High-level thermochemistry for the octasulfur ring: A converged coupled cluster perspective for a challenging second-row system

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Sulfur clusters are challenging targets for high-level ab initio procedures. The heat of formation of the most common and energetically stable S₈ allotrope (α-sulfur) has not been the subject of a high-level ab initio investigation. We apply the Weizmann-n computational thermochemistry protocols to the S₈ sulfur cluster. We show that calculating the heat of formation with sub-chemical accuracy requires accurate treatment of post-CCSD(T), core-valence, scalar relativistic, and zero-point vibrational energy contributions. At the relativistic, all-electron CCSDT(Q)/CBS level of theory we obtain an enthalpy of formation at 0 K of ΔH₂⁰ = 24.44 kcal mol⁻¹, and at 298 K of ΔH₂₉₈ = 23.51 kcal mol⁻¹. These values suggest that the experimental values from Gurvich (ΔH₂⁰ = 25.1 ± 0.5 kcal mol⁻¹) and JANAF (ΔH₂⁰ = 24.95 ± 0.15 and ΔH₂₉₈ = 24.00 ± 0.15 kcal mol⁻¹) represent overestimations and should be revised downward by 0.5–0.7 kcal mol⁻¹. We also show that computationally economical composite ab initio protocols such as G4, G4(MP2), and CBS-QB3 are unable to achieve chemical accuracy relative to our best CCSDT(Q)/CBS heat of formation for S₈.

Introduction

Sulfur has a large number of known allotropes and small sulfur clusters play a key role in the chemistry of next-generation lithium–sulfur batteries. [1,2,3,4,5,6,7] The chemistry of sulfur clusters has been the subject of many experimental [6,9,10,11,12,13,14] and theoretical [15,16,17,18,19,20,21,22,23,24,25,26,27,28,29,30] studies. The most energetically stable allotrope of sulfur is orthorhombic α-sulfur (hereinafter referred to as simply S₈) and perhaps the most fundamental thermochemical property of S₈ is its heat of formation. The experimental heat of formation of S₈ has been obtained by Guthrie et al. in 1954, [31] they arrived at ΔH₀ = 25.23 ± 0.05 kcal mol⁻¹ and ΔH₂₉₈ = 24.35 kcal mol⁻¹ based on the assumption that the saturated sulfur vapour in the experiments consisted of only S₈ and S₉ structures. In 1989, Gurvich et al. revised the value at 0 K slightly downwards to ΔH₀ = 25.1 ± 0.5 kcal mol⁻¹ based on additional data available in the literature. [32]

Despite the importance of the S₈ cluster, its heat of formation has not been the subject of a high-level theoretical investigation. With the advancement of computer hardware and theoretical methods over the past decade, it is now possible to calculate gas-phase thermochemical data with sub-kcal mol⁻¹ (or even sub-kJ mol⁻¹) accuracy using highly accurate composite ab initio methods (e.g., G2, [33]) ccCA, [34] HEAT, [35,36,37] Wn, [38,39,40] Wn-F12, [41,42] and others. [43,44,45] In particular, composite methods that approximate the FCI/CBS energy (i.e., full configuration interaction at the complete basis set limit) are capable of predicting atomization energies (or their cognates, molecular heats of formation) with sub-kJ mol⁻¹ accuracy. [39,39,46,47] This level of accuracy is often better than that associated with many experimental thermochemical determinations, including many of the experimental values in the NIST Chemistry WebBook (i.e., most experimental values are associated with error bars larger than 1 kJ mol⁻¹, and often larger than 1 kcal mol⁻¹). [48] Thus, highly accurate composite theories are instrumental in obtaining new thermochemical data with benchmark accuracy and in critical assessment of published thermochemical data.

In the present work we calculate the total atomization energy (TAE) of the S₈ cluster by means of W4lite theory. [38] This theory includes both secondary energetic contributions (e.g., core-valence, scalar relativistic, atomic spin-orbit, zero-point vibrational energy, and deviations from the Born–Oppenheimer approximation) and post-CCSD(T) contributions up to quasiperturbative quadruple excitations. We show that the T–(T), (Q), core-valence, scalar relativistic, atomic spin-orbit, and zero-point vibrational energy contributions to the TAE can exceed 1 kcal mol⁻¹ and are needed for determining the TAE with sub-chemical accuracy.

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Computational details

In order to obtain an accurate heat of formation for the orthorhombic S8 ring in D_{4h} symmetry we carried high-level, ab initio calculations with the W2.2 (denoted by W2) and W4lite (denoted by W4L) thermo-chemical protocols. [38, 40] Hereinafter, the cc-pV(n+d)-Z and aug-cc-pV (n+d)-Z correlation-consistent basis sets are denoted by VnZ and AVnZ, respectively, and the notation V(X,Y)Z indicates extrapolation from the VXZ and VYZ basis sets. [49,50,51]

In the W4L procedure, the Hartree–Fock (HF) energy is extrapolated from the AV(5,6)Z basis sets, using the Karton–Martin HF extrapolation formula. [52] The valence CCSD correlation contribution is extrapolated from the same basis sets, where the singlet- and triplet-pair energies are extrapolated separately to the infinite basis set limit, using the E(L) = E_∞ + A_L^2 two-point extrapolation formula, with a = 3 and 5 for the singlet- and triplet-pair energies, respectively. [38,39,40] The (T) valence correlation component (i.e., CCSD(T) – CCSD) is extrapolated from the AVQZ and AVSZ basis sets using the above two-point extrapolation formula with a = 3. The CCSD(T) inner-shell contribution is extrapolated from the core-valence weighted correlation-consistent aug-cc-pwCV{T,Q}Z (APWCv{Q,Z}) basis sets of Peterson and Dunning. [53] The scalar relativistic contribution is obtained from second-order Douglas–Kroll–Hess [54,55] CCSD(T)/AVQZ-DK calculations. [56] The diagonal Born–Oppenheimer corrections (DBOCs) are calculated at the HF/AVTZ level of theory.

The CCSD(T) energy is calculated in conjunction with two truncated versions of the VTZ basis set. Namely, the spd part of the VTZ basis (denoted by VTZ(nd)) and the sp part of the VTZ basis set combined with the d function from the VDZ basis set denoted by VTZ(ndd). [40] These two basis sets are used in conjunction with the VTZ basis set to obtain the CCSDT–CCSD(T) component (denoted by T–(T)) using the two-point extrapolation formulas developed in [ref. 40], which do not depend on the highest angular momentum present in the basis set. The CCSD(T) energy is calculated in conjunction with the VTZ basis set and the (Q)/VDZ component is scaled by 1.1 as recommended in [refs. 38] and [40].

In W2 theory, the HF, CCSD, and (T) contributions are extrapolated from smaller basis sets relative to W4L theory (namely, HF/AV(3,5)Z, CCSD/AVQ(5,5)Z, and T/AV(T,Q)Z) and post-CCSD(T) contributions are neglected altogether, for further details see [38].

The S8 geometry was optimized at the B3LYP, [57,58,59] B3LYP-D3BJ, [60] and CCSD(T) levels in conjunction with several valence and core-valence weighted correlation-consistent basis sets. All the large-scale CCSD(T) calculations were performed using the Molpro program suite, [61,62] the post-CCSD(T) calculations were performed with the MRCC program, [63,64] the DBOC calculations were carried out with the CFOUR program, [65] and DFT geometry optimizations and economical composite ab initio calculations were performed with the Gaussian 16 program. [66]

Results and discussion

The principal conformer of the cyclic S8 molecule is the crown-shaped structure in D_{4h} symmetry. Before proceeding to a detailed discussion of the CCSD(T)/CBS results from W4L theory, it is instructive to examine the level of theory used for optimizing the reference geometry. Whilst the higher-level Wn protocols (e.g., W4L, W4, and above) [38,39] use a CCSD(T)/VQZ reference geometry, lower-level Wn theories (e.g., W1 and W2) prescribe the use of B3LYP/VTZ geometries. [40,41] In this context it is important to note that it was found that the CCSD(T)/VQZ level of theory reproduces CCSD(T)/AV(5,6)Z reference bond distances with a root-mean-square deviation of 0.0015 Å for a large set of 108 organic and inorganic molecules. [67] The bond distance and angle obtained at the B3LYP and CCSD(T) levels are depicted in Table 1. Both the B3LYP/VTZ and B3LYP-D3BJ/VTZ levels of theory overestimate our best CCSD(T)/VQZ bond length, namely, by

| Level of theory | r     | θ     | ΔE_{geom}  |
|---------------|-------|-------|------------|
| B3LYP/VTZ     | 2.0719 | 108,77 | 1.17(In)   |
| B3LYP-D3BJ/VTZ| 2.0669 | 108,20 | 0.60(In)   |
| cc-CCSD(T)/VDZ| 2.0869 | 107,41 | 2.34(In)   |
| fc-CCSD(T)/VTZ| 2.0664 | 107,71 | 0.49'(Out), 0.34'(Out) |
| ae-CCSD(T)/pwCVTZ| 2.0994 | 107,75 |            |
| fc-CCSD(T)/VQZ| 2.0545 | 107,77 |            |

Where a = [CCSD(T)/AV(T,Q)Z//Geometry1] – [CCSD(T)/AV(T,Q)Z/CCSD(T)/Geometry2], b = Geometry1 is specified in the first column, geometry2 is fc-CCSD(T)/VQZ. c = Geometry1 is specified in the first column, geometry2 is ae-CCSD(T)/pwCVTZ.

0.017 and 0.012 Å, respectively. These results are consistent with recent observations that the B3LYP/VTZ level of theory tends to overestimate S–S bond distances relative to CCSD(T)/AV(5,6)Z reference values in small sulfur containing molecules such as S2, S2O, and S2H. [68]

We can estimate the effect of using a B3LYP geometry rather than a CCSD(T)/VQZ geometry at the CCSD(T)/AV(T,Q)Z level of theory, i.e., by comparing the CCSD(T)/AV(T,Q)Z//B3LYP/VTZ and CCSD(T)/AV(T,Q)Z//CCSD(T)/VQZ energies. Using a B3LYP geometry rather than a CCSD(T)/VQZ geometry affects the CCSD(T)/AV(T,Q)Z energy by as much as 1.2 (B3LYP/VTZ) and 0.6 (B3LYP-D3BJ/VTZ) kcal mol⁻¹.

Moving to the CCSD(T) geometries, the CCSD(T)/VDZ level of theory significantly overestimates the CCSD(T)/VQZ bond length by 0.032 Å. This difference in geometry affects the CCSD(T)/AV(T,Q)Z energy by a staggering amount of 2.3 (!!) kcal mol⁻¹. This deviation in the S–S bond distance goes down to 0.011 Å at the CCSD(T)/VTZ level of theory. Nevertheless, the CCSD(T)/VTZ reference geometry still leads to a deviation in the CCSD(T)/AV(T,Q)Z energy by 0.5 kcal mol⁻¹ relative to the CCSD(T)/VQZ geometry. The above results illustrate the problems associated with using DFT geometries or CCSD(T) geometries optimized with a double-ζ or even a triple-ζ basis set for a system containing many second-row atoms.

The above results raise the question of the effect of inner-shell correlation on the S8 geometry. It has been shown that inclusion of inner-shell correlation in CCSD(T) geometry optimizations can affect bond distances of small second-row compounds by up to several milli-angstroms. [39,53,69,70,71,72,73,74] The effect of these small geometric changes on the resulting total atomization energy (or heat of formation) has been examined in detail in [39] and [75]. It has been found that the effect of the reference geometry is largely confined to the CCSD(T) component and can affect the final total atomization energy by up to about 0.1 kcal mol⁻¹. Whilst we are unable to optimize the geometry of S8 with all electrons correlated (apart from the 1 s deep-core orbitals) at the CCSD(T)/PWCVQZ level of theory, we can examine the geometry effect in conjunction with the PWCVTZ basis set. Using core-valence correlated CCSD(T)/PWCVDZ reference geometry reduces the S–S bond distance by 0.007 Å relative to the frozen-core CCSD(T)/VTZ bond distance (Table 1). This geometry change affects the CCSD(T)/AV(T,Q)Z energy by an appreciable amount of 0.34 kcal mol⁻¹. It is expected that the geometry effect of correlating the core-electrons will become smaller when moving to a quadruple-ζ basis set.
Table 2
Component breakdown of the W2 and W4L total atomization energy for S₈ at the bottom of the well (TAE₀) and at 0 K (TAE₀) (in kcal mol⁻¹).

| Component | W2 | Component | W4L |
|-----------|----|-----------|-----|
| HF/AV(Q,S)Z | 253.80 | HF/AV(S,6)Z | 254.12 |
| CCSD/AV(Q,S)Z | 225.43 | CCSD/AV(S,6)Z | 224.54 |
| (T)/AV(T,Q)Z | 38.18 | (T)/AV(T,Q)Z | 38.60 |
| N/A | N/A | T-(T)/VTZ(no2d) | -2.99 |
| N/A | N/A | (Q)/VDZ | 2.89 |
| Cv² | 1.88 | Cv² | 1.88 |
| Rel.⁹ | -1.52 | Rel.⁹ | -1.52 |
| SO⁴ | -4.48 | SO⁴ | -4.48 |
| DBOC⁸ | 0.02 | DBOC⁸ | 0.02 |
| N/A | N/A | N/A | 0.09 |
| ∆Egeom⁶ | 0.34 | ∆Egeom⁶ | 0.34 |
| TAE₆ | 513.66 | TAE₆ | 513.45 |
| ZPE | 7.77 | ZPE | 7.77 |
| TAE₀⁴ | 505.89 | TAE₀⁴ | 505.67 |

* Calculated from the VDZ and VTZ(no2d) basis sets. *CCSD(T) core-valence correction extrapolated from the APWCV(T,Q)Z basis sets. *CCSD(T)/AVQZ-DK scalar relativistic correction. *First-order atomic spin-orbit correction. *HF/AVTZ diagonal Born-Oppenheimer correction. *Difference between the MOLPRO and ACES II definitions of the valence ROCCSD(T); one-half of this contribution is added to the final TAE as discussed in the appendix of reference 38. *Effect of correlating the core-valence electrons in the CCSD(T) geometry optimization on the CCSD(T)/CBS energy (see text and Table 1). *Vibrationless, relativistic, all-electron TAE at the CCSD(T)/CBS (from W2 theory) and CCSD(T)/CBS (from W4 theory) levels of theory. *Scaled CCSD(T)/VTZ harmonic frequencies scaled by a scaling factor of 0.9868 taken for elemental sulfur and a B3LYP-D3BJ/AVTZ molecular enthalpy function for S₈; we obtain ∆H₂⁹₈ values of 23.30 (W2) and 23.51 (W4L) kcal mol⁻¹. *Our best W4L value at 0 K (ΔH₂⁹₈ = 24.44 kcal mol⁻¹) suggests that the experimental values from the JANAF tables (ΔH₂⁹₈ = 24.95 ± 0.15), [80,81] Guthrie et al. [31] (ΔH₂⁹₈ = 25.23 ± 0.05), and Gurvich et al. [32] (ΔH₂⁹₈ = 25.1 ± 0.5 kcal mol⁻¹) should be revised downward by 0.5–0.8 kcal mol⁻¹.

The above results demonstrate that, due to error cancelation between various components, the final heat of formation from W2 theory is in good agreement with that obtained from the computationally more intensive W4L theory. In particular, the difference between the two values amounts to just 0.22 kcal mol⁻¹. It is therefore of interest to examine the performance of more approximate composite ab initio procedures for the heat of formation of S₈ in this context it should be pointed out that recent high-level ab initio studies found that the calculation of the total atomization energies of small sulfur clusters (e.g., S₃ and S₄) is a major challenge for high-level composite ab initio methods. [82,83] We consider the following composite ab initio procedures: G4, [84] G4(MP2), [85] G4(MP2)-6X, [86] G3, [87] G3(MP2), [88] G3B3, [89] G3(MP2)B3, [89] and CBS-QB3. [90,91] To enable a more meaningful analysis, apart from S₈, we also include S₃ and S₄ in our error statistics. The TAE₀ reference values are taken from W4L theory for S₈ and from W4L theory for the smaller molecules. [46] Table 3 lists the individual deviations and mean absolute deviations (MADs) for the approximate composite ab initio procedures. Inspections of these results reveals that, consistent with results for other systems containing many second-row atoms, [92] the Gn(MP2)-type procedures outperform the Gn-type procedures. In particular, both G3(MP2) and G3(MP2)B3 attain MADs of 0.9 and 1.0 kcal mol⁻¹, respectively, and G4(MP2)-6X theory clocks in at a slightly higher MAD of 1.2 kcal mol⁻¹. It is noteworthy that the largest deviations for these three methods do not exceed 2.4 kcal mol⁻¹, and therefore they are recommended for the calculation of enthalpies of formation of larger sulfur compounds. The G4 method shows relatively poor performance (MAD = 1.9 kcal mol⁻¹) at a higher computational cost and is therefore not recommended. The other composite ab initio procedures considered give MADs ranging between 2.3 (CBS-QB3) and 4.9 (G3) kcal mol⁻¹. It should be pointed out that MADs reported in Table 3 translate into much larger 95% confidence intervals for the Gn and CBS procedures. In particular, the conversion factors between MADs and 95% confidence intervals range between 2.5–3.5 depending on sample size and distribution [93].
Deviations and mean absolute deviations (MADs) from W4 and W4L total atomization energies (TAE) values for popular G4 and CBS composite ab initio procedures (kcal mol$^{-1}$).

|          | G3(MP2)   | G3(MP2)B3 | G4(MP2)   | G4(MP2)-6X | G3       | G3B3     | G4       | CBS-QB3   |
|----------|-----------|-----------|-----------|------------|----------|----------|----------|-----------|
| S$_8$    | -0.6      | -0.4      | -0.2      | 1.8        | -1.9     | -2.1     | -1.5     | 0.7       |
| S$_4$    | 0.1       | 0.1       | 2.1       | 1.0        | -3.1     | -3.4     | -1.7     | 0.7       |
| S$_3$    | -2.4      | 1.6       | 3.5       | 0.5        | -8.2     | -3.9     | 2.2      | 3.0       |
| S$_6$    | -0.4      | -2.1      | 5.1       | 2.7        | -6.4     | -9.6     | -2.4     | 4.9       |
| MAD      | 0.9       | 1.0       | 2.7       | 1.2        | 4.9      | 4.8      | 1.9      | 2.3       |

Conclusions

We re-examine the heat of formation of the S$_8$ allotrope (α-sulfur) using the high-level Weizmann-n computational thermochromophysics protocols. At the relativistic, all-electron CCSDT(Q)/CBS level of theory we obtain heats of formation of Δ$H_0 = 24.44$ and Δ$H^\circ = 23.51$ kcal mol$^{-1}$. The theoretical Δ$H^\circ$ value suggests that the experimental values by Gurvich (25.1 ± 0.5 kcal mol$^{-1}$) and from the JANAF tables (24.95 ± 0.15 kcal mol$^{-1}$) should be revised downward by 0.5–0.7 kcal mol$^{-1}$. We also examine the ability of computationally economical G3 and CBS composite ab initio procedures to obtain the heats of formation of sulfur compounds (S$_8$, S$_6$, S$_4$, and S$_3$). We find that the G3(MP2), G3(MP2)B3, and G4(MP2)-6X methods attain MADs of 0.9, 1.0, and 1.2 kcal mol$^{-1}$, respectively. However, the computationally more demanding G4, G3B3, and G3 theories gives relatively poor performance with MADs of 1.9, 4.8, and 4.9 kcal mol$^{-1}$, respectively.

Author credit

Amir Karton: Conceptualization, Methodology, Software, Data curation, Investigation, Writing, Reviewing, and Editing.

Supplementary data: Optimized geometries for all the levels of theory considered in Table 1 (Table S1).

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Supplementary materials

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[59] P.J. Stephens, F.J. Devlin, G.F. Chabatowski, M.J. Frisch, J. Phys. Chem. 98 (1994) 11623.
[60] S. Grimme, S. Hrlich, L. Gogriek, J. Comput. Chem. 32 (2011) 1456.
[61] H.-J. Werner, P.J. Knowles, G. Knizia, F.R. Manby, M. Schutz, P. Celani, T. Korona, R. Lindh, A. Mitrushenkov, G. Rauhut, K.R. Shamosanudar, T.B. Adler, R.D. Amos, A. Berndtsson, A. Berndtsson, M.J.O. Deegan, A.J. Dobbs, F. Eckert, E. Goll, C. Hampel, A. Hesselmann, G. Hetzer, T. Herzen, G. Jansen, K. Koppl, V. Liu, A.W. Lloyd, R.A. Mata, A.J. May, S.J. McNicholas, W. Meyer, M.E. Mura, A. Nickla, D.P. O’Neill, P. Palmieri, D. Pitzer, M. Reifer, T. Shiozaki, H. Stoll, A.J. Stone, T. Thorsteinsson, M. Wang, MOLPRO is a package of ab initio programs; available at: http://www.molpro.net.
[62] H.-J. Werner, P.J. Knowles, G. Knizia, F.R. Manby, M. Schutz, WIREs Comput. Mol. Sci. 2 (2012) 242.
[63] M. Kallay, Z. Rolik, J. Csontos, P. Nagy, G. Samu, D. Mester, I. Ladjanszki, L. Szegedy, B. Ladoczki, K. Petrov, M. Farkas, B. Hegely. MRCC: a quantum chemical program suite. See also: http://www.mrcc.hu.
[64] Z. Rolik, L. Szegedy, I. Ladjanszki, B. Ladoczki, M. Kallay, J. Chem. Phys. 139 (2013), 094105.
[65] J.F. Stanton, J. Gaus, M.E. Hardling, P.G. Szalay with contributions from A. A. Auer, R.J. Bartlett, U. Benedikt, C. Berger, D.E. Bernholdt, Y.J. Bomble, L. Cheng, O. Christiansen, M. Heckert, O. Heun, C. Huber, T.-C. Jagau, D. Jonsson, J. Jueliis, K. Klein, W.J. Lauderdale, D.A. Matthews, T. Metzroth, L.A. Mack, D.P. O’Neill, D.R. Price, E. Prochnow, C. Puzzarini, K. Ruud, F. Schiffmann, W. Schwalbach, C. Simmons, S. Stopenkowicz, A. Tajiti, J. Vazquez, F. Wang, J. D. Watts and the integral packages MOLECULE (J. Almlof, P. R. Taylor), PROPS (P. R. Taylor), ABACUS (T. Helgaker, H. J. Aa. Jensen, P. Jørgensen, J. Olsen), and ECP routines by A. V. Mita, C. van Wullen. CFOUR, a Quantum Chemical Program Package; For the current version, see http://www.cfour.de.
[66] M.J. Frisch, G.W. Trucks, H.B. Schlegel, G.E. Scuseria, M.A. Robb, J.R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G.A. Petersson, et al. Gaussian 16, Revision B.01; Gaussian, Inc.: Wallingford CT, 2016.
[67] P.R. Spackman, D. Jayatilaka, A. Karton, J. Chem. Phys. 145 (2016), 104101.
[68] A. Karton, P.R. Spackman, J. Comput. Chem. 42 (2021) 1590.
[69] J.M.L. Martin, P.R. Taylor, Chem. Phys. Lett. 225 (1994) 473.
[70] J.M.L. Martin, Chem. Phys. Lett. 232 (1995) 343.
[71] J.M.L. Martin, P.R. Taylor, Chem. Phys. Lett. 248 (1996) 336.
[72] J.M.L. Martin, J. Chem. Phys. 108 (1998) 2791.
[73] K.L. Bak, J. Gaus, P. Jørgensen, O. Olsen, T. Helgaker, J.F. Stanton, J. Chem. Phys. 114 (2001) 6546.
[74] S. Coriani, D. Marchesan, J. Gaus, C. Hättig, T. Helgaker, P. Jørgensen, J. Chem. Phys. 123 (2005), 184107.
[75] A. Karton, J.M.L. Martin, Mol. Phys. 105 (2007) 2499.
[76] M.K. Keshavarz, B. Brauer, J.M.L. Martin, J. Phys. Chem. A 119 (2015) 1701.
[77] P.W.J.M. Frederix, C.-H. Yang, G.C. Groenenboom, D.H. Parker, K. Alnana, C. M. Western, A.J. Orr-Ewing, J. Phys. Chem. A 113 (2009) 14995.
[78] B. Nagy, P. Szakacs, J. Csontos, Z. Rolik, G. Tasi, M. Kallay, J. Chem. Phys. A 115 (2011) 7822.
[79] J.D. Cox, D.D. Wagman, V.A. Medvedev, CODATA Key Values for Thermodynamics, Hemisphere Publishing Corp., New York, 1985.
[80] M.W. Chase, Jr., C.A. Davies, J.R. Downey Jr., D.J. Frurip, R.A. McDonald, A.N. Syverud, JANAF Thermochemical Tables, third ed.; webified version available as NIST Standard Reference Database at http://kinetics.nist.gov/janaf/, 1985.
[81] R.D. Johnson III, Computational Chemistry Comparison and Benchmark Database, Release 21 (August 2020) Standard Reference Database 101, http://ecchdb.nist.gov/, accessed July 2021.
[82] A. Karton, N. Sylvestyes, J.M.L. Martin, J. Comput. Chem. 38 (2017) 2063.
[83] A. Karton, J. Chem. Phys. 149 (2018), 034102.
[84] L.A. Curtis, P.C. Redfern, K. Raghavachari, J. Chem. Phys. 126 (2007), 084108.
[85] L.A. Curtis, P.C. Redfern, K. Raghavachari, J. Chem. Phys. 127 (2007), 124105.
[86] B. Chan, J. Deng, L. Radom, J. Chem. Theory Comput. 7 (2011) 112.
[87] L.A. Curtis, K. Raghavachari, P.C. Redfern, V. Rassolov, J.A. Pople, J. Chem. Phys. 109 (1998) 7764.
[88] L.A. Curtis, P.C. Redfern, K. Raghavachari, V. Rassolov, J.A. Pople, J. Chem. Phys. 110 (1999) 4703.
[89] L.A. Curtis, P.C. Redfern, K. Raghavachari, V. Rassolov, J.A. Pople, J. Chem. Phys. 110 (1999) 2822.
[90] J.W. Ochterski, G.A. Petersson, J. Chem. Phys. 102 (1995) 2598.
[91] A.G. Baboul, L.A. Curtis, P.C. Redfern, K. Raghavachari, J. Chem. Phys. 110 (1999) 7650.
[92] J.A. Montgomery Jr, M.J. Frisch, J.W. Ochterski, G.A. Petersson, J. Chem. Phys. 110 (1999) 2822.
[93] J.W. Ochterski, G.A. Petersson, J.A. Montgomery Jr, J. Chem. Phys. 104 (1996) 2598.
[94] A.A. Kroeger, A. Karton, Struct. Chem. 30 (2019) 1665.
[95] B. Rusic, Int. J. Quantum Chem. 114 (2014) 1097.