15 August 1997

ELSEVIER

Chemical Physics Letters 274 (1997) 439–444

CHEMICAL
PHYSICS
LETTERS

Vibrational spectra of cyclic C_6 in solid argon

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Received 7 May 1997; in final form 17 June 1997

Abstract

Vapors from solid and powdered carbon emitted from an oven cycled between 2000 and 3000 K were co-condensed with argon onto a CsI substrate maintained at 10 K. The cycling process produced a matrix "sandwich" with regions of high carbon density alternating with layers of argon. FTIR measurements including extensive ^{13}C isotopic data, supported by ab initio calculations, allow the assignment of a band at 1694.7 cm^{-1} to the $\nu_4(e')$ fundamental of cyclic C_6. This represents the first conclusive identification of a small cyclic neutral polycarbon. Additionally, a vibration previously observed at 1710.3 cm^{-1} has been confirmed as the $\nu_9(\sigma_u)$ mode of linear C_8. © 1997 Published by Elsevier Science B.V.

1. Introduction

Pure carbon molecules (polycarbons) have received considerable experimental and theoretical attention over the past forty years. Several reasons were indicated by Weltner and Van Zee in their comprehensive review [1], including the possible role of polycarbons as soot precursors and their signficance in astrophysical processes. More recently, the discovery of methods for producing macroscopic quantities of fullerenes in the laboratory [2,3] and the exploration of mechanisms for their formation have excited new interest. Concomitantly, the capabilities of quantum chemistry have improved substantially; accurate structures, energetics, and spectra of carbon clusters as large as buckminsterfullerene (C_{60}) are now computationally attainable [4].

The US Air Force High Energy Density Matter (HEDM) Program is studying the feasibility of seeding cryogenic rocket propellants with atomic or molecular species to increase their energy content [5]. The present report is an outgrowth of efforts to deposit a few mole percent carbon atoms in cryogenic matrices. In the course of this work a novel condensation chemistry has been observed with cyclic C_6 playing a leading role.

Calculations of C_6 isomers employing extensive electron-correlation treatments [6–9], including single- and double-excitation coupled-cluster calculations with a noniterative treatment of connected triple excitations [10], denoted CCSD(T), indicate that the distorted hexagon ($^1A'_1$, D_{3h} symmetry) is ~ 8 kcal/mol lower in energy than the regular hexagon ($^1A_{1g}$, D_{6h}) and ~ 11 kcal/mol lower than the linear chain ($^3\Sigma_g^-$, $D_{\infty h}$). Additionally, application of density-functional theory (DFT) methods to cyclic C_6 [11,12] yields structures, frequencies, and intensities that are in good accord with the CCSD(T) results [6,9].

Beginning in 1964 Weltner and co-workers pioneered infrared spectroscopy of thermally evaporated carbon species trapped in rare-gas matrices [13–16].

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PII S0009-2614(97)00700-8

Vibrational and electronic spectra of linear C_6 have been extensively studied [16–26], but experimental data concerning possible cyclic forms are sparse. Szczepanski and Vala [21] did find a correlation between the intensities of bands at 1695 cm^{-1} and 586 nm (17065 cm^{-1}) upon matrix annealing, and from kinetic considerations they surmised that these bands may belong to a cyclic cluster containing six or more carbon atoms. Coulomb explosion imaging [27] also seems to provide indirect evidence for the existence of cyclic C_6.

Several researchers have considered the question of why no cyclic forms of any small polycarbons have been directly identified [20,28]; their elusiveness constitutes a long-standing experimental challenge. In this paper we introduce a new method for the abundant production of carbon clusters, focusing on the identification of cyclic C_6. Other cyclic carbon clusters will be discussed in subsequent publications.

2. Computational methods

Harmonic frequencies and infrared intensities for cyclic $^{12}C_6$ have been published [8,9,11,12,29], but the ^{13}C isotopic shifts essential for the definitive identification of matrix-isolated species are not in the literature. Consequently, we performed density-functional (B3LYP) calculations in cc-pVDZ [30], cc-pVTZ [30], and 6-311G(2d) [31] basis sets, as well as CCSD(T) calculations in the cc-pVDZ basis set, largely following the work of Martin and co-workers [9,12]. Additionally, we calculated isotopic shifts of linear C_8 at the B3LYP/cc-pVDZ level. Gaussian [31] and ACES II [32] were used on IBM RS/6000 work stations at Phillips Laboratory and Cray C90 computers at the US Army Corps of Engineers Waterways Experiment Station and the Aeronautical Systems Center.

3. Experimental methods

Carbon vapor from an oven resistively heated to 3000 K was co-condensed with argon onto a CsI substrate at 10 K in a vacuum chamber capable of 10^{-7} Torr. A matrix of 150 μm maximum average thickness was produced in about one hour and FTIR spectra (600–4000 cm^{-1}; resolution 1.2 cm^{-1} FWHM at 1700 cm^{-1}) of several annealed matrices were measured. Except as noted below, the procedures and equipment were identical to those described previously [33].

A cylindrical tantalum cell (2.4 cm long, 0.64 cm diameter, 0.25 mm wall thickness, with a centered 1.0 mm diameter orifice), containing graphite and sealed with 0.6 cm long tantalum end caps, was mounted between water-cooled electrodes. A current of about 700 A was required to reach the highest temperatures. The orifice temperature was 200–400 K above that of the end caps, so the saturated C_3-rich [34] carbon vapor near the cooler graphite surface was considerably dissociated as it exited the orifice.

During deposition, argon condensed onto the substrate at a constant flux no greater than 8×10^{16} atoms cm^{-2} s^{-1}, but the oven current was repeatedly cycled to produce a matrix "sandwich" with ten carbon-rich layers separated by argon layers of approximately equal thickness. The temperature was raised by 300 K/min during a heating phase (from 2000 to 3000 K), taking care to avoid the sputtering of graphite particles. During the transient period between heating and return to steady state, the temperature gradient between the orifice and the graphite surface was largest, and the emitted carbon vapor was significantly atomized. The estimated maximum flux of equivalent carbon atoms through the orifice was 10^{20} cm^{-2} s^{-1} over the course of a deposition. The layered matrix supports average densities in excess of one mole-percent, although these decrease over time with reduction in the graphite surface area.

Varying $^{12}C/^{13}C$ sample ratios were produced by loosely filling a 100 mg solid graphite liner (about 0.5 mm wall thickness, CZR-2 grade, POCO Graphite) with 100 mg powdered carbon of three different isotopic compositions: (a) natural-abundance carbon (99.9995% purity, Johnson Mathey); (b) an equimolar mixture of well-blended ^{12}C and ^{13}C and (c) ^{13}C flakes (99% purity, amorphous, Cambridge Isotope Laboratories). Because the powders evaporate faster than the solid liner, the compositions of the first few layers are nearly identical to the composition of the powder itself, whereas later layers are richer in ^{12}C from the liner.

4. Results and discussion

Fig. 1(a) shows a spectrum of an annealed matrix (27.5 K) containing nearly pure ^{12}C. The most prominent absorption is the 1694.7 cm^{-1} band, previously attributed to a cyclic cluster of six or more atoms by Szczepanski and Vala [21]. The absolute absorbance of this peak in Fig. 1(a), however, is at least three times stronger than they reported (fig. 3 of Ref. [21]), and it undergoes a two- or three-fold intensity increase upon further annealing.

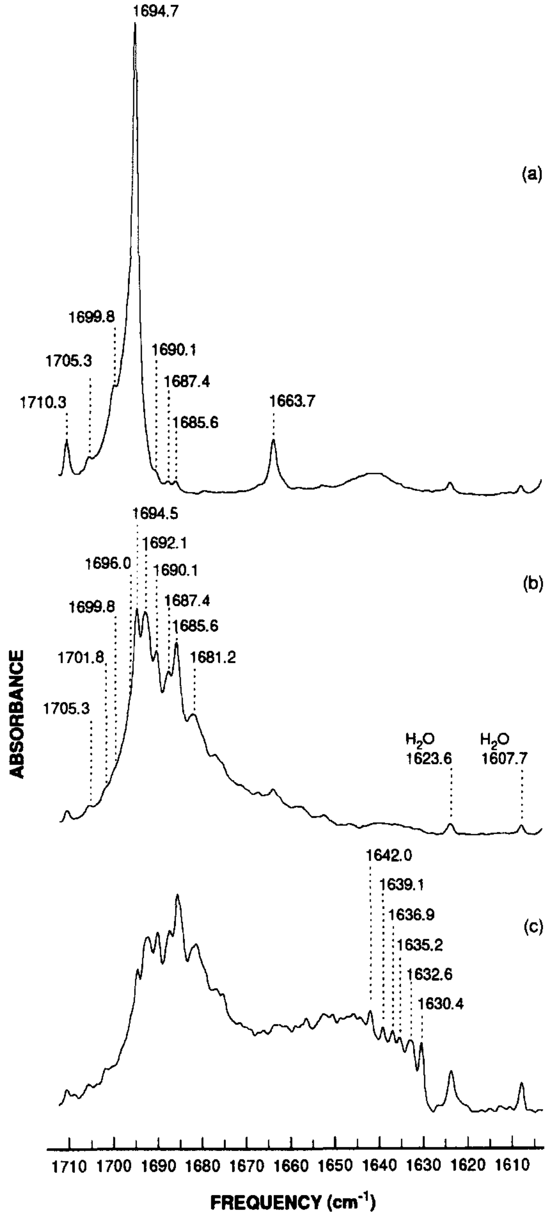

Fig. 1. FTIR spectra of the $\nu_4(e')$ mode of cyclic C_6 and the $\nu_9(\sigma_u)$ mode of linear C_8 produced by evaporating carbon mixtures with average compositions: (a) natural-abundance carbon; (b) 75% ^{12}C and 25% ^{13}C; and (c) 50% ^{12}C and 50% ^{13}C. Integrated absorbances of the 1694.7 cm^{-1} band and its isotopomers are 3.9, 5.7 and 3.5 cm^{-1}, respectively.

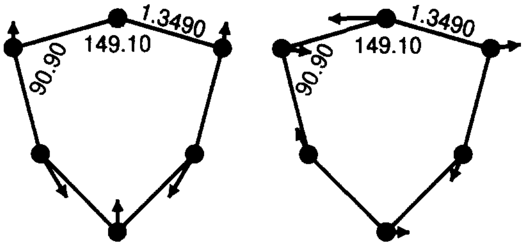

Fig. 2. CCSD(T)/cc-pVDZ equilibrium structure of cyclic C_6 (D_{3h} symmetry) with the bond distance (Å) and angles (degrees) indicated. The arrows illustrate the atomic displacements associated with the degenerate $\nu_4(e')$ normal mode.

Harmonic frequencies calculated [8,9,11,12,29] for the intense $\nu_4(e')$ mode of cyclic $^{12}C_6$ (depicted in Fig. 2) are in reasonable agreement with the 1694.7 cm^{-1} measurement. We computed vibrational frequencies and intensities for the complete set of isotopomers; those for the vibrational modes of cyclic $^{12}C_6$ are reported in Table 1. These data are relatively insensitive to the choice of atomic basis set or correlation treatment, and the B^{3}LYP/cc-pVDZ results are in complete agreement with those from the identical calculation of Martin et al. [12]. Our CCSD(T)/cc-pVDZ frequencies (Table 1), however, differ significantly from those reported by Martin and Taylor [9], even though we obtained the same minimum energy structure (Fig. 2). We confirmed these results using two different program systems [31,32], concluding that the CCSD(T)/cc-pVDZ frequencies for cyclic $^{12}C_6$ reported by Martin and Taylor (table 3 of Ref. [9]) should be replaced by the values listed in Table 1. The scale factor for the $\nu_4(e')$ mode that brings the calculated CCSD(T)/cc-pVDZ frequency into coincidence with the measurement is 0.9762, sufficiently near unity to tentatively assign the 1694.7 cm^{-1} band to cyclic $^{12}C_6$. Conclusive assignment, however, requires examination of the ^{13}C isotopomer data.

Computed isotopomer frequencies and those observed in the spectra of Fig. 1 are listed in Table 2.

Table 1
Calculated harmonic frequencies (cm^{-1}) of cyclic $^{12}C_6$. Infrared intensities (km/mol) of the active modes are given in parentheses

Mode	B3LYP/6-311G(2*d*)	B3LYP/cc-pVDZ	B3LYP/cc-pVTZ	CCSD(T)/cc-pVDZ
$\nu_1(a'_1)$	1218	1222	1223	1183
$\nu_2(a'_1)$	646	659	647	556
$\nu_3(a'_2)$	1393	1437	1412	1371
$\nu_4(e')$	1751 (424)	1769 (404)	1761 (436)	1736 (420)
$\nu_5(e')$	1234 (1)	1219 (1)	1232 (1)	1178 (1)
$\nu_6(e')$	650 (24)	633 (25)	645 (22)	576 (43)
$\nu_7(a''_2)$	425 (7)	419 (8)	435 (6)	380 (7)
$\nu_8(e'')$	534	519	538	492

The cyclic $^{13}C_6$ isotopomer clearly observed at 1630.4 cm^{-1} (Fig. 1c) is shifted by −64.3 cm^{-1} from $^{12}C_6$, in good accord with the scaled calculated shift of −66.8 cm^{-1}. The degeneracy of the $\nu_4(e')$ mode for 16 of the 20 isotopomers is lifted upon ^{13}C substitution, producing modes 4A and 4B (Table 2), for a total of 36 distinct bands contained within only 64.3 cm^{-1}. It should be noted that the current novel matrix preparation technique allows early deposition of highly ^{13}C-substituted isotopomers, even though equal amounts of ^{12}C and ^{13}C were used in sample (c). Fig. 3(a) shows the spectrum from Fig. 1(c) in greater detail, along with spectra (Fig. 3b, c) obtained after two additional annealings of the sample. The features in the congested spectrum between 1675 and 1645 cm^{-1} are well reproduced, whereas

Table 2
Calculated [CCSD(T)/cc-pVDZ] and observed frequencies and shifts (cm^{-1}) for the $\nu_4(e')$ mode of cyclic C_6 isotopomers

Isotopomer	Stat.	Calculated						Observed					
	Wt.	Mode-4A			Mode-4B			Mode-4A			Mode-4B		
		Raw	Scaled [a]	Shift	Raw	Scaled [a]	Shift	Obs.	Shift	Δ [b]	Obs.	Shift	Δ [b]
12-12-12-12-12-12	1	1736.1	1694.7		1736.1	1694.7		1694.7			1694.7		
13-12-12-12-12-12	3	1706.2	1665.5	−29.2	1736.0	1694.6	−0.1	1687.4	−7.3	−21.9	1694.5	−0.2	0.1
12-13-12-12-12-12	3	1727.1	1685.9	−8.8	1731.4	1690.1	−4.6	1685.6	−9.1	0.3	1690.1	−4.6	0.0
13-13-12-12-12-12	6	1698.3	1657.8	−36.9	1730.4	1689.1	−5.6	1657.4	−37.3	0.4	1692.1	−2.6	−3.0
13-12-13-12-12-12	3	1689.7	1649.4	−45.3	1721.5	1680.4	−14.3	1648.6	−46.1	0.8	1681.2	−13.5	−0.8
13-12-12-13-12-12	3	1701.0	1660.4	−34.3	1727.0	1685.8	−8.9	1663.6	−31.1	−3.2	1685.6	−9.1	0.2
12-13-12-13-12-12	3	1719.9	1678.9	−15.8	1724.5	1683.4	−11.3	1679.3	−15.4	−0.4	1682.7	−12.0	0.7
13-13-13-12-12-12	3	1780.5	1638.0	−56.7	1717.3	1676.3	−18.4	1639.1	−55.6	−1.1	1677.0	−17.7	−0.7
13-13-12-13-12-12	6	1692.8	1652.4	−42.3	1721.1	1680.1	−14.6	1652.6	−42.1	−0.2	1681.2	−13.5	−1.1
13-12-13-13-12-12	6	1683.7	1643.5	−51.2	1713.4	1672.5	−22.2	1644.2	−50.5	−0.7	1671.4	−23.3	1.1
13-13-12-12-12-13	3	1690.3	1650.0	−44.7	1724.4	1683.3	−11.4	1650.5	−44.2	−0.5	1682.7	−12.0	0.6
13-12-13-12-13-12	1	1689.6	1649.3	−45.4	1689.6	1649.3	−45.4	1647.2	−47.5	2.1	1647.2	−47.5	2.1
12-13-12-13-12-13	1	1714.9	1674.0	−20.7	1714.9	1674.0	−20.7	1675.2	−19.5	−1.2	1675.2	−19.5	−1.2
13-13-13-13-12-12	6	1674.2	1634.3	−60.4	1709.0	1668.2	−26.5	1635.2	−59.5	−0.9	1666.4	−28.3	1.8
13-13-13-12-13-12	3	1680.4	1640.3	−54.4	1684.8	1644.6	−50.1	1642.0	−52.7	−1.7	1645.9	−48.8	−1.3
13-13-12-13-13-12	3	1677.7	1637.7	−57.0	1704.7	1664.0	−30.7	1636.9	−57.8	0.8	1662.5	−32.2	1.5
13-13-12-13-12-13	3	1684.6	1644.4	−50.3	1714.8	1673.9	−20.8	1644.2	−50.5	0.2	1673.1	−21.6	0.8
13-13-13-13-13-12	3	1673.0	1633.1	−61.6	1677.6	1637.6	−57.1	1632.6	−62.1	0.5	1636.9	−57.8	0.7
13-13-13-13-12-13	3	1667.8	1628.0	−66.7	1700.1	1659.6	−35.1	1630.4	−64.3	−2.4	1661.0	−33.7	−1.4
13-13-13-13-13-13	1	1667.7	1627.9	−66.8	1667.7	1627.9	−66.8	1630.4	−64.3	−2.5	1630.4	−64.3	−2.5

[a] Scale factor is 0.9761534.
[b] Δ = predicted shift − observed shift.

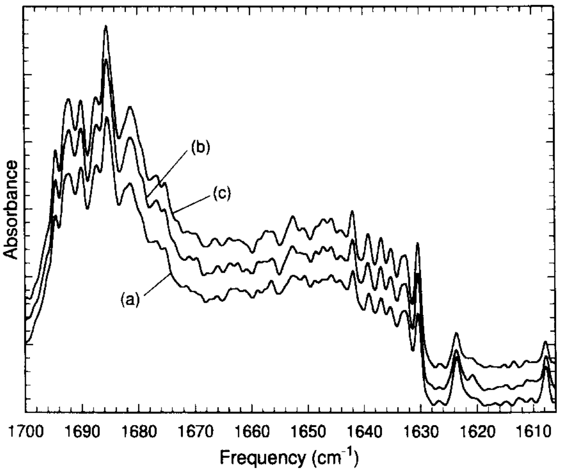

Fig. 3. FTIR spectra of matrix (c) at 10 K after annealing to: (a) 27.5 K for 180 s; (b) 30.0 K for 150 s and (c) 32.5 K for 60 s.

the magnitude of the noise may be gauged from the relatively featureless region between the two H_2O absorptions (Fig. 1b and Fig. 3). Due to the high density of bands in the central portion of this manifold, specific isotopomer assignments are necessarily somewhat provisional, and are sensitive to the accuracy of the ab initio calculations.

The $^{13}C_1{}^{12}C_5$ isotopomers (Table 2) are discernible in Fig. 1(a) at only 1% ^{13}C (natural abundance), and they are prominent in Fig. 1(b, c). The differences (Δ) in Table 2 between predicted (scaled) and observed shifts for 35 of the 36 bands range between -3.2 and 2.1 cm^{-1}, with an RMS average of 1.5 cm^{-1}. Based on these assignments, only one band has a large Δ value (-21.9 cm^{-1}), which could result from any number of spectral perturbations, such as a resonance between the $\nu_5 + \nu_6$ combination band and the ν_4 fundamental. Because each of the 20 isotopomers has a unique vibrational spectrum (indeed, they are divided among three different point groups) and perturbations of this sort occur only among the vibrations of an individual isotopomer, it is not unexpected that a strong interaction arising from a fortuitous near degeneracy might be observed in only a minority of possibilities. The present calculations do not account for such perturbations.

The spectrum in Fig. 1(a) also exhibits an unidentified absorption at 1663.7 cm^{-1}, as well as a band at 1710.3 cm^{-1} that was previously assigned to the $\nu_9(\sigma_u)$ mode of linear C_8 by Szczepanski et al. [26]. Our B3LYP/cc-pVDZ isotopic-shift calculations for this molecule [35] indicate that the bands discernible at 1705.3 and 1699.8 cm^{-1} result from linear $^{13}C_1{}^{12}C_7$ isotopomers at 1% ^{13}C natural abundance. Additional $^{13}C_1{}^{12}C_7$ bands, obscured in Fig. 1(a), appear at 1701.8 and 1696.0 cm^{-1} in Fig. 1(b, c). These results support the assignment of the 1710.3 cm^{-1} band to the $\nu_9(\sigma_u)$ mode of linear C_8.

There are additional reasons to rule out the possibility that the 1694.7 cm^{-1} absorption actually belongs to a fundamental of linear C_8. First, several strong bands in Fig. 1(b, c), most prominently those at 1694.5 and 1692.1 cm^{-1}, could not be accounted for by our calculations on linear C_8. Second, all calculations on linear C_8 [9,11,12,35] predict the $\nu_8(\sigma_u)$ mode at ~ 2100 cm^{-1} to be 2–3 times more intense than the $\nu_9(\sigma_u)$ mode; however, only very weak bands were observed in this spectral region. Third, in agreement with Szczepanski et al. [26], we noticed that a band at 2071.4 cm^{-1} correlated with the 1710.3 cm^{-1} band upon annealing. Specifically, we found that the ratio of the integrated absorbances of these bands was in good accord with the 2.7:1 prediction of theory [12].

Therefore, based on the excellent overall agreement between the cyclic C_6 calculations and measured isotopic shifts, and because all other linear and cyclic C_n clusters ($n \leq 12$), particularly linear C_8, may be dismissed as candidates [9,11,12,29,35], we definitively assign the 1694.7 cm^{-1} band to the $\nu_4(e')$ mode of cyclic $^{12}C_6$. Furthermore, we confirm the assignment of the 1710.3 cm^{-1} band to the $\nu_9(\sigma_u)$ mode of linear C_8.

5. Conclusions

Fourier transform infrared spectroscopy of matrix-isolated carbon vapor has resulted in the first definitive identification of a small cyclic carbon cluster. A new technique was developed to make layered matrices that exhibited novel condensation chemistry. Based on the excellent agreement between the observed isotopomer frequencies and the predictions of ab initio calculations, a band at 1694.7 cm^{-1} is assigned to the $\nu_4(e')$ fundamental of cyclic C_6. Additionally, we have confirmed the assignment of a band at 1710.3 cm^{-1} to the $\nu_9(\sigma_u)$ mode of linear C_8.

Acknowledgements

JDP-M expresses appreciation for partial support from the Air Force Office of Scientific Research, the National Science Foundation through its Associateship Programs Office, and the USAF Phillips Laboratory Propulsion Directorate. JAS acknowledges computational resources provided by the Department of Defense High Performance Computing Modernization Program. The authors thank Dr. Peter Taylor and Dr. Jan Martin for advice and helpful discussions.

References

[1] W. Weltner Jr., R.J. van Zee, Chem. Rev. 89 (1989) 1713.
[2] W. Krätschmer, L.D. Lamb, K. Fostiropoulos, D.R. Huffman, Nature (London) 347 (1990) 354.
[3] H.W. Kroto, J.R. Heath, S.C. O'Brien, R.F. Curl, R.E. Smalley, Nature (London) 318 (1985) 162.
[4] G.E. Scuseria, in: Modern Electronic Structure Theory, Vol. 1, ed. D.R. Yarkony (World Scientific, River Edge, New Jersey, 1995) p. 279.
[5] See, for example, Proceedings of the High Energy Density Matter (HEDM) Contractors Conference Held 5–7 June 1996 in Boulder CO, eds. P.G. Carrick and N.T. Williams (Phillips Laboratory, Edwards AFB, CA, 1997), report PL-TR-96-3037.
[6] J. Hutter, H.P. Lüthi, J. Chem. Phys. 101 (1994) 2213.
[7] V. Pless, H.U. Suter, B. Engels, J. Chem. Phys. 101 (1994) 4042.
[8] K. Raghavachari, R.A. Whiteside, J.A. Pople, J. Chem. Phys. 85 (1986) 6623.
[9] J.M.L. Martin, P.R. Taylor, J. Phys. Chem. 100 (1996) 6047.
[10] K. Raghavachari, G.W. Trucks, J.A. Pople, M. Head-Gordon, Chem. Phys. Lett. 157 (1989) 479.
[11] J. Hutter, H.P. Lüthi, F. Diederich, J. Am. Chem. Soc. 116 (1994) 750.
[12] J.M.L. Martin, J. El-Yazal, J.-P. François, Chem. Phys. Lett. 242 (1995) 570.
[13] W. Weltner Jr., P.N. Walsh, C.L. Angell, J. Chem. Phys. 40 (1964) 1299.
[14] W. Weltner Jr., D. McLeod Jr., J. Chem. Phys. 40 (1964) 1305.
[15] W. Weltner Jr., D. McLeod Jr., J. Chem. Phys. 45 (1966) 3096.
[16] K.R. Thompson, R.L. Dekock, W. Weltner Jr., J. Am. Chem. Soc. 93 (1971) 4688.
[17] M. Vala, T.M. Chandrasekhar, J. Szczepanski, R. Pellow, High Temp. Sci. 27 (1990) 19.
[18] R.H. Kranze, W.R.M. Graham, J. Chem. Phys. 98 (1993) 71.
[19] H.J. Hwang, A. Van Orden, K. Tanaka, E.W. Kuo, J.P. Heath, R.J. Saykally, Mol. Phys. 79 (1993) 769.
[20] R.J. Van Zee, R.F. Ferrante, K.J. Zeringue, W. Weltner Jr., D.W. Ewing, J. Chem. Phys. 88 (1988) 3465.
[21] J. Szczepanski, M. Vala, J. Phys. Chem. 95 (1991) 2792.
[22] D.W. Arnold, S.E. Bradforth, T.N. Kitsopoulos, D.M. Neumark, J. Chem. Phys. 95 (1991) 8753.
[23] C.C. Arnold, Y. Zhao, T.N. Kitsopoulos, D.M. Neumark, J. Chem. Phys. 97 (1992) 6121.
[24] D. Forney, J. Fulara, P. Freivogel, M. Jakobi, D. Lessen, J.P. Maier, J. Chem. Phys. 103 (1995) 48.
[25] P. Freivogel, J. Fulara, M. Jakobi, D. Fomey, J.P. Maier, J. Chem. Phys. 103 (1995) 54.
[26] J. Szczepanski, S. Ekern, C. Chapo, M. Vala, Chem. Phys. 211 (1996) 359.
[27] H. Feldman, D. Kella, E. Malkin, E. Miklazky, Z. Vager, J. Zajfman, R. Naaman, J. Chem. Soc. Faraday Trans. 86 (1990) 2469.
[28] Z. Slanina, Chem. Phys. Lett. 142 (1987) 512.
[29] K. Raghavachari, J.S. Binkley, J. Chem. Phys. 87 (1987) 2191.
[30] T.H. Dunning, J. Chem. Phys. 90 (1989) 1007.
[31] Gaussian 94, Revision D.4, M.J. Frisch, G.W. Trucks, H.B. Schlegel, P.M.W. Gill, B.G. Johnson, M.A. Robb, J.R. Cheeseman, T. Keith, G.A. Petersson, J.A. Montgomery, K. Raghavachari, M.A. Al-Laham, V.G. Zakrzewski, J.V. Ortiz, J.B. Foresman, J. Cioslowski, B.B. Stefanov, A. Nanayakkara, M. Challacombe, C.Y. Peng, P.Y. Ayala, W. Chen, M.W. Wong, J.L. Andres, E.S. Replogle, R. Gomperts, R.L. Martin, D.J. Fox, J.S. Binkley, D.J. DeFrees, J. Baker, J.P. Stewart, M. Head-Gordon, C. Gonzalez and J.A. Pople, Gaussian, Inc., Pittsburgh, PA, 1995.
[32] ACES II, Quantum Theory Project, University of Florida. Authors: J.F. Stanton, J. Gauss, J.D. Watts, M. Nooijen, N. Oliphant, S.A. Perera, P.G. Szalay, W.J. Lauderdale, S.R. Gwaltney, S. Beck, A. Balková, D.E. Bernholdt, K.-K. Baeck, P. Rozyczko, H. Sekino, C. Hober and R.J. Bartlett, Integral packages included are VMOL (J. Almlöf and P.R. Taylor), BPROPS (P.R. Taylor), and ABACUS (T. Helgaker, H.J.Aa. Jensen, P. Jørgensen, J. Olsen and P.R. Taylor).
[33] J.D. Presilla-Márquez, C.W. Larson, P.G. Carrick, C.M.L. Rittby, J. Chem. Phys. 105 (1996) 3398.
[34] J. Drowart, R.P. Burns, G. de Maria, M.G. Inghram, J. Chem. Phys. 31 (1959) 1131.
[35] J.D. Presilla-Márquez, J.A. Sheehy, J.D. Mills and C.W. Larson, to be published.