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ORIGINAL PAPER

A quest for effective polarizability as a function of the radii

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Abstract
Lately we have proposed an atomic polarizability model, viz. $\alpha \propto \left(r^3/Z_{\text{eff}}e^2\right)$, through an empirical approach. As the results obtained using the model were remarkable, we have tried to explore the efficacy of this polarizability model by using four different types of radii for 96 atoms invoking a regression analysis. Further, we have performed a study on molecules by employing additivity property. Although the results are similar in the case of atoms, two of the four radii-based polarizability sets perform better when molecules are considered. In addition, the molecular polarizability is computed for a variety of anaesthetics due to its significance in biochemical interactions. A significant correlation is obtained between the computed and the published data, corroborating the efficacy of polarizability model in the prediction of biological mechanisms. The polarizability model is revealed to be conceptually rigorous even when different types of radii are used, so it can be satisfactorily employed for real-field applications.

Keywords Atomic radius · Theoretical chemistry · Density functional theory (DFT) · Covalent radius · Polarizability

1 Introduction

Evaluation of the polarizability is currently a vigorously expanding field of study. Extensive theoretical, as well as experimental, works are being carried out for its computation in case of atoms, molecules, ions and clusters. By definition, the polarizability is the ease of distortion of an electronic cloud corresponding to a species. Several reviews that have been published on the topic report a wide range of theoretical and experimental approaches for the calculation of polarizabilities [1, 2]. Indeed, the relationship of polarizability to other descriptors has been explored by numerous scientists [3–7]. The effect of polarizability on the nucleus of an atom [8] and the mechanical properties of macro- and nano-dimensional organic cocrystals has been studied, as well [9], and the polarizability has been revealed to be of immense importance in understanding and predicting the nature of chemical–biological interactions [10, 11].

Due to the wide applicability of the polarizability in diverse realms, a polarizability model relying on the mutual effect of the effective atomic nuclear charge (Z_{eff}) and atomic radius (r) was recently proposed by our group [12]. The model is based on an empirical approach and follows all the criteria of a descriptor.

The present work is a quest for assessing the potential of the previously proposed model and exploring its application in molecular polarizability calculations invoking the additivity concept. With an intention of testing the efficacy of the model in different scenarios, we employ different kinds of radii to compute four sets of polarizability. Further, we have tried to study the role of our computed polarizabilities in some biochemical species.

The radius of an atom is a size descriptor. It is a valuable quantity that supports understanding of many physico-chemical properties of different species. It also plays an important role in interpreting various biochemical processes. However, the concept of the radius of an atom is still unclear. Theoretical calculations of atomic and ionic sizes have evolved from an empirical model and have reached up to Self-Consistent Field theory [3, 13–21]. A number of terms, such as the atomic radii, van

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der Waals radii, metallic radii, covalent radii, ionic radii, and absolute radii, and estimation approaches such as empirical, crystallographic, self-consistent field (SCF)-based, orbital-density based, etc., are known to exist for this single property [22–24]. Each of these radii and approaches has some advantages and disadvantages over the others. For instance, covalent radii help in providing information regarding the existence of a chemical bond, but cannot provide a fixed value as it is affected by its surroundings. This radius can be valuable when molecules with different types of bonds, viz. single, double and triple, come into the picture. Similarly, an absolute radius can offer a universal value for each atom, but it may lack in explaining the type of bond in some cases. This radius works best in situations where transferability is highly crucial, such as clusters, nanoparticles, etc. Moreover, an ionic radius keeps changing even if a single electron is gained or lost. Ionic radii are basically useful in understanding the structure of ionic crystals and solvated ions in liquids. An empirical relationship is popular in terms of the minimum requirement for computational resources, whereas SCF has inherent importance in its accurate prediction of atomic and ionic size. Thus, until now, no fixed or universal benchmark for the radius of an atom/ion/molecule has existed. Considering this difficulty, we have tested the validity of our proposed polarizability model for four different kinds of radii.

Numerous studies have utilized chemical reactivity descriptors to explain the mechanisms of chemical–biological interactions [6, 11, 25–34]. One such important descriptor is polarizability. In a study by Agin and others [25], polarizability was used to analyse the potential of various chemicals that hindered action in a frog's muscle. A similar study on frog muscle was performed by Kamlet et al. using several drugs [26]. Hahin and his group studied the effect of alcohols on the nerves of frogs through polarizability [27]. Many phenyl alkane *p*-*ω*-bis(trialkylammonium) compounds were examined by Wien and Mason, who employed polarizability to study their pharmacological activities [28]. Nishimura et al. studied the mechanism of reduction in the action potential in the central nerve cord by means of polarizability [29]. An analysis was made by Tandon et al. to understand the role and the mechanism of polarizability in ligand–substrate biological interactions [11]. It is evident that several biological processes depend on the circulation and dispersal of chemicals within a living organism and such activities are believed to be significantly governed by the polarizability along with some other electronic effects. Thus, we have tried to demonstrate the potential of the polarizability model in providing molecular polarizabilities that can be employed to study electronic interactions in biochemical systems.

2 Method of computation

The polarizability and the radius of an atom, as described above, are important reactivity descriptors [35–38]. Thus, we have used four different sets of radii to explore the efficacy of the polarizability model as proposed by our group previously [12]. Based on the previously proposed model, the polarizability (α) is proportional to the ratio of the cube of atomic radius (r) and the product of effective nuclear charge (Z_{eff}) and the square of electronic charge (e) as follows (Eq. 1),

$$\alpha \propto \left(\frac{r^3}{Z_{\text{eff}}e^2}\right), \tag{1}$$

$$\text{or}\alpha = \left(\frac{r^3}{Z_{\text{eff}}e^2}\right)a + b. \tag{2}$$

Here a and b represent regression parameters. In the present study, we have employed Clementi et al.'s SCF-based radii [39, 40], Desclaux's orbital density-based radii [41], Cordero et al.'s covalent radii [42] and Tandon et al.'s absolute radii [24] to compute the polarizability by using Eq. (2). The reason for selecting these radii is to check the suitability of a variety of radii obtained using diverse methods in the computation of the polarizability.

The polarizability computations are performed for the atoms of 96 elements in the periodic table through a regression approach invoking Eq. (2). For the analysis, the radius and the effective nuclear charge serve as independent variables, whereas polarizability acts as a dependent variable. Reference polarizabilities are obtained from Schwerdtfeger and Nagle's work [43]. Radii are taken from Clementi et al.'s [39, 40], Desclaux's [41], Cordero et al.'s [42] and Tandon et al.'s [24] work while Ghosh and Biswas's effective nuclear charge [15] is used for this purpose. All the radii as mentioned in the report are in units of Å. The procedure involves evaluation of the parameters a and b by using linear regression, performed period-wise, followed by a computation of the atomic polarizability based on the obtained data. The four types of computed polarizabilities are compared with one another and with the Schwerdtfeger and Nagle's [43] polarizabilities in order to test their accuracy and find the most effective amongst all. The relationship of the ionization energy to the polarizability has also been demonstrated by a

number of scientists earlier [7, 23, 43–50]. Accordingly, we have made an attempt to find the correlation between these two properties for each period based on an empirical power relationship [51].

We have also tested the potential of using these polarizabilities for molecules. For this purpose, we have calculated the molecular polarizabilities by using all four computed atomic polarizability values for some simple molecules. The molecular value is calculated employing the property of additivity [52–54] (see Eq. 3). As per the property, "the summation of the polarizabilities of all the isolated atoms present in a system gives an approximate value of the static molecular polarizability (α_m)":

$$\alpha_m \approx \sum_i \alpha_i. \tag{3}$$

The obtained molecular polarizabilities are contrasted against the published theoretical polarizabilities of van Duijnen and Swart [55].

Because polarizability influences the reactivity and the mechanism of various biological molecules, drugs, anaesthetics, etc., as evidenced by the literature [11, 25–29], we have made an effort to study the effect of the computed polarizabilities on some anaesthetics, as well. We have calculated the molecular polarizabilities by using our computed polarizability data based on Desclaux's, Cordero et al.'s and Tandon et al.'s radii, for some anaesthetics that cause nerve inhibition due to their intake leading to an excitability block in a frog's sartorius muscle. In order to verify the validity of the computed values, we performed a comparison with the molecular values published by Tandon et al. [11].

3 Results and discussion

Atomic polarizabilities computed by employing four kinds of radii, viz. Clementi–Raimondi [39] and Clementi et al. radii [40] (α_C), Desclaux radii [41] (α_D), Cordero et al. radii [42] (α_{Co}) and Tandon et al. [24] (α_T), are presented in Table 1 for 96 elements. The magnitude of these polarizabilities is observed to vary from one another; however, such small differences are acceptable. A look at Fig. 1 shows that each polarizability exhibits a similar periodicity trend. This figure further corroborates the fact that the magnitudes of all the values are nearly the same. These results suggest that the model functions suitably for most of the radii when considering atoms. In spite of the radii being calculated through very different approaches and based on different principles, these provide acceptable results for atomic polarizabilities.

We have also correlated all the computed polarizabilities with ionization energy for each period. The empirical power relationships of all the polarizability sets (α_C, α_D, α_{Co} and α_T) to the ionization energy reveal nice correlations ($r^2 > 0.8$) between the descriptors, which suggests the presence of a useful quantitative association between these sets of polarizability and ionization energy.

The efficacy of these polarizabilities is also confirmed for molecules. We have used α_C, α_D, α_{Co} and α_T for calculating the molecular polarizabilities of some simple molecules by invoking the additive property. We observed that the molecular polarizabilities calculated using α_{Co} and α_T present excellent correlations with the corresponding theoretical values. However, molecular data determined using α_C and α_D provide comparatively low correlations with the published theoretical data [55]. The order of decreasing correlation between the theoretical and the computed sets of molecular polarizability is α_{mCo} ($r^2 = 0.9453$) > α_{mT} ($r^2 = 0.8934$) > α_{mC} ($r^2 = 0.7899$) > α_{mD} ($r^2 = 0.7326$). Table 2 lists the theoretical and the calculated molecular polarizabilities for the molecules under study. The molecular polarizability values calculated using α_{Co} and α_T are noted to be more accurate than the values calculated using the other two parameters using the same model. We believe that the variation in the four sets of computed molecular values may be due to the presence of relativistic effect in the polarizability data calculated by Cordero et al. [42] and Tandon et al. radii [24].

The molecular polarizability results are also validated in the case of anaesthetics. Because the polarizability is believed to be associated with the mechanism of anaesthetic action [11], which occurs through an electrically excitable membrane, verifying the results in the case of such molecules is also important. The molecules for the study were selected so that heterogeneity is incorporated in the chemical organization. Table 3 presents the three sets of molecular polarizabilities calculated using the computed Desclaux radii-based polarizability, Cordero et al. radii-based polarizability and Tandon et al. radii-based polarizability along with the theoretical molecular polarizabilities [11] for some anaesthetics. As is evident from the table, the molecular polarizability values for each set are very close to their theoretical counterparts. The correlation plots in Fig. 2 signify an excellent relationship between these computed data and the theoretical data. The same trend is observed again for the theoretical *versus* the computed sets of molecular

Table 1 Atomic polarizabilities for $Z = 1$–96 computed using Clementi–Raimondi [39] and Clementi et al. radii [40] (α_C/Å^3), Desclaux radii [41] (α_D/Å^3), Cordero et al. radii [42] (α_{Co}/Å^3) and Tandon et al. radii [24] (α_T/Å^3)

Elements	α_C	α_D	α_{Co}	α_T	Elements	α_C	α_D	α_{Co}	α_T
H	–	0.667	0.667	0.667	In	7.332	9.819	7.361	8.016
He	–	0.205	0.205	0.205	Sn	6.141	7.649	6.428	5.430
Li	24.365	24.391	24.051	24.242	Sb	5.241	6.574	5.958	4.014
Be	5.520	5.375	6.522	5.935	Te	4.669	5.924	5.496	3.407
B	2.444	2.423	3.109	2.982	I	4.302	5.534	5.259	2.764
C	1.386	1.408	1.705	1.503	Xe	4.045	5.248	5.060	2.340
N	1.073	1.089	1.050	0.878	Cs	62.879	62.634	61.612	61.761
O	0.936	0.962	0.618	0.785	Ba	32.931	31.878	35.035	32.713
F	0.870	0.907	0.201	0.593	La	32.936	34.598	34.961	35.262
Ne	0.839	0.878	0.177	0.515	Ce	28.658	31.511	31.871	31.572
Na	24.612	24.378	24.014	24.434	Pr	25.495	31.117	29.955	29.272
Mg	10.140	9.532	11.786	10.451	Nd	25.321	29.161	28.355	27.708
Al	5.899	8.942	6.457	7.534	Pm	25.299	27.703	27.102	26.601
Si	4.911	5.048	4.486	4.861	Sm	25.365	26.536	26.204	25.781
P	3.968	3.551	3.656	3.495	Eu	25.328	25.635	25.565	25.159
S	3.466	2.866	3.178	3.169	Gd	25.317	23.986	24.846	24.610
Cl	3.153	2.497	2.749	2.693	Tb	25.287	24.253	24.238	24.262
Ar	2.957	2.289	2.777	2.467	Dy	25.283	23.714	23.718	23.936
K	44.249	44.547	42.099	44.101	Ho	25.270	23.250	23.407	23.662
Ca	19.206	19.813	22.077	19.322	Er	25.262	22.877	22.939	23.432
Sc	16.136	16.001	19.160	16.382	Tm	25.249	22.522	22.769	23.235
Ti	13.950	13.427	15.585	14.245	Yb	25.243	22.209	22.391	23.066
V	12.587	11.728	13.307	12.998	Lu	25.231	21.459	22.212	22.981
Cr	11.390	12.476	10.055	11.830	Hf	9.324	8.462	8.742	7.456
Mn	10.336	9.258	9.712	10.144	Ta	8.835	8.127	8.307	7.301
Fe	9.407	8.426	8.306	8.993	W	8.451	7.872	7.784	7.238
Co	8.699	7.754	7.242	8.402	Re	8.182	7.680	7.224	7.193
Ni	8.170	7.211	6.795	8.090	Os	8.004	7.523	6.899	7.107
Cu	7.595	7.848	7.609	7.576	Ir	7.787	7.387	6.741	7.052
Zn	7.168	6.344	6.230	6.173	Pt	7.645	7.374	6.543	7.024
Ga	6.187	7.648	5.655	6.837	Au	7.516	7.276	6.497	6.988
Ge	5.191	5.811	5.047	5.214	Hg	7.398	7.115	6.355	6.923
As	4.492	4.964	4.641	4.317	Tl	9.702	12.199	10.492	12.940
Se	4.000	4.489	4.441	4.108	Pb	9.169	10.086	9.990	10.974
Br	3.696	4.215	4.216	3.731	Bi	8.309	8.994	9.681	10.095
Kr	3.528	4.030	3.811	3.526	Po	7.790	8.324	8.659	9.163
Rb	49.043	50.621	48.273	44.844	At	7.391	7.896	9.080	8.481
Sr	23.183	23.844	26.814	28.084	Rn	7.108	7.595	8.781	8.011
Y	20.424	18.821	23.790	22.818	Fr	–	47.067	47.066	47.066
Zr	18.252	15.797	18.182	19.118	Ra	–	36.433	36.433	36.432
Nb	15.961	15.478	14.686	17.023	Ac	–	31.309	31.068	31.137
Mo	13.989	13.789	12.020	14.917	Th	–	27.566	28.591	29.556
Tc	12.441	11.070	10.330	13.221	Pa	–	24.565	24.377	24.046
Ru	11.366	11.425	9.827	11.934	U	–	22.708	22.814	22.338
Rh	10.410	10.553	8.910	10.833	Np	–	21.298	21.449	21.185
Pd	9.675	4.685	8.228	8.904	Pu	–	20.700	20.269	19.879
Ag	9.012	9.257	8.830	9.141	Am	–	19.893	19.437	19.360
Cd	8.416	7.817	8.452	7.093	Cm	–	18.714	18.751	19.251

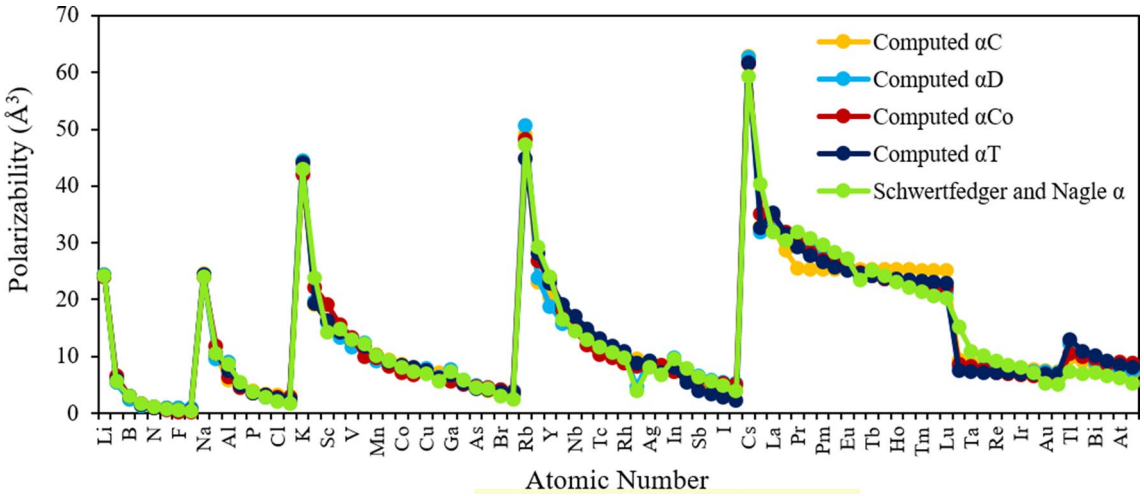

Fig. 1 Comparative plot of polarizabilities computed using Clementi–Raimondi and Clementi et al. radii (α_C/Å^3), Desclaux radii (α_D/Å^3), Cordero et al. radii (α_{Co}/Å^3), Tandon et al. radii (α_T/Å^3), and Schwerdtfeger and Nagle's [43] polarizability (α/Å^3) values

Table 2 Computed molecular polarizabilities calculated using Clementi–Raimondi and Clementi et al. radii-based polarizability (α_{mC}/Å^3), Desclaux radii-based polarizability (α_{mD}/Å^3), Cordero et al. radii-based polarizability (α_{mCo}/Å^3), Tandon et al. radii-based polarizability (α_{mT}/Å^3) and theoretical molecular polarizabilities (α_m/Å^3) [55] for some simple molecules

Diatomics	Computed α_{mC}	Computed α_{mD}	Computed α_{mCo}	Computed α_{mT}	Theoretical α_m
Carbon monoxide	2.322	2.370	2.323	2.288	4.999
Chlorine	6.306	4.994	5.499	5.387	8.412
Nitrogen	2.146	2.178	2.100	1.755	4.275
Nitric oxide	2.009	2.051	1.668	1.663	3.756
Oxygen	1.873	1.925	1.236	1.570	3.185
Carbon dioxide	3.258	3.332	2.941	3.073	6.275
Nitrous oxide	3.082	3.140	2.718	2.540	6.084
Carbon disulphide	8.317	7.141	8.062	7.840	16.005
Sulphur dioxide	5.338	4.791	4.414	4.739	9.439
Sulphur hexafluoride	8.686	8.308	4.385	6.728	9.597

polarizability: α_{mCo} ($r^2 = 0.9987$) > α_{mT} ($r^2 = 0.9969$) > α_{mD} ($r^2 = 0.9968$). This further confirms the suitability of using Cordero et al.'s radii [42] followed by Tandon et al.'s radii [24] for computational purpose for the previously proposed polarizability model [12]. The much smaller variation in these correlations, as well as in the magnitude of polarizability, also indicates the efficacy of the model in different scenarios. This suggests that the computed polarizability model values can be employed to study the mechanism of anaesthetic action solely or in combination with other descriptors.

4 Conclusion

The present work explores the potential of a polarizability model, viz. $\alpha \propto \left(r^3/Z_{eff}e^2\right)$, proposed by our group previously [12]. The efficacy is checked using four different sets of radii for polarizability computations. Suitable similarity in magnitude is observed amongst all the computed polarizabilities. Further molecular polarizabilities are computed invoking the property of additivity, and the results show a valuable correlation with the published data. Both these

Table 3 Computed molecular polarizabilities calculated using Desclaux radii-based polarizability (α_{mD}/Å^3), Cordero et al. radii-based polarizability (α_{mCo}/Å^3), Tandon et al. radii-based polarizability (α_{mT}/Å^3) and theoretical molecular polarizabilities (α_m/Å^3) [11] for some anaesthetic molecules

Anaesthetics	Computed α_{mD}	Computed α_{mCo}	Computed α_{mT}	Theoretical α_m
Methanol	5.039	4.991	4.956	5.570
Ethanol	7.780	8.030	7.793	8.839
Acetone	9.188	9.735	9.296	10.774
2-Propanol	10.522	11.069	10.630	12.108
Propanol	10.522	12.659	10.630	14.583
Urethane	11.906	12.070	11.626	13.392
Ethyl ether	13.264	14.108	13.467	15.377
Butanol	13.264	15.698	13.467	18.528
Antipyrine	26.629	29.475	27.076	32.222
Pyridine	11.463	12.909	11.727	13.993
Chloroform	9.566	10.620	10.250	10.101
Hydroquinone	14.373	15.467	14.590	17.546
Aniline	14.204	15.948	14.564	17.262
Benzyl alcohol	16.153	17.888	16.641	19.847
Acetanilide	19.316	21.310	19.689	23.433
Pentanol	16.006	17.147	16.304	18.646
Phenol	13.411	14.849	13.804	16.578
Toluene	15.190	17.270	15.856	18.879
Benzimidazole	16.034	18.036	16.277	19.514
Hexanol	18.748	20.186	19.141	21.914
Nitrobenzene	14.795	15.850	14.800	17.863
Quinoline	18.427	21.062	19.072	23.066
8-Hydroxyquinoline	19.390	21.680	19.858	24.033
Heptanol	21.490	23.225	21.978	25.183
2-Naphthol	20.375	23.002	21.150	24.400
Methylanthranilate	20.279	21.928	20.474	25.651
Octanol	24.231	26.264	24.815	28.452
Thymol	24.378	27.005	25.152	29.653
Ortho-Phenanthroline	24.406	27.894	25.125	31.304
Ephedrine	26.134	28.722	26.697	30.521
Procaine	35.744	38.840	36.204	42.395
Xylocaine	37.523	41.261	38.256	44.697
Diphenhydramine	39.990	44.658	41.219	48.850
Tetracaine	41.228	44.918	41.878	48.933
Phenyltoloxamine	39.990	44.658	41.219	48.850
Quinine	48.266	53.441	49.392	58.607
Eserine	40.315	43.966	40.754	47.916
Caramiphen	46.363	50.983	47.510	55.754
Dibucaine	52.690	57.827	53.605	62.926

results indicate the accuracy of the model. However, we note that the Cordero et al. [42] radius-based and Tandon et al. [24] radius-based atomic polarizabilities provide superior results in the case of molecules. Molecular data are also calculated for a range of anaesthetics owing to their relevance in chemical–biological interactions. Obtained results reveal significant correlation with the published data, validating the potential for the polarizability model to be used

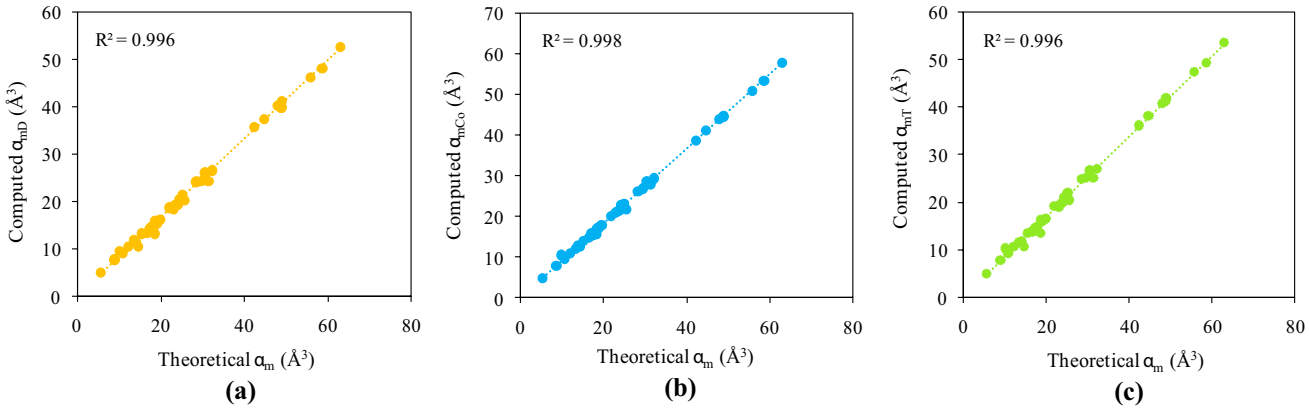

Fig. 2 Correlation plots of theoretical molecular polarizabilities (α_m/Å^3) [11] versus computed molecular polarizabilities calculated using a Desclaux radii-based polarizability (α_{mD}/Å^3); b Cordero et al. radii-based polarizability (α_{mCo}/Å^3), and c Tandon et al. radii-based polarizability (α_{mT}/Å^3) for some anaesthetics

in predicting biological mechanisms as well. Hence, clearly, the polarizability model is conceptually sound and can be satisfactorily employed for real-field applications.

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Author contributions SC: resources, formal analysis, writing—original draft. HT: conceptualization, methodology, formal analysis, investigation, validation, writing—original draft, visualization. TC: conceptualization, supervision, writing—review and editing.

Declarations

Conflict of interest The authors declare that they have no conflict of interest.

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