

Copy of a printed diagram referenced as "Contours of constant density for the attractive and repulsive state"

Contributors

Fuller, Watson, 1935-

Publication/Creation

November 1963

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Wellcome Collection
183 Euston Road
London NW1 2BE UK
T +44 (0)20 7611 8722
E library@wellcomecollection.org
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of a molecule which has been found experimentally (cf. § 1.4), can be calculated theoretically. It is true that H_2^+ is not a chemical species, but it has been found in the discharge tube. Any criticism that we have been using approximate wave functions and therefore getting only approximate energies is met by

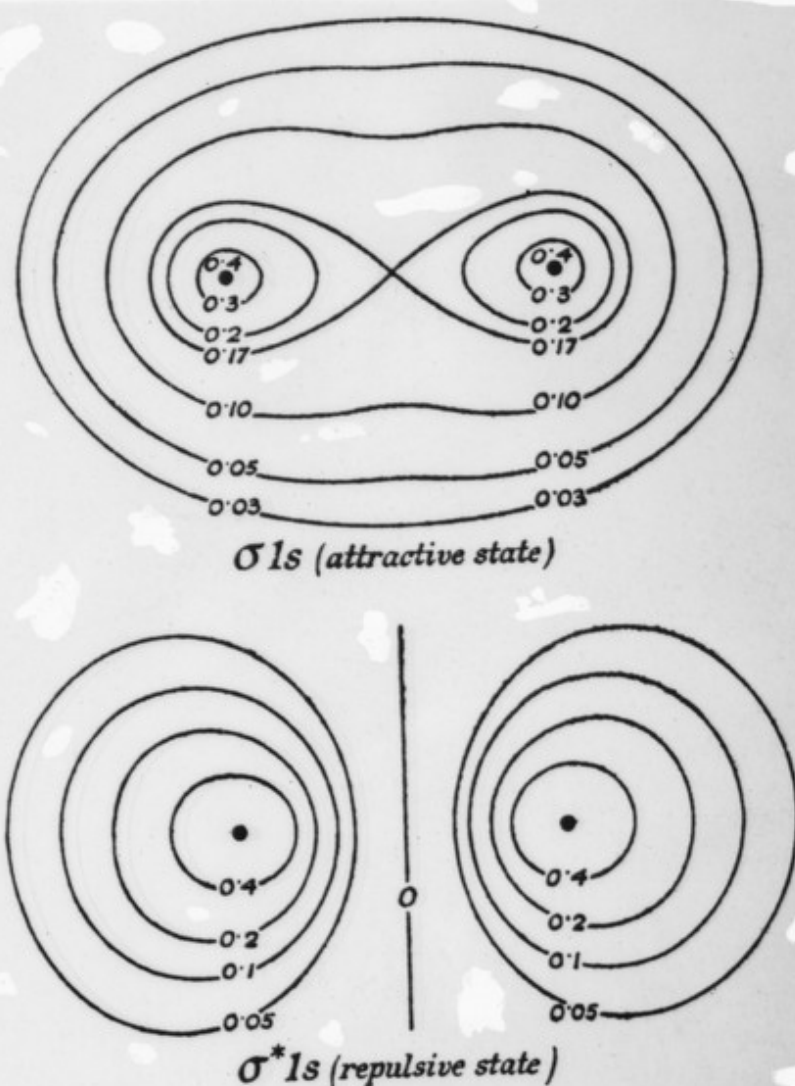


FIG. Contours of constant density ψ^2 for (top) the attractive $\sigma 1s$ state, and (bottom) the repulsive $\sigma^* 1s$ state of H_2^+ .

the observation (§ 3.6) that better wave functions would in fact give us a lower energy and therefore greater stability.

In the second place the final energy curve for $\psi_A - \psi_B$ shows no minimum, so that the molecule would be unstable in such a