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   Evolution of the Early Atmosphere  P V Sukumaran

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    Electrostatic Models for Weak Molecular Complexation
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21  Science and Technology of Ceramics
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A study of electrostatic potential can provide useful guidelines for investigating weak molecular clusters. A variety of models incorporating electrostatics as a principle ingredient have been developed for probing such complexes. The cover page shows a cluster of six water molecules networked by OH...O hydrogen bond. Isosurfaces of MESP values 'X=-105' and 'Y=1050' kJ mol⁻¹ are superposed on the corresponding ball and stick model in order to bring out the complementary lock-and-key arrangement.