

# Professor Sir Harold Walter KROTO

Department of Chemistry and Biochemistry  
The Florida State University  
Tallahassee Florida 32306-4390 USA



**He shared** (with Robert F. Curl Jr. and Richard E. Smalley)

**the 1996 Nobel Prize in Chemistry**

*for the discovery of C<sub>60</sub> Buckminsterfullerene*

*a new form of carbon*

## Main research areas:

- I. Spectroscopy of Unstable Species and Reaction Intermediates (Infrared, Photoelectron, Microwave and Mass Spectrometry)
- II. Astrophysics (Interstellar Molecules and Circumstellar Dust)
- III. Cluster Science (Carbon and Metal Clusters, Microparticles, Nanofibres)
- IV. Fullerene Chemistry, Nanoscience and Nanotechnology

## Research Highlights

1. First detection of  $^1\Delta$  state of a polyatomic free radical (NCN by flash photolysis) [3, 4]
2. Theoretical studies of ground and electronically excited states of small molecules [5, 6]
3. Detection of liquid phase intermolecular interactions using Raman Spectroscopy [7-10]
4. Breakthrough in the detection of new unstable species (thioaldehydes, thiocarbonyls thioborines) using combination of microwave and photoelectron spectroscopy techniques [12, 15, 18-22, 31, 80]
5. Synthesis in 1976 of the first phosphalkenes (compounds containing the free carbon phosphorus double bond) in particular CH<sub>2</sub>=PH (with N P C Simmons and J F Nixon, Sussex), [28, 80]
6. Monograph "Molecular Rotation Spectra" [23]
7. Synthesis in 1976 of the first analogues of HCP, the phosphalkynes which contain the carbon phosphorus triple bond – in particular CH<sub>3</sub>CP (with N P C Simmons and J F Nixon, Sussex), [29, 80]

8. The discovery (1976-8) of the cyanopolyynes, HC<sub>n</sub>N (n = 5, 7, 9), in interstellar space (with D R M Walton A J Alexander and C Kirby (Sussex) and T Oka, L W Avery, N W Broten and J M MacLeod (NRC Ottawa)), Ref 4-6, based on microwave measurements made at Sussex, [27, 30, 35, 80]
9. The discovery of C<sub>60</sub>: Buckminsterfullerene in 1985 (with J R Heath, S C O'Brien, R F Curl and R E Smalley), [100, 112, 139, 239]
10. The detection of endohedral metallofullerene complexes (with J R Heath, S C O'Brien, Q Zhang, Y Liu, R F Curl, F K Tittel and R E Smalley), [101, 139]
11. The prediction that C<sub>60</sub> should be produced in combustion processes and might indicate how soot is formed (with Q L Zhang, S C O'Brien, J R Heath, Y Liu, R F Curl and R E Smalley) [103,139 ]
12. The explanation of why C<sub>70</sub> is the second stable fullerene (after C<sub>60</sub>) and the discovery of the Pentagon Isolation Rule as a criterion for fullerene stability in general [107, 112, 139, 239]
13. The prediction of the tetrahedral structure of C<sub>28</sub> and the possible stability of "tetravalent" derivatives such as C<sub>28</sub>H<sub>4</sub> [107, 112, 139, 239]
14. The prediction that giant fullerenes have quasi-icosahedral shapes and the detailed structure of concentric shell graphite microparticles (with K G McKay), [111, 112, 139, 239]
15. The mass spectrometric identification and solvent extraction (with J P Hare and A Abdul-Sada) of C<sub>60</sub> from arc processed carbon in 1990 – independently from and simultaneously with the Heidelberg/Tucson group; Refs [121, 239]
16. The chromatographic separation/purification of C<sub>60</sub> and C<sub>70</sub> and <sup>13</sup>C NMR measurements which provided unequivocal proof that these species had fullerene cage structures (with J P Hare and R Taylor, Sussex), Refs [121, 139, 239]
17. Crystal structure of C<sub>60</sub> [135, 138]
18. Main Fullerene chemistry breakthroughs: C<sub>60</sub>(ferrocene)<sub>2</sub> [162], characterisation of C<sub>60</sub>Hal<sub>6</sub> [174, 149], C<sub>60</sub>(P<sub>4</sub>)<sub>2</sub> [187, 192]
19. Nanoscience and Nanotechnology advances: Condensed phase nanotubes [205], nanoscale BN structures [224], partly aligned-nanotube bundles [233], nanotube formation mechanisms [161, 238], silicon oxide nanostructures [247], Si surface-deposited fullerene studies [251], insulated carbon nanotube conductors [297]

### *Overview*

Fellow of the Royal Society (1990),  
 Foreign Associate of the National Academy of Sciences (US),  
 President of the Royal Society of Chemistry (2002-2004).  
 Longstaff Medal of the Royal Society of Chemistry (1993),  
 Faraday Lecturer 2001 (Royal Society),  
 Copley Medal of the Royal Society (2002),  
 Erasmus Medal of Academia Europaea,  
 Freeman of the City of Torino,  
 29 Hon Degrees.

## List of publications of Professor Sir Harold Walter KROTO

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2. R N Dixon and H W Kroto, 'The electronic spectrum of nitrosomethane, CH<sub>3</sub>NO', *Roy. Soc.*, 283, 423-432 (1965).
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4. H W Kroto, 'The  $^1\pi_u \leftarrow ^1\Delta_g$  electronic spectrum of NCN', *Can. J. Phys.*, 45, 1439-1450 (1967).
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6. H W Kroto and D P Santry, 'Semiempirical molecular-orbital spectra. II. Approximate open-shell theory', *J. Chem. Phys.*, 47, 2736-2743 (1967).
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12. G H King, H W Kroto and R J Suffolk, 'The photo-electron spectrum of a short-lived species in the decomposition products of CS<sub>2</sub>', *Chem. Phys. Letts.*, 13, 457-458 (1972).
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15. H W Kroto and R J Suffolk, 'The photoelectron spectrum of an unstable species in the pyrolysis products of dimethyldisulphide', *Chem. Phys. Letts.*, 15, 545-548 (1972).
16. C C Costain and H W Kroto, 'Microwave spectrum, structure and dipole moment of cyanogen azide, NCN<sub>3</sub>', *Can. J. Phys.*, 50, 1453-1457 (1972).
17. A J Careless, M C Green and H W Kroto, 'The microwave spectrum of trimethylsilyl isocyanate (CH<sub>3</sub>)<sub>3</sub>SiNCO', *Chem. Phys. Letts.*, 16, 414-418 (1972).
18. H W Kroto and R J Suffolk, 'The photoelectron spectrum of F<sub>2</sub>CS and fluorine substitution shifts', *Chem. Phys. Letts.*, 17, 213-216 (1972).
19. A J Careless, H W Kroto and B M Landsberg, 'The microwave spectrum, structure and dipole moment of thiocarbonyl fluoride, F<sub>2</sub>CS', *Chem. Phys.*, 1, 371-375 (1973).
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24. A J Careless and H W Kroto, 'Rotational transitions in degenerate vibrational states of  $\text{C}_{3v}$  symmetric top molecules with application to  $\text{CH}_3\text{CN}$ ', *J. Mol. Spectrosc.*, 57, 189-197 (1975).
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