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Calculation of bromine nuclear quadrupole coupling constants in gaseous state molecules

W.C. Bailey*, F.M. Gonzalez

Department of Chemistry and Physics, Kean University, Union, NJ 07083, USA

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Abstract

Several DFT and hybrid HF/DFT methods in conjunction with Pople (6-311G) and Ahlrichs (TZV) bases have been investigated for the calculation of ^{79}Br and ^{81}Br nuclear quadrupole coupling constants (nqccs) in gaseous state molecules. The molecules are HBr, BrF, BrCl, Br_2, BrCN, BrBO, HCCBr, CH_3Br, CH_2Br_2, CF_3Br, CH_2CHBr, and CH_3CH_2Br. Assessment of the various models was made by linear regression analysis of calculated electric fields versus experimental nqccs.

The best results are obtained with the B1LYP, B3LYP, and LG1LYP hybrid methods combined with Ahlrichs' TZV bases plus polarization. With the B1LYP/TZV(3df, 3p) model, for example, the residual standard deviation for ^{79}Br is 1.7 MHz (0.42%), and for ^{81}Br, 1.5 MHz (0.42%). The effective nuclear electric quadrupole moments derived from the slopes of the regression lines are, respectively, 330.4 and 276.0 mb.

This B1LYP model is applied to calculation of the ^{79}Br nqccs in SiF_3Br and SiH_3Br for the purpose of investigation of the SiBr bond lengths.

Keywords: ^{79}Br; ^{81}Br; Nuclear quadrupole coupling constants; Density functional theory

1. Introduction

The nuclear quadrupole coupling constant (nqcc) tensor is the spectroscopic measurement of the energy of interaction of the electric quadrupole moment (Q) of the nucleus of the atom with the gradient of the electric field (efg) at the site of the nucleus. In gaseous state molecules, nqcc tensors are measured to a high degree of accuracy by the techniques of microwave Fourier transform spectroscopy [1].

Procedures for accurate and efficient calculation of the nqccs that employ readily available methods and basis sets would be useful for molecular spectroscopists. In a series of recent papers on ^{2}H [2], ^{11}B [3], ^{14}N [4], ^{17}O [5,6], ^{33}S [6], and ^{73} Ge [6], we have shown that accurate nqccs may be obtained from efgs calculated using Becke's [7] hybrid Hartree–Fock/density functional theory (HF/DFT) methods in conjunction with modest sized basis sets. The savings in computational cost of these methods compared to ab initio techniques such as perturbation theory, coupled cluster, etc. can be considerable.

In this work we report the results of our investigation of several DFT and HF/DFT methods

* Corresponding author. Tel.: +1-908-737-3630; fax: +1-908-737-3688.
E-mail address: wbailey@kean.edu (W.C. Bailey).

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for calculation of ^{79}Br and ^{81}Br nqccs in gaseous state molecules. Hartree–Fock (HF) and second-order Møller–Plesset perturbation theory (MP2) results are reported for comparison. The molecules are HBr, BrF, BrCl, Br_2, BrCN, BrBO, HCCBr, CH_3Br, CH_2Br_2, CF_3Br, CH_2CHBr, and CH_3CH_2Br.

MP2 methods have been employed by Palmer et al. [8,9] for calculation of the nqccs on optimized molecular structures of several Br compounds, including most of the above. Their results and ours, however, are not directly comparable as ours are made on the experimental structures.

By way of application, nqccs are calculated in SiF_3Br and SiH_3Br for the purpose of investigation of the SiBr bond lengths.

2. Method

The elements of the nqcc tensor χ_{ij} are related to those of the efg tensor q_{ij} by

$$\chi_{ij} = (eQ/h)q_{ij}, \quad (1)$$

where e is the fundamental electric charge and h is Planck's constant; $i,j = a,b,c$ (principal axes of the inertia tensor).

The procedure in this work follows that previously employed [2–6]. The coefficient eQ/h in Eq. (1) is determined by least-squares linear regression analysis of the calculated efgs versus the experimental nqccs. Although not independent, all three diagonal elements of the efg tensor are plotted against the corresponding elements of the nqcc tensor. This assures, because the tensors are traceless, that the least-squares line passes through (0, 0).

The premise that underlies this procedure is that the errors inherent in the level of theory—model and basis, as well as zero-point vibrations and relativistic effects, are systematic and can be corrected, at least partially, by the best-fit coefficient eQ/h.

Equivalently, a model-dependent effective nuclear moment, Q_{eff}, is derived from $Q_{\text{eff}} = (eQ/h)/234.9649$, where Q_{eff} is in barns (b) and eQ/h in MHz/a.u.

Calculations of the q_{ij} were made using the GAUSSIAN 98 [10] package of programs. Recommended grid for numerical integrations and convergence criteria are discussed in Appendix. Transformation of the calculated q_{ij} from GAUSSIAN 98 standard orientation axes to principal axes of the inertia tensor is discussed in Section 3

The DFT methods investigated are BPW91 (Becke [11] exchange and Perdew–Wang [12] correlation), mPWPW91 (Perdew–Wang exchange modified by Adamo and Barone [13] and Perdew–Wang correlation], BLYP (Becke exchange and Lee–Yang–Parr [14,15] correlation), and LGLYP (Lacks–Gordon [16] exchange and Lee–Yang–Parr correlation).

The hybrid HF/DFT methods are B3LYP (Becke's three-parameter method [7] with Lee–Yang–Parr correlation), B3PW91 (Becke's three-parameter method with Perdew–Wang correlation), B3P86 (Becke's three-parameter method with Perdew [17] correlation), B1LYP (Becke's one-parameter method with Lee–Yang–Parr correlation as implemented by Adamo and Barone [18,19]), mPW1PW91 (Adamo and Barone's one-parameter method with modified Perdew–Wang exchange and Perdew–Wang correlation [13]), and LG1LYP (Adamo and Barone's one-parameter method with Lacks–Gordon exchange and Lee–Yang–Parr correlation [20]).

The bases used are Pople-type 6-311G [21] and Ahlrichs' TZV [22], each augmented with diffuse and polarization functions. The augmenting functions used with both are those recommended for use with the 6-311G bases [21].[1] Schäfer et al. [22] note that the choice of polarization functions is not tightly coupled to that of the remaining basis.

3. Coordinate transformation

For a molecule such as vinyl bromide, it is necessary to transform the calculated q_{ij} from the coordinate axes of the standard orientation of the

[1] Polarization functions were obtained from the Extensible Computational Environment Basis Set Database, Version 7/29/02, as developed and distributed by the Molecular Science Computing Facility, Environmental and Molecular Sciences Laboratory, which is part of the Pacific Northwest Laboratory, P.O. Box 999, Richland, Washington 99352, USA, and funded by the US Department of Energy. The Pacific Northwest Laboratory is a multiprogram laboratory operated by Battelle Memorial Institute for the US Department of Energy under contract DE-AC06-76RLO 1830. Contact David Feller or Karen Schuchardt for further information. http://www.emsl.pnl.gov: 2080/forms/basisform.html.

GAUSSIAN 98 output to the principal coordinate axes a, b, c of the moment of inertia tensor. Experimental microwave nqccs are measured in this latter system.

This is accomplished by translation of the standard orientation coordinates to coordinates (x, y, z) in which the center-of-mass of the molecule lies at (0, 0, 0); followed by rotation to the principal a, b, c, axes. The rotation has a simple form when the nucleus of interest lies in a symmetry plane. Let us choose the z (and c) axis perpendicular to the symmetry plane. Then θ, the angle of rotation about the z-axis that diagonalizes the moment of inertia tensor, is given by

$$\tan 2\theta = 2I_{xy}/(I_{xx} - I_{yy}), \quad (2)$$

where the I_{ij} are elements of the moment of inertia tensor in the x, y, z center-of-mass system. Now,

$$q_{aa} = q_{xx}\cos^2\theta + q_{xy}\sin 2\theta + q_{yy}\sin^2\theta, \quad (3)$$

$$q_{bb} = q_{xx}\sin^2\theta - q_{xy}\sin 2\theta + q_{yy}\cos^2\theta, \quad (4)$$

$$q_{cc} = q_{zz}, \quad (5)$$

$$q_{ab} = [(q_{yy} - q_{xx})/2]\sin 2\theta + q_{xy}(1 - 2\sin^2\theta); \quad (6)$$

where q_{xx}, q_{yy}, and q_{xy} are the efgs calculated by GAUSSIAN 98 (translation to the center-of-mass system does not alter these q_{ij}).

4. Results

The experimental ^{79}Br nqccs [23–34] for the molecules used in this investigation are given in Table 1. Calculations of the efgs were made on the experimental molecular structures [32–41]. Structure types are r_e for HBr, FBr, ClBr, Br_2, CH_3Br, CH_2Br_2, and BrCN; r_z for CF_3Br; and r_s for HCCBr, BrBO, CH_2CHBr, and CH_3CH_2Br.

The results of linear regression analyses of the several methods in conjunction with the 6-311G and TZV bases are shown in Table 2. For these efg calculations, the bases were augmented with one set each of s- and p-diffuse functions plus three sets of d- and one set of f-polarization functions on the heavy atoms; and three sets of p- and one set of d-polarization functions on the hydrogen atoms; that is, 6-311 + G(3df, 3pd) and TZV + G(3df, 3pd).

The linear regression results shown in Table 3 are for the hybrid methods in conjunction with the TZV basis as above but without diffuse functions on the heavy atoms and d-polarization functions on the hydrogen atoms; that is, TZV(3df, 3p).

For the B1LYP/TZV(3df, 3p) model, a plot of the calculated efgs versus the experimental nqccs is shown in Fig. 1. The slopes eQ/h of these regression lines are 77.625(47) MHz/a.u. for ^{79}Br, and 64.853(42) MHz/a.u. for ^{81}Br. These are the coefficients in Eq. (1) used for conversion of the q_{ij} to χ_{ij}.

Table 1
Calculated and experimental ^{79}Br quadrupole coupling constants, χ_{ij} (MHz). Calc. = B1LYP/TZV(3df, 3p). Where two references are given, the first is for the nqcc, the second for the molecular structure

Molecule	ij	Calc.	Expt	Ref.
HBr	zz	532.2	532.2398(57)	[23,35]
FBr	zz	1083.4	1086.8920(12)	[24,35]
ClBr	zz	875.4	875.078(1)	[25,35]
Br_2	zz	809.7	810.0(5)	[26,36]
CH_3Br	zz	574.0	577.1088(57)	[27,37]
$CH_2^{79}Br^{81}Br$	aa	335.9	335.21(42)	[28,38]
	bb	−26.4	−24.93(24)	
	cc	−309.5	−310.28(48)	
	$\|ab\|$	401.2	402.12(79)	
CF_3Br	zz	619.9	618.2628(21)	[29,39]
BrCN	zz	685.5	685.85(2)	[30,40]
HCCBr	zz	652.7	648.113(3)	[31,41]
BrBO	zz	418.6	417.9(35)	[32]
CH_2CHBr	aa	472.5	470.98(9)	[33]
	bb	−220.1	−216.97	
	cc	−252.4	−254.01	
	$\|ab\|$	247.8	246.14(564)	
CH_3CH_2Br	aa	420.0	417.75(20)	[34]
	bb	−146.5	−144.04	
	cc	−273.6	−273.70	
	$\|ab\|$	292.8	294.77(205)	

5. Discussion

The RSD shown in Table 2, with the exception of the Hartree–Fock method, are all less than 1.5% of the average absolute experimental nqcc. Those obtained with the hybrid HF/DFT methods are all about 1% or less.

The RSDs obtained using the TZV basis are consistently smaller than those obtained using the 6-311G basis.

Table 2
Linear regression analysis of calculated efgs versus experimental nqccs. Residual standard deviation, RSD (MHz), and effective nuclear electric quadrupole moment Q_{eff} (mb), as functions of computational model

Nuc.	Method	6-311 + G(3df, 3pd)		TZV + G(3df, 3pd)	
		RSD	Q_{eff}	RSD	Q_{eff}
^{79}Br	HF	14.8	306	14.0	327
	BPW91	5.9	319	5.6	337
	mPWPW91	5.8	319	5.4	337
	BLYP	4.8	318	4.6	334
	LGLYP	5.7	323	4.9	335
	B3P86	3.5	314	2.7	332
	B3PW91	3.5	314	2.8	332
	mPW1PW91	3.5	314	2.7	333
	B3LYP	3.3	313	3.0	330
	B1LYP	3.6	312	3.4	330
	LG1LYP	4.2	316	3.2	330
	MP2(FULL)[a]	6.1	327	4.2	348
^{81}Br	HF	12.6	256	12.1	273
	BPW91	5.1	267	4.9	282
	mPWPW91	5.0	267	4.7	282
	BLYP	4.0	265	4.0	279
	LGLYP	4.8	269	4.3	280
	B3P86	2.8	262	2.3	277
	B3PW91	2.8	262	2.4	278
	mPW1PW91	2.8	262	2.3	278
	B3LYP	2.7	261	2.6	275
	B1LYP	2.9	261	2.9	275
	LG1LYP	3.4	264	2.8	276
	MP2(FULL)[a]	4.8	273	3.2	290

[a] All electron correlation.

The least RSDs are obtained with the hybrid methods in conjunction with Ahlrichs' TZV basis plus polarization. Among these, the RSDs obtained using Perdew and Perdew–Wang correlation are smaller than those obtained using Lee–Yang–Parr correlation.

It is interesting, although likely fortuitous, that the Q_{eff} shown in Table 2 for the hybrid methods with Ahlrichs' basis all lie within the uncertainties in the currently recommended nuclear moments of $Q(^{79}Br) = 331(4)$ mb and $Q(^{81}Br) = 276(4)$ mb [42].

The results given in Table 3 show that going from the TZV + G(3df, 3pd) basis to TZV(3df, 3p) there is notable improvement in the RSDs for the B3LYP, B1LYP, and LG1LYP methods, whereas there is no improvement for the B3P86, B3PW91, and mPW1PW91 methods. Removal of the diffuse functions on the heavy atoms and the d-polarization functions on the hydrogens has a significant positive effect for the B3LYP, B1LYP, and LG1LYP methods.

For the B1LYP/TZV(3df, 3p) model, RSD(^{79}Br) = 1.7 MHz (0.42%) and $Q_{eff}(^{79}Br) = 330.4(2)$ mb, RSD(^{81}Br) = 1.5 MHz (0.42%) and $Q_{eff}(^{81}Br) = 276.0(2)$ mb. Calculated ^{79}Br nqccs are shown in Table 1 along with the experimental values.

The average difference (all three diagonal nqccs for all 12 molecules) between calculated and experimental nqccs is 1.2 MHz, the largest difference is 4.6 MHz (0.71%) for HCCBr.

Calculated ^{81}Br nqccs are not shown, but can be obtained from the calculated ^{79}Br nqccs and the ratio of the slopes of the regression lines, namely 1.1969.

For ^{81}Br, BrBO is not among the molecules used for linear regression analyses (Tables 2 and 3). It is clear that the experimental ^{79}Br and ^{81}Br nqccs cannot both be accurate, as the ratio of nqccs is 1.169 compared with the accurately know ratio of nuclear moments of 1.1970568(15) [43]. Both could be inaccurate, the experimental uncertainties are large. However, for ^{79}Br, the calculated nqcc of 418.6 MHz

Table 3
Linear regression analysis of calculated efgs versus experimental nqccs. RSD (MHz), and effective nuclear electric quadrupole moment, Q_{eff} (mb) as functions of computational model

Nuc.	Method	TZV(3df, 3p)	
		RSD	Q_{eff}
^{79}Br	B3P86	2.7	333
	B3PW91	3.1	334
	mPW1PW91	2.8	334
	B3LYP	1.9	331
	B1LYP	1.7	330
	LG1LYP	2.1	331
^{81}Br	B3P86	2.4	278
	B3PW91	2.7	279
	mPW1PW91	2.4	279
	B3LYP	1.6	276
	B1LYP	1.5	276
	LG1LYP	1.8	276

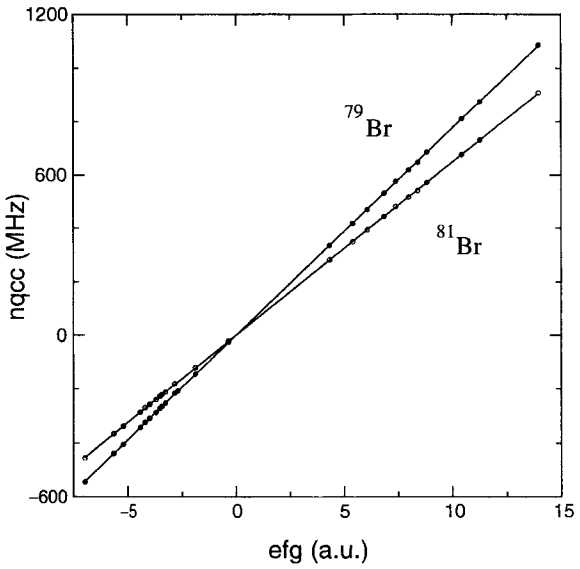

Fig. 1. B1LYP/TZV(3df,3p) efgs versus experimental nqccs. For ^{79}Br, RSD = 1.7 MHz and eQ/h = 77.625(47) MHz/a.u. For ^{81}Br, RSD = 1.5 MHz and eQ/h = 64.853(42) MHz/a.u.

is in good agreement with the experimental value of 417.9(35) MHz. For ^{81}Br, on the other hand, the calculated nqcc of 349.8 MHz differs from the experimental value of 357.4(31) MHz by 7.6 MHz, which lies far outside the experimental uncertainty. A more accurate 'experimental' nqcc for ^{81}Br would be 349.1 MHz, which is obtained from the experimental ^{79}Br nqcc and the ratio of nuclear moments.

This discussion of BrBO is an example of the usefulness of nqcc calculations. Another example is given in Section 6.

6. Bromotrifluorosilane and bromosilane

Cox et al. [44] derived for SiF_3Br an r_z structure in which the SiBr bond length is 2.1559(37) Å. They also determined an r_s bond length of 2.1477(2) Å, which is 0.0082 Å shorter than their r_z value. In SiH_3Br, the r_s SiBr bond length is 2.210 Å [45].

In SiF_3Br and SiH_3Br, respectively, the experimental ^{79}Br nqccs are 344.0(1) [44] and 334.981(8) MHz [46]. The nqcc in SiF_3Br is 9.0 MHz larger than that in SiH_3Br. This difference in nqccs would be due in large part to differences in the SiBr bond length. Therefore, assessment of these structures—particularly the SiBr bond lengths—has been made by calculation of the nqccs.

On the r_z structure of SiF_3Br, the B1LYP/TZV(3df, 3p) calculated nqcc is 353.4 MHz, which is larger than the experimental nqcc by 9.4 MHz (2.7%).

On a structure with the r_z parameters for the SiF_3 geometry but with the r_s parameter for the SiBr bond length, the calculated nqcc is 349.2 MHz, which is larger than the experimental nqcc by 5.2 MHz (1.5%). This is better agreement with the experimental nqcc than that above.

On the r_s structure of SiH_3Br, the calculated nqcc is 338.4 MHz, which is larger than the experimental value by 3.4 MHz (1.0%). This is good agreement with the experimental nqcc.

On the r_s/r_z structure of SiF_3Br, the calculated nqcc is larger than that in SiH_3Br by 10.8 MHz, which is similar to the difference in the experimental nqccs of 9.0 MHz. With the nqcc calculated on the r_z structure, this difference is 15.0 MHz.

A more accurate nqcc is calculated with the r_s bond length for SiBr.

7. Summary

Accurate bromine nqccs have been calculated using hybrid HF/DFT methods with Ahlrichs' TZV bases plus polarization.

Best results are obtained with the B3LYP, B1LYP, and LGLYP methods in conjunction with TZV(3df, 3p) bases. The linear regression RSDs are about 0.5% of the average absolute experimental nqcc.

Good results are obtained with the B3P86, B3PW91, and mPW1PW91 methods with the larger TZV + G(3df, 3pd) bases. The RSDs are less than 0.7%.

The Q_{eff} for all the above hybrid methods are in good agreement with the recommended nuclear moments.

Two examples that demonstrate the usefulness of nqcc calculations are investigations of (1) the accuracy of the nqccs measured in BrBO, and (2) the SiBr bond lengths in SiF_3Br and SiH_3Br.

Appendix A

Calculations for the data presented in Tables 2 and 3 were made using the 'tight' convergence option and the 'ultrafine' integration grid, rather than the less stringent default settings in GAUSSIAN 98 for these parameters.

The B1LYP/TZV(3df, 3p) model was investigated for dependence of the calculated efgs on these parameters.

A.1. Integration grid

The root mean square (rms) difference between efgs calculated using the ultrafine grid (with tight convergence) and those calculated using the default grid (with tight convergence) is 0.0012 a.u. (0.1 MHz). The largest differences are 0.0041 and 0.0036 a.u., respectively, for BrF and BrCl (for which the efgs are 13.9532 and 11.2735 a.u.). The ultrafine grid is not necessary, and in the interest of efficiency not recommended. The default grid consists of 75 radial shells with 302 angular points per shell (75,302), which is pruned to about 7000 points per atom.

A.2. Convergence

The rms difference between efgs calculated using tight convergence (with default grid) and those calculated using default convergence (with default grid) is 0.0059 a.u. (0.5 MHz). The largest differences are 0.0182, 0.0123, and 0.0119 a.u., respectively, for CF_3Br, HCCBr, and BrBO. These correspond to 1.4, 1.0, and 0.9 MHz. Computational errors of this magnitude are not helpful. The default convergence criteria are not recommended.

Tight convergence is 10^{-8} for the rms density matrix, and 10^{-6} for the maximum density matrix. Further tightening the criteria by two orders of magnitude makes no difference in the calculated efgs. Tight convergence is recommended. It is both necessary and sufficient.

Calculations of the efgs for the nqccs presented in Table 1 and those discussed in Section 7 were made using the tight convergence option with the default integration grid.

References

[1] H. Dreizler, Z. Naturforsch. 47a (1992) 342.
[2] W.C. Bailey, J. Mol. Spectrosc. 190 (1998) 318.
[3] W.C. Bailey, J. Mol. Spectrosc. 185 (1997) 403.
[4] W.C. Bailey, Chem. Phys. 252 (2000) 57.
[5] W.C. Bailey, Chem. Phys. Lett. 292 (1998) 71.
[6] W.C. Bailey, F.M. Gonzalez, J. Castiglione, Chem. Phys. 260 (2000) 327.
[7] A.D. Becke, J. Chem. Phys. 98 (1993) 5648.
[8] M.H. Palmer, J.A. Blair-Fish, Z. Naturforsch. 53a (1998) 370.
[9] M.H. Palmer, J.A. Blair-Fish, P. Sherwood, M.F. Guest, Z. Naturforsch. 57a (1998) 383.
[10] M.J. Frisch, G.W. Trucks, H.B. Schlegel, G.E. Scuseria, M.A. Robb, J.R. Cheeseman, V.G. Zakrzewski, J.A. Montgomery Jr., R.E. Stratmann, J.C. Burant, S. Dapprich, J.M. Millam, A.D. Daniels, K.N. Kudin, M.C. Strain, O. Farkas, J. Tomasi, S. Clifford, J. Ochterski, G.A. Petersson, P.Y. Ayala, Q. Cui, K. Morokuma, D.K. Malik, A.D. Rabuck, K. Raghavachari, J.B. Foresman, J. Cioslowski, J.V. Ortiz, A.G. Banoul, B.B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. Gomperts, R.L. Martin, D.J. Fox, T. Keith, M.A. Al-Laham, C.Y. Peng, A. Nanayakkara, M. Challacombe, P.M.W. Gill, B. Johnson, W. Chen, M.W. Wong, J.L. Andres, C. Gonzalez, H. Head-Gordon, E.S. Replogle, J.A. Pople, GAUSSIAN 98, Revision A.9, Gaussian, Inc., Pittsburgh, PA, 1995.
[11] A.D. Becke, Phys. Rev. A 38 (1988) 3098.
[12] J.P. Perdew, K. Burke, Y. Wang, Phys. Rev. B 54 (1996) 16533 and references therein.
[13] C. Adamo, V. Barone, J. Chem. Phys. 108 (1998) 664.
[14] C. Lee, W. Yang, R.G. Parr, Phys. Rev. B 37 (1988) 785.
[15] B. Miehlich, A. Savin, H. Stoll, H. Preuss, Chem. Phys. Lett. 157 (1989) 200.
[16] D.J. Lacks, R.G. Gordon, Phys. Rev. A 47 (1993) 4681.
[17] J.P. Perdew, Phys. Rev. B 33 (1986) 8822.
[18] A.D. Becke, J. Chem. Phys. 104 (1996) 1040.
[19] C. Adamo, V. Barone, Chem. Phys. Lett. 274 (1977) 242.
[20] C. Adamo, V. Barone, J. Comput. Chem. 19 (1998) 418.
[21] W.J. Hehre, L. Random, P.v.R. Schleyer, J.A. Pople, Ab Initio Molecular Orbital Theory, Wiley, New York, 1986, and references therein.
[22] A. Schäfer, C. Huber, R. Ahlrichs, J. Chem. Phys. 100 (1994) 5829.
[23] G. Di Lonardo, L. Fusina, J. Mol. Spectrosc. 148 (1992) 86.
[24] H.S.P. Müller, M.C.L. Gerry, J. Chem. Phys. 103 (1995) 577.
[25] A.C. Legon, J.C. Thorn, Chem. Phys. Lett. 215 (1993) 554.
[26] N. Bettin, H. Knöckel, E. Tiemann, Chem. Phys. Lett. 80 (1981) 386.
[27] S. Carocci, P. Minguzzi, M. Tonelli, A. Di Lieto, J. Mol. Spectrosc. 160 (1993) 359.
[28] Y. Niide, H. Tanaka, I. Ohkoshi, J. Mol. Spectrosc. 139 (1990) 11.
[29] A.J. Gray, R.J. Butcher, J. Mol. Spectrosc. 161 (1993) 351.
[30] C.D. Cogley, S.G. Kukolich, J. Mol. Spectrosc. 97 (1983) 220.
[31] S.M. Bass, R.L. DeLeon, J.S. Muenter, J. Chem. Phys. 92 (1990) 71.

[32] T. Kasuya, T. Okabayashi, S. Watanabe, M. Nomoto, M. Tanimoto, J. Mol. Spectrosc. 191 (1998) 374.
[33] M. Hayashi, C. Ikeda, T. Inagusa, J. Mol. Spectrosc. 139 (1990) 299.
[34] T. Inagusa, M. Hayashi, J. Mol. Spectrosc. 129 (1988) 160.
[35] F.J. Lovas, E. Tiemann, J. Phys. Chem. Ref. Data 3 (1974) 609.
[36] K.P. Huber, G. Herzberg, Constants of Diatomic Molecules, Van Nostrand-Reinhold, New York, 1979.
[37] G. Graner, J. Mol. Spectrosc. 90 (1981) 394.
[38] R. Wellington Davis, M.C.L. Gerry, J. Mol. Spectrosc. 109 (1985) 269.
[39] A.P. Cox, G. Duxbury, J.A. Hardy, Y. Kawashima, J. Chem. Soc. Faraday Trans. II 76 (1980) 339.
[40] M. Le Guennec, G. Wlodarczak, W.D. Chen, R. Bocquet, J. Demaison, J. Mol. Spectrosc. 153 (1992) 117.
[41] H. Jones, J. Sheridan, O.L. Stiefvater, Z. Naturforsch. 32a (1977) 866.
[42] P. Pyykkö, J. Li, 1992 Nuclear Quadrupole Moments, Report HUKI 1-92, ISSN 0784-0365, Helsinki, 1992.
[43] H.H. Brown, J.G. King, Phys. Rev. 142 (1966) 53.
[44] A.P. Cox, I.C. Ewart, T.R. Gayton, J. Mol. Spectrosc. 125 (1987) 76.
[45] R. Kewley, P.M. McKinney, A.G. Robiette, J. Mol. Spectrosc. 34 (1970) 390.
[46] K.F. Dössel, D.H. Sutter, Z. Naturforsch. 34a (1979) 469.