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Book review

Structure and bonding; edited by J.D. Dunitz, J.B. Goodenough, P. Hemmerich, J.A. Ibers, C.K. Jørgensen, J.B. Neilands, D. Reinen and R.J.P. Williams; *Vol. 39, Electrons and transitions*, vi + 120 pages, Springer-Verlag, Berlin-Heidelberg-New York, 1980, DM 64.—; approx. US $ 35.90.

This volume contains two articles on the theory of bonding in transition metal complexes and one on Auger electron spectrometry.

D.W. Clack and K.D. Warren have written a review of molecular orbital calculations on transition metal sandwich complexes. With present computer technology it is possible to carry through an ab-initio calculation of the SCFMO type on a molecule like ferrocene using a minimal basis, but it is a fairly expensive operation. To study a large series of such molecules, or to examine geometry variations of any one, or to use a large basis or to go beyond the SCF level; all of these could not at present be justified unless there was a burning problem to be answered.

This review deals largely with the INDO procedure developed by Clack for transition metal complexes. It is a semi-empirical scheme which has been parameterized for the most part from electronic spectral data. For molecules of this size the molecular orbital energy pattern is rather densely spaced if one includes π and σ orbitals of the ligands and it is difficult to pick out the key features. Clack and Warren largely concentrate on the d orbital sequence and on the orbital populations and bond orders.

The article by S.F. Mason deals with the effect of ligand polarization by the transition metal in transition metal complexes. Ligand field theory describes the effects of metal polarization by the ligands but, as Mason explains, this fails to explain quantitatively the intensities of d—d and f—f transitions and, particularly the strength of optical rotation in chiral compounds. All of these can be encompassed more satisfactorily in a ligand polarization model although the importance of ligand—metal overlap, ignored in the theory, is difficult to judge.

The final article by L.R. Balsenc deals with the Auger spectra of sulphur compounds absorbed on monocrystalline metal faces. It is perhaps a narrower topic than the other two but nicely illustrates the information that can be obtained from modern surface experiments.

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