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Ab initio correlated calculations of rare-gas dimer quadrupoles

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This paper reports *ab initio* calculations of rare gas (RG=Kr, Ar, Ne, and He) dimer quadrupoles at the second order of Møller-Plesset perturbation theory (MP2). The study reveals the crucial role of the dispersion contribution to the RG_2 quadrupole in the neighborhood of the equilibrium dimer separation. The magnitude of the dispersion quadrupole is found to be much larger than that predicted by the approximate model of Hunt. As a result, the total MP2 quadrupole moment is significantly smaller than was assumed in virtually all previous related studies. An analytical model for the distance dependence of the RG_2 quadrupole is proposed. The model is based on the effective-electron approach of Jansen, but replaces the original Gaussian approximation to the electron density in an RG atom by an exponential one. The role of the nonadditive contribution in RG_3 quadrupoles is discussed.

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I. INTRODUCTION

Because of the distortion of its electronic structure, a heteronuclear pair of interacting rare gas (RG) atoms has a nonvanishing dipole moment, whereas a homonuclear RG_2 pair develops a quadrupole Q (the RG_2 dipole is forbidden by symmetry). When the two atoms approach one another closely, their electron clouds distort away from one another to reduce overlap, creating a negative (so-called exchange) quadrupole. At long range, the electronic distortion is related to the attractive dispersion forces, which results in positive values of Q. In the vicinity of the stationary point on the RG_2 dimer potential curve, these two opposite contributions become comparable in magnitude and neither of them can be neglected.

In 1962, Jansen [1] introduced the Gaussian effective-electron model for the RG_2 exchange quadrupole. This model approximates all exchange effects by placing on each atom one "effective" electron with a Gaussian charge distribution proportional to $\exp(-\beta^2 s^2)$, where s stands for the nucleus-electron separation and β is the only adjustable model parameter (it depends on the specific type of the interacting atoms). For a pair of atoms at distance R, Jansen obtained the following formula for the exchange quadrupole:

$$Q(R) = -\frac{1}{2}R^2 \frac{\exp(-\beta^2 R^2/2)}{1-\exp(-\beta^2 R^2/2)}. \tag{1}$$

Although the Gaussian description of the electron distribution in an atom is not very accurate, Eq. (1) has become the most popular approximation to the quadrupole moment of RG_2 dimers.

In 1980, Hunt [2] proposed a model relating the long-range quadrupoles of RG_2 dimers to the characteristics of the interacting atoms,

$$Q(R) = \frac{5BC_6}{2\alpha}R^{-6}, \tag{2}$$

where C_6 and α are, respectively, the usual RG_2 dispersion energy coefficient and the RG atomic dipole polarizability. Less trivially, Eq. (2) involves the coefficient B, which gives the energy E of a system quadratic in an applied field F and linear in the field gradient F': $E \propto BF^2F'$ (see the details in Ref. [2]).

The finite induced dipole moment of a pair of dissimilar RG atoms gives rise to far-infrared absorption [3,4] and a pure rotational microwave spectrum [5–7] in rare gas mixtures. However, in pure (homogeneous) RG clusters or fluid, absorption, which must be very small since it has not been observed thus far, can arise only from many-body effects, because the creation of a dipole moment in a binary collision is forbidden by symmetry.

The exchange-quadrupole-induced dipole (EQID) mechanism is conventionally recognized [8] as the dominant contribution to the three-body dipole moment in RG_3 trimers. In the EQID formalism, the RG_2 quadrupole moment induces a dipole moment on the third atom. Guillot *et al.* [9] estimated the absorption in liquid krypton within the framework of the EQID approach. Cooper *et al.* [10] calculated the transition dipole moments for the lowest allowed vibrational transitions of Ar_3. More recently, the EQID formalism was used in Ref. [11] in calculations of far-infrared absorption spectra and permanent dipole moments for neutral argon clusters up to Ar_{110}.

In atomic systems, the exchange quadrupole produces a relatively small contribution (via the EQID mechanism) to nonadditive forces, if compared, for example, with the many-body dispersion effect [12]. However, in a ternary complex with a polar molecule the nonadditive effect is expected to be significant, because the quadrupole generated on the RG_2 pair can interact directly with the permanent molecular dipole moment.

Such argon complexes were studied in a series of theoretical investigations by Hutson and co-workers: Ar_2-HCl [13], Ar_2-DCl [14], Ar_2-HF [15], Ar_2-DF [16], and, more recently, Ar_n-HF (n=2, 3, 4, and 12) [17]. Significant discrepancies were found between the predictions of pairwise-additive potentials and the experimental results for the frequencies of the intermolecular bending bands, which are very sensitive to three-body forces. In all cases, the exchange quadrupole interaction was found to be the only nonadditive term large enough to explain the discrepancies between the pairwise-additive calculations and the experimental data.

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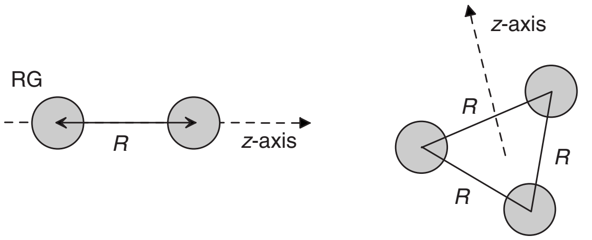

FIG. 1. Choice of the z axis for RG dimer and trimer.

Similar three-body corrections, including an exchange dipole term, are suggested in Ref. [18] to be important also in the NeArHCl trimer. Finally, the attractive interaction between the halide charge and the RG_2 exchange quadrupole is found to be the second most important many-body term (after the induced dipole-induced dipole repulsion) in Ar_n-I^- ($n=2-19$) [19], Ar_n-Br^- ($n=2-9$) [19], Xe_n-I^- ($n=2-14$) [20], and Ar_n-Cl^- ($n=2-15$) [21] complexes.

Thus, the RG_2 quadrupole plays an important role in various physical phenomena. At the same time, there is a lack of reliable *ab initio* investigations of this property. To the best of the author's knowledge, the only published results are those from Ref. [22], where the Ar_2 quadrupole was calculated at the uncorrelated Hartree-Fock (HF) level. Also, in Refs. [10] and [17] the value of the parameter β in Eq. (1) for the Ar_2 dimer was obtained by fitting to HF calculations.

The main goal of the present research is to report the correlated, close to complete basis set limit values of the Kr_2, Ar_2, Ne_2, and He_2 quadrupoles as functions of interatomic separation. In addition, the paper compares the approximate models of Jansen and Hunt with the results of *ab initio* calculations.

II. METHODS

For a system of charges e_i located at $\mathbf{r}_i$, we define the symmetric traceless quadrupole tensor as

$$\mathcal{Q}_{\alpha\beta} = 3\sum_i e_i r_{i\alpha} r_{i\beta} - \sum_i e_i r_i^2 \delta_{\alpha\beta}, \tag{3}$$

where $\alpha,\beta=x,y,z$ and $\delta_{\alpha\beta}$ is the Kronecker symbol. In the case of the RG_2 dimer and the conventional choice of the z axis along the interatomic distance R (see Fig. 1), the quadrupole tensor becomes diagonal,

$$\mathcal{Q} = \mathrm{diag}\{-Q,-Q,2Q\}. \tag{4}$$

Such a definition of the scalar quadrupole Q is equivalent to that of Jansen [1]: $Q=\Sigma_i e_i(z_i^2-x_i^2)$. The same expression (4) also holds for the equilateral configuration of the RG_3 trimer when the z axis is chosen to be normal to the atomic plane (see Fig. 1).

The correlated *ab initio* calculations reported in the present study rely on the second order of the Møller-Plesset perturbation theory (MP2) in the frozen-core approximation. All the quadrupole values were corrected for the basis set superposition error (BSSE) by means of the conventional counterpoise procedure,

$$(\mathrm{BSSE}) = Q(\mathrm{RG}\text{-}X) + Q(X\text{-}\mathrm{RG}), \tag{5}$$

where Q(RG-X) denotes the spurious quadrupole generated on the RG atom in the presence of the ghost orbitals of its partner. All the calculations were performed with the PC GAMESS [23] version of the GAMESS (U.S.) package [24].

The augmented correlation consistent aug-cc-pV5Z (or briefly a5Z) basis set of quintuple quality was used to describe the RG atoms. Unfortunately, the employed version of GAMESS does not support basis functions of higher than g symmetry. Hence the h functions were omitted from the a5Z basis for Kr, Ar, and Ne. Moreover, in the case of Kr and Ar, it was found to be necessary to remove, respectively, two and one of the most diffuse g functions in order to achieve stability in the MP2 density matrix calculations. Additionally, the counterpoise-corrected quadrupole moments were also calculated with the smaller aug-cc-pVQZ (or briefly aQZ) basis set without omission of any basis functions. The difference

$$\Delta Q = Q(\mathrm{aQZ}) - Q(\mathrm{a5Z}) \tag{6}$$

is used as a supplementary quantity indicating (together with the BSSE for the a5Z basis) the closeness of the a5Z values to the complete basis set limit.

III. RESULTS

A. *Ab initio* data

Quadrupole moments for homogeneous Kr, Ar, Ne, and He dimers calculated at both the HF/a5Z and MP2/a5Z levels are summarized in Table I.

In complete agreement with both Eq. (1) and the results of previous uncorrelated calculations [22] of the Ar_2 quadrupole, the present HF data are found to be negative in the whole range of interatomic separation R (the marginally positive $\sim 10^{-5}$ a.u. values for Ar_2 at very large R should be considered as an indication of a slight numerical instability). At the same time, the alternating character of the $Q(R)$ dependence calculated at the MP2 level stems from the (expected) dispersion contribution. Note that for all the RG dimers the MP2 quadrupole goes through zero within ~ 1 a.u. of R_e (the equilibrium value of R at which the dimer energy achieves its minimum). This indicates that in the equilibrium region, which is of primary importance from the experimental point of view, there exists a strong competition between the exchange repulsion and the dispersion attraction of the electron shells of the interacting atoms. Significant mutual cancellation of these two opposite effects results in a remarkable difference between the HF and MP2 values of Q. For example, in the case of the Ar_2 dimer, the MP2 quadrupole at $R=7$ a.u. is found to be just one-half of the HF result.

At short separations $R<R_e$ for all the RG_2 dimers, the BSSE is found to be relatively small, just a few percent or less of the value of Q. However, at long ranges it has a very long tail, which extends much further than that of the counterpoise-corrected HF quadrupole. In the case of Ne_2 at $R>9$ a.u., the BSSE at the MP2 level even exceeds in magnitude the corresponding Q value, resulting in the wrong sign

TABLE I. Quadrupole moments Q (in 10^{-3} a.u.) of RG_2 dimers as functions of interatomic separation R (a.u.). The values of R closest to the equilibrium separations are shown in bold, together with the corresponding values of Q.

	HF			MP2		
R	Q	BSSE	ΔQ	Q	BSSE	ΔQ
			Kr_2			
5.0	−1296.85	−0.06	0.81	−1235.01	8.70	13.33
5.5	−767.88	−0.10	1.72	−700.84	6.40	12.23
6.0	−445.99	−0.16	1.25	−381.70	4.62	9.58
6.5	−251.97	−0.19	0.62	−194.39	3.67	6.74
7.0	−138.05	−0.20	0.32	−88.99	2.47	4.38
7.5	**−73.33**	−0.20	0.28	**−33.23**	1.49	2.67
8.0	−37.83	−0.20	0.31	−6.13	1.06	1.51
8.5	−19.00	−0.20	0.33	5.43	0.72	0.77
9.0	−9.32	−0.19	0.29	9.17	0.38	0.30
9.5	−4.48	−0.18	0.20	9.36	0.15	0.03
10.0	−2.11	−0.18	0.10	8.19	0.07	−0.11
11.0	−0.45	−0.15	0.00	5.30	0.01	−0.16
12.0	−0.09	−0.11	−0.02	3.22	−0.05	−0.14
13.0	−0.02	−0.10	−0.02	1.96	−0.08	−0.10
14.0	0.00	−0.10	−0.01	1.24	−0.10	−0.06
15.0	0.00	−0.09	−0.01	0.80	−0.09	−0.04
			Ar_2			
5.0	−514.35	−0.42	−0.18	−475.47	1.69	3.88
5.5	−286.89	−0.38	0.09	−247.60	1.31	0.95
6.0	−154.82	−0.38	0.24	−121.91	0.61	1.99
6.5	−80.55	−0.48	0.28	−52.26	0.51	0.16
7.0	**−40.46**	−0.49	0.27	**−18.60**	−0.07	0.26
7.5	−19.68	−0.45	0.23	−3.05	−0.12	−0.04
8.0	−9.31	−0.43	0.16	3.05	−0.12	−0.21
8.5	−4.30	−0.47	0.09	4.85	−0.46	−0.39
9.0	−1.95	−0.49	0.05	4.68	−0.54	−0.32
9.5	−0.87	−0.45	0.03	3.93	−0.88	−0.23
10.0	−0.38	−0.36	0.02	3.07	−0.48	−0.13
11.0	−0.06	−0.29	0.02	1.84	−0.38	−0.08
12.0	0.00	−0.29	0.01	1.09	−0.37	−0.05
13.0	0.01	−0.26	0.00	0.67	−0.32	−0.03
14.0	0.01	−0.20	0.00	0.42	−0.25	−0.02
15.0	0.00	−0.16	0.00	0.27	−0.17	−0.02
			Ne_2			
4.0	−93.98	0.29	0.33	−104.88	0.27	−0.52
4.5	−43.05	0.22	0.34	−47.15	0.10	−0.38
5.0	−18.66	0.17	0.25	−19.48	0.01	−0.33
5.5	−7.69	0.16	0.08	−7.19	−0.01	−0.36
6.0	**−3.04**	0.18	0.01	**−2.19**	0.00	−0.30
6.5	−1.16	0.06	0.02	−0.37	−0.12	−0.18
7.0	−0.43	−0.01	0.05	0.20	−0.16	−0.07
7.5	−0.16	0.00	0.06	0.31	−0.11	−0.01
8.0	−0.06	0.00	0.05	0.27	−0.10	0.01
8.5	−0.02	−0.01	0.04	0.21	−0.11	0.01
9.0	−0.01	−0.02	0.03	0.16	−0.12	0.01
9.5	0.00	−0.03	0.02	0.12	−0.14	0.00
10.0	0.00	−0.03	0.01	0.09	−0.13	0.00
11.0	0.00	−0.04	0.00	0.05	−0.11	0.00
			He_2			
4.0	−30.44	−0.20	−0.06	−28.30	−0.22	−0.35
4.5	−12.87	−0.16	−0.03	−11.19	−0.17	−0.24
5.0	−5.20	−0.14	−0.01	−4.02	−0.15	−0.15
5.5	**−2.02**	−0.12	0.00	**−1.24**	−0.13	−0.09
6.0	−0.76	−0.10	0.00	−0.26	−0.11	−0.05
6.5	−0.28	−0.09	0.00	0.04	−0.10	−0.03
7.0	−0.10	−0.08	0.00	0.11	−0.09	−0.02
7.5	−0.03	−0.05	0.00	0.10	−0.06	−0.01
8.0	−0.01	−0.02	0.00	0.08	−0.02	−0.01

of the uncorrected quadrupole moment. Note also the generally alternating character of the BSSE radial dependence, a finding that is in contrast to the always negative BSSE in the interaction energy. All this demonstrates the advantage of the counterpoise procedure when such a delicate property as the interaction quadrupole is considered.

Judging from the rather small differences between the aQZ and a5Z results (ΔQ columns in Table I), we can conclude that the present results (at both the HF and MP2 levels) are practically converged with respect to the basis set size. It is noteworthy that, as a rule, the absolute values of ΔQ are much smaller than the corresponding BSSE.

B. Approximate models

Figure 2 compares the results of the present *ab initio* calculations against the predictions of the approximate models of Jansen [Eq. (1)] and Hunt [Eq. (2)].

The long-range behavior of the RG_2 quadrupole calculated at the MP2 level is found to obey the R^{-6} law [see Fig. 2(a)] as predicted by Hunt's model. However, the latter is found to underestimate the dispersion effect by ~35% in the case of Ar_2 and ~25% for He_2. Such disagreement is not too surprising, keeping in mind that the model of Hunt systematically underestimates, by a factor of 5, the mean-square dipole moments for the ground state of the RG atoms [2].

Jansen's model, despite its incorrect Gaussian asymptotic behavior (instead of an exponential tail), is found to reproduce reasonably well the HF (free from the dispersion effect) values of both the Kr_2 and Ar_2 quadrupoles [Fig. 2(b)], although somewhat overestimating the magnitude of Q_{HF} in the neighborhood of the equilibrium ($7\ \text{a.u.} < R < 8\ \text{a.u.}$).

At the same time, Eq. (1), having only one adjustable parameter, does not provide enough flexibility to fit the full radial dependence of the exchange quadrupole for the lightest He_2 and Ne_2 dimers. As seen in Fig. 2(c), the best (our) fit made in the framework of the model of Jansen fails to reproduce the slope of the *ab initio* curve and overestimates (underestimates) the value of Q_{HF} by a factor of ~3 at the left (right) end of the considered interval of R.

We applied the same effective-electron approach of Jansen, but replacing the original Gaussian approximation to the electron density in an RG atom by an exponential one. In this case, all the integrals in Eq. (7) of Ref. [1] are amenable to evaluation, although the complete analog of the (rather elegant) Eq. (1) is cumbersome and impractical to use. Instead, it is reasonable to retain only the asymptotically leading term which, after addition of the dispersion component, results in the following approximation to the quadrupole:

$$Q(R) = -aR^6 e^{-R/\rho} + bR^{-6}, \tag{7}$$

where a, ρ, and b are adjustable parameters, whose specific values are summarized in Table II.

The values of the parameter b were derived from the long-range part of the $Q_{\mathrm{DS}} \equiv Q_{\mathrm{MP2}} - Q_{\mathrm{HF}}$ curves; cf. Fig. 2(a). Note that at $R \lesssim R_e$ the value of Q_{DS} deviates significantly from the R^{-6} law and even becomes negative for the Ne_2 dimer (see Table I). The remaining parameters, a and ρ, were then fitted to the difference $Q_{\mathrm{MP2}} - bR^{-6}$ (not the Q_{HF} values). Thus, at

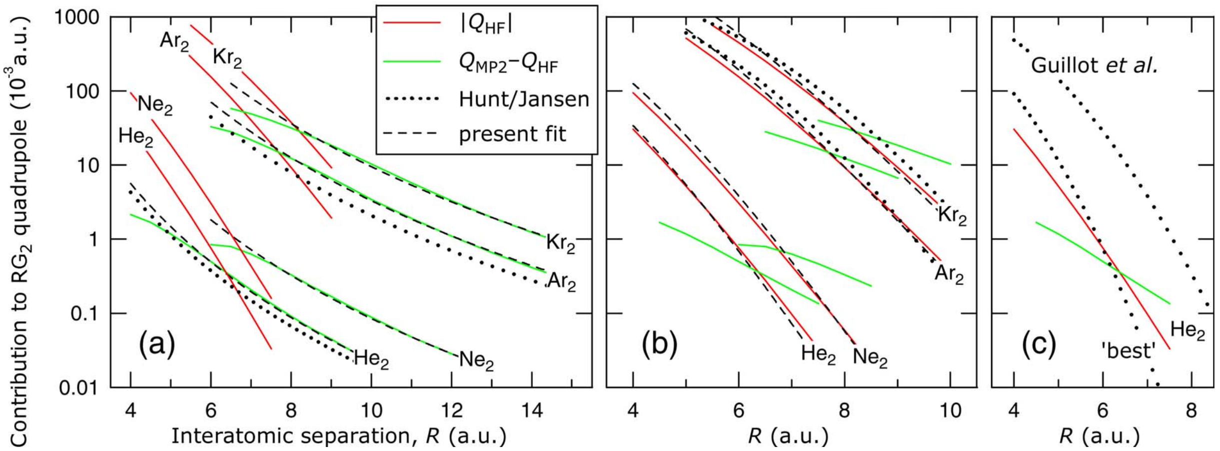

FIG. 2. (Color online) Comparison of the (a) dispersion $Q_{MP2}-Q_{HF}$ and (b) exchange Q_{HF} contributions to RG$_2$ quadrupole with the predictions of models of Hunt (parameters for Ar and He were taken from Refs. [17] and [2], respectively) and Jansen (parameters for Kr and Ar were taken from Refs. [9] and [17], respectively). Also, the results of the present fit [Eq. (7)] are shown: bR^{-6} and $aR^6e^{-R/\rho}$ in (a) and (b), respectively. (c) compares the He$_2$ exchange quadrupole with the predictions of Jansen's model as parametrized by Guillot *et al.* (Ref. [9]) and in the present work (the "best" curve).

close separations the exchange contribution in Eq. (7) systematically exceeds the Q_{HF} values [see Fig. 2(b)].

The present model (7) is compared against the MP2 quadrupoles in Fig. 3. As seen, the matching is almost perfect, particularly as compared with the combination of Eqs. (1) and (2) used for the Ar$_2$ dimer in Ref. [17]. It is worth noting that near the dimer equilibrium separation the parameters from Ref. [17] result in a strong overestimation of the magnitude of Q: by a factor of 2.3 at $R=7.0$ a.u. and as much as a factor of 5.4 at $R=7.5$ a.u.

It is remarkable that the fitted values of the size parameter ρ agree closely (within 2.5%) with the previously reported [25] electrostatic RG sizes w (cf. Table II). The small (systematic) deviation between the ρ and w values might stem from the difference in the basis sets used: a5Z for the former and aQZ for the latter.

C. Nonadditivity in RG$_3$ trimer quadrupoles

Finally, we touch upon the question of a nonadditive contribution to the quadrupole moments of RG$_3$ trimers, using the example of the equilateral configuration. In the pairwise-additive approximation, as is easy to check, the quadrupole of the trimer is opposite in sign and larger in magnitude by exactly a factor of 3/2 than that of the corresponding dimer. Thus, it is convenient to characterize the nonadditivity by the quantity δ defined as

$$Q_{RG_3} \equiv -1.5Q_{RG_2}(1+\delta). \tag{8}$$

As presented in Fig. 4, the nonadditivity decreases the magnitude of the RG$_3$ quadrupole by several percent. For example, in the vicinity of the equilibrium separation, δ amounts to $\sim$3% for He and Ne and $\sim$7% for Ar and Kr. The unpresented MP2 data were found to be, in general features, similar to those in Fig. 4. At the same time, both the alternating character of the $Q_{MP2}(R)$ dependence and the poorer numerical stability of the MP2 calculations in comparison with the HF approach result in much less regularity in the $\delta_{MP2}(R)$ dependence.

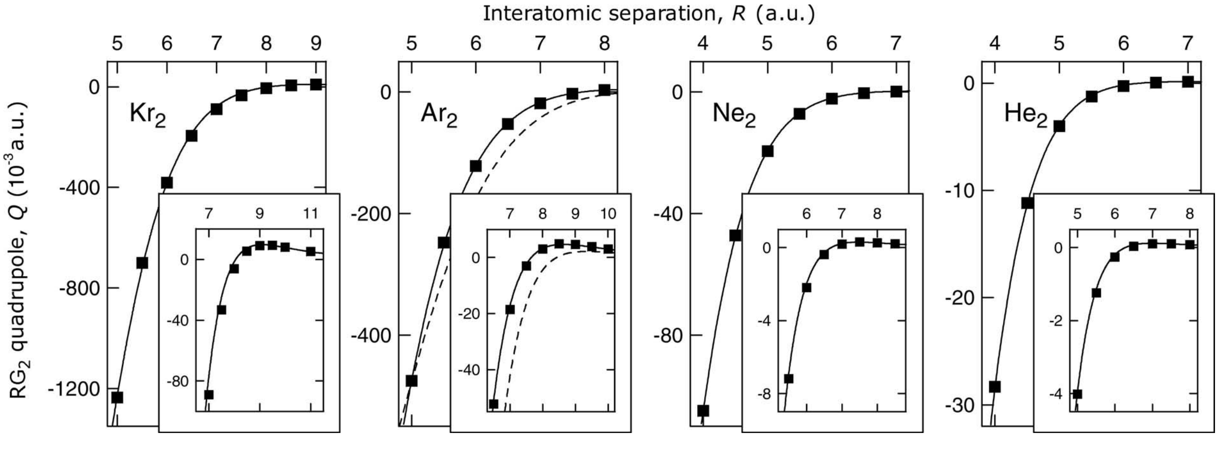

FIG. 3. Comparison of Eq. (7) (solid lines) against the MP2/a5Z values (■) of RG$_2$ quadrupoles. The model for the Ar$_2$ quadrupole used in Ref. [17] is also presented (dashed line).

TABLE II. Fitted parameters in Eq. (7) for RG_2 quadrupoles. Also, for the sake of comparison, electrostatic RG sizes w from Ref. [25] are presented.

RG	a (a.u.)	b (a.u.)	ρ (a.u.)	w (a.u.)
Kr	8.37	9500	0.4475	
Ar	6.19	3300	0.4217	0.4264
Ne	4.32	85	0.3374	0.3460
He	2.67	23	0.3154	0.3229

IV. CONCLUSIONS

The present paper has reported the results of *ab initio* correlated calculations of RG_2 quadrupoles. This study reveals the crucial role of the dispersion contribution to the quadrupole in the neighborhood of the equilibrium dimer separation. The magnitude of the dispersion quadrupole is found to be much larger than that predicted by the (approximate) model of Hunt. As a result, the total quadrupole moment (calculated at the MP2 level of theory) is significantly smaller than it was assumed to be in virtually all previous related studies. This means, for example, that Hutson and co-workers [13–17] have severely overestimated the role of the Ar_2 quadrupole in the three-body effect. Similarly, both the oscillator strengths and permanent dipole moments calculated in Ref. [11] for argon clusters should be reconsidered.

The major source of uncertainty in the reported quadrupoles is the precision of the MP2 approach. As is well known, the post-MP2 correction is crucial for the interaction energy in RG dimers [25]. At the same time, in a recent investigation [26] of RG-Xe dipole moments the difference between coupled cluster singles, doubles, and perturbative triples [CCSD(T)] values and the MP2 results was found to be just a few percent. Thus, we can expect that the CCSD(T) correction to the RG_2 quadrupoles is also small.

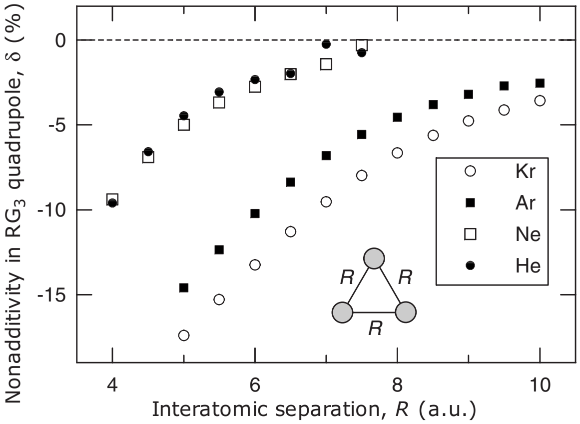

FIG. 4. Nonadditive effect δ [defined by Eq. (8)] in RG_3 quadrupoles calculated at the HF/a5Z level of theory.

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