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Some observations about quantum chemistry software GAUSSIAN

Abstract

When laboratory study of some molecule is not available, one may plan to use data obtained from Quantum Chemistry software, such as GAUSSIAN, MOLPRO, NWCHEM, etc. For our investigation of cosmic molecules, we need reliable data for rotational and centrifugal distortion constants. For some molecules, we have obtained these data with the help of Quantum Chemistry software GAUSSIAN and compared them with those obtained from the laboratory studies. We have found that in some cases, the two sets of data are very close to each other whereas in some cases, they differ very much. As the laboratory measurements provide the most reliable data, one would like to use the GAUSSIAN data only when the laboratory data are available. Thus, an obvious question arises how to decide the reliability of GAUSSIAN data, when for that particular molecule no laboratory data are available. Further, when the laboratory data are available, no one would like to use the GAUSSIAN data.

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Mohit K Sharma
Amity Centre for Astronomy & Astrophysics, Amity Institute of Applied Sciences, Amity University, India

Correspondence: Mohit K Sharma, Amity Centre for Astronomy & Astrophysics, Amity Institute of Applied Sciences, Amity University, Noida 201313, India,
Email mksharma4@amity.edu, mohitkuamrsharma32@yahoo.in

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Introduction

In a cosmic object having molecules, kinetic temperature in general is very low; few tens of Kelvin. Thus, one is concerned with the rotational levels in the ground vibrational state and ground electronic state. The rotational and centrifugal distortion constants, electric dipole moment can be used for calculation of energies of rotational levels and radiative transition probabilities (Einstein A-coefficients) for radiative transitions between the levels. We have investigated some molecules where laboratory data are available and for the same molecules we have obtained the data with the help of GAUSSIAN also. We have found that for some molecules, the two sets of data are in good agreement whereas for some molecules, they differ very much. As the laboratory data are the most reliable, one would like to use the GAUSSIAN data only in absence of the laboratory data. Thus, an obvious question arises how to decide the reliability of GAUSSIAN data. We are aware of the fact that the frequencies of spectral lines obtained from the GAUSSIAN data are not as accurate as required by the astronomers. However, the GAUSSIAN data can play important role in getting qualitative results about a molecule. We could not succeed in running the CCSD and CCSD (T) methods for the GAUSSIAN, as the computer program broke down each time during the execution. Therefore, we have employed the functional B3LYP method, i.e., Becke's three parameter exchange function B3 (Becke[1]) with Lee, Yang and Parr's gradient corrected exchange-correlation functional.[2]

Investigation

In the present discussion, we have considered the following molecules following sections.-to be deleted.

Cyclopropenone

Guillemin et al.,[3] have recorded spectrum of cyclopropenone (c-C_3H_2O) and have derived rotational and centrifugal distortion constants for Watson's rotational operator written in I^r representation and - to be deleted with A-type reduction, given in Table 1 (column 2). Sharma et al.[4] have optimized the cyclopropenone with the help of GAUSSIAN 2009 Frisch et al.[5] using B3LYP method and cc-pVDZ basis set. The values are given in Table 1 (column 3). The two sets of data are in good agreement. The deviations of rotational constants A, B and C, with respect to their experimental values are 0.46%, 1.18% and 0.90%, respectively.

Table 1 Rotational and centrifugal distortion constants in MHz of c-C_3H_2O

Constant	Laboratory	cc-pVDZ
A	32040.73	31894.85
B	7825.046	7733.81
C	6280.685	6224.503
ΔJ	1.79362×10^{-3}	1.651250766×10^{-3}
ΔJK	33.7882×10^{-3}	3.271020188×10^{-2}
ΔK	50.65×10^{-3}	4.379488485×10^{-2}
δJ	0.38536×10^{-3}	3.533088298×10^{-4}
δK	$22.156\times10_{-3}$	2.093510188×10^{-2}
H_J		$2.937852086\times10^{-10}$
H_{JK}		6.851055671×10^{-8}
H_{KJ}		$-1.128055614\times10^{-7}$
H_K		9.251718141×10^{-8}
h_J		$2.362038947\times10^{-10}$
h_{JK}		3.968188988×10^{-8}
h_K		1.205246347×10^{-6}

Titanium dihydride

Inspired with good agreement between two sets of data for c-C_3H_2O, Sharma et al.,[6] decided to go for the investigation of titanium dihydride (TiH_2) for which laboratory data are not available. They[6] have optimized the molecule TiH_2 with the help of GAUSSIAN 2009 Frisch et al.,[5] where B3LYP method and cc-pVTZ basis set are used. The rotational and centrifugal distortion constants obtained for Watson's rotational operator written in I^r representation and - to be deleted with A-type reduction are given in Table 2. The outcome of the investigation is very exciting.

Table 2 Rotational and centrifugal distortion constants in MHz of TiH_2

Constant	cc-pVTZ	Constant	cc-pVTZ
A	2.8589602×10^5	ΦJ	$2.037108491 \times 10^{-3}$
B	1.2520818×10^5	ΦJK	$-1.928681064 \times 10^{-2}$
C	8.707408×10^4	ΦKJ	$-1.946479675 \times 10^{-2}$
ΔJ	6.004343	ΦK	$5.110638046 \times 10^{-1}$
ΔJK	-4.186548023×10^1	φJ	$1.014000418 \times 10^{-3}$
ΔK	2.549058853×10^2	φJK	$-3.557138924 \times 10^{-3}$
δJ	2.465123	φK	$1.085768474 \times 10^{-1}$
δK	2.332384		

Ethylene oxide

Pan et al.[7] recorded spectrum of ethylene oxide (c-C_2H_4O) and have derived rotational and centrifugal distortion constants for Watson's rotational operator written in I^r representation and – to be deleted with A-type reduction, given in Table 3 (column 2). Sharma et al.[8] have optimized the ethylene oxide with the help of GAUSSIAN 2009 Frisch et al.[5] bf using B3LYP method and cc-pVDZ basis set. The values of data are given in Table 3 (column 3). The two sets of data are in good agreement. The deviations of rotational constants A, B and C, with respect to their experimental values are -0.79%, -0.58% and -0.70%, respectively. It again provided us a confidence about our investigation of TiH_2 Sharma et al.[6]

Vinylidene

Inspired with good agreement between two sets of data for c-C_3H_2O and for c-C_2H_4O, we decided to go for the investigation of vinylidene (H_2CC) for which also laboratory data are not available. bf Sharma et al.[9] have optimized the molecule H_2CC with the help of GAUSSIAN 2009 Frisch et al.[5] employing the B3LYP method in conjunction with four basis sets, cc-pVTZ, aug-cc-pVDZ, aug-cc- pVTZ and aug-cc-pVQZ. The resulting rotational and centrifugal distortion constants for Watson's rotational operator written in I^r representation and - to be deleted with S-type reduction are given in Table 4. There is good agreement between the data obtained from different basis sets.

Silanone

Bailleux et al.[10] have recorded spectrum of silanone (H_2SiO) and derived rotational and centrifugal distortion constants for Watson's rotational operator written in I^r representation and - to be deleted with A-type reduction, given in Table 5 (column 2). Sharma et al.[11] have optimized the molecule H_2SiO with the help of GAUSSIAN 2009 Frisch et al.[5] bf employing B3LYP method in conjunction with three basis sets, aug-cc-pVDZ, aug-cc-pVTZ and aug-cc-pVQZ. The values are given in Table 5 (columns 3-5). There is very good agreement between the four sets of data. The deviations of rotational constants A, B and C obtained for the basis set aug-cc-pVQZ, with respect to their experimental values are 0.24%, 0.53% and 0.18%, respectively.

cis-Formic acid

Winnerwisser et al.[12] have recorded spectrum of cis-Formic acid (cis-HCOOH) and derived rotational and centrifugal distortion constants for Watson's rotational operator written in I^r representation and - to be deleted with A-type reduction, given in Table 6 (column 2). Sharma et al.[13] have optimized the molecule cis-HCOOH with the help of GAUSSIAN 2009 Frisch et al.[5] bf employing B3LYP method in conjunction with three basis sets, aug-cc-pVDZ, aug-cc-pVTZ and aug-cc-pVQZ. The values are given in Table 6 (columns 3-5). There is very good agreement between the four sets of data. The deviations of rotational constants A, B and C obtained for the basis set aug-cc-pVQZ, with respect to their experimental values are -1.16%, -0.22% and -0.46%, respectively. All these data provided us a encouragement about our investigations of TiH_2 and H_2CC molecules.

Table 3 Rotational and centrifugal distortion constants (MHz) of c-C_2H_4O

Constant	Laboratory	cc-pVDZ
A	25483.89	25685.72
B	22120.85	22249.95
C	14097.84	14197.62
ΔJ	51.1883×10^{-3}	$50.79096319 \times 10^{-3}$
ΔJK	-70.4938×10^{-3}	$-71.09013012 \times 10^{-3}$
ΔK	27.6541×10^{-3}	$28.41532834 \times 10^{-3}$
δJ	-9.01689×10^{-3}	$8.836730565 \times 10^{-3}$
δK	3.3491×10^{-3}	$-6.556467036 \times 10^{-3}$
ΦJ	0.2456×10^{-6}	$-5.960452772 \times 10^{-8}$
ΦJK	-5.2164×10^{-6}	$-4.838170644 \times 10^{-6}$
ΦKJ	15.7370×10^{-6}	$15.30527314 \times 10^{-6}$
ΦK	-10.638×10^{-6}	$-10.40655085 \times 10^{-6}$
ΦJ	-0.05097×10^{-6}	$-2.887999339 \times 10^{-8}$
ΦJK	1.4297×10^{-6}	$-1.411514955 \times 10^{-6}$
φK	-17.8633×10^{-6}	$1.713117251 \times 10^{-5}$
L_J	-0.1210×10^{-9}	
L_{JJK}	-0.1288×10^{-9}	
L_{JK}	0.624×10^{-9}	
L_{KKJ}	-0.800×10^{-9}	
L_K	0.892×10^{-9}	
l_J	-0.00367×10^{-9}	
l_{JK}	0.0921×10^{-9}	
l_{KJ}	-0.448×10^{-9}	
l_K	0.679×10^{-9}	
P_K	-1.114×10^{-12}	

Disilicon

McCarthy et al.[14] has recorded spectrum of disilicon (Si_2C) and have derived rotational and centrifugal distortion constants for Watson's rotational operator written in I^r representation and - to be deleted with S-type reduction, given in Table 7 (column 2). Sharma et al.[15] have optimized the molecule Si_2C with the help of GAUSSIAN 2009 Frisch et al.[5] employing the B3LYP method in conjunction with three basis sets, aug-cc-pVDZ, aug-cc-pVTZ and aug-cc-pVQZ. The values are given in Table 7 (columns 3-5). There is large disagreement between the laboratory data and those obtained from GAUSSIAN. The deviations of rotational constants A, B and C obtained for the basis set aug-cc-pVQZ, with respect to their experimental values are -51.89%, 20.23% and 15.28%, respectively. These large deviations perturbed us and lead to a question about the reliability of GAUSSIAN data.

Table 4 Rotational and centrifugal distortion constants in MHz of H_2CC

Constant	cc-pVTZ	aug-cc-pVDZ	aug-cc-pVTZ	aug-cc-pVQZ
$A \times 10^{-5}$	2.858903	2.858903	2.858903	2.858903
$B \times 10^{-4}$	3.993411	3.993411	3.993411	3.993411
$C \times 10^{-4}$	3.503965	3.503965	3.503965	3.503965
$D_J \times 10^3$	42.70791	43.44087	44.28356	44.55227
D_{JK}	20.98798	18.94745	20.44459	20.4197
D_K	5.317725	6.440168	5.879314	5.933398
$d_1 \times 10^2$	−1.442126677	−1.373607832	−1.445080323	−1.452037644
$d^2 \times 10^2$	−2.675152631	−2.408896481	−2.609261594	−2.613141728
$H_J \times 10^6$	−9.085110924	−7.573403608	−8.601743486	−8.655849617
$H_{JK} \times 10^3$	2.717971	2.280665	2.564823	2.580959
$H_{KJ} \times 10^2$	−1.854934803	−1.597951879	−1.709596957	−1.731162015
$H_K \times 10^2$	2.401038	2.151629	2.272677	2.29427
$h_1 \times 10^6$	−1.524539329	−1.248551723	−1.444404960	−1.443374339
$h_2 \times 10^6$	4.698862	3.929762	4.456302	4.485417
$h_3 \times 10^6$	1.651997	1.367133	1.5717	1.57211

Table 5 Rotational and centrifugal distortion constants in MHz of H_2SiO

Constant	Experiment	cc-pVDZ	aug-cc-pVDZ	aug-cc-pVTZ	aug-cc-pVQZ
$A \times 10^5$	1.666573	1.62688	1.62316	1.658067	1.662584
$B \times 10^{-4}$	1.867939	1.787253	1.78186	1.842979	1.858002
$C \times 10^{-4}$	1.674277	1.610344	1.605601	1.65862	1.671235
$\Delta J \times 10^2$	1.75216	1.631609	1.647716	1.66202	1.676962
$\Delta JK \times 10^1$	6.02486	5.543688	5.632878	5.839659	5.871728
ΔK	7.5	8.199677	8.090008	8.443277	8374.246
$\delta J \times 10^3$	2.0811	1.822749	1.836778	1.876133	1.906645
$\delta K \times 10^1$	4.13	3.503961	3.550486	3.660305	3.689542
$\Phi J \times 10^9$		6.733706	6.296932	5.253595	5.657116
$\Phi JK \times 10^6$	4.757	7.800663	7.879044	8.266248	8.41835
$\Phi KJ \times 10^5$	-4.774	-1.57875	-1.796	-2.14959	-2.2458
$\Phi K \times 10^3$		1.443688	1.377452	1.435596	1.415752
$\varphi J \times 10^9$		3.572809	3.531365	3.408102	3.524366
$\varphi JK \times 10^6$		4.031514	4.065714	4.256998	4.334719
$\varphi K \times 10^4$		4.511626	4.605502	4.727325	4.732419

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Table 6 Rotational and centrifugal distortion constants (MHz) of cis-HCOOH

Constant	Lab	Optimization		
		aug-cc-pVDZ	aug-cc-pVTZ	aug-cc-pVQZ
A	86461.62	85967.44	87387.25	87478.32
B	11689.18	11617.78	11690.94	11715.35
C	10284	10234.65	10311.44	10331.7
$\Delta J \times 10^3$	8.35515	6.594446	6.564108	6.564716
$\Delta JK \times 10^3$	−71.4412	259.8124	274.8887	275.2381
$K \times 10^3$	2361.672	2176.623	2296.741	2303.991
$\delta J \times 10^3$	1.41773	0.592251	0.556347	0.55381
$\delta K \times 10^3$	40.747	115.2922	118.6733	118.4331
$\Phi J \times 10^8$	1.064	−0.4527703926	−0.4722888293	−0.4808865771
$\Phi JK \times 10^6$	−0.2974	9.566051	10.98867	11.10552
$\Phi KJ \times 10^6$	−9.673	108.8903	119.0774	119.4857
$\Phi K \times 10^6$	185.11	1.389687	1.452612	1.434686
$\varphi J \times 10^9$	2.317	0.108608	0.08907	0.084311
$\varphi JK \times 10^6$	−0.73	0.746964	0.783595	0.775275
$\varphi K \times 10^6$		37.1677	39.04597	38.76245
$L_K \times 10^9$	−20.2			
$l_{JK} \times 10^9$	0.558			

Table 7 Rotational and centrifugal distortion constants of Si_2C in MHz

Constant	Experimental	aug-cc-pVDZ	aug-cc-pVTZ	aug-cc-pVQZ
A	64074.34	115272.4	141935.4	133191.5
B	4395.621	3648.742	3597.055	3655.86
C	4102.028	3536.791	3508.148	3558.194
$D_J \times 10^3$	9.7315	18.02061	28.55172	17.97574
D_{JK}	−0.8572075	−7.016988202	−17.432464312	−9.250582631
$D_K \times 10^{-2}$	0.235881	7.258966	27.69195	12.60339
$d_1 \times 10^3$	1.519832	2.2482	3.425177	2.169344
$d_2 \times 10^1$	0.51591	1.269923	2.405429	1.420247
$H_J \times 10^7$	−0.41349	−6.979665512	−26.90729235	−4.538089470
$H_{JK} \times 10^4$	0.93298	9.032487	48.46837	10.80401
$H_{KJ} \times 10^1$	−0.0188755	−2.856368246	−22.85802143	−4.878977881
H_K	0.044863	26.42362	320.7195	61.69333
$h_j \times 10^8$	−0.5231	−11.16426814	−43.12215486	−6.341531159
$h_k \times 10^2$		1.388191	7.346143	3.083056
$h_{jk} \times 10^5$	−0.6586	−2.147381766	−9.373151002	−1.964934254

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Discussion

When got good agreement between the laboratory data and those obtained with the help of GAUS- SION for c-C_3H_2O, c-C_2H_4O, H_2SiO and cis-HCOOH, we felt encouraged that in absence of lab- oratory data for a particular molecule, at least qualitative analysis of the molecule could be done with the help of the GAUSSIAN data. But, a large disagreement between the two sets of data for Si_2C has shattered down all the confidence. Thus, an obvious question irises how to decide the reliability of GAUSSIAN data, when laboratory data are not available. Further, when the laboratory data are available, no one would like to use the GAUSSIAN data. We Sharma et al.[16] have earlier presented some observations about the Quantum Chemistry software MOLPRO. Werner et al.[17] About the computer code MOLSCAT Hutson et al.,[18] we Sharma et al.[19] have presented some observations. About the observations, someone may respond. - to be deleted These observations however - to be deleted provide some awareness to the users of the GAUSSIAN, MOLPRO and MOLSCAT.

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Conflicts of interest

The author declares there is no conflict of interest.

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