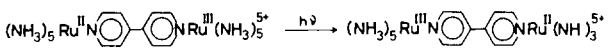
Intervalence Transfer (IT) absorption bands can appear (*e.g.* eqn. 1). The properties of IT absorption bands can be understood based on the early work of



(1)

Hush and later theoretical developments. Perhaps most important is the information available in IT bands concerning related thermal electron transfer processes.

Experimentally, it has been possible to probe the role of molecular and solvent vibrations and of the distance between redox sites on the energy of the transition. Although a continuum model for the solvent has been successful in some cases, it is clear that specific solvent effects are important in others.

In more recent work, it has been possible to explore the relationship between IT and related, excited state transitions, to calculate thermal electron transfer rate constants from the properties of IT bands, and to extend the treatment involved to both metal–ligand and donor–acceptor charge transfer transitions.

Jahn–Teller Effect and Stereochemistry

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The main theoretical aspects of the Jahn–Teller effect (JTE) are outlined and particular attention is paid to a correct understanding of the related statements about the electronic degeneracy and the spontaneous distortion.

The 'static' and 'dynamic' limits and their connections by tunneling mechanism are considered. Moreover the role played by the JTE in quenching electronic operators (Ham effect) and in amplifying distorting perturbations is shown.

Successively the most significant results for the linear coupling in the 'static' approximation are summarized following Öpik and Pryce's analysis. On the other hand it is stressed how the introduction of second order and/or anharmonic terms can yield simultaneous stable distortions thus overcoming Öpik and Pryce's 'dichotomy'. Real systems, for which such a coexistence has been proved by experiments, are presented.

Finally, it is shown how a straightforward evaluation of the Jahn–Teller coupling constants is possible following the angular overlap model and some applications to molecules containing transition metal ions are reported.

Vibronic Model for Mixed Valence Compounds and Spin Crossover Systems

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The vibronic coupling model for mixed valence systems recently proposed by Piepho, Krausz and Schatz [1] is described. Using the model, it is a simple process to obtain the vibronic energy levels and eigenfunctions relevant to an intervalence band. Calculations are essentially exact within the context of the model, and are not limited to the cases of very strong or very weak interactions. The eigenvalues and eigenvectors obtained may be used to determine properties associated with the mixed valence band. These include, for example, the absorption profile of the band, the degrees of delocalization and valence-trapping, and the electron transfer kinetics for the system.

Very similar formalism applies to both mixed valence and spin crossover systems. Thus the applicability of the model to single-center systems with two different spin states with intersecting potential surfaces is discussed.

Finally, the limitations of the mixed valence model are discussed, and methods of improving the model by more explicit consideration of the nature of the interacting centers are considered.

References

1 S. B. Piepho, E. R. Krausz and P. N. Schatz, *J. Am. Chem. Soc., 100,* 2996 (1978).

Low Spin Co(II) Complexes in Various Solvents as Studied by ESR Spectroscopy

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Four-coordinated, low spin, Co(II)-complexes of the Co(salen) type, have a $^2A_2$ ground state, the