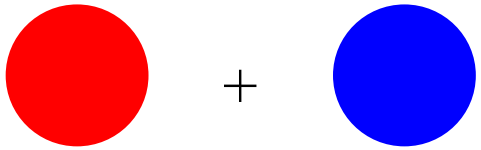
分子軌道法

＝1s軌道どうしの相互作用＝

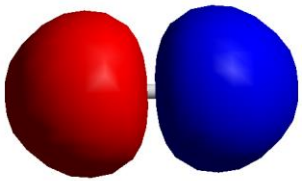
text p.64

逆位相



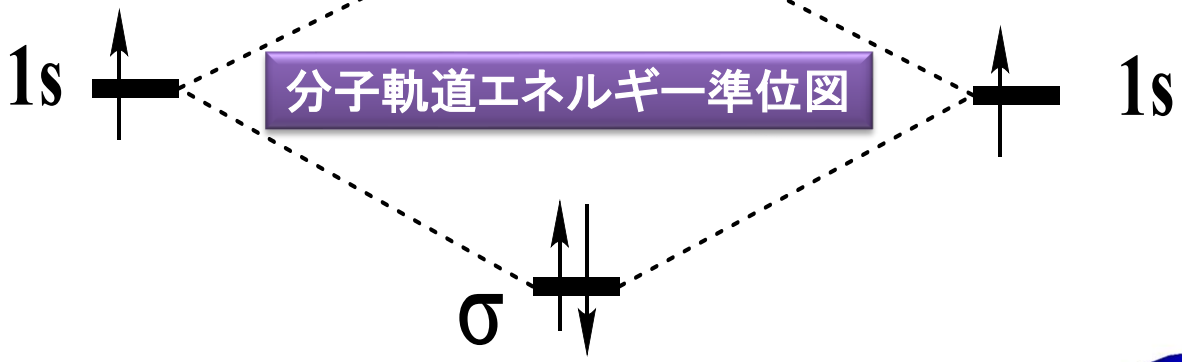
s　　s

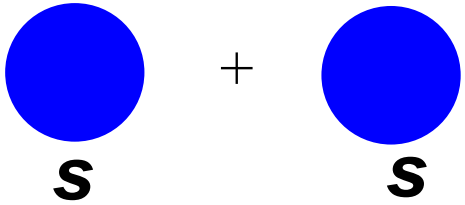
⟹ 反結合性軌道



σ*（アスタリスクで
ラベルされる）

H—H





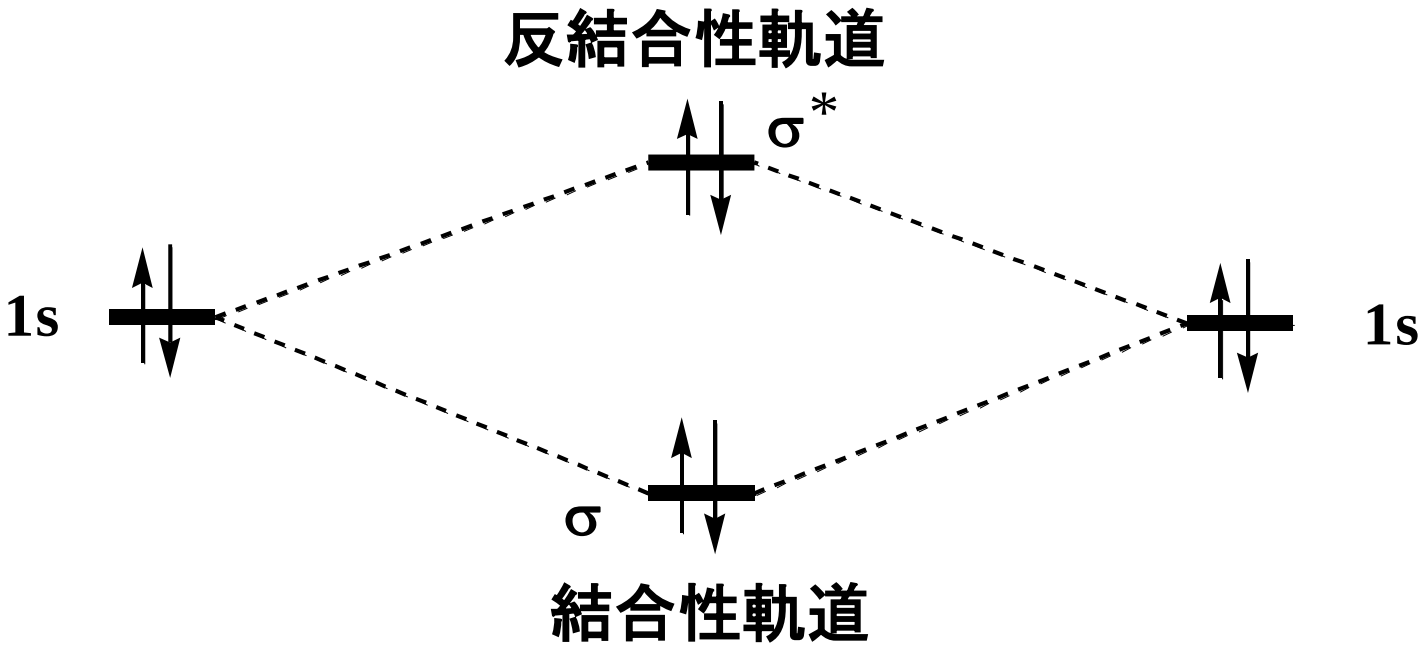
s　　s

⟹ 結合性軌道

同位相

分子軌道法

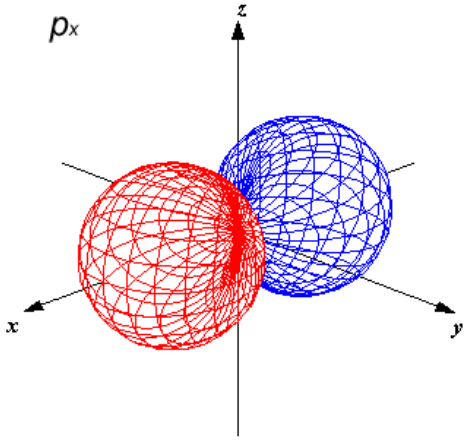
＝He_2が存在しない理由＝

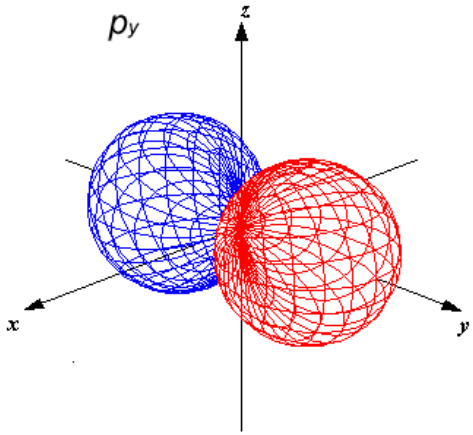


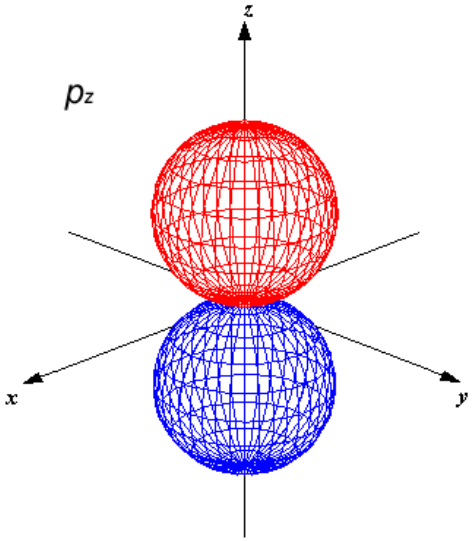
安定化と不安定化の両方が相殺する

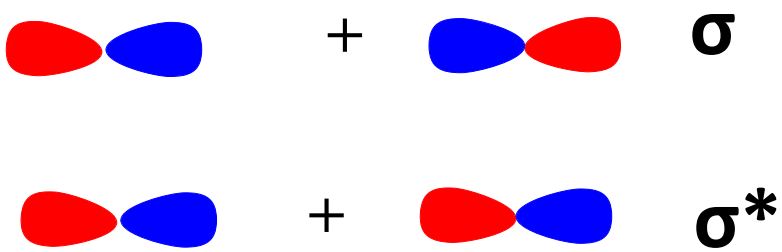
BO = ＿＿＿＿＿＿ = ＿＿

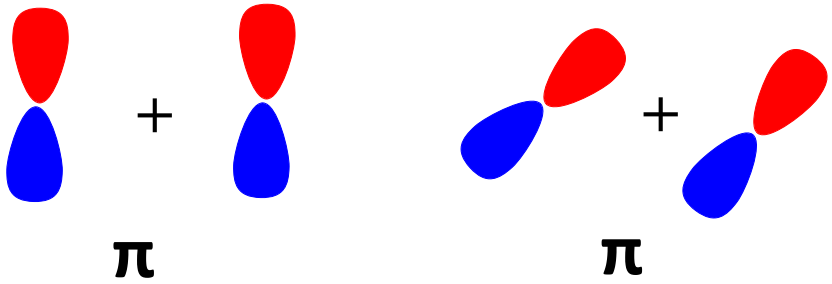
P軌道同士の相互作用

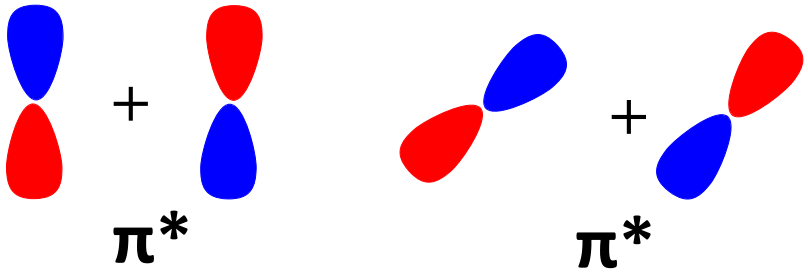




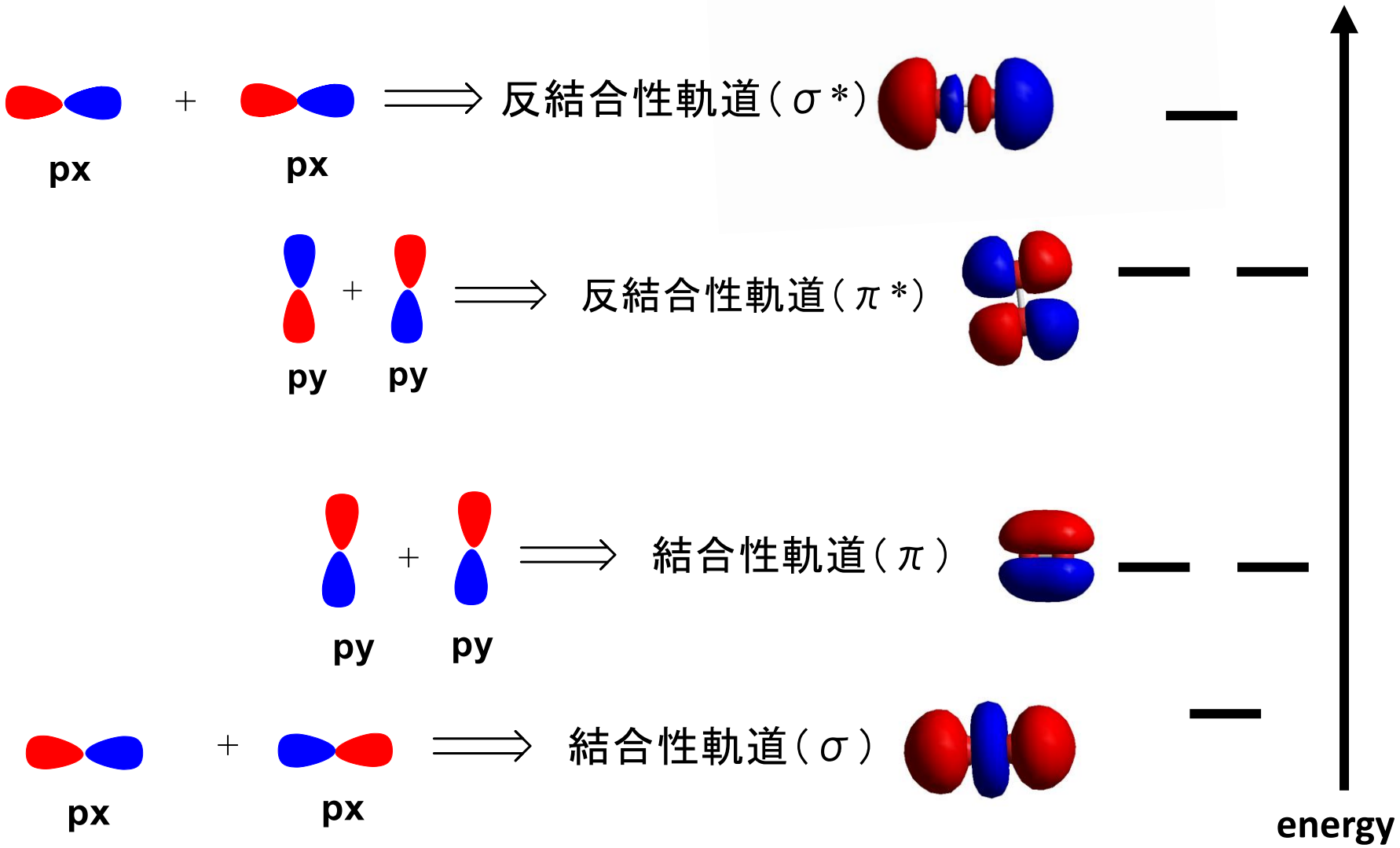




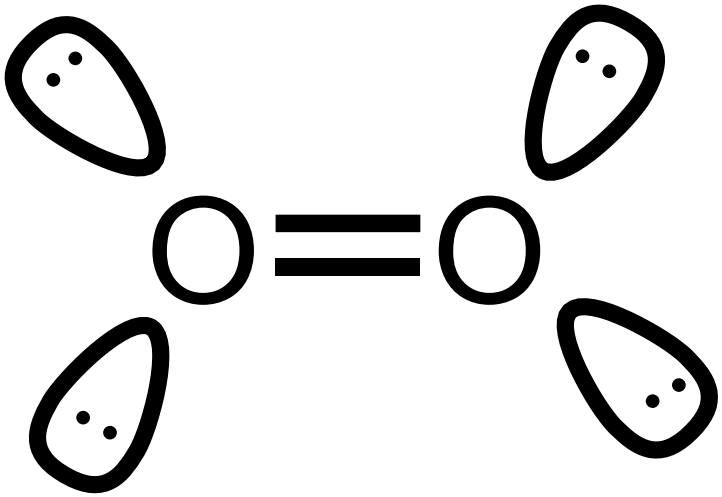




P軌道同士の相互作用から生成される分子軌道

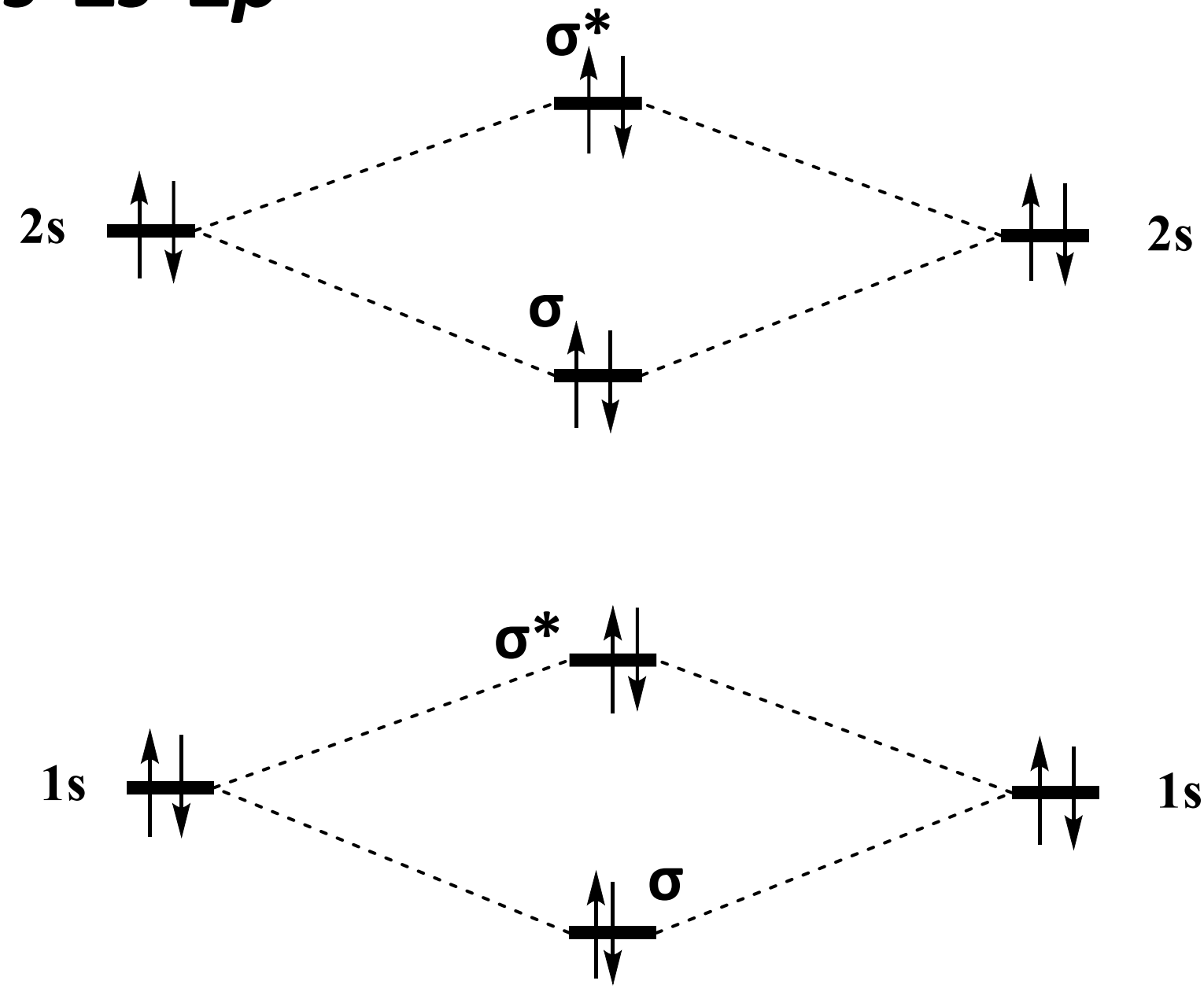


等核二原子分子

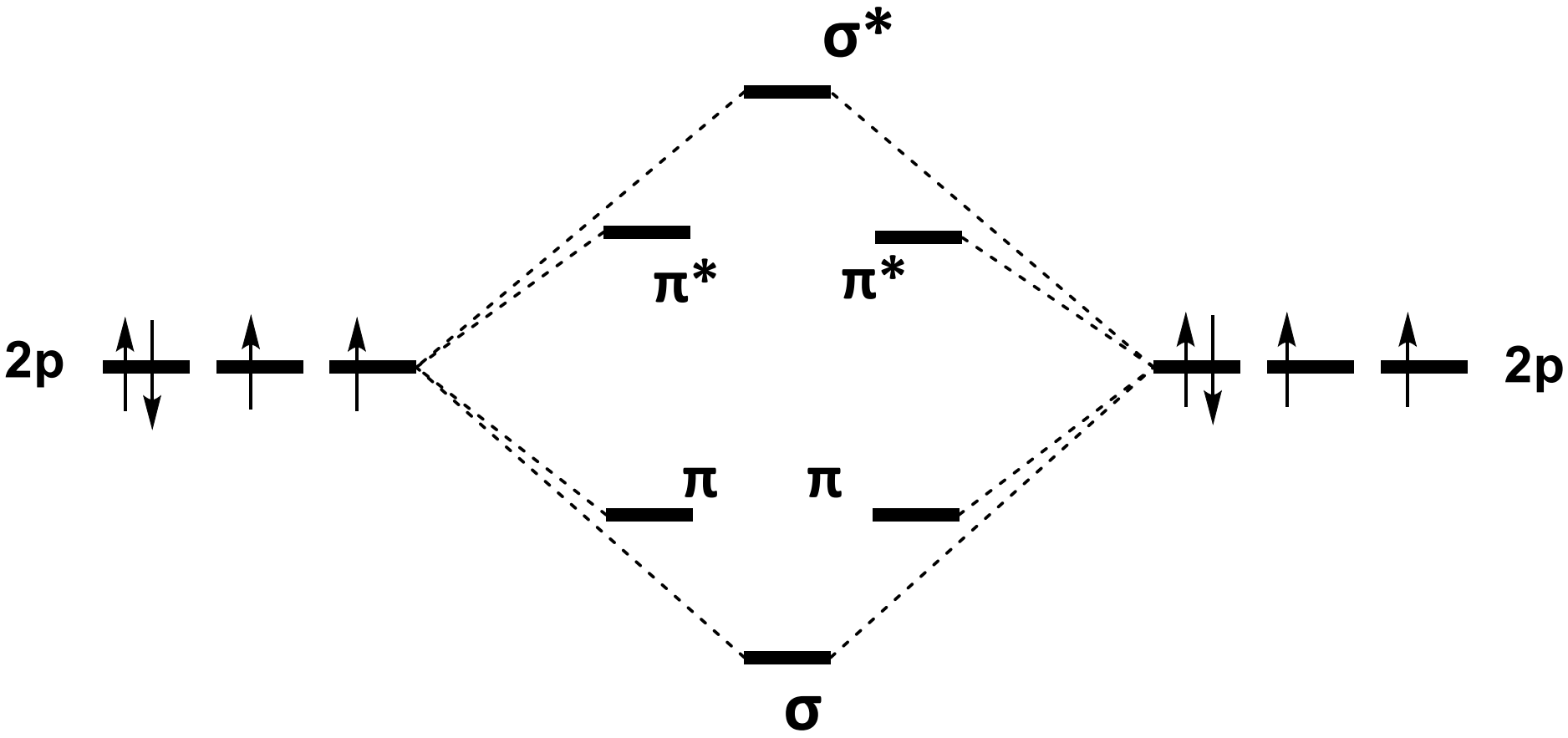


酸素分子の
分子軌道エネルギー準位図
を考える

${}_8O\ 1s^2 2s^2 2p^4$

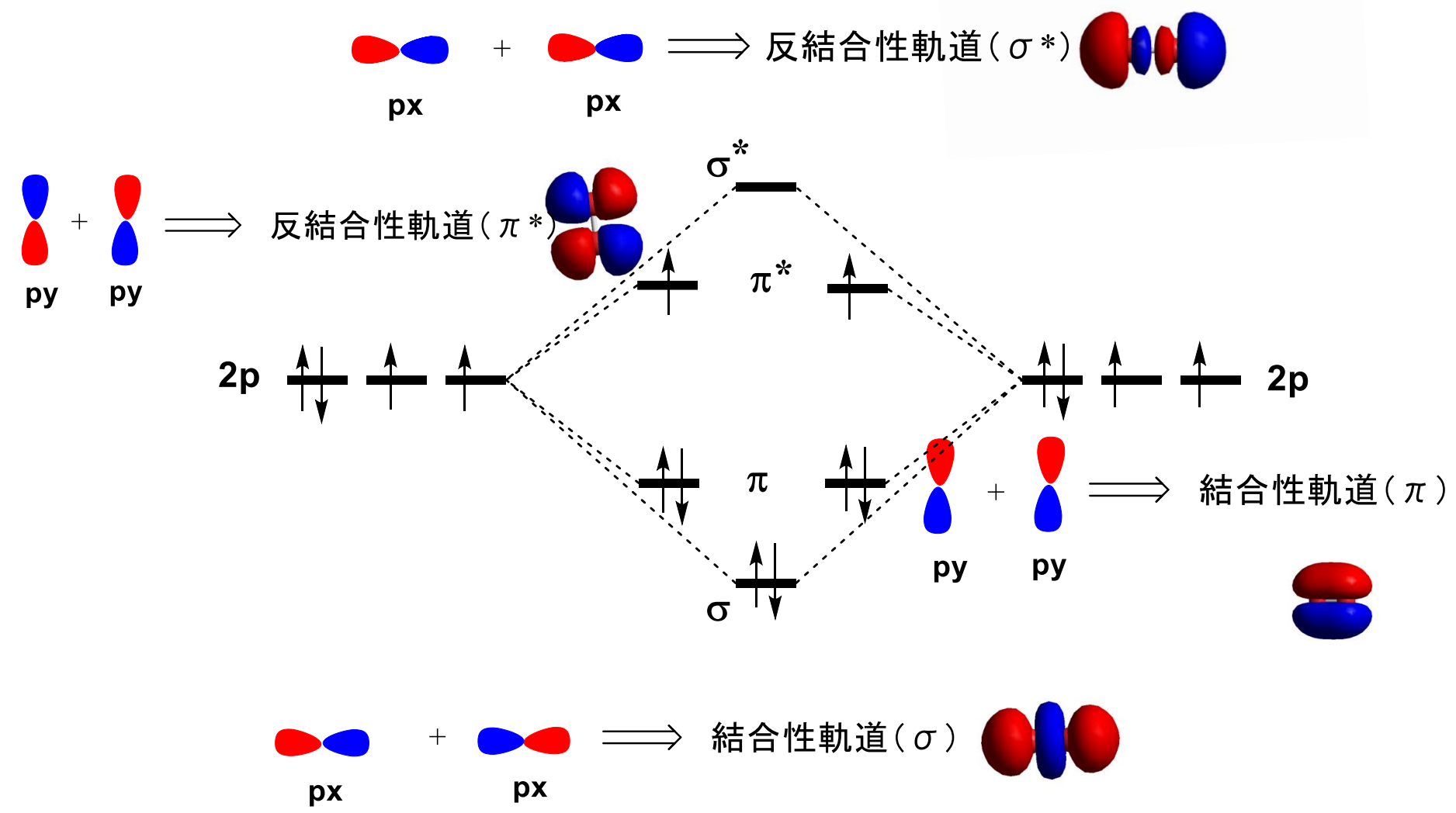


${}_8\mathrm{O}\ 1s^2 2s^2 2p^4$



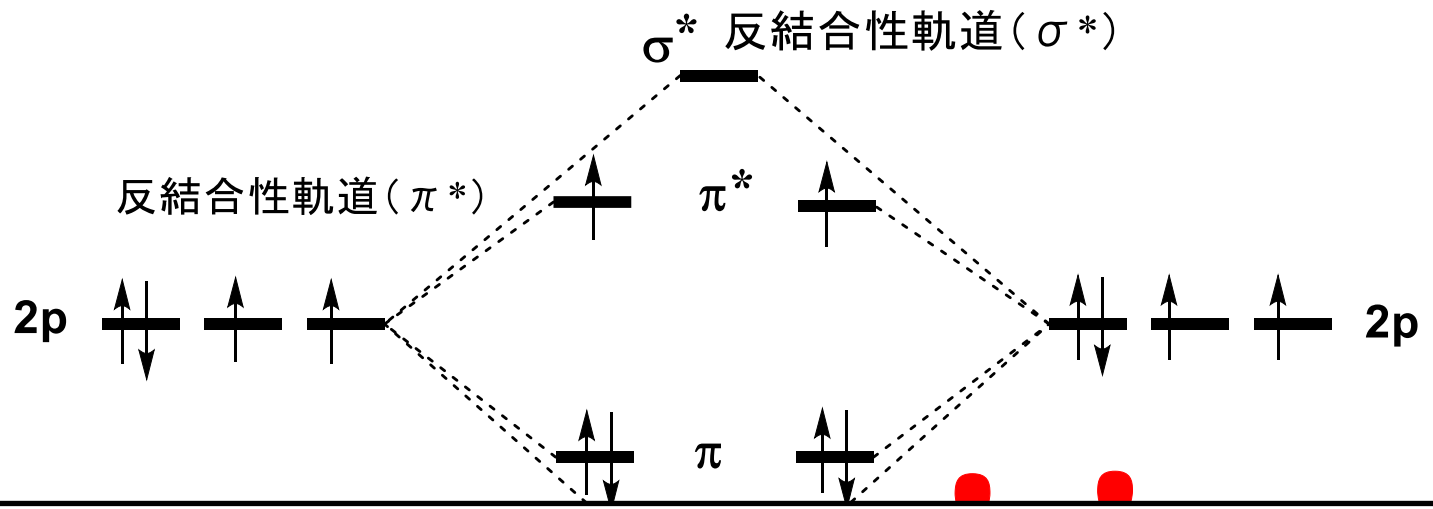
＝2p軌道どうしの相互作用＝ O_2

Text p.66



＝2p軌道どうしの相互作用＝ O_2

Text p.66



$O_2 \xrightarrow{e^-} {\bullet}O_2^- \xrightarrow{e^-} O_2^{2-} \xrightarrow{2e^-} 2O^{2-}$

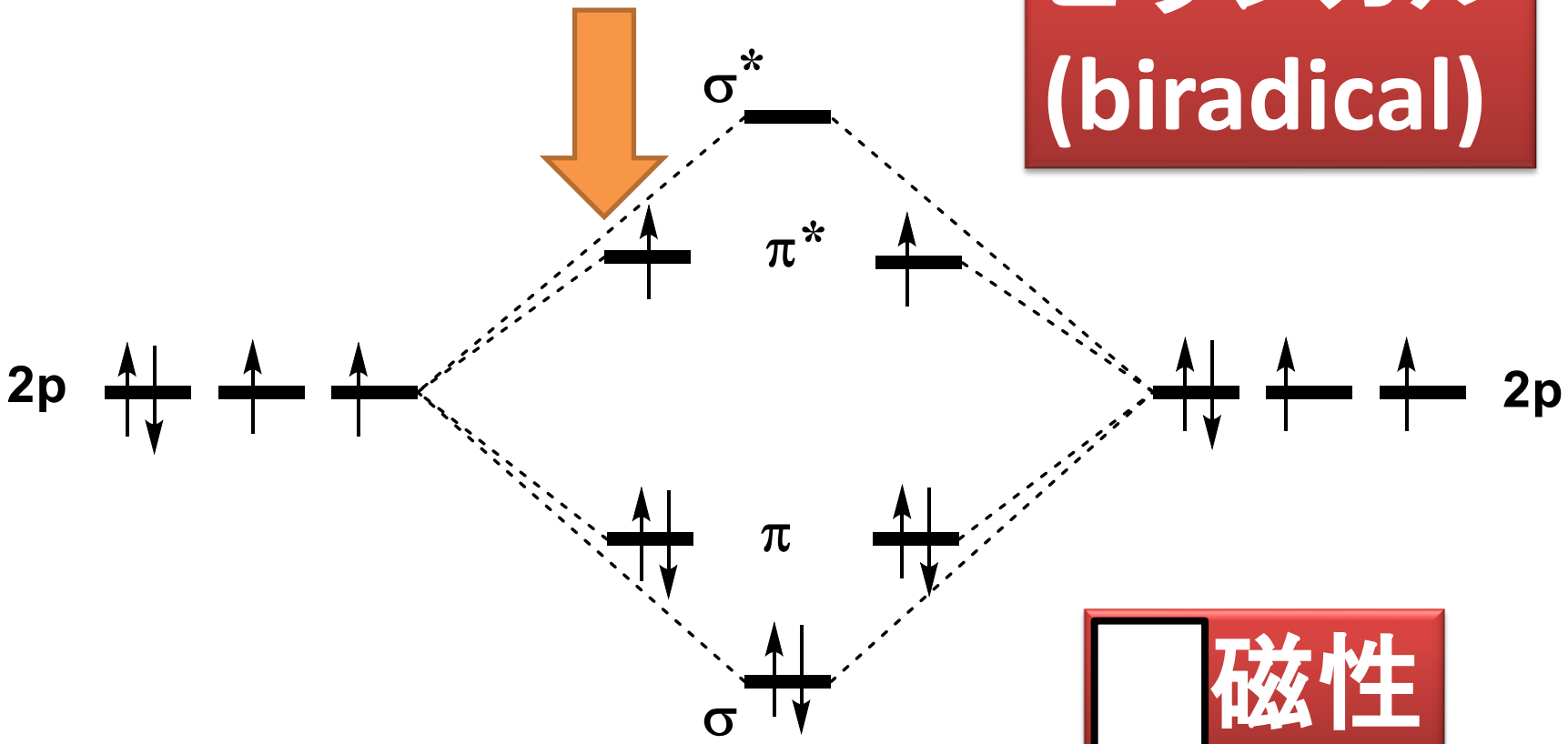
superoxide　peroxide　oxide

O═O　<　[O—O]$^-$　<　[O—O]$^{2-}$

1.20 Å　1.5重結合　1.28 Å　1重結合　1.49 Å

電子を取り込みやすい

ビラジカル
(biradical)



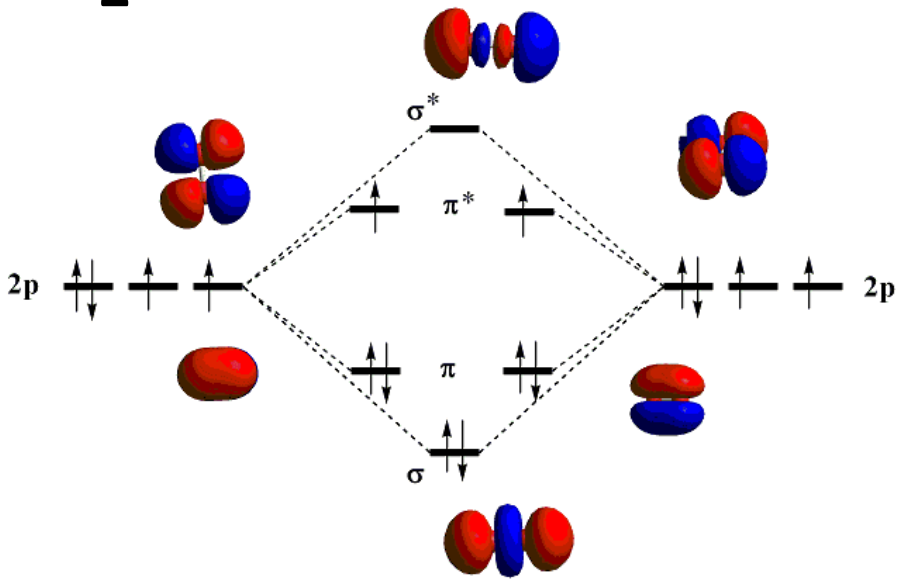
□磁性

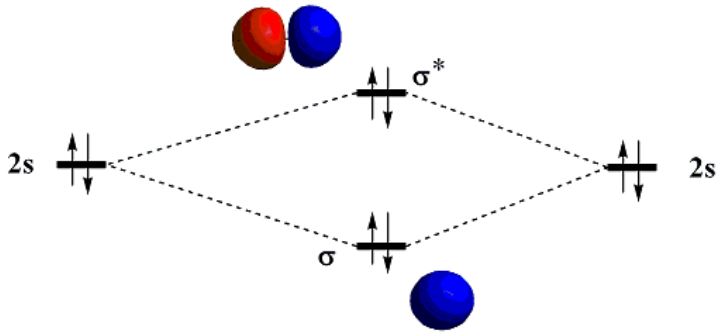
結合次数　(BO)

BO: bond order

Text p.65

$$BO = \frac{1}{2}\,(\text{結合性軌道中の電子数} - \text{反結合性軌道中の電子数})$$





三重項酸素のbond order

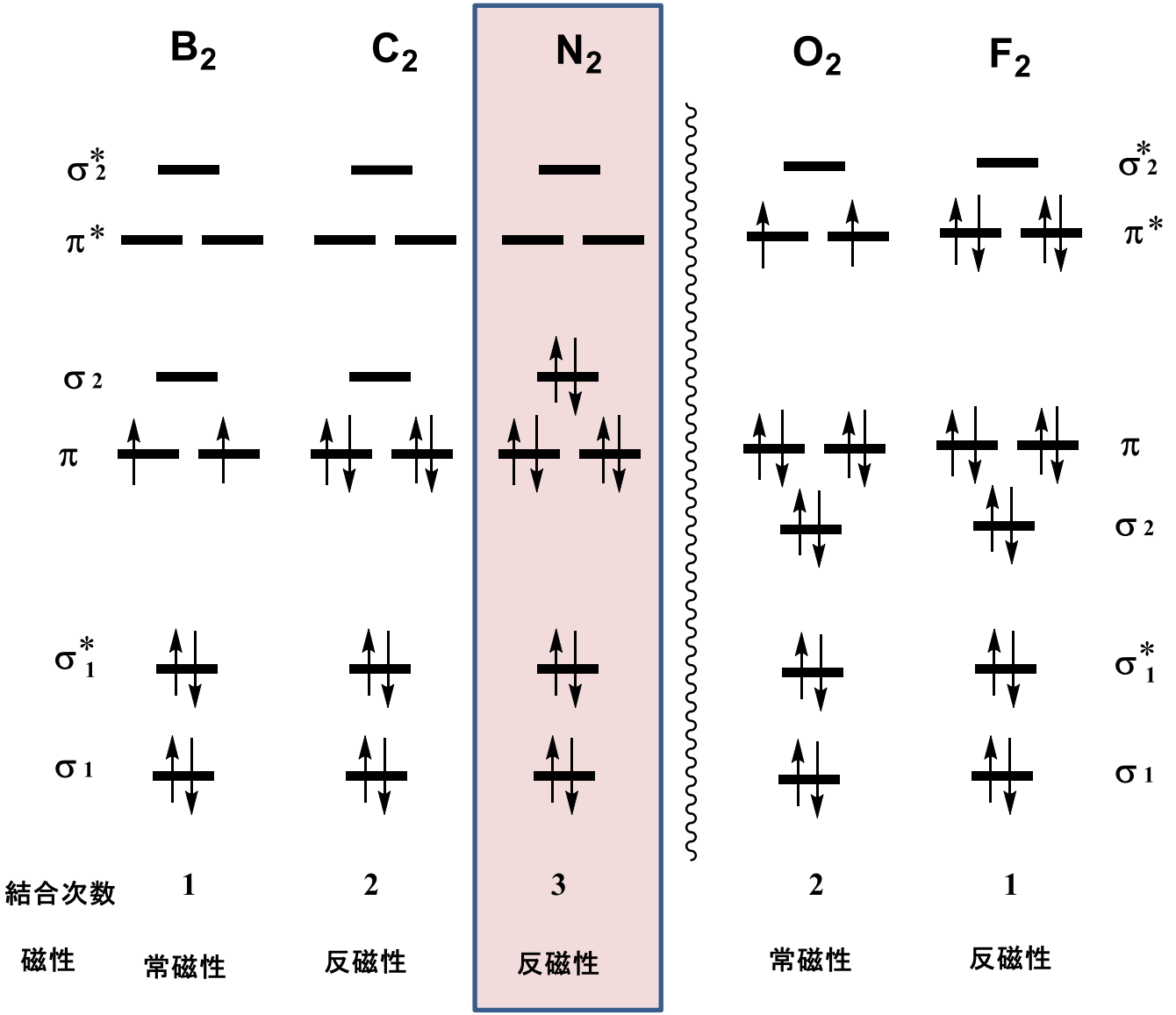
BO = □

= □

O═O

第2周期元素の等核二原子分子の軌道占有状態と結合の性質

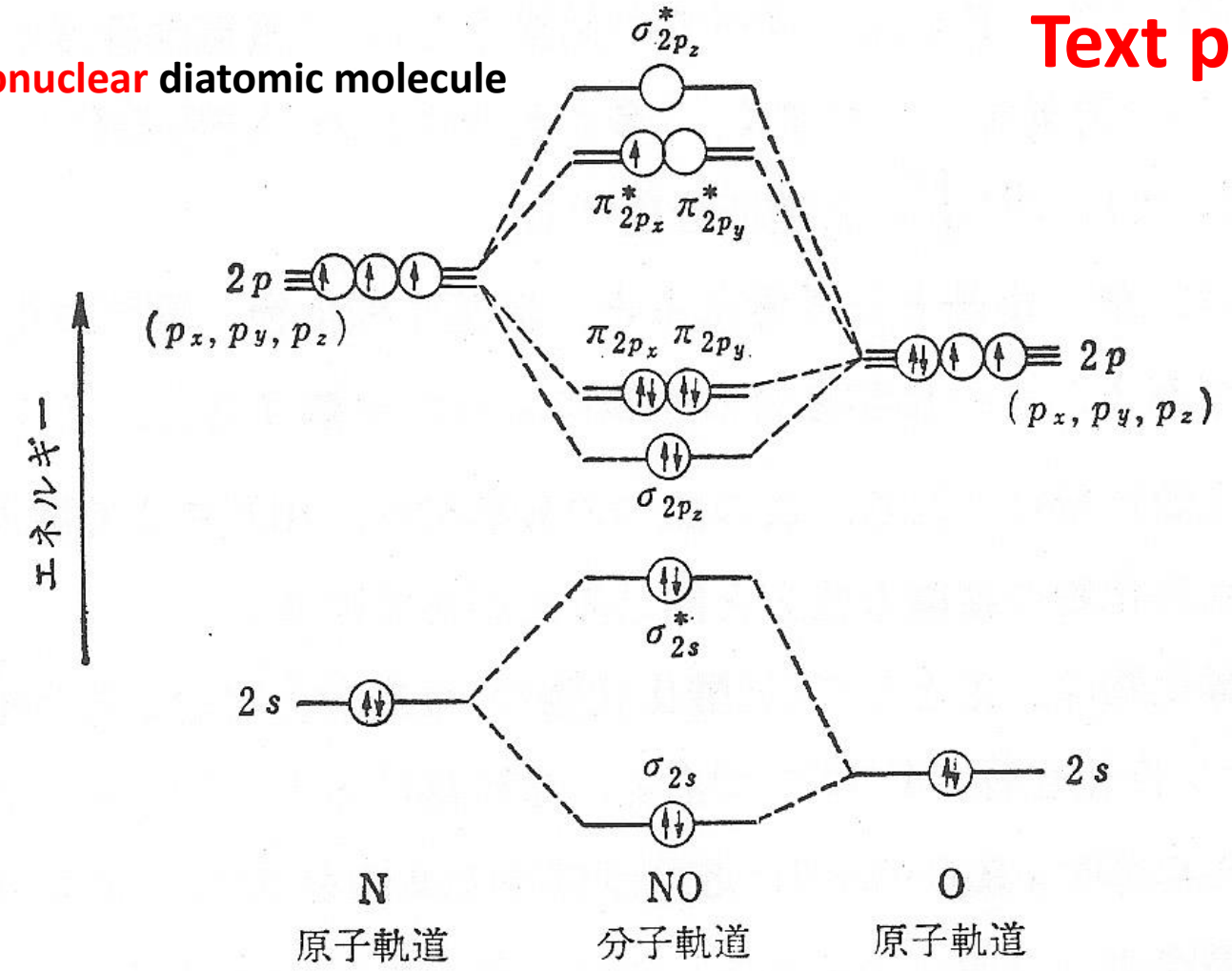
テキスト
p.67
図3.48



MO Diagram for NO (nitrogen monoxide)

Heteronuclear diatomic molecule

Text p.69



NO 分子の分子軌道エネルギー準位図