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The electronic and molecular structure of carbon clusters: C_8 and C_{10}*

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Summary. The equilibrium geometries of C_8 and C_{10} have been determined from electronic structure calculations, using a variety of correlated methods and large basis sets of atomic natural orbitals. For C_8, a cyclic form with C_{4h} symmetry (^1A_g) and a linear, cumulene-like form ($^3\Sigma_g^-$) are isoenergetic candidates for the electronic ground state. For C_{10}, the ground-state equilibrium structure is definitely monocyclic. Three different cyclic structures have been considered here, i.e. cumulenic D_{10h}, distorted-cumulenic D_{5h} and acetylenic D_{5h}. These are all essentially isoenergetic, and are about 50 kcal/mol below the linear $^3\Sigma_g^-$ state. The choice of basis sets and methods used has a strong impact on the predicted ground-state structures.

Key words: Carbon clusters – C_8/C_{10} – Equilibrium geometries – Electronic structure calculations

1. Introduction

Ground-state structures of small- and medium-sized carbon clusters (C_n, $n < 10$) are generally assumed to have linear shapes, whereas a monocyclic form is assigned to C_{10} and the larger clusters [1]. So far, this general prediction has agreed well with experimental results [2–7] but has shown only modest agreement with *ab-initio* theory. Several calculations have shown a preference for monocyclic structures even for the smaller clusters C_4 and C_6 [8–12], although these calculations also indicated that the linear and monocyclic forms are nearly isoenergetic and might coexist under certain circumstances. With the conditions under which the experiments were performed, it is possible that the monocyclic forms would elude detection, and the computed energies are not necessarily in disagreement with experiment.

While a large number of theoretical and experimental investigations on small carbon clusters (C_n, $n \leqslant 6$), have been reported [2–7], fewer studies have been conducted for larger clusters, such as C_8 and C_{10} [6, 7, 13–17]. Most theoretical

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* Dedicated to Prof. Klaus Ruedenberg

calculations on these larger systems have been carried out using semi-empirical [13] or SCF [14, 15] methods. Very recently, correlated calculations based on double-zeta quality basis sets and a single-reference CI approach [16, 17] have been performed for both C_8 and C_{10}, and monocyclic ground states were predicted. These results contradict experimental findings of linear or slightly bent structures [6, 7].

Past experience from calculations on C_4 and C_6 [18, 19] indicates that the linear and monocyclic conformers are close in energy, and that the relative energies of these forms depends strongly on the basis sets used. If these findings are representative also for the larger carbon clusters, then basis sets much larger than those used in recent calculations are needed to achieve the required accuracy in calculations on C_8 and C_{10}. Previous work on C_4 and C_6 also indicated a possible multi-reference character of the wavefunction, due to a near degeneracy of several electronic states. This problem, too, is likely to be aggravated in the larger clusters, and a multi-reference correlation approach would therefore also be desirable. Furthermore, the calculations on C_4 and C_6 show that, in order to achieve sufficient accuracy *all* valence electrons must be correlated, i.e., 32 and 40 electrons for C_8 and C_{10} respectively, which raises concerns about size-consistency (or lack thereof) for the correlation methods used.

Here, we have carried out calculations using methods such as multi-reference CI (MRCI) and modified coupled-pair functional [20] (MCPF) on C_8 and C_{10} using large basis sets.

2. Computational details

In the present calculations, a $13s8p$ Gaussian basis set [21] was augmented with four d-type functions to form the primitive set. The polarization functions were chosen as an even-tempered sequence with a ratio of 2.5 and a geometric mean of 1.806. The basis was then contracted to $4s3p1d$ (Set *A*), $5s4p2d$ (Set ***B***) and $6s5p4d$ (Set *C*), using a general contraction to atomic natural orbitals (ANOs) [22]. Retaining only the pure $5d$ components of the Cartesian d-functions, these basis sets yielded 18, 27, and 41 contracted functions per carbon atom respectively. For technical reasons, some of the calculations were not carried out with full symmetry constraints but in an abelian subgroup (i.e. D_{2h} and C_{2h} rather than $D_{\infty h}$ and C_{4h}, respectively).

Liang and Schaefer [23] have recently found the cumulene $^3\Sigma_g^-$ state to be the lowest linear structure for both C_8 and C_{10} from *ab-initio* calculations. Accordingly, we felt justified in considering only that state for the optimization of the linear form. For the cyclic structures, our preliminary calculations indicated that electronic states other than the totally symmetric are not favorable. Therefore, geometries of the cyclic C_8 and C_{10} were optimized only for the $^1A_{1g}$ electronic state. The optimization was carried out with basis set *A* and a multi-reference CI procedure, using an iterative natural orbital (INO) scheme. In this scheme, successive MRCI calculations were performed for each geometry, using the natural orbitals obtained from the previous iteration. Starting the procedure with CASSCF orbitals, two INO iterations in each point were considered sufficient to obtain an adequate orbital space, even though the INO procedure is not fully converged at that stage. In these MRCI calculations, only the outer valence electrons were correlated, i.e. 16 and 18 electrons for the cyclic and linear forms of C_8 and 20 and 22 for the cyclic and linear forms of C_{10}. The reference spaces included the three configurations with largest coefficient in a preceding CASSCF calculation.

For additional estimates of the energies, MCPF and SDCI calculations correlating all valence electrons (i.e. 32 electrons for C_8 and 40 electrons for C_{10}) were carried out using basis set *A* at the optimized geometries. For C_8 the results were confirmed by performing SDCI and MCPF calculations using the larger basis set ***B***. In addition, we also carried out MRCI calculations for C_8 in which all valence electrons were correlated.

The first step in the MRCI procedure is usually a CASSCF (or other MCSCF) calculation. In addition to providing orbitals, the CASSCF also indicates the dominating configurations, which are the ones to be used as reference configurations in the MRCI treatment. The reference configurations used in this work for the two forms of C_8 are given in the following:

the linear form ($D_{\infty h}$ symmetry)

(core) + (inner valence) +
$(2\pi_u)^4(2\pi_g)^2$ (leading configuration)
$(2\pi_u)^2(2\pi_g)^4$
$(2\pi_u)^3(2\pi_g)^2(3\pi_u)^1$ (2 distinct configurations)
$(2\pi_u)^4(3\pi_u)^2$

where

$$\text{core} \equiv (1\sigma_g)^2(1\sigma_u)^2(2\sigma_g)^2(2\sigma_u)^2(3\sigma_u)^2(3\sigma_g)^2(4\sigma_g)^2(4\sigma_u)^2$$

and

$$\text{inner valence} \equiv (5\sigma_g)^2(5\sigma_u)^2(6\sigma_g)^2(6\sigma_u)^2(7\sigma_g)^2(7\sigma_u)^2(8\sigma_g)^2 \\ (1\pi_u)^4(1\pi_g)^4(8\sigma_u)^2(9\sigma_g)^2$$

the cyclic form (C_{4h} symmetry)

(core) + (inner valence) +
$(5b_g)^2(1b_u)^2$ (leading configuration)
$(6a_g)^2(1b_u)^2$
$(5b_g)^2(2a_u)^2$
$(5b_g)^2(1b_u)^2(6e_u)(2e_g)$ (2 distinct configurations)
$(5b_g)^2(2e_g)^2$ (2 configurations in C_{2h} symmetry)

where

$$\text{core} \equiv (1a_g)^2(1e_u)^4(1b_g)^2(2a_g)^2(2e_u)^4(2b_g)^2$$

and

$$\text{inner valence} \equiv (3a_g)^2(3e_u)^4(3b_g)^2(4b_g)^2(4e_u)^4(4a_g)^2(1a_u)^2(5a_g)^2(1e_g)^4(5e_u)^4.$$

Using these reference configurations and basis set *A*, about 9.1 and 8.4 million of total configurations were generated for the linear and cyclic forms respectively.

The MOLECULE-SWEDEN [24] program system was used in the calculations presented here. The correlation effects in C_{10} were further studied in single-reference, coupled-cluster calculations (CCSD), using the TITAN code [25]. All valence electrons were correlated in these calculations. To assess the residual basis set effect, MP2 calculations were performed with basis sets ***A***, ***B***, and ***C***, using the program DISCO [26]. These MP2 calculations were of spin-restricted nature, and the open-shell MP2 calculations were carried out using a symmetry-restricted formalism similar to the one proposed by Hubac and Çarsky [27]. The OS-MP2 formalism used here is based on a single set of orbitals obtained from the ROHF calculation, whereas different sets of orbital energies are defined for the α- and β-orbitals as expectation values of the different Fock operators. While not formally rigorous, the approach has been found to remedy many of the anomalities seen in UMP schemes due to severe spin contamination. In general, the approach gives results which fall between the usual UMP method and the ROMP2 scheme recently proposed by Handy and co-workers [28], while being less expensive than any of those since only one set of orbitals is used.

3. Results

Optimized geometries of the different structures of C_8 and C_{10} are shown in Figs. 1 and 2, respectively. Geometrical parameters are given in the figures. Cyclic C_8 has alternating bond distances *and* angles, corresponding to C_{4h} symmetry. The SDCI, MRCI, and MCPF energies of C_8 calculated with basis sets ***A*** and ***B*** are listed in Table 1, along with their relative energies. Table 2 shows basis set effects on the relative energy of the cyclic and linear C_8 at the SCF and MP2 level. For C_{10}, the three cyclic structures studied here are very close in energy. Total energies of these structures and the linear form, calculated at the MCPF and SDCI levels are provided in Table 3. Energies of different structures of C_{10} relative to the $^1A_{1g}$ cumulenic D_{10h} are given in Table 4.

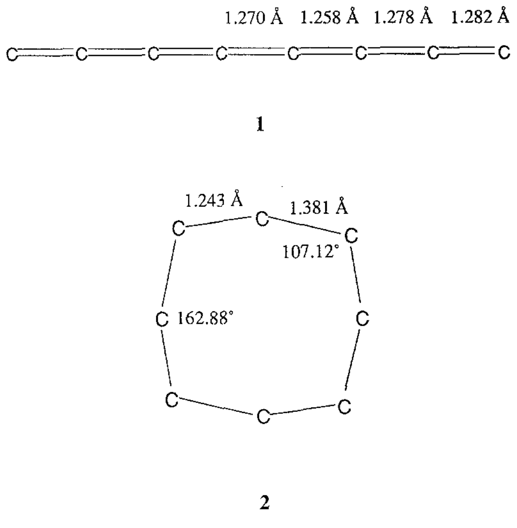

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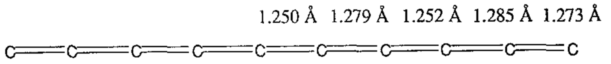
Fig. 1. Optimized geometries of different C_8 structures, i.e. cumulene **1** and monocyclic **2**



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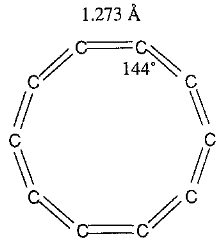

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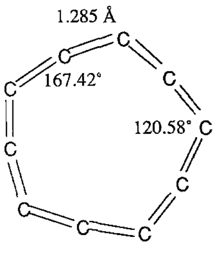

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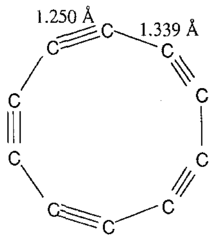

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Fig. 2. Optimized geometries of different C_{10} structures, i.e. cumulene **3**, cumulenic D_{10h} **4**, distorted-cumulenic D_{5h} **5** and acetylenic D_{5h} **6**

Table 1. Total energies (in Hartree) and relative energies (in kcal/mol) of the cyclic and linear forms of C_8

Basis	Method	Structure **2**	Structure **1**	*E*(*cyc.*)-*E*(*lin.*)
A	SDCI	−303.38683	−303.38515	−1.05
A	SDCI + DVD	−303.54731	−303.54596	−0.85
A	MCPF	−303.65216	−303.64673	−3.41
A	MRCI	−303.40303	−303.41453	7.22
B	SDCI	−303.43603	−303.41606	−12.53
B	SDCI + DVD	−303.64296	−303.62515	−11.17
B	MCPF	−303.70960	−303.69359	−10.04

Table 2. Relative energies of linear and cyclic forms of C_8 at the SCF and MP2 level (in kcal/mol) using various basis sets

Contracted basis	*E*(*cyc.*)-*E*(*lin.*) SCF	MP2
A	5.38	4.69
B	1.74	−3.39
C	1.74	−4.86

Table 3. Total energies (in Hartree) of different structures of C_{10}, and with different correlation methods. 40 electrons were correlated in all calculations

Basis	Method	Structure **3**	Structure **4**	Structure **5**	Structure **6**
A	SDCI	−379.22803	−379.30903	−379.33414	−379.30510
A	SDCI + DVD	−379.49840	−379.58699	−379.60247	−379.58583
A	MCPF	−379.60480	−379.69391	−379.70212	−379.69781
A	CCSD		−379.66468	−379.67579	−379.66897
A	CCSD(T)		−379.77669	−379.77867	−379.77745

Table 4. Energies of different C_{10} structures relative to the ${}^1A_1'$ state of the distorted-cumulenic D_{5h} structure **5** (in kcal/mol).

Basis	Method	Structure **3**	Structure **4**	Structure **6**
A	SDCI	66.57	15.75	18.21
A	SDCI + DVD	65.30	9.71	10.44
A	MCPF	61.10	5.19	3.46
A	CCSD		6.97	4.28
A	CCSD(T)		1.24	0.76

4. Discussion

4.1. The ground-state conformation of C_8

Using basis set *A*, the relative energies obtained from the three methods, i.e SDCI, MCPF, and MRCI, are quite different (see Table 1). The SDCI calculations find the cyclic form 1.0 kcal/mol more stable than the linear form. When the MCPF method is used, that energy gap is slightly increased to 3.4 kcal/mol, still favoring the cyclic form. Apparently, the lack of size-consistency, which ought to be considerable for a 32 electron SDCI calculation and is largely remedied in the MCPF method, has only affected the relative energy slightly. In contrast, the MRCI calculations predict the linear (${}^3\Sigma_g^-$) state to be 7.2 kcal/mol *lower* in energy than the cyclic structure. The difference between the SDCI and MRCI relative energies must be ascribed to near-degeneracy effects. Since the selection of reference states has a certain element of arbitrariness the result must be regarded as uncertain, but it would appear that in this case, and for this particular comparison, near-degeneracy correlation is more important than size-consistency. The difference in relative energy obtained by single- and multi-reference approaches also indicates the deficiency of the single-reference correlation treatment for the linear structure. Although the Davidson correction lowers the SDCI energies significantly, it is rather unimportant for the relative energy. This is also the case for C_{10}.

Using basis set *B*, the relative energies obtained from MCPF and SDCI calculations on C_8 are −10.0 and −12.5 kcal/mol respectively. Thus, extending the basis set from *A* to *B* favors the cyclic form by 7–8 kcal/mol. A similar basis set trend is also observed in the MP2 calculations (see Table 2). At the MP2 level, a further increase of the basis set size from *B* to *C* only recovered an additional 1.5 kcal/mol. Increasing the basis set further is not likely to affect the relative energy by more than 1–2 kcal/mol, a conclusion which ought to pertain also to the more advanced correlation methods.

The MP2 and MCPF calculations with large basis sets both suggest a cyclic ground state for C_8. However, both methods are based on a single-reference approach. Adding a tentative correction of 8–10 kcal/mol for multi-reference effects would make the two forms practically isoenergetic within realistic error bars.

4.2. The ground-state conformation of C_{10}

Using basis set A, SDCI and MCPF calculations predict all three cyclic structures (i.e. cumulenic D_{10h} **4**, distorted-cumulenic D_{5h} **5**, and acetylenic D_{5h} **6**) to be about 50 kcal/mol more stable than the linear ${}^3\Sigma_g^-$ form **3**. This energy difference is certainly outside any estimated error bars due to truncation of the one- and many-electron basis set. Thus, unlike the smaller clusters in the series C_{10} definitely has a cyclic ground state with the linear form much higher in energy.

According to the SDCI calculations, the cyclic structure **5** is the most stable form. The energies of **4** and **6** relative to **5** are 15.7 and 18.2 kcal/mol, respectively. At the MCPF level, these energy differences (in the same order) are significantly reduced, to 5.2 and 3.5 kcal/mol. This behavior has also been observed in recent calculations on C_{10} by Liang and Schaefer [17]. A more accurate correlation treatment would be necessary in order to determine energy differences between these cyclic structures. We have therefore carried out coupled-cluster calculations with single and double excitations (CCSD) including also an estimate of connected triples (CCSD(T)) for these three cyclic structures using basis set A. Total and relative energies of the three cyclic structures obtained from these calculations are also provided in Tables 3 and 4. CCSD calculations indicate that **4** and **6** are 7.0 and 4.3 kcal/mol above **5**, respectively, while these differences in energy (in the same order) are only 1.2 and 0.8 kcal/mol when connected triples are included at the CCSD(T) level. These differences are further lowered by 1.0 and 0.4 kcal/mol at the MP2 level when extending the basis from A to $\boldsymbol{B}$. It is likely that the three cyclic structures considered here would become essentially isoenergetic if more accurate correlation treatments and larger basis sets were employed. In any case, the small differences in energy between these three cyclic structures indicate that the potential surface for cyclic C_{10} is very flat.

4.3. Convergence of the perturbation series

The relative energy between the structures **5** and **4** (ΔE_1 in Table 5), obtained from MP2 calculations with Set A basis is -35.8 kcal/mol, a 30 kcal/mol difference from those obtained from MCPF, CCSD, and CCSD(T) calculations. The accuracy of the MP2 method might, therefore, be questionable. Moreover, SCF calculations carried out using the same basis gave ΔE_1 of 31.0 kcal/mol, a difference of 60 kcal/mol from the MP2 calculations. The failure of SCF and MP2 calculations in determining the relative energy indicates a poor convergence of the perturbation series. To investigate this problem further, we performed MP4 calculations using the $(7s3p)/[3s2p]$ basis of van Duijneveldt [21] (Set $\boldsymbol{D}$) on the cyclic structures **4**, **5**, and **6**. The result is given in Table 5.

Table 5. Energies of the cyclic C_{10} structures **4** and **6** relative to the $^1A_1'$ state of **5** in kcal/mol

Basis	Method	ΔE_1 $E(\mathbf{4})-E(\mathbf{5})$	ΔE_2 $E(\mathbf{6})-E(\mathbf{5})$
D	SCF	2.30	1.77
D	MP2	−52.07	−49.99
D	MP3	−16.41	−25.58
D	MP4 (SDQ)	−22.57	−28.21
D	MP4 (SDTQ)	−40.33	−36.79
E	SCF	30.31	
E	MP2	−31.46	
E	MP3	13.11	
E	MP4 (SDQ)	6.54	
E	MP4 (SDTQ)	−21.37	
E	MCPF	8.55	6.05
E	CCSD	8.13	5.10
E	CCSD(T)	3.27	2.51
A	SCF	31.00	29.78
A	MP2	−35.79	−24.75
B	SCF	30.78	29.59
B	MP2	−36.77	−25.14

With Set ***D***, the MP4 (SDTQ) favored **4** by −40.3 kcal/mol. However, the same basis set also gave ΔE_1 of 2.3 and −52.1 kcal/mol at the SCF and MP2 levels, respectively. Set ***D*** is of course far too small to estimate the relative energy accurately, and a *d*-exponent of 0.8 was added. This $(7s3p1d)/[3s2p1d]$ basis is labelled Set ***E***. Using this basis, the values obtained for ΔE_1 at the SCF and MP2 level are 30.3 and −31.5 kcal/mol. These results are comparable to those obtained with set ***A***. MP4 (SDTQ) calculations with Set ***E*** gave ΔE_1 of −21.4 kcal/mol compared to the value of 3.3 kcal/mol obtained from CCSD(T) calculations (see Table 5). This suggests that the energies of structures **4** and **5** are not yet converged in the fourth order perturbation calculations, and the accuracy of the single-reference based method is, therefore, questionable. Lee and Taylor have suggested the norm of the T_1 amplitudes obtained from the CCSD calculation as a diagnostic of the reliability of a single-reference correlation treatment [29]. They also concluded that a T_1 value of 0.02 or greater would indicate a large degree of multi-reference character and the single-reference method might not be sufficient for the correlation treatment. The T_1 value for the calculation on **4** was 0.014 whereas a value of 0.034 was obtained for **5**. Thus, while the Hartree–Fock provides a reasonable zeroth-order wavefunction for **4**, it is rather a poor choice for **5**. This would explain why the convergence of the perturbation series on the relative energy of these two structures is so poor. However, the total energies for **4** and **5** shown in Fig. 3 would suggest that the convergence is actually somewhat better for **5** than for **4**, although both are rather disappointing.

This behavior is not strongly dependent on the basis set. Figure 4 shows the same convergence pattern with basis set ***D***, and also indicates that the convergence of the MPn series for **6** is similarly unsatisfactory. Our calculations indicate that the slow convergence of the perturbation series is responsible for

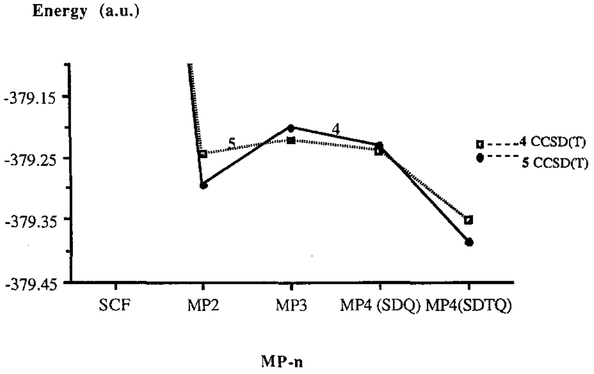

Fig. 3. Total energies of the cumulenic D_{10h} (**4**) and distorted-cumulenic D_{5h} (**5**) forms of C_{10} calculated using Møller–Plesset and CCSD(T) methods with basis Set *E*

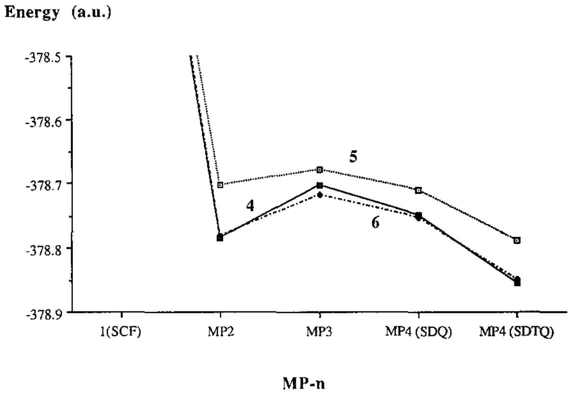

Fig. 4. Convergence of the perturbation series for total energies of cumulenic D_{10h} (**4**), distorted-cumulenic D_{5h} (**5**) and acetylenic D_{5h} (**6**) forms of C_{10}. Møller–Plesset calculations were carried out using basis Set *D*

the disagreement between results obtained from MP4 and other correlated calculations.

Another interesting observation is the difference between ΔE_1 obtained at MP4 (SDQ) and MP4 (SDTQ) levels. Using Set *E*, MP4 (SDQ) calculations yielded ΔE_1 of 6.5 kcal/mol which differs by 27 kcal/mol from that of MP4 (SDTQ). On the other hand, using the same basis set MCPF and CCSD calculations gave ΔE_1 of 8.1 and 8.5 respectively. The agreement between MP4 (SDQ) and MCPF/CCSD calculations suggests that the contribution of triple excitations is overestimated at MP4 level. This overestimation is largely corrected in the CCSD(T) calculation. The contribution of connected triples in CCSD(T) is obtained by estimating MP4(T) and MP5(T) energies [30, 31]. In many systems, the MP4(T) and MP5(T) terms have opposite signs [26], and the contributions of the triple excitations partly cancel.

It is worth noting that the slow convergence of the perturbation series is observed only on the carbon cluster with $4n + 2\pi$ electrons. This seems to be due to a poor choice of the zeroth-order wavefunction. One might expect a similar, slow convergence also for other carbon clusters with $4n + 2\pi$ electrons such as $C_{14}, C_{18}, \ldots$, etc. Raghavachari et al. carried out MP4 calculations on C_6 [12] and a similar convergence pattern was obtained. Moreover, recent calculations on C_{18} also indicate a similar behavior [32]. For C_4 and C_8, in contrast, results obtained from MP2 calculations are in good agreement with those from other methods (see Tables 1 and 2).

5. Conclusions

The linear and cyclic forms of C_8 are isoenergetic. Cyclic C_8 has C_{4h} symmetry and a ^1A_g electronic ground state while linear C_8 is cumulene-like with $^3\Sigma_g^-$ state. The choice of basis sets and methods heavily affects the difference in energy between the linear and cyclic forms of C_8.

The ground-state structure of C_{10} is undisputable monocyclic but it remains unclear which cyclic structure has the lowest energy. Three cyclic structures considered are practically isoenergetic with energy differences of less than 2 kcal/mol, indicating that cyclic C_{10} is a very non-rigid molecule. The level of correlation treatment is important in determining the energy differences between the three cyclic structures.

Along with previously studied carbon clusters [18, 19, 33, 34], these results demonstrate some general mechanisms governing the stability of cyclic carbon clusters relative to the linear ones. As discussed by, e.g., Pitzer and Clementi [1] the ring strain is inversely proportional to the size of the cluster, and with one more bond formed, the rings are expected to be the preferred forms for larger clusters. Among the rings, the systems with $4n+2$ atoms show additional aromatic stabilization, both for the in-plane and the out-of-plane π-electron system, thus illustrating the "double aromaticity" suggested by Schleyer and co-workers [35]. It has also been hypothesized [35] that 4n-electron systems might show double aromaticity due to a redistribution of electrons between the in-plane and the out-of-plane π-systems. While such terms certainly occur in the configuration expansion for C_8, they are not among the leading configurations. In the 4n-electron cyclic clusters for $n > 2$, the ground states have been found to be high-spin ($S = 2$) states, at least at the Hartree–Fock level of approximation [33]. From the accumulated experience available so far, the clusters with more than nine atoms are cyclic, while for the smaller ones the linear structures are equally or more stable.

Finally, we have found that the effect of triple excitations is severely overestimated at the MP4 level, and for these systems the MP4 (SDQ) method is probably more reliable than MP4 (SDTQ).

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References

1. Pitzer KS, Clementi E (1959) J Am Chem Soc 81:4477
2. Weltner Jr. W, McLeod Jr D (1966) J Chem Phys 45:3096
3. Thompson KR, DeKock KL, Weltner Jr W (1971) J Am Chem Soc 93:4688
4. Graham WRM, Dismuke KJ, Weltner JR W (1976) Astrophysical J 204:301
5. Shen LN, Graham WRM (1989) J Chem Phys 91:5115
6. Van Zee RJ, Ferrante RF, Zeringue KJ, Weltner Jr W, Ewing DW (1988) J Chem Phys 88:3465
7. Vala M, Chandrasekhar TM, Sczepanski J, Pellow R (private communication)
8. Whiteside RA, Krishnan R, Defrees DJ, Pople JA, Schleyer PvR (1981) Chem Phys Lett 80:547
9. Magers DH, Harrison RJ, Bartlett RJ (1986) J Chem Phys 84:3284
10. Ritchie JP, King HF, Young WS (1986) J Chem Phys 85:5157

11. Bernholdt DE, Magers DH, Bartlett RJ (1988) J Chem Phys 89:3612
12. Raghavachari K, Whiteside RA, Pople JA (1986) J Chem Phys 85:6623
13. Slanina Z, Zahradnik R (1977) J Phys Chem 81:2252
14. Ray AK (1987) Mol Phys 20:5233
15. Fan Q, Pfeiffer GV (1989) Chem Phys Lett 162:472
16. Raghavachari K, Binkley JS (1987) J Chem Phys 87:2191
17. Liang C, Schaefer HF (1990) J Chem Phys 93:8844
18. Parasuk V, Almlöf J (1991) J Chem Phys 94:8172
19. Parasuk V, Almlöf J (1989) J Chem Phys 91:1137
20. Chong DP, Langhoff SR (1986) J Chem Phys 84:5606
21. van Duijneveldt FB (1971) IBM Research Report RJ945
22. Almlöf J, Taylor PR (1987) J Chem Phys 86:4070
23. Liang C, Schaefer III HF (1990) Chem Phys Lett 169:150
24. Siegbahn PEM, Bauschlicher Jr CW, Roos BO, Heiberg A, Taylor PR, Almlöf J, SWEDEN, a vectorized MC SCF and CI program
25. TITAN is a set of electronic structure programs written by Lee TJ, Rendell AP, Rice JE
26. Almlöf J, Faegri Jr K, Feyereisen M, Korsell K; DISCO, a Direct SCF and MP2 Program
27. Hubac I, Çarsky P (1980) Phys Rev A 22:2392
28. Knowles PJ, Andrews JS, Amos RD, Handy NC, Pople JA (1991) Chem Phys Lett 186:130; Amos RD, Andrews JS, Handy NC, Knowles PJ (1991) Chem Phys Lett 185:256
29. Lee TJ, Taylor PR (1989) Int J Quant Chem S23:199
30. Lee TJ, Rendell AP, Taylor PR (1990) J Phys Chem 94:5463
31. Raghavachari K, Trucks GW, Pople JA, Head-Gordon M (1989) Chem Phys Lett 157:479
32. Parasuk V, Almlöf J, Feyereisen MW (1991) J Am Chem Soc 113:1049
33. Feyereisen MW, Gutowski M, Simons J, Almlöf J (1992) J Chem Phys 96:2926
34. Martin JML, François JP, Gijbels R, Almlöf J (1991) Chem Phys Lett 187:367
35. McEwen AB, Schleyer PvR (1986) J Org Chem 51:4357
36. Chandarsekhar J, Jemmis ED, Schleyer PvR (1979) Tetrahedron Lett 39:3707