On the Electric Multipole Moments of Carbon Monoxide

George Maroulis
Department of Chemistry, University of Patras, GR-26110 Patras, Greece

Z. Naturforsch. **47a**, 480–484 (1992); received October 11, 1991

The electric dipole, quadrupole, octopole and hexadecapole moment of carbon monoxide has been obtained from finite-field SCF and Moeller-Plesset perturbation theory calculations. The resulting values for the octopole and hexadecapole moments of CO($X\,^1\Sigma^+$) are 3.59 $e a_0^3$ and -9.01 $e a_0^4$, respectively.

Key words: Carbon monoxide, Electric moments, Octopole moment, Hexadecapole moment.

1. Introduction

Electric moments are relevant for many phenomena caused by intermolecular interactions [1–4]. Recent work [5–13] has provided evidence that models relying on the knowledge of the electric moments of the monomers can be used to predict molecular structures and properties of weakly bonded van der Waals systems. Not all electric moments are easily amenable to experiment [2]. Experimental determinations of electric moments beyond the quadrupole are extremely rare. Theory can contribute to the field by predicting these properties.

The electric moments of carbon monoxide have been the object of numerous experimental or theoretical studies [14–27]. Of particular interest to theory is the determination of Hartree-Fock values for the dipole (μ), quadrupole (Θ), octopole (Ω) and hexadecapole (Φ) moments from fully numerical calculations (NHF) by Laaksonen, Pyykkö and Sundholm [22]. This makes possible the construction of Gaussian-type basis sets of near Hartree-Fock quality and the subsequent prediction of accurate electric moments via theoretical methods that take into account electron correlation. In this work we report self-consistent field (SCF) and finite-field Moeller-Plesset perturbation theory (MP) calculations of μ, Θ, Ω, and Φ. The higher moments are extracted from the energies of the molecule perturbed by strategically placed electric point charges. This approach has been followed successfully in previous work on N_2 [28], F_2 [29], HCl [30] and HCCH [31]. Previous correlated values of Ω and Φ for carbon monoxide have been obtained as expectation values of the relevant operators using SD-CI (single and double excitations configuration interaction) wavefunctions. Our approach to the subject has distinct advantages over the SD-CI method [21].

Atomic units are used throughout this work. The conversion factors from atomic to SI units are:

Energy,	$1\,E_h = 4.3597482 \times 10^{-18}$ J,
Length,	$1\,a_0 = 0.529177249 \times 10^{-11}$ m,
Dipole moment,	$1\,e a_0 = 8.478358 \times 10^{-30}$ Cm,
Quadrupole moment,	$1\,e a_0^2 = 4.486554 \times 10^{-40}$ Cm^2,
Octopole moment,	$1\,e a_0^3 = 2.374182 \times 10^{-50}$ Cm^3,
Hexadecapole moment.	$1\,e a_0^4 = 1.256363 \times 10^{-60}$ Cm^4.

2. Theory

The energy of an uncharged molecule in a weak electric field can be written as [1, 32]

$$\begin{aligned} E = E^0 &- \mu_\alpha F_\alpha - (1/3)\,\Theta_{\alpha\beta} - (1/15)\,\Omega_{\alpha\beta\gamma} \\ &- (1/105)\,\Phi_{\alpha\beta\gamma\delta} + \dots \\ &- (1/2)\,\alpha_{\alpha\beta} F_\alpha F_\beta - (1/3)\,A_{\alpha,\beta\gamma} F_\alpha F_{\beta\gamma} \\ &- (1/6)\,C_{\alpha\beta,\gamma\delta} F_{\alpha\beta} F_{\gamma\delta} - (1/15)\,E_{\alpha,\beta\gamma\delta} F_\alpha F_{\beta\gamma\delta} + \dots \\ &- (1/6)\,\beta_{\alpha\beta\gamma} F_\alpha F_\beta F_\gamma - (1/6)\,B_{\alpha\beta,\gamma\delta} F_\alpha F_\alpha F_{\gamma\delta} + \dots \\ &- (1/24)\,\gamma_{\alpha\beta\gamma\delta} F_\alpha F_\beta F_\gamma F_\delta + \dots, \end{aligned} \tag{1}$$

where F_α, $F_{\alpha\beta}$, … are the field, field gradient, etc. at the origin, E^0, μ_α, $\Theta_{\alpha\beta}$, $\Omega_{\alpha\beta\gamma}$ and $\Phi_{\alpha\beta\gamma\delta}$ the energy and permanent moments of the free molecule and $\alpha_{\alpha\beta}$, $\beta_{\alpha\beta\gamma}$, $\gamma_{\alpha\beta\gamma\delta}$, $A_{\alpha,\beta\gamma}$, $C_{\alpha\beta,\gamma\delta}$, $E_{\alpha,\beta\gamma\delta}$ and $B_{\alpha\beta,\gamma\delta}$ the molec-

---

Reprint requests to Prof. George Maroulis, Department of Chemistry, University of Patras, GR-26110 Patras, Greece.

0932-0784 / 92 / 0300-0480 $ 01.30/0. – Please order a reprint rather than making your own copy.

ular polarizabilities. The greek suffixes denote Cartesian components and a repeated suffix implies summation over x, y, and z.

For a polar linear molecule like CO there is only one independent component for an electric moment tensor of any order, μ_α, $\Theta_{\alpha\beta}$, $\Omega_{\alpha\beta\gamma}$ or $\Phi_{\alpha\beta\gamma\delta}$ [1]. Therefore we shall simply write μ, Θ, Ω and Φ for the respective properties. The dipole moment is independent of the choice of the origin but the higher moments are not [1].

The electric moments are extracted from (1) by using suitable electric fields. Using a homogeneous electric field, all field-gradient terms are eliminated from (1) and the dipole moment is easily obtained. We give here a description of the calculation of Θ, Ω, and Φ. We simulate a weak quadrupolar field by placing an array of four charges $-32\,Q$, Q, Q, $-32\,Q$ at $(2R, \pi)$, (R, π), $(R, 0)$, and $(R, 0)$ on the molecular axis. Using very distant charges we ensure that higher terms make a negligible contribution to the perturbed energy $E_{\mathrm{qd}}(Q, R)$, so that

$$E_{\mathrm{qd}}(Q,R) \approx E^0 - 6\,\Theta\,(Q/R^3) \tag{2}$$

and

$$\Theta \approx [E_{\mathrm{qd}}(-Q,R) - E_{\mathrm{qd}}(Q,R)]/(12\,Q/R^3)\,. \tag{3}$$

Placing an array of $4\,Q$, $-Q$, Q, $-4\,Q$ at the same positions as above we simulate a very weak octopolar field, so that

$$E_{\mathrm{oc}}(Q,R) \approx E^0 + (3/2)\,\Omega\,(Q/R^4)\,, \tag{4}$$

hence

$$\Omega \approx (2/3)\,[E_{\mathrm{oc}}(Q,R) - E^0]/(Q/R^4)\,. \tag{5}$$

Last, a very weak hexadecapolar field is obtained by placing charges of $-8\,Q$, Q, Q, $-8\,Q$ at the same positions as above. The perturbed energy $E_{\mathrm{hx}}(Q, R)$ can be written in this case as

$$E_{\mathrm{hx}}(Q,R) \approx E^0 + (3/2)\,\Phi\,(Q/R^5)\,, \tag{6}$$

and the hexadecapole moment is calculated as

$$\Phi \approx (2/3)\,[E_{\mathrm{hx}}(Q,R) - E^0]/(Q/R^5)]\,. \tag{7}$$

Both SCF and MP values of μ, Θ, Ω, and Φ are calculated from E_{qd}, E_{oc}, and E_{hx}. Electron correlation corrections are obtained from the fourth-order MP approximation to the perturbed molecucular energy. The use of many-body perturbation theory techniques in molecular property calculations has been presented in many comprehensive reviews [33–36].

The fourth-order approximation to the energy is written as

$$\mathrm{MP4} = \mathrm{SCF} + \mathrm{D2} + \mathrm{D3} + \mathrm{S4} + \mathrm{D4} + \mathrm{T4} + \mathrm{Q4} + \mathrm{R4}\,, \tag{8}$$

where the fourth order terms are contributions from single, double, triple and quadruple substitutions from the zeroth order wave function and R the renormalization term. Lower order approximations are defined as

$$\begin{aligned}
\mathrm{MP2} &= \mathrm{SCF} + \mathrm{D2}\,, && (9)\\
\mathrm{MP3} &= \mathrm{SCF} + \mathrm{D2} + \mathrm{D3}\,, && (10)\\
\mathrm{DQ\text{-}MP4} &= \mathrm{MP3} + \mathrm{D4} + \mathrm{Q4} + \mathrm{R4} &&\\
&= \mathrm{MP3} + \mathrm{DQR4}\,, && (11)\\
\mathrm{SDQ\text{-}MP4} &= \mathrm{DQ\text{-}MP4} + \mathrm{S4}\,. && (12)
\end{aligned}$$

By virtue of (8)–(12) we adopt analogous expressions for the molecular properties.

3. Computational Details

All calculations were carried out with a large gaussian-type basis set (11s 7p 4d 2f) contracted to [6s 4p 4d 2f] and consisting of 104 CGTF. The d-GTF and f-GTF are five and seven-membered, respectively. This basis set is the carefully optimized (11s 7p 3d 2f) [6s 4p 3d 2f] one used in the calculation of the quadrupole polarizability of CO [26], augmented by one tight d-GTF on carbon and oxygen. The respective exponents are 2.228519 and 2.706063 a_0^{-2}.

A homogeneous field of 0.01 $e^{-1}\,a_0^{-1}\,E_{\mathrm{h}}$ was used in the calculation of the dipole moment. Calculations of $E(F_z)$, $E(-F_z)$, $E(2F_z)$ and $E(-2F_z)$ were performed in order to eliminate the contribution of the dipole polarizability and hyperpolarizability and obtain μ_z. For the calculation of the quadrupole moment from (3) the values of Q and R were 200 e and 100 a_0, respectively. For the octopole moment $Q = 1000\ e$ and $R = 200\ a_0$. A very weak octopolar field is produced from this arrangement, as evidenced by the value of $(Q/R^4) = 6.25 \times 10^{-7}\ e^{-1}\,a_0^{-3}\,E_{\mathrm{h}}$. For the hexadecapole moment $Q = 10\,000\ e$ and $R = 200\ a_0$, so that $(Q/R^5) = 3.125 \times 10^{-7}\ e^{-1}\,a_0^{-4}\,E_{\mathrm{h}}$.

The SDQ-MP4 approximation to MP4 was adopted in this work. Inclusion of the T4 term would increase dramatically the cost of calculations. The quality of the predictions based on the SDQ-MP4 approximation has been tested in previous work [28, 29, 37].

All calculations were performed with Gaussian 86 [38].

Table 1. Dependence of the SCF electric moments on the bond length. The quadrupole, octopole and hexadecapole moments are relative to the centre of mass.

R	μ	Θ	Ω	Φ
1.932221	0.0885	−1.70	3.86	−8.91
2.132221	−0.1066	−1.52	4.42	−10.61
2.332221	−0.3181	−1.28	4.88	−12.15

Table 2. Electron correlation corrections to the electric multipole moments of $CO(X^1\Sigma^+)$ at the experimental geometry *. The quadrupole, octopole and hexadecapole moments are relative to the centre of mass.

Method	μ	Θ	Ω	Φ
SCF	−0.1067	−1.52	4.42	−10.62
D2	0.2265	0.03	−0.93	1.66
D3	−0.0880	0.05	0.16	−0.25
S4	0.0160	−0.04	−0.01	0.09
D4	0.0216	0.01	−0.12	0.26
QR4	−0.0115	−0.01	0.07	−0.15
MP2	0.1199	−1.49	3.49	−8.95
MP3	0.0319	−1.44	3.66	−9.20
DQ-MP4	0.0420	−1.44	3.60	−9.10
SDQ-MP4	0.0580	−1.48	3.59	−9.01

* Bond length 2.132221 a_0. Atomic cartesian coordinates: C (0.0, 0.0, −1.218246) and O (0.0, 0.0, 0.913975).

4. Results and Discussion

SCF results: SCF values for μ, Θ, Ω, and Φ were calculated at three different internuclear separations: the experimental one, $r_e = 2.132221\ a_0$ [39] and two others, 1.932221 and 2.332221 a_0. These values are given in Table 1. Our values at r_e are $-0.1067\ e a_0$, $-1.52\ e a_0^2$, $4.42\ e a_0^3$ and $-10.62\ e a_0^4$. They compare quite well to the numerical Hartree-Fock values [23] of $-0.104245\ e a_0$, $-1.53001\ e a_0^2$, $4.42239\ e a_0^3$ and $-10.6883\ e a_0^4$, calculated at 2.132 a_0. Agreement is better than 1% for the higher electric moments. Using our values at $r_e - 0.2$, r_e and $r_e + 0.2$ we obtained, via a parabolic fit, estimates of the first derivatives of the electric moments at r_e: $(\mathrm{d}\mu/\mathrm{d}r) = -1.0165\ e$, $(\mathrm{d}\Theta/\mathrm{d}r) = 1.05\ e a_0$, $(\mathrm{d}\Omega/\mathrm{d}r) = 22.55\ e a_0^2$ and $(\mathrm{d}\Phi/\mathrm{d}r) = -8.10\ e a_0^3$ for μ, Θ, Ω, and Φ, respectively.

Correlated results: Electron correlation corrections to the electric moments of CO were calculated at the SDQ-MP4 level and are given in Table 2. The behaviour of the MP series for μ and Θ displays quite different patterns from those present in the case of Ω or Φ. The D2 correction for μ is quite large, more important in size than the SCF value and of opposite sign. Consequently, MP2, MP3, DQ-MP4, and SDQ-MP4 are positive. Electron correlation changes only slightly the SCF Θ result. Convergence is rather slow for this property, as D2, D3, and S4+D4+QR4 are roughly of the same size at 0.03, 0.05, and $-0.04\ e a_0^2$. Convergence is quite good for either Ω or Φ. Electron correlation reduces the magnitude of both properties. The SDQ-MP4 values are $3.59\ e a_0^3$ and $-9.01\ e a_0^4$, 19 and 15% lower (in absolute terms) than the respective SCF ones.

Comparison to other predictions and experiment. Theoretical predictions and experimental data for the electric moments of CO are presented in Table 3. It is easily seen that the SCF values are close enough to the respective NHF limits for all fairly large basis sets.

Electron correlation changes the sign of the dipole moment. Correlated methods invariably predict the correct sign but fail to produce a close agreement with the experimental value of $0.04881\ e a_0$ [16]. A SD-CI calculation by Amos [19] gave $0.1370\ e a_0$. The MBPT(4) (complete fourth-order many-body perturbation theory) result of Diercksen and Sadlej [21] is still far from the experimental one at $0.1024\ e a_0$. The same authors have also reported a SD-CI value of $0.0435\ e a_0$, calculated with the same basis set as the above, quite close to the experimental one. Feller, Boyle, and Davidson [24] reported SD-CI and MRSD-CI (multireference SD-CI) values of 0.0205 and $0.0400\ e a_0$, respectively. An approximate coupled-cluster doubles (ACCD) calculation by Dykstra, Liu, and Malik [25] gave $0.0357\ e a_0$. The most accurate theoretical prediction is presumably the $0.0492\ e a_0$ reported by Scuseria et al. [27] who used a large [10s 9p 4d 2f 1g] basis set and the CCSD(T) (coupled-cluster single, double and connected triple excitations). Our SDQ-MP4 value of $0.0580\ e a_0$ is $0.01\ e a_0$ above the experimental value. We predict a total correlation correction of $0.1647\ e a_0$, to be compared with the $0.1536\ e a_0$ of Scuseria et al. [27].

The theoretical methods fare better in the prediction of the quadrupole moment. Theory predicts the value of Θ in the region of -1.45 to $-1.52\ e a_0^2$. The present claculation gave $-1.48\ e a_0^2$. This is quite close to a value of $-1.502\ e a_0^2$ obtained by Maroulis

Table 3. Comparison of theoretical and experimental values of the electric multipole moments of $CO(X^1\Sigma^+)$.

Method	μ	Θ	Ω	Φ
SCF [a]	−0.1016	−1.5016	4.4070	−10.5742
SCF [b]	−0.1040	−1.5078	4.4453	−10.3074
SCF [c]	−0.0993	−1.5238	4.433	−10.785
SCF [d]	−0.106	−1.540	4.435	−10.73
SCF [e]	−0.1045	−1.5355		
SCF [f]	−0.0911	−1.5486	4.4205	
SCF [g]	−0.112	−1.537	4.403	−10.552
SCF [h]	−0.1044			
SCF [i]	−0.105	−1.547	4.354	−10.403
SCF [i]	−0.101	−1.508	4.438	−10.689
SCF [i]	−0.102	−1.513	4.422	−10.631
SCF [i]	−0.107	−1.537	4.394	−10.695
SCF [j]	−0.1067	−1.52	4.42	−10.62
NHF [k]	−0.104245	−1.53001	4.42239	−10.6883
SD-CI [a]	0.1370	−1.4499	3.7710	−9.4185
MBPT(4) [c]	0.1024	−1.5195		
SD-CI [c]	0.0435	−1.5164	3.903	−9.848
SD-CI [e]	0.0205	−1.5160		
MRSD-CI [e]	0.0400	−1.5219		
ACCD [f]	0.0357	−1.4902	3.8196	
CCD + ST(CCD) [g]		−1.502		
CCSD(T) [h]	0.0492			
SDQ-MP4 [j]	0.0580	−1.48	3.59	−9.01
Experiment	0.0481 [l]	−1.5 ± 0.7 [m] −1.4 ± 0.1 [n] −1.44 ± 0.3 [p] −1.5 [o]		

[a] Basis set [5s 4p 2d] at 2.132 a_0 [19].
[b] Basis set [24s 12p 4d] at 2.13263 a_0 [20].
[c] Basis set [8s 5p 3d 1f] at 2.132 a_0 [21].
[d] Basis set [6s 5p 3d 2f] [22].
[e] Basis set [10s 6p 4d 2f] at 2.132 a_0 [24].
[f] ELP basis set at 2.132221 a_0 [25].
[g] Basis set [6s 4p 3d 2f] at 2.132221 a_0 [26].
[h] Basis set [10s 9p 4d 2f 1g] at 2.1316 a_0 [27].
[i] Basis sets [6s 4p 3d 1f], [6s 4p 4d 1f], [6s 4p 4p 1f] and [6s 4p 3d 2f] at 2.132221 a_0. Unpublished results by Maroulis and Thakkar.
[j] Present investigation. Basis set [6s 4p 4d 2f] at 2.132221 a_0.
[k] Fully numerical values at a bond length of 2.132 a_0 [23].
[l] Stark effect measurements [16].
[m] Microwave asymmetric Zeeman shifts [14].
[n] Far IR rotational spectra [15].
[o] Molecular beam electric resonance Stark-Zeeman spectra [17].
[p] Ion molecule scattering cross sections [18].

and Thakkar [26] via the CCD + ST(CCD), coupled-cluster doubles corrected by fourth-order contributions from single and triple excitations computed with CCD amplitudes. Comparison with experiment would necessitate averaging over the ground vibrational and rotational state. This correction has been estimated at 0.08 $e a_0^2$ in previous work [26] and brings the theoretical predictions quite close to the experimental results.

To our knowledge, no experimental estimates of the octopole and hexadecapole are available. The SD-CI values of Ω are 3.7710 $e a_0^3$ [19] and 3.903 $e a_0^3$ [21]. The ACCD [25] result of 3.8196 $e a_0^3$ is 6.4% higher than our SDQ-MP4 one of 3.59 $e a_0^3$. We use a more flexible basis set than the ELP one used in the ACCD calculation, but both sets lead to almost identical SCF values. We estimate the octopole moment of carbon monoxide at $3.6 \pm 0.2\, e a_0^3$.

Our value for the hexadecapole moment is −9.01 $e a_0^4$, smaller than both the SD-CI ones of −9.4185 $e a_0^4$ [19] and −9.848 $e a_0^4$ [21]. We expect our value to be more accurate and we estimate the hexadecapole moment of carbon monoxide at $-9.0 \pm 0.5\, e a_0^4$.

5. Conclusions

We have reported SDQ-MP4 values for the electric dipole, quadrupole, octopole and hexadecapole moments of ground state carbon monoxide. Our values for Ω and Φ should be the most accurate currently available. Our estimates for these properties are $\Omega = 3.6 \pm 0.2\, e a_0^3$ and $\Phi = -9.0 \pm 0.5\, e a_0^4$.

Acknowledgements

The author is happy to acknowledge the generous hospitality of the Computer Centre of the Computer Technology Institute (ITY) of Patras.

[1] A. D. Buckingham, Adv. Chem. Phys. **12,** 107 (1967).
[2] A. D. Buckingham, in: Physical Chemistry an Advanced Treaty, Vol. 1 (H. Eyring, W. Jost, and D. Henderson, eds.), Academic Press, New York 1970.
[3] A. D. Buckingham, in: Intermolecular Interactions, from Diatomics to Biopolymers (B. Pullman, ed.), Wiley, New York 1978.
[4] C. G. Gray and K. E. Gubbins, Theory of Molecular Fluids, Vol. 1, Clarendon Press, Oxford 1984.
[5] A. D. Buckingham and P. W. Fowler, J. Chem. Phys. **79,** 6426 (1983).
[6] A. D. Buckingham and P. W. Fowler, Can. J. Chem. **63,** 2018 (1985).
[7] J. E. Bohr and K. L. C. Hunt, J. Chem. Phys. **87,** 3821 (1987).
[8] M. O. Bulanin, V. P. Bulychev, and K. G. Tokhadze, J. Mol. Struct. **161,** 321 (1987).
[9] V. Magnasco, G. Figari, and C. Costa, J. Mol. Struct. **164,** 49 (1988).
[10] V. Magnasco, C. Costa, and G. Figari, J. Mol. Struct. **169,** 105 (1988).

[11] M. O. Bulanin, V. P. Bulychev, and K. G. Tokhadze, Opt. Spectrosc. **67,** 336 (1989).
[12] C. E. Dykstra, J. Phys. Chem. **94,** 180 (1990).
[13] A. van der Pol, A. van der Avoird, and P. E. S. Wormer, J. Chem. Phys. **92,** 7498 (1990).
[14] S. Gustafson and W. Gordy, J. Chem. Phys. **52,** 579 (1970).
[15] U. Buontempo, S. Cunsolo, and G. Jacucci, J. Chem. Phys. **59,** 3750 (1973).
[16] J. S. Muenter, J. Mol. Spectrosc. **55,** 490 (1975).
[17] W. L. Meerts, F. H. De Leeuw, and A. Dymanus, Chem. Phys. **22,** 319 (1977).
[18] F. E. Budenholzer, E. A. Gislason, A. D. Jorgensen, and J. G. Sachs, Chem. Phys. Lett. **47,** 429 (1977).
[19] R. D. Amos, Chem. Phys. Lett. **68,** 536 (1979).
[20] D. G. Bounds and S. Wilson, Mol. Phys. **54,** 445 (1985).
[21] G. H. F. Diercksen and A. J. Sadlej, Chem. Phys. **96,** 17 (1985).
[22] F. Visser and P. E. S. Wormer, Chem. Phys. **92,** 129 (1985).
[23] L. Laaksonen, P. Pyykkö, and D. Sundholm, Comp. Phys. Rep. **4,** 313 (1986).
[24] D. Feller, C. M. Boyle, and E. R. Davidson, J. Chem. Phys. **86,** 3424 (1987).
[25] C. E. Dykstra, S. Y. Liu, and D. J. Malik, Adv. Chem. Phys. **75,** 37 (1989).
[26] G. Maroulis and A. J. Thakkar, J. Chem. Phys. **92,** 812 (1990).
[27] G. E. Scuseria, M. D. Miller, F. Jensen, and J. Geertsen, J. Chem. Phys. **94,** 6660 (1991).
[28] G. Maroulis and A. J. Thakkar, J. Chem. Phys. **88,** 7623 (1988).
[29] G. Maroulis and A. J. Thakkar, J. Chem. Phys. **90,** 366 (1989).
[30] G. Maroulis, J. Phys. B **24,** L117 (1991).
[31] G. Maroulis, Chem. Phys. Lett. **177,** 352 (1991).
[32] A. D. McLean and M. Yoshimine, J. Chem. Phys. **47,** 1927 (1967).
[33] I. Hubač and P. Čársky, Topics Current Chem. **75,** 97 (1978).
[34] R. J. Bartlett, Annu. Rev. Phys. Chem. **32,** 359 (1981).
[35] A. Szabo and N. S. Ostlund, Modern Quantum Chemistry, McMillan, New York 1982.
[36] M. Urban, I. Černušák, V. Kellö, and J. Noga, Methods Comput. Chem. **1,** 117 (1987).
[37] G. Maroulis and A. J. Thakkar, J. Chem. Phys. **93,** 4164 (1990).
[38] M. J. Frisch, J. S. Binkley, H. B. Schlegel, K. Raghavachari, C. F. Melius, R. L. Martin, J. J. P. Stewart, F. W. Bobrowicz, C. M. Rohlfing, L. R. Kahn, D. J. Defrees, R. Seeger, R. A. Whiteside, D. J. Fos, E. M. Fleuder, and J. A. Pople, Gaussian 86 (Carnegie-Mellon University, Pittsburgh 1984).
[39] K. P. Huber and G. Herzberg, Molecular Spectra and Molecular Structure. IV. Constants of Diatomic Molecules, Van Nostrand, New York 1979.