3.92980800	2.99713800
C	0.99964900	-2.52310200	1.73007000
H	1.92678100	-2.05681200	1.40817900
C	-0.99198500	1.76174900	-2.12965400
C	-0.80720800	2.81484900	-3.06482400
H	-1.65380900	3.48296300	-3.21832400
C	0.37012200	2.96255200	-3.76655700
C	1.39146500	2.02772700	-3.54226200
H	2.33295200	2.06621400	-4.09070400
C	1.19187200	1.03203300	-2.60337500
H	1.97168300	0.29482500	-2.42790800
C	2.79593200	-1.63115400	-1.04594100
H	2.21533000	-2.39495300	-1.56724300
C	4.18133400	-1.63372900	-1.08992400
H	4.69677400	-2.41189000	-1.64778900
C	4.87968500	-0.61902700	-0.40952100
C	4.14044100	0.34372600	0.29418600
H	4.67981300	1.12149200	0.83272200
C	2.75226600	0.28344700	0.29956900
C	1.89425800	1.21454800	1.04179400
C	2.37985500	2.27677100	1.79360300
H	3.44558200	2.49420700	1.84488200
C	1.49360700	3.09751300	2.50649200
C	0.11899200	2.80668500	2.44502100
H	-0.61873300	3.39848500	2.98155000
C	-0.30208400	1.73785400	1.66999200
H	-1.36094500	1.48587200	1.60035000
C	-1.01304300	-2.24472300	-2.70106200
H	-0.95255100	-3.23175400	-3.21532600
O	-0.28159000	-2.20401200	-1.64734600
O	-1.73135800	-1.36071400	-3.18657100
H	-0.17968900	-5.01784900	3.71298800
H	0.49441400	3.77128800	-4.48922100
O	6.23227200	-0.48243100	-0.36309000
O	2.05797700	4.11645800	3.20764000
C	1.12427400	4.95715000	3.94533100
H	1.75533500	5.71559800	4.42593200
H	0.40730300	5.44150600	3.26127300
H	0.58913100	4.37085500	4.71111700
C	6.98622300	-1.49840200	-1.08513800
H	6.74798700	-1.47505400	-2.16183400
H	8.03785500	-1.22674300	-0.92734000
H	6.79112800	-2.50200100	-0.67082800

TS = [Ru(Bid)(4,4'-OMe_2Bpy)(---OCOH)]

Ru	0.03898200	-0.46158400	0.26642200
N	2.02995300	-0.17968600	0.13768800
N	2.39534700	1.42475600	1.94641000
N	0.00193500	0.81492900	1.94867000
N	2.59798600	-1.68230400	-1.70949500
N	0.14567100	-1.68624200	-1.44513100
N	-2.01268900	-0.71234000	0.38299200
N	-0.60133600	1.07337500	-0.83115300
C	2.77894300	0.64428500	0.96248900
C	4.19452900	0.53541200	0.56744600
C	4.25384700	-0.38031000	-0.49114000
C	2.87396200	-0.82376600	-0.75458500
C	5.34276000	1.14305100	1.06015800

H	5.29092800	1.85446100	1.88734400
C	6.56675500	0.81298500	0.46116900
H	7.48819600	1.27375800	0.82391200
C	6.62609700	-0.10468600	-0.59882900
H	7.59280700	-0.34605500	-1.04628200
C	5.46283500	-0.71517100	-1.08832900
H	5.50339000	-1.43247600	-1.91104300
C	1.33014100	-2.09181500	-2.05256100
C	1.30257200	-2.99208400	-3.15083400
H	2.26733000	-3.27880800	-3.56732900
C	0.11731100	-3.46718900	-3.66868900
H	0.11013900	-4.15864000	-4.51347400
C	-1.07752000	-3.02734500	-3.08121900
H	-2.05025700	-3.35587600	-3.44814100
C	-1.01550500	-2.16293700	-2.00405700
H	-1.93580400	-1.82675200	-1.53624700
C	1.10594400	1.52124500	2.41770300
C	0.97133800	2.42705500	3.50440600
H	1.87537300	2.94988500	3.81391000
C	-0.23486700	2.62239200	4.14061800
H	-0.32315000	3.31876600	4.97660100
C	-1.33990000	1.88861500	3.68713200
H	-2.31915200	1.97856500	4.15792600
C	-1.17762000	1.02394900	2.62020200
H	-2.02707100	0.44071000	2.27759100
C	-2.66928100	-1.71230500	1.02567200
H	-2.03153700	-2.46545000	1.49389700
C	-4.05145800	-1.79069900	1.10684000
H	-4.50875200	-2.61880800	1.64305000
C	-4.82313300	-0.78650700	0.49255500
C	-4.16004500	0.24734900	-0.18827600
H	-4.75479900	1.02207900	-0.67032200
C	-2.77319900	0.26183000	-0.23063700
C	-1.97034000	1.27550000	-0.91681600
C	-2.50035100	2.35341400	-1.61151900
H	-3.57660300	2.50903900	-1.66877300
C	-1.65012400	3.26744300	-2.25135700
C	-0.26144200	3.05615800	-2.17072800
H	0.45056400	3.72554400	-2.64743500
C	0.21204500	1.96497100	-1.46155400
H	1.28137800	1.77189500	-1.37838600
C	0.90905200	-3.03865000	2.32706200
H	1.19537400	-3.88531700	3.00405100
O	0.55471200	-3.34228300	1.15881900
O	0.97109200	-1.89092000	2.83450400
O	-2.25726500	4.29261400	-2.90373700
O	-6.18022500	-0.71922800	0.49470300
C	-1.35780200	5.23998100	-3.54998400
H	-2.02221100	5.98595900	-4.00443200
H	-0.69841200	5.72280000	-2.80941500
H	-0.75894100	4.74245400	-4.33113600
C	-6.85768700	-1.79020000	1.21402200
H	-7.92575700	-1.55947900	1.11133900
H	-6.63800000	-2.77032000	0.75858600
H	-6.57196300	-1.78892600	2.27932800

TS = [Ru(Bid)(4,4'-OMe_2Bpy)(H--H--OCOH)]

Ru	-0.00533100	0.38019600	-0.55581600
N	1.99849800	0.19775500	-0.39261100
N	2.45058100	-1.48258600	-2.11387600
N	0.02610500	-1.02270600	-2.12695800
N	2.45559800	1.66872300	1.51006300
N	0.04345400	1.79984200	1.00888600

N	-2.09845100	0.37506100	-0.53220400
N	-0.43631500	-1.13209000	0.83491200
C	2.78143800	-0.67066600	-1.13348400
C	4.16524100	-0.59767300	-0.63114900
C	4.16551800	0.31626500	0.43037700
C	2.78300200	0.80738700	0.57373300
C	5.32891000	-1.24780600	-1.02324400
H	5.32289600	-1.96106800	-1.85054900
C	6.50912000	-0.95723600	-0.32354400
H	7.44158700	-1.45029300	-0.60745100
C	6.50981500	-0.04006800	0.73815600
H	7.44269100	0.16863000	1.26655400
C	5.32984900	0.60973700	1.12906700
H	5.32477300	1.32499200	1.95458800
C	1.19065000	2.17385100	1.70254600
C	1.12988600	3.17380500	2.71030000
H	2.06788800	3.42086700	3.20591100
C	-0.05138100	3.80367500	3.03478500
H	-0.08289500	4.57676600	3.80498700
C	-1.20969900	3.42008400	2.34354400
H	-2.17741400	3.87766300	2.55050600
C	-1.11554300	2.44233500	1.37027700
H	-2.00414200	2.15364500	0.81700700
C	1.17694300	-1.64579700	-2.60470100
C	1.10087000	-2.55983000	-3.69120300
H	2.04034200	-3.00512400	-4.01607400
C	-0.09646100	-2.86647200	-4.29893000
H	-0.13980600	-3.57020200	-5.13247200
C	-1.25633500	-2.24556400	-3.81200900
H	-2.23640200	-2.44190200	-4.24753600
C	-1.14808200	-1.35834800	-2.75756700
H	-2.03820600	-0.86160600	-2.38370000
C	-2.92058800	1.17816200	-1.26257200
H	-2.41684500	1.86840200	-1.94060400
C	-4.30391100	1.15485200	-1.18002300
H	-4.88666300	1.83392500	-1.79821500
C	-4.91025800	0.24865900	-0.29132700
C	-4.08246800	-0.59596200	0.46271300
H	-4.55027500	-1.29995400	1.14917000
C	-2.70146600	-0.52042200	0.32862600
C	-1.77074100	-1.37553300	1.07906400
C	-2.18173700	-2.36087600	1.96813500
H	-3.23617200	-2.55427300	2.15666100
C	-1.22877300	-3.13406900	2.64844000
C	0.13299700	-2.88584900	2.40148200
H	0.92084100	-3.44923000	2.89570300
C	0.47236600	-1.89018600	1.49796500
H	1.51968500	-1.67387300	1.28163900
H	-0.04750300	2.33946700	-1.56592700
H	0.32564500	1.50808200	-1.81539100
C	0.44467100	4.30730100	-0.96675900
H	0.09059700	5.32642700	-0.68815900
O	-0.48419200	3.57216200	-1.47611000
O	1.62419800	3.99492400	-0.77585600
O	-1.72185800	-4.07104700	3.50016000
O	-6.24737400	0.10866600	-0.08840000
C	-0.72151400	-4.84542800	4.22328500
H	-1.30446400	-5.52538800	4.85749800
H	-0.09342100	-5.42571900	3.52673800
H	-0.09491000	-4.18873900	4.84998000
C	-7.09423200	0.99650500	-0.87397400
H	-6.96065800	0.81371900	-1.95353700
H	-8.11823200	0.73877200	-0.57468000

H	-6.88536400	2.05278800	-0.63464400

7.5 Optimized geometries for catalytic system of Iw

[Ru(Bid)(4,4'-(COOMe)$_2$Bpy)(Cl)]

Ru	0.56208600	-0.85838400	0.19545600
N	2.52233800	-0.38141700	0.19008700
N	2.70493900	0.85667500	2.28915500
N	0.46056600	-0.16140400	2.18791600
N	3.23049500	-1.36526600	-1.93227400
N	0.77673000	-1.56721000	-1.77656100
N	-1.46213800	-1.16859800	0.18797900
N	-0.08626300	0.95506300	-0.40201800
C	3.16951600	0.35095200	1.16824700
C	4.57890000	0.51766900	0.76719000
C	4.73924100	-0.15547500	-0.45094900
C	3.42139900	-0.71063300	-0.81137800
C	5.64415500	1.16605600	1.37851000
H	5.51381700	1.68805200	2.32897300
C	6.88970200	1.12818200	0.73489600
H	7.74774100	1.62964900	1.18787000
C	7.05034100	0.45362800	-0.48453000

H	8.03150600	0.43744600	-0.96394600
C	5.96919200	-0.19911300	-1.09432800
H	6.08910600	-0.72650300	-2.04322400
C	2.00116400	-1.78042900	-2.39775800
C	2.05858600	-2.42910400	-3.65844300
H	3.05006500	-2.58342000	-4.08215000
C	-0.32112900	-2.54467700	-3.72384400
H	-1.26260200	-2.80588300	-4.20748500
C	-0.34065700	-1.93365400	-2.48248500
H	-1.29331400	-1.72307700	-2.00359300
C	1.44426100	0.61471300	2.78908300
C	1.21356200	1.19510900	4.06405200
H	2.01487500	1.81004000	4.47170400
C	-0.91210600	0.12272400	4.18401200
H	-1.83977800	-0.12687500	4.69929900
C	-0.66738900	-0.40498000	2.92874100
H	-1.39635300	-1.07181700	2.47496600
C	-2.11456500	-2.34586800	0.41964200
H	-1.46511100	-3.20726700	0.58715300
C	-3.49491000	-2.44510300	0.46002000
H	-3.96562500	-3.40784800	0.65474800
C	-4.27023500	-1.29480800	0.25591100
C	-3.62256200	-0.08836700	0.00232900
H	-4.22143800	0.80583600	-0.17074700
C	-2.23038800	-0.04145500	-0.03941500
C	-1.45666700	1.15157400	-0.36732700
C	-2.02103400	2.39127500	-0.66855300
H	-3.10067700	2.52638300	-0.62473100
C	-1.20144000	3.45737700	-1.02982900
C	0.18248400	3.24889500	-1.09235800
H	0.84264000	4.06654300	-1.38174800
C	0.70091500	2.00623500	-0.77802900
H	1.77180000	1.80915000	-0.81476000
C	0.04627500	0.96694400	4.76121400
H	-0.11603700	1.41573400	5.74303600
C	0.91500300	-2.82057700	-4.32269700
H	0.97313500	-3.31644500	-5.29342200
C	-5.75357300	-1.30137100	0.28357800
C	-1.73447800	4.80225200	-1.35771100
O	-6.45195200	-0.30332400	0.11100600
O	-1.03738000	5.75729900	-1.69486800
O	-6.24383100	-2.54937500	0.51736900
O	-3.09060700	4.84807900	-1.23815900
C	-7.70654400	-2.58959100	0.53197600
H	-8.10542300	-2.26111300	-0.44019700
H	-7.95326000	-3.64127000	0.72163800
H	-8.10003700	-1.94468200	1.33272100
C	-3.64090400	6.16499500	-1.56105500
H	-3.41246800	6.42718100	-2.60572300
H	-4.72211600	6.05972700	-1.41106600
H	-3.22384000	6.92871200	-0.88665700
Cl	1.16226000	-3.12564300	0.99424800

[Ru(Bid)(4,4'-(COOMe)$_2$Bpy)]$^+$

Ru	0.58271500	-0.93345500	0.32851400
N	2.56684700	-0.57069500	0.30540300
N	2.79955500	0.85861400	2.27315800
N	0.51503900	-0.07458500	2.25717400
N	3.24226600	-1.79924600	-1.69815900
N	0.78103200	-1.88553100	-1.53674700
N	-1.44335200	-1.23199000	0.36164900
N	-0.03619100	0.76464200	-0.43057400
C	3.24738800	0.22735500	1.21401000

C	4.66412900	0.27862400	0.81469400
C	4.79786400	-0.51752800	-0.32993700
C	3.45835100	-1.03862900	-0.65320400
C	5.75836600	0.92181000	1.37878000
H	5.64831500	1.53804000	2.27360200
C	7.00514600	0.75217900	0.76086300
H	7.88602600	1.24570100	1.17683500
C	7.13929000	-0.04496700	-0.38600400
H	8.12287500	-0.16154700	-0.84592600
C	6.02988900	-0.69317800	-0.94685200
H	6.12913300	-1.31681000	-1.83779800
C	1.99913100	-2.21365600	-2.12425600
C	2.03275900	-2.99965800	-3.30446900
H	3.01798300	-3.24441600	-3.69878800
C	-0.34969600	-2.99886100	-3.38999900
H	-1.29861000	-3.25585500	-3.86100400
C	-0.35015400	-2.25838000	-2.22315000
H	-1.29415900	-1.93991400	-1.79003800
C	1.52830200	0.71964000	2.78500800
C	1.32007600	1.43093600	3.99491000
H	2.14583900	2.04868100	4.34487400
C	-0.85401200	0.47426700	4.20047000
H	-1.79534800	0.32245700	4.72861400
C	-0.63215000	-0.18409100	3.00587200
H	-1.39230200	-0.85490500	2.61391400
C	-2.09612500	-2.37540400	0.71210100
H	-1.45682500	-3.22370800	0.96232500
C	-3.47872800	-2.46254700	0.75724700
H	-3.95622400	-3.39900800	1.04210700
C	-4.24473400	-1.33247000	0.44039600
C	-3.59209300	-0.15887600	0.06959000
H	-4.18425100	0.72006100	-0.18670700
C	-2.20105300	-0.13009700	0.02298700
C	-1.40291500	1.00299100	-0.42180100
C	-1.92560200	2.22028000	-0.85461700
H	-3.00115900	2.38932200	-0.82704600
C	-1.07183000	3.21433200	-1.32423800
C	0.30382000	2.95778500	-1.36064400
H	0.98832500	3.71817700	-1.73673500
C	0.78913600	1.74299400	-0.91410300
H	1.85245500	1.51182600	-0.92655500
C	0.14115700	1.32457000	4.70136600
H	-0.00502600	1.87437600	5.63283700
C	0.87573000	-3.40347400	-3.93649000
H	0.91532000	-4.00225500	-4.84812900
C	-5.73058700	-1.32321800	0.46750600
C	-1.55887100	4.53452600	-1.79706900
O	-6.41423300	-0.33689400	0.19996400
O	-0.82461000	5.42340800	-2.22244800
O	-6.23426400	-2.53627900	0.81626900
O	-2.91202800	4.63357100	-1.70089900
C	-7.69874300	-2.55368900	0.83617800
H	-8.09438200	-2.28640100	-0.15572300
H	-7.96056300	-3.58557400	1.09914100
H	-8.07781600	-1.84689800	1.59047600
C	-3.41569600	5.92622300	-2.16892400
H	-3.17537500	6.06497600	-3.23427300
H	-4.50026400	5.87442500	-2.01562000
H	-2.97397500	6.74362600	-1.57875800

[Ru(Bid)(4,4'-(COOMe)$_2$Bpy)(H$_2$)]$^+$

Ru	0.53925700	-1.16324900	0.16199100
N	2.53268100	-0.75554900	0.09330600

N	2.97338300	-0.19696800	2.43488800
N	0.60296600	-0.86420000	2.26411900
N	2.96725800	-0.94798900	-2.30670500
N	0.59166700	-1.50655400	-1.93329100
N	-1.53709700	-1.24516400	0.18011700
N	0.04557600	0.82096900	-0.11670800
C	3.29985300	-0.35115000	1.17544700
C	4.65769400	-0.04883200	0.68746100
C	4.65575000	-0.26621600	-0.69502200
C	3.29677200	-0.70347200	-1.06261900
C	5.80052300	0.38024800	1.34997100
H	5.79539400	0.55041600	2.42861200
C	6.95759200	0.58711300	0.58624400
H	7.87446800	0.92388200	1.07457700
C	6.95572300	0.36886800	-0.79996000
H	7.87134500	0.53855900	-1.37038500
C	5.79668800	-0.06192800	-1.46017600
H	5.78934000	-0.23251700	-2.53876500
C	1.71652800	-1.34393700	-2.73072700
C	1.64636200	-1.59618400	-4.12474900
H	2.56264000	-1.44385800	-4.69294500
C	-0.64920900	-2.19766700	-3.91652600
H	-1.60020700	-2.53812600	-4.32591800
C	-0.54875900	-1.93637300	-2.56192100
H	-1.41586400	-2.08457400	-1.92512300
C	1.72508100	-0.44443700	2.96544700
C	1.65428300	-0.23644300	4.36655700
H	2.56756700	0.09969500	4.85512000
C	-0.63404800	-0.90012500	4.36573000
H	-1.58135000	-1.10289300	4.86528500
C	-0.53327700	-1.08678700	2.99874000
H	-1.39606000	-1.44313100	2.44307200
C	-2.30602400	-2.36352800	0.33013600
H	-1.76134100	-3.29829000	0.46505900
C	-3.69079300	-2.33522900	0.31341800
H	-4.25455300	-3.25879600	0.43606500
C	-4.34332300	-1.11030300	0.13764500
C	-3.57632800	0.04071900	-0.01283400
H	-4.08368100	0.99471100	-0.15460500
C	-2.18444700	-0.04108600	0.01094600
C	-1.30002500	1.11270600	-0.13961800
C	-1.75607900	2.42271200	-0.29424700
H	-2.82281400	2.63779000	-0.30356400
C	-0.83913100	3.45980000	-0.43516500
C	0.52474300	3.16005500	-0.41753300
H	1.26070600	3.95655200	-0.52616700
C	0.93003400	1.84525300	-0.25701300
H	1.98600700	1.58275100	-0.23655000
H	1.27517400	-2.72723000	0.40153900
H	0.45413500	-2.89180500	0.39701000
C	0.47930500	-2.01842000	-4.72552400
H	0.44018300	-2.21166100	-5.79902900
C	0.48993000	-0.45498900	5.07202900
H	0.44973100	-0.29045000	6.15026700
C	-5.82417500	-0.97607300	0.10199700
C	-1.25468200	4.87879800	-0.60357000
O	-0.46620500	5.80967800	-0.74344800
O	-6.41156700	0.09736800	-0.01231100
O	-6.43525500	-2.18458900	0.20455900
O	-2.60667800	5.00669700	-0.58107800
C	-7.89636700	-2.08669900	0.15881000
H	-8.24538900	-3.12485300	0.21027700
H	-8.26393500	-1.50528300	1.01825100

H	-8.21542000	-1.60812600	-0.77966900
C	-3.04813400	6.39442800	-0.74019800
H	-4.14248300	6.34420200	-0.69284800
H	-2.64556300	7.01622500	0.07400100
H	-2.71507100	6.78979600	-1.71205900

[Ru(Bid)(4,4'-(COOMe)$_2$Bpy)(H)]

Ru	0.62149900	-1.02228200	0.41718000
H	0.95332000	-2.39159500	1.26197900
N	2.58554700	-0.55562600	0.40102400
N	2.66837100	1.13988700	2.16273200
N	0.44446300	0.07515500	2.21042300
N	3.37721600	-1.95215600	-1.44251900
N	0.92223800	-2.15267500	-1.32675400
N	-1.40140000	-1.25638900	0.35774900
N	-0.01438200	0.78026800	-0.58072800
C	3.18044900	0.41057700	1.19356700
C	4.59096300	0.54174900	0.78751700
C	4.80556100	-0.37761500	-0.24867700
C	3.51957800	-1.05493300	-0.49300100
C	5.61644400	1.35520400	1.25305500
H	5.44397300	2.06924600	2.06139000
C	6.87722900	1.22896300	0.65167400
H	7.70448700	1.85491200	0.99353600
C	7.09208000	0.30887800	-0.38519900
H	8.08404300	0.22929500	-0.83529000
C	6.05092800	-0.50821500	-0.85001100
H	6.21244700	-1.22577100	-1.65752100
C	2.17446600	-2.49465500	-1.83356000
C	2.28574400	-3.43131200	-2.89523400
H	3.29524700	-3.67497300	-3.22422500
C	-0.08874100	-3.57393600	-3.03753400
H	-1.00853100	-3.94688000	-3.48881300
C	-0.16290100	-2.68371200	-1.98255500
H	-1.13485300	-2.36871300	-1.61154500
C	1.39945300	0.97925100	2.66892500
C	1.11751200	1.81041800	3.78604200
H	1.89959400	2.50838700	4.08218100
C	-1.00574800	0.75939500	4.05190800
H	-1.95157800	0.61321900	4.57406000
C	-0.71087900	-0.01924600	2.94831400
H	-1.41528900	-0.78137500	2.62231800
C	-2.09531700	-2.37148100	0.75601100
H	-1.47706200	-3.21447600	1.06390900
C	-3.47547000	-2.44032200	0.78706200
H	-3.96588800	-3.35349400	1.12177400
C	-4.22694600	-1.32247400	0.39287800
C	-3.54520600	-0.18840900	-0.04080000
H	-4.12330200	0.67793200	-0.36218700
C	-2.15183600	-0.16721900	-0.06612000
C	-1.37594900	0.97165000	-0.56391600
C	-1.95171700	2.16244800	-1.01785300
H	-3.03052600	2.30683900	-0.98991400
C	-1.13277800	3.17639800	-1.50859300
C	0.25243000	2.97428200	-1.54113500
H	0.90679600	3.75668800	-1.92607400
C	0.76734400	1.77668200	-1.07233800
H	1.84059500	1.57676200	-1.07793700
C	-0.07295200	1.71849600	4.47414400
H	-0.27487100	2.36010200	5.33402300
C	1.17319700	-3.98113600	-3.49519400
H	1.27250800	-4.69717600	-4.31316900
C	-5.70687400	-1.29106100	0.40732600

C	-1.67094400	4.46903600	-2.00408700
O	-6.38381000	-0.32637700	0.05066200
O	-0.97516600	5.37552500	-2.45714600
O	-6.22923800	-2.46328700	0.86682600
O	-3.02701500	4.52591900	-1.89499700
C	-7.69166100	-2.46022900	0.89355800
H	-8.09334000	-2.31473700	-0.12124700
H	-7.96481800	-3.44874800	1.28234600
H	-8.06058200	-1.66300400	1.55728200
C	-3.57767200	5.79048300	-2.38432800
H	-3.35803100	5.91230500	-3.45628300
H	-4.65790000	5.70911500	-2.21359000
H	-3.15365300	6.63537200	-1.82024000

TS = [Ru(Bid)(4,4'-(COOMe)$_2$Bpy)(H—H—NMe$_2$)]

N	2.33949600	0.07985500	0.11030300
N	3.00977100	-0.09554900	2.45329700
N	0.61753800	-0.67520700	2.29685600
N	2.47776500	0.70160500	-2.25078600
N	0.43110000	-0.63333400	-1.91665100
N	-1.53317000	-1.14713700	0.22036800
N	-0.43632800	1.22838300	0.17702700
C	3.19180700	0.22338800	1.19399300
C	4.43324600	0.86431500	0.72198400
C	4.26287100	1.12842400	-0.64377400
C	2.93123600	0.61778400	-1.01873200
C	5.60386300	1.21238600	1.38367800
H	5.73233300	1.00374000	2.44792600
C	6.61465900	1.83697700	0.63888900
H	7.54847200	2.12207000	1.12818300
C	6.44371600	2.10235700	-0.72790600
H	7.24621600	2.59207200	-1.28360800
C	5.25867700	1.74731600	-1.38837700
H	5.12112700	1.95117000	-2.45241500
C	1.32669100	0.08640600	-2.69691100
C	1.13774800	0.16962500	-4.10068300
H	1.85731600	0.76913900	-4.65638900
C	-0.73661600	-1.29918600	-3.94977800
H	-1.54095700	-1.88559400	-4.39389800
C	-0.54686900	-1.32905700	-2.57989000
H	-1.19377100	-1.94426200	-1.95800700
C	1.81442600	-0.53031100	2.98777300
C	1.86459800	-0.77225500	4.38463200
H	2.83619700	-0.66380300	4.86479600
C	-0.48624500	-1.17028900	4.41433700
H	-1.42122600	-1.39322600	4.92854600
C	-0.49550100	-0.95764100	3.04733100
H	-1.43206700	-1.01804800	2.49867800
C	-2.04999800	-2.40957200	0.31369000
H	-1.31671300	-3.20799000	0.43703200
C	-3.40644200	-2.67684800	0.24732600
H	-3.76454700	-3.70246100	0.32721600
C	-4.30344600	-1.61528100	0.06873700
C	-3.79776500	-0.32086000	-0.01596400
H	-4.49439000	0.50719500	-0.14665100
C	-2.42484100	-0.10061600	0.07437400
C	-1.81000800	1.22623700	0.06685100
C	-2.53455200	2.41740400	-0.00389400
H	-3.61968100	2.39867000	-0.09039200
C	-1.86278000	3.63604900	0.04291600
C	-0.46995200	3.63556400	0.16811100
H	0.07325800	4.57957300	0.21055500
C	0.20439600	2.42738600	0.23521900

H	1.28841300	2.38667300	0.34292300
H	1.57589700	-2.31951900	-0.21799600
H	0.87523700	-2.30434600	0.33588500
N	2.68067600	-3.14074000	-0.89691300
Ru	0.44986200	-0.64128600	0.19437100
C	2.09610200	-4.48711900	-0.78577300
H	1.84666100	-4.68826700	0.26964100
H	1.16950300	-4.53030800	-1.38347600
H	2.79313300	-5.26887900	-1.14445500
C	3.87425000	-3.02175100	-0.04448500
H	4.32445200	-2.02612400	-0.18176700
H	3.58044400	-3.14156800	1.01240500
H	4.63121200	-3.79191600	-0.29330300
C	2.99912100	-2.82756800	-2.29895400
H	2.08182400	-2.88459100	-2.90711500
H	3.41498200	-1.81026900	-2.36453900
H	3.74142300	-3.54073500	-2.71147100
C	0.11501700	-0.50686700	-4.73213000
H	-0.01347000	-0.44274400	-5.81419500
C	0.73241800	-1.09870000	5.10191200
H	0.78328200	-1.27793400	6.17739600
C	-5.77241900	-1.80334800	-0.02630800
C	-2.57213900	4.94142500	-0.02208200
O	-6.57542000	-0.88698900	-0.19362800
O	-2.00974700	6.03279700	0.02268500
O	-6.11627800	-3.11349200	0.09880100
O	-3.91668900	4.76990500	-0.12993900
C	-7.56131600	-3.32888300	0.01058900
H	-7.69045700	-4.40900300	0.14932100
H	-8.07926600	-2.76624000	0.80252300
H	-7.93421600	-3.01235200	-0.97571400
C	-4.65072600	6.03540600	-0.17892100
H	-4.35048600	6.61548500	-1.06507900
H	-5.70554600	5.74257000	-0.24254500
H	-4.46072300	6.62172200	0.73313200

TS = [Ru(Bid)(4,4'-(COOMe)$_2$Bpy)(H—CO$_2$)]

Ru	0.61324800	-0.72398400	-0.00801000
H	1.18875000	-2.25211200	0.40748200
N	2.54068400	-0.12915700	-0.03025100
N	2.69150600	1.06945300	2.09365400
N	0.49526400	-0.04326900	1.99183500
N	3.30068100	-1.16542500	-2.11012100
N	0.84365100	-1.34940400	-1.99741400
N	-1.36339700	-1.21259700	0.00746000
N	-0.29077700	1.11611300	-0.51380800
C	3.17527000	0.58061100	0.97219200
C	4.59985000	0.71394800	0.61799800
C	4.78615900	0.02538000	-0.58827400
C	3.46857800	-0.49792500	-0.99094200
C	5.65988200	1.33950400	1.26169500
H	5.50994300	1.87362000	2.20248100
C	6.92639400	1.26260400	0.66400100
H	7.78074100	1.74507900	1.14390500
C	7.11284700	0.57253000	-0.54307100
H	8.11023200	0.52471400	-0.98554800
C	6.03695500	-0.05616700	-1.18653600
H	6.17651500	-0.59540600	-2.12605300
C	2.07522500	-1.53912200	-2.61716800
C	2.14181600	-2.11822100	-3.91072500
H	3.13746100	-2.26497600	-4.32753400
C	-0.23844300	-2.18087100	-4.02144000
H	-1.17587300	-2.39056500	-4.53704400

C	-0.26931600	-1.64747600	-2.74554900
H	-1.22541000	-1.44495400	-2.26943900
C	1.43173800	0.80256600	2.57825700
C	1.15158600	1.42061200	3.82637500
H	1.91639800	2.08786800	4.22195700
C	-0.92257000	0.25194400	3.95615800
H	-1.84533100	-0.02231200	4.46775400
C	-0.63150700	-0.31395000	2.72874800
H	-1.31837100	-1.03557200	2.29291000
C	-1.87326700	-2.47075100	0.18384700
H	-1.13184400	-3.26587600	0.26733200
C	-3.22914100	-2.73143300	0.27243900
H	-3.57802900	-3.75251200	0.42132600
C	-4.13918400	-1.66786300	0.18114600
C	-3.64244600	-0.38323700	-0.02881400
H	-4.34691500	0.44427700	-0.11638500
C	-2.26947900	-0.17079900	-0.12794100
C	-1.66286200	1.13211500	-0.40549400
C	-2.39168400	2.31215400	-0.57490700
H	-3.47665500	2.31067400	-0.48394600
C	-1.72028300	3.49868000	-0.85905100
C	-0.32557800	3.47803700	-0.97841500
H	0.21454200	4.39790000	-1.20325100
C	0.34819700	2.28034200	-0.80202100
H	1.43421300	2.21503200	-0.88471400
C	1.68666700	-2.74233700	1.93384500
O	2.83708400	-2.43225700	1.97408500
O	0.70516100	-3.26055800	2.37302400
C	1.00291000	-2.44696600	-4.61561300
H	1.06811800	-2.88435100	-5.61355400
C	-0.01580500	1.16596100	4.51299200
H	-0.21746700	1.64601700	5.47251500
C	-2.42794300	4.79277400	-1.04046400
C	-5.60565100	-1.84373800	0.29377500
O	-6.41990100	-0.92206800	0.24357500
O	-1.86352000	5.85783400	-1.28065400
O	-5.94143200	-3.15349800	0.46026200
O	-3.77495400	4.65095900	-0.90850800
C	-4.49542500	5.91126000	-1.09609700
H	-4.32175900	6.30038900	-2.11133400
H	-5.55131800	5.65309600	-0.95123900
H	-4.16667700	6.65285100	-0.35203400
C	-7.38520200	-3.35557600	0.58172000
H	-7.90083700	-2.98041600	-0.31575200
H	-7.50764400	-4.44107300	0.67858200
H	-7.76819900	-2.83693800	1.47427100

[Ru(Bid)(4,4'-(COOMe)$_2$Bpy)(H-CO$_2$)]

Ru	0.41885900	-0.79737900	0.09297600
N	2.39803600	-0.37250300	0.10427800
N	2.72771900	0.24886400	2.44605800
N	0.40437100	-0.54506900	2.19407000
N	2.99462000	-0.82323400	-2.22360900
N	0.55803400	-1.13437300	-1.99201500
N	-1.60850100	-1.07188700	0.07158700
N	-0.21642700	1.10368200	-0.16359500
C	3.11567200	0.05868900	1.20698800
C	4.50995400	0.29505500	0.79071900
C	4.59172700	-0.03293500	-0.56748400
C	3.24429200	-0.45525700	-0.99013500
C	5.62304400	0.73462700	1.49534500
H	5.55486100	0.98511300	2.55613600
C	6.83513800	0.84491700	0.79879500

H	7.72957800	1.18994300	1.32195900
C	6.91703000	0.51597800	-0.56255000
H	7.87416800	0.60875800	-1.08030100
C	5.78861400	0.06890400	-1.26460900
H	5.84671900	-0.19217600	-2.32342500
C	1.74990900	-1.16228300	-2.70645600
C	1.75677500	-1.53813700	-4.07450100
H	2.72679700	-1.55365400	-4.56919300
C	0.59423800	-1.85686900	-4.74289400
H	0.61333600	-2.14555600	-5.79534300
C	-0.61135400	-1.78653500	-4.03322400
H	-1.56786300	-2.01098700	-4.50552700
C	-0.58158900	-1.43129800	-2.69710500
H	-1.51212900	-1.38539400	-2.13970800
C	1.47396200	-0.04926300	2.93030900
C	1.33894500	0.17057900	4.32631300
H	2.21169800	0.56928300	4.84130500
C	0.16934300	-0.11919300	4.99490400
H	0.08046900	0.05293100	6.06912600
C	-0.89573900	-0.65219900	4.25676800
H	-1.84131400	-0.92128000	4.72757600
C	-0.73686800	-0.84272500	2.89664500
H	-1.55242400	-1.26821400	2.31891300
C	-2.26069900	-2.26851900	0.15211300
H	-1.61871500	-3.14994200	0.20130800
C	-3.64183700	-2.36863600	0.17278800
H	-4.11578900	-3.34643300	0.24429400
C	-4.41206100	-1.19984000	0.10557000
C	-3.76218800	0.02802800	0.00404100
H	-4.35888400	0.93833000	-0.05739500
C	-2.37025900	0.07543400	-0.01742000
C	-1.58489300	1.29797000	-0.15581900
C	-2.13017300	2.57263600	-0.29687100
H	-3.21004300	2.72320700	-0.29469400
C	-1.29333200	3.67443000	-0.45066700
C	0.09190100	3.47393500	-0.45863400
H	0.77751000	4.31163200	-0.57560400
C	0.59207200	2.19012100	-0.31422200
H	1.66326300	1.99209600	-0.31792300
C	1.56136500	-3.31170400	0.24313200
H	0.67143600	-2.57190000	0.51411700
O	1.33715000	-3.97202300	-0.78110000
O	2.45519200	-3.32748000	1.10005300
C	-5.89674900	-1.20646800	0.13526500
C	-1.91701900	5.01465400	-0.60709100
O	-6.59056500	-0.19366800	0.06514000
O	-3.12959200	5.21557700	-0.59023400
O	-6.38640500	-2.46968700	0.25304500
O	-0.97673200	5.98154900	-0.77620000
C	-7.84888600	-2.50953500	0.30333400
H	-8.27394000	-2.10697900	-0.62883600
H	-8.09361100	-3.57255300	0.41663500
H	-8.21628000	-1.92843600	1.16305800
C	-1.55505500	7.31558100	-0.94602800
H	-2.12349500	7.60229700	-0.04802500
H	-0.69066000	7.97511200	-1.08834300
H	-2.21348500	7.33612100	-1.82802500

[Ru(Bid)(4,4'-(COOMe)$_2$Bpy)(O-COH)]

Ru	0.52780900	-0.84152900	0.06118300
N	2.44509900	-0.23074200	0.07667500
N	2.50581700	1.00826100	2.17964800

N	0.38472900	-0.24496500	2.07101400
N	3.25289400	-1.21035100	-2.00957700
N	0.79859000	-1.44634400	-1.93524800
N	-1.45228900	-1.32508300	0.04742000
N	-0.28353300	0.94245900	-0.42325600
C	3.02671200	0.54029500	1.06716100
C	4.43532300	0.77443800	0.70090000
C	4.66523500	0.08717600	-0.49940500
C	3.38619100	-0.53299800	-0.89159800
C	5.45105800	1.48130900	1.33161300
H	5.26850700	2.01334600	2.26776700
C	6.71665900	1.48921700	0.72714500
H	7.53638400	2.03707200	1.19693700
C	6.94649200	0.80082100	-0.47317300
H	7.94250400	0.82026500	-0.92079900
C	5.91576100	0.08847100	-1.10336000
H	6.08934200	-0.45076800	-2.03709000
C	2.04520400	-1.64063100	-2.51870100
C	2.14533900	-2.26823400	-3.78698600
H	3.15000300	-2.41634100	-4.18105700
C	-0.23357400	-2.36466600	-3.94333600
H	-1.15684200	-2.60455900	-4.47099700
C	-0.29617900	-1.78244400	-2.68979500
H	-1.26326600	-1.56689500	-2.24105700
C	1.27468000	0.63532800	2.67502200
C	0.98219700	1.17004800	3.95612400
H	1.70239500	1.87648800	4.36672000
C	-0.98015900	-0.18074900	4.08805400
H	-1.85587800	-0.56164700	4.61365100
C	-0.68726900	-0.65278200	2.82066200
H	-1.32616600	-1.40517200	2.36279500
C	-1.98667800	-2.57456200	0.18484000
H	-1.25953900	-3.38538600	0.25613500
C	-3.35009600	-2.79688400	0.25383900
H	-3.74423500	-3.80669300	0.37079200
C	-4.23063500	-1.70732700	0.18605800
C	-3.70373200	-0.42810200	0.01980700
H	-4.37020700	0.43004200	-0.05387200
C	-2.32233100	-0.25645200	-0.06212200
C	-1.66303800	1.01988900	-0.32227600
C	-2.33430500	2.22621900	-0.51070700
H	-3.41898500	2.28450400	-0.41719700
C	-1.62099800	3.37914100	-0.82839200
C	-0.22888000	3.29366300	-0.96486200
H	0.36187600	4.17149900	-1.22311600
C	0.39752900	2.07681000	-0.75683000
H	1.47815100	1.96852600	-0.84793900
C	1.91378200	-3.16496800	1.48039800
H	2.07183000	-4.26715100	1.51298100
O	1.12760500	-2.82090300	0.52303900
O	2.47393700	-2.44938500	2.31874700
C	1.02349900	-2.64042800	-4.49840800
H	1.11446000	-3.11779200	-5.47587400
C	-0.13749500	0.78106300	4.66201500
H	-0.34651000	1.19325000	5.65096700
O	-6.19081400	-3.08007400	0.37818600
O	-3.59682100	4.74108100	-0.88560100
O	-6.40138300	-0.80104800	0.25059800
O	-1.55246400	5.67517800	-1.33578300
C	-2.37711200	4.64268400	-1.01134600
C	-5.68843200	-1.96184600	0.28180700
C	-2.27032600	6.93452700	-1.53484500
H	-1.49205700	7.65874300	-1.80378600

H	-3.00716600	6.83015600	-2.34627400
H	-2.77966000	7.23442900	-0.60587600
C	-7.84530800	-1.02023200	0.33373400
H	-8.28056200	-0.01396900	0.31049500
H	-8.19044400	-1.61532100	-0.52586800
H	-8.10183900	-1.53755400	1.27107700

TS = [Ru(Bid)(4,4'-(COOMe)$_2$Bpy)(--O-COH)]

Ru	0.46670900	-0.70721400	0.07217400
N	2.44033500	-0.27010700	0.06798700
N	2.67578800	0.83072400	2.23684800
N	0.38435400	-0.07057500	2.09451900
N	3.11698800	-1.20741200	-2.08557600
N	0.65350800	-1.28033300	-1.94525000
N	-1.52171100	-1.13392700	0.08988700
N	-0.27748800	1.06058200	-0.37220000
C	3.12343400	0.35462800	1.09896100
C	4.54923000	0.42588200	0.73187900
C	4.68276000	-0.19626600	-0.51599900
C	3.33473600	-0.62378200	-0.93158600
C	5.64860500	0.95394900	1.39629700
H	5.53840300	1.43672100	2.36968700
C	6.90118500	0.84573400	0.77586800
H	7.78626800	1.25169700	1.27037500
C	7.03542900	0.22077000	-0.47302100
H	8.02337800	0.14707600	-0.93260000
C	5.92005300	-0.30950900	-1.13689100
H	6.01905600	-0.79794300	-2.10866100
C	1.86703300	-1.50517000	-2.58532900
C	1.89110100	-2.04362800	-3.89685300
H	2.87364400	-2.21894500	-4.33293600
C	0.72955500	-2.30388800	-4.59329900
H	0.76288800	-2.71346100	-5.60446400
C	-0.49087800	-2.00592000	-3.97370300
H	-1.44354200	-2.16332100	-4.47968700
C	-0.48114100	-1.50894500	-2.68282400
H	-1.42248100	-1.28132700	-2.18966900
C	1.39434600	0.65590600	2.71254500
C	1.17321000	1.24014300	3.98680500
H	1.99649200	1.81422000	4.40969000
C	-0.01401100	1.06443700	4.66574500
H	-0.16948900	1.51646700	5.64711600
C	-1.00119900	0.26664900	4.07218300
H	-1.94485500	0.05472100	4.57505600
C	-0.76378700	-0.26708900	2.81807700
H	-1.51327500	-0.90385300	2.35503200
C	-2.07626200	-2.36755700	0.25772500
H	-1.36535700	-3.19009600	0.35906900
C	-3.44697900	-2.56366800	0.31408000
H	-3.84884800	-3.56600900	0.45571000
C	-4.30237500	-1.45861200	0.19786400
C	-3.74898500	-0.19352300	0.00856500
H	-4.40917100	0.66819100	-0.09298800
C	-2.36594900	-0.05102700	-0.05187200
C	-1.65740500	1.19624600	-0.30063800
C	-2.26754900	2.43229600	-0.49121100
H	-3.35111900	2.53213200	-0.42034100
C	-1.49672800	3.55616400	-0.77538300
C	-0.10671700	3.41112500	-0.87511300
H	0.52882400	4.26565600	-1.10315300
C	0.46637700	2.16783600	-0.66984800
H	1.54270700	2.01482400	-0.73233400
C	1.90610400	-3.70065400	1.20868100

H	2.44503900	-4.66893400	1.37889400
O	1.37778600	-3.56955600	0.06996800
O	1.89733400	-2.88750800	2.16216600
C	-5.78119900	-1.57059900	0.26641200
C	-2.19362100	4.85438800	-0.95540100
O	-3.40999800	5.00116700	-0.84966800
O	-6.54883200	-0.61363100	0.18120600
O	-6.17815600	-2.86036300	0.43662300
O	-1.32059800	5.85445300	-1.24979400
C	-1.98248800	7.14784700	-1.43028300
H	-1.17250700	7.84143700	-1.68568000
H	-2.72227100	7.08756700	-2.24334500
H	-2.48088600	7.45315700	-0.49716900
C	-7.63310800	-2.99588700	0.52393000
H	-7.80458500	-4.07123400	0.65357400
H	-8.01614500	-2.43042900	1.38736300
H	-8.10673300	-2.62969600	-0.39989600

TS = [Ru(Bid)(4,4'-(COOMe)$_2$Bpy)(H--H--O-COH)]

Ru	-0.08913100	-0.35257000	-0.27492800
N	-0.21585800	1.64771500	-0.07574100
N	2.14718500	2.23003600	0.16823600
N	1.99942500	-0.15487600	-0.46139400
N	-2.63458000	1.98619500	-0.20645800
N	-2.19439100	-0.44168700	-0.14851800
N	0.08715500	-2.39829500	-0.31261700
N	0.19486200	-0.75044200	1.68850500
C	0.86112200	2.49332200	0.12902000
C	0.34543500	3.86437300	0.30254500
C	-1.04710200	3.79872300	0.16009200
C	-1.38940500	2.38113700	-0.06815200
C	0.98927000	5.07148500	0.54111800
H	2.07526700	5.11671800	0.64836000
C	0.20042200	6.22711700	0.63970500
H	0.67623700	7.19190400	0.82919200
C	-1.19319200	6.16193300	0.49529600
H	-1.78425000	7.07719600	0.57292800
C	-1.83527700	4.93849600	0.25206400
H	-2.92004000	4.88250800	0.13683700
C	-3.03326600	0.66535500	-0.26967200
C	-4.42561600	0.49695800	-0.40475200
H	-5.04258900	1.38673500	-0.50942900
C	-5.01644600	-0.76236500	-0.37688600
C	-4.17603100	-1.87509800	-0.17747800
H	-4.56071800	-2.88975300	-0.10795800
C	-2.81408500	-1.65900100	-0.07578900
H	-2.15753400	-2.51347000	0.07127700
C	2.70444200	1.00442000	-0.13958800
C	4.11310900	1.01275500	-0.15964100
H	4.62520900	1.93510700	0.10556400
C	4.84708100	-0.10594600	-0.54059700
C	4.13288500	-1.25563800	-0.92807900
H	4.62738900	-2.16051200	-1.27249900
C	2.75143900	-1.22130000	-0.86881500
H	2.19455200	-2.10364500	-1.17691900
C	-0.06403200	-3.20207900	-1.40350900
H	-0.35560800	-2.68658500	-2.32061100
C	0.15282000	-4.57195900	-1.36324400
H	0.02309900	-5.16556900	-2.26884200
C	0.54414400	-5.16603800	-0.15767700
H	0.73310900	-6.23894100	-0.09972500
C	0.68437900	-4.36589100	0.97094800
H	0.97845500	-4.80796900	1.92280500

C	0.44418600	-2.98954600	0.88284000
C	0.50390200	-2.06177000	2.00895900
C	0.80686400	-2.43515900	3.32348500
H	1.05313800	-3.47299900	3.54814900
C	0.79165400	-1.48500400	4.33789500
H	1.03067100	-1.76817400	5.36381400
C	0.45959200	-0.16460700	4.01725800
H	0.42891000	0.61155700	4.78257600
C	0.17007500	0.16344300	2.70087300
H	-0.09371300	1.18064400	2.41067900
C	0.01997428	0.60058101	-3.84395873
H	-0.37036772	0.45664101	-4.87836873
O	-0.54973572	-0.18127599	-3.00098773
O	0.90512028	1.44511401	-3.65109273
O	-6.37176600	-0.80891400	-0.52456600
O	6.20575600	0.01584500	-0.52234200
C	-6.95619600	-2.13980100	-0.46525900
H	-6.78093700	-2.60624100	0.51920000
H	-8.03160600	-1.97717700	-0.61495600
H	-6.55929000	-2.78383900	-1.26833800
C	6.94078400	-1.16961600	-0.93579000
H	7.99789600	-0.88684000	-0.84615600
H	6.72289200	-2.02361000	-0.27185800
H	6.71083700	-1.43237000	-1.98242200

7.6 Optimized geometries for catalytic system of 1d'

[Ru(4,4'-(OMe)$_2$ Bid)(Bpy)(Cl)]

Ru	-0.04718000	-0.31400300	-0.37389300
N	-0.22164100	1.68705100	-0.19857900
N	2.12789500	2.34861100	-0.01451800
N	2.04478500	-0.05857200	-0.55300500
N	-2.65434100	1.95382600	-0.23444000
N	-2.14506600	-0.46253600	-0.22063400
N	0.19204300	-2.36169000	-0.37512500
N	0.23085400	-0.66928900	1.59575500
C	0.83305800	2.57080800	-0.05202900
C	0.28212300	3.93302100	0.08466900
C	-1.11129800	3.82090600	-0.00332200
C	-1.41729500	2.38657000	-0.16874900
C	0.89652000	5.16685300	0.25513700
H	1.98366100	5.24854000	0.32127200
C	0.07619900	6.30168500	0.33778700
H	0.52820400	7.28694700	0.47209300
C	-1.31916400	6.18955300	0.24836800
H	-1.93516600	7.08920900	0.31327900
C	-1.93116900	4.93904900	0.07663800
H	-3.01717700	4.84562600	0.00605100
C	-3.01896900	0.62197500	-0.26714500
C	-4.41307500	0.41946100	-0.30294600
H	-5.05675100	1.29529800	-0.34492700
C	-4.96950100	-0.85491900	-0.26260000
C	-4.08827700	-1.94899300	-0.16980600
H	-4.43971500	-2.97646500	-0.11528800
C	-2.72836200	-1.69759700	-0.15373400
H	-2.04313300	-2.53874200	-0.08700500
C	2.71868100	1.12438200	-0.25490600

C	4.12785400	1.16021800	-0.23039700
H	4.61318400	2.10224800	0.01555500
C	4.89378500	0.04160300	-0.54133800
C	4.21262900	-1.13418000	-0.91131900
H	4.73376300	-2.04120200	-1.20730900
C	2.82992100	-1.12345100	-0.89853600
H	2.29874200	-2.02477200	-1.19560500
C	0.08449400	-3.19703200	-1.44809400
H	-0.20406000	-2.70890100	-2.38154100
C	0.33931100	-4.55898500	-1.37144400
H	0.24240800	-5.17616100	-2.26534800
C	0.72425100	-5.11455000	-0.14612200
H	0.94023700	-6.18036900	-0.05849100
C	0.82249400	-4.28363700	0.96420500
H	1.11111600	-4.69418100	1.93149200
C	0.54646600	-2.91696000	0.83892400
C	0.56700100	-1.96602600	1.94621900
C	0.86227200	-2.30501500	3.27201900
H	1.13195800	-3.33153300	3.52075700
C	0.81007500	-1.33605900	4.26702000
H	1.04278400	-1.59281800	5.30129300
C	0.44838100	-0.03132700	3.91546600
H	0.38730700	0.75881100	4.66454400
C	0.16824400	0.26398800	2.58947300
H	-0.11586000	1.26854900	2.27627800
O	-6.33103800	-0.93399200	-0.30109200
O	6.24913800	0.18656700	-0.47944300
C	-6.87484700	-2.28161500	-0.23238100
H	-7.96357400	-2.14366100	-0.26463400
H	-6.54790500	-2.88614800	-1.09552800
H	-6.58772200	-2.77724500	0.71065300
C	7.01526000	-0.99737500	-0.83742600
H	8.06447300	-0.69531800	-0.72155000
H	6.78963000	-1.83754500	-0.15870300
H	6.82336200	-1.29085100	-1.88350000
Cl	-0.31721900	-0.08351100	-2.84213200

[Ru(4,4'-(OMe)$_2$ Bid)(Bpy)]$^+$

Ru	-0.05500900	-0.31837300	-0.49734000
N	-0.19089700	1.69490100	-0.38464200
N	2.16943600	2.31898300	-0.18031500
N	2.05446800	-0.09778500	-0.67250700
N	-2.61873400	2.00257200	-0.37939100
N	-2.15275300	-0.42569400	-0.41170000
N	0.13259700	-2.37301700	-0.53581500
N	0.16718600	-0.71150700	1.42014900
C	0.88230600	2.56300500	-0.22451100
C	0.35207200	3.93078100	-0.07710700
C	-1.04317500	3.84219900	-0.15178600
C	-1.37691500	2.41635000	-0.32520000
C	0.98955900	5.15209800	0.09954800
H	2.07839400	5.21417600	0.15660000
C	0.18924500	6.29838400	0.20311700
H	0.65842600	7.27443000	0.34461400
C	-1.20907100	6.21003400	0.12717300
H	-1.80891400	7.11894700	0.21014100
C	-1.84398400	4.97286400	-0.05201200
H	-2.93201400	4.89830300	-0.11055000
C	-3.00743800	0.67881400	-0.43718800
C	-4.40362300	0.50547400	-0.48644400
H	-5.02839400	1.39527400	-0.51490700
C	-4.98735500	-0.75729700	-0.47197500
C	-4.12881000	-1.87093400	-0.38697600

H	-4.50289300	-2.89090400	-0.34464600
C	-2.76577200	-1.65161700	-0.35801800
H	-2.10126700	-2.50883000	-0.29455800
C	2.74446600	1.08256000	-0.39813600
C	4.15196800	1.10201700	-0.36874100
H	4.64756800	2.04437700	-0.14653000
C	4.90575900	-0.03650200	-0.63683600
C	4.21031200	-1.21794400	-0.96108400
H	4.72138500	-2.14412500	-1.21163500
C	2.82942600	-1.19061800	-0.95865400
H	2.29091400	-2.09875000	-1.21714700
C	0.04386200	-3.17015500	-1.63558400
H	-0.19363200	-2.65567800	-2.56875300
C	0.24824900	-4.54246900	-1.58390500
H	0.16805300	-5.13482400	-2.49574100
C	0.56016600	-5.13903700	-0.35744200
H	0.73370500	-6.21383100	-0.28939400
C	0.64399900	-4.34109800	0.77884200
H	0.87954900	-4.78317100	1.74668100
C	0.42215600	-2.96450500	0.67326900
C	0.44175100	-2.02185800	1.78285000
C	0.68341900	-2.36537000	3.11627800
H	0.90459500	-3.40228400	3.37077000
C	0.63904500	-1.39159700	4.10661300
H	0.82967700	-1.65290300	5.14810100
C	0.33952100	-0.07583300	3.74083600
H	0.28591000	0.71904700	4.48512900
C	0.11090900	0.23144900	2.40803100
H	-0.12257000	1.24552300	2.08802100
O	-6.34676800	-0.80699400	-0.52450400
O	6.25959800	0.09370700	-0.57652800
C	-6.92294300	-2.14346300	-0.48391600
H	-8.00728500	-1.97788400	-0.52655200
H	-6.59941200	-2.74004100	-1.35358600
H	-6.65928000	-2.65993200	0.45439900
C	7.01449900	-1.10926900	-0.89885900
H	8.06636600	-0.81287600	-0.79509700
H	6.78235600	-1.92459400	-0.19314000
H	6.81581300	-1.43270500	-1.93458100

[Ru(4,4'-(OMe)$_2$ Bid)(Bpy)(H$_2$)]$^+$

Ru	0.00222500	-0.35494900	-0.57446800
N	0.01568500	1.67505800	-0.43113900
N	2.42047100	2.12010200	-0.29538900
N	2.12393700	-0.31522700	-0.59155300
N	-2.38361700	2.15289700	-0.30067900
N	-2.12332900	-0.28469900	-0.61347500
N	-0.02302000	-2.43020500	-0.36440900
N	-0.00894600	-0.56993800	1.48359600
C	1.15445500	2.45496700	-0.29342800
C	0.72938500	3.85371900	-0.09229100
C	-0.66977100	3.86286100	-0.09434100
C	-1.11296100	2.47009600	-0.29702800
C	1.45891000	5.02268400	0.08237100
H	2.55097700	5.00913400	0.08395800
C	0.74609400	6.21757400	0.25426500
H	1.28818900	7.15553800	0.39254700
C	-0.65701000	6.22665500	0.25234600
H	-1.18740700	7.17149500	0.38919900
C	-1.38466600	5.04112800	0.07836700
H	-2.47681700	5.04141500	0.07695800
C	-2.88182300	0.87393900	-0.46678100
C	-4.28779200	0.81820400	-0.48290700

H	-4.83837000	1.74817800	-0.36155900
C	-4.97208300	-0.38199900	-0.65497300
C	-4.20523600	-1.55047400	-0.82188200
H	-4.65775600	-2.52708200	-0.97341900
C	-2.82775600	-1.44274300	-0.79365800
H	-2.23325200	-2.34154800	-0.93415000
C	2.89964000	0.83342300	-0.45895100
C	4.30432100	0.75748900	-0.48729900
H	4.86936300	1.68035800	-0.37868000
C	4.96970300	-0.45362200	-0.65737600
C	4.18518500	-1.61299300	-0.80467100
H	4.62305600	-2.59720400	-0.95006600
C	2.80961300	-1.48550000	-0.76547300
H	2.20012600	-2.37640500	-0.89196600
C	-0.03668200	-3.35002000	-1.37227000
H	-0.02767700	-2.94350000	-2.38449500
C	-0.06332500	-4.71901900	-1.14621800
H	-0.07207500	-5.40384500	-1.99448800
C	-0.08143400	-5.19172200	0.16840700
H	-0.10620400	-6.26173300	0.37879900
C	-0.06832000	-4.27106500	1.20943900
H	-0.08632300	-4.61570500	2.24256700
C	-0.03507900	-2.90021700	0.92960600
C	-0.01347400	-1.86191800	1.95933800
C	0.00352300	-2.12730500	3.33278500
H	0.00915700	-3.15695200	3.68749100
C	0.01692600	-1.07601200	4.24213300
H	0.03014000	-1.27560800	5.31440400
C	0.01421200	0.23253700	3.75684200
H	0.02352100	1.08736900	4.43318200
C	0.00335900	0.44768100	2.38472300
H	0.00547500	1.45564200	1.97276600
H	-0.01304100	0.14403400	-2.24078600
H	0.07879600	-0.69254500	-2.27654000
O	-6.33152500	-0.32058100	-0.65269800
O	6.32960600	-0.41050400	-0.67211600
C	6.98978600	-1.69421300	-0.86810500
H	8.06171800	-1.45762100	-0.86073800
H	6.75259300	-2.38840600	-0.04447800
H	6.70938000	-2.13764400	-1.83815600
C	-7.01038900	-1.59531400	-0.84432600
H	-8.07919900	-1.34604800	-0.82077900
H	-6.74944900	-2.03807600	-1.82004900
H	-6.76961600	-2.29565700	-0.02694300

[Ru(4,4'-(OMe)$_2$ Bid)(Bpy)(H)]

Ru	-0.07002200	-0.32618600	-0.56202600
H	-0.23546300	-0.23864900	-2.20412200
N	-0.25270700	1.68078100	-0.41651400
N	2.09747700	2.35052100	-0.22816100
N	2.02080600	-0.06345900	-0.73603500
N	-2.68892600	1.93475900	-0.38389400
N	-2.16929300	-0.47725000	-0.43460800
N	0.18606300	-2.36493100	-0.44701100
N	0.23161300	-0.64295100	1.54788800
C	0.79925500	2.56603300	-0.24692800
C	0.24442800	3.91876100	-0.05434800
C	-1.15054100	3.80058100	-0.11595300
C	-1.45061500	2.37243300	-0.32806700
C	0.85437400	5.15021700	0.14878600
H	1.94223700	5.23667600	0.19524500
C	0.02933400	6.27616400	0.29090900
H	0.47849900	7.25888900	0.45143400

C	-1.36699300	6.15776700	0.22854000
H	-1.98715100	7.04992900	0.34097700
C	-1.97486100	4.90975500	0.02431900
H	-3.06172000	4.81122400	-0.02416100
C	-3.05012600	0.60679800	-0.45387200
C	-4.44569500	0.40063200	-0.50036300
H	-5.09048900	1.27649500	-0.52406200
C	-4.99926200	-0.87378400	-0.49427700
C	-4.11456800	-1.96804300	-0.42361900
H	-4.46367500	-2.99746600	-0.39415400
C	-2.75590300	-1.71491300	-0.39672900
H	-2.06879200	-2.55588700	-0.35306400
C	2.69253900	1.13203500	-0.47157000
C	4.10359400	1.17861600	-0.46862000
H	4.58349700	2.13063400	-0.25196500
C	4.87455900	0.05877500	-0.75485500
C	4.19756400	-1.13522900	-1.07365500
H	4.72253700	-2.04910300	-1.34067000
C	2.81556900	-1.13398900	-1.04935100
H	2.28825200	-2.04785700	-1.31296700
C	0.09759500	-3.24182800	-1.49602400
H	-0.19018200	-2.79417000	-2.44751500
C	0.35979300	-4.59812800	-1.38367500
H	0.27531500	-5.23662100	-2.26380900
C	0.73510900	-5.12070500	-0.14077500
H	0.95677300	-6.18211200	-0.02112300
C	0.81454100	-4.25673100	0.94434700
H	1.09511600	-4.64186400	1.92417600
C	0.53398500	-2.89318900	0.78624800
C	0.56371700	-1.93226400	1.89273900
C	0.88105000	-2.27310400	3.21569000
H	1.14592800	-3.29842500	3.47269500
C	0.85813500	-1.29565500	4.20423200
H	1.10613200	-1.55103400	5.23574000
C	0.51092500	0.01316200	3.85522300
H	0.47854300	0.80708900	4.60217700
C	0.20775600	0.29523900	2.52915600
H	-0.07140500	1.30230100	2.21192200
O	-6.36244400	-0.95678400	-0.54284100
O	6.23151500	0.21572400	-0.71831900
C	-6.89987700	-2.30737500	-0.51808400
H	-7.98905100	-2.17442700	-0.55909900
H	-6.56010800	-2.88635500	-1.39390200
H	-6.62205200	-2.82959600	0.41352100
C	6.99927300	-0.97188700	-1.05624300
H	8.04833600	-0.65759500	-0.97618100
H	6.79867700	-1.79247700	-0.34623200
H	6.78549700	-1.30205700	-2.08721200

TS = [Ru(4,4'-$(OMe)_2$ Bid)(Bpy)(H—H—NMe_3)]$^+$

N	0.16135800	1.54280900	0.18261700
N	2.56019700	2.00721400	0.05260300
N	2.24400900	-0.43165600	-0.16040100
N	-2.20943100	1.96405500	0.62769600
N	-1.97871800	-0.32849400	-0.26083900
N	0.04280300	-2.50011600	-0.31427700
N	-0.00473100	-0.98391800	1.81891400
C	1.30406700	2.32379500	0.25895900
C	0.90584800	3.68693200	0.66194800
C	-0.48133500	3.66591700	0.85809000
C	-0.94034100	2.29850900	0.54560400
C	1.64505900	4.84549400	0.86296300
H	2.72621600	4.85670500	0.70877800

C	0.95751200	5.99912200	1.26753800
H	1.50889400	6.92728000	1.43288500
C	-0.43121200	5.97808600	1.46398800
H	-0.94226000	6.88971400	1.78142600
C	-1.17013900	4.80359700	1.25936400
H	-2.25141000	4.78211000	1.41171900
C	-2.72344900	0.74959200	0.21267600
C	-4.13032100	0.69001900	0.24047700
H	-4.67402100	1.55091900	0.62323800
C	-4.82549700	-0.41776800	-0.23543000
C	-4.07367500	-1.48278000	-0.76942100
H	-4.53941200	-2.37100300	-1.18921500
C	-2.69465800	-1.38449600	-0.75362400
H	-2.10615600	-2.19906700	-1.17111500
C	3.02338600	0.72389100	-0.16997900
C	4.41773000	0.64835000	-0.35454200
H	4.98572100	1.57597600	-0.36634300
C	5.07279600	-0.57240900	-0.48708900
C	4.29411700	-1.74297100	-0.40688400
H	4.73013900	-2.73687100	-0.46791700
C	2.92662000	-1.61400900	-0.24918600
H	2.31947500	-2.51456500	-0.19601600
C	0.11860200	-3.23965100	-1.46023400
H	0.27885200	-2.66693000	-2.37528800
C	-0.00425500	-4.62130800	-1.47941900
H	0.06447200	-5.15519600	-2.42778100
C	-0.21856100	-5.30353700	-0.27745500
H	-0.32579800	-6.38895200	-0.26125400
C	-0.29060300	-4.57200000	0.90246000
H	-0.45058600	-5.08359000	1.85147400
C	-0.15305400	-3.17918600	0.87241200
C	-0.17229300	-2.33005200	2.06418100
C	-0.32324800	-2.81494100	3.36859700
H	-0.45674300	-3.88205800	3.54195600
C	-0.30119300	-1.93227800	4.44267300
H	-0.42029900	-2.30241400	5.46195700
C	-0.11857500	-0.56993900	4.19301500
H	-0.08929200	0.15555000	5.00641200
C	0.02562200	-0.13631500	2.88152000
H	0.17610700	0.91779100	2.64609000
H	-0.15357400	0.43051700	-2.10221200
H	0.33274700	-0.31809700	-1.88638900
N	-0.65793000	1.37864100	-3.09519800
Ru	0.13014300	-0.44660400	-0.18393800
C	-0.53445600	0.57292300	-4.32229800
H	0.50484600	0.21826700	-4.42103900
H	-1.20254200	-0.30165800	-4.24638200
H	-0.80363400	1.15763600	-5.22187600
C	0.27847900	2.51555100	-3.12102700
H	0.12441200	3.13395800	-2.22356300
H	1.31355700	2.13377000	-3.12206200
H	0.12619900	3.14322000	-4.02017800
C	-2.04627900	1.83515900	-2.91252000
H	-2.71483100	0.96193200	-2.84550400
H	-2.12159200	2.42402100	-1.98579600
H	-2.37122000	2.46669100	-3.76293600
O	6.42360800	-0.52994900	-0.66337400
O	-6.18521500	-0.36679900	-0.16081700
C	7.07188000	-1.82683000	-0.79518100
H	6.68810900	-2.37203300	-1.67415300
H	8.13525400	-1.59274200	-0.93528100
H	6.93663700	-2.43014100	0.11833100
C	-6.88149100	-1.54170000	-0.66411200

H	-7.94560200	-1.31876000	-0.51159200
H	-6.67990100	-1.69333500	-1.73806500
H	-6.60158400	-2.44242900	-0.09168100

TS = [Ru(4,4'-$(OMe)_2$ Bid)(Bpy)(H—CO_2)]

Ru	-0.12686800	-0.31496600	-0.32042900
H	-0.31328600	-0.06359300	-1.97922200
N	-0.30359600	1.67929200	-0.07251700
N	2.03943700	2.33401100	0.20991200
N	1.97682400	-0.06158200	-0.38209700
N	-2.73138400	1.95875400	-0.22757700
N	-2.22871500	-0.45790100	-0.24829600
N	0.09988300	-2.35753200	-0.39902300
N	0.09904100	-0.82036700	1.72100900
C	0.74572500	2.55806900	0.13552700
C	0.19342900	3.91875200	0.27371100
C	-1.19490800	3.81374900	0.11876100
C	-1.49622400	2.38452400	-0.08858200
C	0.80254200	5.14692700	0.49709600
H	1.88559200	5.22314800	0.61604900
C	-0.01741700	6.28320500	0.56407400
H	0.43084700	7.26387800	0.73883200
C	-1.40732600	6.17832200	0.40727100
H	-2.02308400	7.07893300	0.46099400
C	-2.01422000	4.93358400	0.18236000
H	-3.09603200	4.84592200	0.05895200
C	-3.10019500	0.63107200	-0.29472400
C	-4.49431400	0.43358500	-0.37022300
H	-5.13343900	1.31254700	-0.41690000
C	-5.05614600	-0.83818000	-0.35679400
C	-4.18103000	-1.93658900	-0.24896400
H	-4.53790600	-2.96286900	-0.20787900
C	-2.82104000	-1.69179400	-0.20047400
H	-2.14004600	-2.53564200	-0.12551100
C	2.63880900	1.11576600	-0.02960700
C	4.04657400	1.14945700	0.05986000
H	4.51878500	2.08787700	0.34220000
C	4.82595400	0.03507900	-0.22797100
C	4.16131100	-1.13798000	-0.63700800
H	4.69535900	-2.04406400	-0.91193400
C	2.78049900	-1.12578400	-0.69387900
H	2.26588300	-2.02405800	-1.02678400
C	0.01334300	-3.12683900	-1.52559600
H	-0.25678000	-2.58917000	-2.43495000
C	0.26114600	-4.49160100	-1.53392300
H	0.18161200	-5.04711900	-2.46908200
C	0.61589500	-5.12937500	-0.34006400
H	0.82731600	-6.19933100	-0.31778700
C	0.68564000	-4.37294700	0.82418400
H	0.94494100	-4.85076700	1.76904700
C	0.41818000	-2.99913700	0.78607900
C	0.42274200	-2.13501800	1.96861700
C	0.70487100	-2.57939600	3.26727300
H	0.96551500	-3.62226200	3.44514100
C	0.65347300	-1.68383800	4.32988900
H	0.87619000	-2.02006700	5.34371500
C	0.31114900	-0.35185000	4.07812300
H	0.25694700	0.38017400	4.88452800
C	0.04259700	0.03764000	2.77213600
H	-0.22904000	1.06589400	2.52660900
C	0.93485500	0.38320800	-3.07138500
O	0.94758100	1.57269900	-3.01261900
O	1.27321600	-0.67163000	-3.51178900

O	-6.41743200	-0.91242300	-0.43254800
O	6.17825900	0.17824400	-0.10520000
C	-6.96635100	-2.25845600	-0.38996400
H	-6.71068900	-2.76223700	0.55784200
H	-8.05328700	-2.11763000	-0.45493300
H	-6.61417700	-2.85813700	-1.24663300
C	6.95848200	-0.99971500	-0.45130200
H	8.00241400	-0.69863700	-0.29274900
H	6.71063900	-1.84954100	0.20741300
H	6.80621400	-1.27924400	-1.50773100

[Ru(4,4'-$(OMe)_2$ Bid)(Bpy)(H-CO_2)]

Ru	-0.00716600	-0.34429400	-0.25369300
N	-0.12337700	1.65834900	-0.00801200
N	2.24707900	2.26911200	0.04105900
N	2.08815600	-0.13473300	-0.49882000
N	-2.54763500	1.99531400	0.01982700
N	-2.11150600	-0.43265200	-0.07866300
N	0.14575400	-2.39487700	-0.35816700
N	0.28989900	-0.81145800	1.68902500
C	0.95933800	2.51636700	0.08923100
C	0.44937200	3.88853100	0.27113800
C	-0.94791800	3.81234300	0.24924100
C	-1.29881900	2.39011900	0.07352200
C	1.10406000	5.10347400	0.42577400
H	2.19487300	5.15612100	0.43793100
C	0.31830400	6.25672600	0.56350800
H	0.80113800	7.22845000	0.68828500
C	-1.08236100	6.18069000	0.54067700
H	-1.67083200	7.09464900	0.64729700
C	-1.73448400	4.94932600	0.38154900
H	-2.82455200	4.88467700	0.36015200
C	-2.95326100	0.67779700	-0.06972600
C	-4.35130000	0.52103400	-0.12306300
H	-4.96741800	1.41729700	-0.12415800
C	-4.94607800	-0.73600400	-0.16506900
C	-4.09846300	-1.85937400	-0.12457000
H	-4.48069100	-2.87710300	-0.13105700
C	-2.73286000	-1.65185100	-0.08155400
H	-2.07674900	-2.51736600	-0.05473100
C	2.79906000	1.03639300	-0.24373200
C	4.20636500	1.04882500	-0.30495500
H	4.72023800	1.98437700	-0.09600300
C	4.93517500	-0.08584600	-0.64588700
C	4.21500800	-1.25787400	-0.94754200
H	4.70404700	-2.18023400	-1.25065000
C	2.83645500	-1.22276900	-0.85912400
H	2.27679400	-2.12198200	-1.10361000
C	-0.00239400	-3.15630900	-1.47941600
H	-0.26925400	-2.60760000	-2.38504200
C	0.17415200	-4.53315000	-1.47900400
H	0.04672100	-5.09301200	-2.40594500
C	0.65636700	-4.41838700	0.87240100
H	0.91498100	-4.90007800	1.81543900
C	0.46047000	-3.03408700	0.82239300
C	0.54312200	-2.14000800	1.97412700
C	0.83200600	-2.55297400	3.27922800
H	1.03076500	-3.60509500	3.48178500
C	0.59695400	-0.28227800	4.02079300
H	0.60744400	0.47939100	4.80077700
C	0.31650100	0.08696300	2.71264900
H	0.10283200	1.12080600	2.44261500
C	-0.69553500	0.44180500	-2.83016800

H	-0.01676000	-0.20688400	-2.11298400
O	-1.71938300	-0.15457800	-3.20166300
O	-0.18704400	1.53015400	-3.13884600
C	0.51834600	-5.17672300	-0.28547000
H	0.67260400	-6.25626600	-0.25829200
C	0.86340600	-1.62286800	4.31213100
H	1.09078500	-1.93823300	5.33120700
O	-6.30689600	-0.77113500	-0.22638700
O	6.29155700	0.03959800	-0.67189300
C	7.02040900	-1.16382400	-1.04546600
H	8.07780700	-0.87154000	-1.00563900
H	6.82925600	-1.98201700	-0.33060200
H	6.75764100	-1.48231000	-2.06843300
C	-6.89073600	-2.10270100	-0.29104800
H	-6.65270100	-2.68598900	0.61456900
H	-7.97309900	-1.92781400	-0.34688200
H	-6.54897200	-2.63919100	-1.19236900

[Ru(4,4'-(OMe)$_2$ Bid)(Bpy)(O-COH)]

Ru	-0.08913100	-0.35257000	-0.27492800
N	-0.21585800	1.64771500	-0.07574100
N	2.14718500	2.23003600	0.16823600
N	1.99942500	-0.15487600	-0.46139400
N	-2.63458000	1.98619500	-0.20645800
N	-2.19439100	-0.44168700	-0.14851800
N	0.08715500	-2.39829500	-0.31261700
N	0.19486200	-0.75044200	1.68850500
C	0.86112200	2.49332200	0.12902000
C	0.34543500	3.86437300	0.30254500
C	-1.04710200	3.79872300	0.16009200
C	-1.38940500	2.38113700	-0.06815200
C	0.98927000	5.07148500	0.54111800
H	2.07526700	5.11671800	0.64836000
C	0.20042200	6.22711700	0.63970500
H	0.67623700	7.19190400	0.82919200
C	-1.19319200	6.16193300	0.49529600
H	-1.78425000	7.07719600	0.57292800
C	-1.83527700	4.93849600	0.25206400
H	-2.92004000	4.88250800	0.13683700
C	-3.03326600	0.66535500	-0.26967200
C	-4.42561600	0.49695800	-0.40475200
H	-5.04258900	1.38673500	-0.50942900
C	-5.01644600	-0.76236500	-0.37688600
C	-4.17603100	-1.87509800	-0.17747800
H	-4.56071800	-2.88975300	-0.10795800
C	-2.81408500	-1.65900100	-0.07578900
H	-2.15753400	-2.51347000	0.07127700
C	2.70444200	1.00442000	-0.13958800
C	4.11310900	1.01275500	-0.15964100
H	4.62520900	1.93510700	0.10556400
C	4.84708100	-0.10594600	-0.54059700
C	4.13288500	-1.25563800	-0.92807900
H	4.62738900	-2.16051200	-1.27249900
C	2.75143900	-1.22130000	-0.86881500
H	2.19455200	-2.10364500	-1.17691900
C	-0.06403200	-3.20207900	-1.40350900
H	-0.35560800	-2.68658500	-2.32061100
C	0.15282000	-4.57195900	-1.36324400
H	0.02309900	-5.16556900	-2.26884200
C	0.54414400	-5.16603800	-0.15767700
H	0.73310900	-6.23894100	-0.09972500
C	0.68437900	-4.36589100	0.97094800
H	0.97845500	-4.80796900	1.92280500

C	0.44418600	-2.98954600	0.88284000
C	0.50390200	-2.06177000	2.00895900
C	0.80686400	-2.43515900	3.32348500
H	1.05313800	-3.47299900	3.54814900
C	0.79165400	-1.48500400	4.33789500
H	1.03067100	-1.76817400	5.36381400
C	0.45959200	-0.16460700	4.01725800
H	0.42891000	0.61155700	4.78257600
C	0.17007500	0.16344300	2.70087300
H	-0.09371300	1.18064400	2.41067900
C	0.12526100	0.56142600	-3.22082600
H	-0.26508100	0.41748600	-4.25523600
O	-0.44444900	-0.22043100	-2.37785500
O	1.01040700	1.40595900	-3.02796000
O	-6.37176600	-0.80891400	-0.52456600
O	6.20575600	0.01584500	-0.52234200
C	-6.95619600	-2.13980100	-0.46525900
H	-6.78093700	-2.60624100	0.51920000
H	-8.03160600	-1.97117700	-0.61495600
H	-6.55929000	-2.78383900	-1.26833800
C	6.94078400	-1.16961600	-0.93579000
H	7.99789600	-0.88684000	-0.84615600
H	6.72289200	-2.02361000	-0.27185800
H	6.71083700	-1.43237000	-1.98242200

TS = [Ru(4,4'-(OMe)$_2$ Bid)(Bpy)(--OCO$_3$)]

Ru	-0.03399100	-0.31886600	-0.28837100
N	-0.14340900	1.69389900	-0.13259900
N	2.22425100	2.29322900	0.05394800
N	2.09241900	-0.13651400	-0.36494800
N	-2.56965700	2.02679200	-0.11030700
N	-2.13548200	-0.40376900	-0.13479000
N	0.11819200	-2.36314400	-0.37952700
N	0.15775900	-0.76135600	1.62726300
C	0.93793600	2.54773100	0.01986000
C	0.42295400	3.92143200	0.17620000
C	-0.97355700	3.84712500	0.11148200
C	-1.32167400	2.42458900	-0.06627100
C	1.07318400	5.13505100	0.35968400
H	2.16302600	5.18596500	0.40938400
C	0.28495500	6.28832000	0.48031400
H	0.76473000	7.25840400	0.62796200
C	-1.11464600	6.21417800	0.41433200
H	-1.70530500	7.12784600	0.51118200
C	-1.76248500	4.98453500	0.22817400
H	-2.85166600	4.92066400	0.17771500
C	-2.97562500	0.70746100	-0.15524700
C	-4.37470000	0.55019400	-0.18272700
H	-4.99074200	1.44628400	-0.20526300
C	-4.97092500	-0.70686100	-0.16491800
C	-4.12376500	-1.82873200	-0.09656600
H	-4.50647600	-2.84568200	-0.05995400
C	-2.75652600	-1.62068600	-0.08348100
H	-2.09994700	-2.48554400	-0.03944700
C	2.78831200	1.04768000	-0.13957100
C	4.19742700	1.06322700	-0.12513700
H	4.69761800	2.01134000	0.05906500
C	4.94442400	-0.08433300	-0.36886500
C	4.24134300	-1.27388700	-0.63743500
H	4.74520800	-2.21012400	-0.86399100
C	2.85899800	-1.23875100	-0.62127900
H	2.31780100	-2.15365300	-0.84817100
C	0.02661400	-3.12196100	-1.50685400

H	-0.19293100	-2.57276600	-2.42512600
C	0.21200700	-4.49800000	-1.49598900
H	0.13355700	-5.06025400	-2.42691700
C	0.50346500	-5.13832000	-0.28607500
H	0.66232100	-6.21706100	-0.25194600
C	0.58575400	-4.37964300	0.87736800
H	0.80453100	-4.85787000	1.83217500
C	0.38474300	-2.99691500	0.81539300
C	0.40613400	-2.08765100	1.95375600
C	0.62544900	-2.47481000	3.27949500
H	0.82639100	-3.52230700	3.50573900
C	0.58547400	-1.53036400	4.29826300
H	0.75928600	-1.82585600	5.33356300
C	0.31237800	-0.19856100	3.96850400
H	0.26361800	0.57430800	4.73607400
C	0.10469800	0.15131400	2.64287400
H	-0.10742200	1.17818300	2.34769000
C	-0.28794300	0.23217200	-3.54337200
H	-0.37515200	0.42227700	-4.64430500
O	-1.37391100	0.10462300	-2.92349300
O	0.87209200	0.16065600	-3.06302600
C	-6.91899100	-2.07414500	-0.17494300
H	-6.60731600	-2.66005400	-1.05634600
H	-6.65207800	-2.60880700	0.75254400
H	-8.00267800	-1.90080000	-0.20603800
C	7.04488000	-1.16468100	-0.65721500
H	6.84364300	-1.96032900	0.08003800
H	6.80613900	-1.51909400	-1.67430000
H	8.09976200	-0.86502900	-0.60462400
O	-6.33362700	-0.74254300	-0.19938000
O	6.30161800	0.04549700	-0.34037300

TS = [Ru(4,4'-$(OMe)_2$ Bid)(Bpy)(H—H—OCHO)]

Ru	-0.15431900	-0.34544000	-0.28696100
N	-0.22105200	1.67261800	-0.15496300
N	2.13474900	2.19884500	0.25977600
N	1.96157900	-0.22052700	-0.20408800
N	-2.62860700	2.07832500	-0.35395500
N	-2.26693800	-0.36313000	-0.40019700
N	-0.05738800	-2.40019700	-0.18074100
N	-0.16969500	-0.66291800	1.76482600
C	0.86266400	2.49040400	0.12469400
C	0.37368400	3.87457000	0.27419900
C	-1.01146800	3.84284800	0.07309800
C	-1.37726000	2.43567000	-0.17929500
C	1.03582000	5.06444100	0.54700600
H	2.11687000	5.08265100	0.70154300
C	0.27138000	6.23834500	0.61670700
H	0.76152000	7.19099200	0.82958600
C	-1.11645000	6.20678800	0.41440000
H	-1.68829800	7.13565700	0.47159600
C	-1.77656700	5.00019500	0.13901000
H	-2.85662100	4.96979100	-0.02093300
C	-3.06695300	0.77615900	-0.48065300
C	-4.46007600	0.66401200	-0.66526600
H	-5.04325000	1.57982200	-0.73291300
C	-5.09141800	-0.57222800	-0.74662400
C	-4.28987700	-1.72334600	-0.62151500
H	-4.70423900	-2.72783000	-0.65583400
C	-2.92716700	-1.56045500	-0.45546900
H	-2.30325900	-2.44630200	-0.37109400
C	2.67758700	0.94529400	0.05974200
C	4.08600000	0.93107900	0.10570700

H	4.60105800	1.86690600	0.31029100
C	4.81437200	-0.22860800	-0.13484600
C	4.09344800	-1.40405200	-0.41862400
H	4.58258300	-2.35210200	-0.62749300
C	2.71226300	-1.34030300	-0.43390900
H	2.15519300	-2.24284800	-0.66917300
C	-0.05347400	-3.26147300	-1.24109800
H	-0.16986200	-2.79515600	-2.22006700
C	0.09258800	-4.63398400	-1.10122200
H	0.09321600	-5.26818800	-1.98837600
C	0.24173400	-5.17752400	0.17917300
H	0.36781500	-6.25181400	0.32040300
C	0.21944900	-4.32173600	1.27459100
H	0.32131500	-4.72273000	2.28280700
C	0.06295700	-2.94389100	1.08349600
C	-0.01322200	-1.97033200	2.17234600
C	0.03583800	-2.30536500	3.53093600
H	0.16431000	-3.34457200	3.83242700
C	-0.08197700	-1.30960700	4.49405100
H	-0.04316000	-1.56180600	5.55472700
C	-0.25547300	0.01366300	4.07914000
H	-0.35686400	0.82395200	4.80161600
C	-0.29444100	0.29670700	2.72010800
H	-0.42783300	1.31566500	2.35472200
C	2.33392200	0.08865700	-3.34578700
H	3.27708700	-0.25216200	-3.83177500
O	1.47139200	-0.85876700	-3.19998400
O	2.20655300	1.27247900	-3.01727100
O	-6.44328600	-0.56360100	-0.92837700
O	6.17385300	-0.12536300	-0.08265700
C	-7.06270400	-1.87689000	-1.02344500
H	-6.92313100	-2.44957000	-0.09085600
H	-8.12969300	-1.67005000	-1.17894600
H	-6.66095600	-2.44130800	-1.88203900
C	6.89817800	-1.35012900	-0.38546800
H	7.95790100	-1.07433900	-0.30527600
H	6.66117900	-2.14381300	0.34330500
H	6.67736800	-1.69645800	-1.40948300
H	0.50398800	-0.44765700	-2.40956200
H	-0.28099400	-0.12991400	-2.00231800

7.7 Optimized geometries for catalytic system of 1w'

[Ru(4,4'-(COOMe)$_2$ Bid)(Bpy)(Cl)]

Ru	0.56208600	-0.85838400	0.19545600
N	2.52233800	-0.38141700	0.19008700
N	2.70493900	0.85667500	2.28915500
N	0.46056600	-0.16140400	2.18791600
N	3.23049500	-1.36526600	-1.93227400
N	0.77673000	-1.56721000	-1.77656100
N	-1.46213800	-1.16859800	0.18797900
N	-0.08626300	0.95506300	-0.40201800
C	3.16951600	0.35095200	1.16824700
C	4.57890000	0.51766900	0.76719000
C	4.73924100	-0.15547500	-0.45094900
C	3.42139900	-0.71063300	-0.81137800
C	5.64415500	1.16605600	1.37851000
H	5.51381700	1.68805200	2.32897300
C	6.88970200	1.12818200	0.73489600
H	7.74774100	1.62964900	1.18787000
C	7.05034100	0.45362800	-0.48453000
H	8.03150600	0.43744600	-0.96394600
C	5.96919200	-0.19911300	-1.09432800
H	6.08910600	-0.72650300	-2.04322400
C	2.00116400	-1.78042900	-2.39775800
C	2.05858600	-2.42910400	-3.65844300
H	3.05006500	-2.58342000	-4.08215000
C	-0.32112900	-2.54467700	-3.72384400
H	-1.26260200	-2.80588300	-4.20748500
C	-0.34065700	-1.93365400	-2.48248500
H	-1.29331400	-1.72307700	-2.00359300
C	1.44426100	0.61471300	2.78908300
C	1.21356200	1.19510900	4.06405200
H	2.01487500	1.81004000	4.47170400
C	-0.91210600	0.12272400	4.18401200
H	-1.83977800	-0.12687500	4.69929900
C	-0.66738900	-0.40498000	2.92874100
H	-1.39635300	-1.07181700	2.47496600
C	-2.11456500	-2.34586800	0.41964200
H	-1.46511100	-3.20726700	0.58715300
C	-3.49491000	-2.44510300	0.46002000
H	-3.96562500	-3.40784800	0.65474800
C	-4.27023500	-1.29480800	0.25591100
C	-3.62256200	-0.08836700	0.00232900
H	-4.22143800	0.80583600	-0.17074700

C	-2.23038800	-0.04145500	-0.03941500
C	-1.45666700	1.15157400	-0.36732700
C	-2.02103400	2.39127500	-0.66855300
H	-3.10067700	2.52638300	-0.62473100
C	-1.20144000	3.45737700	-1.02982900
C	0.18248400	3.24889500	-1.09235800
H	0.84264000	4.06654300	-1.38174800
C	0.70091500	2.00623500	-0.77802900
H	1.77180000	1.80915000	-0.81476000
C	0.04627500	0.96694400	4.76121400
H	-0.11603700	1.41573400	5.74303600
C	0.91500300	-2.82057700	-4.32269700
H	0.97313500	-3.31644500	-5.29342200
C	-5.75357300	-1.30137100	0.28357800
C	-1.73447800	4.80225200	-1.35771100
O	-6.45195200	-0.30332400	0.11100600
O	-1.03738000	5.75729900	-1.69486800
O	-6.24383100	-2.54937500	0.51736900
O	-3.09060700	4.84807900	-1.23815900
C	-7.70654400	-2.58959100	0.53197600
H	-8.10542300	-2.26111300	-0.44019700
H	-7.95326000	-3.64127000	0.72163800
H	-8.10003700	-1.94468200	1.33272100
C	-3.64090400	6.16499500	-1.56105500
H	-3.41246800	6.42718100	-2.60572300
H	-4.72211600	6.05972700	-1.41106600
H	-3.22384000	6.92871200	-0.88665700
Cl	1.16226000	-3.12564300	0.99424800

[Ru(4,4'-(COOMe)$_2$ Bid)(Bpy)]$^+$

Ru	-0.02572400	-0.25714600	-0.47376000
N	-0.03483100	1.75730400	-0.34517300
N	2.35763500	2.23278700	-0.15948200
N	2.09040400	-0.19513700	-0.52866500
N	-2.43667500	2.21843700	-0.35619500
N	-2.12583200	-0.23026800	-0.46239800
N	0.00260800	-2.33028200	-0.54739100
N	0.04273400	-0.71387500	1.45335100
C	1.08830300	2.56081300	-0.19598200
C	0.64730400	3.95877300	-0.05650600
C	-0.75091900	3.95598400	-0.12511100
C	-1.17092700	2.55519100	-0.29440200
C	1.35973700	5.13912500	0.11321400
H	2.45052500	5.13551800	0.16574300
C	0.63054600	6.33200900	0.21673200
H	1.15864900	7.27798500	0.35413000
C	-0.77096000	6.32921700	0.14746700
H	-1.31379800	7.27309400	0.23162400
C	-1.48160300	5.13321600	-0.02562300
H	-2.57234300	5.12485300	-0.07878800
C	-2.90165500	0.92824100	-0.43635700
C	-4.31479200	0.84274600	-0.46210800
H	-4.87805700	1.77438600	-0.45285900
C	-4.96950000	-0.37029600	-0.47087900
C	-4.19054300	-1.53830900	-0.45781400
H	-4.65022600	-2.52495000	-0.45377000
C	-2.81687000	-1.42221300	-0.45389700
H	-2.21044000	-2.32198900	-0.45216100
C	2.84459100	0.95870300	-0.32540600
C	4.25888500	0.89190500	-0.29692400
H	4.80556200	1.81800300	-0.12765600
C	4.93354900	-0.29536400	-0.48461400
C	4.17512900	-1.45610500	-0.70531000

H	4.65147000	-2.42057500	-0.87161300
C	2.79955200	-1.36023000	-0.71433900
H	2.20901900	-2.25216000	-0.89847300
C	-0.05168300	-3.08921600	-1.67377300
H	-0.13702100	-2.53507600	-2.61040000
C	0.00140700	-4.47685200	-1.64158700
H	-0.04493800	-5.04057900	-2.57351900
C	0.11814700	-5.12483900	-0.40809300
H	0.16730000	-6.21313900	-0.35397200
C	0.16892400	-4.36207000	0.75469600
H	0.25704500	-4.84526100	1.72742800
C	0.10543600	-2.96859000	0.66636700
C	0.12437100	-2.05164400	1.79928600
C	0.20243000	-2.44307700	3.13867600
H	0.26686500	-3.50270800	3.38558200
C	0.19604800	-1.48466900	4.14526000
H	0.25721100	-1.78406700	5.19212500
C	0.10814500	-0.13626500	3.79097800
H	0.09773600	0.64813200	4.54780400
C	0.03377900	0.21643500	2.45105400
H	-0.03728000	1.25675000	2.13780900
C	-6.45480700	-0.38065300	-0.46960200
C	6.41928200	-0.28597700	-0.45192300
O	-7.15433400	0.62946200	-0.50052500
O	7.10152100	0.71669300	-0.25249200
O	6.92814700	-1.52907800	-0.67286600
O	-6.94268800	-1.65062200	-0.41773600
C	-8.40530400	-1.69273200	-0.37814000
H	-8.65145300	-2.75894400	-0.30370400
H	-8.77748500	-1.14054700	0.49849800
H	-8.82553300	-1.25805400	-1.29811900
C	8.39105200	-1.55686100	-0.63756300
H	8.75385400	-1.24493900	0.35399800
H	8.65390900	-2.60231600	-0.83961900
H	8.80550100	-0.89177500	-1.41069400

[Ru(4,4'-(COOMe)$_2$ Bid)(Bpy)(H$_2$)]$^+$

Ru	-0.01077500	-0.29615600	-0.53915700
N	-0.01216300	1.73129700	-0.38802100
N	2.38762700	2.18603000	-0.27481300
N	2.10204900	-0.24916300	-0.58242200
N	-2.40961100	2.18350800	-0.23786900
N	-2.12122800	-0.25351900	-0.52901700
N	0.00028800	-2.38000100	-0.33917200
N	0.03518200	-0.52551900	1.52327900
C	1.12007500	2.52185000	-0.27489400
C	0.68933300	3.91987900	-0.09555600
C	-0.71045300	3.91924100	-0.08260700
C	-1.14277800	2.52080500	-0.25435200
C	1.41270800	5.09652000	0.04964900
H	2.50471900	5.09106400	0.04030300
C	0.69251600	6.28909800	0.20642900
H	1.22921200	7.23324800	0.32104300
C	-0.71044000	6.28847100	0.21919400
H	-1.24584300	7.23212600	0.34340200
C	-1.43219200	5.09516700	0.07557200
H	-2.52419200	5.08869900	0.08570200
C	-2.88454600	0.89905900	-0.37894500
C	-4.29762600	0.81917900	-0.37036000
H	-4.85676300	1.74403600	-0.23954700
C	-4.95736400	-0.38166100	-0.53039800
C	-4.18657900	-1.54005200	-0.70527300
H	-4.65053900	-2.51407200	-0.84906200

C	-2.81070700	-1.42874300	-0.69675700
H	-2.20441700	-2.31723900	-0.84434500
C	2.86406100	0.90290100	-0.42155800
C	4.27716200	0.82347200	-0.40761800
H	4.83567900	1.74709900	-0.26573800
C	4.93802100	-0.37597800	-0.57338700
C	4.16850000	-1.53251100	-0.76603300
H	4.63346100	-2.50488300	-0.91762600
C	2.79257500	-1.42177400	-0.76255900
H	2.18712000	-2.30874100	-0.92260300
C	-0.01677900	-3.29237300	-1.35195600
H	-0.02184900	-2.88052300	-2.36201800
C	-0.02760100	-4.66302700	-1.13230100
H	-0.04140100	-5.34403700	-1.98344300
C	-0.02412200	-5.14107200	0.17993000
H	-0.03741600	-6.21215100	0.38576100
C	-0.00353200	-4.22579600	1.22588400
H	-0.00275100	-4.57606800	2.25710300
C	0.01309400	-2.85377200	0.95207100
C	0.04561100	-1.82003400	1.98823700
C	0.08852400	-2.09327300	3.35918400
H	0.10284700	-3.12440200	3.70903000
C	0.11617300	-1.04627000	4.27369100
H	0.14874300	-1.25230300	5.34434600
C	0.10253500	0.26488700	3.79759100
H	0.12295900	1.11551300	4.47880300
C	0.06389400	0.48780600	2.42679900
H	0.05369900	1.49796600	2.02025100
H	-0.00486200	0.21568900	-2.20587800
H	-0.12248200	-0.61514100	-2.24802000
C	6.42474000	-0.38145500	-0.54472000
C	-6.44434000	-0.38664300	-0.51673400
O	-7.13777100	0.61453800	-0.35363600
O	7.11638600	0.61831600	-0.36592500
O	6.91985900	-1.63369300	-0.74067100
O	-6.93725300	-1.64030600	-0.70882600
C	8.38273300	-1.67640800	-0.70749100
H	8.63401400	-2.72819100	-0.89035900
H	8.80210600	-1.03038700	-1.49393900
H	8.75064800	-1.35022300	0.27754700
C	-8.40044400	-1.68234400	-0.69508400
H	-8.64961900	-2.73544300	-0.87318200
H	-8.78123000	-1.34845700	0.28241300
H	-8.80903500	-1.04250000	-1.49220600

[Ru(4,4'-(COOMe)$_2$ Bid)(Bpy)(H)]

Ru	-0.09512100	-0.24226500	-0.50747700
H	-0.27621800	-0.06361800	-2.13057500
N	-0.13801300	1.76347700	-0.33528600
N	2.24536900	2.26473000	-0.13526800
N	1.99140800	-0.13224200	-0.67923400
N	-2.54506600	2.17173800	-0.40827100
N	-2.16849400	-0.26910500	-0.35156700
N	0.01354000	-2.30686600	-0.45700800
N	0.22574800	-0.66395500	1.60185200
C	0.96635400	2.57822600	-0.16400300
C	0.50244500	3.96660000	0.00017700
C	-0.89597700	3.94361500	-0.10201900
C	-1.28569400	2.53756700	-0.30316700
C	1.19017200	5.15558800	0.20720300
H	2.27954900	5.16810600	0.28566300
C	0.44080000	6.33684100	0.31182400
H	0.95172000	7.28825000	0.47569800

C	-0.95785200	6.31426800	0.20727300
H	-1.51742300	7.24869300	0.28982200
C	-1.64514000	5.10905900	-0.00071800
H	-2.73417800	5.08588000	-0.08182000
C	-2.97720100	0.86896200	-0.43717600
C	-4.38595600	0.73955200	-0.49989700
H	-4.97387500	1.65068800	-0.60181800
C	-4.20144500	-1.62398600	-0.22712400
H	-4.63663600	-2.61546800	-0.11321100
C	-2.83208900	-1.46967100	-0.20936900
H	-2.19736800	-2.34276000	-0.08854600
C	2.74149700	1.00965200	-0.38531000
C	4.15699000	0.94542100	-0.35960800
H	4.69860900	1.85613400	-0.10867200
C	4.08652200	-1.35063100	-1.00546900
H	4.56891900	-2.28750500	-1.27876100
C	2.71116300	-1.26028900	-1.00671400
H	2.12019700	-2.12379300	-1.29989300
C	-0.16912500	-3.13004900	-1.53308300
H	-0.44645500	-2.62621200	-2.45927800
C	-0.00739500	-4.50625800	-1.47546200
H	-0.16372200	-5.10436400	-2.37385800
C	0.36238000	-5.09853900	-0.26390300
C	0.53438500	-4.28493300	0.84980200
H	0.81298300	-4.72761300	1.80570700
C	0.34941500	-2.90031900	0.74696400
C	0.47352900	-1.98346400	1.88749000
C	0.80053100	-2.39432900	3.18724700
H	0.99571000	-3.44408600	3.40278500
C	0.87726700	-1.45236800	4.20775200
C	0.62205500	-0.11030100	3.91556400
H	0.67131400	0.65660100	4.68911000
C	0.30254100	0.23975700	2.60873800
H	0.09152800	1.27500100	2.33172200
C	4.84011400	-0.21541100	-0.65529700
H	5.90917585	-0.23446892	-0.61475614
C	-5.01086400	-0.48672700	-0.40308500
H	-6.07719309	-0.55290760	-0.46192715
C	0.57015062	-6.62073330	-0.15733898
C	1.23916013	-1.89026896	5.63914157
O	0.90290927	-7.13942586	0.93983934
O	1.30896219	-1.03917693	6.56344703
O	0.38430778	-7.44761413	-1.30913347
O	1.49676741	-3.26877269	5.91890212
C	0.65966900	-8.80897408	-0.96887581
H	-0.01119861	-9.12670663	-0.19823798
H	0.52823890	-9.42618227	-1.83298240
H	1.66800617	-8.89267287	-0.62080878
C	1.82110007	-3.42241557	7.30313555
H	0.99929309	-3.08807567	7.90125770
H	2.01741086	-4.45347813	7.51115499
H	2.68927869	-2.84065641	7.53274861

TS = [Ru(4,4'-(COOMe)$_2$ Bid)(Bpy)(H—H—NMe$_3$)]$^+$

N	0.13650000	1.61009900	0.21468600
N	2.52288600	2.10490600	0.07649500
N	2.23788700	-0.34391300	-0.07573600
N	-2.24137100	1.98956600	0.62906400
N	-1.95591500	-0.30898900	-0.22870600
N	0.08869600	-2.44511000	-0.25492300
N	-0.01658400	-0.92007900	1.87905800
C	1.26202200	2.41457300	0.27137900
C	0.83866000	3.77989600	0.63167800

C	-0.54953000	3.73876000	0.82219800
C	-0.97969500	2.35555000	0.54743000
C	1.55598900	4.95692000	0.80156700
H	2.63742900	4.98375400	0.65183500
C	0.84497300	6.10852100	1.16916100
H	1.37831700	7.05112200	1.30957100
C	-0.54399600	6.06753500	1.36009400
H	-1.07318900	6.97851700	1.64804000
C	-1.26105300	4.87455300	1.18704200
H	-2.34241700	4.83860800	1.33537900
C	-2.71819300	0.76031500	0.23300100
C	-4.13056300	0.66444500	0.25759300
H	-4.68988300	1.51346900	0.64707700
C	-4.79079800	-0.44470000	-0.23025100
C	-4.02093700	-1.49425800	-0.75849900
H	-4.48782900	-2.38117400	-1.18289200
C	-2.64545800	-1.38493400	-0.73220400
H	-2.03609000	-2.18561300	-1.14423300
C	2.99663500	0.82422600	-0.09860400
C	4.40158800	0.75626300	-0.25550500
H	4.95370100	1.69390700	-0.29216400
C	5.06550400	-0.45101500	-0.33397000
C	4.30678800	-1.62840300	-0.23713300
H	4.77783200	-2.60932900	-0.26459900
C	2.93616300	-1.52738000	-0.11222500
H	2.33721300	-2.43154300	-0.04744600
C	0.19202600	-3.18169500	-1.39801400
H	0.35605900	-2.60766000	-2.31174200
C	0.09067300	-4.56578300	-1.41536200
H	0.18211200	-5.10139200	-2.36068300
C	-0.13217800	-5.24631100	-0.21503400
H	-0.22360300	-6.33312700	-0.19717500
C	-0.23374600	-4.51389600	0.96268700
H	-0.40161000	-5.02609900	1.90986100
C	-0.11493600	-3.11990200	0.93014700
C	-0.16286500	-2.26717600	2.12103500
C	-0.32041900	-2.75262600	3.42382100
H	-0.43548900	-3.82135200	3.59931700
C	-0.32779000	-1.86627000	4.49565900
H	-0.45188000	-2.23711200	5.51409600
C	-0.16907000	-0.50180400	4.24714600
H	-0.16407100	0.22529500	5.05939700
C	-0.01663600	-0.06812500	2.93588700
H	0.11608600	0.98800400	2.69877100
H	-0.15316400	0.42792600	-2.01432900
H	0.41169300	-0.24584600	-1.82347300
N	-0.74695000	1.32557400	-3.08127700
Ru	0.14302600	-0.37941400	-0.13178500
C	-0.63796200	0.43148900	-4.24587900
H	0.40069900	0.07016600	-4.33093300
H	-1.30373000	-0.43560300	-4.09566100
H	-0.91844200	0.94465800	-5.18552700
C	0.18569200	2.45772300	-3.20195800
H	0.05049800	3.13355200	-2.34318800
H	1.22152600	2.07693900	-3.20084600
H	0.01702700	3.02805700	-4.13651600
C	-2.13224000	1.79481800	-2.91631100
H	-2.79992700	0.92853100	-2.78375200
H	-2.19867900	2.44622000	-2.03123700
H	-2.46815200	2.36774300	-3.80408200
C	6.54180100	-0.44575300	-0.49880900
C	-6.27627200	-0.46322300	-0.19713500
O	7.22939600	0.57063900	-0.57201700

O	-6.97159500	0.43076300	0.28076500
O	7.03873000	-1.71232900	-0.56041200
O	-6.77186800	-1.59499700	-0.77027200
C	8.49239600	-1.74283600	-0.72268000
H	8.74538500	-2.80909000	-0.76864000
H	8.78408900	-1.22912400	-1.65186100
H	8.98367000	-1.26139700	0.13701100
C	-8.23458600	-1.64059800	-0.75890000
H	-8.48870000	-2.58060200	-1.26363500
H	-8.60732000	-1.63882900	0.27697700
H	-8.64758500	-0.77773600	-1.30365200

TS = [Ru(4,4'-(COOMe)$_2$ Bid)(Bpy)(H—CO$_2$)]

Ru	-0.12766300	-0.35341300	-0.29403600
H	-0.35906200	0.01396300	-1.91830000
N	-0.15600200	1.63546900	0.02161800
N	2.23254200	2.11901200	0.19034300
N	1.96650800	-0.25702400	-0.42905600
N	-2.55636700	2.07717500	-0.09863700
N	-2.20939600	-0.36696800	-0.14728400
N	-0.07349000	-2.41039000	-0.48644300
N	0.14132800	-1.00258500	1.71976200
C	0.95657500	2.44088200	0.17780200
C	0.50768300	3.83638500	0.32513100
C	-0.88932000	3.82785300	0.21357000
C	-1.29382500	2.42393500	0.02421900
C	1.20817400	5.02031000	0.51701200
H	2.29716300	5.02207800	0.60075800
C	0.47145000	6.21121600	0.59837600
H	0.99199400	7.15941100	0.74984100
C	-0.92666600	6.20282500	0.48506100
H	-1.47596500	7.14472000	0.54851300
C	-1.62631400	5.00260900	0.29089300
H	-2.71473400	4.99043800	0.20052200
C	-3.00487500	0.77989900	-0.16091100
C	-4.41820000	0.67347600	-0.19952200
H	-4.98259700	1.60297900	-0.23517900
C	-5.05170200	-0.55214000	-0.16885600
C	-4.25137100	-1.70373700	-0.08470000
H	-4.71106000	-2.69021200	-0.03247800
C	-2.88071400	-1.56816800	-0.07362800
H	-2.25636300	-2.45452200	-0.01432100
C	2.72082700	0.86558700	-0.08544600
C	4.13714900	0.79130800	-0.03911200
H	4.66907300	1.69576500	0.24823800
C	4.81103000	-0.36840900	-0.35988700
C	4.05189600	-1.48284500	-0.75607800
H	4.54482900	-2.41069000	-1.04442500
C	2.67855100	-1.38298200	-0.77898000
H	2.08680300	-2.23498000	-1.10167500
C	-0.25993000	-3.09286800	-1.65304600
H	-0.46369700	-2.47418800	-2.52770200
C	-0.19052200	-4.47632600	-1.73906900
H	-0.34645400	-4.96479800	-2.70143800
C	0.08197000	-5.21834200	-0.58592600
H	0.14715900	-6.30662000	-0.62269900
C	0.26237500	-4.54345400	0.61661900
H	0.46354700	-5.10256600	1.52996400
C	0.17707300	-3.14737400	0.65514600
C	0.31494200	-2.35588700	1.88223200
C	0.58833300	-2.90369000	3.14221200
H	0.73013600	-3.97804200	3.25613800
C	0.68607900	-2.06818300	4.24988700

H	0.90199400	-2.48567800	5.23460300
C	0.50554900	-0.69301400	4.08202000
H	0.57439900	-0.00626200	4.92592000
C	0.23811300	-0.20143100	2.80962600
H	0.08819300	0.86427000	2.62791000
C	0.79238600	0.47222200	-3.04239800
O	0.85369700	1.65698500	-2.92512400
O	1.07261900	-0.56502300	-3.56202500
C	-6.52516900	-0.70861400	-0.20562100
C	6.28848400	-0.48686900	-0.32094800
O	-7.10291200	-1.79503000	-0.20885600
O	6.90714200	-1.51254200	-0.60197000
O	6.88097600	0.67770200	0.06619700
O	-7.16375800	0.49489400	-0.23301300
C	8.33897600	0.57847800	0.11756500
H	8.74059100	0.32275800	-0.87514700
H	8.67503200	1.57431100	0.43141200
H	8.64454300	-0.18665900	0.84810200
C	-8.61980000	0.36072300	-0.27081600
H	-8.97646700	-0.18191400	0.61848100
H	-8.99340700	1.39185200	-0.27638900
H	-8.93171200	-0.17421700	-1.18142900

[Ru(4,4'-(COOMe)$_2$ Bid)(Bpy)(H-CO$_2$)]

Ru	-0.00473300	-0.27781600	-0.23524500
N	-0.03157700	1.72758100	-0.01995500
N	2.36076000	2.22232400	0.04805900
N	2.09493900	-0.18867400	-0.41789400
N	-2.43613900	2.16579300	0.01088500
N	-2.09832300	-0.27734000	-0.09950500
N	0.06182200	-2.34792900	-0.31523400
N	0.21636900	-0.75435700	1.73001000
C	1.08602300	2.53814300	0.07503600
C	0.63991300	3.93340300	0.23366900
C	-0.75982200	3.91879600	0.21264800
C	-1.17177000	2.51301100	0.05567100
C	1.34794600	5.12018100	0.37167400
H	2.43999600	5.12575100	0.38392500
C	0.61309800	6.30842700	0.49263800
H	1.13811800	7.25963100	0.60387500
C	-0.78947900	6.29399000	0.47074300
H	-1.33703300	7.23430300	0.56443800
C	-1.49586900	5.09078400	0.32909800
H	-2.58767000	5.07399300	0.30901000
C	-2.88793100	0.86969100	-0.07175900
C	-4.29928900	0.76537200	-0.10282300
H	-4.87589100	1.68888600	-0.09623900
C	-4.93651700	-0.45742000	-0.13383900
C	-4.14151100	-1.61433800	-0.11659600
H	-4.58624000	-2.60781700	-0.12336400
C	-2.76910700	-1.47759200	-0.09667200
H	-2.14812000	-2.36790200	-0.08977000
C	2.84867300	0.95939400	-0.18666600
C	4.26377500	0.89997400	-0.21345600
H	4.81113200	1.81945100	-0.01352200
C	4.93700400	-0.26970900	-0.49507700
C	4.17615900	-1.41710900	-0.77118500
H	4.64939500	-2.36382600	-1.02519100
C	2.80040800	-1.32909400	-0.72297100
H	2.20565100	-2.20735800	-0.95440700
C	-0.07451500	-3.10577800	-1.43769400
H	-0.29628200	-2.55096900	-2.35245900
C	0.05234600	-4.48883400	-1.42500800

H	-0.06332500	-5.04930600	-2.35301500
C	0.45793600	-4.37737200	0.94157700
H	0.66779900	-4.86307100	1.89445000
C	0.31479900	-2.98778900	0.87724700
C	0.39886300	-2.08886100	2.02716900
C	0.62601000	-2.50598200	3.34270400
H	0.76937500	-3.56420000	3.55890500
C	0.47126000	-0.22082600	4.06409100
H	0.49089100	0.54461800	4.83996300
C	0.25092600	0.15097000	2.74448600
H	0.09420100	1.19163300	2.46122700
C	-0.77295200	0.38136400	-2.85816600
H	0.03984700	-0.01648400	-2.08859600
O	-1.53751400	-0.50654300	-3.26450600
O	-0.62175400	1.57680300	-3.13952000
C	0.33081100	-5.13631500	-0.21764600
H	0.44397700	-6.22061800	-0.17975100
C	0.66605700	-1.56952600	4.36998200
H	0.84494100	-1.88785100	5.39781400
C	6.42254900	-0.25566200	-0.50403000
C	-6.42047700	-0.48783400	-0.17960200
O	7.10963200	0.73648300	-0.27016300
O	-7.13569100	0.51174100	-0.15864700
O	-6.89017400	-1.76416000	-0.25563700
O	6.92980300	-1.48422900	-0.80068800
C	-8.35029600	-1.82601200	-0.32879700
H	-8.57907500	-2.89438500	-0.42504800
H	-8.79723600	-1.41169300	0.58812700
H	-8.71200800	-1.26606600	-1.20485100
C	8.39287400	-1.50431000	-0.80566000
H	8.78043700	-1.21149300	0.18239100
H	8.65595700	-2.54332500	-1.03855900
H	8.78267800	-0.81937500	-1.57457800

[Ru(4,4'-(COOMe)$_2$ Bid)(Bpy)(D-COH)]

Ru	-0.10184200	-0.38757900	-0.30767500
N	-0.14315500	1.60655600	-0.05408800
N	2.23993500	2.08013900	0.18308500
N	1.97753400	-0.28027200	-0.49472700
N	-2.54558400	2.03066100	-0.14628100
N	-2.18449300	-0.41224200	-0.12782400
N	-0.01023400	-2.44896000	-0.41013800
N	0.19439100	-0.87178500	1.65256600
C	0.96768700	2.40865200	0.13835400
C	0.51176900	3.79999200	0.30360300
C	-0.88442000	3.78941500	0.17603900
C	-1.28465400	2.38675400	-0.03499900
C	1.20604700	4.98243600	0.52442500
H	2.29392600	4.98593000	0.62120600
C	0.46475200	6.16944100	0.61787800
H	0.98066300	7.11628500	0.79164100
C	-0.93190700	6.15896800	0.48859800
H	-1.48472100	7.09804600	0.56208400
C	-1.62570100	4.96042400	0.26595400
H	-2.71302400	4.94680400	0.16376200
C	-2.98434400	0.72758500	-0.18442300
C	-4.39653400	0.60817300	-0.22647600
H	-4.96988100	1.53079300	-0.28784300
C	-5.01836700	-0.62237400	-0.16526500
C	-4.21087100	-1.76538100	-0.04653100
H	-4.66347800	-2.75367600	0.02822200
C	-2.84094400	-1.61687300	-0.02805300
H	-2.20673500	-2.49384900	0.06495200

C	2.73016700	0.83204500	-0.12331700
C	4.14518300	0.75893800	-0.09632500
H	4.68054600	1.64941600	0.22599100
C	4.81668500	-0.37884900	-0.49679800
C	4.05596300	-1.46860300	-0.94988200
H	4.54705200	-2.37131800	-1.31163100
C	2.68048800	-1.37777000	-0.93023600
H	2.08298100	-2.21197500	-1.28899800
C	-0.20447400	-3.20627900	-1.52492900
H	-0.47920900	-2.64997800	-2.42299900
C	-0.04958200	-4.58590900	-1.53011500
H	-0.21292900	-5.14415000	-2.45239100
C	0.32423800	-5.23370900	-0.34817600
H	0.46608300	-6.31510000	-0.32552700
C	0.50861400	-4.47784100	0.80479900
H	0.79105300	-4.96440600	1.73835100
C	0.32849700	-3.09090500	0.76198100
C	0.44171000	-2.20403100	1.91994300
C	0.74350700	-2.63606200	3.21611700
H	0.93833600	-3.69124900	3.40529500
C	0.79256500	-1.71843500	4.25968900
H	1.03110800	-2.04776500	5.27188200
C	0.52822000	-0.37340600	3.98900900
H	0.55078300	0.37803900	4.77862300
C	0.23552500	0.01073500	2.68755100
H	0.02164200	1.04909000	2.43302500
C	0.18379600	0.57563500	-3.20789700
H	-0.22654100	0.51727300	-4.24180200
O	-0.48748300	-0.14609900	-2.38304800
O	1.17972800	1.27689600	-2.99268900
C	6.29597900	-0.49035900	-0.49635500
C	-6.49198500	-0.79081800	-0.19851000
O	-7.06057600	-1.88150600	-0.17973300
O	6.91356400	-1.47557200	-0.89782700
O	6.88689900	0.62948900	0.00680900
O	-7.13855600	0.40707200	-0.24527300
C	-8.59416300	0.26310900	-0.27029500
H	-8.93995600	-0.27205700	0.62775500
H	-8.97437100	1.29169800	-0.28451900
H	-8.90922500	-0.28364800	-1.17266100
C	8.34711600	0.54692700	0.01463500
H	8.67569300	1.48392400	0.48046400
H	8.67948900	-0.32197200	0.60316000
H	8.73103900	0.46664300	-1.01436400

TS = [Ru(4,4'-(COOMe)$_2$ Bid)(Bpy)(--OCOH)]

Ru	-0.03837700	-0.25831100	-0.25876100
N	-0.03684100	1.72860000	0.09933600
N	2.36233000	2.19641100	0.16271300
N	2.07540100	-0.21818900	-0.26997600
N	-2.43426500	2.20646600	0.07046600
N	-2.13590900	-0.23483400	-0.17026100
N	-0.03960300	-2.27387100	-0.62701800
N	0.06855500	-0.98199600	1.58734500
C	1.09318400	2.52773000	0.18368700
C	0.66414000	3.93124600	0.31330600
C	-0.73533700	3.93479100	0.28000900
C	-1.16487100	2.53312800	0.13738000
C	1.38638600	5.11164200	0.43379500
H	2.47829300	5.10349000	0.45415500
C	0.66623100	6.31126800	0.52528100
H	1.20265500	7.25774700	0.62158700
C	-0.73645200	6.31470300	0.49179800

H	-1.27240500	7.26370100	0.56225400
C	-1.45705900	5.11843700	0.36674500
H	-2.54877000	5.11517200	0.33646000
C	-2.90548200	0.92101800	-0.04457800
C	-4.31897200	0.83889800	-0.02031200
H	-4.87781300	1.76914200	0.06844500
C	-4.97945800	-0.36912300	-0.09822900
C	-4.20512400	-1.53563100	-0.19778600
H	-4.66759700	-2.51901100	-0.25971600
C	-2.83097000	-1.42149800	-0.22549600
H	-2.23150600	-2.32180800	-0.31106200
C	2.83758600	0.92010000	-0.01951800
C	4.25020900	0.83675900	0.03441800
H	4.80350000	1.75315100	0.23276300
C	4.91663200	-0.35394400	-0.16438000
C	4.14970400	-1.49946700	-0.42818000
H	4.61721900	-2.46594500	-0.60765800
C	2.77529500	-1.38452100	-0.46848200
H	2.18116200	-2.26438800	-0.69369400
C	-0.12278200	-2.84493100	-1.85799500
H	-0.18906300	-2.14515900	-2.69402500
C	-0.12132200	-4.22252600	-2.03841100
H	-0.18979600	-4.63461100	-3.04532900
C	-0.03104300	-5.05697600	-0.91993300
H	-0.02719900	-6.14166400	-1.03476400
C	0.05341100	-4.48673100	0.34734000
H	0.12122700	-5.12042800	1.23149400
C	0.04624400	-3.09542100	0.47655000
C	0.11692600	-2.35798300	1.73370100
C	0.22413600	-2.93856300	3.00089500
H	0.26453000	-4.02355800	3.09498100
C	0.28342900	-2.13326000	4.13264800
H	0.36949400	-2.58101800	5.12335000
C	0.23342900	-0.74533100	3.97761600
H	0.27836200	-0.07790200	4.83826500
C	0.12744000	-0.20367800	2.70458200
H	0.08764600	0.87203700	2.53681300
C	0.09553500	1.10315500	-3.47776500
H	-0.02050600	1.56861600	-4.49123700
O	-0.95214300	0.59195800	-2.99390600
O	1.23771700	1.15127800	-2.96533200
C	-6.46370300	-0.37686600	-0.07040900
C	6.40031900	-0.36123100	-0.10206100
O	-7.16139600	0.62820000	0.04924400
O	7.09015300	0.63009700	0.12767900
O	-6.95573300	-1.64099800	-0.19757700
O	6.90270500	-1.60603200	-0.33376000
C	-8.41805900	-1.68449700	-0.18026600
H	-8.66653700	-2.74305100	-0.32457900
H	-8.79950500	-1.32152800	0.78671400
H	-8.82880300	-1.07074000	-0.99664700
C	8.36420800	-1.64540900	-0.27643500
H	8.71586200	-1.34231100	0.72191400
H	8.62240100	-2.69145900	-0.48173900
H	8.79478300	-0.97866100	-1.03936400

TS = [Ru(4,4'-(COOMe)$_2$ Bid)(Bpy)(H—H—OCOH)]

Ru	-0.15901700	-0.38193100	-0.27530400
N	-0.17098000	1.62514400	-0.03980500
N	2.21142000	2.08046800	0.25318300
N	1.94645300	-0.32155100	-0.26205100
N	-2.56537700	2.09022100	-0.19502500
N	-2.25760400	-0.35939400	-0.26765400

N	-0.12451000	-2.45124900	-0.32701400
N	-0.07795900	-0.86377100	1.75234500
C	0.94387500	2.41603400	0.17827100
C	0.50185500	3.81448600	0.32703000
C	-0.89033700	3.81969700	0.17263700
C	-1.30223200	2.42195400	-0.04755000
C	1.20646000	4.98911100	0.55564700
H	2.29229500	4.98004100	0.67251800
C	0.47767700	6.18530700	0.62860800
H	1.00138000	7.12707500	0.80642900
C	-0.91640800	6.19048800	0.47294900
H	-1.45933600	7.13638700	0.53092000
C	-1.61999400	4.99931300	0.24260400
H	-2.70506100	4.99763500	0.11825400
C	-3.03059900	0.80069700	-0.29081100
C	-4.44407400	0.71976100	-0.37854000
H	-4.99114800	1.65952600	-0.41285000
C	-5.09797000	-0.49467600	-0.39853800
C	-4.32073600	-1.66145100	-0.32341500
H	-4.79721200	-2.64111000	-0.31928900
C	-2.94913900	-1.54927600	-0.25962200
H	-2.34255100	-2.44813600	-0.20952900
C	2.69797000	0.81555900	0.02139900
C	4.11437400	0.75213000	0.04990600
H	4.64485800	1.67366300	0.27872300
C	4.78999000	-0.41867800	-0.22279100
C	4.03207000	-1.55935800	-0.52971000
H	4.52491100	-2.50229800	-0.76395400
C	2.65676500	-1.46742000	-0.53303800
H	2.06703600	-2.34326200	-0.78522800
C	-0.20829300	-3.22218300	-1.44850300
H	-0.34149500	-2.67642300	-2.38311300
C	-0.12907300	-4.60776200	-1.41818900
H	-0.19976600	-5.17132000	-2.34892300
C	0.04416800	-5.25392500	-0.19086600
H	0.11756000	-6.34091800	-0.13666700
C	0.11547200	-4.48646800	0.96683500
H	0.24015200	-4.96994000	1.93557900
C	0.02280400	-3.09290000	0.88600100
C	0.04490800	-2.20166900	2.04847900
C	0.15738900	-2.63958200	3.37329700
H	0.25575400	-3.70235200	3.59162500
C	0.14182600	-1.71281000	4.41029400
H	0.23087100	-2.04541800	5.44549100
C	0.00764900	-0.35639700	4.10570100
H	-0.01172400	0.40072500	4.88982800
C	-0.09890600	0.02851500	2.77501900
H	-0.20691100	1.07582000	2.48994900
C	2.19647000	0.11117400	-3.41788700
H	3.09097900	-0.25165800	-3.97564600
O	1.28832600	-0.79110500	-3.27554000
O	2.16263200	1.27917800	-3.01483400
C	6.27029500	-0.52238600	-0.21828300
C	-6.57353000	-0.62469000	-0.48069500
O	-7.16793600	-1.70071000	-0.52530900
O	6.89039300	-1.55311700	-0.47497800
O	6.85961300	0.66221000	0.10424100
O	-7.19016000	0.58942900	-0.49582900
C	-8.64721700	0.48147100	-0.57335700
H	-9.03522400	-0.07160800	0.29610000
H	-9.00273300	1.51890500	-0.56809700
H	-8.94473400	-0.03081600	-1.50159400
C	8.31992300	0.58368800	0.10703100

H	8.65192400	1.59471100	0.37251000
H	8.66252900	-0.15032000	0.85303100
H	8.68831000	0.29785700	-0.89036200
H	0.36867700	-0.35159000	-2.39948500
H	-0.35624000	0.00712000	-1.95217500