EngineeringRise

Molecular orbital theory and hydrogen bonding

Formulas and units, JEE Main. Status: Reviewed on 2026-11-20.

Result	Formula	Units or note
Bond order	BO = (Nb - Na) / 2 Valid when: homonuclear diatomic species; Nb, Na = bonding and antibonding electrons	dimensionless
B2, C2, N2 order	sigma 2s < sigma* 2s < pi 2p < sigma 2p < pi* 2p < sigma* 2p Valid when: diatomics up to N2 (14 electrons or fewer), including their ions	n/a (energy order)
O2, F2 order	sigma 2s < sigma* 2s < sigma 2p < pi 2p < pi* 2p < sigma* 2p Valid when: O2, F2 and their ions (more than 14 electrons)	n/a (energy order)
Spin-only magnetic moment	mu = square root of n(n + 2) Valid when: free species, n unpaired electrons; orbital contribution ignored	Bohr magneton (n unpaired electrons)
Bond order values	O2^+ 2.5; O2 2; O2^- 1.5; O2^2- 1; N2 3; N2^+ 2.5; C2 2; B2 1 Valid when: valence electron counts filled in the correct order for each species	dimensionless
Bond order and bond length	higher bond order, shorter bond, higher bond energy	n/a (qualitative)
Hydrogen bonds in ice	each molecule 4 contacts, each bond shared: 2 H bonds per molecule Valid when: ice, where every molecule is tetrahedrally bonded	count per molecule
Hydrogen bonding conditions	H on N, O or F; lone pair on N, O or F of a neighbour	n/a (qualitative)

Full lesson with worked examples:
https://www.engineeringrise.in/learn/learn/jee-main/chemistry/chemical-bonding-and-molecular-structure/molecular-orbital-theory-ar

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