Copy of a printed graphs referenced as "Energy curves for H+2"

Contributors

Fuller, Watson, 1935-

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Wellcome Collection
183 Euston Road
London NW1 2BE UK
T +44 (0)20 7611 8722
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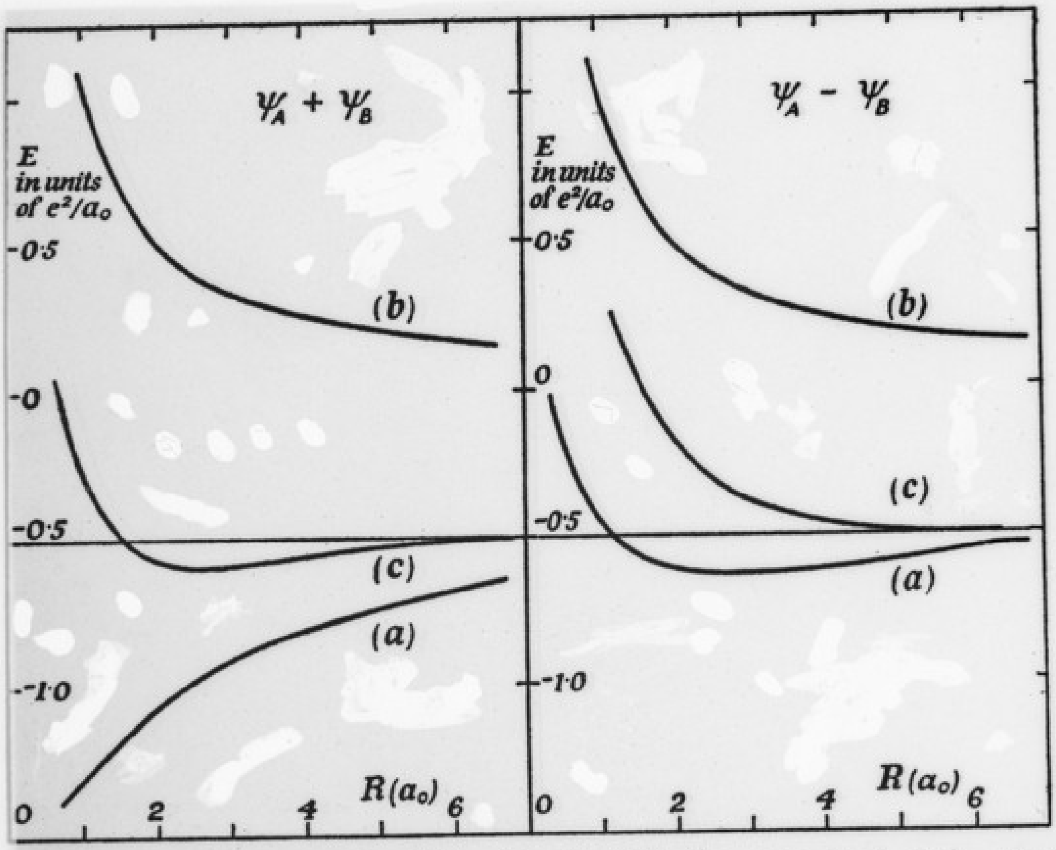
account of the term $1 \pm S$ in the denominator it follows that the top energy exceeds E_A by a greater amount than the bottom energy lies below it.

We have so far left undecided the particular choices of ψ_A and ψ_B. If we are interested in the ground state, this will arise by choosing for ψ_A and ψ_B the lowest a.o.'s for a hydrogen atom.



Energy curves for H_2^+. On the left the m.o. is $\psi_A + \psi_B$, on the right it is $\psi_A - \psi_B$. On both diagrams (a) is the electronic energy; (b) is the nuclear Coulomb repulsion energy; (c) is the total energy curve of the molecule.

These are the wave functions of (2.7), from which β and S may be calculated for any chosen internuclear distance R. In this way the electronic energy is obtained, and so, by adding the nuclear Coulomb energy [redacted] y curve for the molecule. The r[redacted] left is the energy curve for the m.o. $\psi_A + \psi_B$ and on the right for $\psi_A - \psi_B$. The first of these is the ene[redacted] its ground state.

[redacted] urves. In the first