



Figure 9.37

The correct molecular orbital energy-level diagram for the B_2 molecule. When $p-s$ mixing is allowed, the energies of the σ_{2p} and π_{2p} orbitals are reversed. The two electrons from the B $2p$ orbitals now occupy separate, degenerate π_{2p} molecular orbitals and thus have parallel spins. Therefore, this diagram explains the observed paramagnetism of B_2 .

	B_2	C_2	N_2	O_2	F_2
σ_{2p}^*	—	—	—	—	—
π_{2p}^*	—	—	—	$\uparrow \uparrow$	$\uparrow \uparrow$
σ_{2p}	—	—	$\uparrow \downarrow$	$\uparrow \downarrow$	$\uparrow \downarrow$
π_{2p}	$\uparrow \uparrow$	$\uparrow \uparrow$	$\uparrow \uparrow$	$\uparrow \uparrow$	$\uparrow \uparrow$
σ_{2s}^*	$\uparrow \downarrow$	$\uparrow \downarrow$	$\uparrow \downarrow$	$\uparrow \downarrow$	$\uparrow \downarrow$
σ_{2s}	$\uparrow \downarrow$	$\uparrow \downarrow$	$\uparrow \downarrow$	$\uparrow \downarrow$	$\uparrow \downarrow$
Magnetism	Para-magnetic	Dia-magnetic	Dia-magnetic	Para-magnetic	Dia-magnetic
Bond order	1	2	3	2	1
Observed bond dissociation energy (kJ/mol)	290	620	942	495	154
Observed bond length (Å)	1.59	1.31	1.10	1.21	1.43

Bond energy increases with bond order; bond length decreases with increasing bond order.