

REPRESENTATION OF ORBITAL SHAPES

H.M.N. Bandara, H.A.U. Gunasekera
Dept. of Chemistry, University of Peradeniya.

Polar plots and contour diagrams are often used to illustrate the shapes of atomic orbitals¹. A clear understanding of orbital shapes is a prerequisite for the comprehension of chemical bonding.

Problems arise when polar plots are used to represent hybrid orbitals¹. We have observed that diagrams in a number of elementary textbooks do not represent the shapes of hybrid orbitals correctly², and we have therefore developed computer programmes for quick display of the exact shapes of these orbitals. These programmes are useful in the teaching of chemistry to undergraduates. A convenient method is also described to construct molecular orbitals using polar-type diagrams.

References

1. Osamu Kikuchi and Keizo Suzuki (1985) J.Chem.Educ. 62 (3) : 206
2. Scaife, D.B. J.Chem Educ 55 (7): 442

E₁-30 : 10th Dec. 1987 (Thursday) 02.00 p.m. - 02.15 p.m.

E₁-31 : 10th Dec. 1987 (Thursday) 02.15 p.m. - 02.30 p.m.