

Fig. 5 Model of the (110) face, showing one metal atom in the next layer, and three locations for hydrogen atoms

Fig. 5 shows three locations for hydrogen atoms on the (110) plane. The atoms on the left and right are bonded simply by the normal-emergent t_{2g} orbitals: the one on the right is, however, bonded to a metal atom in a layer one below the surface, but both should be weak states of binding. The position of the atom in the centre is more complicated: it is bonded by two t_{2g} orbitals emerging from the atoms below it and by two e_g orbitals emerging from the atoms below it and by two e_g orbitals from the atoms on either side of it. This should therefore be a strongly bound state.

Space does not permit the elaboration of these ideas to the adsorption of other atoms and molecules. The same basic concept can also be applied to metals crystallising in other habits, but this development has not yet been fully exploited.

References

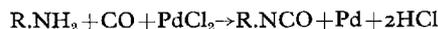
- 1 S. L. Altmann, C. A. Coulson and W. Hume-Rothery, *Proc. Roy. Soc. A*, 1957, **240**, 145
- 2 J. B. Goodenough, *Magnetism and the Chemical Bond*, (Interscience, New York, 1963)
- 3 D. A. Dowden, in *Coloquio sobre Química Física de Processos en Superficies Sólidas*, (Liberia Científica Medinaceli, Madrid, 1965), p. 177

Isocyanate Preparation with Palladium Chloride

The manufacture of numerous plastics and synthetic surface coatings involves the production on a large scale of several important isocyanates. These are generally produced by treating a primary amine or its salt with phosgene, resulting in the intermediate formation of a carbonyl chloride from which HCl is eliminated to yield the isocyanate.

Research carried out by E. W. Stern and M. L. Spector of the M. W. Kellogg Company, New Market, New Jersey (*J. Org. Chem.*, 1966, **31**, (2), 596), has yielded a new route to isocyanates that is unusual in that it employs palladium chloride as a reactant. In this method, the primary aliphatic or aromatic amine reacts with carbon monoxide in the presence of palladium

chloride at, or very slightly above, atmospheric pressure and in the temperature range 65 to 85°C, yielding the isocyanate while the salt is reduced to metallic palladium:



A detailed mechanism of the reaction has not yet been worked out; the *in situ* formation of phosgene from $PdCl_2$ and the carbon monoxide, however, has been ruled out, since no reduction of the salt to metal occurs in the absence of the amine. It seems possible that both the amine and the carbon monoxide combine with the palladium chloride to form a complex that leads to isocyanate formation on decomposition.

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