

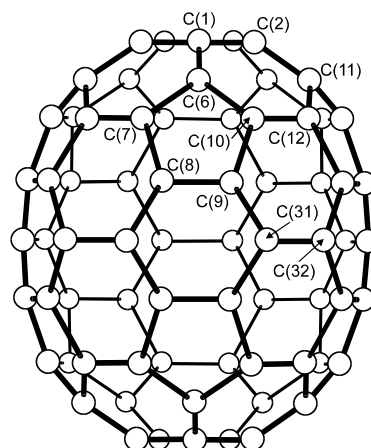
957

 $C_{70}$ 

ED, neutron and X-ray  
diffraction,  $^{13}\text{C}$  NMR,  
*ab initio* and DFT  
calculations

**[5,6]Fullerene- $C_{70}$ - $D_{5h}$**  $C_{70}$ - $D_{5h}(6)$  [5,6]Fullerene $D_{5h}$  assumed $C_{70}$ 

| $r_a$       | $\text{\AA}^a$ |
|-------------|----------------|
| C(1)–C(2)   | 1.461(8)       |
| C(1)–C(6)   | 1.388(17)      |
| C(6)–C(7)   | 1.453(11)      |
| C(10)–C(12) | 1.386(25)      |
| C(7)–C(8)   | 1.468(11)      |
| C(8)–C(9)   | 1.425(14)      |
| C(9)–C(31)  | 1.405(13)      |
| C(31)–C(32) | 1.538(19)      |
| $l^b$       | 3.590(25)      |
| $h^c$       | 3.953(32)      |



Six molecular models with different equatorial bonds were found that give excellent fits to the ED intensities. The best model was selected from considerations of theoretical energies (BP86/TZP level of DFT) and by comparison of computed  $^{13}\text{C}$  NMR chemical shifts (gauge-including atomic orbitals, GIAO-HF/TZP) with those from experiment. This model is in good agreement with structures determined in the crystal by neutron and X-ray diffraction and with results of theoretical calculations (HF/DZP, BP86/TZP), with one important difference: the equatorial bond is some 0.06 Å longer.

The ED measurements were made at 810...835 °C.

<sup>a</sup>) Twice the estimated standard errors.

<sup>b</sup>) Distance from the center of the molecule to an equatorial atom.

<sup>c</sup>) Distance from the center of the molecule to the center of a capping pentagon.

Hedberg, K., Hedberg, L., Bühl, M., Bethune, D.S., Brown, C.A., Johnson, R.D.: J. Am. Chem. Soc. **119** (1997) 5314.