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Differences between Gaussian and GAMESS Basis Sets (II)—6-31G and 6-31G*—

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Gaussian and GAMESS, which are calculation codes for the ab initio molecular orbital method, can be used by simply specifying a basis set name such as 6-31G. However, if an individual basis set with a common name does not have the same parameter set, the calculations with the two codes will each produce a different result. Previously, we used Gaussian and GAMESS for STO-3G calculations of hydrides containing third-period elements and compared the results [1]. In this study, we used 6-31G and 6-31G* for 36 molecules containing a first- to fourth-period element (H, Be, N, Ne, Na-Kr) and compared the results calculated using the two codes. For molecules containing a first- to third-period element (H, Be, N, Ne, Na-Ar) except Si, the optimized structure and total energy obtained with Gaussian and GAMESS were almost the same, whereas the two codes gave different results for K, Ca, and Ga-Kr because the basis parameters used in the two codes are different. On the other hand, the results for the Sc-Zn were in agreement. When the results calculated using Gaussian and GAMESS codes are compared or combined, it is necessary to severely check whether or not the input data produces a sufficiently accurate calculation result.

Keyword: Basis set, Gaussian, GAMESS, 6-31G, 6-31G*, Total energy

1 INTRODUCTION

The basis set is one of the important parameters in the ab initio SCF-MO calculation. In most conventional basis sets, a linear combination of Gaussian type orbitals (GTOs) is used as an atomic orbital. This is referred to as a contracted GTO (CGTO). Program codes such as Gaussian [1] and GAMESS [2] have a database of basis sets and can be used by simply specifying a basis set name in the input.

In various studies, the minimal basis set STO-NG (STO-3G is the most popular) [3, 4] and the split-valence-type basis set N-31G (6-31G is the most popular) [5–14] have been widely used as the de facto standards for basis sets. Both were developed by Pople et al. and are still used today, nearly 30 years since their introduction. Relatively accurate calculations can be performed by using STO-3G and 6-31G, and the calculation cost is low because of the small numbers of GTOs and CGTOs.

To the best of our knowledge, Gaussian is the oldest general-purpose calculation code for the ab initio molecular orbital method, and GAMESS was developed thereafter. Both codes are reliable and have been widely used by many researchers. The two codes are designed so that STO-NG and N-31G can be used in a very simple setting, and experimental results can be consistently reproduced even by researchers who are not familiar with quantum chemistry and molecular orbital methods. In that sense, it is becoming common place to use Gaussian and GAMESS as tools for furthering research. If a basis set name specified in a Gaussian input is the same as that of GAMESS and the calculated results are the same, there is no confusion. However, this is not always the case. When the scope of the code is expanded or improved, each code development group may make a different parameter set without changing the basis set name, which can confuse users. We have already performed STO-3G calculations using Gaussian and GAMESS for hydrides containing a third-period element and showed that the two codes produce different calculation results [15]. In this paper, we compare the results of 6-31G and 6-31G* obtained by using Gaussian and GAMESS. The 6-31G is the first split-valence-type basis sets and continues to be widely used as it produces accurate results in spite of the low calculation cost. Polarization functions are added to 6-31G to create 6-31G*, which has also been widely used.

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### Table 1. Comparison of 6-31G and 6-31G* basis set structures and input settings of Gaussian and GAMESS.

| Element Code | Input Setting * | CGTO structure b,c,d | GTO * | CGTO |
|--------------|-----------------|-----------------------|-------|-------|
| 1st row H, He | Gaussian 6-31G** | (4s1p)[2s1p]: 31G(p)  | 7    | 5 |
|               | GAMESS NPFUNC=1 | (4s1p)[2s1p]: 31G(p)  | 7    | 5 |
| 2nd row Li-Ne | Gaussian 6-31G* | (6s)(4sp1d)[1s][2sp1d]: 6-31G(d) | 28 | 15 |
|               | GAMESS NDFUNC=1 | (6s)(4sp1d)[1s][2sp1d]: 6-31G(d) | 28 | 15 |
| 3rd row Na-Ar | Gaussian 6-31G* | (6s)(6sp4s)[1s][1sp][2sp][3sp][2sp]: 66-31G(d) | 52 | 19 |
|               | GAMESS NDFUNC=1 | (6s)(6sp4s)[1s][1sp][2sp][3sp]: 66-31G(d) | 52 | 19 |
| 4th row Sc-Zn | Gaussian 6-31G* | (6s)(6sp4s)[1s][1sp][2sp][3sp][4sp]: 666-31G(d) | 49 | 29 |
|               | GAMESS NDFUNC=0 | (6s)(6sp4s)[1s][1sp][2sp][3sp][4sp]: 666-31G(d) | 49 | 29 |
| Ga-Kr         | Gaussian 6-31G* | (14s1p5d)[6s4p1d]: 666-31G(d) | 77 | 24 |
|               | GAMESS NDFUNC=0 | (14s1p5d)[6s4p1d]: 666-31G(d) | 77 | 24 |

a GBASIS=N31 and NGAUSS=6 for all input setting with GAMESS.

b (primitive GTO)/[CGTO]: Pople's expression.

c Superscript "d" means a d-type orbital included in a valence orbital, and **bold** text indicates the polarization function (see text).

d nsp has the same exponents and different coefficients for s-type and p-type CGTO.

A Cartesian basis set (6d, 10f) is used.

### 2 VERIFYING PARAMETERS FOR 6-31G AND 6-31G*

#### 2.1 General remarks

In this section, we compare Gaussian and GAMESS with regard to the CGTO parameter values of 6-31G and 6-31G*. We refer to the codes’ manuals and the numerical values in the log files actually output by executing the two codes. In the Gaussian and GAMESS manuals, the descriptions of the basis function are summarized in the sections titled “Basis Sets” [16] and “Section 4 Further Information” [17], respectively.

#### 2.2 Origin of 6-31G name and CGTO structure

The inner K shell of the second period element is expressed by six primitive GTOs, which are contracted into one CGTO. The valence L shell is expressed by four primitive GTOs, which are divided into three GTOs and one GTO. These two groups are used as CGTOs. The name 6-31G comes from these contractions. In other words, when 6-31G was developed, only the species containing second-period elements were targeted in the calculation. However, in the basis sets for the third- and fourth-period elements, which have M and N shells, the designation 6-31G is largely irrelevant to the CGTO structure. Table 1 shows CGTO structures in various elements. For example, (4s1p)[2s1p] for H and He means that four s-type GTOs and one p-type GTO (bold text indicates the polarization function) are contracted to two s-type CGTOs and one p-type CGTO. For another example, (6s)(4sp1d)[1s][1sp][2sp][3sp][4sp][2d] for Li-Ne means that six s-type GTOs for K-shell is contracted to one s-type CGTO, and two s-type GTOs and one d-type CGTO (the polarization function) are contracted to two s-type CGTOs, two p-type CGTOs and one d-type CGTO. The CGTO structure in each period row is explained in detail below.

#### 2.3 First and second period elements: H-Ne

As seen in Table 1, Gaussian and GAMESS have the same CGTO structures and assign the same CGTO parameter values for nine elements within the first- and the second-period elements;
H-Ne. The Gaussian website lists 10 papers for 6-31G [5–14] and the oldest one is written by Ditchfield et al. in 1971 [5]. However, the paper does not refer to 6-31G, because the 6-31G was not developed yet. So it describes 4-31G parameters of C, N, O, F and 31G parameters of H. When 6-31G is set in the latest version of Gaussian and GAMESS, the value of 31G from this paper is used for H. On the other hand, for Li, B, and Be, the values listed in Table 1 from Dill and Popele’s paper [18] are applied in both codes. However, this paper is not included in the above 10 papers listed on the Gaussian site [16] but referred to in the GAMESS manual [17]. For C, N, O, and F, the parameters value listed in the paper by Hehre et al. in 1972 [6] are used in Gaussian and GAMESS. Descriptions of the rare gas elements He and Ne cannot be found in the papers listed on the Gaussian site, though the GAMESS manual [17] states that the descriptions about the elements are “unpublished, copied out of GAUSSIAN 82.” As a result, Gaussian and GAMESS have used the same parameters. Consequently, Gaussian and GAMESS assign the same CGTO parameter values for the first- and second-period elements H-Ne.

2.4 Third-period elements: Na-Ar

For third-period elements, both Gaussian and GAMESS have the same CGTO structures, which are (6s)(6sp)(4sp1d)/[1s][1sp][2sp1d] for 6-31G*. And they use the same CGTO parameter values come from Francl et al. paper in 1982 [10] for Na, Mg, Al, and Si. However, for S, Ga, GAMESS uses different CGTO values from those of Gaussian [19]. The GAMESS manual [17] includes the following remark: “Note that the built in 6-31G basis for Si is not that given by Pople in reference 22 (ref. 10 in this paper). The Gordon basis gives a better wavefunction, for a ROHF calculation in full atomic (Kh) symmetry.” That is, the GAMESS manual indicates that Gordon basis was determined to yield better values than Pople’s for both of energy and virial. The parameters of the polarization function of Si in Gaussian are also different from those of GAMESS. However, it should be noted that GAMESS is not always superior for all Si-contained molecules to Gaussian, as shown in the results below.

2.5 Fourth-period elements: K-Kr

CGTO’s differences between Gaussian and GAMESS are complicated in fourth-period elements. First, for K, Ca, and Sc-Zn when 6-31G is specified, Gaussian uses CGTO structures and parameters which are derived from Rassolov et al.’s paper published in 1998 [13]. The structures are (6s)(6sp)(6sp)(4sp)/[1s][1sp][1sp][2sp] for K, and (6s)(6sp)(6sp)(4sp4d)/[1s][1sp][1sp2d][2sp] for Sc-Zn, respectively (Table 1). However, 6-31G* is specified for K and Ca, Gaussian uses the polarization function’s exponent values from Blaudeau et al.’s parameters published in 1997 [12], even though Rassolov et al. in 1998 [13] provided the exponent values of polarization function. The Blaudeau’s et al. paper includes both the base function parameters and polarization function’s exponent values, but Gaussian only adopts the polarization function part. On the one hand, for Sc-Zn Gaussian uses the exponent values in Rassolov et al.’s paper in 1998 [13]. The reason for this mixture is unknown.

In GAMESS, for Sc-Zn Rassolov et al.’s parameters in 1998 [13] are used for both the base function and polarization function as in Gaussian, but for K and Ca, GAMES uses Rassolov et al’s newer parameter set in 2001 [14]. Regarding this difference, the GAMESS manual states, “Note that reference 27 (ref. 14 in this paper) renames basis sets published earlier as ‘6-31G*’ in references 25 and 32. GAMESS was changed to use the 6-31G* basis sets from reference 27 for K, Ca, and Ga-Kr in September 2006. Sc-Zn remain those of ref. 21” (ref. 13 in this paper). The difference between the Rassolov et al.’s first parameter set and the newer set is that the latter includes two CGTOs with d-type orbitals as base functions, not polarization functions. All s-type and p-type CGTOs have the exactly same structures and parameters. Therefore, as shown in Table 1, GAMESS implicitly includes two d-type CGTOs containing four GTOs ((4d)/(2d)) when the calculation is performed without setting polarization functions for K and Ca. Naturally, GAMESS represents the wave function more accurately than Gaussian because GAMESS uses more basis sets than Gaussian. If GAMESS is set to add a polarization function (NDFUNC = 1) for K and Ca, one more d-type orbital is added, and a total of three d-type CGTOs are used i.e., (4sp4d1d)/(2sp2d1d).

Next, for Ga-Kr Gaussian uses the values listed in Binning et al.’s parameter sets [11]. This basis has structure of (14s11p5d)/[6s4p1d], which is different from the 6–31 structure. All s-orbital and p-orbital primitive GTOs have different exponents. Note that the coefficient of the primitive GTO output to the Gaussian log file uniformly scales the values listed in Binning et al.’s paper [11], so care must be taken when comparing the two. On the other hand, GAMESS uses all CGTO structures and parameters from Rassolov et al.’s newer parameter set in 2001 [14]. In conclusion, both program codes use completely different basis sets for Ga-Kr.

3 Calculation conditions and results

3.1 Calculation conditions

The following molecules are used in the calculation: H2, Be, N2, Ne, NaH, MgH2, AlH3, SiH4, PH3, H2S, Cl2, Ar, SiH4, SiF4, SiCl4, Si(H2)4, SiH2OH, Si(OH)4, including a first-, second-, or third-period element, in addition to K2, CaH, ScF3, TiCl4, VOCI3, Cr(CO)6, MnH, Fe(CO)5, CoF3, Ni(CO)4, CuF, ZnH, GaH, GeH4, AsH3, SeH2, Br2, and KrF2 containing a fourth-period element. First, the molecular structures were optimized by MOPAC/PM3. Then, structural optimization was performed for all the molecules by Gaussian (Gaussian 16: ES64L-G16RevA.03 25-Dec-2016) and GAMESS (VERSION = 20 APR 2017 (R1)). The basis set was specified as 6-31G** (GBASIS = N31 NGAUSS = 6 NDFUNC = 1 in GAMESS setting) for H2, 6-31G* (GBASIS = N31 NGAUSS = 6 NDFUNC = 1 in GAMESS setting) for molecules including a second-, third-, or fourth-period element, and 6-31G (GBASIS = N31 NGAUSS = 6 in GAMESS setting) for molecules including Si or a fourth-period element. The initial coordinates are given in Cartesian coordinates, singlet molecules are handled by RHF, and multiplet molecules are handled by UHF. In addition, “opt = very tight” was set for Gaussian as an option for the structural optimization. Note that in GAMESS d-type and f-type GTOs always have Cartesian form (6d, 10f). On the other hand, in Gaussian, the form is automatically selected depending on the basis set. For example, in the case of 6-31G, the d-type orbital is in Cartesian form (6d) and...
the f-type orbital is in pure form \((7f)\). Therefore, the user should be careful when comparing the results of Gaussian and GAMESS. To unify the handling of f-type orbital with the Cartesian basis in this study, we set an optional parameter 10f in Gaussian. For all other calculation conditions, the default settings were used for both codes.

### 3.2 First, second, and third period elements: H-Ar

| Molecule | Code | Input Setting | SCF Energy | \(\Delta E / \%\) | Length | \(\Delta Length / \%\) |
|----------|------|---------------|------------|-----------------|--------|---------------------|
| 1st row  |      |               |            |                 |        |                     |
| H\(_2\)  | Gaussian | 6-31G**        | −1.131333588 | 0.0000         | 0.7326 | −0.0011            |
|          | GAMESS  | NPFUNC=1       | −1.131333588 | 0.0000         | 0.7326 | −0.0011            |
| Be       | Gaussian | 6-31G*         | −14.566944381 | 0.0000  | −        | −                  |
|          | GAMESS  | NDFUNC=1       | −14.566944381 | 0.0000  | −        | −                  |
| N\(_2\)  | Gaussian | 6-31G*         | −108.943949471 | 0.0000  | 1.0784  | 0.0000             |
|          | GAMESS  | NDFUNC=1       | −108.943949471 | 0.0000  | 1.0784  | 0.0000             |
| Ne       | Gaussian | 6-31G*         | −128.474406520 | 0.0000  | −        | −                  |
|          | GAMESS  | NDFUNC=1       | −128.474406520 | 0.0000  | −        | −                  |
| NaH      | Gaussian | 6-31G*         | −162.372451652 | 0.0000  | 1.9144  | −0.0106            |
|          | GAMESS  | NDFUNC=1       | −162.372451649 | 0.0000  | 1.9142  | −0.0106            |
| MgH\(_2\)| Gaussian | 6-31G*         | −200.715570043 | 0.0000  | 1.7176  | 0.0144             |
|          | GAMESS  | NDFUNC=1       | −200.715570052 | 0.0000  | 1.7178  | 0.0144             |
| AlH\(_3\)| Gaussian | 6-31G*         | −243.616255403 | 0.0000  | 1.5840  | 0.0018             |
|          | GAMESS  | NDFUNC=1       | −243.616255403 | 0.0000  | 1.5840  | 0.0018             |
| SiH\(_4\)| Gaussian | 6-31G*         | −291.225134321 | 0.0002  | 1.4753  | 0.3628             |
|          | GAMESS  | NDFUNC=1       | −291.224611365 | 0.0002  | 1.4806  | 0.3628             |
| PH\(_3\)| Gaussian | 6-31G*         | −342.447958883 | 0.0000  | 1.4029  | 0.0003             |
|          | GAMESS  | NDFUNC=1       | −342.447958875 | 0.0000  | 1.4029  | 0.0003             |
| H\(_2\)S | Gaussian | 6-31G*         | −398.667322858 | 0.0000  | 1.3264  | 0.0008             |
|          | GAMESS  | NDFUNC=1       | −398.667322858 | 0.0000  | 1.3264  | 0.0008             |
| Cl\(_2\)| Gaussian | 6-31G*         | −918.912817034 | 0.0000  | 1.9898  | −0.0029            |
|          | GAMESS  | NDFUNC=1       | −918.912817000 | 0.0000  | 1.9897  | −0.0029            |
| Ar       | Gaussian | 6-31G*         | −526.773744921 | 0.0000  | −        | −                  |
|          | GAMESS  | NDFUNC=1       | −526.773744921 | 0.0000  | −        | −                  |

\(a\) GBASIS=N31 and NGAUSS=6 for all input setting with GAMESS.

\(b\) \(\Delta E = \frac{[(\text{GAMESS})-(\text{Gaussian})]}{(\text{Gaussian})}\).

\(c\) \(\Delta Length = \frac{[(\text{GAMESS})-(\text{Gaussian})]}{(\text{Gaussian})}\).

Table 2. Comparison between results obtained by using Gaussian and GAMESS with 6-31G* basis sets for H-Ar. The units of energy and length are a.u. and Å, respectively.

3.2 First, second, and third period elements: H-Ar

Table 2 shows the input settings and the calculation results for molecules containing a first, second, and third period element. In all the molecules except SiH\(_4\), the total energies obtained with Gaussian and GAMESS agreed well with each other within the calculation error range. The optimized structures obtained with the two codes also agreed with each other within 0.015%. However for SiH\(_4\), the total energies obtained with the two codes were different from each other, so we performed additional calculations on five kinds of molecules containing Si with both 6-31G and 6-31G* under the same conditions. The results are shown in Table 3. The energies obtained with GAMESS were 0.00006–0.00079% lower for 6-31G and 0.00018–0.00106% lower for 6-31G* than those with Gaussian except SiCl\(_4\) for 6-31G*. As described in Section 2.4, the GAMESS manual states that the CGTO parameters used for Si in GAMESS are improved from the original one in Gaussian. However, in our calculations, the original Gaussian parameters gave lower energies except in one case, so the GAMESS parameters have not been improved. Meanwhile, the energy difference between the two codes was at most 0.00106%. The difference in interatomic distance between the optimized structures obtained with the two codes was very small (< 0.01Å).

### 3.3 Fourth-period elements: K-Kr

Table 4 shows the input settings and the calculation results of the molecules containing a fourth-period element. The energy differences \(\Delta E\) are from −0.0001 to −0.0023% for K\(_2\) and CaH. GAMESS gives lower energies than Gaussian. As shown in Table 1, GAMESS uses more basis set and the wave function is represented well.

Next, for molecules containing Sc-Zn except CoF\(_3\), all the calculation results obtained with Gaussian and GAMESS were the same for 6-31G and 6-31G* because the basis sets used in the two codes are the same as described in Section 2.4 and Table 1. As for CoF\(_3\), different results were obtained with the two codes for 6-31G and
6-31G* even though the parameters of the given basis set were the same for both. In the optimized structure obtained with Gaussian, three F atoms formed an equilateral triangle, but with GAMESS three F atoms formed an isosceles triangle. The energies of the two were different from each other, and the result using GAMESS had a slightly lower energy in 6-31G and 6-31G* than that of Gaussian.

For Ga-Kr, the results obtained from Gaussian and GAMESS were different because the two codes used different basis sets as shown in Table 5. Gaussian uses Binning et al.'s parameter set [11], which has a different CGTO structure from Rassolov et al.'s in 2001 [14] adopted in GAMESS. The CGTO number used in Gaussian is smaller than that in GAMESS as shown in Table 1. Therefore, the energies obtained with Gaussian for all molecules and complexes including Ga-Kr were 0.089% and 0.086% higher in average in 6-31G and 6-31G*, respectively, than those with GAMESS. The difference in molecular structure ranged from 0.002 to 0.020 Å in bond distance and 0.4° to 2.3° in bond angle. The reproducibility of the experimental values in Gaussian is slightly lower than that in GAMESS.

In this study, we performed calculations using 6-31G and 6-31G* for 36 molecules containing a first- to fourth-period element (H, Be, N, Ne, Na-Kr) with Gaussian and GAMESS and compared the calculation results. We found that up to the third-period elements (H, Be, N, Ne, Na-Ar) except Si, the optimized structure and total energy were the same for both codes. While the results for the fourth-period element Sc-Zn agreed with each other, the two codes yielded different results for K, Ca, and Ga-Kr as a result of differences in the two codes' parameters. Thus, it is crucial to read the manuals and related papers thoroughly before determining the calculation parameters conditions. In addition, when evaluating the results published by other researchers, users should not equate the results of using 6-31G with Gaussian with those using GAMESS. In the case of a large molecule calculation, the number of parameters that make up CGTO increases, making it difficult to verify them. However, this process should not be avoided.

### Table 3. Comparison of SCF energy (in a.u.) for Si compounds between Gaussian and GAMESS.

| Molecule     | Code     | SCF Energy | ΔE / % a |
|--------------|----------|------------|----------|
| (a) 6-31G    |          |            |          |
| SiH₄         | Gaussian | −291.173295916 | 0.00061  |
|              | GAMESS   | −291.172164084 |          |
| SiF₄         | Gaussian | −686.733707300 | 0.00079  |
|              | GAMESS   | −686.728308072 |          |
| SiCl₄        | Gaussian | −2126.870504330 | 0.00006  |
|              | GAMESS   | −2126.869152257 |          |
| Si(CH₃)₄     | Gaussian | −447.316724328 | 0.00047  |
|              | GAMESS   | −447.314613828 |          |
| SiH₂O        | Gaussian | −366.04353785  | 0.00056  |
|              | GAMESS   | −366.041483974 |          |
| Si(OH)₄      | Gaussian | −590.705379975 | 0.00037  |
|              | GAMESS   | −590.703195272 |          |
| (b) 6-31G*   |          |            |          |
| SiH₄         | Gaussian | −291.225134321 | 0.00018  |
|              | GAMESS   | −291.224611290 |          |
| SiF₄         | Gaussian | −686.949843700 | 0.00096  |
|              | GAMESS   | −686.943219231 |          |
| SiCl₄        | Gaussian | −2127.046879770 | −0.00011 |
|              | GAMESS   | −2127.049121153 |          |
| Si(CH₂)₄     | Gaussian | −447.413554900 | 0.00059  |
|              | GAMESS   | −447.410925267 |          |
| SiH₂O        | Gaussian | −366.130395900 | 0.00054  |
|              | GAMESS   | −366.128436415 |          |
| Si(OH)₄      | Gaussian | −590.891687800 | 0.00106  |
|              | GAMESS   | −590.885420587 |          |

ΔE = [(GAMESS)-(Gaussian)]/(Gaussian).
Table 4. Comparison between results obtained by using Gaussian and GAMESS with 6-31G and 6-31G* basis sets for K-Zn. The units of energy and length are a.u. and Å, respectively.

| Molecule | Code | Input Setting | M | SCF Energy | ΔE / % | Length | Δ | Length (Expt.) |
|----------|------|---------------|---|------------|--------|--------|---|----------------|
| K₂       | Gaussian | 6–31G  | 1  | -1198.232384430 | -0.0002 | 4.1920 | 0.0079 | 3.9051 |
|          | GAMESS | NDFUNC=0    |    | -1198.235335151 |        | 4.1999 |          |        |
|          | Gaussian | 6–31G* | 1  | -1198.2338199910 | -0.0001 | 4.2031 | -0.0010 |        |
|          | GAMESS | NDFUNC=1    |    | -1198.235468452 |        | 4.2021 |          |        |
| CaH      | Gaussian | 6–31G  | 2  | -677.243153651  | 0.0023  | 2.1676 | -0.1184 | 2.0025 |
|          | GAMESS | NDFUNC=0    |    | -677.258865954  |        | 2.0492 |          |        |
|          | Gaussian | 6–31G* | 2  | -677.250513665  | -0.0014 | 2.1240 | -0.0658 |        |
|          | GAMESS | NDFUNC=1    |    | -677.260043581  |        | 2.0582 |          |        |
| ScF₃     | Gaussian | 6–31G  | 1  | -1058.247031010 | 0.0000  | 1.8590 | 0.0000 | (no data) |
|          | GAMESS | NDFUNC=0    |    | -1058.247032260 |        | 1.8590 |          |        |
|          | Gaussian | 6–31G* | 1  | -1058.297280220 | 0.0000  | 1.8370 | 0.0000 |          |
|          | GAMESS | NDFUNC=1    |    | -1058.297281572 |        | 1.8370 |          |        |
| TiCl₄    | Gaussian | NDFUNC=0   | 1  | -2686.435456190 | 0.0000  | 2.2013 | 0.0009 | 2.170  |
|          | Gaussian | 6–31G  | 1  | -2686.435457539 | 0.0000  | 2.2022 |          |        |
|          | Gaussian | 6–31G* | 1  | -2686.512799320 | 0.0000  | 2.1734 | 0.0003 |        |
|          | GAMESS | NDFUNC=1    |    | -2686.512799518 |        | 2.1737 |          |        |
| VOCl₃    | Gaussian | NDFUNC=0   | 1  | -2396.052641560 | 0.0000  | (VO)=1.515 (VCl)=2.162 | 0.003 | (VO)=1.570 (VCl)=2.142 |
|          | Gaussian | 6–31G  | 1  | -2396.052641722 | 0.0000  | (VO)=1.483 (VCl)=2.140 | 0.007 |          |
|          | Gaussian | 6–31G* | 1  | -2396.163941380 | 0.0000  | (VO)=1.490 (VCl)=2.138 | -0.002 |          |
| Cr(CO)₆  | Gaussian | 6–31G  | 1  | -1719.14648060  | 0.0000  | (CrC)=1.968 (CO)=1.137 | 0.000 | (CrC)=1.92 (CO)=1.16 |
|          | Gaussian | 6–31G* | 1  | -1719.552456180 | 0.0000  | (CrC)=1.987 (CO)=1.119 | 0.000 |          |
|          | GAMESS | NDFUNC=0    |    | -1719.146448015 |        | (CrC)=1.968 (CO)=1.137 | 0.000 |          |
|          | GAMESS | NDFUNC=1    |    | -1719.552426580 |        | (CrC)=1.987 (C−O)=1.119 | 0.000 |          |
| MnH      | Gaussian | 6–31G  | 7  | -1150.265262840 | 0.0000  | 1.7888 | 0.00 | 1.731  |
|          | Gaussian | 6–31G* | 7  | -1150.269449100 | 0.0000  | 1.7888 | 0.00 |          |
### Table 4. (continued)

| Molecule     | Code   | Input Setting | M | SCF Energy | ΔE / % | Length (Expt.) | Δ | Length (Expt.) |
|--------------|--------|---------------|---|------------|--------|----------------|---|----------------|
| **Fe(CO)₅** | [3Dh]  | Gaussian      | 1 | -1825.431516880 | 0.0000 | (FeC)ₐₓ=2.052 (FeC)ₑᵧ=1.829 (CO)=1.134 | 0.000 | 0.000 |
|              |        | GAMESS NDFUNC=0 | 1 | -1825.431516939 | 0.0000 | (FeC)ₐₓ=2.052 (FeC)ₑᵧ=1.829 (CO)=1.134 | 0.000 | 0.000 |
|              |        | Gaussian      | 6–31G | -1825.783473950 | 0.0000 | (FeC)ₐₓ=2.035 (FeC)ₑᵧ=1.859 (CO)=1.117 | 0.000 | 0.000 |
|              |        | GAMESS NDFUNC=1 | 1 | -1825.783474002 | 0.0000 | (FeC)ₐₓ=2.035 (FeC)ₑᵧ=1.859 (CO)=1.117 | 0.000 | 0.000 |
|              |        | Gaussian      | 6–31G | -1679.275683260 | -0.0046 | (NiC)=1.850 (CO)=1.134 | 1.666 | 0.044 |
|              |        | GAMESS NDFUNC=0 | 1 | -1679.353732361 | 0.0000 | (NiC)=1.850 (CO)=1.134 | 1.71, 1.75 | 0.084 |
|              |        | Gaussian      | 6–31G* | -1679.352372880 | -0.0040 | (NiC)=1.886 (CO)=1.117 | 1.722, 1.693 | 0.052 |
|              |        | GAMESS NDFUNC=1 | 1 | -1679.420675189 | 0.0000 | (NiC)=1.886 (CO)=1.117 | 1.722, 1.693 | 0.052 |
| **CoF₃**     |        | Gaussian      | 6–31G | -1957.178142860 | 0.0000 | (NiC)=1.838 (CO)=1.141 | 1.641 | 0.081 |
|              |        | GAMESS NDFUNC=0 | 1 | -1957.178142479 | 0.0000 | (NiC)=1.838 (CO)=1.141 | 1.722, 1.693 | 0.052 |
|              |        | Gaussian      | 6–31G* | -1957.466238010 | 0.0000 | (NiC)=1.866 (CO)=1.117 | 1.722, 1.693 | 0.052 |
|              |        | GAMESS NDFUNC=1 | 1 | -1957.466237789 | 0.0000 | (NiC)=1.866 (CO)=1.117 | 1.722, 1.693 | 0.052 |
| **Ni(CO)₄** |        | Gaussian      | 6–31G | -1738.032855100 | 0.0000 | (NiC)=1.838 (CO)=1.141 | 1.641 | 0.081 |
|              |        | GAMESS NDFUNC=0 | 1 | -1738.032855147 | 0.0000 | (NiC)=1.838 (CO)=1.141 | 1.722, 1.693 | 0.052 |
|              |        | Gaussian      | 6–31G* | -1738.048742120 | 0.0000 | (NiC)=1.866 (CO)=1.117 | 1.722, 1.693 | 0.052 |
|              |        | GAMESS NDFUNC=1 | 1 | -1738.048742120 | 0.0000 | (NiC)=1.866 (CO)=1.117 | 1.722, 1.693 | 0.052 |
| **CuF**      |        | Gaussian      | 6–31G | -1778.013187530 | 0.0000 | (NiC)=1.838 (CO)=1.141 | 1.641 | 0.081 |
|              |        | GAMESS NDFUNC=0 | 1 | -1778.013187527 | 0.0000 | (NiC)=1.838 (CO)=1.141 | 1.722, 1.693 | 0.052 |
|              |        | Gaussian      | 6–31G* | -1778.014810230 | 0.0000 | (NiC)=1.866 (CO)=1.117 | 1.722, 1.693 | 0.052 |
|              |        | GAMESS NDFUNC=1 | 1 | -1778.014810231 | 0.0000 | (NiC)=1.866 (CO)=1.117 | 1.722, 1.693 | 0.052 |

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| Molecule     | Code   | Input Setting | M | SCF Energy | ΔE / % | Length (Expt.) | Δ | Length (Expt.) |
|--------------|--------|---------------|---|------------|--------|----------------|---|----------------|
| **ZnH**      |        | Gaussian      | 6–31G | -1738.032855100 | 0.0000 | (NiC)=1.838 (CO)=1.141 | 1.641 | 0.081 |
|              |        | GAMESS NDFUNC=0 | 1 | -1738.032855147 | 0.0000 | (NiC)=1.838 (CO)=1.141 | 1.722, 1.693 | 0.052 |
|              |        | Gaussian      | 6–31G* | -1738.048742120 | 0.0000 | (NiC)=1.866 (CO)=1.117 | 1.722, 1.693 | 0.052 |
|              |        | GAMESS NDFUNC=1 | 1 | -1738.048742120 | 0.0000 | (NiC)=1.866 (CO)=1.117 | 1.722, 1.693 | 0.052 |

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a GBASIS=N31 and NGAUSS=6 for all input setting of GAMESS.
b Multiplicity.
c ΔE = [(GAMESS)-(Gaussian)]/(Gaussian).
d Δ = [(GAMESS)-(Gaussian)]/(Gaussian).
e ref. 14.
f ref. 13.
Table 5. Comparison between results obtained by using Gaussian and GAMESS with 6-31G and 6-31G* basis sets for Ga-Kr. The units of energy, length, and angle are a.u, Å, and degrees, respectively.

| Molecule | Code     | Input Setting | M | SCF Energy  | ΔE / % | Length/Angle | Δ | Length (Expt.) |
|----------|----------|---------------|---|-------------|-------|--------------|---|----------------|
| GaH      | Gaussian | 6–31G        | 1 | -1921.709263540 | -0.0914 | 1.676        |   | 0.017          | 1.663 |
|          | GAMESS   | NDFUNC=0     | 1 | -1923.466230414 | -0.0908 | 1.674        |   | 0.008          |
|          | Gaussian | 6–31G*       | 1 | -1921.771684660 | -0.0914 | 1.674        |   | 0.017          |
|          | GAMESS   | NDFUNC=1     | 1 | -1923.517238939 | -0.0908 | 1.682        |   | 0.008          |
| GeH₄     | Gaussian | 6–31G        | 1 | -2075.406674100 | -0.0919 | 1.531        |   | 0.004          | 1.514 |
|          | GAMESS   | NDFUNC=0     | 1 | -2077.314578279 | -0.0919 | 1.535        |   | 0.002          |
|          | Gaussian | 6–31G*       | 1 | -2075.541283840 | -0.0886 | 1.535        |   | 0.002          |
|          | GAMESS   | NDFUNC=1     | 1 | -2077.380408954 | -0.0886 | 1.537        |   | 0.002          |
| AsH₃     | [C₃v]   | Gaussian     | 6–31G | -2233.506370560 | -0.0918 | 1.507        |   | 0.008          | 2.3 |
|          |          | GAMESS       | NDFUNC=0 | -2235.557434790 | -0.0918 | 1.515        |   | 0.007          | 2.3 |
|          | Gaussian | 6–31G*       | 1 | -2233.704565870 | -0.0862 | 1.507        |   | 0.001          | 0.7 |
|          | GAMESS   | NDFUNC=1     | 1 | -2235.630113727 | -0.0862 | 1.512        |   | 0.001          | 0.7 |
| SeH₂     | Gaussian | 6–31G        | 1 | -2398.505037250 | -0.0883 | 1.453        |   | 0.013          | 0.4 |
|          | GAMESS   | NDFUNC=0     | 1 | -2400.624092548 | -0.0883 | 1.466        |   | 0.008          | 0.4 |
|          | Gaussian | 6–31G*       | 1 | -2398.726324320 | -0.0820 | 1.453        |   | 0.008          | 0.4 |
|          | GAMESS   | NDFUNC=1     | 1 | -2400.693870763 | -0.0820 | 1.466        |   | 0.008          | 0.4 |
| Br₂      | Gaussian | 6–31G        | 1 | -5139.496613650 | -0.0891 | 2.426        |   | 0.020          | 2.281 |
|          | GAMESS   | NDFUNC=0     | 1 | -5144.076275856 | -0.0891 | 2.406        |   | 0.020          |
|          | Gaussian | 6–31G*       | 1 | -5139.764659470 | -0.0862 | 2.286        |   | 0.004          | 2.281 |
|          | GAMESS   | NDFUNC=1     | 1 | -5144.196853695 | -0.0862 | 2.286        |   | 0.004          |
| KrF₂     | Gaussian | 6–31G        | 1 | -2947.710656110 | -0.0834 | 1.923        |   | 0.020          | 1.875 |
|          | GAMESS   | NDFUNC=0     | 1 | -2950.170025401 | -0.0834 | 1.903        |   | 0.020          |
|          | Gaussian | 6–31G*       | 1 | -2947.846883530 | -0.0826 | 1.834        |   | 0.018          |
|          | GAMESS   | NDFUNC=1     | 1 | -2950.281145831 | -0.0826 | 1.816        |   | 0.018          |

a GBASIS=N31 and NGAUSS=6 for all GAMESS input settings.
b Multiplicity.
c ΔE = [(GAMESS)-(Gaussian)]/(Gaussian).
d Δ = [(GAMESS)-(Gaussian)]/(Gaussian).
e ref. 15.
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