Supporting information

Experimental and Theoretical Studies on Radical Trifluoromethylation of Ti ate and Li Enolates

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Contents

General experimental methods

Chemical shift of ^{1}H NMR was expressed in parts per million downfield from tetramethylsilane as an internal standard (δ=0) in $CDCl_3$. Chemical shifts of ^{13}C NMR were expressed in parts per million downfield from $CDCl_3$ as an internal standard (δ=77.0) in $CDCl_3$. Chemical shifts of ^{19}F NMR were expressed in parts per million downfield from BTF as an internal standard (δ=-63.24) in $CDCl_3$. Analytical thin layer chromatographies (TLC) were performed on a glass plates sheets pre-coated with silica gel. Visualization was accomplished by UV light (254 nm), anisaldehyde, $KMnO_4$ and phosphomolybdic acid. Column chromatography was performed on silica gel (spherical, neutral), employing hexane and dichloromethane mixture as an eluent unless otherwise noted. THF was distilled from benzophenone-kethyl under Ar prior to use. All experiments were carried out under argon atmosphere unless otherwise noted.

Typical experimental procedure for trifluoromethylation

The reaction of titanium ate enolate. To a solution of $^{i}Pr_2NH$ (44.9 μL, 0.32 mmol) in THF (2.0 mL) was added $^{n}BuLi$ (205.1 μL of 1.56 M solution in hexane, 0.32 mmol) at -78 °C. The reaction mixture was stirred at 0 °C for 30 minutes and then cooled to -78 °C. To the solution was added cyclohexanone (20.7 μL, 0.2 mmol) and stirred for 30 minutes at the temperature. Then $Ti(O^{i}Pr)_4$ (94.5 μL, 0.32 mmol) was added to the solution. After stirred for 30 minutes at -78 °C, gaseous CF_3I (ca. 200 mg, ca. 1.0 mmol) was added with a cannula followed by Et_3B (0.2 mL of 1.0 M solution in hexane, 0.2 mmol). The reaction mixture was stirred for 2 hours at -78 °C and then quenched by acetic acid (0.12 mL of 5 M solution in THF) at the temperature. After warming to room temperature, BTF (10 μL, 0.082 mmol) was added as an internal standard. The yield was determined by ^{19}F NMR of the crude mixture (81%).

The reaction of lithium enolate. To a solution of $^{i}Pr_2NH$ (28.0 μL, 0.20 mmol) in THF (2.0 mL) was added $^{n}BuLi$ (126.3 μL of 1.58 M solution in hexane, 0.20 mmol) at -78 °C. The reaction mixture was stirred at 0 °C for 30 minutes and then cooled to -78 °C. To the solution was added cyclohexanone (20.7 μL, 0.2 mmol) and stirred for 60 minutes at the temperature. Then, gaseous CF_3I (ca. 200 mg, ca. 1.0 mmol) was added

with a cannula. Next, a syringe, which was filled with 0.12 mL of 5M solution of acetic acid in THF, was set to the reaction vessel and kept untouched till quenching the reaction. Then Et_3B (0.2 mL of 1.0 M solution in hexane, 0.2 mmol) was added in flat 15 s to start the radical addition reaction. The reaction mixture was immediately quenched (in ~1 s) by acetic acid solution, which was set beforehand, at -78 °C. After warming to room temperature, BTF (10 μL, 0.082 mmol) was added as an internal standard. The yield was determined by ^{19}F NMR of the crude mixture (81%).

2-Trifluoromethyl-cyclohexanone (1): ^1H NMR ($CDCl_3$, 400 MHz) δ 1.62~1.88 (m, 3H), 1.92~2.14 (m, 2H), 2.24~2.39 (m, 2H), 2.42~2.53 (m, 1H), 2.98~3.13 (m, 1H). ^{13}C NMR ($CDCl_3$, 75 Hz) δ 23.7, 27.1, 27.5 (q, *J*=2.4 Hz), 42.2, 53.6(q, *J*=25.7 Hz), 124.6(q, *J*=279.5 Hz), 203.0. ^{19}F NMR ($CDCl_3$, 376 Hz) δ -69.3(d, 7.9 Hz) (ppm). IR (neat) 2954, 2876, 2364, 1729, 1272, 1170, 1125, 1060 (cm^{-1}). EI-MS m/z=166 [$M^{+\bullet}$]

Gaussian 03 reference (Ref. 13)

Gaussian 03, Revision C.02, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, Jr., J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; and Pople, J. A.; Gaussian, Inc., Wallingford CT, 2004.

Computational Methods

All the calculations were performed with GAUSSIAN 03 program package. All the structures were optimized at UB3LYP/631+LAN (LANL2DZ for Ti, I, 6-31+G* for others) level (E). Gibbs free energies (G) contain zero-point, thermal and entropy effects at 298.15 K and 1 atm pressure. Then the energies were recalculated in the presence of dielectric field (THF, ε=7.58) as described by the CPCM model at UB3LYP/6311+LAN (LANL2DZ for Ti, I, 6-311+G* for others) level (E(sol)). Gibbs free energies (G(sol)) contain zero-point, thermal and entropy effects at 195.15 K and 1 atm pressure.

Molecular Geometries and Energies

3: Li radical

Charge=0, Multiplicity=2

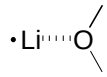
E(UB3LYP/631+LAN)= -7.49111328996 a.u.

G(UB3LYP/631+LAN)= -7.504516 a.u.

G(sol)(UB3LYP/6311+LAN//UB3LYP/631+LAN)= -7.524294 a.u.

4: Li radical with one dimethyl ether

Charge=0, Multiplicity=2



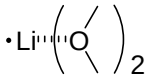
E(UB3LYP/631+LAN)= -162.540264501 a.u.

G(UB3LYP/631+LAN)= -162.487524 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	3	0	-0.013338	2.239848	0.000000
2	8	0	0.000000	0.330203	0.000000
3	6	0	1.197847	-0.454594	0.000000
4	1	0	1.239245	-1.082862	0.898823
5	1	0	1.239245	-1.082862	-0.898823
6	1	0	2.038350	0.244348	0.000000
7	6	0	-1.193732	-0.461071	0.000000
8	1	0	-1.231729	-1.089553	0.898824
9	1	0	-2.038058	0.233306	0.000000
10	1	0	-1.231729	-1.089553	-0.898824

5: Li radical with two dimethyl ethers

Charge=0, Multiplicity=2



E(UB3LYP/631+LAN)= -317.585341556 a.u.

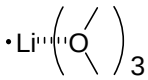
G(UB3LYP/631+LAN)= -317.462352 a.u.

G(sol)(UB3LYP/6311+LAN//UB3LYP/631+LAN)= -317.529107 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	3	0	-0.055546	-0.054371	-1.270073
2	8	0	1.533741	-0.007939	-0.125303
3	6	0	2.228501	1.229180	0.066180
4	1	0	1.486165	2.029074	0.000730
5	1	0	2.706226	1.242325	1.055325
6	1	0	2.984158	1.369698	-0.717614
7	6	0	2.403299	-1.144974	-0.076542
8	1	0	2.870817	-1.216422	0.915072
9	1	0	1.787524	-2.028593	-0.264145
10	1	0	3.176342	-1.070137	-0.852368
11	8	0	-1.618526	-0.006345	-0.139263
12	6	0	-1.624232	-0.116899	1.284776
13	1	0	-2.118676	0.755083	1.733498
14	1	0	-2.144227	-1.032976	1.595449
15	1	0	-0.580910	-0.156921	1.605395
16	6	0	-2.933565	0.059119	-0.703748
17	1	0	-3.496519	-0.850966	-0.456457
18	1	0	-3.462599	0.944116	-0.324927
19	1	0	-2.807395	0.134549	-1.787204

6: Li radical with three dimethyl ethers

Charge=0, Multiplicity=2



E(UB3LYP/631+LAN)= -472.628763985 a.u.

G(UB3LYP/631+LAN)= -472.432311 a.u.

G(sol)(UB3LYP/6311+LAN//UB3LYP/631+LAN)= -472.534280 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	3	0	0.004195	-0.002530	-0.669307
2	8	0	-1.525450	-1.035941	-0.046170
3	6	0	-2.010143	-2.148537	-0.807331
4	1	0	-1.238604	-2.392512	-1.543676

5	1	0	-2.189032	-3.007953	-0.145067
6	1	0	-2.936529	-1.875803	-1.330776
7	6	0	-2.467827	-0.572272	0.922010
8	1	0	-2.696470	-1.369460	1.642170
9	1	0	-2.009683	0.274809	1.438499
10	1	0	-3.393766	-0.246391	0.428348
11	8	0	1.671387	-0.796145	-0.035472
12	6	0	1.731790	-1.908042	0.859817
13	1	0	2.530299	-1.758288	1.598960
14	1	0	0.764509	-1.968503	1.364479
15	1	0	1.915336	-2.837776	0.303721
16	6	0	2.885498	-0.610360	-0.773767
17	1	0	3.713321	-0.386478	-0.085512
18	1	0	3.114803	-1.509896	-1.360773
19	1	0	2.721284	0.230247	-1.454237
20	8	0	-0.145261	1.835423	-0.036044
21	6	0	-0.925924	2.786466	-0.770235
22	1	0	-1.540359	3.382315	-0.079764
23	1	0	-0.270884	3.445016	-1.356102
24	1	0	-1.565348	2.217577	-1.451663
25	6	0	0.785046	2.451319	0.856845
26	1	0	1.491978	3.080645	0.298856
27	1	0	0.252581	3.063741	1.597149
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7: Li radical with four dimethyl ethers

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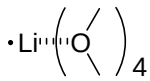

E(UB3LYP/631+LAN)= -627.673050021 a.u.

G(UB3LYP/631+LAN)= -627.401664 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	3	0	-0.000330	-0.001610	0.001252
2	8	0	1.199075	0.792698	-1.342109
3	6	0	1.134505	2.147099	-1.797999
4	1	0	0.280128	2.616968	-1.305316
5	1	0	2.053703	2.684798	-1.526530
6	1	0	0.997404	2.176920	-2.888015
7	6	0	2.313789	0.083208	-1.889268
8	1	0	3.256694	0.562048	-1.589504
9	1	0	2.281051	-0.936178	-1.494660
10	1	0	2.249289	0.056476	-2.986115
11	8	0	-1.194826	1.345093	0.795482
12	6	0	-1.129189	1.801661	2.149657
13	1	0	-0.997236	2.892336	2.178751
14	1	0	-2.045612	1.525714	2.689809
15	1	0	-0.271064	1.313627	2.617712

16	6	0	-2.312698	1.888574	0.088032
17	1	0	-3.253774	1.585958	0.568652
18	1	0	-2.251635	2.985595	0.061171
19	1	0	-2.280577	1.493988	-0.931386
20	8	0	-1.212244	-1.328486	-0.797258
21	6	0	-1.135288	-1.801208	-2.145259
22	1	0	-0.974095	-2.888268	-2.160679
23	1	0	-2.059518	-1.557267	-2.687424
24	1	0	-0.291404	-1.295678	-2.620514
25	6	0	-2.318815	-1.886045	-0.083218
26	1	0	-3.264971	-1.615721	-0.572973
27	1	0	-2.231229	-2.980597	-0.034594
28	1	0	-2.300435	-1.471063	0.928501
29	8	0	1.209537	-0.802060	1.327950
30	6	0	1.129974	-2.149030	1.803294
31	1	0	2.053356	-2.693297	1.560826
32	1	0	0.968001	-2.162068	2.890283
33	1	0	0.285462	-2.623943	1.298363
34	6	0	2.316748	-0.088761	1.885225
35	1	0	2.300885	0.921900	1.467611
36	1	0	2.227772	-0.037325	2.979527
37	1	0	3.262301	-0.581047	1.617447

8: Li cation

Charge=1, Multiplicity=1

Li^+

E(UB3LYP/631+LAN)= -7.28456710192 a.u.

G(UB3LYP/631+LAN)= -7.297315 a.u.

G(sol)(UB3LYP/6311+LAN//UB3LYP/631+LAN)= -7.479987 a.u.

9: Li cation with one dimethyl ether

Charge=1, Multiplicity=1

E(UB3LYP/631+LAN)= -162.378864248 a.u.

G(UB3LYP/631+LAN)= -162.324303 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	3	0	0.012597	2.163533	-0.000001
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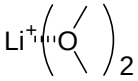
3	6	0	-1.206703	-0.450337	-0.000002
4	1	0	-1.233093	-1.073528	0.898939
5	1	0	-2.058880	0.233426	-0.000234
6	1	0	-1.232849	-1.073998	-0.898646

7	6	0	1.202216	-0.458972	0.000004
8	1	0	1.224360	-1.082588	-0.898824
9	1	0	2.059436	0.218554	0.000276
10	1	0	1.224094	-1.082925	0.898599

10: Li cation with two dimethyl ethers

Charge=1, Multiplicity=1



E(UB3LYP/631+LAN)= -317.463877779 a.u.

G(UB3LYP/631+LAN)= -317.337579 a.u.

G(sol)(UB3LYP/6311+LAN//UB3LYP/631+LAN)= -317.458589 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	3	0	0.000000	-0.000111	-0.000165
2	8	0	1.838476	0.000009	-0.000022
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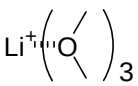
5	1	0	1.959200	1.451462	1.453011
6	1	0	3.269074	0.235228	1.503147
7	6	0	2.641962	-0.849452	-0.848726
8	1	0	3.266401	-1.505920	-0.233846
9	1	0	1.959451	-1.451443	-1.453042
10	1	0	3.269283	-0.235164	-1.503007
11	8	0	-1.838476	-0.000036	-0.000038
12	6	0	-2.641872	-0.848814	0.849430
13	1	0	-3.266256	-0.233992	1.506005
14	1	0	-3.269247	-1.503045	0.235144
15	1	0	-1.959299	-1.453171	1.451306
16	6	0	-2.641904	0.848822	-0.849398
17	1	0	-3.266499	0.234059	-1.505827
18	1	0	-3.269068	1.503181	-0.235032
19	1	0	-1.959352	1.453046	-1.451434

11: Li cation with three dimethyl ethers

Charge=1, Multiplicity=1



E(UB3LYP/631+LAN)= -472.531328303 a.u.

G(UB3LYP/631+LAN)= -472.332090 a.u.

G(sol)(UB3LYP/6311+LAN//UB3LYP/631+LAN)= -472.480714 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	3	0	0.000111	-0.000191	-0.001175
2	8	0	0.505031	1.824112	0.000748
3	6	0	-0.161893	2.839516	-0.768896
4	6	0	1.604073	2.346870	0.766933
5	8	0	1.326587	-1.348678	0.001694
6	6	0	2.524332	-1.298104	-0.792756
7	6	0	1.244286	-2.543414	0.798124
8	8	0	-1.832736	-0.471229	-0.003409
9	6	0	-2.824535	0.171689	0.815826
10	6	0	-2.385536	-1.519413	-0.818233
11	1	0	0.537080	3.293281	-1.480961
12	1	0	-0.976323	2.355251	-1.311607
13	1	0	-0.567582	3.611846	-0.105065
14	1	0	1.245720	3.106939	1.470752
15	1	0	2.042669	1.513235	1.319292
16	1	0	2.355790	2.785068	0.100051
17	1	0	2.505870	-0.360034	-1.351395
18	1	0	3.408854	-1.326171	-0.145863
19	1	0	2.549512	-2.142623	-1.491067
20	1	0	1.251603	-3.429568	0.152856
21	1	0	2.086161	-2.588361	1.498649
22	1	0	0.305512	-2.500703	1.354274
23	1	0	-3.605292	0.614921	0.186817
24	1	0	-3.271970	-0.553059	1.505837
25	1	0	-2.319835	0.956271	1.383401
26	1	0	-2.838249	-2.291709	-0.185546
27	1	0	-3.140068	-1.109633	-1.499583
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12: Li cation with four dimethyl ethers

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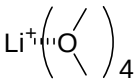

E(UB3LYP/631+LAN)= -627.584655641 a.u.

G(UB3LYP/631+LAN)= -627.311971 a.u.

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1	3	0	0.000752	-0.002758	-0.010741
2	8	0	-1.144381	-0.229016	1.585785
3	6	0	-0.802394	-1.072716	2.692554
4	1	0	0.070030	-1.656507	2.395919
5	1	0	-0.564448	-0.468450	3.577259
6	1	0	-1.633386	-1.749789	2.926266
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9	1	0	-2.513062	1.145411	0.943618
10	1	0	-3.181520	-0.119497	2.017339
11	8	0	-1.288482	0.153376	-1.491497
12	6	0	-2.396812	-0.736841	-1.670117
13	1	0	-2.423611	-1.401026	-0.804029
14	1	0	-3.335352	-0.171381	-1.727588
15	1	0	-2.273267	-1.325939	-2.587906
16	6	0	-1.175183	1.105063	-2.556931
17	1	0	-1.002907	0.594058	-3.512577
18	1	0	-2.088224	1.709499	-2.625636
19	1	0	-0.327535	1.751553	-2.325436
20	8	0	1.170526	1.578982	0.124026
21	6	0	0.947126	2.656086	1.043076
22	1	0	1.827359	2.801497	1.681692
23	1	0	0.732207	3.585445	0.500729
24	1	0	0.089841	2.382934	1.660043
25	6	0	2.295341	1.817009	-0.730675
26	1	0	2.137829	2.722640	-1.330348
27	1	0	3.209836	1.932236	-0.135483
28	1	0	2.394414	0.951854	-1.389060
29	8	0	1.228096	-1.540176	-0.204301
30	6	0	1.015626	-2.618449	-1.123878
31	1	0	0.058472	-2.441557	-1.616486
32	1	0	1.815518	-2.643515	-1.874730
33	1	0	0.985321	-3.576610	-0.590241
34	6	0	2.465597	-1.666591	0.505759
35	1	0	2.481159	-2.598423	1.085160
36	1	0	3.311683	-1.661047	-0.193131
37	1	0	2.542705	-0.811639	1.180064

13: $Ti^{-}(III)(OMe)_4$

Charge=-1, Multiplicity=2

$Ti^{-}(III)(OMe)_4$

E(UB3LYP/631+LAN)= -518.840710058 a.u.

G(UB3LYP/631+LAN)= -518.727741 a.u.

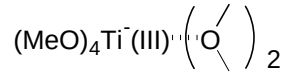
G(sol)(UB3LYP/6311+LAN//UB3LYP/631+LAN)= -518.890711 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	22	0	-0.046055	0.000358	-0.002429
2	8	0	-1.184757	1.530963	-0.203629
3	8	0	-1.201377	-1.518372	0.194965
4	8	0	1.137962	0.146528	1.501546
5	8	0	1.150675	-0.151941	-1.495409
6	6	0	2.043813	0.797401	-1.989294
7	6	0	-1.935508	2.220123	0.744958
8	6	0	-1.947810	-2.209582	-0.755384
9	6	0	2.012801	-0.813878	2.006860
10	1	0	2.762209	1.137249	-1.218156

11	1	0	1.528787	1.698297	-2.375482
12	1	0	2.636252	0.376468	-2.824614
13	1	0	2.768258	-1.126046	1.259689
14	1	0	1.486621	-1.729033	2.341051
15	1	0	2.563613	-0.416451	2.881311
16	1	0	-2.124463	-3.253703	-0.431255
17	1	0	-1.446296	-2.255546	-1.741415
18	1	0	-2.942135	-1.747822	-0.914942
19	1	0	-1.439584	2.261428	1.733994
20	1	0	-2.931606	1.759722	0.897119
21	1	0	-2.108241	3.265738	0.423518

14: $Ti^{-}(III)(OMe)_4$ with two dimethyl ethers

Charge=-1, Multiplicity=2



E(UB3LYP/631+LAN)= -828.886666499 a.u.

G(UB3LYP/631+LAN)= -828.617087 a.u.

This structure has imaginary frequency (-8 cm^{-1}) corresponding to the vibration of ether.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	22	0	-0.098666	0.085784	-0.026261
2	8	0	-2.330123	0.008063	-0.047378
3	8	0	0.076852	-0.420018	-1.895918
4	8	0	-0.058894	-1.932009	0.464649
5	8	0	2.280034	0.121923	0.009891
6	8	0	0.107023	0.492948	1.871688
7	8	0	-0.337571	2.034615	-0.484693
8	6	0	-3.154216	1.131495	-0.332539
9	1	0	-3.669682	0.985353	-1.294745
10	1	0	-3.902750	1.258961	0.465776
11	1	0	-2.477637	1.987411	-0.391598
12	6	0	-3.016620	-1.236779	-0.024254
13	1	0	-3.749547	-1.248945	0.797673
14	1	0	-3.539022	-1.395929	-0.980544
15	1	0	-2.246742	-1.997488	0.121092
16	6	0	2.976344	-0.102244	-1.206705
17	1	0	2.420244	0.410607	-1.991327
18	1	0	4.002825	0.293275	-1.129494
19	1	0	3.012988	-1.176445	-1.437818
20	6	0	2.858857	-0.568334	1.112593
21	1	0	2.875789	-1.649860	0.919139
22	1	0	3.884043	-0.201119	1.285634
23	1	0	2.214641	-0.361590	1.968038
24	6	0	0.137521	1.698409	2.556411
25	1	0	-0.571548	1.692495	3.410225

26	1	0	1.142322	1.899638	2.988586
27	1	0	-0.120001	2.550563	1.903473
28	6	0	0.574249	2.854017	-1.123080
29	1	0	0.184146	3.889463	-1.234124
30	1	0	1.538915	2.940548	-0.576361
31	1	0	0.818456	2.497239	-2.146850
32	6	0	-0.128169	-2.556705	1.690209
33	1	0	0.149408	-1.888912	2.529616
34	1	0	-1.152657	-2.940017	1.931036
35	1	0	0.537546	-3.449754	1.740392
36	6	0	0.151318	-1.632723	-2.562112
37	1	0	1.095376	-1.722655	-3.143532
38	1	0	0.101522	-2.488354	-1.866339
39	1	0	-0.672264	-1.738708	-3.299258

15: $Ti(IV)(OMe)_4$

Charge=0, Multiplicity=1

$Ti(IV)(OMe)_4$

E(UB3LYP/631+LAN)= -518.825262428 a.u.

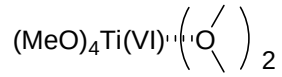
G(UB3LYP/631+LAN)= -518.708669 a.u.

G(sol)(UB3LYP/6311+LAN//UB3LYP/631+LAN)= -518.809260 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	22	0	-0.013181	0.018412	-0.019730
2	8	0	-1.141358	1.221388	0.696364
3	8	0	1.139643	0.860095	-1.117957
4	8	0	0.939777	-0.812207	1.261696
5	8	0	-0.970880	-1.215939	-0.913231
6	6	0	-1.422865	2.466058	1.277614
7	1	0	-0.951441	3.277501	0.705666
8	1	0	-2.508853	2.627185	1.288379
9	1	0	-1.052821	2.498404	2.311795
10	6	0	1.201836	-2.007787	1.951914
11	1	0	0.731737	-2.863371	1.447565
12	1	0	2.285893	-2.175667	1.999355
13	1	0	0.812462	-1.940655	2.976679
14	6	0	-2.176576	-1.564980	-1.543287
15	1	0	-2.093992	-1.409852	-2.627620
16	1	0	-2.393967	-2.624793	-1.356179
17	1	0	-3.008940	-0.959106	-1.159039
18	6	0	2.451101	1.025831	-1.588083
19	1	0	2.648931	2.092375	-1.759144
20	1	0	3.179866	0.642804	-0.859793
21	1	0	2.582660	0.488691	-2.537518

16: Ti(IV)$(OMe)_4$ with two dimethyl ethers

Charge=0, Multiplicity=1



E(UB3LYP/631+LAN)= -828.874080343 a.u.

G(UB3LYP/631+LAN)= -828.594978 a.u.

This structure has imaginary frequencies (-35, -28 cm^{-1}) corresponding to the vibration of ether.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	22	0	-0.003097	0.000000	0.000000
2	8	0	2.233934	-0.000001	0.000001
3	8	0	-0.188098	1.856755	-0.202041
4	8	0	0.188150	0.201537	1.855891
5	8	0	-2.236776	0.000001	0.000000
6	8	0	-0.188099	-1.856756	0.202038
7	8	0	0.188151	-0.201537	-1.855890
8	6	0	3.013899	-0.861669	-0.829864
9	1	0	3.691361	-0.266545	-1.456663
10	1	0	3.597179	-1.550944	-0.205112
11	1	0	2.314827	-1.414372	-1.455859
12	6	0	3.013899	0.861667	0.829865
13	1	0	3.691364	0.266545	1.456663
14	1	0	3.597177	1.550944	0.205112
15	1	0	2.314827	1.414369	1.455861
16	6	0	-3.015817	0.830319	-0.862075
17	1	0	-2.316300	1.458688	-1.411677
18	1	0	-3.596112	0.205970	-1.554185
19	1	0	-3.695784	1.454742	-0.267377
20	6	0	-3.015818	-0.830317	0.862076
21	1	0	-3.596113	-0.205968	1.554185
22	1	0	-3.695785	-1.454740	0.267377
23	1	0	-2.316302	-1.458686	1.411677
24	6	0	-0.521338	-2.905179	-0.662999
25	1	0	0.052261	-3.807287	-0.398968
26	1	0	-1.592255	-3.157486	-0.581307
27	1	0	-0.310928	-2.636063	-1.709354
28	6	0	0.527618	0.663095	-2.902673
29	1	0	1.598845	0.577384	-3.152221
30	1	0	-0.044628	0.401880	-3.806448
31	1	0	0.320377	1.709979	-2.633306
32	6	0	0.527616	-0.663095	2.902673
33	1	0	0.320373	-1.709979	2.633307
34	1	0	1.598843	-0.577385	3.152221
35	1	0	-0.044629	-0.401879	3.806449
36	6	0	-0.521335	2.905179	0.662997
37	1	0	-1.592252	3.157487	0.581305
38	1	0	-0.310926	2.636063	1.709352

39	1	0	0.052265	3.807287	0.398965

17: CF_3I

Charge=0, Multiplicity=1

CF_3I

E(UB3LYP/631+LAN)= -349.018444593 a.u.

E(UB3LYP/6311+LAN//UB3LYP/631+LAN)= -349.114136646 a.u.

G(sol)(UB3LYP/6311+LAN//UB3LYP/631+LAN)= -349.121674 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.195600	0.000040	-0.000022
2	53	0	0.984300	0.000015	0.000024
3	9	0	-1.666640	-0.080729	1.250908
4	9	0	-1.666242	-1.043150	-0.695391
5	9	0	-1.666483	1.123767	-0.555643

18: anion radical of CF_3I

Charge=-1, Multiplicity=2

$CF_3I^{\bullet-}$

E(UB3LYP/631+LAN)= -349.076225064 a.u.

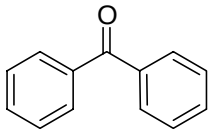
E(UB3LYP/6311+LAN//UB3LYP/631+LAN)= -349.172090437 a.u.

G(sol)(UB3LYP/6311+LAN//UB3LYP/631+LAN)= -349.253018 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	-1.654211
2	9	0	0.000000	1.262126	-2.192298
3	9	0	1.093033	-0.631063	-2.192298
4	9	0	-1.093033	-0.631063	-2.192298
5	53	0	0.000000	0.000000	1.304100

19: benzophenone

Charge=0, Multiplicity=1



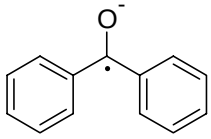
E(UB3LYP/631+LAN)= -576.643660499 a.u.

E(UB3LYP/6311+LAN//UB3LYP/631+LAN)= -576.764580737 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000015	1.094974	-0.000245
2	8	0	0.000015	2.323310	-0.000055
3	6	0	-1.301785	0.348291	-0.026655
4	6	0	-1.445814	-0.897559	-0.659778
5	6	0	-2.431306	0.963085	0.540710
6	6	0	-2.696553	-1.517594	-0.720527
7	1	0	-0.588081	-1.370857	-1.128198
8	6	0	-3.673780	0.332631	0.499550
9	1	0	-2.315373	1.936250	1.008107
10	6	0	-3.809365	-0.909163	-0.133034
11	1	0	-2.801120	-2.473641	-1.226948
12	1	0	-4.538448	0.809631	0.953729
13	1	0	-4.780071	-1.397012	-0.172218
14	6	0	1.301802	0.348279	0.026439
15	6	0	1.445700	-0.897540	0.659655
16	6	0	2.431433	0.963025	-0.540758
17	6	0	2.696416	-1.517597	0.720649
18	1	0	0.587874	-1.370799	1.127946
19	6	0	3.673888	0.332548	-0.499352
20	1	0	2.315598	1.936167	-1.008228
21	6	0	3.809341	-0.909216	0.133318
22	1	0	2.800878	-2.473622	1.227135
23	1	0	4.538643	0.809508	-0.953408
24	1	0	4.780030	-1.397082	0.172695

20: anion radical of benzophenone

Charge=-1, Multiplicity=2



E(UB3LYP/631+LAN)= -576.669092230 a.u.

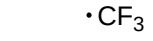
E(UB3LYP/6311+LAN//UB3LYP/631+LAN)= -576.790650971 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.000009	1.017926	0.000191
2	8	0	-0.000005	2.298555	-0.000036
3	6	0	1.292564	0.310920	0.011236
4	6	0	1.507300	-1.024924	0.452659
5	6	0	2.456276	1.046178	-0.357531
6	6	0	2.780694	-1.591265	0.479555
7	1	0	0.671582	-1.608894	0.824746
8	6	0	3.723368	0.473350	-0.338419
9	1	0	2.315220	2.080876	-0.654708

10	6	0	3.908674	-0.858987	0.071874
11	1	0	2.899420	-2.613899	0.838201
12	1	0	4.583905	1.069222	-0.643891
13	1	0	4.900682	-1.306462	0.089723
14	6	0	-1.292575	0.310911	-0.011044
15	6	0	-1.507232	-1.024931	-0.452514
16	6	0	-2.456350	1.046156	0.357551
17	6	0	-2.780614	-1.591287	-0.479602
18	1	0	-0.671451	-1.608888	-0.824481
19	6	0	-3.723433	0.473313	0.338244
20	1	0	-2.315348	2.080851	0.654762
21	6	0	-3.908664	-0.859023	-0.072086
22	1	0	-2.899276	-2.613922	-0.838269
23	1	0	-4.584022	1.069173	0.643593
24	1	0	-4.900664	-1.306508	-0.090085

21: CF_3 radical

Charge=0, Multiplicity=2



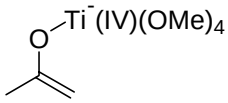
E(UB3LYP/631+LAN)= -337.575706492 a.u.

G(sol)(UB3LYP/6311+LAN//UB3LYP/631+LAN)= -337.676881 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000213	0.330477
2	9	0	-1.096968	-0.633102	-0.073424
3	9	0	1.096928	-0.633171	-0.073424
4	9	0	0.000040	1.266130	-0.073469

22: Ti ate enolate

Charge=-1, Multiplicity=1



E(UB3LYP/631+LAN)= -711.435921430 a.u.

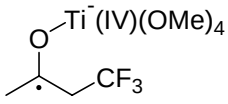
G(sol)(UB3LYP/6311+LAN//UB3LYP/631+LAN)= -711.450729 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.101738	-0.753450	-0.556630
2	6	0	2.424185	-0.678294	-0.425117
3	6	0	2.949362	-0.973443	0.965385
4	6	0	3.252016	-0.407531	-1.464800

5	22	0	-0.436419	0.150776	0.239732
6	8	0	-1.461617	-1.124914	-0.749385
7	6	0	-1.261352	-1.896130	-1.886656
8	1	0	-1.810159	-2.853516	-1.807798
9	1	0	-0.191949	-2.118490	-2.032188
10	1	0	-1.628751	-1.384658	-2.798399
11	8	0	-1.333702	1.566691	-0.622761
12	6	0	-2.440277	1.586523	-1.470585
13	1	0	-2.173058	2.029411	-2.447721
14	1	0	-3.246442	2.207248	-1.037786
15	1	0	-2.838677	0.574692	-1.643528
16	8	0	0.709384	1.431475	1.001165
17	6	0	1.237455	2.641390	0.565399
18	1	0	1.565922	3.247646	1.429248
19	1	0	0.480839	3.216268	0.003545
20	1	0	2.112674	2.489923	-0.090690
21	8	0	-1.126825	-0.454094	1.850528
22	6	0	-2.040739	-1.457754	2.176266
23	1	0	-2.410220	-1.966162	1.272318
24	1	0	-2.902055	-1.030942	2.720107
25	1	0	-1.568650	-2.207195	2.835902
26	1	0	2.609259	-1.966509	1.290202
27	1	0	2.539427	-0.240212	1.669658
28	1	0	4.045053	-0.944126	1.004831
29	1	0	2.851957	-0.190877	-2.451830
30	1	0	4.330312	-0.393801	-1.332675

23: Ti ate ketyl radical

Charge=-1, Multiplicity=2



E(UB3LYP/631+LAN)= -1049.078676760 a.u.

G(sol)(UB3LYP/6311+LAN//UB3LYP/631+LAN)= -1049.172280 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.479992	0.030411	-0.475963
2	6	0	-1.460690	-0.827764	-0.440569
3	6	0	-1.302583	-2.173519	0.209354
4	6	0	-2.795869	-0.373302	-0.971713
5	22	0	1.484252	0.098495	-0.130361
6	8	0	1.409293	1.938090	-0.487046
7	6	0	0.392013	2.892421	-0.512613
8	1	0	0.362848	3.465590	0.431485
9	1	0	-0.594336	2.427285	-0.659125
10	1	0	0.567296	3.610920	-1.333225
11	8	0	3.375821	0.226826	0.084059

12	6	0	4.135521	1.270719	0.603026
13	1	0	5.195761	1.159910	0.309328
14	1	0	4.102107	1.296896	1.709806
15	1	0	3.770135	2.245203	0.236427
16	8	0	1.729670	-1.242422	-1.424641
17	6	0	2.871588	-1.823221	-1.979032
18	1	0	2.851600	-2.919931	-1.840983
19	1	0	3.788800	-1.428083	-1.515361
20	1	0	2.916533	-1.629306	-3.066307
21	8	0	1.202354	-0.502736	1.623073
22	6	0	2.067870	-1.104373	2.537825
23	1	0	1.978215	-0.618621	3.526048
24	1	0	3.118381	-1.041535	2.211280
25	1	0	1.814605	-2.172129	2.671877
26	1	0	-1.339969	-2.117331	1.310579
27	1	0	-0.326184	-2.599294	-0.053081
28	1	0	-2.093263	-2.866404	-0.112440
29	1	0	-2.639017	0.425903	-1.706903
30	6	0	-3.773627	0.181974	0.054565
31	1	0	-3.336241	-1.195582	-1.465597
32	9	0	-4.114890	-0.732718	1.006439
33	9	0	-4.959785	0.563733	-0.532657
34	9	0	-3.313470	1.272389	0.709908

24: Li enolate without solvent

Charge=0, Multiplicity=1

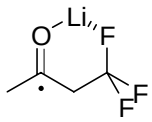
E(UB3LYP/631+LAN)= -200.106838202 a.u.

G(sol)(UB3LYP/6311+LAN//UB3LYP/631+LAN)= -200.155226 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.133263	-0.048423	0.013214
2	6	0	0.182432	0.123535	0.002514
3	6	0	0.787623	1.335337	-0.003290
4	3	0	-2.748241	-0.178463	-0.021793
5	1	0	0.202685	2.251609	0.002020
6	1	0	1.869119	1.424389	-0.011698
7	6	0	0.982806	-1.164804	-0.002529
8	1	0	0.722698	-1.768765	-0.882797
9	1	0	0.736727	-1.766259	0.883386
10	1	0	2.062434	-0.982616	-0.011413

25: Li ketyl radical without solvent

Charge=0, Multiplicity=2



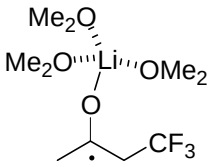
E(UB3LYP/631+LAN)= -537.752166162 a.u.

G(sol)(UB3LYP/6311+LAN//UB3LYP/631+LAN)= -537.867652 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.537134	1.258773	-0.008221
2	6	0	1.447203	-0.060938	0.070010
3	6	0	2.720848	-0.860929	0.064988
4	6	0	0.224922	-0.697904	-0.565396
5	3	0	0.218800	2.326840	-0.102047
6	1	0	3.436657	-0.428428	0.773925
7	1	0	3.213165	-0.848355	-0.929197
8	1	0	2.555759	-1.910943	0.338087
9	1	0	0.163551	-0.493813	-1.656655
10	6	0	-1.098474	-0.233224	0.003697
11	1	0	0.229250	-1.787183	-0.443217
12	9	0	-1.237431	-0.419693	1.324643
13	9	0	-2.164291	-0.795988	-0.601446
14	9	0	-1.300372	1.164124	-0.184401

26: Li ketyl radical with three dimethyl ether

Charge=0, Multiplicity=2



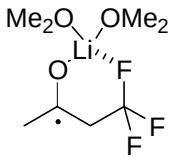
E(UB3LYP/631+LAN)= -1002.90755121 a.u.

G(sol)(UB3LYP/6311+LAN//UB3LYP/631+LAN)= -1002.872851 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.218648	1.231941	-0.268084
2	6	0	1.450117	1.689553	-0.170878
3	6	0	1.640211	3.184523	-0.067899
4	6	0	2.540882	0.904335	-0.877043
5	3	0	-1.083264	0.065486	-0.030916
6	1	0	0.969844	3.603746	0.693624
7	1	0	1.397103	3.702722	-1.021388

8	1	0	2.668836	3.458680	0.198866
9	1	0	2.204955	0.577735	-1.879736
10	6	0	2.995845	-0.352358	-0.162941
11	1	0	3.446817	1.506893	-1.014058
12	9	0	3.578501	-0.101049	1.038886
13	9	0	3.923892	-1.041878	-0.896538
14	9	0	1.985621	-1.235968	0.079331
15	8	0	-1.390420	-1.622580	-1.127031
16	6	0	-0.709358	-2.833050	-0.801227
17	6	0	-1.497014	-1.418018	-2.533995
18	1	0	0.299236	-2.840012	-1.232726
19	1	0	-0.631725	-2.874100	0.286334
20	1	0	-1.276104	-3.700407	-1.169598
21	1	0	-2.082055	-2.226640	-2.996040
22	1	0	-2.004100	-0.462742	-2.680919
23	1	0	-0.501635	-1.377274	-2.996697
24	8	0	-2.831225	1.017242	-0.492121
25	6	0	-4.167738	0.544844	-0.457654
26	6	0	-2.733941	2.441290	-0.568873
27	1	0	-4.719434	0.866499	-1.353682
28	1	0	-4.126259	-0.546875	-0.432591
29	1	0	-4.694238	0.914934	0.435007
30	1	0	-3.216459	2.905089	0.303799
31	1	0	-1.666576	2.669125	-0.579303
32	1	0	-3.217622	2.805966	-1.486611
33	8	0	-1.159188	-0.599549	1.878492
34	6	0	-2.152974	-1.347961	2.559114
35	6	0	-0.155475	-0.070749	2.751366
36	1	0	-2.688247	-0.719737	3.286703
37	1	0	-2.858540	-1.714813	1.809345
38	1	0	-1.707117	-2.203483	3.088237
39	1	0	0.386508	-0.888828	3.245602
40	1	0	0.526378	0.512002	2.131174
41	1	0	-0.617746	0.574231	3.512424

27: Li ketyl radical with two dimethyl ethers and internal corrdination
Charge=0, Multiplicity=2



E(UB3LYP/631+LAN)= -847.865727235 a.u.

G(sol)(UB3LYP/6311+LAN//UB3LYP/631+LAN)= -847.869804 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.320944	-0.820916	1.268313
2	6	0	-1.638628	-0.762525	1.178350

3	6	0	-2.449404	-1.368605	2.296660
4	6	0	-2.240650	-0.874101	-0.213096
5	1	0	-2.049601	-1.050027	3.266922
6	1	0	-2.404561	-2.479133	2.287217
7	1	0	-3.508764	-1.084240	2.249511
8	1	0	-1.983731	-1.839332	-0.699600
9	6	0	-1.797744	0.194461	-1.188278
10	1	0	-3.334466	-0.813043	-0.180090
11	9	0	-2.088942	1.454970	-0.792067
12	9	0	-2.357790	0.034267	-2.416847
13	9	0	-0.429144	0.183953	-1.417549
14	3	0	0.912951	-0.072748	0.235292
15	8	0	2.346615	-1.294246	-0.292561
16	6	0	3.485579	-1.160319	-1.130251
17	6	0	2.189342	-2.612115	0.247370
18	8	0	1.380925	1.776426	0.699932
19	6	0	2.067928	2.795104	-0.012912
20	6	0	0.615548	2.279047	1.803219
21	1	0	3.418966	-1.842828	-1.989247
22	1	0	3.509540	-0.128968	-1.490893
23	1	0	4.407765	-1.371510	-0.570377
24	1	0	3.061264	-2.873814	0.862659
25	1	0	1.283562	-2.587337	0.857267
26	1	0	2.081086	-3.342934	-0.565995
27	1	0	2.775920	3.318610	0.645329
28	1	0	2.618723	2.314879	-0.825719
29	1	0	1.359610	3.521673	-0.435148
30	1	0	-0.119219	3.014680	1.450277
31	1	0	0.100210	1.421123	2.237772
32	1	0	1.283133	2.745940	2.540566

28: dimethyl ether

Charge=0, Multiplicity=1

OMe_2

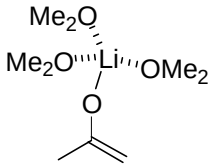
E(UB3LYP/631+LAN)= -155.031474215 a.u.

G(sol)(UB3LYP/6311+LAN//UB3LYP/631+LAN)= -155.008580 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.000000	0.587414	0.000000
2	6	0	1.177447	-0.195599	0.000000
3	1	0	1.234172	-0.836088	-0.895386
4	1	0	2.023739	0.496096	-0.000011
5	1	0	1.234182	-0.836072	0.895397
6	6	0	-1.177447	-0.195599	0.000000
7	1	0	-1.234176	-0.836081	0.895390
8	1	0	-2.023739	0.496096	0.000002
9	1	0	-1.234178	-0.836078	-0.895393

29: Li enolate with three dimethyl ethers

Charge=0, Multiplicity=1



E(UB3LYP/631+LAN)= -665.272285045 a.u.

G(sol)(UB3LYP/6311+LAN//UB3LYP/631+LAN)= -665.153754 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.623695	-0.013774	-0.128250
2	6	0	-2.984413	0.108764	-1.442028
3	8	0	-1.390430	-0.060862	0.313965
4	3	0	0.349422	0.000979	0.061788
5	6	0	-3.694307	-0.108957	0.950828
6	1	0	-4.027009	0.139288	-1.743493
7	1	0	-2.233261	0.175651	-2.227179
8	8	0	0.978950	1.750579	-0.695672
9	8	0	1.279184	-0.145578	1.872715
10	8	0	1.028758	-1.591155	-0.965668
11	6	0	-0.063710	2.585544	-1.210821
12	6	0	2.280357	2.204837	-1.029773
13	1	0	0.015086	3.595136	-0.782775
14	1	0	0.006131	2.648658	-2.305885
15	1	0	-1.010099	2.123183	-0.926925
16	1	0	2.450480	3.221531	-0.645471
17	1	0	2.995106	1.520570	-0.565350
18	1	0	2.428822	2.206387	-2.119866
19	6	0	0.891883	-1.374589	2.489183
20	6	0	0.945806	0.983437	2.680124
21	6	0	2.345749	-1.987954	-1.311173
22	6	0	0.013525	-2.353231	-1.626934
23	1	0	1.399457	-1.490810	3.457609
24	1	0	-0.196542	-1.406813	2.625450
25	1	0	1.196483	-2.178530	1.816229
26	1	0	2.534288	-1.835396	-2.384382
27	1	0	3.036189	-1.373137	-0.728068
28	1	0	2.511570	-3.047953	-1.067722
29	1	0	1.464029	0.925796	3.648246
30	1	0	1.276937	1.872272	2.139308
31	1	0	-0.139288	1.035431	2.837858
32	1	0	0.113559	-2.254552	-2.717129
33	1	0	0.096365	-3.413863	-1.349355
34	1	0	-0.946422	-1.949076	-1.302790
35	1	0	-3.580010	-1.049290	1.507663
36	1	0	-4.710592	-0.063481	0.543899
37	1	0	-3.568410	0.707728	1.675107

30: naked enolate

Charge=-1, Multiplicity=1

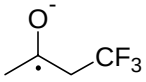
E(UB3LYP/631+LAN)= -192.564643602 a.u.

G(sol)(UB3LYP/6311+LAN//UB3LYP/631+LAN)= -192.645291 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.194521	1.387578	-0.000050
2	6	0	-0.133951	0.110626	0.000187
3	6	0	-1.192702	-0.790016	-0.000012
4	1	0	-2.221202	-0.430819	-0.000163
5	1	0	-1.028681	-1.866350	-0.000065
6	6	0	1.295130	-0.483702	-0.000032
7	1	0	1.841205	-0.121043	0.883155
8	1	0	1.841157	-0.120499	-0.883023
9	1	0	1.312823	-1.583356	-0.000368

31: naked ketyl raadical

Charge=-1, Multiplicity=2



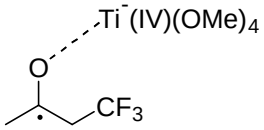
E(UB3LYP/631+LAN)= -530.207588448 a.u.

G(sol)(UB3LYP/6311+LAN//UB3LYP/631+LAN)= -530.361880 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-2.354705	-1.189699	0.098145
2	6	0	-1.513439	-0.210218	0.072558
3	6	0	-2.045998	1.209800	-0.008869
4	6	0	-0.204228	-0.451378	-0.682975
5	1	0	-2.908821	1.324660	0.657393
6	1	0	-2.405745	1.439192	-1.047134
7	1	0	-1.300157	1.974067	0.244005
8	1	0	-0.119105	-1.529098	-0.858546
9	6	0	1.076731	-0.028193	-0.010126
10	1	0	-0.192619	0.046912	-1.685007
11	9	0	1.160452	1.313307	0.237061
12	9	0	2.185881	-0.316179	-0.784801
13	9	0	1.307632	-0.648039	1.178919

32: TS of Ti(III) elimination from Ti ate ketyl radical(**23**)

Charge=-1, Multiplicity=2



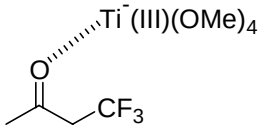
E(UB3LYP/631+LAN)= -1049.065633820 a.u.

G(sol)(UB3LYP/6311+LAN//UB3LYP/631+LAN)= -1049.166297 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.670896	0.614106	-0.965456
2	6	0	1.399868	-0.255104	-0.487095
3	6	0	1.357529	-1.686399	-0.968879
4	6	0	2.411735	0.133465	0.599539
5	22	0	-1.733732	0.187793	-0.103562
6	8	0	-1.950233	1.954916	-0.709443
7	6	0	-1.433269	3.228141	-0.521346
8	1	0	-1.951181	3.956929	-1.172369
9	1	0	-0.356954	3.269263	-0.764883
10	1	0	-1.555424	3.578058	0.522063
11	8	0	-3.190046	0.059620	1.156796
12	6	0	-4.523066	0.320465	0.846727
13	1	0	-5.184701	-0.012906	1.669482
14	1	0	-4.863655	-0.198634	-0.072428
15	1	0	-4.706443	1.400701	0.691397
16	8	0	-0.453629	-0.489030	1.204034
17	6	0	-0.717791	-1.241979	2.350912
18	1	0	-0.576926	-2.326351	2.168658
19	1	0	-1.748954	-1.091991	2.707533
20	1	0	-0.026432	-0.960060	3.169762
21	8	0	-1.999953	-1.189141	-1.395116
22	6	0	-2.811458	-2.321169	-1.396729
23	1	0	-3.377800	-2.398047	-2.344060
24	1	0	-3.543713	-2.320311	-0.569553
25	1	0	-2.210971	-3.247137	-1.302772
26	1	0	2.074742	-1.820936	-1.793045
27	1	0	0.349129	-1.893990	-1.341084
28	1	0	1.623855	-2.393285	-0.175244
29	1	0	2.157767	1.136222	0.950751
30	6	0	3.858056	0.148807	0.161591
31	1	0	2.333501	-0.560597	1.442810
32	9	0	4.322512	-1.082768	-0.196941
33	9	0	4.680934	0.580404	1.166298
34	9	0	4.089928	0.967977	-0.896413

33: $Ti^{-}(III)(OMe)_4$ coordinated with α-CF_3 ketone

Charge=-1, Multiplicity=2



E(UB3LYP/631+LAN)= -1049.07971125 a.u.

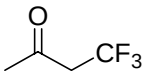
G(sol)(UB3LYP/6311+LAN//UB3LYP/631+LAN)= -1049.180602 a.u.

This structure has imaginary frequency (-29 cm^{-1}) corresponding to the rotation of Me group on the ligand.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	2.846884	-2.527250	-0.703254
2	6	0	2.377956	-1.591007	-0.074169
3	6	0	1.762876	-1.762733	1.292086
4	6	0	2.350953	-0.190776	-0.705231
5	22	0	-1.961143	-0.132467	-0.035390
6	8	0	-2.286743	-1.303431	-1.490118
7	6	0	-2.599010	-1.084140	-2.831852
8	1	0	-3.122352	-1.961049	-3.254468
9	1	0	-1.690816	-0.919127	-3.440164
10	1	0	-3.256828	-0.206970	-2.975536
11	8	0	-3.454898	1.070052	0.148984
12	6	0	-4.763032	0.738742	0.504789
13	1	0	-5.101333	1.332941	1.375240
14	1	0	-4.884328	-0.329171	0.774957
15	1	0	-5.468970	0.945708	-0.322173
16	8	0	-0.496040	1.077117	-0.425227
17	6	0	-0.539959	2.478836	-0.469410
18	1	0	0.097167	2.923362	0.317791
19	1	0	-1.564570	2.860419	-0.330610
20	1	0	-0.165678	2.854563	-1.439894
21	8	0	-1.557221	-0.975153	1.633482
22	6	0	-1.508666	-0.442315	2.924066
23	1	0	-1.763908	-1.215066	3.671858
24	1	0	-2.214564	0.396648	3.061740
25	1	0	-0.498865	-0.065158	3.173043
26	1	0	1.943626	-2.779190	1.651320
27	1	0	0.677636	-1.576445	1.244612
28	1	0	2.170273	-1.031406	1.999792
29	1	0	2.578027	-0.301280	-1.769308
30	6	0	3.377296	0.760321	-0.137401
31	1	0	1.353289	0.278635	-0.590125
32	9	0	3.154706	1.092610	1.162938
33	9	0	3.407103	1.929089	-0.833949
34	9	0	4.648301	0.259923	-0.184287

34: α-CF_3 ketone

Charge=0, Multiplicity=1



E(UB3LYP/631+LAN)= -530.215605952 a.u.

G(sol)(UB3LYP/6311+LAN//UB3LYP/631+LAN)= -530.297350 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.405038	1.316070	-0.012039
2	6	0	-1.480468	0.105218	-0.032304
3	6	0	-2.805060	-0.631361	0.025441
4	6	0	-0.241329	-0.795666	-0.114842
5	6	0	1.094891	-0.086418	0.001002
6	9	0	2.105865	-1.000771	-0.052875
7	9	0	1.227464	0.573511	1.171927
8	9	0	1.308092	0.791229	-1.000563
9	1	0	-2.863738	-1.409806	-0.745233
10	1	0	-3.626252	0.077928	-0.097795
11	1	0	-2.907360	-1.131634	0.997971
12	1	0	-0.287778	-1.559035	0.670956
13	1	0	-0.255572	-1.332369	-1.071750

35: Ti(III)$(OMe)_3$

Charge=0, Multiplicity=2

Ti(III)$(OMe)_3$

E(UB3LYP/631+LAN)= -403.632481061 a.u.

G(sol)(UB3LYP/6311+LAN//UB3LYP/631+LAN)= -403.632335 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	22	0	-0.001843	-0.003350	0.003542
2	8	0	-0.823010	1.600055	0.006221
3	8	0	1.797063	-0.093163	-0.003746
4	8	0	-0.978698	-1.516959	0.004608
5	6	0	-1.514598	2.815303	0.002614
6	1	0	-1.132418	3.467675	-0.794652
7	1	0	-2.587787	2.647382	-0.163780
8	1	0	-1.384409	3.327686	0.965791
9	6	0	-1.681052	-2.725998	0.000760
10	1	0	-0.994211	-3.570402	-0.150399
11	1	0	-2.202158	-2.864021	0.958154
12	1	0	-2.426543	-2.729615	-0.806400
13	6	0	3.195309	-0.088346	-0.009221
14	1	0	3.572547	-0.595450	-0.907968

15	1	0	3.577219	0.942041	-0.000046
16	1	0	3.579682	-0.614034	0.875714

36: methoxide anion

Charge=-1, Multiplicity=1

$^{-}$OMe

E(UB3LYP/631+LAN)= -115.109825010 a.u.

G(sol)(UB3LYP/6311+LAN//UB3LYP/631+LAN)= -115.221350 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000013	0.543555	0.000000
2	1	0	1.030803	1.036913	0.000000
3	1	0	-0.515494	1.036729	0.892694
4	1	0	-0.515494	1.036729	-0.892694
5	8	0	0.000013	-0.796463	0.000000

37: $Ti(IV)(OMe)_4$

Charge=0, Multiplicity=1

$Ti(IV)(OMe)_4$

E(UB3LYP/631+LAN)= -518.825262428 a.u.

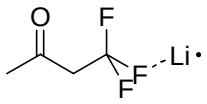
G(sol)(UB3LYP/6311+LAN//UB3LYP/631+LAN)= -518.809260 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	22	0	-0.013181	0.018412	-0.019730
2	8	0	-1.141358	1.221388	0.696364
3	8	0	1.139643	0.860095	-1.117957
4	8	0	0.939777	-0.812207	1.261696
5	8	0	-0.970880	-1.215939	-0.913231
6	6	0	-1.422865	2.466058	1.277614
7	1	0	-0.951441	3.277501	0.705666
8	1	0	-2.508853	2.627185	1.288379
9	1	0	-1.052821	2.498404	2.311795
10	6	0	1.201836	-2.007787	1.951914
11	1	0	0.731737	-2.863371	1.447565
12	1	0	2.285893	-2.175667	1.999355
13	1	0	0.812462	-1.940655	2.976679
14	6	0	-2.176576	-1.564980	-1.543287
15	1	0	-2.093992	-1.409852	-2.627620
16	1	0	-2.393967	-2.624793	-1.356179
17	1	0	-3.008940	-0.959106	-1.159039
18	6	0	2.451101	1.025831	-1.588083
19	1	0	2.648931	2.092375	-1.759144

20	1	0	3.179866	0.642804	-0.859793
21	1	0	2.582660	0.488691	-2.537518

38: Li radical coordinated to fluorine of α-CF_3 ketone

Charge=0, Multiplicity=2



E(UB3LYP/631+LAN)= -537.707925331 a.u.

G(sol)(UB3LYP/6311+LAN//UB3LYP/631+LAN)= -537.822498 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.722161	-1.158558	0.262627
2	6	0	-1.634076	0.029640	0.033059
3	6	0	-2.837880	0.943198	-0.063787
4	6	0	-0.276267	0.721458	-0.172293
5	3	0	3.208297	2.099953	0.484469
6	6	0	0.921300	-0.197522	-0.063543
7	9	0	0.948992	-1.155108	-0.996983
8	9	0	1.058446	-0.762396	1.142077
9	9	0	2.095106	0.553936	-0.267198
10	1	0	-3.751143	0.361988	0.079080
11	1	0	-2.868018	1.442338	-1.040779
12	1	0	-2.782143	1.731606	0.698148
13	1	0	-0.251265	1.198949	-1.158693
14	1	0	-0.156395	1.525189	0.566147

42: $Ti(IV)(OMe)_4$ with I^-

Charge=-1, Multiplicity=1

$Ti^-(IV)(OMe)_4$-I

E(UB3LYP/631+LAN)= -530.309596934 a.u.

G(sol)(UB3LYP/6311+LAN//UB3LYP/631+LAN)= -530.356199 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	53	0	2.139617	-0.090753	-0.047275
2	22	0	-0.960405	0.022731	-0.077527
3	8	0	-0.763480	-1.767782	0.317522
4	6	0	-0.141993	-2.738556	1.093136
5	1	0	-0.509353	-3.739839	0.808742
6	1	0	-0.363112	-2.583808	2.163447
7	1	0	0.949229	-2.708483	0.957830

8	8	0	-2.159049	-0.275487	-1.451545
9	6	0	-2.940035	-1.404777	-1.726812
10	1	0	-3.030387	-1.531595	-2.818412
11	1	0	-3.956414	-1.283388	-1.314548
12	1	0	-2.496384	-2.314176	-1.295444
13	8	0	-0.631872	1.774887	-0.522543
14	6	0	0.148816	2.903733	-0.728861
15	1	0	0.034537	3.617866	0.105872
16	1	0	-0.163575	3.413348	-1.656614
17	1	0	1.211663	2.634437	-0.808701
18	8	0	-1.896256	0.391180	1.476367
19	6	0	-2.471683	1.587085	1.921035
20	1	0	-2.083062	2.457520	1.372391
21	1	0	-2.261970	1.722191	2.995203
22	1	0	-3.567335	1.558488	1.791995

43: iodide ion

Charge=-1, Multiplicity=1

I^-

E(UB3LYP/631+LAN)= -11.4721100599 a.u.

G(sol)(UB3LYP/6311+LAN//UB3LYP/631+LAN)= -11.574630 a.u.

44: lithium iodide

Charge=0, Multiplicity=1

Li-I

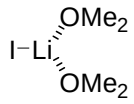
E(UB3LYP/631+LAN)= -18.9856260611 a.u.

G(sol)(UB3LYP/6311+LAN//UB3LYP/631+LAN)= -19.069770 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	3	0	0.000000	0.000000	-2.304908
2	53	0	0.000000	0.000000	0.130466

45: lithium iodide with two ethers

Charge=0, Multiplicity=1



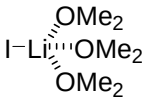
E(UB3LYP/631+LAN)= -329.111276397 a.u.

G(sol)(UB3LYP/6311+LAN//UB3LYP/631+LAN)= -329.068807 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	3	0	0.705191	0.017632	-0.041124
2	8	0	1.508216	1.786119	-0.032824
3	6	0	1.379520	2.472743	1.218100
4	1	0	1.698078	1.780303	2.000951
5	1	0	2.027623	3.358813	1.228428
6	1	0	0.336710	2.765835	1.390696
7	6	0	1.126716	2.606072	-1.145548
8	1	0	1.765975	3.497517	-1.188966
9	1	0	1.270045	2.009888	-2.049477
10	1	0	0.072502	2.896269	-1.063996
11	8	0	1.962111	-1.416199	-0.012816
12	6	0	3.381695	-1.323806	-0.103257
13	1	0	3.853164	-1.782680	0.776390
14	1	0	3.742201	-1.825205	-1.011673
15	1	0	3.635178	-0.262170	-0.144223
16	6	0	1.479777	-2.765986	0.046181
17	1	0	1.779391	-3.311932	-0.857831
18	1	0	1.881985	-3.269704	0.934755
19	1	0	0.391174	-2.708779	0.105378
20	53	0	-1.821480	-0.228199	0.005193

46: lithium iodide with three ethers

Charge=0, Multiplicity=1



E(UB3LYP/631+LAN)= -484.157595545 a.u.

G(sol)(UB3LYP/6311+LAN//UB3LYP/631+LAN)= -484.075546 a.u.

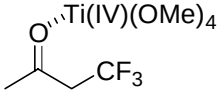
This structure has imaginary frequencies (-30, -13 cm^{-1}) cooresponding to vibration of ether.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	3	0	0.554592	0.003410	-0.000159
2	8	0	1.349977	-1.601561	-0.889571
3	6	0	0.591525	-2.253378	-1.913921
4	1	0	-0.186647	-1.556792	-2.228388
5	1	0	1.245705	-2.516132	-2.757297
6	1	0	0.114715	-3.158465	-1.516580
7	6	0	2.336305	-2.446463	-0.308424
8	1	0	3.075449	-2.754370	-1.062135
9	1	0	2.829093	-1.874663	0.480352
10	1	0	1.871385	-3.342598	0.126196
11	8	0	1.328991	1.593900	-0.933611
12	6	0	2.258125	1.516861	-2.008591
13	1	0	3.001967	2.323382	-1.935971
14	1	0	2.755402	0.547596	-1.937855
15	1	0	1.739318	1.591261	-2.974686
16	6	0	0.570813	2.808282	-0.940736
17	1	0	1.236311	3.668480	-0.780923
18	1	0	0.040066	2.919790	-1.894644
19	1	0	-0.163845	2.732402	-0.138151
20	8	0	1.319927	0.025251	1.846623
21	6	0	0.580605	-0.624854	2.885313
22	1	0	1.265932	-1.164180	3.554556
23	1	0	0.001458	0.110670	3.457466
24	1	0	-0.112280	-1.315773	2.403462
25	6	0	2.186956	1.041125	2.338006
26	1	0	1.617173	1.804294	2.886523
27	1	0	2.948210	0.610800	3.004609
28	1	0	2.669587	1.499794	1.472827
29	53	0	-2.089621	-0.009922	-0.012383

50: Ti(IV)$(OMe)_4$ coordinated to α-CF_3 ketone

Charge=0, Multiplicity=1



E(UB3LYP/631+LAN)= -1049.04423485 a.u.

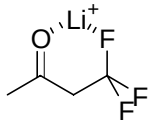
G(sol)(UB3LYP/6311+LAN//UB3LYP/631+LAN)= -1049.085490 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.598111	0.442411	-0.620787
2	6	0	-1.573640	-0.290997	-0.571671
3	6	0	-1.487279	-1.738896	-0.170753
4	6	0	-2.932486	0.299605	-0.972384
5	22	0	1.819124	0.031830	0.006851
6	8	0	1.898262	1.749724	-0.543667
7	6	0	1.324912	2.988238	-0.861020
8	8	0	3.540258	-0.235124	0.476668

9	6	0	4.736669	0.506481	0.533388
10	8	0	1.594354	-1.262406	-1.278870
11	6	0	2.460944	-2.078037	-2.031161
12	8	0	0.950852	-0.343465	1.573539
13	6	0	1.336232	-0.699813	2.880003
14	6	0	-4.028350	0.176637	0.071607
15	9	0	-4.401140	-1.109505	0.293952
16	9	0	-5.139830	0.845824	-0.321272
17	9	0	-3.649523	0.691857	1.265351
18	1	0	-1.671636	-1.812408	0.909217
19	1	0	-0.479934	-2.106126	-0.374782
20	1	0	-2.241559	-2.346960	-0.678717
21	1	0	-2.794422	1.361066	-1.190718
22	1	0	-3.290544	-0.202326	-1.879837
23	1	0	1.259365	3.622002	0.034628
24	1	0	0.315557	2.849195	-1.269752
25	1	0	1.944553	3.500742	-1.609647
26	1	0	5.096277	0.551867	1.570131
27	1	0	4.574845	1.527964	0.162903
28	1	0	5.504776	0.017547	-0.080553
29	1	0	2.006963	-3.070219	-2.167303
30	1	0	3.429727	-2.202127	-1.526144
31	1	0	2.634523	-1.639276	-3.024590
32	1	0	1.083715	0.109040	3.580188
33	1	0	2.416439	-0.895422	2.937656
34	1	0	0.798150	-1.606829	3.191206

51: Li^+ coordinated to α-CF_3 ketone

Charge=1, Multiplicity=1



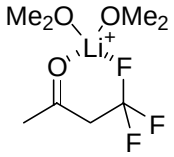
E(UB3LYP/631+LAN)= -537.578593175 a.u.

G(sol)(UB3LYP/6311+LAN//UB3LYP/631+LAN)= -537.762120 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.354071	1.199231	0.046080
2	6	0	1.464499	-0.024579	-0.066764
3	6	0	2.788408	-0.708284	0.035955
4	6	0	0.240491	-0.899114	-0.330145
5	3	0	-0.051013	2.386487	-0.138242
6	6	0	-1.088406	-0.255366	0.018738
7	9	0	-1.167336	0.088325	1.317074
8	9	0	-2.124496	-1.016402	-0.298172
9	9	0	-1.263672	0.957433	-0.684509
10	1	0	3.602563	0.011717	-0.065155
11	1	0	2.884094	-1.510573	-0.704809

12	1	0	2.858121	-1.184071	1.026119
13	1	0	0.231186	-1.171128	-1.394833
14	1	0	0.314095	-1.839397	0.228519

52: Li^+ coordinated to α-CF_3 ketone with two dimethyl ethers
Charge=1, Multiplicity=1



E(UB3LYP/631+LAN)= -847.721222700 a.u.

G(sol)(UB3LYP/6311+LAN//UB3LYP/631+LAN)= -847.769066 a.u.

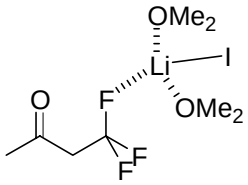
This structure has imaginary frequency (-17 cm^{-1}) cooresponding to vibration of ether

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.583984	0.948132	1.090125
2	6	0	1.798148	1.095690	0.985318
3	6	0	2.596069	1.864852	1.995687
4	6	0	2.567515	0.519881	-0.203151
5	1	0	1.936169	2.422341	2.662830
6	1	0	3.307508	2.540882	1.506185
7	1	0	3.192476	1.158039	2.590454
8	1	0	2.705660	1.321427	-0.941648
9	6	0	1.894510	-0.653514	-0.889483
10	1	0	3.569703	0.201922	0.103604
11	9	0	1.727111	-1.698898	-0.052193
12	9	0	2.594930	-1.071600	-1.949567
13	9	0	0.634486	-0.325479	-1.351965
14	3	0	-0.902762	0.154120	0.133826
15	8	0	-2.127578	1.402720	-0.610922
16	6	0	-3.276682	0.988696	-1.366372
17	6	0	-1.988822	2.829595	-0.557819
18	8	0	-1.691188	-1.469268	0.760065
19	6	0	-1.542602	-2.781877	0.197123
20	6	0	-2.385094	-1.484439	2.016972
21	1	0	-3.185272	1.318942	-2.408028
22	1	0	-3.316072	-0.101380	-1.325618
23	1	0	-4.189406	1.405860	-0.924539
24	1	0	-2.878567	3.279086	-0.100967
25	1	0	-1.114203	3.048815	0.057573
26	1	0	-1.846988	3.236180	-1.566613
27	1	0	-2.527656	-3.233973	0.030794
28	1	0	-1.023066	-2.673250	-0.756366
29	1	0	-0.951666	-3.417548	0.867074
30	1	0	-1.831771	-2.084701	2.749164

31	1	0	-2.453819	-0.451755	2.366325
32	1	0	-3.393476	-1.895439	1.888017

53: Li-I coordinated to fluorine of α-CF_3 ketone with two dimethyl ethers

Charge=0, Multiplicity=1

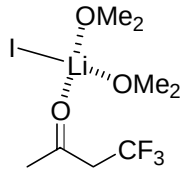


E(UB3LYP/631+LAN)= -847.721222700 a.u.

G(sol)(UB3LYP/6311+LAN//UB3LYP/631+LAN)= -847.769066 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	2.730238	0.255257	1.649798
2	6	0	2.907694	-0.302975	0.582525
3	6	0	3.506797	-1.684309	0.466831
4	6	0	2.497935	0.333597	-0.748780
5	6	0	1.812446	1.675281	-0.639586
6	9	0	1.436075	2.126866	-1.863757
7	9	0	2.579176	2.632847	-0.085636
8	9	0	0.658398	1.616533	0.108491
9	1	0	2.711149	-2.382225	0.170874
10	1	0	3.921278	-1.991902	1.429318
11	1	0	4.281590	-1.722842	-0.308540
12	1	0	3.381727	0.460969	-1.385828
13	1	0	1.814525	-0.355593	-1.263996
14	3	0	-1.144588	0.321320	0.270190
15	8	0	-2.342281	1.498406	-0.688962
16	6	0	-2.583317	2.851330	-0.308262
17	6	0	-2.744340	1.206674	-2.032159
18	8	0	-1.504062	0.511700	2.175533
19	6	0	-2.755840	-0.043534	2.587323
20	6	0	-0.449922	0.232550	3.108042
21	53	0	-0.617631	-2.056927	-0.687309
22	1	0	-2.253973	2.959291	0.727391
23	1	0	-2.016825	3.540071	-0.949481
24	1	0	-3.654710	3.083373	-0.381221
25	1	0	-2.199349	1.846815	-2.738588
26	1	0	-2.498546	0.159014	-2.214359
27	1	0	-3.824785	1.368327	-2.144402
28	1	0	-2.689833	-1.137095	2.651988
29	1	0	-3.049917	0.371169	3.560917
30	1	0	-3.496670	0.232121	1.833399
31	1	0	-0.693272	0.671363	4.084719
32	1	0	-0.311085	-0.851031	3.209266
33	1	0	0.464164	0.680516	2.716920

54: Li-I coordinated to oxygen of α-CF_3 ketone with two dimethyl ethers
Charge=0, Multiplicity=1



E(UB3LYP/631+LAN)= -859.345202220 a.u.

G(sol)(UB3LYP/6311+LAN//UB3LYP/631+LAN)= -859.360817 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.981457	0.140277	0.765316
2	6	0	1.738172	-0.822288	0.761189
3	6	0	1.317477	-2.206443	0.362736
4	6	0	3.191217	-0.607847	1.210396
5	3	0	-0.866018	0.622059	0.117678
6	1	0	0.280356	-2.214623	0.015859
7	1	0	1.415285	-2.873166	1.231486
8	1	0	1.992447	-2.597329	-0.409295
9	1	0	3.219258	0.201735	1.944554
10	6	0	4.110343	-0.213219	0.063873
11	1	0	3.604937	-1.517909	1.655104
12	9	0	4.161896	-1.169416	-0.897944
13	9	0	5.375193	-0.024318	0.507863
14	9	0	3.718490	0.933133	-0.536945
15	8	0	-0.476453	1.761129	-1.439844
16	6	0	-0.868529	1.411154	-2.769546
17	6	0	0.448284	2.842693	-1.389414
18	1	0	0.007986	1.104558	-3.357275
19	1	0	-1.570307	0.579582	-2.682274
20	1	0	-1.354166	2.267252	-3.258267
21	1	0	0.012511	3.742243	-1.846889
22	1	0	0.663955	3.035416	-0.336533
23	1	0	1.378766	2.583296	-1.913162
24	8	0	-1.563177	1.890786	1.490877
25	6	0	-2.820010	2.469433	1.125896
26	6	0	-1.562386	1.403624	2.832812
27	1	0	-3.053074	3.311278	1.792657
28	1	0	-2.718640	2.828844	0.100136
29	1	0	-3.615989	1.716229	1.169888
30	1	0	-2.306449	0.605892	2.955468
31	1	0	-0.563560	1.007499	3.028851
32	1	0	-1.773788	2.223540	3.533432
33	53	0	-2.588372	-1.349534	-0.289660

55: anion radical of Me-I

Charge=-1, Multiplicity=2

MeI$^{\bullet-}$

E(UB3LYP/631+LAN)= -51.3194021287 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.100062	-0.000178	0.000000
2	53	0	-0.518041	0.000022	0.000000
3	1	0	2.950556	-0.557268	-0.917711
4	1	0	2.950638	-0.516529	0.941224
5	1	0	2.954594	1.073673	-0.023509