Supporting Information

GaCl₃-Catalyzed Skeletal Rearrangement of α,α,α -Trisubstituted Aldehydes

Masayuki Oshita,[†] Takao Okazaki,[‡] Kouichi Ohe,[‡] and Naoto Chatani,^{*,†}

[†] *Department of Applied Chemistry, Faculty of Engineering, Osaka University,
Suita, Osaka 565-0871, Japan*

[‡] *Department of Energy and Hydrocarbon Chemistry, Graduate School of Engineering,
Kyoto University,
Nishikyo-ku, Kyoto 615-8510, Japan*

Materials. Toluene and methylcyclohexane were distilled from CaH₂. Anhydrous 1,2-dichloroethane and tetrahydrofuran was purchased from Aldrich Chemical Co. and dried under MS 4A. GaCl₃ was purchased from Aldrich Chemical Co. and used as a 1.0 M stock solution in methylcyclohexane. 2,2-diphenylpropionaldehyde **1** was prepared by reduction of the corresponding nitrile with DIBAL. Aldehydes **4** and **7** were prepared by the reduction of nitriles which were synthesized by a method of Caron¹. Pivalaldehyde **10** was purchased from Aldrich Chemical Co. and was used after distillation from CaSO₄.

Typical Procedure . The reaction was carried out in a 10 mL two necked flask equipped with a reflux condenser and a septum inlet. The flask was charged with GaCl₃ (1.0 M in methylcyclohexane, 0.2 mmol, 200 μ L) by means of a syringe and the methylcyclohexane was removed in vacuo. The residue was dissolved in 1,2-dichloroethane (3 mL) and 2,2-diphenylpropionaldehyde (**1**) (1 mmol, 210 mg) was added. The system was immersed in an oil bath at 80 °C. After 1 hour, the vessel was removed from the oil bath and allowed to cool to room temperature. The mixture was treated with saturated aqueous Na₂CO₃ and the aqueous layer was extracted with ether. The combined organic layers were dried over MgSO₄ and concentrated under reduced pressure. The residue was subjected to column chromatography on silica gel (eluent; hexane/Et₂O = 20/1) to give 1,2-diphenylpropan-1-one (**2**) (183 mg, 87 % yield) as a colorless oil and 1,1-diphenylpropan-2-one (**3**) (19 mg, 9 % yield) as a colorless oil.

2-Methyl-1-[4-(trifluoromethyl)phenyl]-1-propanone (5c). Colorless oil; R_f 0.43 (hexane/ether = 25/1); ¹H NMR (CDCl₃) δ 1.24 (d, *J* = 6.9 Hz, 6H), 3.55 (hept, *J* = 6.9 Hz, 1H), 7.73 (d, *J* = 8.1 Hz, 2H), 8.5 (d, *J* = 8.1 Hz, 2H); ¹³C NMR (CDCl₃) δ 18.9, 35.8, 123.5 (q, *J* = 272 Hz), 125.5 (q, *J* = 3.9 Hz), 128.5, 133.9 (q, *J* = 32.4 Hz), 138.8, 203.1; IR (KBr) 3363 w, 3068 w, 2977 s, 2937 s, 2877 m, 1691 s, 1581 m, 1511 m, 1465 s, 1409 s, 1384 m, 1328 s, 1222 s, 1174 s, 1133 s, 1116 s, 1068 s, 1016 m, 983 s, 854 s, 767 s, 723 s, 698 s, 593 m, 501 m; MS, *m/z* (relative intensity, %) 216 (M⁺, 3.0),

187 (0.3), 173 (100), 159 (0.6), 145 (37), 119 (0.8), 95 (6.8), 75 (5.5), 50 (4.2); Exact Mass Calcd for $C_{11}H_{11}F_3O$: 216.0762, found 216.0747.

DFT calculations. Structures were optimized using a molecular point group of C_1 except $GaCl_3$ (C_{3v}) and Ga_2Cl_6 (C_{2v}) by the density functional theory (DFT) method at B3LYP/6-31G(d) levels using the Gaussian 98 program.² Transition structures of methyl and hydride shifts are located by changing bond angles of C(1)-C(2)-C(3) in **12Ts** and **12aTs** or H-C(2)-C(3) in **13Ts** and **13aTs**. Computed geometries were verified by frequency calculations. Furthermore, global minima were checked by manually changing initial geometries and by comparing the resulting optimized structures and their energies. Table S1 summarizes the total energies (E), zero point energies (ZPE), for the **10-14**, $GaCl_3$, and Ga_2Cl_6 . Figures 1 and S1 summarize energy profile of the isomerization from **10** to **11**. Computer geometries and Cartesian coordinated are shown in Figure 1 and Tables S2-S15.

Figure S1. Optimized structures for the studied molecules.

Table S1. Total Electronic Energies (E) and Zero Point Energies (ZPE) Derived by DFT Calculations at the B3LYP/6-31G (d)

Level

Compd	E, hartree ^a	ZPE, hartree ^a	ΔE , kcal/mol
GaCl ₃ (C _{3v})	-3303.6813268	0.003841	
Ga ₂ Cl ₆ (C _{2v})	-6607.3954090	0.008649	
10	-271.7737386	0.141293	
11	-271.7832180	0.141681	
12	-6879.1932802	0.154363	(0) ^c
12Ts	-6879.1623940	0.151230 ^b	19.4 ^c
13	-6879.2068506	0.154546	-8.5 ^c
13Ts	-6879.1758896	0.148448 ^b	10.9 ^c
14	-6879.2017658	0.154101	-5.3 ^c
12a	-3575.5010918	0.147591	(0) ^d
12aTs	-3575.4406054	0.145134 ^b	38.0 ^d
13a	-3575.4642250	0.148626	23.1 ^d
13aTs	-3575.4437699	0.143401 ^b	36.0 ^d
14a	-3575.5145242	0.147844	-8.4 ^d

^a 1 hartree = 627.5096 kcal/mol. ^b Number of imaginary frequency is 1. ^c Relative electronic energies to **12**. ^d Relative energies to **12a**.

Table S2. Cartesian Coordinates of the Optimized Structure for GaCl₃ by B3LYP/6-31G(d)^a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	31	0	0.000000	0.000000	0.000000
2	17	0	0.000000	2.132343	0.000000
3	17	0	1.846664	-1.066172	0.000000
4	17	0	-1.846664	-1.066172	0.000000

^a Number of imaginary frequencies is 0.

Table S3. Cartesian Coordinates of the Optimized Structure for Ga₂Cl₆ by B3LYP/6-31G(d)^a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	31	0	0.000000	1.640067	-0.019594
2	17	0	0.000000	2.296805	2.011959
3	17	0	0.000000	2.986161	-1.673666
4	17	0	1.661767	0.000000	-0.302563
5	17	0	-1.661767	0.000000	-0.302563
6	31	0	0.000000	-1.640067	-0.019594
7	17	0	0.000000	-2.296805	2.011959
8	17	0	0.000000	-2.986161	-1.673666

^a Number of imaginary frequencies is 0.

Table S4. Cartesian Coordinates of the Optimized Structure for **10** by B3LYP/6-31G(d)^a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	8	0	2.105376	-0.088914	0.000000
2	6	0	1.034423	-0.653336	-0.000024
3	6	0	-0.330123	0.026828	0.000000
4	6	0	-1.081739	-0.454067	-1.261531
5	1	0	0.983825	-1.768917	-0.000065
6	1	0	-0.580075	-0.118295	-2.176213
7	1	0	-1.154730	-1.548064	-1.295166
8	1	0	-2.101424	-0.051911	-1.267136
9	6	0	-0.169573	1.551197	-0.000130
10	6	0	-1.081608	-0.453863	1.261684
11	1	0	0.383414	1.887950	-0.882606
12	1	0	-1.150842	2.039529	0.000323
13	1	0	0.384275	1.887999	0.881784
14	1	0	-0.580192	-0.117405	2.176248
15	1	0	-2.101505	-0.052242	1.267013
16	1	0	-1.154034	-1.547883	1.295829

^a Number of imaginary frequencies is 0.

Table S5. Cartesian Coordinates of the Optimized Structure for **11** by B3LYP/6-31G(d)^a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	8	0	-0.875904	-1.175467	-0.837322
2	6	0	-0.753374	-0.245236	-0.062284
3	6	0	-1.960484	0.507550	0.472504
4	6	0	0.626873	0.232804	0.405135
5	1	0	-2.097746	0.265669	1.535048
6	1	0	-1.817383	1.592795	0.410848
7	1	0	-2.857793	0.216476	-0.077506
8	6	0	1.112277	1.341990	-0.554331
9	1	0	0.513049	0.677321	1.404104
10	6	0	1.626097	-0.927145	0.467826
11	1	0	0.413426	2.185240	-0.598822
12	1	0	2.082900	1.729264	-0.225422
13	1	0	1.229172	0.943818	-1.568426
14	1	0	1.707762	-1.411869	-0.509315
15	1	0	2.616989	-0.566783	0.765766
16	1	0	1.308521	-1.687982	1.189200

^a Number of imaginary frequencies is 0.

Table S6. Cartesian Coordinates of the Optimized Structure for **12** by B3LYP/6-31G(d)^a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	31	0	1.740355	-0.210910	-0.091825
2	8	0	-0.138229	0.372972	-0.115190
3	31	0	-1.167076	-1.282544	0.017022
4	6	0	-0.431526	1.625604	0.514284
5	1	0	-0.577728	1.464621	1.584954
6	6	0	-1.616555	2.387647	-0.111369
7	6	0	-2.910689	1.600545	0.203606
8	6	0	-1.725679	3.768091	0.571464
9	6	0	-1.448594	2.547314	-1.631987
10	1	0	-1.415832	1.578526	-2.139607
11	1	0	-2.298706	3.107667	-2.035353
12	1	0	-0.534642	3.095849	-1.879894
13	1	0	-3.001834	1.374326	1.271745
14	1	0	-3.776769	2.204213	-0.086703
15	1	0	-2.984886	0.667098	-0.360024
16	1	0	-0.879726	4.414807	0.324607
17	1	0	-2.640445	4.265465	0.233688
18	1	0	-1.780646	3.676557	1.663113
19	17	0	2.858938	0.200504	-1.867717
20	17	0	1.139623	2.574740	0.403840
21	17	0	2.563736	-0.357938	1.887047
22	17	0	-2.496419	-1.686814	-1.621815
23	17	0	0.792312	-2.392481	-0.425504
24	17	0	-1.797974	-1.521013	2.058729

a Number of imaginary frequencies is 0.

Table S7. Cartesian Coordinates of the Optimized Structure for **12a** by B3LYP/6-31G(d)^a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	31	0	-1.165771	0.069075	-0.052285
2	17	0	-1.650970	-0.802348	1.885011
3	17	0	-1.259011	-1.310785	-1.736974
4	17	0	-1.882110	2.070301	-0.414798
5	8	0	0.808526	0.381795	0.118142
6	6	0	1.772369	-0.380024	0.319321
7	6	0	3.159456	0.210977	0.344711
8	6	0	3.879260	-0.204756	-0.966457
9	6	0	3.155766	1.729582	0.538954
10	1	0	3.375048	0.229285	-1.836160
11	1	0	4.906081	0.172288	-0.942795
12	1	0	3.920295	-1.290885	-1.095494
13	1	0	2.646447	2.012879	1.465101
14	1	0	4.185028	2.098745	0.585901
15	1	0	2.645107	2.230944	-0.288131
16	6	0	1.578392	-1.853109	0.508677
17	1	0	3.686810	-0.276616	1.177562
18	1	0	0.913396	-2.013178	1.366537
19	1	0	1.064197	-2.271588	-0.364825
20	1	0	2.522379	-2.375412	0.671704

a Number of imaginary frequencies is 0.

Table S8. Cartesian Coordinates of the Optimized Structure for **12Ts** by B3LYP/6-31G(d)^a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.487931	1.578227	-0.587464
2	6	0	-1.284285	2.527591	0.077747
3	31	0	1.893783	-0.114675	0.002030
4	17	0	2.032749	-2.244017	0.205653
5	17	0	2.668383	0.991824	1.718637
6	17	0	2.511083	0.719741	-1.928631
7	8	0	-0.061141	0.451556	0.022596
8	31	0	-1.470809	-1.044766	-0.000767
9	17	0	-1.280589	-1.876149	1.976060
10	17	0	-1.029416	-2.111549	-1.822533
11	17	0	-3.342452	0.088554	-0.264812
12	6	0	-1.523006	2.448936	1.557618
13	6	0	-2.134299	3.465762	-0.733578
14	1	0	-0.479378	1.559521	-1.677454
15	1	0	-1.470545	3.442712	2.013596
16	1	0	-2.538696	2.063885	1.702702
17	1	0	-0.829633	1.768885	2.054909
18	1	0	-1.799589	3.544981	-1.771482
19	1	0	-3.146397	3.044577	-0.738333
20	1	0	-2.180196	4.461468	-0.282874
21	6	0	0.561444	3.007850	-0.162669
22	1	0	1.247958	2.760086	-0.978563
23	1	0	0.253209	4.044867	-0.290649
24	1	0	1.012780	2.806156	0.803944

^a Number of imaginary frequencies is 1.

Table S9. Cartesian Coordinates of the Optimized Structure for **12aTs** by B3LYP/6-31G(d)^a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	31	0	1.069209	-0.018936	0.007684
2	17	0	0.199745	-0.031677	2.057329
3	17	0	1.530291	2.009325	-0.662730
4	17	0	2.647255	-1.477989	-0.280968
5	8	0	-0.424691	-0.581409	-1.057628
6	6	0	-1.575909	-0.897911	-0.496873
7	6	0	-2.446400	0.075730	0.068290
8	6	0	-2.191212	1.527436	-0.148286
9	6	0	-3.550190	-0.333446	0.985398
10	6	0	-2.847535	-0.873941	-1.717971
11	1	0	-1.686335	-1.916340	-0.101302
12	1	0	-1.679151	1.888830	0.754405
13	1	0	-1.516241	1.708542	-0.986031
14	1	0	-3.120940	2.094936	-0.254910
15	1	0	-3.252197	-0.001451	1.989542
16	1	0	-4.494652	0.164725	0.742789
17	1	0	-3.692616	-1.416340	1.022171
18	1	0	-2.210022	-1.378636	-2.446707
19	1	0	-3.707636	-1.482241	-1.445166
20	1	0	-3.134627	0.094867	-2.127059

^a Number of imaginary frequencies is 1.

Table S10. Cartesian Coordinates of the Optimized Structure for **13** by B3LYP/6-31G(d)^a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	31	0	-1.955513	0.132801	0.024591
2	17	0	-1.525777	-2.067735	-0.167799
3	17	0	-3.029770	1.001706	-1.631490
4	17	0	-2.545922	0.751926	2.002492
5	8	0	-0.054638	0.456643	-0.190832
6	31	0	0.882221	-1.215558	-0.025401
7	17	0	1.704853	-2.107087	-1.796434
8	17	0	1.273416	-1.869740	1.986438
9	17	0	2.932797	0.676014	0.130704
10	6	0	0.511628	1.724156	-0.618914
11	6	0	1.702980	2.087636	0.294547
12	6	0	2.418286	3.356189	-0.165699
13	6	0	1.306220	2.169519	1.768158
14	6	0	0.780538	1.689758	-2.119556
15	1	0	-0.258958	2.477700	-0.410528
16	1	0	1.706504	4.191305	-0.161488
17	1	0	3.230284	3.601877	0.523682
18	1	0	2.834208	3.258382	-1.170240
19	1	0	0.855772	1.245770	2.134479
20	1	0	2.180807	2.397875	2.382774
21	1	0	0.576766	2.979238	1.893634
22	1	0	-0.124540	1.361262	-2.636884
23	1	0	1.034890	2.687129	-2.490040
24	1	0	1.592357	1.001787	-2.371316

a Number of imaginary frequencies is 0.

Table S11. Cartesian Coordinates of the Optimized Structure for **13a** by B3LYP/6-31G(d)^a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	31	0	1.063276	-0.002503	-0.182961
2	17	0	-0.849742	-0.295638	1.474858
3	17	0	2.074474	1.779180	0.500114
4	17	0	2.212260	-1.824192	-0.157230
5	8	0	-0.236413	0.065124	-1.462981
6	6	0	-1.511505	0.530539	-1.096264
7	6	0	-2.126401	-0.354074	0.023968
8	6	0	-3.430885	0.173336	0.603188
9	6	0	-2.211549	-1.819957	-0.380881
10	6	0	-1.513626	2.035548	-0.815712
11	1	0	-2.169618	0.339969	-1.960810
12	1	0	-4.167786	0.235172	-0.207879
13	1	0	-3.825689	-0.505651	1.364155
14	1	0	-3.319461	1.166839	1.041667
15	1	0	-1.259753	-2.183184	-0.771973
16	1	0	-2.523671	-2.445707	0.459254
17	1	0	-2.964782	-1.910837	-1.173958
18	1	0	-0.966267	2.530131	-1.622622
19	1	0	-2.527511	2.447628	-0.785200
20	1	0	-1.010782	2.280949	0.125595

a Number of imaginary frequencies is 0.

Table S12. Cartesian Coordinates of the Optimized Structure for **13Ts** by B3LYP/6-31G(d)^a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.891355	2.546059	0.333114
2	6	0	-0.229995	1.659236	-0.544843
3	31	0	1.905884	-0.208235	0.108716
4	17	0	1.896061	-1.700781	1.649044
5	17	0	2.657105	1.782361	0.767035
6	17	0	2.662305	-0.704654	-1.854981
7	8	0	-0.009304	0.374976	-0.114001
8	31	0	-1.580039	-0.900231	-0.077903
9	17	0	-1.904003	-1.384601	2.006689
10	17	0	-0.989557	-2.463372	-1.432081
11	17	0	-3.155844	0.440684	-0.839996
12	6	0	-1.338766	3.904545	-0.106975
13	6	0	-1.164329	2.161653	1.750556
14	6	0	-0.054828	1.875431	-2.032351
15	1	0	-2.428649	3.832670	-0.235100
16	1	0	-1.146604	4.653848	0.665294
17	1	0	-0.915908	4.232612	-1.055538
18	1	0	-1.055080	3.021442	2.416815
19	1	0	-2.210188	1.826611	1.798679
20	1	0	-0.549791	1.330010	2.094651
21	1	0	0.044720	2.926070	-2.306968
22	1	0	0.827514	1.332420	-2.376561
23	1	0	-0.935110	1.456397	-2.531962
24	1	0	0.594820	2.385198	0.063437

^a Number of imaginary frequencies is 1.

Table S13. Cartesian Coordinates of the Optimized Structure for **13aTs** by B3LYP/6-31G(d)^a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	31	0	-0.981741	0.025912	-0.001418
2	17	0	0.241645	-0.002716	1.886883
3	17	0	-2.419976	-1.597359	-0.070208
4	17	0	-1.774942	2.020457	-0.381056
5	8	0	0.363581	-0.273260	-1.314388
6	6	0	1.595626	-0.649483	-0.934533
7	6	0	2.432893	0.349582	-0.281276
8	6	0	3.701066	-0.006093	0.405296
9	6	0	2.076740	1.780124	-0.435340
10	6	0	1.736719	-2.136886	-0.599475
11	1	0	2.349657	-0.435197	-1.812304
12	1	0	3.447485	-0.027112	1.477674
13	1	0	4.078743	-0.996425	0.148152
14	1	0	4.477717	0.750558	0.266116
15	1	0	1.592329	2.094376	0.501307
16	1	0	2.962760	2.406815	-0.574302
17	1	0	1.338903	1.929414	-1.226133
18	1	0	1.158304	-2.695032	-1.337675
19	1	0	2.767548	-2.500413	-0.605293
20	1	0	1.299231	-2.314111	0.387969

^a Number of imaginary frequencies is 1.

Table S14. Cartesian Coordinates of the Optimized Structure for **14** by B3LYP/6-31G(d)^a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	31	0	-1.538806	-0.720583	0.114360
2	8	0	0.052216	0.363938	-0.135216
3	31	0	1.599937	-0.809094	0.027615
4	6	0	-0.029474	1.723068	-0.617345
5	6	0	0.287465	1.756029	-2.104930
6	6	0	0.827541	2.642653	0.274879
7	6	0	0.876554	4.088787	-0.243767
8	6	0	0.433347	2.608991	1.759167
9	1	0	-0.123169	4.536898	-0.256282
10	1	0	1.501570	4.689854	0.423952
11	1	0	1.302771	4.162404	-1.248382
12	1	0	0.371013	1.593137	2.155606
13	1	0	1.189181	3.145186	2.341594
14	1	0	-0.530664	3.101059	1.920724
15	17	0	-2.494675	-0.544434	2.023536
16	17	0	-1.829372	2.147696	-0.432787
17	17	0	-2.543723	-1.259024	-1.704202
18	17	0	2.782988	-0.370068	1.767515
19	17	0	0.093820	-2.481744	0.438221
20	17	0	2.617448	-1.088598	-1.846938
21	1	0	-0.297365	0.997053	-2.629916
22	1	0	0.057761	2.734455	-2.530003
23	1	0	1.350554	1.542575	-2.259927
24	1	0	1.842716	2.223623	0.184250

a Number of imaginary frequencies is 0.

Table S15. Cartesian Coordinates of the Optimized Structure for **14a** by B3LYP/6-31G(d)^a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	31	0	1.130388	0.064115	0.055359
2	17	0	2.755327	-1.123991	-0.718475
3	17	0	0.812561	-0.019202	2.209438
4	17	0	0.859617	2.028098	-0.845376
5	8	0	-0.454135	-0.972735	-0.629215
6	6	0	-1.684508	-0.846026	-0.498318
7	6	0	-2.309818	0.332971	0.204646
8	6	0	-2.900565	1.293530	-0.856484
9	6	0	-3.365279	-0.104552	1.237036
10	6	0	-2.545499	-1.928566	-1.081578
11	1	0	-1.506167	0.860218	0.725474
12	1	0	-3.725200	0.832223	-1.410953
13	1	0	-3.292653	2.177738	-0.344352
14	1	0	-2.134487	1.625469	-1.562724
15	1	0	-2.936081	-0.774081	1.989659
16	1	0	-3.742657	0.781575	1.756671
17	1	0	-4.219687	-0.603830	0.767270
18	1	0	-2.850427	-2.601716	-0.268910
19	1	0	-3.458999	-1.526499	-1.528186
20	1	0	-1.976182	-2.504319	-1.813152

a Number of imaginary frequencies is 0.

References

- 1) Caron, S.; Vazquez, E.; Wojcik, J. M. *J. Am. Chem. Soc.* **2000**, *122*, 712.
- 2) Gaussian 98 A9: Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Zakrzewski, V. G.; Montgomery, J. A., Jr.; Stratmann, R. E.; Burant, J. C.; Dapprich, S.; Millam, J. M.; Daniels, A. D.; Kudin, K. N.; Strain, M. C.; Farkas, O.; Tomasi, J.; Barone, V.; Cossi, M.; Cammi, R.; Mennucci, B.; Pomelli, C.; Adamo, C.; Clifford, S.; Ochterski, J.; Petersson, G. A.; Ayala, P. Y.; Morokuma, Q. Cui; K.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B. ; Cioslowski, J.; Ortiz, J. V.; Baboul, A. G.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Gomperts, R.; 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.; Andres, J. L.; Gonzalez, C.; Head-Gordon, M.; Replogle, E. S.; Pople, J. A.; Gaussian, Inc., Pittsburgh PA, 1998.