

**RaH as a potential candidate for electron electric-dipole-moment searches**N. M. Fazil,<sup>1</sup> V. S. Prasanna,<sup>2</sup> K. V. P. Latha,<sup>1,\*</sup> M. Abe,<sup>3</sup> and B. P. Das<sup>4</sup><sup>1</sup>*Department of Physics, Pondicherry University, Ramaswamy Venkataraman Nagar, Kalapet 605 014, India*<sup>2</sup>*Physical Research Laboratory, Atomic, Molecular and Optical Physics Division, Navrangpura, Ahmedabad 380009, India*<sup>3</sup>*Tokyo Metropolitan University, 1-1, Minami-Osawa, Hachioji-city, Tokyo 192-0397, Japan*<sup>4</sup>*Department of Physics, Tokyo Institute of Technology, 2-1-1-H86 Ookayama, Meguro-ku, Tokyo 152-8550, Japan*

(Received 20 December 2018; published 3 May 2019)

Diatomic polar molecules have been the focus of research in the recent past as candidates for electron electric dipole moment (eEDM),  $d_e$ , measurements. In the present work, we focus on RaH molecule and have calculated three of its properties (in the  $X^2\Sigma^+$  state) the effective electric field ( $E_{\text{eff}}$ ), the scalar-pseudoscalar (S-PS) interaction coefficient ( $W_{s,A}$ ), and permanent electric dipole moment (PDM) that play crucial roles in probing fundamental symmetry violations. The calculations were based on the relativistic coupled-cluster singles and doubles (RCCSD) frame work. Our results for  $|E_{\text{eff}}|$ ,  $W_{s,A}$ , and PDM are 80.31 GV/cm, 216.82 kHz, and 4.44 D respectively. In addition to possessing high magnitudes of  $E_{\text{eff}}$  and  $W_{s,A}$ , RaH also has a large PDM, which is a highly desirable criterion for eEDM experiments. The analysis of our results clearly indicates the spectacular role of electron correlation in enhancing their magnitudes  $\approx 16\%$  for PDM and  $\approx 31\%$  for  $E_{\text{eff}}$  and  $W_{s,A}$ . The ratio of  $E_{\text{eff}}$  to  $W_{s,A}$  for RaH is  $89.56 \times 10^{18} e^{-1} \text{ cm}^{-1}$ . Based on our results and other experimental considerations, we propose RaH as a future candidate for experiments in this field.

DOI: [10.1103/PhysRevA.99.052502](https://doi.org/10.1103/PhysRevA.99.052502)**I. INTRODUCTION**

Fundamental symmetry violations have profound implications to physics in general and for exploring physics beyond the standard model (SM). An electric dipole moment (EDM) of a nondegenerate quantum system [1] originates from parity ( $\mathcal{P}$ ) and time-reversal ( $\mathcal{T}$ ) violating interactions in the system. In other words, if parity and/or time reversal were exact symmetries, the EDM of a nondegenerate system would not exist. An accurate determination of the effective electric field ( $E_{\text{eff}}$ ), which can only be calculated theoretically, together with an observed energy shift ( $\Delta E = -d_e E_{\text{eff}}$ ), can provide an estimate of the eEDM,  $d_e$ . The existence of a large  $E_{\text{eff}}$  and the alignment of molecules in eEDM experiments, which depends on the PDM of the molecules, besides other factors, leads to a better statistical sensitivity. Therefore, molecules with reasonably large  $E_{\text{eff}}$  and PDM are preferred. This would enable a better interaction of  $E_{\text{eff}}$  with an eEDM. Recent studies on the molecules HgH and YbH [2] show a relatively large value of  $E_{\text{eff}}$  in comparison with their fluoride derivatives. In contrast, magnitudes of PDM in HgH and YbH are relatively small due to the less anionic nature of lighter atom (H), which in turn makes them less polar. RaH has a surprisingly large PDM, thereby making it the only hydride system to the best of our knowledge with a large PDM and  $E_{\text{eff}}$  and therefore a good polar candidate. It is difficult to attain the field required to polarize a diatomic molecule with low PDM and high rotational constant in a laboratory. Recently, Gao and coworkers [3] reported that because they possess highly diagonal Franck-Condon factor, short lifetimes, and no intervening electronic

states, the alkaline-earth-metal monohydrides (AEMH; BeH, MgH, CaH, SrH, and BaH) can be laser cooled. The “electron in lone orbital” character of AEMH and alkaline-earth-metal monofluoride (AEMF) systems [4] further facilitates the direct laser cooling of RaH. Recent advances in cryogenic buffer-gas-cooled BaH [5] and experiments on CaH [6] and SrF [7–9] are highly encouraging. Hence, the ability to cool RaH may not be too far fetched, as it belongs to the same AEMH group.

In diatomic polar molecules,  $E_{\text{eff}}$  is much larger than it would be in the constituent atoms due to the strong polarization of atomic orbitals along the internuclear axis,  $\hat{\lambda}$  [10]. To utilize the  $E_{\text{eff}}$ , which is averaged to zero in the absence of an external electric field, a field of the order of kV/cm needs to be applied. Although an applied electric field can lead to a larger extent of interaction of the eEDM with  $E_{\text{eff}}$  [11], a continued increase does not imply a higher sensitivity. This is because a larger field disrupts the internal structure of the molecule. Because of the nearness of rotational states in molecules, rather than the electronic states in atoms, the polarizing external electric field should be modest [12].

Even though the SM predictions of eEDM are not realized yet, many extensions of this model predict estimates of eEDM that are feasible to be measured with the present experimental technology. Each experimental result is enhancing the upper bound of the eEDM in spite of a null result. Some of the reported upper bounds using molecules are  $|d_e| < 1.1 \times 10^{-29} e \text{ cm}$  in the ThO molecule (ACME) [13] and  $|d_e| < 10.5 \times 10^{-28} e \text{ cm}$  with YbF molecule [14]. Some extensions of the SM predict much larger values; for example, supersymmetric theories give  $d_e \approx 10^{-26} - 10^{-28} e \text{ cm}$  [15,16].

In a recent work [17], PDMs of AEMHs excluding RaH were studied. Among the AEMH molecules, RaH is the

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most polar molecule and possesses relatively smaller rotational constant than its immediate predecessor, BaH. Polar molecules trapped in a cryogenic solid matrix of inert-gas atoms is the latest approach for eEDM searches [18]. The matrix distribution of argon atoms prevents molecular rotations and hence the candidate molecules either orient themselves accordingly or sustain the orientation even after the removal of applied external field [18]. This method is suitable for molecules with radio active elements as well [18] and a seven-to nine-order increase in experimental sensitivity than the current limit [18] is expected. The application of an electric field of the order of  $10^8$  V/m in the case of polar molecules leads to perfect orientation of the molecules embedded in the argon matrix [19]. These techniques in measurement scenario may help to overcome the obstacles in connection with the rotational constant of RaH molecule. We focus on exploring molecules with enhanced  $E_{\text{eff}}$  as well as PDM. In this paper, besides identifying RaH as a potential eEDM candidate, we highlight the role of electron correlation in determining the magnitudes of the  $E_{\text{eff}}$ , the scalar-pseudoscalar (S-PS) interaction coefficient ( $W_{s,A}$ ), and PDM of RaH molecule and perform a comprehensive comparison with other predicted eEDM candidates.

We categorize the paper into three sections. Section II discusses the parity-violating operators related to  $E_{\text{eff}}$  and  $W_{s,A}$  and a brief discussion about PDM. In Sec. III, the computational details are discussed and Sec. IV deals with the results obtained for RaH and its important implications.

## II. THEORY

We determine the ground-state wave function using the relativistic coupled-cluster singles and doubles method (RCCSD). We employ Dirac-Fock ground-state wave function  $|\Phi_0\rangle$  as the reference state. The state  $|\Phi_0\rangle$  is built from single-particle four-component Dirac spinors which is a single determinant of an open-shell doublet configuration. The wave function  $|\Phi_0\rangle$  corresponds to an ionic configuration,  $\text{Ra}^+$  and  $\text{H}^-$ . The coupled-cluster wave function is represented as

$$|\Psi\rangle = e^T |\Phi_0\rangle, \quad (1)$$

where  $T$  is the cluster operator. The cluster operator ( $T$ ) is truncated to single and double excitations,  $T = T_1 + T_2$ .

In an eEDM experiment, the signature of  $\mathcal{P}$  and  $\mathcal{T}$  violation can arise from both eEDM and S-PS interaction. If  $d_e$  exists, then, the relativistic interaction Hamiltonian,  $H_{\text{eEDM}}$ , is given by [20]

$$H_{\text{eEDM}} = -d_e \sum_{j=1}^{N_e} \beta \vec{\Sigma}_j \cdot \vec{E}_{j,\text{int}}, \quad (2)$$

where the summation index  $j$  runs over the total number of electrons in the system,  $N_e$ ,  $\beta$  and  $\vec{\Sigma}$  are the Dirac matrices, and  $\vec{E}_{j,\text{int}}$  is the internal electric field acting on the  $j$ th electron due to the other electrons and the nuclei in the molecule. The operator,  $H_{\text{eEDM}}$ , can be rewritten in a one-body form as

$$H_{\text{eEDM}} = 2ic \frac{d_e}{e} \sum_{j=1}^{N_e} \beta \gamma_5 p_j^2, \quad (3)$$

where,  $\gamma_5$  represents the product of the Dirac matrices,  $p_j$  is the momentum of  $j$ th electron, and  $c$  is the velocity of light. The energy shift due to the eEDM is given by  $\Delta E = \langle \Psi | H_{\text{eEDM}} | \Psi \rangle = -d_e E_{\text{eff}}$ , where  $\Psi$  is the ground-state molecular wave function. Using this expression for energy shift and Eq. (3), we arrive at an expression for  $E_{\text{eff}}$  in the one-body form

$$E_{\text{eff}} = -\frac{2ic}{e} \sum_{j=1}^{N_e} \langle \Psi | \beta \gamma_5 p_j^2 | \Psi \rangle. \quad (4)$$

In addition to eEDM, the electron-nuclear S-PS interaction contributes to an additional shift in the energy. The Hamiltonian for this interaction is given by

$$H_{S-PS} = i \frac{G_F}{\sqrt{2}} \sum_{A=1}^{N_n} \sum_{j=1}^{N_e} k_{s,A} Z_A \beta \gamma_5 \rho_A(\mathbf{r}_{Aj}), \quad (5)$$

where the summation index  $A$  runs over the total number of nuclei,  $N_n$ , in the molecule. The abbreviations,  $k_{s,A}$ ,  $Z_A$ , and  $\rho$  represent the S-PS interaction constant, the atomic number of  $A$ th nucleus, and the unit normalized nuclear charge density respectively. The quantity  $G_F$  represents Fermi coupling constant ( $2.22249 \times 10^{-14}$  a.u.) and the remaining symbols have the same meaning as before. Readers can refer to Refs. [21,22] and the references therein for further details about  $k_{s,A}$  and  $\rho$ . The S-PS interaction produces an energy shift of the form

$$\Delta E = 2 \langle \Psi | H_{S-PS} | \Psi \rangle = \sum_{A=1}^{N_n} k_{s,A} W_{s,A}. \quad (6)$$

Ignoring the contribution from the light nucleus, one can drop the summation from Eq. (6) and we get

$$W_{s,Ra} = \frac{2}{k_{s,Ra}} \langle \Psi | H_{S-PS} | \Psi \rangle, \quad (7)$$

where the second subscript on  $k$  refers to atomic radium, Ra. We calculate the PDM of RaH molecule by the expectation value approach [17] as detailed below [23]:

$$d = \langle \Phi_0 | e^{T\dagger} D_N e^T | \Phi_0 \rangle_c + \langle \Phi_0 | \left( - \sum_{j=1}^{N_e} er_j \right) | \Phi_0 \rangle + \sum_{A=1}^{N_n} Z_A er_A, \quad (8)$$

where  $D_N$  is the normal ordered electric dipole operator and the subscript  $c$  represents the terms that are connected [24]. In Eq. (8), the first two terms constitute the electronic part and the third term is the nuclear part of PDM. The full nonlinear CCSD calculation was employed to calculate the cluster amplitudes. The expectation value of the quantities of

TABLE I. Particulars of the basis sets.

Ra	H
Dyall-DZ: 26s, 23p, 14d, 8f	cc-pVDZ: 4s, 1p
Dyall-TZ: 33s, 29p, 17d, 11f	cc-pVTZ: 5s, 2p, 1d
Dyall-QZ: 37s, 34p, 21d, 14f	cc-pVQZ: 6s, 3p, 2d, 1f

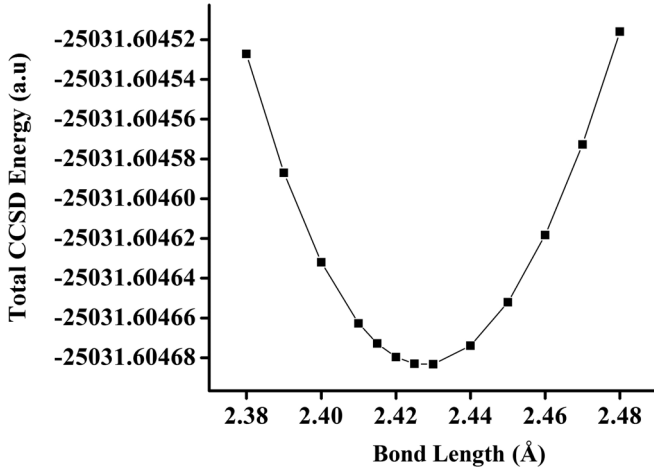


FIG. 1. Potential energy curve using DZ basis set. The minimum is found to occur at 2.43 Å.

interest were calculated at the linear level (in T). By using normal ordering, an operator  $X$  can be represented as [24]

$$\langle X \rangle = \langle X_N \rangle + \langle DF \rangle, \quad (9)$$

where  $\langle DF \rangle$  stands for the expectation value of the operator with the reference state. In the RCCSD linear expectation (LE) value approach,  $\langle X_N \rangle$  is expanded as

$$\langle X_N \rangle = \langle \Phi_0 | (1 + T_1^\dagger + T_2^\dagger) X_N (1 + T_1 + T_2) | \Phi_0 \rangle_c. \quad (10)$$

The expectation value of a normal ordered operator on reference wave function ( $\langle \Phi_0 | X_N | \Phi_0 \rangle_c$ ) is zero by definition. Due to Slater-Condon rules,  $\langle \Phi_0 | X_N T_2 | \Phi_0 \rangle_c$  and  $\langle \Phi_0 | T_2^\dagger X_N | \Phi_0 \rangle_c$  do not contribute either, for the one-body operator,  $X$ . From here onward, the subscripts  $N$  and  $c$  and the bra and ket notations are dropped. Hence,  $X T_1$  represents  $\langle \Phi_0 | X_N T_1 | \Phi_0 \rangle_c$  and so on.

### III. COMPUTATIONAL DETAILS

We employ the REL4D code from UTCHEM [25,26] and DIRAC08 [27] for our calculations. The generation of Dirac-Fock (DF) coefficients and integral transformations from atomic to molecular orbitals were performed with UTCHEM. DIRAC08 was used to compute the  $T_1$  and  $T_2$  amplitudes.

The bond length of the RaH molecule was found with the potential energy curve using Dunning's correlation consistent polarized valence double- $\zeta$  (cc-pVDZ) [28,29] basis set for atomic hydrogen and Dyall's [30] double- $\zeta$  basis function for atomic radium. Using this bond length, we performed the electronic structure calculations with triple- $\zeta$  (TZ) and quadruple- $\zeta$  (QZ) quality basis sets. In the QZ CCSD calculation, the virtual molecular spinors were truncated at a

TABLE II. The PDMs (D) of lighter AEMH molecules [17] from the LE approach. The PDM of the RaH molecule is obtained from LE and also extrapolation (EP).

Molecule	CaH	SrH	BaH	RaH	RaH (EP)
QZ PDM	2.60	3.31	3.77	4.44	4.50

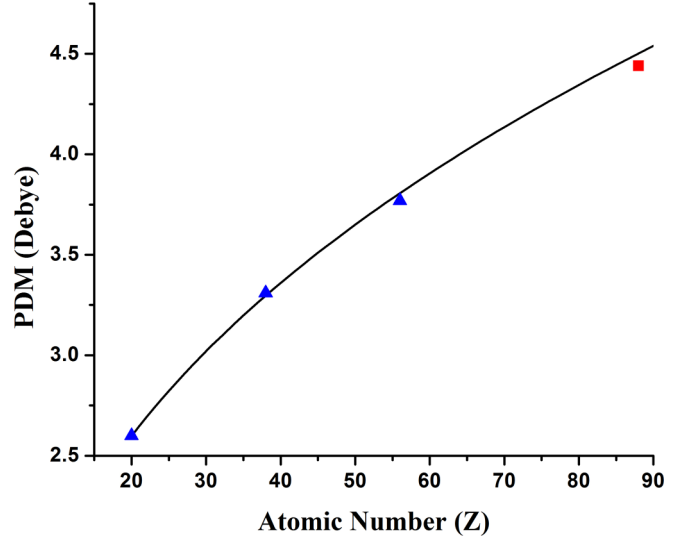


FIG. 2. The solid curve corresponds to the function [Eq. (11)]. The triangle and square (RaH) symbols represent the PDMs of AEMHs in the LE approach.

certain energy cutoff ( $\approx 9000$  a.u.) for faster convergence. The root-mean-squared nuclear charge radii are 5.662 and 1.408 fm for Ra and H respectively [31]. The details of the basis sets used are given in Table I.

### IV. RESULTS AND DISCUSSION

The equilibrium bond length (2.43 Å) of RaH was determined from the minimum of the potential energy curve because of the absence of the experimental bond length. Figure 1 shows total CCSD energy as a function of the bond length.

We also perform an extrapolation of PDMs of AEMH molecules with respect to atomic number,  $Z$  (heavier element), and obtain an estimate for PDM of RaH  $\approx 4.50$  D. For extrapolation, the following function was employed:

$$\mu = 0.855 Z^{0.371}, \quad (11)$$

where,  $\mu$  represents PDM, the coefficient and the exponent are calculated using the least squared fitting to the PDMs of CaH, SrH, and BaH (see Table II). The value of PDM obtained from the LE approach differs from its extrapolated estimate (see Fig. 2) by  $\approx 0.06$  D. This ensures the reliability of bond length used in the present calculation.

In Table III, we list the calculated PDMs,  $E_{\text{eff}}$  and  $W_{s, \text{Ra}}$ , of RaH using different quality basis sets. The total QZ CCSD

TABLE III. List of the calculated total CCSD energy ( $E$ ), PDM (D),  $E_{\text{eff}}$  (GV/cm), and  $W_{s, \text{Ra}}$  (kHz) values of RaH.

Method	Basis	$E$ (a.u)	PDM	$E_{\text{eff}}$	$W_{s, \text{Ra}}$
DF	DZ	-25 028.707	3.81	-60.12	162.19
	TZ	-25 028.729	3.69	-56.50	152.49
	QZ	-25 028.733	3.73	-55.48	149.70
CCSD	DZ	-25 031.604	3.88	-87.88	236.51
	TZ	-25 031.746	4.29	-81.86	221.09
	QZ	-25 031.731	4.44	-80.31	216.82

TABLE IV. Contributions to PDM,  $E_{\text{eff}}$ , and  $W_{s, \text{Ra}}$  from the individual terms of RaH at the RCCSD level.

Term	PDM (D)	$E_{\text{eff}}$ (GV/cm)	$W_{s, \text{Ra}}$ (kHz)
DF	3.73	-55.48	149.70
$XT_1$	0.39	-13.34	35.66
$T_1^\dagger X$	0.39	-13.34	35.66
$T_1^\dagger XT_1$	-0.06	1.47	-3.97
$T_1^\dagger XT_2$	0.01	-0.66	1.77
$T_2^\dagger XT_1$	0.01	-0.66	1.77
$T_2^\dagger XT_2$	-0.03	1.70	-3.77

energy slightly deviates in its trend from DZ to TZ, which may be due to the truncated number of virtuals at the QZ level. There is a significant change in magnitude of PDM,  $E_{\text{eff}}$  and  $W_{s, \text{Ra}}$ , on moving from DF to CCSD level. This reflects the importance of electron correlation effects. The calculated CCSD contributions of PDM,  $E_{\text{eff}}$  and  $W_{s, \text{Ra}}$ , show a trend of convergence on moving to higher quality basis set. In general, the results show saturation with QZ basis set, in spite of truncating virtuals.

In Table IV, the individual contributions from correlation terms calculated using the QZ basis set along with the DF results are tabulated. As expected, the term  $XT_1$  and its Hermitian conjugate contribute as the major correlation corrections to the DF result for all three properties. The term  $XT_1$  encapsulates the many-body correlation terms involving single-hole and single-particle excitations to all orders of perturbation in the residual Coulomb interaction. Therefore, the terms  $XT_1$  and  $T_1^\dagger X$  subsume in them a class of effects called the Brueckner pair correlation effects. The  $XT_1$  contribution for PDM,  $E_{\text{eff}}$ , and  $W_{s, \text{Ra}}$  are 17.5%, 33.2%, and 32.9% respectively.

In Table V, our results of  $E_{\text{eff}}$  and  $W_{s, \text{A}}$  for RaH are compared with those of the other hydride derivatives [2,22] and also with other proposed eEDM candidates. The magnitudes of  $E_{\text{eff}}$  and PDM are larger in RaH than in RaF and YbF. Some molecules like CnH [32] have exceptionally high magnitudes of  $E_{\text{eff}}$  and  $W_{s, \text{Ra}}$ , but possess a small PDM. However, the reasonably large magnitudes of all the three properties make

TABLE V. Comparison with other candidates. The ratio,  $R$ , expressed in units of  $(10^{18} e^{-1} \text{ cm}^{-1})$ .

Molecule	PDM (D)	$ E_{\text{eff}} $ (GV/cm)	$ W_{s, \text{A}} $ (kHz)	$R$
HgF [34]	2.61	115.42		
HgCl [34]	2.72	113.56		
HgBr [34]	2.36	109.29		
HgI [34]	1.64	109.30		
WC [35]		36		
YbH [2]	2.93	31.3		
YbF [21]	3.59	23.2	40.5	139
HgH [2]	0.15	118.5		
HgH [22]	0.27	123.2	284.2	105
CnH [32]	0.11	1105	5551	48
RaF [36]	3.85	52.5	141.2	89.9
RaH (DF)	<b>3.73</b>	<b>55.48</b>	<b>149.70</b>	<b>89.61</b>
RaH (CCSD)	<b>4.44</b>	<b>80.31</b>	<b>216.82</b>	<b>89.56</b>

TABLE VI. Comparison between the LE and the FFCCSD with FFCCSD(T) results of RaH molecule.

RaH	LE	FFCCSD	FFCCSD(T)
DZ-PDM (D)	3.88	3.90	3.81
TZ-PDM (D)	4.29	4.26	4.20
DZ- $ E_{\text{eff}} $ (GV/cm)	87.88	86.85	85.22
TZ- $ E_{\text{eff}} $ (GV/cm)	81.86	81.12	80.01

RaH a good choice for eEDM experiments. Moreover, a combination of at least two experiments is required to extract both eEDM and S-PS interaction coefficient. Because of the similarities of RaH and RaF, these two could form one such combination. The ratio of  $E_{\text{eff}}$  to  $W_{s, \text{A}}$  defined as  $R$ , is useful to get independent limits of  $d_e$  and  $k_s$  through such combination experiments [33].

The error estimation is carried out using finite field coupled cluster singles and doubles (FFCCSD) method and with partial triples [FFCCSD(T)] at DZ and TZ basis set levels. The FFCCSD(T) approach can accommodate nonlinear terms at the CCSD level and, in addition, contributions from partial triples. The FFCCSD(T) magnitude of  $E_{\text{eff}}$  at the TZ level changes by  $\approx 2.3\%$  in comparison with the LE method (see Table VI). In addition, basis set incompleteness (2%) and choice of bond length (0.4%) causes an overall error of  $\approx 4.7\%$  in the magnitude of  $E_{\text{eff}}$ . The uncertainty in PDM is less than that for  $E_{\text{eff}}$ , which is a result of the less prominent electron correlation effect for PDM property in the present class of molecules. Lastly, we comment on the error due to the exclusion of the Breit and quantum electrodynamic (QED) effects. In comparison with the Coulomb interaction, the Breit interaction is of the order of  $\alpha^2$  and QED effects are expected to be even weaker. Recent work on YbOH and BaOH [37] included the Gaunt interaction in their calculation, which alters the final result only by less than 2%. Therefore, we expect these interactions to account for an additional uncertainty of 3% in RaH over other estimates due to its relatively large correlation effects. Then, with the error estimate of  $E_{\text{eff}}$  at the TZ basis set level as a representative case, the maximum uncertainty in the present calculation is within 8%.

## V. CONCLUSION

We have reported calculations of PDM,  $E_{\text{eff}}$ , and  $W_{s, \text{A}}$  for RaH molecule in the framework of RCCSD. We demonstrate the remarkable role of electron correlation effects in enhancing the magnitudes of these properties. We found that the most dominant contribution to the correlation terms arises from the all order pair correlation effects. They contribute to the final magnitude of  $E_{\text{eff}}$  and  $W_{s, \text{A}}$  by 33.2% and 32.9%, respectively, which is quite significant. Of the AEMH molecules, the RaH molecule possesses relatively large magnitudes of PDM,  $E_{\text{eff}}$ , and  $W_{s, \text{A}}$ , the theoretical parameters that scrutinize its suitability for eEDM and S-PS interaction studies. Hence, we reiterate that RaH could be one of the future candidates for the  $\mathcal{P}$ - and  $\mathcal{T}$ -violation experiments and further search of the physics beyond the SM.

## ACKNOWLEDGMENTS

One of the authors, N.M.F. acknowledges the UGC, India for his Senior Research Fellowship (Ref. No. 21/06/2015 (i) EU-V). We would like to thank Dr. A. C. Vutha for valuable

discussions. Calculations were carried out on the Tokyo Tech Computer Cluster (CHIYO), Tokyo, Japan; Inter-University Accelerator Centre, New Delhi, India; and National PARAM Supercomputing Facility, C-DAC, Pune, India.

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