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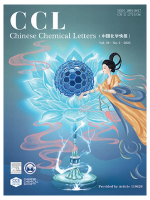

Benchmarking model chemistry composite calculations for vertical ionization potential of molecular systems

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ABSTRACT

In chemical science, the vertical ionization potential (VIP) is a crucial metric for understanding the electronegativity, hardness and softness of chemical material systems as well as the electronic structure and stability of molecules. Ever since the last century, the model chemistry composite methods have witnessed tremendous developments in computing the thermodynamic properties as well as the barrier heights. However, their performance in realm of the vertical electron processes of molecular systems has been rarely explored. In this study, we for the first time benchmarked the model chemistry composite methods (*e.g.*, CBS-QB3, G4 and W1BD) in comparison with the commonly used Koopmans's theorem (KT), electron propagator theory (*e.g.*, OVGF, D2, P3 and P3+) and CCSD(T) methods in calculating the VIP for up to 613 molecular systems with available experimental measurements. The large-scale test calculations strongly showed that the CBS-QB3 model chemistry composite technique can be well recommended to calculate VIP from the perspectives of accuracy, economy and applicability. Notably, the VIP values of up to 7 molecules were identified to have the absolute errors of larger than 0.3 eV at all calculation levels, which have strong hints that their VIP experimental values should be re-investigated.

Cations play a crucial role in various fields, including electron transfer (*i.e.*, redox reactions), interstellar chemistry, catalytic coordination, structural regulation of lithium batteries, stability of solar cells, determination of photoelectric and physicochemical properties of organic light-emitting polymers [1–10]. Additionally, cations are integral to the emerging class of functional materials known as ionic liquids [11]. Moreover, cations have significant impacts on medicine [12], biology [13] and robotics [14]. Cations can usually be expressed by the level of vertical ionization potential, and have attractive applications in the so-called superalkali field, as well as in atomic, molecular and cluster science [15,16]. The vertical ionization potential (VIP) is a crucial parameter that quantifies the energy required to remove an electron from a neutral atom or molecule, resulting in the formation of a cation in the neutral state. This value holds significant importance in various aspects, serving as a key metric for assessing cluster stability, predicting complex stability, redox potentials and evaluating the charge transport capacity of organic compounds [17–19]. Additionally, VIP is a vital indicator utilized for identifying species, determining chemical states and understanding the environmental conditions in which bonding occurs [20,21]. It serves as a fundamental chemical property, playing a pivotal role in assessing Mulliken electronegativity, hardness and softness [22–29]. Undoubtedly, VIP is significant in the chemical sciences [30].

Obviously, accurate determination of VIP is an important task. Experimentally, the two most common types of experiments are (1) photoelectron spectroscopy (PES), in which a molecule is ionized at a fixed ultraviolet wavelength and the kinetic energy of the measured emission electrons is subtracted from the photon energy to calculate IP. Nevertheless, the majority of earlier studies utilized He photoelectron spectroscopy with low energy resolution for the detected electrons, constraining the precision in attributing accurate ionization energy (IE) values [31], but their complexity hinders the study of larger clusters [13]; (2) Photoionization mass spectrometry, in which the generation of +1 molecular ions is monitored during the process of the scanning ultraviolet wavelengths [32]. However, one must note that the above experimental techniques can not directly deduce the structural, electronic and suborbital information, which have to be aided by the quantum chemical calculations.

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Hopefully, with the rapid and continuous development of quantum chemistry methods and computers, theoretical calculations offer a highly efficient means of predicting molecular spectra, states, and VIP. The selection of a reliable calculation method serves as the initial critical step in VIP prediction. It has been demonstrated that by employing appropriate quantum chemistry methods [33], the accuracy of VIP predictions can reach within 0.3 eV, providing robust theoretical evidence for studying molecular stability. Up to now, a series of computational methods have been developed to predict thermochemical properties (*e.g.*, dissociation energies, ionization potentials, electron affinities and proton affinities), such as CCSD(T), G4, P3, D2, OVGF, W1BD, and some of them have also been used for VIPs [34–37]. Among these methods, OVGF (Outer Valence Green's Function, a method based on advanced ab initio wavefunction methods) is frequently used and usually considered to be able to compute time-savingly [38–41]. The electron propagator theory (EPT) approach provides a conceptual basis for accurate calculations of ionization potentials (IPs), single-electron properties and total energies of molecules [42–44]. Unfortunately, the EPT methods are only applicable if the ionization orbital map embodied in Koopman's theorem is still qualitatively valid [45]. Alternatively, CCSD(T) is generally considered to be a highly accurate calculation method, but is rather expensive in computational facilities.

Model chemistry composite algorithms such as CBS-QB3, G4 and W1BD have been found very successful in various fields, being able to accurately predict thermochemical properties. Concerning the computational cost, CBS-QB3 is superior to the latter two ones. Very recently, the application of CBS-QB3 has been shown to perform very well for the vertical detachment energies (VDEs) of molecular species, playing the one-stone-two-birds role to reach the accuracy and economy balance [46]. However, although the good performance of the CBS-QB3 model chemistry composite algorithm has been well demonstrated in VIP prediction of atomic species, it has been rarely applied to compute the molecular species' VIP [47–49]. One should note that the process of VDE (anion → neutral) and VIP (neutral → cation) have quite different charge states, which would influence the energy changes of the process significantly. Therefore, it is highly desirable to test the feasibility of the model chemistry composite algorithms (here we considered CBS-QB3, G4 and W1BD) in calculating VIP in the large-scale benchmarking studies. The commonly used CCSD(T) and EPT (*e.g.*, OVGF, D2, P3, P3+) methods were also compared. Our VIP benchmark test covers a total of 613 molecules, whose experimental values are all available. After comparing and weighing the accuracy, economy and applicability, the CBS-QB3 method, which is the most cost-effective and leading among the methods in terms of mean absolute errors (MAEs), root mean square error (RMSE) and computational speed, is highly recommended for calculating VIP.

The formula for calculating VIPs in this work is as follows:

$$\mathrm{VIP} = E(\text{cation at optimized neutral geometry}) - E(\text{neutral}) \tag{1}$$

E(cation at optimized neutral geometry) and *E*(neutral) represent the energy of the cation (optimized structure based on neutral) and the neutral molecule, respectively, including zero-point energy correction. Three model chemistry composite methods, *i.e.*, CBS-QB3 [50], G4 [51] and W1BD [52] were employed. These methods integrate a series of single-point energy calculations based on geometries optimized using DFT methods (specifically, B3LYP/6–311G(2d,d,p), B3LYP/6–31G(2df,p) and B3LYP/cc-pV(T + d)Z, respectively). Additionally, singlet-point energy calculations based on the commonly used CCSD(T) (coupled with aug-cc-pVTZ) and EPT (*e.g.*, OVGF, D2, P3, P3+) [53–56] (coupled with 6–311++G(3df,3pd)) methods were carried out at the B3LYP/6–311++G(d,p) geometries. All calculations are performed using the Gaussian 16 package [57].

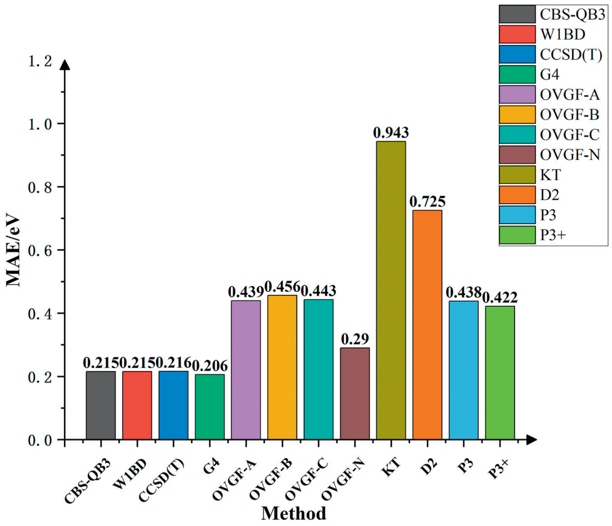

Fig. 1. Mean absolute errors (MAEs) (eV) for 613 VIP (CBS-QB3, G4, KT, EPT) and 265 VIP (W1BD, CCSD(T)).

In this work, 613 neutral molecular systems containing main group elements in rows 1–3 of the periodic table were studied. Their experimental VIP values range from 7.43 eV to 16.5 eV. The experimental vertical ionization potentials used are taken from the NIST Basic Atomic Spectroscopy Database. The detailed geometries of all the molecular systems and the theoretical values of VIP calculated at all computational levels (CBS-QB3, G4, W1BD, CCSD(T), KT and EPT methods (OVGF, D2, P3, P3+) as well as the experimental values of the systems are listed in Tables S1–S4 (Supporting information). Note that due to the high computational cost, only 265 molecular systems were tested at the W1BD and CCSD(T) levels, whereas the 613 systems were considered for all the other levels. The MAEs, RMSE and absolute errors (AEs) were calculated to compare with the reported experimental values. MAEs, RMSE and AEs values are often used to assess the accuracy or reliability of a design method. In addition, the time costs of the computational levels were compared to evaluate the economics of the methodology.

The MAEs are the average of the absolute error. MAEs are used to represent the average difference between the predicted value and the true value (in this case, the experimental value). Therefore, MAEs can be a good indicator of the accuracy of the test method. As shown in Fig. 1, the MAEs values in descending order were KT (0.912 eV) > D2 (0.594 eV) > P3 (0.401 eV) > OVGF-C (0.381 eV) > OVGF-B (0.373 eV) > P3+ (0.363 eV) > OVGF-A (0.344 eV) > OVGF-N (0.325 eV) > CBS-QB3 (0.235 eV) > CCSD(T) (0.216 eV) > W1BD (0.215 eV) > G4 (0.211 eV). Understandably, the KT method produces the largest MAEs. Among all the methods, the MAEs of the model chemistry composite methods G4 (0.211 eV), CBS-QB3 (0.235 eV), W1BD (0.215 eV) and gold standard method CCSD(T) (0.216 eV) were lower than those of the best-performing EPT method, *i.e.*, OVGF-N (0.325 eV), by 0.114, 0.09, 0.11 and 0.109 eV, respectively. Notably, the MAEs values predicted by CBS-QB3, G4, W1BD and CCSD(T) are closer to each other, and are all smaller than 0.3 eV, whereas the EPT methods showed MAEs larger than 0.3 eV except OVGF-N (0.29 eV). Clearly, in terms of MAEs in VIP calculations, the CBS-QB3, G4, W1BD and CCSD(T) are superior to the other applied methods. Comparisons at the level of 265 systems are presented in Fig. S1 (Supporting information).

The RMSE, which is the square root of the ratio of the square of the deviation of an observation from the true value to the ratio of the number of observations N, is very sensitive to

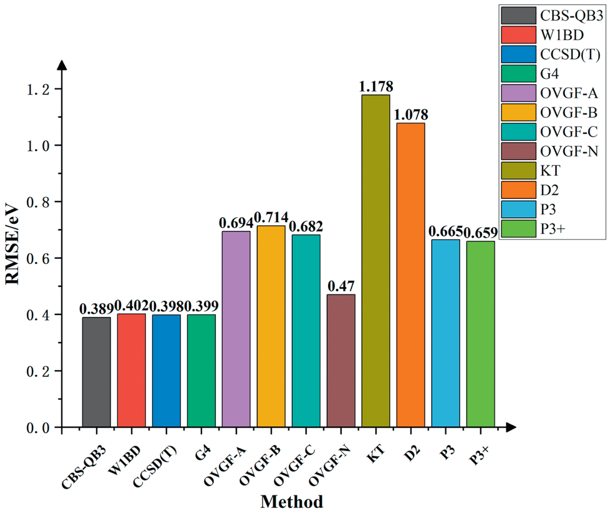

Fig. 2. The root-mean-square deviation (RMSE) values (eV) for 613 VIP (CBS-QB3, G4, KT, EPT) and 265 VIP (W1BD, CCSD(T)).

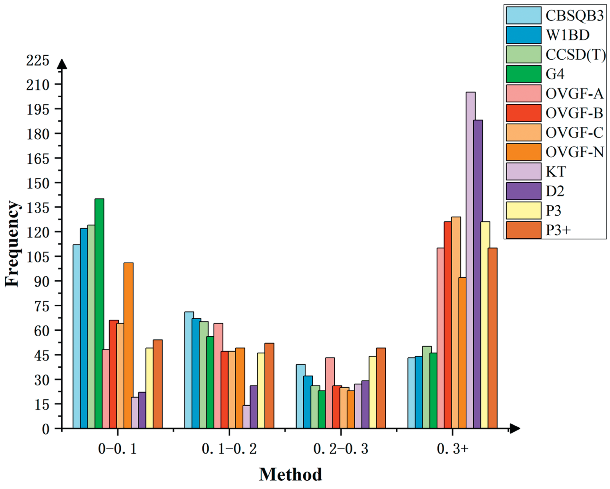

Fig. 3. Absolute errors (AEs) (eV) for 265 VIP in 0–0.3 eV (CBS-QB3, G4, W1BD, OVGF, CCSD(T), KT, EPT).

large or small errors in a set of measurements. Thus, the RMSE error gives a good indication of the accuracy of the measurement. As shown in Fig. 2, the RMSD values in descending order are KT (1.122 eV) > D2 (0.92 eV) > OVGF-N (0.661 eV) > OVGF-B (0.586 eV) > OVGF-C (0.577 eV) > P3 (0.576 eV) > OVGF-A (0.558 eV) > P3+ (0.555 eV) > W1BD (0.402 eV) > CCSD(T) (0.398 eV) > G4 (0.397 eV) > CBS-QB3 (0.395 eV). Similarly, among all the methods, the model chemistry composite methods CBS-QB3 (0.395 eV), G4 (0.397 eV), W1BD (0.402 eV) and the gold standard method CCSD(T) (0.398 eV) have RMSEs that were lower than the best-performing EPT method P3+ (0.555 eV) by 0.16, 0.158, 0.153 and 0.157 eV, respectively. It is evident that CBS-QB3, G4, W1BD and CCSD(T) are superior to several other methods in terms of RMSE for calculating VIPs. Comparisons at the level of 265 systems are presented in Fig. S1.

AEs are the absolute magnitude of the deviation of the measured value from the true value. The distribution histogram of the absolute errors (AEs) between theoretical and experimental values at 6 theoretical levels in the range of 0–0.3 eV is shown in Fig. 3. Detailed theoretical, experimental, and AEs values are listed in Supporting information. Within the scope of 0–0.3 eV, AEs distribution order: CBS-QB3 (83.7%) > W1BD (83.3%) > G4 (82.6%) > CCSD(T) (81.1%) > OVGF-N (65.2%) > OVGF-A (58.4%) = P3+ (58.4%) > OVGF-B (52.4%) = P3 (52.4%) > OVGF-C (51.3%) > D2 (29.0%) > KT (22.0%). This distribution once again proves that among the applied methods, CBS-QB3, W1BD, G4 and CCSD(T) are more reliable than others in computing VIPs.

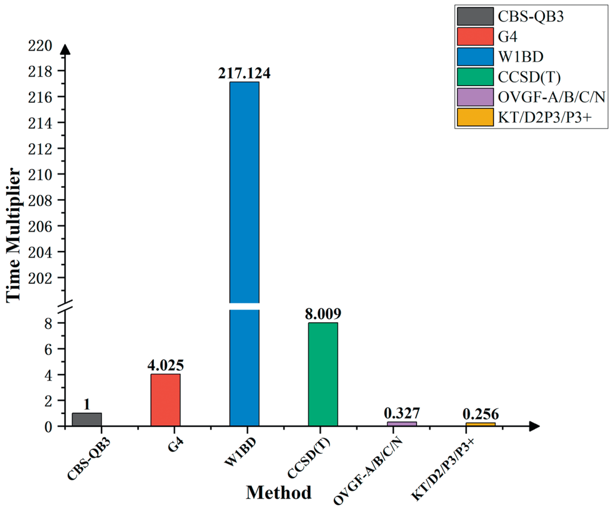

Fig. 4. Comparison of time-consumption (average time) of 7 systems, H_2O, CO_2, OCS, CH_3CClO, $C_2H_2Cl_2$, $CFCl_3$ and CCl_4 at various levels.

To evaluate the computational economics of different theoretical approaches, we selected 7 molecular systems of different sizes, namely H_2O, CO_2, OCS, CH_3CClO, $C_2H_2Cl_2$, $CFCl_3$ and CCl_4, to be tested on the same computational server (Gaussian16, 48 GB memory, 64 core machine). Using CPU time of CBS-QB3 as reference 1, the time multiples of the 6 levels are plotted in Fig. 4. Here, for simplicity, we compare the average time of the seven neutral systems. In these systems, the average time multiplier of W1BD, CCSD(T), G4, OVGF and P3+ is 217.124, 8.009, 4.025, 0.327 and 0.332 times of CBS-QB3, respectively. W1BD takes the most time and KT, D2, P3, P3+ take the least time. Therefore, we can say that in computing VIPs, the economy of CBS-QB3 is significantly better than that of W1BD, CCSD(T) and G4, and is closer to OVGF.

The applicability of these methods to various chemical systems needs to be considered. Our large-scale benchmark tests of the 12 methods on up to 613 molecular VIPs showed that the three model chemistry (CBS-QB3, G4 and W1BD) and gold standard CCSD(T) methods all perform much better than the 7 EPT and the KT methods in light of the MAEs, RMSE and AEs criteria. Firstly, as is known, the EPT calculations are fast, and have a low computational complexity. Yet, they might lose validity when the ionization orbital map breaks down. In addition, some EPT studies have reported that unexpectedly large errors can occur though pole strength (PS) values are reasonable [58]. Secondly, despite the accuracy (comparable to CBS-QB3 in the present VIP calculations), the W1BD method (originally designed as a high-precision wave function method) has to face high computational complexity, and consumes very high computational resources. As a result, W1BD can usually be only suitable for smaller systems. The CCSD(T) and G4 methods are also computationally much more expensive than CBS-QB3, though both are much cheaper than W1BD. In all, the model chemistry method, CBS-QB3, appears to have the good virtues of being accurate and economic for computing the molecular VIPs.

Although the model chemistry composite methods have shown great success in predicting the thermochemistry of a large number of systems [59–61], to the best of our knowledge, none of them have been applied to systematically study and benchmark the VIP of molecular systems. In this work, we have tried for the first time to apply the model chemistry composite methods, CBS-QB3, G4 and W1BD, together with the widely used CCSD(T) and EPT methods, to calculations of VIPs (up to 613 molecules) in comparison with the experimental values. Among the CBS-QB3, G4, W1BD and CCSD(T) methods, which have all been shown to be "more accurate" in computing VIP of molecules, CBS-QB3 most worthy of attention and recommendation because of its balanced accuracy and economy.

We are aware that CCSD(T), as the gold standard method, is often used as a benchmark in testing studies of a large number of chemical systems. We strongly suggest that for VIP calculations, the expensive CCSD(T) can be replaced by the accurate and economical CBS-QB3, which can provide benchmark VIP values to aid in the development of cheaper methods (*e.g.*, DFT [62,63] and semiempirical methods [64]) for use in large-size systems.

For the small chemical systems, the predictive accuracy for calculation of ionization potentials and electronic energy spectra should be well realized, and therefore the calculated and experimental data could be very close to each other [65,66]. However, in our work, at all of the applied 12 computational levels, the 7 systems, *i.e.*, BF_2 (difluoroboryl radical), B_2H_4 (diborane (4)), B_2F_4 (diboron tetra-fluoride), CH_2N_2 (3*H*-diazirine), C_5H_6 (1,2,4-pentatriene), C_5H_6 (cyclopropylacetylene), HNO_2 (nitrous acid), encounter the larger AEs between theoretical and experimental values to surpass the thresholds of 0.3 eV (even by as much as 0.5–0.7 eV). Considering the facts that (1) it is now known that due to the restriction of technical resolution, many of the early results could be misleading [67], and (2) many VIP experimental values were obtained a long period of time ago, we appeal that in future, VIP experiments for the 7 systems should be performed for improvement.

Finding a method to perform in a balanced manner between accuracy and economy is always very appealing. While the model chemistry composite methods have been proven very successful in a number of fields, their applications in the realm of molecular VIPs have been largely limited, to our best knowledge. In this work, for the first time, we systematically benchmarked the performances of three model chemistry composite methods, *i.e.*, CBS-QB3, G4 and W1BD, in computing VIPs of a large set of molecules (up to 613), in comparison of the gold standard CCSD(T), KT and a series of EPT methods (OVGF-A/B/C/N, D2, P3, P3+) together with the experimental measurements. Based on the criteria of MAEs, RMSE, AEs and time-consumption, the present work clearly showed that CBS-QB3 is the best choice for computing VIPs to meet the accuracy and economy balance. Besides, we identified 7 systems to possess unusually larger AEs (>0.3 eV) at all applied methods, indicative of a great need to future experimental re-investigation.

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

Supplementary material associated with this article can be found, in the online version, at doi:10.1016/j.cclet.2024.109721.

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