TABLE I
Comparison of g Factors

Molecule X_2	g_r	$g_r(H_2)\frac{M_H}{M_X}$
$^{7}Li_2$	0.10797 ± 0.00011	0.1268
$^{23}Na_2$	0.03892 ± 0.00010	0.0387
$^{39}K_2$	0.02163 ± 0.00006	0.0228
$^{85}Rb_2$	0.00953 ± 0.00004	0.0105
$^{133}Cs_2$	0.00547 ± 0.00003	0.0067

compared their g factors with that of H_2 divided by the ratio of atomic masses (Table I). The roughly parallel trends shown by these quantities are consistent with both this interpretation and the ideas on which Eq. (5.1) is based.

For strongly electrically dipolar molecules $^{+}AB^{-}$ the nuclear contribution to the rotational g factor has an upper limit

$$g_r^n = 1/M_a - 1/M_b \tag{5.2}$$

This limit applies in the case that the electric dipolar moment at the equilibrium internuclear distance has the magnitude eR_e; being negative, an electronic contribution must decrease an actual value from that upper limit, for which one assumes implicitly that a formal charge displaced from the cationic atomic center to the anionic center of the molecule cannot exceed one electron. For even the most polar diatomic molecules the actual electric dipolar moment is less than about five-sixths of this limiting value; for this reason, apart from neglect of electronic contribution, the above formula is only a rough indicator of g_r for the most polar diatomic molecules.

TABLE II
Comparison of Electric Dipolar Moment and Irreducible Nonadiabatic Contribution to Rotational g Factors

$^{+}AB^{-}$	g_r^{irr}	$\frac{m_p}{eR} d_z \left(\frac{1}{m_a} - \frac{1}{m_b}\right)$	g_r
$^{7}Li^{1}H$	−0.0022	0.6930	−0.6952
$^{7}Li^{19}F$	−0.0034	−0.0773	0.0739
$^{1}H^{11}B$	−8.5414	−0.2663	−8.2751
$^{27}Al^{1}H$	−3.4294	0.0324	−3.4618
$^{69}Ga^{1}H$	−3.1811	0.0625	−3.2436
$^{19}F^{11}B$	−0.2278	0.0056	−0.2334
$^{27}Al^{19}F$	−0.0783	0.0033	−0.0816
$^{69}Ga^{19}F$	−0.0485	0.0121	−0.0606

Using Eq. (1.42), Sauer [22] analyzed the importance of electric dipolar moment d_z and the irreducible nonadiabatic contribution g_r^{irr} to rotational g factors of hydrides and fluorides of Li, B, Al, and Ga. The results are summarized in Table II.

For hydrides and to a lesser extent also for fluorides of B, Al, and Ga, the irreducible nonadiabatic contribution dominates, whereas for Li compounds the electric dipolar contribution is paramount [22]. This pattern conforms to an observation that the paramagnetic contribution to magnetizability exceeds the diamagnetic contribution [see Eq. (1.9)] in BH and AlH as discussed in Section IV.B.

B. Rotational and Vibrational Dependences of g_r

In alluding to rotational and vibrational dependences of the rotational g factor, we suggest that they are slight. We justify this trend here with reference to analytic properties of expectation values, starting with the definition [139]

$$\begin{aligned}\langle vJ|g_r(R)|vJ\rangle = g_r(R_e) + \left(v+\frac{1}{2}\right)\gamma\left\{-\frac{3}{4}(c_1-1)\left(\frac{\partial g_r(x)}{\partial x}\right)_{x=0}\right.\\ \left.+\frac{1}{2}\left(\frac{\partial^2 g_r(x)}{\partial x^2}\right)_{x=0}\right\} + \frac{1}{4}\gamma^2[J(J+1)]\left(\frac{\partial g_r(x)}{\partial x}\right)_{x=0} + \cdots\end{aligned} \tag{5.3}$$

in which $\gamma \equiv 2\frac{B_e}{\omega_e}$ with B_e and ω_e being the equilibrium rotational and vibrational parameters, respectively; c_1, defined in Eq. (2.21) typically has a value about -1.5. If $g_r(R_e)$ and its first and second derivatives with respect to $x \equiv (R-R_e)/R_e$ evaluated at R_e or $x=0$ have comparable magnitudes, an expected variation between adjacent vibrational states is of the order $2\gamma g_r(R_e)$, whereas an expected variation between rotational states with $J=1$ and $J=2$ is $\gamma^2 g_r(R_e)$. Typical values of γ are, roughly, for $^1H_2$, 0.026; for $^1H^{19}F$ and $^7Li^1H$, 0.010; for $^{12}C^{16}O$, 0.002; for $^{28}Si^{32}S$, 0.001; and for $^{127}I_2$, 0.00033.

For molecules of only two diatomic species is the rotational dependence of g_r measured; for $^1H_2$, the difference of g_r between $|0,1\rangle$ and $|0,2\rangle$ is 0.00064 [36], compared with $\gamma^2 g_r \sim 0.00062$. For $^7Li^1H$, a rotational dependence of a form $g_r = (-0.0654 \pm 0.007) + (1.2 \pm 0.6) \times 10^{-4} J(J+1)$ is deduced [37], of which the magnitude of the coefficient of $J(J+1)$ is comparable with $\gamma^2 g_r \sim 7 \times 10^{-5}$. Vibrational dependences of g_r are measured for several molecules, among which is $^{28}Si^{32}S$ [140]; in this case, $2\gamma g_r$ (with g_r for $v=0$) is 0.0002, to be compared with the linear coefficient 0.0003 in an expansion for g_r as a function of $(v+\frac{1}{2})$. In all these instances, the magnitudes of variation with v or $J(J+1)$ are as expected; much larger apparent variations might be suspect, and might then, if significant, indicate presence of a perturbing electronic state.

C. Remarks on g_r in Electronic States Other Than $^1\Sigma^+$ or 0^+

In this article, we attempt to present a comprehensive survey of the rotational g factor for molecular species in an electronic state of class $^1\Sigma^+$ or 0^+. The reason for doing so is that both calculations and experiments for such species have attained a mature state. For molecular species in other states, experimental work to produce these data on new species continues apace, but calculations are few or nonexistent. Mizushima [141] has considered the analysis of rotational spectra to produce values of g_r, and includes a summary of values from the literature before 1975. In their 1995 version the Landolt–Börnstein tables [142] present values of g_r from experiments that show a range from -73.78 ± 0.18 for ^{58}Ni^{1}H in the state $X\ ^2\Delta$, $v = 0$, to 51.4 ± 0.4 for ^{59}Co^{1}H in the state $X\ ^3\Phi_4$, $v = 0$; the unusual nature of these values was there remarked upon, but most remaining values fall in an expected range, from -5 to 1. Notable exceptions are for ^{even}Se^{16}O in state $a\ ^1\Delta$, $v = 0$, $g_r \sim 2.0 \pm 0.6$ [143] and for Br$_2$ in a few electronically and vibrationally excited states $A\ ^3\Pi^+_{0u}$: ^{79}Br$_2$, $v = 42$, $g_r = 3.76 \pm 0.24$; ^{81}Br$_2$, $v = 40$, $g_r = 2.19 \pm 0.18$ and $v = 45$, $g_r = 5.35 \pm 0.22$ [144]. For an electronic state of class other than $^1\Sigma$ or 0, net angular momentum due to electronic orbital motion or to spin, or to both, produces a permanent magnetic dipolar moment apart from any such moment induced on molecular rotation, but the values specified above pertain specifically to the rotational g factor. Eq. (1.27) in its second form shows that the nuclear contribution to g_r takes values in the range less than unity, with known magnitudes between 0.4 and 1 [141]. For molecules in a state of class $^1\Sigma^+$ or 0^+, the electronic contribution to g_r can take only negative values, according to Eq. (1.26); for such species the value of g_r^n then provides an upper limit to g_r, namely one in a range less than unity.

D. Accuracy of Experimental and Computed Rotational g Factors

Whether derived from experiment or calculation, any numerical value of g_r has a finite accuracy, arising from either random or systematic sources of error, or likely from both to some extent.

Both molecular beams with electric resonance on spectral transitions and microwave spectra with Zeeman effect yield precise and accurate data, with uncertainties about ± 0.00001 in the best cases (see the Appendix for examples of many such instances). Magnetic resonance in the far infrared region might be expected to produce results of comparable accuracy. Unless spectra with optical resolution much better than reported heretofore for samples in intense magnetic fields become available, magnetic circular dichroism on vibration–rotational transitions seems limited to a precision about ±0.01; such a relative accuracy about one part per hundred is characteristic of intensity measurements.

For frequency data from vibration–rotational and pure rotational spectra of samples without applied fields, two limitations arise. One is an ambiguity of extramechanical effects, such that data available from only measurements of wave numbers or frequencies of such transitions are almost inevitably inadequate to enable separation of all contributing adiabatic and nonadiabatic effects, as discussed in Section II.E. A second impediment is less fundamental in that accuracy of frequency measurements bears directly on values of g_r deduced therefrom. To ensure maximum precision of auxiliary parameters u_j, t_j, and s_j in Eqs. (2.22)–(2.24), one should include within a global analysis spectral data from isotopic variants of atomic centers of both A and B with atomic masses over a broad range: this condition is obviously fulfilled most readily for H, having M_H with masses 1, 2, or even 3 u, whereas for bromine, which has a mass intermediate in a range of masses for stable nuclides of chemical elements between hydrogen and bismuth, the range is only 79–81 u, corresponding to variation of only a few parts per hundred [32]. If one seeks to evaluate g_r with a relative uncertainty about one part per hundred, corresponding uncertainties in both t_a and t_b in Eq. (2.29) must be at least as small. If for atomic centers A and B spectral data for isotopic variants of only one species, either A or B, are available, estimates of g_r from only t_0 of only the other species are likely to be unreliable, because large correlations inevitably exist between that t_0 and other fitting coefficients to which spectral data are much more sensitive than to parameters with factors m_e/M; the latter is a ratio of electronic and atomic masses. If, as in the case of BrCl, atomic masses are of order 50 u, a ratio m_e/M has an order 10^{-5}; then one needs to evaluate $Y_{1,0}$ and $Y_{0,1}$ in Eq. (2.18) with relative uncertainties $|\delta Y_{1,0}/Y_{1,0}|$ and $|\delta Y_{0,1}/Y_{0,1}|$ both about 10^{-7}, and measured frequencies require both this precision and comparable consistency from all sources of spectral data included in an analysis for the purpose of deriving a value of g_r. Because wave numbers can be almost routinely measured with precision about a few parts in 10^8 [145], with conventional commercial instruments and with precisions and absolute accuracy about parts in 10^{10} at current frontiers of metrological standards in the mid infrared region [146], there arises the prospect of obtaining increasingly precise results for g_r from spectral analyses of samples without externally applied fields.

For purposes of quantum–chemical computations, assessment of uncertainty of calculated values of rotational g factors is more subtle than for experimental data because there at least two principal factors determine the level of accuracy of computed values: the completeness of a one-electron basis set used, and the level of electronic correlation included; of the two, the latter is the easier one to estimate. For instance, within perturbative propagator approaches the accuracy increases in an order RPA = CHF < SOPPA < CCSDPPA ~ SOPPA(CCSD); CASSCF and RASSCF methods having active spaces of moderate size yield a level of accuracy comparable to that of SOPPA-like methods. The same condition holds for correlated MP2, MP3, and L-CCD methods (the latter being a method based on linearized coupled-cluster doubles) also applied to calculation of rotational *g* factors [73,147]. With regard to the fine distinctions between various correlated methods, guidance about relative accuracy is generally difficult to formulate. The relative accuracy depends on the nature of the particular state of interest, for instance whether its nature is singly or multiconfigurational, but many other factors also come into play.

Most important for the level of accuracy of a computed *g* factor is the completeness of the one-electron basis set. There is no simple measure of quality of a basis set. For instance, the size of the basis set is not necessarily an effective indication of its level of completeness, and a basis set that is well suited for calculation of other properties, such as total energy, might not be optimal for calculation of an electronic *g* factor. As a rough rule of thumb one should distrust a calculation employing a basis set that includes less than three one-electron functions per occupied atomic orbital (having quality so called triple zeta), one moreover that fails to contain polarization functions, i.e., basis functions describing virtual atomic orbitals of low energy. That effects of basis set and electronic correlation are coupled is a further complication. For instance, for a particular molecular species one might find a large effect of electronic correlation in a small basis set but a small effect with a more nearly complete basis set, or even vice versa!

In the Appendix, calculations at various levels of approximation for many molecular species are listed; from them the reader can assess the effect of including electron correlation. On comparing rotational *g* factors computed by the same authors for a given species, one can obtain a good estimate of the effect of electronic correlation, as the same basis set is generally used. Conversely, when one compares results from disparate authors, the effect of basis set might well be a major cause of discrepancy; only consultation of pertinent publications can indicate whether this condition is applicable.

E. Zeeman Effect and Rotational *g* Factor in Molecular Research

Experimental measurement of the Zeeman effect on spectral transitions between rotational states of diatomic molecules (and, more generally, polyatomic molecules) is practiced much less than use of the Stark effect. The latter method enables estimate of primarily the magnitude of a permanent electric dipolar moment defined with respect to the molecular frame; despite this property being conventionally attributed to a nonrotating molecule, by parity no molecule in a particular nondegenerate quantum state can possess such a moment with respect to a frame fixed in the laboratory or in space moving with the center of mass [131]. In contrast, a molecule in an electronic state of class $^1\Sigma^+$ or 0^+ can intrinsically possess a molecular magnetic dipolar moment but only if this property arises purely by virtue of molecular rotation, apart from possible intrinsic nuclear angular momenta. In that sense the molecular magnetic dipolar moment is as fundamental as the molecular electric dipolar moment, and the Zeeman effect might therefore warrant experimental practice just as much as the Stark effect. Despite these circumstances, some textbooks on molecular spectroscopy neglect to provide sufficient emphasis of the Zeeman effect, and correspondingly the rotational g factor, or, in some cases, might even omit entirely. Measurement of microwave spectra with a Fourier-transform technique, employing a conventional waveguide rather than a beam or jet of gaseous sample, enables resolution and precision of frequencies of transitions to be enhanced, but to apply external fields in the same experiment proves to be a difficult task, and to attempt its extension with supersonic jets has been impracticable. Success of the Fourier-transform experiment with the Stark effect [148] preceded that with the Zeeman effect [47] by several years; no application of the latter technique on a diatomic molecular compound has been reported, although this approach is expected to be a generally satisfactory method with which to measure the rotational g factor over various rotational and vibrational states. Even for those diatomic molecular species for which g_r has been measured experimentally, in only a few cases have results been obtained for other than the lowest vibrational state or at most a few vibrational states, and for one rotational state, generally $J = 1$. Although theoretical methods, already powerful, continue to be developed, there remains much scope for use of experimental measurements to complement computational work.

APPENDIX

A table of experimental and calculated rotational *g* factors, indicating the nature of the experiment or calculation, is presented here. The relative accuracy of experimental and theoretical methods is discussed in Section V.D.

TABLE A.I
Measured and Calculated Rotational g Factors[a]

Molecule	Condition	Value	Experiment	Calculation	Refs.
$^{27}\mathrm{Al}^{35}\mathrm{Cl}$	R_e	-0.084 ± 0.08	IR		[149]
$^{27}\mathrm{Al}^{19}\mathrm{F}$	$v=0$	-0.08051 ± 0.0008	RZ–MW		[150]
	R_e	-0.0839		RPA	[22]
$^{27}\mathrm{Al}^{1}\mathrm{H}$	R_e	-3.46		CHF	[151]
	R_e	-2.25 ± 0.25	IR		[114]
	R_e	-2.7 ± 0.5	IR		[113]
	R_e	-3.370		CCSDPPA	[113]
$^{40}\mathrm{Ar}^{1}\mathrm{H}^{+}$	$v=0$	0.6638 ± 0.0034	RZ–MW		[152]
	R_e	0.6874		RPA	[25]
	R_e	0.6839		SOPPA	[25]
	R_e	0.6830		CCSDPPA	[25]
	R_e	0.6876		RPA	[104,105]
	R_e	0.6803		SOPPA	[104,105]
	R_e	0.6783		CASSCF	[104,105]
$^{40}\mathrm{Ar}^{2}\mathrm{H}^{+}$	$v=0$	0.3295 ± 0.0016	RZ–MW		[152]
	R_e	0.3439		RPA	[25]
	R_e	0.3423		SOPPA	[25]
	R_e	0.3420		CCSDPPA	[25]
$^{138}\mathrm{Ba}^{16}\mathrm{O}$	$v=0$	(0.103 ± 0.001)[b]	MB–MR		[153]
$^{11}\mathrm{B}^{19}\mathrm{F}$	R_e	-0.21		CHF	[154]
	R_e	-0.2339		RPA	[22]
$^{11}\mathrm{B}^{1}\mathrm{H}$	R_e	-8.17		CHF	[117]
	R_e	-8.30		CHF	[118]
	R_e	-8.3		CHF	[123]
	R_e	-8.2070		CHF	[124]
	$v=0, J=0$	-8.1019		CHF	[124]
	R_e	-7.3371		CCSDPPA	[124]
	$v=0, J=0$	-7.2430		CCSDPPA	[124]
$^{79}\mathrm{Br}^{35}\mathrm{Cl}$	R_e	-0.02509 ± 0.00070	IR		[112]
$^{79}\mathrm{Br}^{19}\mathrm{F}$	$v=0$	-0.1008 ± 0.0002	RZ–MW		[98]
$^{81}\mathrm{Br}^{19}\mathrm{F}$	$v=0$	-0.1004 ± 0.0002	RZ–MW		[98]
$^{12}\mathrm{C}^{1}\mathrm{H}^{+}$	R_e	-11.41		CHF	[123]
$^{35}\mathrm{Cl}^{19}\mathrm{F}$	$v=0$	-0.1089 ± 0.0002	RZ–MW		[98]
	R_e	-0.103		CHF	[155]
	$v=0, J=1$	-0.109202 ± 0.000016	MB–ER		[103]

cating the
e relative
ussed in

Refs.
[149]
[150]
[22]
[151]
[114]
[113]
[113]
[152]
[25]
[25]
[25]
[104,105]
[104,105]
[104,105]
[152]
[25]
[25]
[25]
[153]
[154]
[22]
[117]
[118]
[123]
[124]
[124]
[124]
[124]
[112]
[98]
[98]
[123]
[98]
[155]
[103]

TABLE A.I (*Continued*)

Molecule	Condition	Value	Experiment	Calculation	Refs.
$^{37}Cl^{19}F$	$v=0$	-0.1062 ± 0.0002	RZ–MW		[98]
	R_e	-0.101		CHF	[155]
	$v=0, J=1$	-0.107348 ± 0.000022	MB–ER		[103]
$^{12}C^{16}O$	$v=0$	$(0.26910 \pm 0.0005)^b$	RZ–MW		[96]
	$v=0, J=1$	$(0.267 \pm 0.003)^b$	RZ–MW		[156]
	$v=0$	-0.26890 ± 0.00010	MB–MR		[55]
	R_e	-0.242		CHF	[157]
	$v=0$	-0.26895 ± 0.00005	MB–ER		[158]
	$v=0,1$	-0.262 ± 0.026	MVCD		[50]
	R_e	-0.2800		CHF	[73]
	$v=0$	-0.2821		CHF	[73]
	R_e	-0.2583		MP2	[73]
	$v=0$	-0.2587		MP2	[73]
	R_e	-0.280		CHF	[88]
	R_e	-0.2686		MP3	[147]
	R_e	-0.2642		L-CCD	[147]
	R_e	-0.2801		CHF	[89]
	R_e	-0.2592		CASSCF	[89]
$^{12}C^{18}O$	$v=0$	$(0.25622 \pm 0.0005)^b$	RZ–MW		[96]
	$v=0$	-0.25625 ± 0.00005	MB–ER		[158]
$^{13}C^{16}O$	$v=0$	$(0.25704 \pm 0.0005)^b$	RZ–MW		[96]
	$v=0$	-0.25691 ± 0.00020	MB–MR		[159]
	$v=0$	-0.2595 ± 0.0030	MB–ER		[158]
$^{14}C^{16}O$	$v=0$	$(0.24664 \pm 0.0005)^b$	RZ–MW		[96]
$^{12}C^{32}S$	$v=0$	-0.2702 ± 0.0004	RZ–MW		[160]
$^{12}C^{34}S$	$v=0$	-0.2659 ± 0.0007	RZ–MW		[160]
$^{12}C^{32}S$	$v=0$	-0.2529 ± 0.005	RZ–MW		[160]
$^{133}Cs^{79}Br$	$v=0$	-0.0099 ± 0.0010^c	RZ–MR		[161]
$^{133}Cs^{133}Cs$	$v=0$	$(0.00545 \pm 0.00005)^b$	MB–MR		[137]
	$v=0$	$(0.00547 \pm 0.00003)^b$	MB–MR		[138]
$^{133}Cs^{35}Cl$	$v=0$	$(0.0212 \pm 0.0011)^b(?)$	MB–MR		[40]
	$v=0$	-0.02803 ± 0.00007^c	RZ–MR		[161]
	$v=1$	-0.02756 ± 0.00017^c	RZ–MR		[161]
	$v=2$	-0.02699 ± 0.00025^c	RZ–MR		[161]
	$v=3$	-0.02699 ± 0.00023^c	RZ–MR		[161]
	$v=4$	-0.02669 ± 0.00026^c	RZ–MR		[161]
	$v=5$	-0.02648 ± 0.00028^c	RZ–MR		[161]
	$v=6$	-0.02630 ± 0.00023^c	RZ–MR		[161]
$^{12}C^{80}Se$	$v=0$	-0.2431 ± 0.0016	RZ–MW		[160]
$^{133}Cs^{19}F$	$v=0$	-0.064203 ± 0.000024	MB–MR		[162]
	$v=1$	-0.063940 ± 0.000048	MB–MR		[162]
	$v=0$	$(0.0621 \pm 0.0055)^b(?)$	MB–MR		[40]
	$v=0$	-0.06413 ± 0.00018^c	RZ–MR		[161]
	$v=1$	-0.06444 ± 0.00030^c	RZ–MR		[161]
	$v=2$	-0.06384 ± 0.00022^c	RZ–MR		[161]
	$v=3$	-0.06355 ± 0.00021^c	RZ–MR		[161]

TABLE A.I (*Continued*)

Molecule	Condition	Value	Experiment	Calculation	Refs.
	$v=4$	-0.06421 ± 0.00088^c	RZ–MR		[161]
$^{133}Cs^{127}I$	$v=0$	< 0.0036	RZ–MW		[152]
$^{63}Cu^{19}F$	$v=0$	-0.0628 ± 0.0002	RZ–MR		[163]
$^{19}F^{19}F$	$v=0$	-0.1208 ± 0.001	MB–MR		[164]
	R_e	-0.101		CHF	[165]
	R_e	-0.0900		CHF	[73]
	$v=0$	-0.0923		CHF	[73]
	R_e	-0.1074		MP2	[73]
	$v=0$	-0.1102		MP2	[73]
	R_e	-0.1048		MP3	[147]
	R_e	-0.1136		L-CCD	[147]
$^{68}Ga^{19}F$	$v=0$	-0.06012 ± 0.00012	RZ–MR		[163]
	R_e	-0.0620		RPA	[22]
$^{69}Ga^{1}H$	R_e	-3.22 ± 0.1	IR		[110]
	R_e	-3.2452		RPA	[26]
	R_e	-3.4440		SOPPA	[26]
	R_e	-3.3798		SOPPA(CCSD)	[26]
	$v=0, J=1$	-3.3369		SOPPA(CCSD)	[26]
	$v=1, J=1$	-3.2556		SOPPA(CCSD)	[26]
	R_e	-2.9457		RASSCF	[26]
	$v=0, J=1$	-2.9111		RASSCF	[26]
	$v=1, J=1$	-2.8448		RASSCF	[26]
$^{69}Ga^{2}H$	R_e	-1.6471		RPA	[26]
	R_e	-1.7479		SOPPA	[26]
	R_e	-1.7163		SOPPA(CCSD)	[26]
	$v=0, J=1$	-1.7007		SOPPA(CCSD)	[26]
	$v=1, J=1$	-1.6707		SOPPA(CCSD)	[26]
	R_e	-1.4949		RASSCF	[26]
	$v=0, J=1$	-1.4824		RASSCF	[26]
	$v=1, J=1$	-1.4583		RASSCF	[26]
$^{71}Ga^{1}H$	R_e	-3.2439		RPA	[26]
	R_e	-3.4426		SOPPA	[26]
	R_e	-3.3784		SOPPA(CCSD)	[26]
	$v=0, J=1$	-3.3355		SOPPA(CCSD)	[26]
	$v=1, J=1$	-3.2543		SOPPA(CCSD)	[26]
	R_e	-2.9445		RASSCF	[26]
	$v=0, J=1$	-2.9099		RASSCF	[26]
	$v=1, J=1$	-2.8437		RASSCF	[26]
$^{71}Ga^{2}H$	R_e	-1.6458		RPA	[26]
	R_e	-1.7465		SOPPA	[26]
	R_e	-1.7149		SOPPA(CCSD)	[26]
	$v=0, J=1$	-1.6993		SOPPA(CCSD)	[26]
	$v=1, J=1$	-1.6693		SOPPA(CCSD)	[26]
	R_e	-1.4937		RASSCF	[26]
	$v=0, J=1$	-1.4812		RASSCF	[26]
	$v=1, J=1$	-1.4572		RASSCF	[26]

Refs.
[161]
[152]
[163]
[164]
[165]
[73]
[73]
[73]
[73]
[147]
[147]
[163]
[22]
[110]
[26]
[26]
[26]
[26]
[26]
[26]
[26]
[26]
[26]
[26]
[26]
[26]
[26]
[26]
[26]
[26]
[26]
[26]
[26]
[26]
[26]
[26]
[26]
[26]
[26]
[26]
[26]
[26]
[26]
[26]
[26]
[26]

TABLE A.I (*Continued*)

Molecule	Condition	Value	Experiment	Calculation	Refs.
$^{70}Ge^{16}O$	$v=0, J=1$	(0.14179 ± 0.00010)	MB–ER		[166]
	$v=1, J=1$	(0.14254 ± 0.00012)	MB–ER		[166]
$^{72}Ge^{16}O$	$v=0, J=1$	(0.14134 ± 0.00011)	MB–ER		[166]
	$v=1, J=1$	(0.14208 ± 0.00010)	MB–ER		[166]
$^{74}Ge^{16}O$	$v=0, J=1$	$-0.141369 \pm 0.000151^{c}$	RZ–MW		[140]
	$v=1, J=1$	$-0.142034 \pm 0.000203^{c}$	RZ–MW		[140]
	$v=2, J=1$	$-0.142686 \pm 0.000292^{c}$	RZ–MW		[140]
	$J=1$	$(-0.141040 \pm 0.000112)^{c}$ $-(6.60 \pm 0.06)\times 10^{-4}\ (v+1/2)$	RZ–MW		[140]
	$v=0, J=1$	-0.14089 ± 0.00010^{c}	MB–ER		[166]
	$v=1, J=1$	-0.14164 ± 0.00012^{c}	MB–ER		[166]
$^{72}Ge^{32}S$	$v=0$	-0.06828 ± 0.00011	RZ–MW		[167]
	R_e	-0.07702 ± 0.0044	IR		[111]
$^{74}Ge^{80}Se$	$v=0$	-0.03765 ± 0.00006	RZ–MW		[167]
$^{74}Ge^{130}Te$	$v=0$	-0.03193 ± 0.00010	RZ–MW		[167]
$^{1}H^{1}H$	$v=0, J=1$	0.8787 ± 0.0070	MB–MR		[11]
	$v=0, J=2$	0.8786 ± 0.0070	MB–MR		[11]
	$v=0, J=1$	0.88291 ± 0.00007	MB–MR		[35]
	$v=0, J=1$	0.88291 ± 0.00007	MB–MR		[36]
	$v=0, J=2$	0.882265 ± 0.000035	MB–MR		[36]
	R_e	0.9103		CHF	[73]
	$v=0$	0.9055		CHF	[73]
	R_e	0.9013		MP2	[73]
	$v=0$	0.8955		MP2	[73]
	$v=0, J=1$	0.8816 ± 0.0002		Full CI	[168]
	R_e	0.8970		MP3	[147]
	R_e	0.8899		L-CCD	[147]
$^{1}H^{2}H$	$v=0, J=1$	0.6601 ± 0.0050	MB–MR		[11]
	$v=0, J=1$	0.663211 ± 0.000012	MB–MR		[169]
	$v=0, J=1$	0.66323		Full CI	[170]
$^{2}H^{2}H$	$v=0, J=1$	0.4406 ± 0.0030	MB–MR		[11]
	$v=0, J=1$	0.442884 ± 0.000052	MB–MR		[36]
	$v=0, J=1$	0.44254		Full CI	[170]
$^{1}H^{79}Br$	R_e	0.3832		RPA	[104,105]
	R_e	0.3926		SOPPA	[104,105]
	R_e	0.3902		CASSCF	[104,105]
$^{1}H^{81}Br$	$v=0, J=1$	0.37122 ± 0.00008	MB–ER		[171]
$^{2}H^{79}Br$	$v=0, J=1$	0.181 ± 0.015	RZ–MW		[156]
$^{2}H^{81}Br$	$v=0, J=1$	0.184 ± 0.015	RZ–MW		[156]
$^{1}H^{35}Cl$	$v=0, J=1$	0.45935 ± 0.00009	MB–ER		[172]
	$v=0$	0.450 ± 0.017	MVCD		[51]
	R_e	0.4886		RPA	[104,105]
	R_e	0.4908		SOPPA	[104,105]
	R_e	0.5023		CASSCF	[104,105]
$^{1}H^{37}Cl$	$v=0$	0.467 ± 0.022	MVCD		[51]
$^{2}H^{35}Cl$	$v=0$	0.235 ± 0.012	MVCD		[51]

TABLE A.I (*Continued*)

Molecule	Condition	Value	Experiment	Calculation	Refs.
$^{2}H^{37}Cl$	$v=0$	0.243 ± 0.014	MVCD		[51]
$^{4}He^{1}H^{+}$	$v=0,\ J=1$	0.5574		SOS	[68]
	$v=0,\ J=2$	0.5568		SOS	[68]
	$v=0,\ J=3$	0.5558		SOS	[68]
	$v=0,\ J=4$	0.5545		SOS	[68]
$^{1}H^{19}F$	$v=0$	0.7392 ± 0.0005	MB–MR		[173]
	R_e	0.749		CHF	[174]
	$v=0$	0.738		CHF	[174]
	$v=0,\ J=1$	0.74104 ± 0.00015	MB–ER		[172]
	R_e	0.760		CHF	[175]
	$v=0,\ J=1$	0.741599 ± 0.000005	MB–ER		[176]
	$v=1,\ J=1$	0.715825 ± 0.000006	MB–ER		[176]
	R_e	0.75449	extrapol.		[176]
	R_e	0.7624		CHF	[73]
	$v=0$	0.7535		CHF	[73]
	R_e	0.7619		MP2	[73]
	$v=0$	0.7524		MP2	[73]
	R_e	0.763		CHF	[88]
	R_e	0.7527		MP3	[147]
	R_e	0.7488		L-CCD	[147]
	R_e	0.7583		CHF	[89]
	R_e	0.7539		CASSCF	[89]
	R_e	0.7513		RASSCF	[177]
	$v=0$	0.7391		RASSCF	[177]
	R_e	0.7671		RPA	[104,105]
	R_e	0.7505		SOPPA	[104,105]
	R_e	0.7635		CASSCF	[104,105]
$^{2}H^{19}F$	$v=0$	0.3695 ± 0.005	MB–MR		[173]
	R_e	0.3744		RASSCF	[177]
	$v=0$	0.3697		RASSCF	[177]
$^{1}H^{127}I$	R_e	0.1952		RPA	[104,105]
	R_e	0.2213		SOPPA	[104,105]
	R_e	0.2154		CASSCF	[104,105]
	R_e	0.2567		RASSCF	[104,105]
$^{2}H^{127}I$	$v=0,\ J=1$	0.096 ± 0.010	RZ–MW		[156]
$^{127}I^{127}I$	$v=0$ $J=12, 14$	-0.000913	RZ–MW		[178]
$^{115}In^{19}F$	R_e	-0.0556 ± 0.0020	IR		[64]
$^{39}K^{39}K$	$v=0$	$(0.02122 \pm 0.00020)^{b}$	MB–MR		[137]
	$v=0$	$(0.02163 \pm 0.00006)^{b}$	MB–MR		[138]
$^{39}K^{19}F$	$v=0$	$(0.0364 \pm 0.0012)^{b}$(?)	MB–MR		[40]
$^{84}Kr^{1}H^{+}$	$v=0$	-0.554489 ± 0.000050	RZ–MW		[108]
	R_e	0.6085		RPA	[104,105]
	R_e	0.5971		SOPPA	[104,105]
	R_e	0.5879		CASSCF	[104,105]
$^{84}Kr^{2}H^{+}$	$v=0$	-0.279113 ± 0.000030	RZ–MW		[108]

Refs.
[51]
[68]
[68]
[68]
[68]
[173]
[174]
[174]
[172]
[175]
[176]
[176]
[176]
[73]
[73]
[73]
[73]
[88]
[147]
[147]
[89]
[89]
[177]
[177]
[104,105]
[104,105]
[104,105]
[173]
[177]
[177]
[104,105]
[104,105]
[104,105]
[104,105]
[156]
[178]
[64]
[137]
[138]
[40]
[108]
[104,105]
[104,105]
[104,105]
[108]

TABLE A.I (*Continued*)

Molecule	Condition	Value	Experiment	Calculation	Refs.
$^{7}\mathrm{Li}^{7}\mathrm{Li}$	$v=0$	$(0.10797 \pm 0.00012)^{b}$	MB–MR		[137]
	$v=0$	0.10797 ± 0.00011	MB–MR		[138]
	R_e	0.1100		CHF	[155]
$^{7}\mathrm{Li}^{79}\mathrm{Br}$	$v=0$	$(0.0911 \pm 0.0039)^{b}(?)$	MB–MR		[40]
$^{7}\mathrm{Li}^{79}\mathrm{Br}$	$v=0$	(0.112056 ± 0.000064)	MB–ER		[42]
$^{7}\mathrm{Li}^{81}\mathrm{Br}$	$v=0$	(0.112217 ± 0.000064)	MB–ER		[42]
$^{6}\mathrm{Li}^{35}\mathrm{Cl}$	$v=0$	$(0.1042 \pm 0.0033)^{b}$	MB–MR		[40]
$^{7}\mathrm{Li}^{35}\mathrm{Cl}$	$v=0$	$(0.0848 \pm 0.0032)^{b}$	MB–MR		[40]
$^{7}\mathrm{Li}^{35}\mathrm{Cl}$	$v=0$	(0.100419 ± 0.000031)	MB–ER		[41]
	$v=1,\ J=1$	$+0.100642 \pm 0.000080$	MB–ER		[41]
$^{7}\mathrm{Li}^{37}\mathrm{Cl}$	$v=0$	(0.101336 ± 0.000040)	MB–ER		[41]
$^{6}\mathrm{Li}^{19}\mathrm{F}$	$v=0$	$(0.0818 \pm 0.0005)^{b}$	MB–MR		[179]
$^{7}\mathrm{Li}^{19}\mathrm{F}$	$v=0$	$(0.0642 \pm 0.0004)^{b}$	MB–MR		[179]
	$v=0$	$(0.07367 \pm 0.00050)^{b}$	MB–MR		[40]
	R_e	0.0729		RPA	[22]
$^{7}\mathrm{Li}^{1}\mathrm{H}$	$v=0$	$-(0.654 \pm 0.007)$ $+(1.2 \pm 0.6) \times 10^{-4}\ J(J+1)$	MB–MR		[37]
	R_e	-0.674		CHF	[180]
	$v=0$	-0.6677		CHF	[181]
	$v=1$	-0.6536		CHF	[181]
	$v=0,\ J=1$	-0.65842 ± 0.00017	MB–ER		[182]
	$v=0,\ J=1$	0.6898		CHF	[129]
	$v=0,\ J=1$	0.6962		SOPPA	[129]
	$v=0,\ J=1$	0.6717		CCDPPA	[129]
	R_e	0.6430		CCSDPPA	[129]
	$v=0,\ J=1$	0.6351		CCSDPPA	[129]
	R_e	0.6973		CHF	[89]
	R_e	0.6594		CASSCF	[89]
$^{7}\mathrm{Li}^{2}\mathrm{H}$	$v=0$	$-(0.272 \pm 0.005)$ $+(3.4 \pm 1.7) \times 10^{-5}\ J(J+1)$	MB–MR		[37]
	$v=0,\ J=1$	-0.27674 ± 0.00011	MB–ER		[182]
$^{7}\mathrm{Li}^{127}\mathrm{I}$	$v=0$	$(0.1068 \pm 0.0089)^{b}(?)$	MB–MR		[40]
$^{14}\mathrm{N}^{14}\mathrm{N}$	R_e	-0.240		CHF	[151]
	R_e	-0.288		CHF	[88]
	R_e	-0.2872		CHF	[147]
	R_e	-0.2653		MP2	[147]
	R_e	-0.2784		MP3	[147]
	R_e	-0.2739		L-CCD	[147]
$^{15}\mathrm{N}^{15}\mathrm{N}$	$v=0$	$(0.2593 \pm 0.0005)^{b}$	MB–MR		[38]
	R_e	-0.224		CHF	[151]
	R_e	-0.2681		CHF	[73]
	$v=0$	-0.2711		CHF	[73]
	R_e	-0.2477		MP2	[73]
	$v=0$	-0.2478		MP2	[73]
	R_e	-0.2599		MP3	[147]
	R_e	-0.2557		L-CCD	[147]

TABLE A.I (*Continued*)

Molecule	Condition	Value	Experiment	Calculation	Refs.
$^{23}Na^{19}F$	$v=0$	$-0.00536 \pm 0.00006)^b$			[183]
$^{23}Na^{23}Na$	$v=0$	$(0.03860 \pm 0.00009)^b$	MB–MR		[137]
	$v=0$	$(0.03892 \pm 0.00010)^b$	MB–MR		[138]
$^{23}Na^{127}I$	$v=0$	$(0.0268 \pm 0.0047)^b$(?)	MB–MR		[40]
$^{23}Na^{39}K$	$v=0$	$(0.0253 \pm 0.0029)^b$	MB–MR		[40]
$^{20}Ne^{1}H^{+}$	R_e	0.8805		RPA	[104,105]
	R_e	0.8649		SOPPA	[104,105]
	R_e	0.8714		CASSCF	[104,105]
$^{208}Pb^{16}O$	$v=0$	-0.16233 ± 0.00039	RZ–MW		[184]
$^{208}Pb^{32}S$	$v=0$	-0.06440 ± 0.00004	RZ–MW		[167]
$^{208}Pb^{80}Se$	$v=0$	-0.02764 ± 0.00007	RZ–MW		[167]
$^{208}Pb^{130}Te$	$v=0$	(-0.01800 ± 0.00004)	RZ–MW		[185]
$^{85}Rb^{85}Rb$	$v=0$	$(0.00953 \pm 0.00006)^b$	MB–MR		[137]
	$v=0$	$(0.00953 \pm 0.00004)^b$	MB–MR		[138]
$^{85}Rb^{87}Rb$	$v=0$	$(0.00940 \pm 0.00006)^b$	MB–MR		[138]
$^{85}Rb^{35}Cl$	$v=0$	$(0.0183 \pm 0.0018)^b$(?)	MB–MR		[40]
$^{85}Rb^{19}F$	$v=0$	-0.05471 ± 0.00004^b	MB–ER		[186]
$^{85}Rb^{19}F$	$v=0$	$(0.0441 \pm 0.0028)^b$(?)	MB–MR		[40]
$^{28}Si^{16}O$	$v=0,\ J=1$	-0.15359 ± 0.00012^c	MB–ER		[166]
	$v=1,\ J=1$	-0.15450 ± 0.00011^c	MB–ER		[166]
	$v=2,\ J=1$	-0.15539 ± 0.00012^c	MB–ER		[166]
$^{28}Si^{32}S$	$v=0,\ J=1$	-0.091131 ± 0.000108^c	RZ–MW		[140]
	$v=1,\ J=1$	-0.091451 ± 0.000132^c	RZ–MW		[140]
	$v=2,\ J=1$	-0.091632 ± 0.000117^c	RZ–MW		[140]
	$v=3,\ J=1$	-0.092176 ± 0.000220^c	RZ–MW		[140]
	$J=1$	$(-0.090974 \pm 0.000065)^c$ $-(2.96 \pm 0.24) \times 10^{-4}\ (v+1/2)$	RZ–MW		[140]
$^{120}Sn^{16}O$	$v=0$	-0.14631 ± 0.00038	RZ–MW		[184]
$^{120}Sn^{32}S$	$v=0$	-0.06120 ± 0.00007	RZ–MW		[167]
$^{120}Sn^{80}Se$	$v=0$	-0.03007 ± 0.00010	RZ–MW		[167]
$^{120}Sn^{130}Te$	$v=0$	-0.02212 ± 0.00013	RZ–MW		[167]
$^{130}Te^{130}Te$	$v=6,\ J=52$	-0.308 ± 0.009	beat resonance		[187]
$^{203}Tl^{35}Cl$	$v=0,\ J=1$	-0.02798 ± 0.00007^c	MB–ER		[188]
$^{205}Tl^{35}Cl$	$v=0,\ J=1$	-0.02806 ± 0.00004^c	MB–ER		[188]
	$v=1,\ J=1$	-0.02801 ± 0.00005	MB–ER		[188]
	$v=2,\ J=1$	-0.02788 ± 0.00008	MB–ER		[188]
$^{205}Tl^{37}Cl$	$v=0,\ J=1$	-0.02661 ± 0.00007^c	MB–ER		[188]
$^{203}Tl^{19}F$	$v=0,\ J=1$	-0.053568 ± 0.000080	MB–ER		[189]
$^{205}Tl^{19}F$	$v=0,\ J=1$	-0.053556 ± 0.00072^c	MB–ER		[189]
$^{205}Tl^{19}F$	$v=0$	-0.05370 ± 0.00015^c	RZ–MR		[161]
	$v=1,\ J=1$	-0.053507 ± 0.000035	MB–ER		[189]
	$v=2,\ J=1$	-0.053469 ± 0.000059	MB–ER		[189]
	$v=0,\ J=2$	-0.053580 ± 0.000079	MB–ER		[189]
$^{132}Xe^{1}H^{+}$	$v=0$	(0.30 ± 0.05)	line broadening		[107]

TABLE A.I (*Continued*)

Molecule	Condition	Value	Experiment	Calculation	Refs.
	R_e	0.4351		RPA	[104,105]
	R_e	0.4423		SOPPA	[104,105]
	R_e	0.4288		CASSCF	[104,105]

[a] RZ–MW, microwave rotational Zeeman effect; MB–MR, molecular beam and magnetic resonance; MB–ER, molecular beam and electric resonance; MVCD, magnetic vibrational circular dichroism; RPA, random-phase approximation; CHF, coupled Hartree–Fock; SOPPA, second-order polarization propagator approximation; CCSDPPA and SOPPA(CCSD) coupled-cluster singles- and doubles-based SOPPA; CASSCF, response method based on a complete active-space self-consistent field; RASSCF, response method based on a restricted active-space self-consistent field; MP2 and MP3, methods based on second- and third-order, respectively, Møller–Plesset perturbation theory; L-CCD, method based on linearization of the coupled-cluster doubles method; SOS, sum-over-states method; full CI, full configuration interaction.

[b] Values in parentheses signify that the sign is not determined; a question mark in parentheses signifies that the value is suspect (see Section II.A).

[c] The sign is assumed.

Acknowledgments

J. F. O. thanks Professor M. C. L. Gerry for helpful comments on microwave spectroscopy and the Department of Chemistry at Odense University for hospitality during his visits in August 1996, 1998, and 1999. This work was supported in by part by grants from the Danish Natural Science Research Council to J. O. (grant no. 9600856) and to S.P.A.S. (grant no. 9701136).

References

1. W. Gordy and R. L. Cook, *Microwave Molecular Spectra*, Wiley, New York, 1984.
2. C. H. Townes and A. L. Schawlow, *Microwave Spectroscopy*, McGraw-Hill, New York, 1955.
3. W. H. Flygare, *Molecular Structure and Dynamics*, Prentice-Hall, Englewood Cliffs, NJ, 1978.
4. D. H. Sutter and W. H. Flygare, *Top. Curr. Chem.* **63**, 89 (1976).
5. P. R. Bunker, *J. Mol. Spectrosc.* **35**, 306 (1970).
6. J. F. Ogilvie, *The Vibrational and Rotational Spectrometry of Diatomic Molecules*, Academic, London, 1998.
7. J. Oddershede and J. R. Sabin, *Chem. Phys.* **122**, 291 (1988).
8. R. Frisch and O. Stern, *Z. Phys.* **85**, 4 (1933).
9. I. Estermann and O. Stern, *Z. Phys.* **85**, 17 (1933).
10. E. U. Condon, *Phys. Rev.* **30**, 781 (1927).
11. N. F. Ramsey, *Phys. Rev.* **58**, 226 (1940).
12. G. C. Wick, *Z. Phys.* **85**, 25 (1933).
13. G. C. Wick, *Nuovo Cimento* **10**, 118 (1933).
14. G. C. Wick, *Phys. Rev.* **73**, 51 (1948).
15. N. F. Ramsey, *Molecular Beams*, Oxford University Press, London, 1969.

16. D. K. Coles and W. E. Good, *Phys. Rev.* **70**, 979 (1946).
17. J. T. Cox and W. Gordy, *Phys. Rev.* **101**, 1298 (1956).
18. C. K. Jen, *Phys. Rev.* **81**, 197 (1951).
19. J. R. Eshbach and M. W. P. Strandberg, *Phys. Rev.* **85**, 24 (1952).
20. I. M. Mills, T. Cvitaš, K. Homann, N. Kallay, and K. Kuchitsu, *Quantities, Units and Symbols in Physical Chemistry*, 2nd Ed., Blackwell, Oxford, U.K., 1993.
21. J. H. van Vleck, *The Theory of Electric and Magnetic Susceptibilities*, Oxford University Press, London, 1932.
22. S. P. A. Sauer, *Chem. Phys. Lett.* **297**, 475 (1998).
23. J. K. G. Watson, *J. Mol. Spectrosc.* **45**, 99 (1973).
24. C. H. Townes, G. C. Dousmanis, R. L. White, and R. F. Schwarz, *Discuss. Faraday Soc.* **19**, 56 (1955).
25. J. Geertsen and G. E. Scuseria, *J. Chem. Phys.* **90**, 6486 (1989).
26. S. P. A. Sauer, *Chem. Phys. Lett.* **260**, 271 (1996).
27. J. T. Hougen, *J. Chem. Phys.* **36**, 519 (1962).
28. J. K. G. Watson, *Mol. Phys.* **19**, 465 (1970).
29. B. J. Howard and R. E. Moss, *Mol. Phys.* **20**, 147 (1971).
30. P. R. Bunker and R. E. Moss, *Mol. Phys.* **33**, 417 (1977).
31. J. K. G. Watson, *J. Mol. Spectrosc.* **80**, 411 (1980).
32. R. M. Herman and J. F. Ogilvie, *Adv. Chem. Phys.* **103**, 187 (1998).
33. R. M. Herman and A. Asgharian, *J. Mol. Spectrosc.* **19**, 305 (1966).
34. F. Knauer and O. Stern, *Z. Phys.* **39**, 780 (1926).
35. N. J. Harrick and N. F. Ramsey, *Phys. Rev.* **88**, 228 (1952).
36. R. G. Barnes, P. J. Bray, and N. F. Ramsey, *Phys. Rev.* **94**, 893 (1954).
37. T. R. Lawrence, C. H. Anderson, and N. F. Ramsey, *Phys. Rev.* **130**, 1865 (1963).
38. S. I. Chan, M. R. Baker, and N. F. Ramsey, *Phys. Rev.* **A136**, 1224 (1964).
39. J. W. Cederberg and N. F. Ramsey, *Phys. Rev.* **A135**, 39 (1964).
40. F. Mehran, R. A. Brooks, and N. F. Ramsey, *Phys. Rev.* **141**, 93 (1966).
41. R. R. Freeman, D. W. Johnson, and N. F. Ramsey, *J. Chem. Phys.* **61**, 3471 (1974).
42. J. L. Cecchi and N. F. Ramsey, *J. Chem. Phys.* **60**, 53 (1974).
43. R. E. Moss and A. J. Perry, *Mol. Phys.* **25**, 1121 (1973).
44. R. H. Hughes and E. B. Wilson, *Phys. Rev.* **71**, 562 (1947).
45. C. A. Burrus, *J. Chem. Phys.* **28**, 427 (1958).
46. T. J. Balle and W. H. Flygare, *Rev. Sci. Instrum.* **52**, 33 (1981).
47. A. Klesing and D. H. Sutter, *Z. Naturforsch.* **48a**, 968 (1993).
48. K. M. Evenson, R. J. Saykally, D. A. Jennings, R. F. Curl, and J. M. Brown, in *Chemical and Biochemical Applications of Lasers*, (C. B. Moore, ed.), Vol. 5, p. 95, Academic, New York, 1980.
49. T. D. Varberg, K. M. Evenson, and J. M. Brown, *J. Chem. Phys.* **100**, 2487 (1994).
50. B. Wang and T. A. Keiderling, *J. Chem. Phys.* **98**, 903 (1993).
51. C. N. Tam and T. A. Keiderling, *J. Mol. Spectrosc.* **157**, 391 (1993).
52. P. J. Stephens, *Adv. Chem. Phys.* **35**, 197 (1976).
53. B. Wang, R. K. Yoo, P. V. Croatto, and T. A. Keiderling, *Chem. Phys. Lett.* **180**, 339 (1991).

54. B. Wang, R. K. Yoo, P. V. Croatto, and T. A. Keiderling, *J. Phys. Chem.* **96**, 2422 (1992).
55. I. Ozier, P. Yi, A. Khosla, and N. F. Ramsey, *J. Chem. Phys.* **46**, 1530 (1967).
56. J. L. Dunham, *Phys. Rev.* **41**, 721 (1932).
57. J. F. Ogilvie, *J. Phys. B: At. Mol. Opt. Phys.* **27**, 47 (1994).
58. J. F. Ogilvie, *Proc. Royal Soc. London* **A378**, 287 (1981).
59. J. F. Ogilvie, *Proc. Royal Soc. London* **A381**, 479 (1982).
60. J. F. Ogilvie, *J. Chem. Phys.* **88**, 2804 (1988).
61. J. H. van Vleck, *J. Chem. Phys.* **4**, 327 (1936).
62. J. F. Ogilvie, in *Fundamental Principles of Molecular Modeling*, (W. Gans, A. Amman, and J. C. A. Boeyens, eds.), p. 41, Plenum, New York, 1996.
63. E. Tiemann, H. Arnst, W. U. Stieda, T. Törring, and J. Hoeft, *Chem. Phys.* **67**, 133 (1982).
64. J. F. Ogilvie, H. Uehara, and K. Horiai, *J. Chem. Soc. Faraday Trans.* **91**, 3007 (1995).
65. J. Oddershede and J. Geertsen, *J. Chem. Phys.* **92**, 6036 (1990).
66. M. J. Packer, S. P. A. Sauer, and J. Oddershede, *J. Chem. Phys.* **100**, 8969 (1994).
67. D. M. Bishop and L. M. Cheung, *J. Chem. Phys.* **72**, 5125 (1980).
68. D. M. Bishop and L. M. Cheung, *J. Chem. Phys.* **74**, 1817 (1981).
69. J. Oddershede, *Adv. Chem. Phys.* **69**, 201 (1987).
70. J. Olsen and P. Jørgensen, *J. Chem. Phys.* **82**, 3235 (1985).
71. H. Hellmann, *Z. Phys.* **85**, 180 (1933).
72. R. P. Feynman, *Phys. Rev.* **56**, 340 (1939).
73. S. M. Cybulski and D. M. Bishop, *J. Chem. Phys.* **100**, 2019 (1994).
74. S. P. A. Sauer and J. Oddershede, *Int. J. Quantum Chem.* **50**, 317 (1994).
75. J. Fagerström and J. Oddershede, *J. Chem. Phys.* **101**, 10775 (1994).
76. J. Oddershede, in *Methods in Computational Molecular Physics*, (G. H. F. Diercksen and S. Wilson, eds.), p. 249, Reidel, Dordrecht, The Netherlands, 1983.
77. J. Linderberg and Y. Öhrn, *Propagators in Quantum Chemistry*, Academic, London, 1973.
78. J. Oddershede, P. Jørgensen, and D. L. Yeager, *Comput. Phys. Rep.* **2**, 33 (1984).
79. J. Oddershede, *Int. J. Quantum Chem. Symp.* **16**, 583 (1982).
80. E. S. Nielsen, P. Jørgensen, and J. Oddershede, *J. Chem. Phys.* **73**, 6238 (1980).
81. J. Geertsen and J. Oddershede, *J. Chem. Phys.* **85**, 2112 (1986).
82. J. Geertsen, S. Eriksen, and J. Oddershede, *Adv. Quantum Chem.* **22**, 167 (1991).
83. R. J. Bartlett, *Ann. Rev. Phys. Chem.* **32**, 359 (1981).
84. S. P. A. Sauer, *J. Phys. B: At. Mol. Opt. Phys.* **30**, 3773 (1997).
85. M. J. Packer, E. K. Dalskov, T. Enevoldsen, H. J. Aa. Jensen, and J. Oddershede, *J. Chem. Phys.* **105**, 5886 (1996).
86. P. Pulay, *Adv. Chem. Phys.* **69**, 241 (1987).
87. T. Helgaker and P. Jørgensen, *Adv. Quantum Chem.* **19**, 183 (1988).
88. J. Gauss, K. Ruud, and T. Helgaker, *J. Chem. Phys.* **105**, 2804 (1996).
89. K. Ruud, T. Helgaker, and P. Jørgensen, *J. Chem. Phys.* **107**, 10599 (1997).
90. K. Ruud, T. Helgaker, K. L. Bȧk, P. Jørgensen, and H. J. Aa. Jensen, *J. Chem. Phys.* **99**, 3847 (1993).
91. F. London, *J. Phys. Radium* **8**, 397 (1937).

92. R. Ditchfield, *Mol. Phys.* **27**, 789 (1974).
93. Aa. E. Hansen and T. D. Bouman, *J. Chem. Phys.* **82**, 5035 (1985).
94. T. Helgaker and P. Jørgensen, *J. Chem. Phys.* **95**, 2595 (1991).
95. J. Olsen, K. L. Bak, K. Ruud, T. Helgaker, and P. Jørgensen, *Theor. Chim. Acta* **90**, 421 (1995).
96. B. Rosenblum, A. H. Nethercot, and C. H. Townes, *Phys. Rev.* **109**, 400 (1958).
97. R. K. Nesbet, *J. Chem. Phys.* **40**, 3619 (1964).
98. J. J. Ewing, H. L. Tigelaar, and W. H. Flygare, *J. Chem. Phys.* **56**, 1957 (1972).
99. G. H. Cheesman, A. J. T. Finney, and I. K. Snook, *Theor. Chim. Acta* **16**, 33 (1970).
100. S. Green, *Adv. Chem. Phys.* **25**, 179 (1974).
101. J. McGurk, C. L. Norris, H. L. Tigelaar, and W. H. Flygare, *J. Chem. Phys.* **58**, 3118 (1973).
102. K. C. Janda, W. Klemperer, and S. E. Novick, *J. Chem. Phys.* **64**, 2698 (1976).
103. B. Fabricant and J. S. Muenter, *J. Chem. Phys.* **66**, 5274 (1977).
104. T. Rasmussen, *Calculation of Rotational g Factors*, Master's thesis, Odense University, Odense, Denmark, 1997.
105. T. Rasmussen and S. P. A. Sauer, to be published.
106. K. B. Laughlin, G. A. Blake, R. C. Cohen, D. C. Hovde, and R. J. Saykally, *Phil. Trans. Royal Soc. London* **A234**, 109 (1988).
107. K. A. Peterson, R. H. Petrmichl, R. L. McClain, and R. C. Woods, *J. Chem. Phys.* **95**, 2352 (1991).
108. H. Linnartz, M. Havenith, E. Zwart, W. L. Meerts, and J. J. ter Meulen, *J. Mol. Spectrosc.* **153**, 710 (1992).
109. P. Rosmus and E. A. Reinsch, *Z. Naturforsch.* **35a**, 1066 (1980).
110. J. F. Ogilvie and S. C. Liao, *Chem. Phys. Lett.* **226**, 281 (1994).
111. J. F. Ogilvie, *Mol. Phys.* **88**, 1055 (1996).
112. J. F. Ogilvie, *J. Chem. Soc. Faraday Trans.* **91**, 3005 (1995).
113. S. P. A. Sauer and J. F. Ogilvie, *J. Phys. Chem.* **98**, 8617 (1994).
114. J. F. Ogilvie, *J. Chin. Chem. Soc.* **39**, 381 (1992).
115. J. L. Deutsch, W. S. Neil, and D. A. Ramsay, *J. Mol. Spectrosc.* **125**, 115 (1987).
116. J. B. White, M. Dulick, and P. F. Bernath, *J. Chem. Phys.* **99**, 8371 (1993).
117. R. M. Stevens and W. N. Lipscomb, *J. Chem. Phys.* **42**, 3666 (1965).
118. R. A. Hegstrom and W. N. Lipscomb, *J. Chem. Phys.* **45**, 2378 (1966).
119. M. Jaszuński, *Theoret. Chim. Acta* **48**, 323 (1978).
120. G. Boucekkine-Yaker, A. Boucekkine, M. Żaucer, and G. Berthier, *Int. J. Quantum Chem.* **23**, 365 (1983).
121. G. T. Daborn and N. C. Handy, *Mol. Phys.* **49**, 1277 (1983).
122. M. Iwai and A. Saika, *Int. J. Quantum Chem.* **24**, 627 (1983).
123. P. W. Fowler and E. Steiner, *Mol. Phys.* **74**, 1147 (1991).
124. S. P. A. Sauer, J. Oddershede, and J. Geertsen, *Mol. Phys.* **76**, 445 (1992).
125. S. P. A. Sauer, T. Enevoldsen, and J. Oddershede, *J. Chem. Phys.* **98**, 9748 (1993).
126. C. van Wüllen, *Theoret. Chim. Acta* **87**, 89 (1993).
127. K. Ruud, T. Helgaker, K. L. Bak, P. Jørgensen, and J. Olsen, *Chem. Phys.* **195**, 157 (1995).
128. G. Audi and A. H. Wapstra, *Nucl. Phys.* **A595**, 409 (1995).
129. J. F. Ogilvie, J. Oddershede, and S. P. A. Sauer, *Chem. Phys. Lett.* **228**, 183 (1994).

130. M. Dulick, K. Q. Zhang, B. Guo, and P. F. Bernath, *J. Mol. Spectrosc.* **188**, 14 (1998).
131. R. G. Woolley, *Adv. Phys.* **25**, 27 (1976).
132. N. C. Handy and A. M. Lee, *Chem. Phys. Lett.* **252**, 425 (1996).
133. R. D. Amos, J. F. Gaw, N. C. Handy, and S. Carter, *J. Chem. Soc. Faraday Trans. 2* **84**, 1247 (1988).
134. J. F. Ogilvie, *Ber. Bunsenges. Phys. Chem.* **100**, 1906 (1996).
135. J. F. Ogilvie, *Chem. Phys. Lett.* **267**, 590 (1997).
136. I. Espe, *Phys. Rev.* **103**, 1254 (1956).
137. R. A. Brooks, C. H. Anderson, and N. F. Ramsey, *Phys. Rev. Lett.* **10**, 441 (1963).
138. R. A. Brooks, C. H. Anderson, and N. F. Ramsey, *Phys. Rev.* **A136**, 62 (1964).
139. R. H. Tipping and J. F. Ogilvie, *J. Mol. Struct.* **35**, 1 (1976).
140. R. Honerjäger and R. Tischer, *Z. Naturforsch.* **28a**, 1374 (1973).
141. M. Mizushima, *The Theory of Rotating Diatomic Molecules*, Wiley, New York, 1975.
142. E. Tiemann, in *Molecular Constants*, (W. Huttner, ed.), Vol. 19D, Springer, Berlin, 1995.
143. A. Carrington, G. N. Currie, D. H. Levy, and T. A. Miller, *Mol. Phys.* **17**, 535 (1969).
144. R. Luypaert, J. van Craen, J. Coremans, and G. de Vlieger, *J. Phys.* **B14**, 2575 (1981).
145. S. Klee and J. F. Ogilvie, *Spectrochim. Acta* **A49**, 345 (1993).
146. S. Saupe, B. Meyer, M. H. Wappelhorst, W. Urban, and A. G. Maki, *J. Mol. Spectrosc.* **179**, 13 (1996).
147. S. M. Cybulski and D. M. Bishop, *J. Chem. Phys.* **106**, 4082 (1997).
148. W. Kasten, W. Stahl, and H. Dreizler, *Z. Naturforsch.* **39a**, 511 (1984).
149. J. F. Ogilvie and S. C. Liao, *Acta Phys. Hung.* **74**, 365 (1994).
150. R. Honerjäger and R. Tischer, *Z. Naturforsch.* **29a**, 342 (1974).
151. E. A. Laws, R. M. Stevens, and W. N. Lipscomb, *J. Chem. Phys.* **54**, 4269 (1971).
152. K. B. Laughlin, G. A. Blake, R. C. Cohen, and R. J. Saykally, *J. Chem. Phys.* **90**, 1358 (1989).
153. R. Brooks and M. Kaufman, *J. Chem. Phys.* **43**, 3406 (1965).
154. R. A. Hegstrom and W. N. Lipscomb, *J. Chem. Phys.* **48**, 809 (1968).
155. W. N. Lipscomb, *MTP Int. Rev. Sci. Phys. Chem.* **1**, 167 (1972).
156. C. A. Burrus, *J. Chem. Phys.* **30**, 976 (1959).
157. R. M. Stevens and M. Karplus, *J. Chem. Phys.* **49**, 1094 (1968).
158. W. L. Meerts, F. H. De Leeuw, and A. Dymanus, *Chem. Phys.* **22**, 319 (1977).
159. I. Ozier, L. M. Crapo, and N. F. Ramsey, *J. Chem. Phys.* **49**, 2314 (1968).
160. J. McGurk, H. L. Tigelaar, S. L. Rock, C. L. Norris, and W. H. Flygare, *J. Chem. Phys.* **58**, 1420 (1973).
161. R. Honerjäger and R. Tischer, *Z. Naturforsch.* **28a**, 458 (1973).
162. G. Gräff and Ö. Runólfsson, *Z. Phys.* **187**, 140 (1965).
163. R. Honerjäger and R. Tischer, *Z. Naturforsch.* **29a**, 1919 (1974).
164. I. Ozier, L. M. Crapo, J. W. Cederberg, and N. F. Ramsey, *Phys. Rev. Lett.* **13**, 482 (1964).
165. R. M. Stevens and W. N. Lipscomb, *J. Chem. Phys.* **41**, 3710 (1964).
166. R. E. Davis and J. S. Muenter, *J. Chem. Phys.* **61**, 2940 (1974).
167. R. Honerjäger and R. Tischer, *Z. Naturforsch.* **32a**, 1 (1977).
168. K. Ruud, P.-O. Åstrand, T. Helgaker, and K. V. Mikkelsen, *J. Mol. Struct.* **388**, 231 (1996).

169. W. E. Quinn, J. M. Baker, J. T. LaTourrette, and N. F. Ramsey, *Phys. Rev.* **112**, 1929 (1958).
170. P.-O. Åstrand, K. Ruud, K. V. Mikkelsen, and T. Helgaker, *Chem. Phys. Lett.* **271**, 163 (1997).
171. O. D. Dabbousi, W. L. Meerts, F. H. de Leeuw, and A. Dymanus, *Chem. Phys.* **2**, 473 (1973).
172. F. H. De Leeuw and A. Dymanus, *J. Mol. Spectrosc.* **48**, 427 (1973).
173. M. R. Baker, C. H. Anderson, J. Pinkerton, and N. F. Ramsey, *Bull. Am. Phys. Soc.* **6**, 19 (1961).
174. R. M. Stevens and W. N. Lipscomb, *J. Chem. Phys.* **41**, 184 (1964).
175. P. Swanstrøm, W. P. Kraemer, and G. H. F. Diercksen, *Theoret. Chim. Acta* **44**, 109 (1977).
176. S. M. Bass, R. L. DeLeon, and J. S. Muenter, *J. Chem. Phys.* **86**, 4305 (1987).
177. P.-O. Åstrand, K. Ruud, K. V. Mikkelsen, and T. Helgaker, *J. Chem. Phys.* **110**, 9463 (1999).
178. R. Solarz and D. H. Levy, *Chem. Phys. Lett.* **17**, 35 (1972).
179. A. M. Russell, *Phys. Rev.* **111**, 1558 (1958).
180. R. M. Stevens, R. M. Pitzer, and W. N. Lipscomb, *J. Chem. Phys.* **38**, 550 (1963).
181. R. M. Stevens and W. N. Lipscomb, *J. Chem. Phys.* **40**, 2238 (1964).
182. R. R. Freeman, A. R. Jacobsen, D. W. Johnson, and N. F. Ramsey, *J. Chem. Phys.* **63**, 2597 (1975).
183. G. Gräff and G. Werth, *Z. Phys.* **183**, 223 (1965).
184. R. Honerjäger and R. Tischer, *Z. Naturforsch.* **28a**, 1372 (1973).
185. R. Honerjäger and R. Tischer, *Z. Naturforsch.* **29a**, 1695 (1974).
186. G. Gräff, R. Schönwasser, and M. Tonutti, *Z. Phys.* **199**, 157 (1967).
187. R. S. Ferber, A. I. Okunevich, O. A. Shmit, and M. Y. Tamanis, *Chem. Phys. Lett.* **90**, 476 (1982).
188. R. Ley and W. Schauer, *Z. Naturforsch.* **27a**, 77 (1972).
189. R. V. Boeckh, G. Gräff, and R. Ley, *Z. Phys.* **179**, 285 (1964).