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## THERMODYNAMICAL AND KINETICAL INVESTIGATIONS ON THE TUNGSTEN-FLUORINE CYCLE

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The simultaneous reaction equilibria in the heterogeneous system tungsten-fluorine and its influence by bromine, oxygen, hydrogen, molybdenum and argon has been investigated by means of thermochemical computer programs.
By an analysis of the temperature dependence of the mass-balance of tungsten the chemical transport in these systems and the burning behaviour of halogen-incandescent lamps may be predicted.
Results for the chemical transport reactions are compared to lamp experiments.
The influence of concentration diffusion on local stoichiometry, the effect of reaction kinetic and the processes through which low temperature reactions at the bulb wall control the halogen cycle are delineated.

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## AN ELECTROSTATIC APPROACH TO THE THERMOCHEMISTRY OF FLUOROCARBONS

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The often used predictive schemes, notably bond and group additivites, work well for the prediction of heats of formation of compounds not containing polar groups. However, as halogens are introduced into the molecule, the additivity schemes may be in error by as much as 7-10 kcal $mol^{-1}$. An electrostatic point charge model will be described which shows marked improvement in the prediction of heats of formation of fluorine and chlorine containing organic molecules. Intrinsic point charges are assigned to each atom at infinite distances. As these charges are brought to molecular dimensions, polarization occurs due to the electric fields generated. The heats of formation are then considered to be the sum of three terms - a bond contribution, an electrostatic work contribution, and a polarization work contribution.