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QUANTUM CHEMISTRY, SOLID STATE PHYSICS AND QUANTUM BIOLOGY

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THE 1964 International Summer Institute in Quantum Chemistry, Solid State Physics and Quantum Biology, where discussions ranged from linear algebra and chemical reactivity to ageing and heredity provided a good illustration of the intermixing between various disciplines in science that has become a happy feature in contemporary research. The institute was one of the series arranged by the Uppsala Quantum Chemistry Group and the Quantum Theory project at the University of Florida, and about 800 scientists have participated in and contributed to these institutes since the first one held in 1958. The present one which was attended by about hundred persons from seventeen different countries was held in two parts: the first one was held at Abisko in Northern Lappland between July 19 and July 31 and the second part at Uppsala between August 6 and August 22.

Abisko is a summer resort in Northern Lappland about 200 kilometres north of the arctic circle and can be reached only by train. It is situated in a real wilderness and due to the intense sunlight, the vegetation in Abisko valley is exceedingly rich and has a pseudo-tropical character. We however missed the midnight sun which could be seen from Abisko only until July 4. The institute was held in the tourist station and this was the only habitation for miles around. Five lectures a day was the minimum and nine hours a day was not uncommon since the weather at Abisko was quite unpredictable.

Uppsala, one of the oldest universities in Europe (1477), where the second part of the institute was held, provided an appropriate environment for serious study in an academic atmosphere. At Uppsala it was normal to have eight lectures a day which were very often followed in the evenings by discussions and question hours.

The entire course was directed by Professor Per-Olov Lowdin of the Quantum Chemistry Group, Uppsala, and the Quantum Theory Project, University of Florida. The other lecturers were: Raymond Daudel (Sorbonne and CNRS, Paris), Frank E. Harris (Stanford University), Masao Kotani (University of Tokyo), Laurens Jansen (Batelle Memorial Institute, Geneva), Bela Lengyel (San Fernando Valley College, California), Andrew Liehr (Mellon Institute, Pittsburgh) and Ruben Pauncz (Technion, Haifa). The problem sessions were handled by the Uppsala Quantum Chemistry Group led by Dr. Jean Louis Calais.

The lectures of Lowdin started with a brief history of Quantum Theory and led on to the application of the methods of linear algebra to quantum theory. Great emphasis was laid on projection operators, the way to derive them from the Cayley-Hamilton equation and their use in component analysis. Cyclic operators, nilpotent operators and normal operators were discussed with examples of their occurrence in quantum theory. Heisenberg's uncertainty relations were derived from the concept of the

width of an operator and these led to Heisenberg's equation of motion and Ehrenfest's relations. These methods were applied in a series of lectures to atomic, molecular and solid state systems and led to a study of the exchange effects, spin effects and the Hartree-Fock schemes for atoms. Crystals were discussed in a brief way and the use of projection operator techniques to derive the Bloch functions from the Born-von Karman conditions was demonstrated. A discussion of the "Tunnelling Effect" was followed by a proposition that tunnelling effect may play an important role in what Lowdin calls "Quantum Genetics", tunnelling of protons could affect gene, DNA, RNA and protein syntheses. Proton tunnelling between the hydrogen-bonded base pairs of the DNA molecule leads to an inversion and hence a mistake in the code and this may be one of the methods of incorporating coding mistakes. Such coding mistakes will have a direct consequence on mutation and ageing; perhaps this may be one of the answers to the problem of evolution and inception of cancer.

A major portion of the second half of Lowdin's lecture series was devoted to a serious study of the time dependent and time independent perturbation theories. The lectures of Lowdin closed with a discussion of bond order and bond lengths, the derivation of the expression for the spin-orbit and Fermi contact couplings and an excellent discussion on density matrices.

Pauncz treated the general theory of angular momentum with the projection operator techniques and applied the results to the treatment of spin and orbital angular momenta and LS-, jj- and intermediate-coupling schemes in atoms. The treatment of theory of the conjugated systems included the simple MO-LCAO method, the pairing theorem for alternant hydrocarbons, a discussion of the reactivity index in aromatic molecules, the Parisier-Parr Pople method and other semi-empirical approaches. His lectures ended with a treatment of the alternant M.O. method where different orbitals are permitted for different spins.

Lengyel had the difficult task of connecting quantum theory with the theory of Hilbert space and for quite a few of the participants this was their first contact with abstract mathematics. Starting from the theory of linear spaces, Lengyel dealt with the concept of norm,

scalar products, bounded self-adjoint operators and the spectral resolution theorem. Harris in the course of his lectures dealt with the expansion of total wave functions in terms of Hartree products and Slater determinants and went through the procedure of evaluating matrix elements between Slater determinants for the various terms of the Hamiltonian. This led to the treatment of the Hartree-Fock scheme and the ASP-MO-LCAO-SCF method; the last four lectures were devoted to an examination of the available computational methods to evaluate correlation terms in the Hartree-Fock Scheme.

Jansen dealt with the problem of crystal stability and put forward a convincing theory to explain why Ne, Ar, Kr crystallized in fcc and He⁴ crystallized in hcp and similarly NaCl and most alkali halides crystallized in two interpenetrating fcc lattices while CsCl, CsBr, CsI crystallized in two interpenetrating simple cubic lattices.

Kotani dealt with many electron atoms in fields of various symmetries and derived many theorems using group theory. The case of spherical symmetry and cubic symmetry were considered and matrix elements were calculated.

Daudel discussed the quantum theory of chemical reactivity and indicated how equilibrium constants (pK values) for acid-base pairs, tautomeric system and singlet-triplet equilibria in biradical and biradicaloid systems, could be calculated. It was postulated that the pK values for tautomerism of the DNA bases being more favourable in their excited state may be one of the reasons for mutagenesis under irradiation. Daudel indicated briefly how the problem of chemical carcinogenesis could be studied by consideration of localization energy.

Liehr's lectures were on Ligand Field Theory. To sum up, the Summer Institute served its purpose by focusing our attention on the trends of recent research in the field of quantum chemistry and one returned with a feeling that a lot still remains to be done both in the fundamental basis of quantum theory and in its applications to physics, chemistry and biology.

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