

**Amidinate bromogermylene resulting from carbodiimide insertion into Ar-GeBr bond**

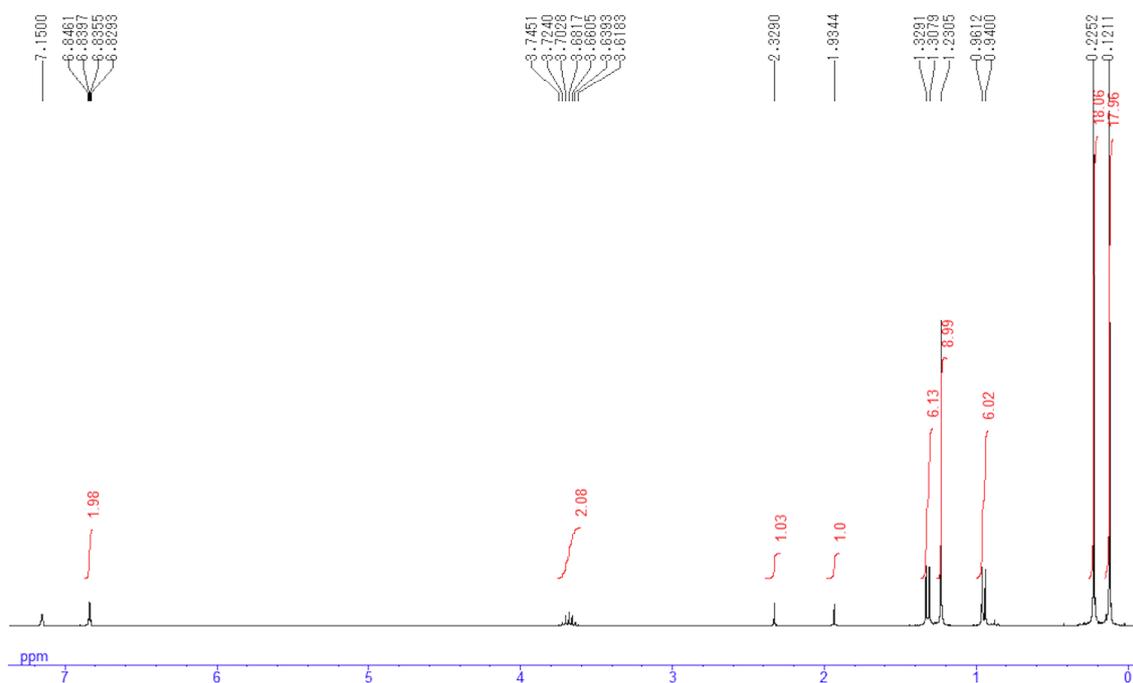
**Takahiro Sasamori, Tomohiro Sugahara and Norihiro Tokitoh**

**Experimental Procedure**

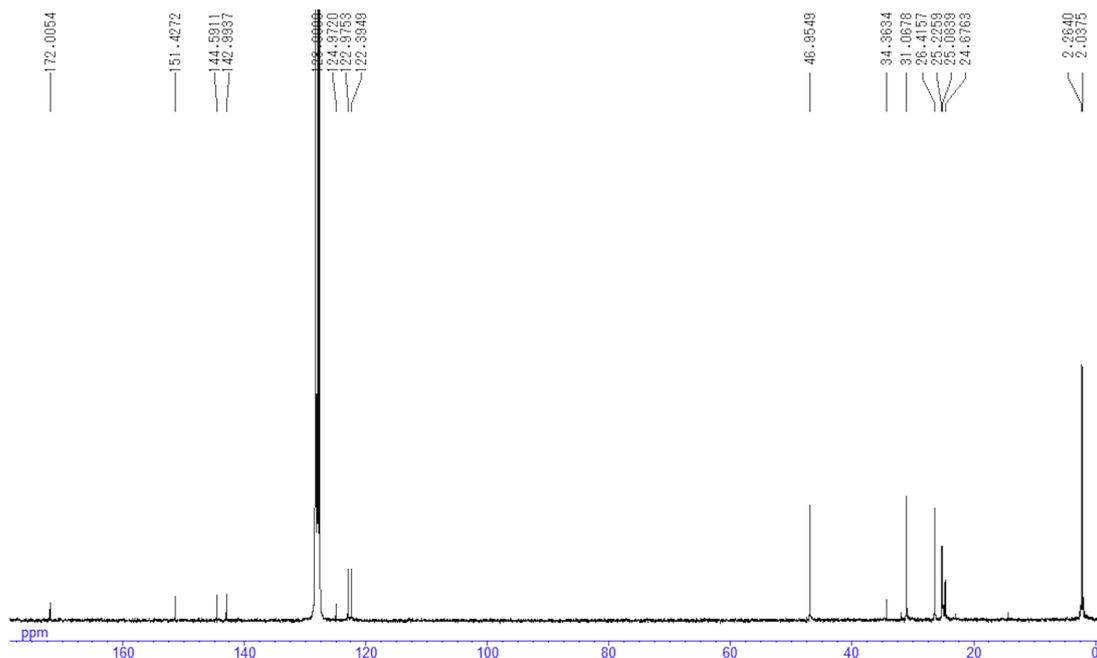
**General remarks:** All manipulations were carried out under an argon atmosphere using Schlenk-line techniques. All solvents were purified by standard methods.  $^1\text{H}$  (300 MHz) and  $^{13}\text{C}$  (75 MHz) NMR spectra were measured on a JEOL AL-300 spectrometer. Signals arising from residual  $\text{C}_6\text{D}_5\text{H}$  (7.16 ppm in the  $^1\text{H}$  NMR spectra) and  $\text{C}_6\text{D}_6$  (128.0 ppm in the  $^{13}\text{C}$  NMR spectra) in  $\text{C}_6\text{D}_6$  were used to reference the spectra. Multiplicity of signals in the  $^{13}\text{C}$  NMR spectra were determined by DEPT techniques. High-resolution mass spectra (HRMS) were obtained from a Bruker micrOTOF focus-Kci mass spectrometer (DART). All melting points were determined on a Büchi Melting Point Apparatus M-565 and are uncorrected. Elemental analyses were carried out at the Microanalytical Laboratory (Institute for Chemical Research of Kyoto University).

**Synthesis of bromogermylene 4:** Heating a  $\text{C}_6\text{D}_6$  solution of dibromodigermene **3** (11.1 mg, 9.2  $\mu\text{mol}$ , 0.018 M) and *N,N'*-diisopropylcarbodiimide (2.9 mg, 23.0  $\mu\text{mol}$ , 2.5 equiv.) in a *J*-Young NMR tube at 70 °C for 7 hours resulted in the formation of bromogermylene **4** as the main product, as evident from the  $^1\text{H}$  NMR spectrum. After removal of the solvent and any other residual reagents under reduced pressure, the resulting substance was recrystallized from hexane to afford product **4** as stable colourless crystals in 84% yield (10.3 mg, 7.7  $\mu\text{mol}$ ). Colourless crystals, mp 112.3–113.3 °C;  $^1\text{H}$  NMR (300 MHz, 298 K,  $\text{C}_6\text{D}_6$ )  $\delta$  0.12 (s, 18H,  $\text{CH}(\text{SiMe}_3)_2$ ), 0.22 (s, 18H,  $\text{CH}(\text{SiMe}_3)_2$ ), 0.95 (d, 6H,  $J = 6.3$  Hz,  $\text{CHCH}_3$ ), 1.23 (s, 9 H,

$C(Me)_3$ ), 1.32 (d, 6H,  $J = 6.3$  Hz,  $CHCH_3$ ), 1.93 (s, 1H,  $CHSi$ ), 2.33 (s, 1H,  $CHSi$ ), 3.68 (sep, 2H,  $J = 6.3$  Hz,  $CHCH_3$ ), 6.83 (d, 1H,  $J = 1.8$  Hz,  $ArH$ ), 6.84 (d, 1H,  $J = 1.8$  Hz,  $ArH$ );  $^{13}C$  NMR (75 MHz, 298 K,  $C_6D_6$ )  $\delta$  2.04 (q), 2.26 (q), 24.68 (s), 25.08 (q), 25.23 (q) 26.42 (d), 31.07 (q), 34.36 (s), 46.95 (d), 122.39 (d), 122.98 (d), 124.97 (s), 142.99 (s), 144.59 (s), 151.43 (s), 172.01 (s). MS (DART-TOF, positive mode):  $m/z$  calcd for  $C_{31}H_{64}^{79}Br^{74}GeN_2Si_4$  729.2542 ( $[M+H]^+$ ), found 729.2541 ( $[M+H]^+$ ).



**Figure S1.**  $^1H$  NMR spectrum of **4** in  $C_6D_6$ .



**Figure S2.**  $^{13}\text{C}$  NMR spectrum of **4** in  $\text{C}_6\text{D}_6$ .

**X-ray crystallographic analysis:** Single crystals of **4** were obtained upon recrystallization from hexane at room temperature. Intensity data were collected on a RIGAKU Mercury CCD(system) with VariMax Mo Optics using  $\text{MoK}_\alpha$  radiation (0.71073 Å). The structures were solved using the SHELXT<sup>S1</sup> program and refined by a full-matrix least square method on  $F^2$  for all reflections (SHELXL).<sup>S1</sup> All hydrogen atoms were placed using AFIX instructions, while all other atoms were refined anisotropically. Crystallographic data for **4**:  $\text{C}_{31}\text{H}_{63}\text{BrGeN}_2\text{Si}_4$ , FW 728.69, crystal size  $0.05 \times 0.05 \times 0.02$  mm<sup>3</sup>, temperature  $-170$  °C,  $\lambda = 0.71073$  Å, monoclinic, space group  $Pbcn$  (#60),  $a = 19.0423(5)$  Å,  $b = 13.8557(4)$  Å,  $c = 14.9376(4)$  Å,  $V = 3941.20(19)$  Å<sup>3</sup>,  $Z = 4$ ,  $D_{\text{calcd}} = 1.228$  g cm<sup>-3</sup>,  $\mu = 1.934$  mm<sup>-1</sup>,  $\theta_{\text{max}} = 28.223^\circ$ , 32529 reflections measured, 4513 independent reflections ( $R_{\text{int}} = 0.0693$ ), 201 parameters refined, GOF = 1.188, completeness to  $\theta_{\text{max}} = 97.1\%$ ,  $R_1 [I > 2\sigma(I)] = 0.0530$ ,  $wR_2$  (all data) = 0.1180, largest diff. peak and hole 0.335 and  $-0.348$  e Å<sup>-3</sup>. The cif file including the crystallographic data for **4** was deposited at the Cambridge Crystallographic Data Centre (CCDC) under reference number CCDC-2103198, which is freely available via [www.ccdc.cam.ac.uk/data\\_request/cif](http://www.ccdc.cam.ac.uk/data_request/cif).

**Computational calculations:** Structural optimization and potential energy surface search calculations for model compounds (**4'**, **5'**, **6<sub>imi'</sub>**, **7'**, **8'**, **9<sub>imi'</sub>**, **10'**, **TS67**, **TS78**, **TS84**, **TS910**, **TS104**) were carried out at the B3PW91/3-21G level of theory. The molecular geometries for the transition states were first estimated by Reaction plus software package (Software to optimize reaction paths along the user's expected ones, HPC Systems Inc., <http://www.hpc.co.jp/chem/react2.html> (written in Japanese)), based on the nudged elastic band (NEB) method,<sup>S2</sup> and were subsequently re-optimized using *Gaussian 16* software package.<sup>S3</sup> Harmonic frequency calculations verified the nature of ground or transition states by all positive frequencies or only one negative frequency, respectively. From these optimized geometries, all reported data were obtained by means of single-point (SP) calculations at the B3PW91/6-311G(2d) level of theory. The structural optimization of **4** was performed at the B3PW91/6-311G(2d) level of theory. Frequency calculations confirmed minimum energies for all optimized structures. All calculations were carried out using the *Gaussian 16* program package.<sup>S3</sup> Computational time was generously provided by the Supercomputer Laboratory in the Institute for Chemical Research of Kyoto University.

**<coordinates of the optimized structures as the .xyz format>**

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C  0.000005 -0.279184 -0.000004
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H -2.186583  1.047582  0.908522
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C	2.353433	-1.342790	0.353813
N	1.197653	-0.894807	0.564300
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H	5.398262	-2.158490	0.526686
H	5.065816	-1.737491	-1.164717
H	5.006622	-0.463249	0.090726
C	0.642466	-0.810563	1.960006
H	0.614375	0.251043	2.220987
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C	-1.478390	-0.110037	-0.152998
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H	-3.913722	1.169918	1.856580
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H	0.544493	0.837414	-3.531840
H	1.843789	1.797629	-2.770488
C	2.214368	-2.708342	0.386347
H	2.811657	-2.334622	1.228336
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H	2.872729	-3.258316	-0.293133

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C	3.716980	0.361221	-0.608682
C	4.046157	-0.984824	-0.492675
C	3.040901	-1.908782	-0.207271
C	1.720989	-1.503157	-0.016120
H	4.485564	1.093746	-0.836020
H	5.070777	-1.313215	-0.624860
H	3.272646	-2.967883	-0.145602
Ge	-0.678622	0.164762	-0.438067
C	0.634454	-2.532166	0.168620
H	-0.023251	-2.318621	1.019743
H	0.004406	-2.572823	-0.735512
H	1.061864	-3.529224	0.316907
C	2.103524	2.280627	-0.556814
H	1.345257	2.453998	-1.334598
H	1.688408	2.671440	0.389731
H	3.006431	2.839610	-0.820225
Br	-2.846247	-0.977949	-0.255723
N	-0.936304	1.906858	0.247220
C	-0.076740	1.846846	1.302043
N	0.190367	0.372547	1.258466
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H	-2.545095	3.100690	-0.389469
C	0.656432	-0.226726	2.509236
H	1.096522	0.570447	3.116582
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H	1.410985	-0.992600	2.305547

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C	1.764756	-0.039981	0.196490
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C	4.138465	0.332674	-0.032400
C	4.330079	-0.988273	-0.417658
C	3.241914	-1.849445	-0.455053
C	1.955074	-1.396893	-0.144225
H	4.987942	1.004826	0.032916
H	5.323079	-1.347345	-0.665600

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Ge	-0.996436	-0.071530	-0.955229
C	0.834043	-2.421020	-0.188405
H	-0.014399	-2.177075	0.458226
H	0.459716	-2.542928	-1.213215
H	1.219272	-3.393626	0.139829
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H	2.330694	2.916745	0.001897
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N	-1.040431	1.781004	-0.451632
C	0.020588	1.957203	0.311721
N	0.377776	0.380868	0.495349
C	-1.879594	2.919441	-0.843597
H	-1.446022	3.840117	-0.442148
H	-1.938763	2.979604	-1.935361
H	-2.886621	2.774679	-0.439666
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H	0.370219	-0.903653	2.203280
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C	-3.671904	-1.160667	-0.726416
C	-2.305622	-1.074082	-0.436371
H	-4.694139	1.931934	0.190233
H	-5.579025	-0.165257	-0.801765
H	-4.055708	-2.101919	-1.107934
Ge	1.356551	-0.980062	-0.402290
C	-1.452134	-2.294123	-0.647747
H	-0.771680	-2.177338	-1.502500
H	-0.845253	-2.509342	0.241134
H	-2.083459	-3.166964	-0.843802
C	-2.244450	2.478557	1.069908
H	-1.416499	2.180792	1.731865
H	-1.893009	3.299261	0.432230
H	-3.081418	2.861465	1.664620
Br	3.182700	0.726080	-0.237414
N	0.543513	-0.697161	1.344432
C	-0.311154	0.286048	1.051081
N	-0.116894	0.441346	-0.393440
C	0.565430	-1.360266	2.650073
H	-0.169017	-0.887796	3.308777
H	0.325992	-2.425654	2.552097
H	1.562059	-1.263768	3.093726
C	-0.060587	1.710361	-1.152033
H	0.990349	1.915779	-1.379628
H	-0.630816	1.585601	-2.076182
H	-0.463357	2.540486	-0.577411
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C	2.621317	-1.984018	0.312570
C	3.653853	-1.195410	-0.183281
C	3.343096	-0.047697	-0.907743
C	2.009605	0.314251	-1.123783
H	2.851774	-2.891376	0.863000
H	4.689100	-1.481700	-0.025051
H	4.136172	0.567779	-1.323132
Ge	-0.848161	0.266319	-1.087336
C	1.741489	1.559922	-1.955629
H	1.199759	1.306339	-2.876447
H	1.140903	2.298370	-1.411799
H	2.684726	2.038114	-2.242444
C	0.232788	-2.570905	0.680846
H	-0.384146	-2.071065	1.433612
H	-0.453300	-2.922993	-0.096456
H	0.713055	-3.442671	1.138430
Br	-2.675534	-0.890998	0.284254
N	0.979605	1.265712	2.109052
C	0.190688	1.510080	1.259447
N	-0.677413	1.656763	0.350559
C	2.371240	1.203877	2.507700
H	2.881969	0.501905	1.839018
H	2.837760	2.191580	2.428773
H	2.434021	0.847908	3.537382
C	-1.733388	2.711672	0.416356
H	-1.826143	3.156167	-0.577550
H	-2.674803	2.222134	0.684682
H	-1.479202	3.478539	1.152982

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C	2.507709	-2.048890	0.206509
C	3.489727	-1.493861	-0.607017
C	3.234303	-0.293198	-1.266138
C	1.986556	0.321045	-1.163185
H	2.709897	-2.967455	0.749343
H	4.453502	-1.981355	-0.712364
H	4.003608	0.165588	-1.880077
Ge	-0.903449	0.398599	-0.979581
C	1.738581	1.590444	-1.951175
H	1.061446	1.390180	-2.795625
H	1.270923	2.367606	-1.336613
H	2.676175	1.986608	-2.355386
C	0.287647	-2.046634	1.341751
H	0.030617	-1.324652	2.127032
H	-0.654468	-2.331751	0.861447
H	0.728612	-2.929454	1.816256
Br	-2.747118	-0.995943	0.057168
N	1.162844	1.288737	2.038479
C	0.414518	1.264081	1.085333
N	-0.637107	1.664549	0.442226
C	2.489371	0.821682	2.377594
H	2.706477	-0.087343	1.801770
H	3.235846	1.588106	2.142082
H	2.531384	0.599436	3.446879
C	-1.428078	2.837178	0.864615
H	-2.062871	3.128488	0.023330

H -2.061611 2.581227 1.720640  
H -0.772674 3.672402 1.133125  
30

8, electronic energy = -5188.78380166 a.u

C 1.707119 0.031738 0.000136  
C 2.119394 -0.526867 1.225582  
C 2.907331 -1.680922 1.209558  
C 3.295979 -2.256366 0.000933  
C 2.908347 -1.681052 -1.208078  
C 2.120419 -0.526999 -1.224898  
H 3.214998 -2.128285 2.149351  
H 3.903664 -3.155221 0.001233  
H 3.216791 -2.128532 -2.147562  
Ge -1.031138 -0.692245 -0.001276  
C 1.697250 0.111477 -2.530376  
H 0.610474 0.260345 -2.554269  
H 2.167711 1.094938 -2.651720  
H 1.980328 -0.516780 -3.380444  
C 1.694732 0.111545 2.530603  
H 2.161538 1.096895 2.650545  
H 0.607401 0.256418 2.554977  
H 1.980579 -0.514718 3.381209  
Br -3.489930 -0.366874 0.000465  
N 1.322693 2.493796 0.000158  
C 0.887645 1.290481 -0.000189  
N -0.505681 1.055531 -0.000577  
C 2.770314 2.758176 0.000790  
H 3.398294 1.856015 0.000720  
H 3.012536 3.363415 -0.881064  
H 3.011941 3.362803 0.883235  
C -1.324399 2.287444 -0.000372  
H -2.377684 2.007060 -0.001330  
H -1.084968 2.889837 0.881478  
H -1.083482 2.891027 -0.880984

30

TS82, electronic energy = -5188.76195642 a.u

C -1.924272 0.020293 -0.037048  
C -2.667531 0.820824 -0.929550  
C -3.634332 0.219051 -1.742548  
C -3.883562 -1.147557 -1.666054  
C -3.187106 -1.924325 -0.745240  
C -2.214409 -1.355761 0.083728  
H -4.203165 0.837883 -2.430124  
H -4.635483 -1.600992 -2.303284  
H -3.404438 -2.984092 -0.652223  
Ge 1.549442 -0.773573 0.462160  
C -1.515298 -2.238503 1.097258  
H -1.132227 -1.659529 1.943443  
H -2.211478 -2.991322 1.484622  
H -0.668183 -2.769077 0.641559  
C -2.482509 2.323503 -1.019207  
H -1.958465 2.718143 -0.144800  
H -1.909736 2.593923 -1.915462  
H -3.459065 2.817213 -1.085979  
Br 3.610376 0.034893 -0.631592  
N -1.014491 1.150873 1.983534  
C -0.858119 0.637805 0.827591  
N 0.484675 0.665451 0.255331

C	-2.357167	1.184971	2.598413
H	-3.145156	0.732759	1.983104
H	-2.297487	0.666616	3.561686
H	-2.606319	2.231808	2.804983
C	0.830175	1.999814	-0.294135
H	1.889688	2.009611	-0.557739
H	0.239080	2.211920	-1.190904
H	0.630617	2.763296	0.466431

### References:

- S1 (a) G. M. Sheldrick, *Acta Crystallogr.*, 2015, **C71**, 3; (b) I. Usón and G. M. Sheldrick, *Acta Crystallogr.*, 2018, **D74**, 106.
- S2 G. Henkelman and H. Jónsson, *J. Chem. Phys.* 2000, **113**, 9978.
- S3 M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, *Gaussian 16, Revision C.01*, Gaussian, Wallingford, CT, 2016.