

## NOVEL RARE GAS CHEMISTRY

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UV-Photolysis of rare gas matrices doped with hydrogen halides yield H and Y (Y=halogen) atoms, and further excitation of the charge-transfer transition of XY pairs (X=Ar, Kr, Xe) results in mobilised holes. Permanent trapping of the holes may occur for instance in centers of type (XHX)<sup>+</sup>. Annealing of the UV-irradiated H-containing matrices results in extremely strong IR-absorptions, which could by doping experiments be shown to belong to neutral species of type HXY. The novel rare-gas containing species found so far are HXeCl, HXeBr, HXeI, HKrCl and HXeH. All these species are strongly polar and their common structure is (HX)<sup>+</sup>Y<sup>-</sup>. In order to learn more about the potential surface, detailed spectroscopic studies are performed on HXeI. This species can be photodecomposed into neutral atoms by infrared irradiation in the 3  $\mu\text{m}$  region, and recovered quantitatively thermally at temperatures below 30 K. An Arrhenius analysis propose for the barrier from neutral atoms to HXeI a value of 700  $\text{cm}^{-1}$ . We suggest that this barrier originates from an avoided crossing between two singlet surfaces limiting either to separated atoms H + Xe + I or to ionic species (HXe)<sup>+</sup> + I<sup>-</sup>.

### References:

- Neutral rare-gas containing charge-transfer molecules in solid matrices. I. HXeCl, HXeBr, HXeI and HKrCl in Kr and Xe. M.Pettersson, J.Lundell, M.Räsänen, *J.Chem.Phys.* 102 (1995) 6423-31.
- Neutral rare gas containing charge-transfer molecules in solid matrices. II. HXeH, HXeD and DXeD in Xe. M.Pettersson, J.Lundell, M.Räsänen, *J.Chem.Phys.* 103 (1995) 205-10.
- The mechanism of formation and IR-induced decomposition of HXeI in solid Xe. M.Pettersson, J.Nieminen, L.Khriachtchev, M.Räsänen, *J.Chem.Phys.* to be submitted.