The Heat of Formation of Buckminsterfullerene, C_{60}

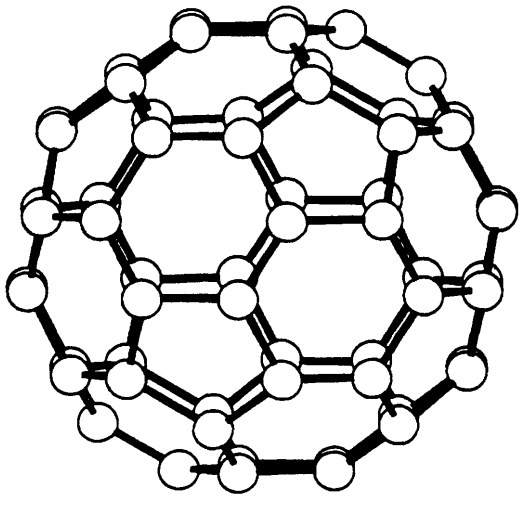
Jerome M. Schulman* and Raymond L. Disch

Department of Chemistry, Queens College, City University of New York, Flushing, New York 11367, USA

The heat of formation of C_{60} (buckminsterfullerene) has been calculated to be 672 kcal mol^{-1} or 11.2 kcal (mol C)$^{-1}$; this may be compared with the value of 1.5 kcal (mol C)$^{-1}$ for a graphite monolayer (1 cal = 4.184 J).

The recent synthesis and isolation of C_{60} (buckminsterfullerene, **1**),[1] a molecule proposed by Kroto, Heath, O'Brien, Curl and Smalley,[2,3] has stimulated interest in its properties and chemical reactivity.[4] For example, its ^{13}C NMR spectrum has been found to contain a single sharp line.[5,6] Clearly, a key thermodynamic property of C_{60} is its heat of formation. We have recently shown that accurate heats of formation of benzenoid aromatics can be obtained from their *ab initio* SCF total energies by means of a group equivalent method. The method has been applied both to planar aromatics and to the non-planar benzo[*c*]phenanthrene **2** and corannulene **3** molecules.[7,8] It is applied here to C_{60}.

We previously reported *ab initio* calculations which optimized the geometry of C_{60} in I_h symmetry.[9] The lengths of the CC bonds exocyclic and endocyclic to the (twelve) regular pentagonal rings were found to be 1.361 and 1.423 Å, respectively. Similar radialene-like geometries have been found by subsequent *ab initio* calculations performed in larger basis sets.[10,11] The 6-31G* SCF energy of C_{60} at our STO-3G



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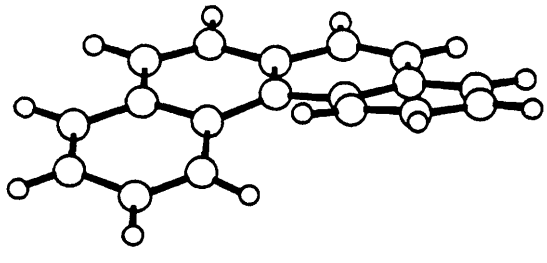

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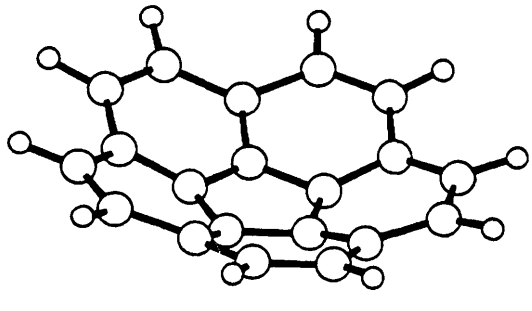

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geometry[9] is −2271.81875 au.[11] This basis, which contains d functions, should be adequate for the energetics of C_{60}, a molecule with considerable angle strain. Combination of the *ab initio* 6-31G* energy with sixty $=C_b<$ group equivalents of energy −37.88150 au[8] furnishes the value in eqn. (1). This value, 672 kcal mol^{-1}, equivalent to 11.2 kcal (mol C)$^{-1}$, is significantly larger than that of graphite (zero) and a graphitic monolayer [1.5 kcal (mol C)$^{-1}$].[12] On the other hand, the more highly strained C_{24} (O_h) cluster has $\Delta_f H^\circ \approx 30$ kcal (mol C)$^{-1}$.[13]

$$\Delta_f H^\circ (298\ \text{K}) = -2271.81875 + 60 \times 37.88150 = 1.0713\ \text{au} \quad (1)$$

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