Highly Efficient Methyl Ketone Synthesis with Photoactivated Acetone and Olefins Assisted by Mg(II)-Exchanged Zeolite Y

Daijiro Tsukamoto, Yasuhiro Shiraishi, and Takayuki Hirai.*

Research Center for Solar Energy Chemistry, and Division of Chemical Engineering, Graduate School of Engineering Science, Osaka University, Toyonaka 560-8531, Japan

shiraish@cheng.es.osaka-u.ac.jp

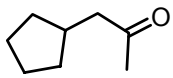
Supporting Information

Contents

Synthesis of standard methyl ketones

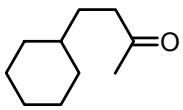
The standard methyl ketones (**2′**, **3′**, **4′**, **6′**, and **8′**) were synthesized according to a literature procedure (Linker, U.; Kersten, B.; Linker, T. *Tetrahedron Lett.* **1995**, *51*, 9917–9926), as follows: Potassium acetate (1.75 g, 18 mmol) and manganese(II) acetate tetrahydrate (12.5 mg, 0.05 mmol) were added to a mixture of acetone (20 mL) and acetic anhydride (15 mL) and heated to 70°C under nitrogen atmosphere. Olefin (**2**, **3**, **4**, **6**, or **8**; 5.0 mmol) was added to the mixture. Potassium permanganate (0.321 g, 0.02 mmol) was added slowly to the mixture and stirred for 10 h. Water (100 mL) was added to the mixture and extracted with CH_2Cl_2 (100 mL × 2) and diethyl ether (100 mL). The combined organic layer was washed with a saturated $NaHCO_3$ solution (100 mL × 2) and water (100 mL) and dried with Na_2SO_4. The solution was concentrated by evaporation and purified by silica gel column chromatography. The elution conditions for the respective products are summarized as below. ^1H and ^{13}C NMR charts of the methyl ketones are summarized in Figures S3–S8.

1-cyclopentyl-propan-2-one (**2′**): a cyclohexane/ethyl acetate (97/3 v/v) elution affords **2′** as a colorless oil with 32% yield (201 mg, 1.60 mmol). ^1H NMR (270 MHz, $CDCl_3$): δ (ppm) = 2.47 (d, 2H), 2.29–2.17 (m, 1H), 2.13 (s, 3H), 1.90–1.00 (m, 8H).



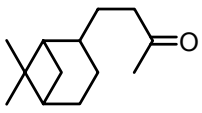
2′

4-cyclohexyl-2-butanone (**3′**): a cyclohexane/ethyl acetate (95/5 v/v) elution affords **3′** as a colorless oil with 45% yield (347 mg, 2.25 mmol). ^1H NMR (270 MHz, $CDCl_3$): δ (ppm) = 2.42 (t, 2H), 2.13 (s, 3H), 1.75–1.63 (m, 5H), 1.52–1.42 (m, 2H), 1.30–1.10 (m, 4H), 0.97–0.80 (m, 2H).



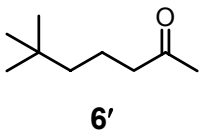
3′

4-(6,6-Dimethyl-bicyclo[3.1.1]hept-2-yl)-butan-2-one (**4′**): a cyclohexane/ethyl acetate (95/5 v/v) elution affords **4′** as a colorless oil with 25% yield (243 mg, 1.25 mmol). ^1H NMR (270 MHz, $CDCl_3$): δ (ppm) = 2.52 (t, 2H), 2.20 (t, 2H), 2.15 (s, 3H), 2.10–1.15 (m, 9H), 0.88 (m, 6H). ^{13}C NMR (68 MHz, $CDCl_3$): δ (ppm) = 208.4, 136.0, 121.1, 42.1, 40.1, 32.2, 31.5, 29.8, 29.2, 28.9, 26.4, 19.9, 19.6.



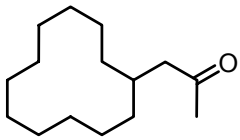
4′

6,6-dimethyl-heptan-2-one (**6′**): an *n*-hexane/ethyl acetate (97/3 v/v) elution affords **6′** as a colorless oil with 12% yield (85 mg, 0.6 mmol). ^{1}H NMR (270 MHz, $CDCl_3$): δ (ppm) = 2.38 (t, 2H), 2.13 (s, 3H), 1.62–1.45 (m, 2H), 1.20–1.08 (m, 2H), 0.88 (s, 9H).



6′

1-cyclododecyl-propan-2-one (**8′**): a cyclohexane/ethyl acetate (95/5 v/v) elution affords **8′** as a colorless oil with 11% yield (123 mg, 0.55 mmol). ^{1}H NMR (270 MHz, $CDCl_3$): δ (ppm) = 2.35 (d, 2H), 2.12 (s, 3H), 1.60 (m, 1H), 1.55–1.18 (m, 22H).



8′

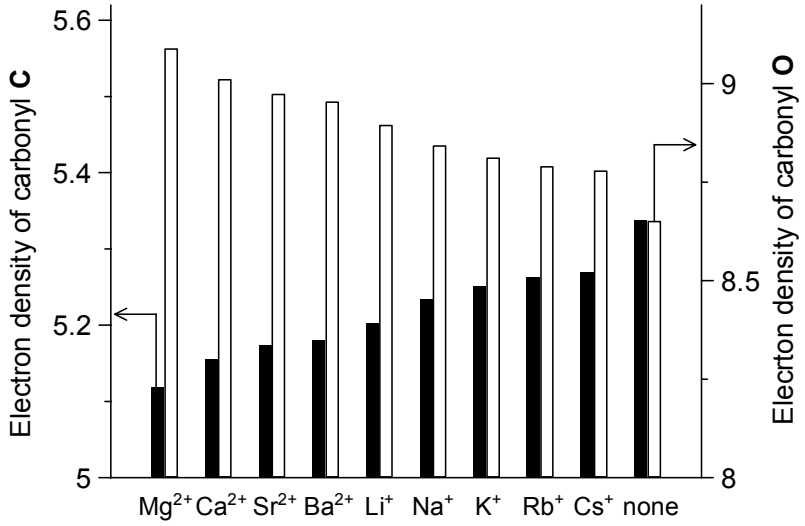


Figure S1. Calculated electron densities of carbonyl carbon and oxygen atoms of S_0 acetone, when associated with alkali or alkaline earth metal cations. The detailed electron density data are summarized in Table S1.

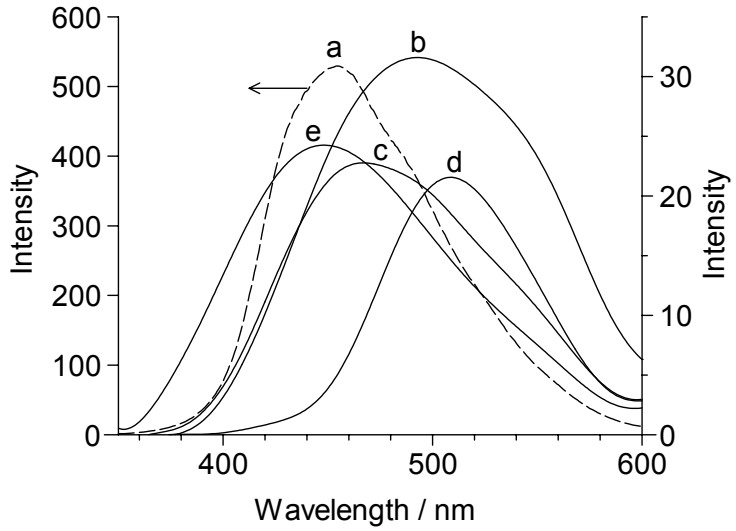


Figure S2. Phosphorescence spectra of acetone measured at 77 K in (a) diethyl ether/2-propanol (3/1 v/v) glass, (b) dry MgY, (c) MgY with water, (d) dry HY, (e) dry CsY.

The sample (a) was measured within a 4 mm cylindrical quartz tube. The samples (a)–(e) were measured as follows: each catalyst (100 mg) was placed in a cylindrical quartz tube (capacity, 6 cm^3) and treated with 75 Torr O_2 at 673 K for 2 h. The tube was evacuated at 473 K for 3 h and then cooled to room temperature. Acetone (6 Torr, 2 μmol) [and water (16 Torr, 5.8 μmol)] was introduced to the tube and the measurement was performed at 77 K.

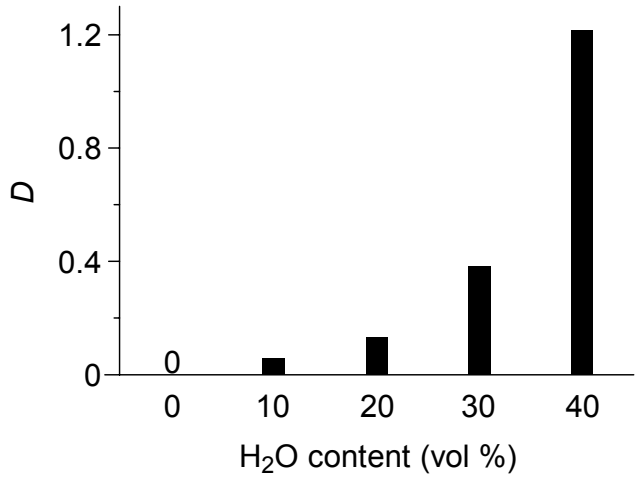


Figure S3. The distribution ratio, *D*, of 1-hexene (**1**) obtained during adsorption experiments with MgY in acetone solutions with different water content.

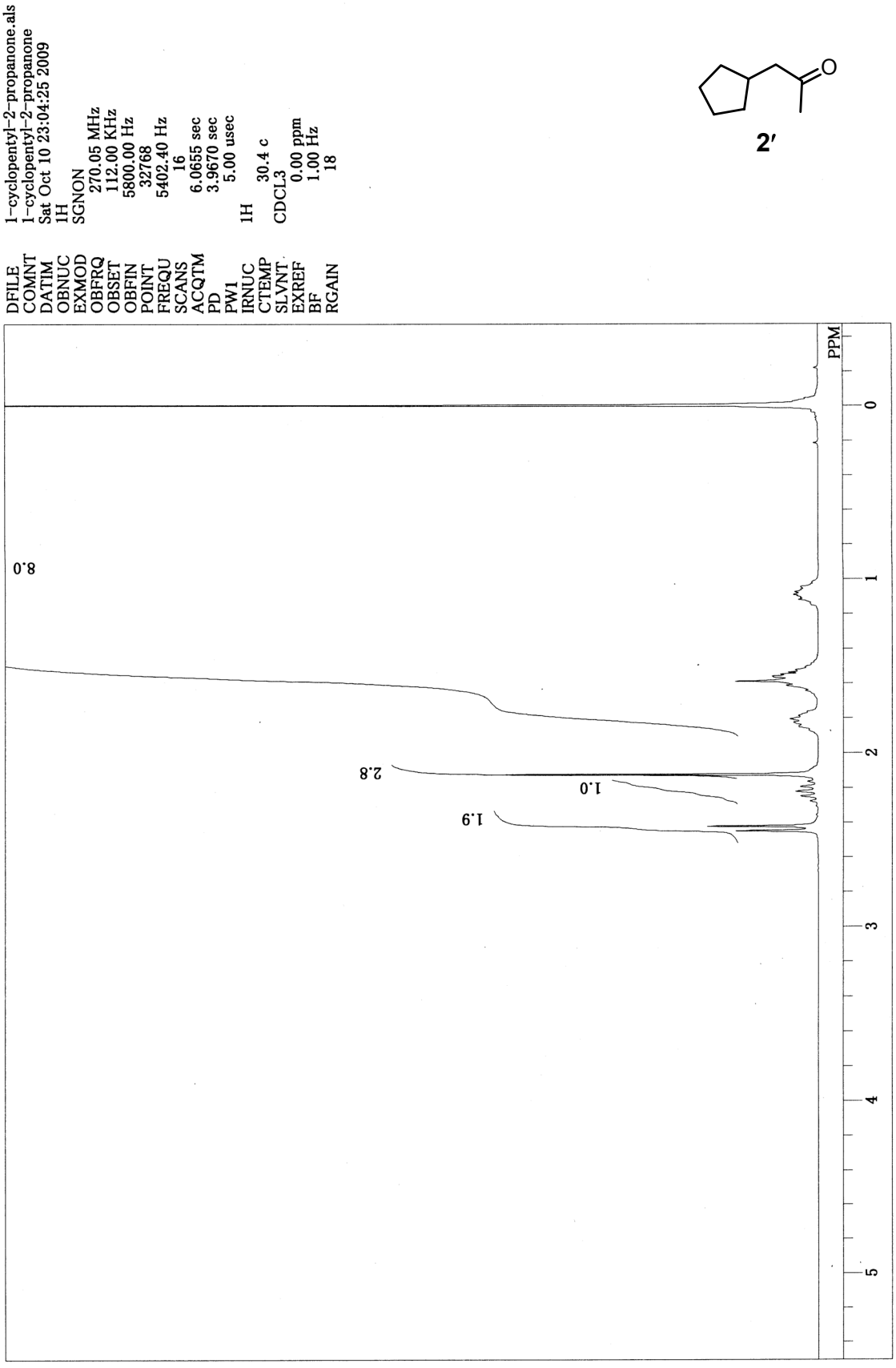


Figure S4. ^{1}H NMR chart of **2′** ($CDCl_3$, 270 MHz).

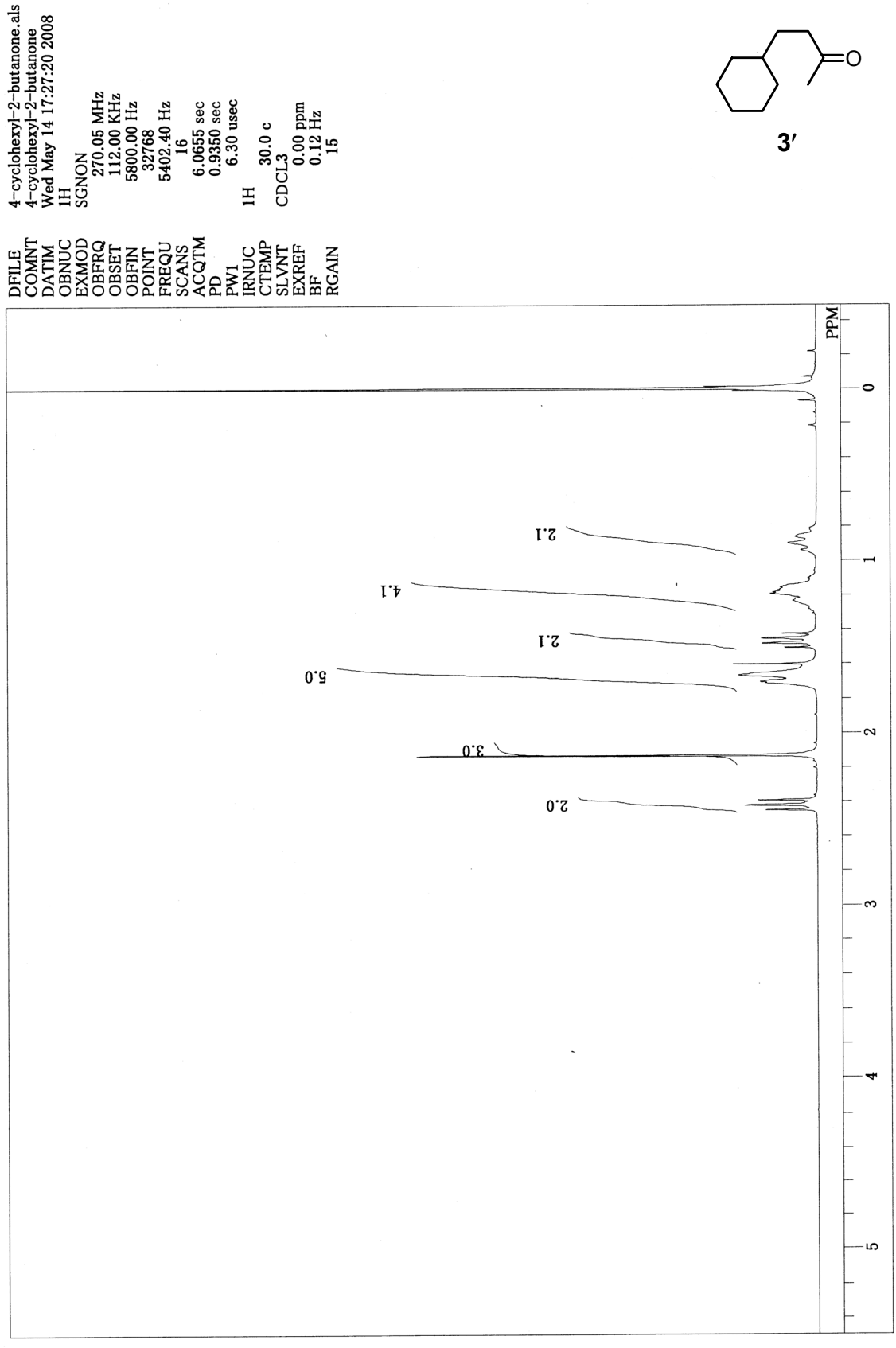


Figure S5. ^{1}H NMR chart of **3′** ($CDCl_3$, 270 MHz).

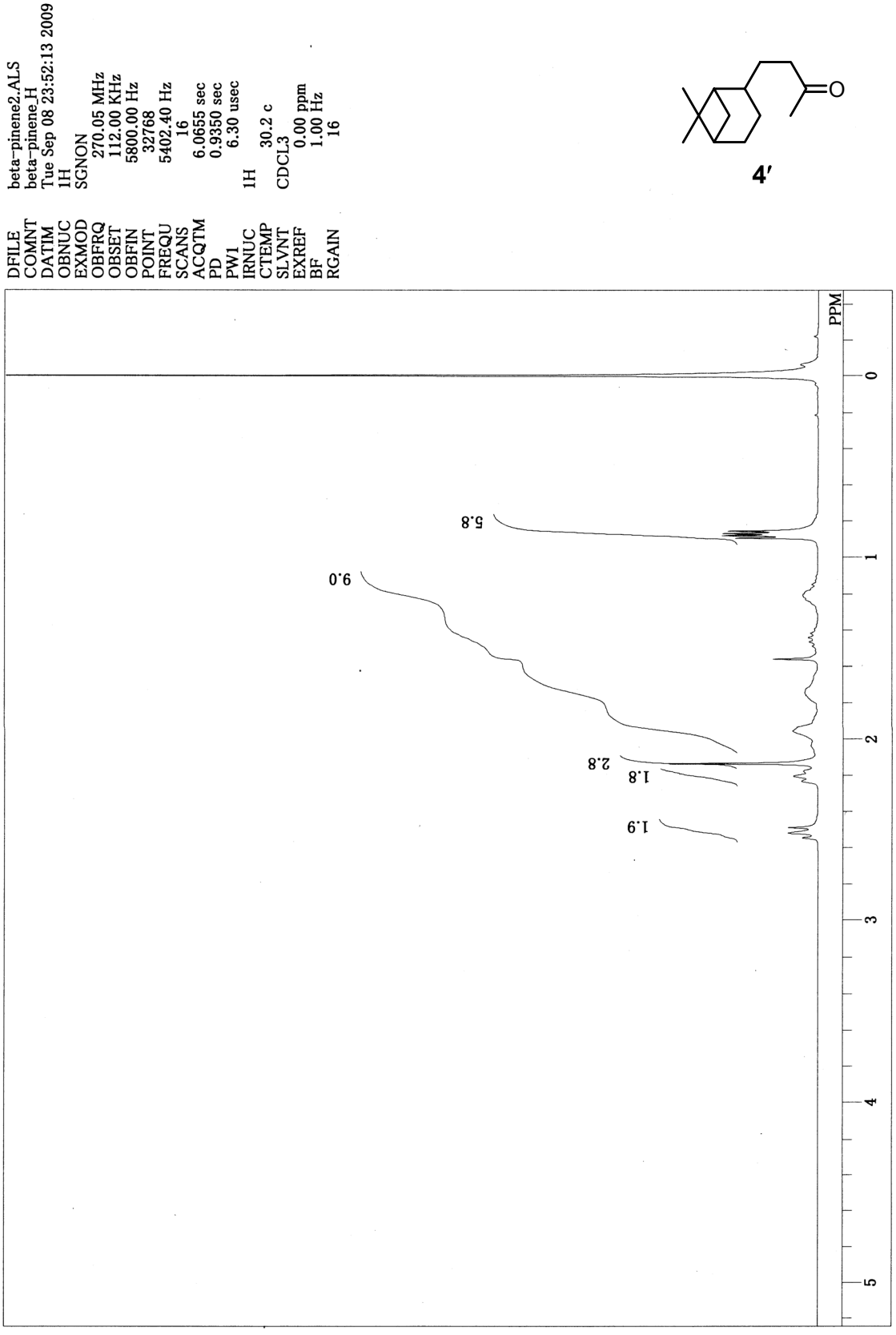


Figure S6. ^{1}H NMR chart of **4′** ($CDCl_3$, 270 MHz).

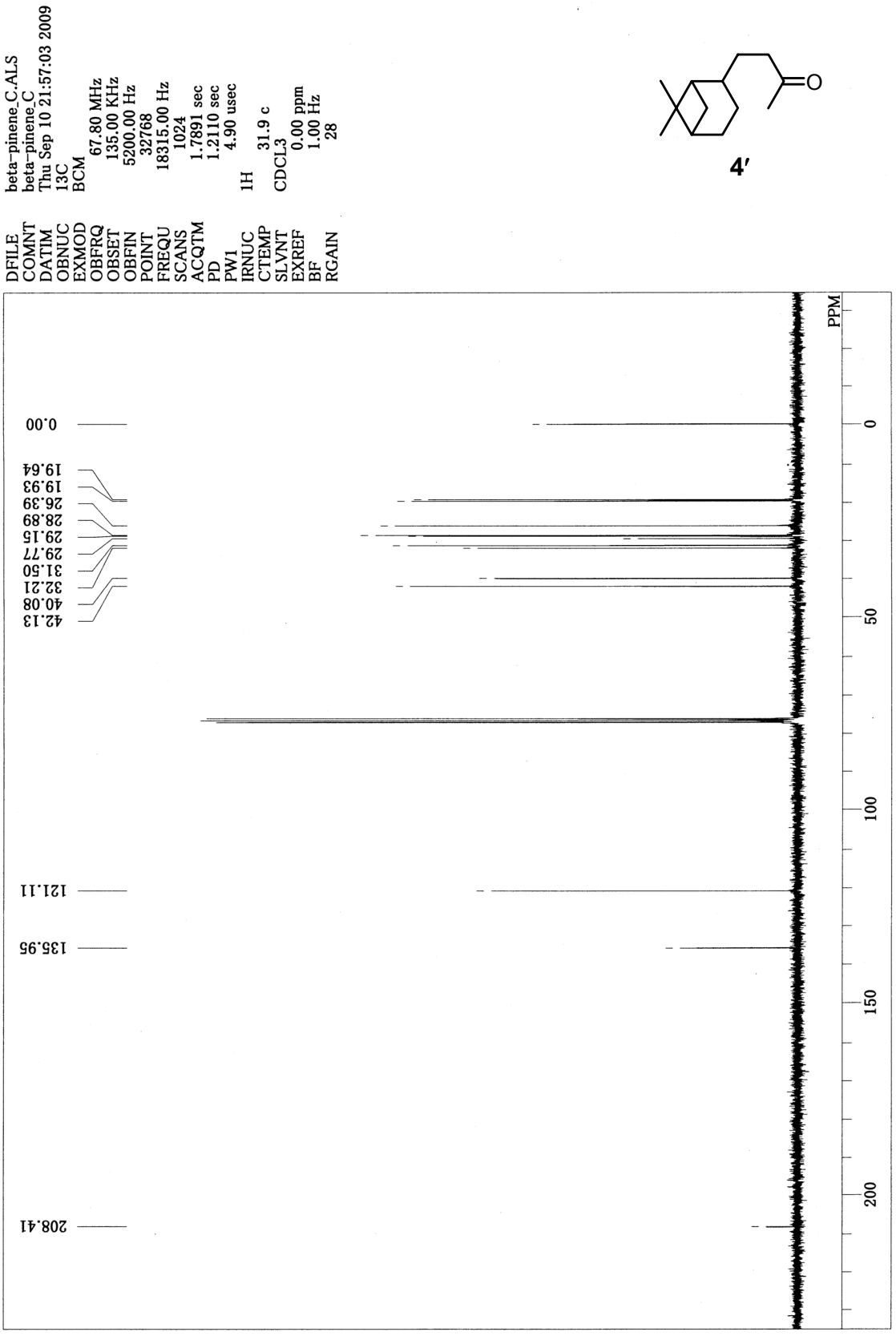


Figure S7. ^{13}C NMR chart of **4′** ($CDCl_3$, 68 MHz).

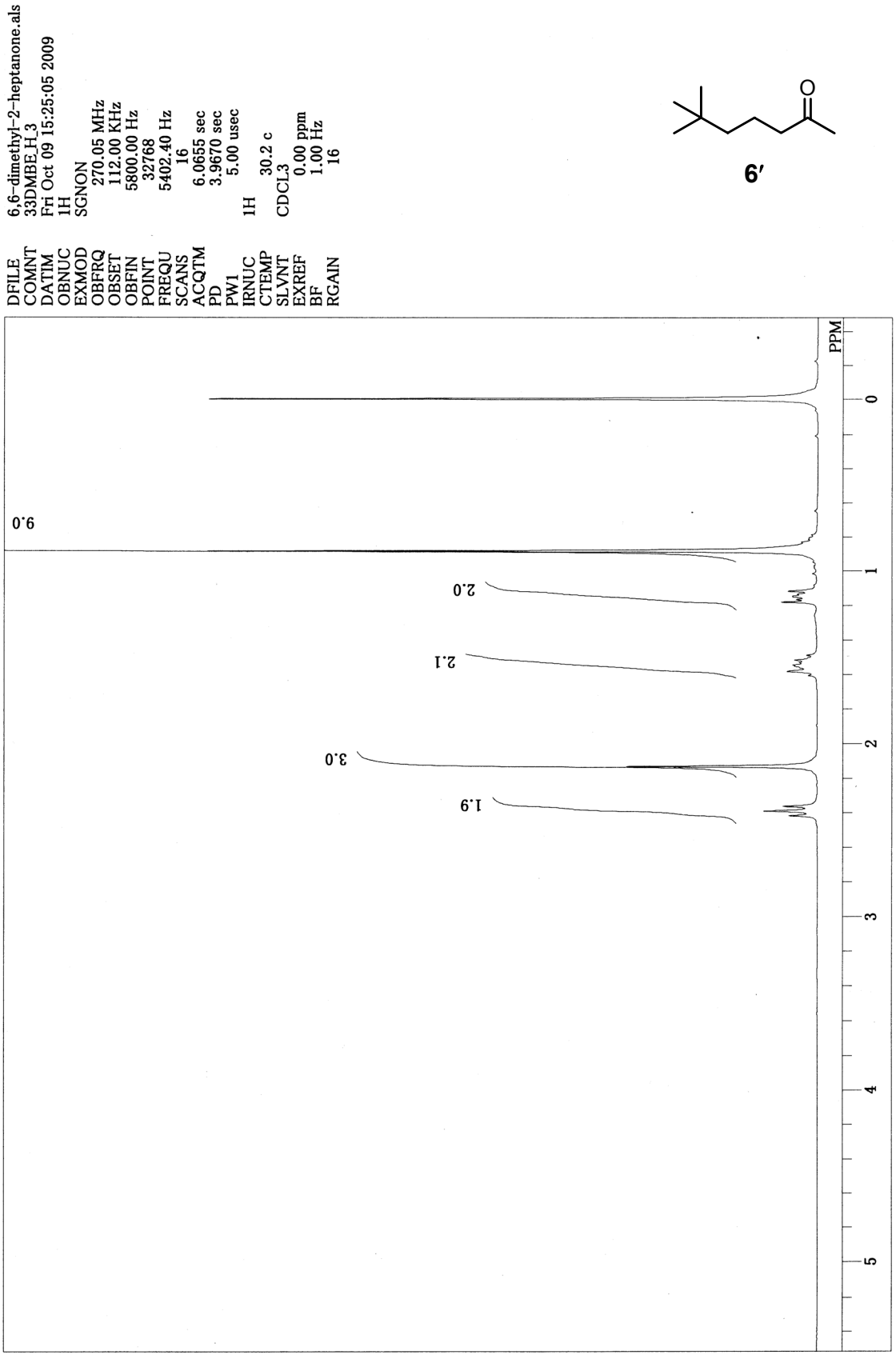


Figure S8. ^{1}H NMR chart of **6′** ($CDCl_3$, 270 MHz).

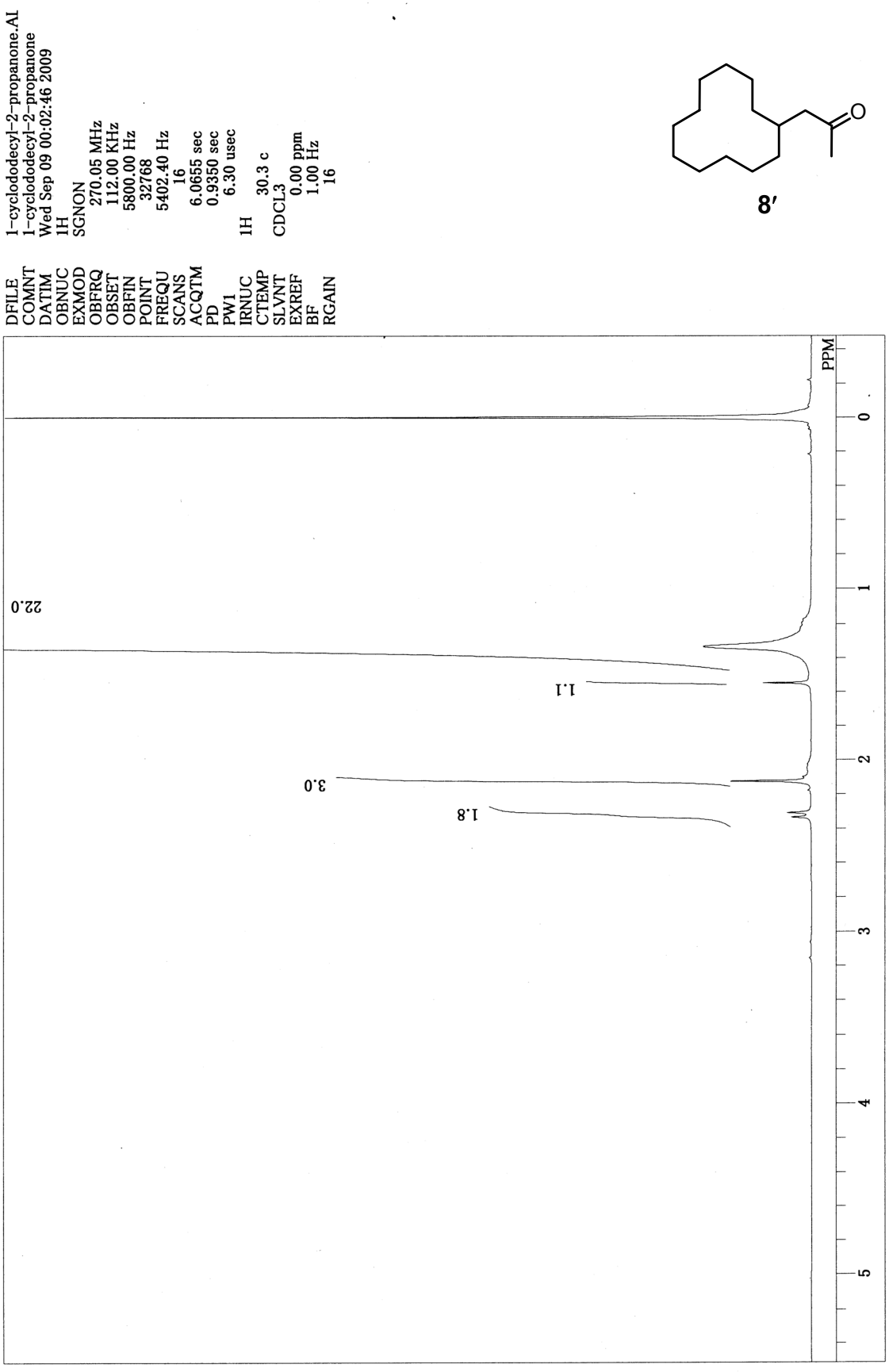


Figure S9. ^{1}H NMR chart of **8′** ($CDCl_3$, 270 MHz).

Table S1. Detailed electron density data for (a) S_0 acetone...M^{n+} and (b) T_1 acetone...M^{n+} systems.

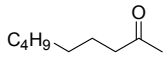
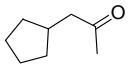
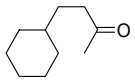
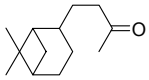
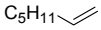
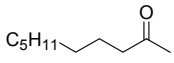
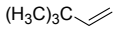
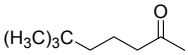
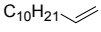
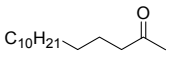
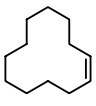
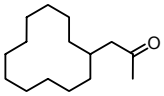
(a) S_0 acetone...M^{n+}

cations	electron density		
	carbonyl carbon	carbonyl oxygen	M^{n+}
Mg^{2+}	5.119	9.088	10.024
Ca^{2+}	5.155	9.010	18.010
Sr^{2+}	5.174	8.973	36.003
Ba^{2+}	5.181	8.953	54.001
Li^{+}	5.203	8.894	2.009
Na^{+}	5.234	8.842	10.004
K^{+}	5.251	8.811	18.002
Rb^{+}	5.263	8.789	36.001
Cs^{+}	5.269	8.778	54.001
none	5.337	8.650	

(b) T_1 acetone...M^{n+}

cations	electron density		
	carbonyl carbon	carbonyl oxygen	M^{n+}
Mg^{2+}	5.503	9.003	10.034
Ca^{2+}	5.549	8.897	18.001
Sr^{2+}	5.576	8.841	36.004
Ba^{2+}	5.675	8.425	54.002
Li^{+}	5.681	8.385	2.011
Na^{+}	5.689	8.359	10.005
K^{+}	5.689	8.344	18.003
Rb^{+}	5.695	8.331	36.002
Cs^{+}	5.698	8.324	54.001
none	5.719	8.257	

Table S2. Results of Photoreaction of Various Olefins in an Acetone/water Mixture with and without MgY.[a]

entry	additive	olefin	conv. (%)	product	GC yield (%)	Y_{MgY}/Y_{none} (–) [b]	D (–) [c]
1			67		47	1.70	
2	MgY	**1**	> 99	**1′**	80		1.21
3			83		46	1.30	
4	MgY	**2**	99	**2′**	60		0.68
5			33		15 [d]	2.73	
6	MgY	**3**	64	**3′**	41 [d]		1.42
7			60		33	1.94	
8	MgY	**4**	84	**4′**	64		1.03
9			96		52	1.36	
10	MgY	**5**	99	**5′**	71		1.31
11			55		44	1.43	
12	MgY	**6**	70	**6′**	63		0.76
13			100		93 [e]	0.90	
14	MgY	**7**	99	**7′**	84 [e]		0.09
15			76		26 [e]	1.02	
16	MgY	**8**	74	**8′**	26 [e]		0.10

[a] Reaction conditions: acetone/water (6/4 v/v) mixture (10 mL), olefin (0.2 mmol), MgY (5 mg), nitrogen (1 atm), λ >300 nm, photoirradiation time (6 h). [b] Y_{MgY}/Y_{none} denotes the ratio of methyl ketone yields obtained with and without MgY. [c] Distribution ratio of olefins determined by adsorption experiments. [d] Photoirradiation time (2 h). [e] Olefin (0.05 mmol).

Cartesian Coordinates

Free S_0 acetone

E(RHF) = -191.9649 a.u.

Center Number	Atom	Cartesian Coordinates(Å) X	Y	Z
1	C	-1.287284	-0.616325	-0.000065
2	C	0.000000	0.176763	-0.000056
3	O	-0.000001	1.408530	0.000011
4	C	1.287285	-0.616324	0.000057
5	H	-1.328637	-1.269297	-0.878998
6	H	-2.139703	0.064554	-0.004647
7	H	-1.332593	-1.261719	0.884296
8	H	2.139705	0.064558	0.003828
9	H	1.332298	-1.262494	-0.883743
10	H	1.328932	-1.268525	0.879558

S_0 acetone...Li^+

E(RHF) = -199.2782 a.u.

Center Number	Atom	Cartesian Coordinates(Å) X	Y	Z
1	C	-0.890036	-1.279511	-0.000010
2	C	-0.118264	-0.000522	-0.000036
3	C	-0.867562	1.291827	-0.000011
4	O	1.130117	-0.011913	-0.000004
5	H	-0.223608	-2.142098	-0.000467
6	H	-1.545012	-1.311940	-0.877919
7	H	-1.544153	-1.312289	0.878543
8	H	-0.186467	2.142905	-0.000552
9	H	-1.520946	1.336016	0.878584
10	H	-1.521952	1.335613	-0.877861
11	Li	2.918791	-0.007890	0.000013

S_0 acetone...Na^+

E(RHF) = -353.6801 a.u.

Center Number	Atom	Cartesian Coordinates(Å) X	Y	Z
1	C	1.526484	-1.285139	-0.000009
2	C	0.756843	-0.000005	0.000008
3	C	1.526329	1.285223	-0.000018
4	O	-0.488457	-0.000083	-0.000001
5	H	0.853541	-2.142986	-0.000145
6	H	2.179733	-1.324377	0.878673
7	H	2.179984	-1.324264	-0.878501
8	H	0.853286	2.142991	-0.000662
9	H	2.180248	1.324209	-0.878201
10	H	2.17915	1.324756	0.878972
11	Na	-2.670566	-0.000013	-0.000001

S_0 acetone...K^+

E(RHF) = - 790.9775 a.u.

Center Number	Atom	Cartesian Coordinates(Å) X	Y	Z
1	C	-2.082915	1.284800	-0.000013
2	C	-1.308105	-0.000023	-0.000006
3	C	-2.083582	-1.284441	0.000012
4	O	-0.064571	-0.000358	-0.000001
5	H	-1.409636	2.142538	-0.000842
6	H	-2.735058	1.324927	0.879331
7	H	-2.736441	1.324223	-0.878350
8	H	-1.410739	-2.142521	0.000725
9	H	-2.735854	-1.324188	-0.879253
10	H	-2.737021	-1.323569	0.878429
11	K	2.480470	-0.000029	0

S_0 acetone...Rb^+

E(RHF) = -215.4420 a.u.

Center Number	Atom	Cartesian Coordinates(Å) X	Y	Z
1	C	-2.886685	1.285415	0.000003
2	C	-2.108099	-0.000014	-0.000027
3	C	-2.887052	-1.285219	-0.000014
4	O	-0.865440	-0.000196	0.000012
5	H	-2.212975	2.143178	0.000281
6	H	-3.539315	1.325560	0.879158
7	H	-3.538913	1.325829	-0.879439
8	H	-2.213582	-2.143170	-0.000774
9	H	-3.540146	-1.325000	-0.878835
10	H	-3.538838	-1.325626	0.879763
11	Rb	1.967522	-0.000008	-0.000001

S_0 acetone...Cs^+

E(RHF) = -211.4731 a.u.

Center Number	Atom	Cartesian Coordinates(Å) X	Y	Z
1	C	-3.433327	1.286904	-0.000041
2	C	-2.655940	-0.000240	0.000049
3	C	-3.439349	-1.283710	-0.000021
4	O	-1.413995	-0.003223	0.000044
5	H	-2.757314	2.142880	-0.001032
6	H	-4.084664	1.329457	0.880027
7	H	-4.086267	1.328568	-0.878945
8	H	-2.767284	-2.142783	0.000252
9	H	-4.091436	-1.322872	-0.879682
10	H	-4.091913	-1.322674	0.879296
11	Cs	1.642955	-0.000082	-0.000003

S_0 acetone...Mg^{2+}

E(RHF) = -390.9665 a.u.

Center Number	Atom	Cartesian Coordinates(Å) X	Y	Z
1	C	-1.485562	1.282915	0.007365
2	C	-0.759769	0.000001	-0.000388
3	C	-1.485600	-1.282898	-0.007153
4	O	0.522236	-0.000019	-0.000190
5	H	-0.852550	2.125555	0.285977
6	H	-2.367151	1.219690	0.654821
7	H	-1.874625	1.445025	-1.011545
8	H	-0.852769	-2.125651	-0.285834
9	H	-2.367582	-1.219883	-0.654086
10	H	-1.874043	-1.444661	1.012055
11	Mg	2.366368	-0.000002	0.000099

S_0 acetone...Ca^{2+}

E(RHF) = -868.1978 a.u.

Center Number	Atom	Cartesian Coordinates(Å) X	Y	Z
1	C	-1.994988	1.282358	0.000028
2	C	-1.249635	0.000000	-0.000050
3	C	-1.994988	-1.282358	0.000032
4	O	0.019054	0.000000	-0.000092
5	H	-1.330695	2.146132	-0.000025
6	H	-2.657000	1.317420	0.874637
7	H	-2.657157	1.317429	-0.874460
8	H	-1.330695	-2.146132	0.000099
9	H	-2.657051	-1.317480	-0.874536
10	H	-2.657106	-1.317369	0.874560
11	Ca	2.228747	0.000000	0.000020

S_0 acetone...Sr^{2+}

E(RHF) = -221.6127 a.u.

Center Number	Atom	Cartesian Coordinates(Å) X	Y	Z
1	C	2.686366	-1.281256	-0.000032
2	C	1.929373	-0.000124	0.000024
3	C	2.681913	1.283662	-0.000004
4	O	0.666147	-0.002473	0.000023
5	H	2.023156	-2.146290	-0.000909
6	H	3.345801	-1.316273	0.875923
7	H	3.347281	-1.315519	-0.874878
8	H	2.015818	2.146493	0.000446
9	H	3.341569	1.320772	-0.875694
10	H	3.342346	1.320414	0.875109
11	Sr	-1.750817	-0.000092	-0.000003

S_0 acetone...Ba^{2+}

E(RHF) = -216.4437 a.u.

Center Number	Atom	Cartesian Coordinates(Å) X	Y	Z
1	C	3.168694	1.283003	-0.000052
2	C	2.410176	-0.000065	0.000092
3	C	3.170742	-1.281905	-0.000052
4	O	1.150052	-0.001126	0.000080
5	H	2.502869	2.146192	-0.000486
6	H	3.828047	1.319638	-0.875606
7	H	3.827390	1.320080	0.875993
8	H	2.506253	-2.146116	-0.000476
9	H	3.829508	-1.317922	0.875986
10	H	3.830147	-1.317488	-0.875612
11	Ba	-1.464684	-0.000028	-0.000007

Free T_1 acetone

E(RHF) = -193.1556 a.u.

Center Number	Atom	Cartesian Coordinates(Å) X	Y	Z
1	C	-1.299264	-0.589672	0.041764
2	C	0.000000	0.093965	-0.294042
3	O	0.000002	1.391246	0.064476
4	C	1.299262	-0.589675	0.041764
5	H	-1.311088	-1.578889	-0.422880
6	H	-2.153043	-0.019570	-0.332960
7	H	-1.413185	-0.710376	1.129477
8	H	2.153041	-0.019575	-0.332961
9	H	1.311084	-1.578892	-0.422880
10	H	1.413184	-0.710379	1.129477

T_1 acetone...Li^+

E(RHF) = -199.1659 a.u.

Center Number	Atom	Cartesian Coordinates(Å) X	Y	Z
1	C	-0.864927	-1.305445	0.003036
2	C	-0.150916	-0.000013	-0.273572
3	C	-0.863942	1.305964	0.003070
4	O	1.101579	-0.000436	0.248276
5	H	-0.280702	-2.167933	-0.324407
6	H	-1.803884	-1.290711	-0.554842
7	H	-1.085210	-1.405185	1.073338
8	H	-0.279079	2.168025	-0.324362
9	H	-1.084160	1.405852	1.073370
10	H	-1.802906	1.291935	-0.554819
11	Li	2.934006	-0.000510	-0.256561

T_1 acetone...Na^+

E(RHF) = -353.5753 a.u.

Center Number	Atom	Cartesian Coordinates(Å) X	Y	Z
1	C	-1.520889	1.304189	-0.009474
2	C	-0.802959	0.000000	-0.264215
3	C	-1.520913	-1.304177	-0.009476
4	O	0.441082	-0.000011	0.276772
5	H	-0.925763	2.164687	-0.323493
6	H	-1.768357	1.410957	1.054855
7	H	-2.447039	1.296579	-0.588542
8	H	-0.925798	-2.164685	-0.323492
9	H	-2.447059	-1.296549	-0.588548
10	H	-1.768385	-1.410939	1.054852
11	Na	2.711120	-0.000003	-0.072801

T_1 acetone...K^+

E(RHF) = -790.8779 a.u.

Center Number	Atom	Cartesian Coordinates(Å) X	Y	Z
1	C	-2.097337	1.303924	0.045840
2	C	-1.421222	0.000000	-0.298869
3	C	-2.097374	-1.303905	0.045840
4	O	-0.114971	-0.000018	0.056185
5	H	-1.549134	2.160790	-0.352662
6	H	-2.196719	1.419198	1.133724
7	H	-3.094893	1.297968	-0.399032
8	H	-1.549193	-2.160786	-0.352660
9	H	-3.094929	-1.297922	-0.399034
10	H	-2.196761	-1.419175	1.133724
11	K	2.541947	-0.000002	0.001558

T_1 acetone...Rb^+

E(RHF) = -215.3451 a.u.

Center Number	Atom	Cartesian Coordinates(Å) X	Y	Z
1	C	-2.921711	1.303550	0.023052
2	C	-2.227442	-0.000011	-0.284285
3	C	-2.922837	-1.302975	0.023019
4	O	-0.940475	-0.000554	0.136599
5	H	-2.351350	2.160647	-0.343424
6	H	-3.079647	1.419490	1.104271
7	H	-3.894166	1.300634	-0.474757
8	H	-2.353189	-2.160549	-0.343447
9	H	-3.895279	-1.299225	-0.474809
10	H	-3.080889	-1.418788	1.104234
11	Rb	2.016494	-0.000031	-0.006367

T_1 acetone...Cs^+

E(RHF) = -211.3779 a.u.

Center Number	Atom	Cartesian Coordinates(Å) X	Y	Z
1	C	-3.487121	1.303590	0.024540
2	C	-2.794551	-0.000033	-0.285186
3	C	-3.490339	-1.301953	0.024454
4	O	-1.505983	-0.001601	0.128954
5	H	-2.916522	2.160107	-0.343099
6	H	-3.641489	1.419905	1.106401
7	H	-4.461368	1.302719	-0.469860
8	H	-2.921790	-2.159837	-0.343163
9	H	-4.464556	-1.298688	-0.469996
10	H	-3.645035	-1.417912	1.106306
11	Cs	1.686013	-0.000057	-0.003656

T_1 acetone...Mg^{2+}

E(RHF) = -390.8158 a.u.

Center Number	Atom	Cartesian Coordinates(Å) X	Y	Z
1	C	-0.110661	-1.563900	1.273552
2	C	0.315279	-0.688541	0.000000
3	C	-0.110661	-1.563900	-1.273552
4	O	-0.110661	0.546834	0.000000
5	H	0.288237	-1.012884	2.129723
6	H	0.374820	-2.532099	1.158769
7	H	-1.200073	-1.650169	1.303595
8	H	0.288237	-1.012884	-2.129723
9	H	-1.200073	-1.650169	-1.303595
10	H	0.374820	-2.532099	-1.158769
11	Mg	0.116298	2.409474	0.000000

T_1 acetone...Ca^{2+}

E(RHF) = -868.0481 a.u.

Center Number	Atom	Cartesian Coordinates(Å) X	Y	Z
1	C	0.060440	2.088343	1.257148
2	C	-0.402671	1.180314	0.000000
3	C	0.060440	2.088343	-1.257148
4	O	-0.038709	-0.053471	0.000000
5	H	-0.350062	1.532975	2.104564
6	H	-0.405237	3.065566	1.152278
7	H	1.151114	2.145441	1.278092
8	H	-0.350062	1.532975	-2.104564
9	H	1.151114	2.145441	-1.278092
10	H	-0.405237	3.065566	-1.152278
11	Ca	0.060440	-2.260110	0.000000

T_1 acetone...Sr^{2+}

E(RHF) = -221.4632 a.u.

Center Number	Atom	Cartesian Coordinates(Å) X	Y	Z
1	C	-2.786509	-1.247595	0.092155
2	C	-1.853603	-0.001241	-0.395058
3	C	-2.785485	1.248862	0.092000
4	O	-0.631194	-0.000055	-0.036857
5	H	-2.228030	-2.095081	-0.312857
6	H	-3.764019	-1.146533	-0.372507
7	H	-2.835574	-1.256375	1.182843
8	H	-2.227702	2.093944	-0.318800
9	H	-2.828960	1.260097	1.182844
10	H	-3.764876	1.145905	-0.368163
11	Sr	1.769797	-0.000044	0.014919

T_1 acetone...Ba^{2+}

E(RHF) = -216.3226 a.u.

Center Number	Atom	Cartesian Coordinates(Å) X	Y	Z
1	C	3.222556	1.305572	0.046691
2	C	2.526630	-0.000021	-0.307899
3	C	3.222928	-1.305394	0.046693
4	O	1.231637	-0.000135	0.066587
5	H	2.689982	2.173276	-0.347735
6	H	4.213672	1.272698	-0.412168
7	H	3.334035	1.402758	1.133761
8	H	2.690532	-2.173242	-0.347658
9	H	3.334509	-1.402517	1.133760
10	H	4.214006	-1.272295	-0.412225
11	Ba	-1.502902	-0.000010	0.000119

Free S_0 1-hexene

E(RHF) = -234.1791 a.u.

Center Number	Atom	Cartesian Coordinates(Å) X	Y	Z
1	C	3.056887	-0.218439	-0.449229
2	C	2.030655	-0.170507	0.415588
3	C	0.770739	0.614009	0.200438
4	C	-0.467278	-0.286012	0.117020
5	C	-1.764647	0.498651	-0.065893
6	C	-2.992407	-0.405887	-0.150751
7	H	3.941405	-0.816736	-0.251556
8	H	3.040493	0.344538	-1.379675
9	H	2.089149	-0.752444	1.337367
10	H	0.860609	1.203912	-0.721534
11	H	0.634267	1.328740	1.025078
12	H	-0.537255	-0.894796	1.029775
13	H	-0.340793	-0.988049	-0.718379
14	H	-1.691154	1.107004	-0.977202
15	H	-1.880930	1.201772	0.769711
16	H	-3.910524	0.175818	-0.283493
17	H	-3.100918	-1.001967	0.761884
18	H	-2.908037	-1.098686	-0.995018

S_0 1-hexene...Li^+

E(RHF) = -241.4525 a.u.

Center Number	Atom	Cartesian Coordinates(Å) X	Y	Z
1	C	2.847621	-0.622163	-0.430647
2	C	1.858878	-0.334410	0.444612
3	C	0.647115	0.498406	0.111708
4	C	-0.649436	-0.332504	0.168591
5	C	-1.892323	0.499180	-0.142191
6	C	-3.166937	-0.340771	-0.092383
7	H	3.681603	-1.262017	-0.158040
8	H	2.801669	-0.299519	-1.474071
9	H	1.905373	-0.749797	1.452277
10	H	0.729702	0.923358	-0.905736
11	H	0.521388	1.330137	0.830552
12	H	-0.739334	-0.778353	1.167040
13	H	-0.558764	-1.158637	-0.546995
14	H	-1.787971	0.951262	-1.137273
15	H	-1.966306	1.325208	0.577396
16	H	-4.045171	0.269865	-0.318675
17	H	-3.309576	-0.778837	0.900365
18	H	-3.128124	-1.155993	-0.821534
19	Li	2.675334	1.725632	0.025520

S_0 1-hexene...Na^+

E(RHF) = -395.8646 a.u.

Center Number	Atom	Cartesian Coordinates(Å) X	Y	Z
1	C	-2.048748	1.300501	-0.374886
2	C	-1.202286	0.622212	0.433561
3	C	-0.116944	-0.300525	-0.039244
4	C	1.269396	0.318014	0.212206
5	C	2.406452	-0.602033	-0.229130
6	C	3.778821	0.023450	0.010381
7	H	-2.726742	2.055780	0.017700
8	H	-1.988122	1.208211	-1.459789
9	H	-1.232320	0.827472	1.507257
10	H	-0.233228	-0.505143	-1.112439
11	H	-0.160891	-1.262332	0.493413
12	H	1.377063	0.547736	1.280622
13	H	1.332012	1.271850	-0.327097
14	H	2.288663	-0.836619	-1.295072
15	H	2.333628	-1.553353	0.314175
16	H	4.578554	-0.649189	-0.312364
17	H	3.930964	0.240246	1.072591
18	H	3.884408	0.960887	-0.544934
19	Na	-3.445831	-0.952297	0.026237

S_0 1-hexene...K^+

E(RHF) = -833.1654 a.u.

Center Number	Atom	Cartesian Coordinates(Å) X	Y	Z
1	C	-1.443336	1.852267	-0.395264
2	C	-0.698238	1.114489	0.451403
3	C	0.220248	0.003939	0.027411
4	C	1.697085	0.393104	0.199395
5	C	2.652030	-0.729942	-0.199106
6	C	4.116719	-0.330992	-0.033146
7	H	-2.022386	2.704118	-0.049510
8	H	-1.420351	1.677569	-1.470948
9	H	-0.687860	1.380629	1.510646
10	H	0.042552	-0.251086	-1.028336
11	H	0.045964	-0.903356	0.629460
12	H	1.876764	0.675288	1.245228
13	H	1.894494	1.285215	-0.408190
14	H	2.463221	-1.011474	-1.243615
15	H	2.440782	-1.618425	0.411126
16	H	4.782747	-1.148099	-0.324685
17	H	4.336790	-0.073409	1.007806
18	H	4.358389	0.537132	-0.654570
19	K	-3.019903	-0.898489	0.003759

S_0 1-hexene...Rb^+

E(RHF) = -257.6332 a.u.

Center Number	Atom	Cartesian Coordinates(Å) X	Y	Z
1	C	-0.365284	2.118915	-0.376492
2	C	0.292713	1.274182	0.442270
3	C	1.112936	0.104065	-0.019565
4	C	2.613775	0.342784	0.207516
5	C	3.472718	-0.844085	-0.225179
6	C	4.962839	-0.595824	0.000944
7	H	-0.864392	3.006657	0.003252
8	H	-0.343878	1.990704	-1.458139
9	H	0.309450	1.488589	1.513409
10	H	0.936175	-0.078783	-1.089281
11	H	0.829868	-0.810041	0.526369
12	H	2.790700	0.554760	1.270716
13	H	2.913283	1.240844	-0.347914
14	H	3.291077	-1.053051	-1.287946
15	H	3.159770	-1.738706	0.330236
16	H	5.559252	-1.456336	-0.316544
17	H	5.172863	-0.413765	1.060057
18	H	5.304045	0.276706	-0.565682
19	Rb	-2.745848	-0.470481	0.004987

S_0 1-hexene...Cs^+

E(RHF) = -253.6666 a.u.

Center Number	Atom	Cartesian Coordinates(Å) X	Y	Z
1	C	0.362355	2.271637	-0.372878
2	C	0.974726	1.388636	0.439682
3	C	1.727816	0.177437	-0.029678
4	C	3.238332	0.319813	0.210970
5	C	4.026282	-0.912183	-0.230753
6	C	5.527382	-0.759397	0.007404
7	H	-0.091241	3.180941	0.012771
8	H	0.371464	2.146282	-1.454820
9	H	1.002107	1.593774	1.512345
10	H	1.546995	0.017891	-1.102313
11	H	1.383197	-0.723557	0.502564
12	H	3.420037	0.507436	1.278038
13	H	3.597627	1.204429	-0.330532
14	H	3.839446	-1.096970	-1.297144
15	H	3.654955	-1.792579	0.311433
16	H	6.072112	-1.651172	-0.316913
17	H	5.740992	-0.602997	1.069956
18	H	5.925539	0.097230	-0.546267
19	Cs	-2.392811	-0.323570	0.003862

S_0 1-hexene...Mg^{2+}

E(RHF) = -433.1310 a.u.

Center Number	Atom	Cartesian Coordinates(Å) X	Y	Z
1	C	-2.229736	1.180972	-0.467833
2	C	-1.353527	0.791821	0.512961
3	C	-0.278406	-0.254314	0.318966
4	C	1.115332	0.437996	0.140843
5	C	2.238881	-0.579327	-0.060729
6	C	3.589346	0.124518	-0.200723
7	H	-2.957354	1.975275	-0.309122
8	H	-2.093923	0.851410	-1.512531
9	H	-1.392980	1.284585	1.488127
10	H	-0.401524	-0.847951	-0.630116
11	H	-0.182111	-0.936193	1.180459
12	H	1.296626	1.036361	1.042243
13	H	1.044051	1.120712	-0.713769
14	H	2.038855	-1.175435	-0.960937
15	H	2.268039	-1.268379	0.792591
16	H	4.381763	-0.612621	-0.350901
17	H	3.831732	0.697312	0.698765
18	H	3.596916	0.803331	-1.058240
19	Mg	-2.493452	-1.094867	-0.093957

S_0 1-hexene...Ca^{2+}

E(RHF) = -910.3567 a.u.

Center Number	Atom	Cartesian Coordinates(Å) X	Y	Z
1	C	-1.660800	1.745594	-0.428197
2	C	-0.854857	1.120173	0.467604
3	C	0.086511	-0.007586	0.118800
4	C	1.563967	0.456106	0.187391
5	C	2.540596	-0.668826	-0.152264
6	C	3.989748	-0.186841	-0.094757
7	H	-2.241685	2.622068	-0.150278
8	H	-1.624685	1.507172	-1.497368
9	H	-0.803603	1.503794	1.489695
10	H	-0.078309	-0.371395	-0.916503
11	H	0.020329	-0.854615	0.832415
12	H	1.761274	0.836614	1.196602
13	H	1.683935	1.292675	-0.510850
14	H	2.321258	-1.052887	-1.157487
15	H	2.400727	-1.499499	0.552535
16	H	4.673440	-1.002908	-0.340891
17	H	4.245588	0.174317	0.905494
18	H	4.164230	0.623086	-0.808861
19	Ca	-2.525675	-0.926507	-0.009298

S_0 1-hexene...Sr^{2+}

E(RHF) = -263.7735 a.u.

Center Number	Atom	Cartesian Coordinates(Å) X	Y	Z
1	C	-0.628312	2.094641	-0.396016
2	C	-0.003493	1.259575	0.471832
3	C	0.828336	0.073608	0.058020
4	C	2.335562	0.394924	0.196622
5	C	3.219123	-0.792667	-0.183715
6	C	4.704174	-0.456495	-0.053128
7	H	-1.093015	3.017447	-0.055718
8	H	-0.547749	1.954421	-1.476913
9	H	0.021969	1.534150	1.530568
10	H	0.643748	-0.195622	-0.996538
11	H	0.648168	-0.809882	0.697246
12	H	2.539955	0.696390	1.231409
13	H	2.557864	1.256371	-0.444439
14	H	2.999724	-1.094740	-1.216517
15	H	2.977334	-1.647912	0.461791
16	H	5.319470	-1.316866	-0.328687
17	H	4.956131	-0.179672	0.975039
18	H	4.978417	0.375178	-0.709069
19	Sr	-2.335115	-0.500810	-0.006049

S_0 1-hexene...Ba^{2+}

E(RHF) = -258.6080 a.u.

Center Number	Atom	Cartesian Coordinates(Å) X	Y	Z
1	C	0.039749	2.270323	-0.393336
2	C	0.600041	1.390922	0.470002
3	C	1.355403	0.157177	0.054170
4	C	2.878667	0.374990	0.191995
5	C	3.682249	-0.868776	-0.185043
6	C	5.186309	-0.636124	-0.048180
7	H	-0.366222	3.219043	-0.050044
8	H	0.110709	2.128836	-1.473867
9	H	0.632908	1.652754	1.531422
10	H	1.147968	-0.096418	-0.999317
11	H	1.110261	-0.713465	0.689081
12	H	3.104281	0.664797	1.225897
13	H	3.160863	1.218408	-0.449480
14	H	3.446807	-1.155371	-1.218870
15	H	3.379973	-1.706310	0.458540
16	H	5.743621	-1.535718	-0.322235
17	H	5.451960	-0.377587	0.981379
18	H	5.519215	0.176144	-0.701395
19	Ba	-2.051730	-0.350110	-0.003728