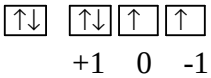
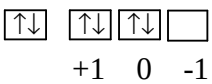
Term Symbols and Molecular Spectroscopy

Atomic Term Symbols - Oxygen

L	0	1	2	3
Term	S	P	D	F

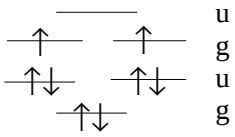
ground state: $(1s)^2\ (2s)^2\ (2p)^4$ — 

$L = M_{L,max} = +1+1+0-1 = 1 \Rightarrow {}^3P$

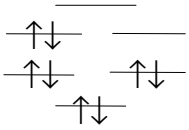
excited states: $(1s)^2\ (2s)^2\ (2p)^4$ — 

$L = M_{L,max} = +1+1+0+0 = 2 \Rightarrow {}^1D$ and ${}^1S$

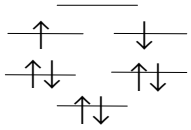
Homonuclear Diatomics* – O_2 ground state: KK $(\sigma_{g,2s})^2(\sigma^*_{u,2s})^2(\sigma_{g,2pz})^2(\pi_{u,2p})^4(\pi^*_{g,2p})^2$



$\Lambda = +1+1-1-1+1-1 = 0$ $\quad {}^3\Sigma^-_g$

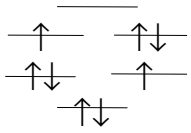


$\Lambda = +1+1-1-1+1+1 = 2$ $\quad {}^1\Delta_g$

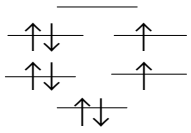


$\Lambda = +1+1-1-1+1-1 = 0$ $\quad {}^1\Sigma^+_g$

$\ldots(\sigma_{g,2pz})^2(\pi_{u,2p})^3(\pi^*_{g,2p})^3$



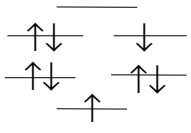
$\Lambda = +1+1-1+1-1-1 = 0$



$\Lambda = +1+1-1+1+1-1 = 2$

$${}^3\Sigma^+_u + {}^3\Sigma^-_u + {}^3\Delta_u$$

$\ldots(\sigma_{g,2pz})^1(\pi_{u,2p})^4(\pi^*_{g,2p})^3$



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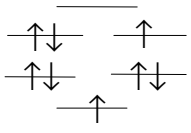

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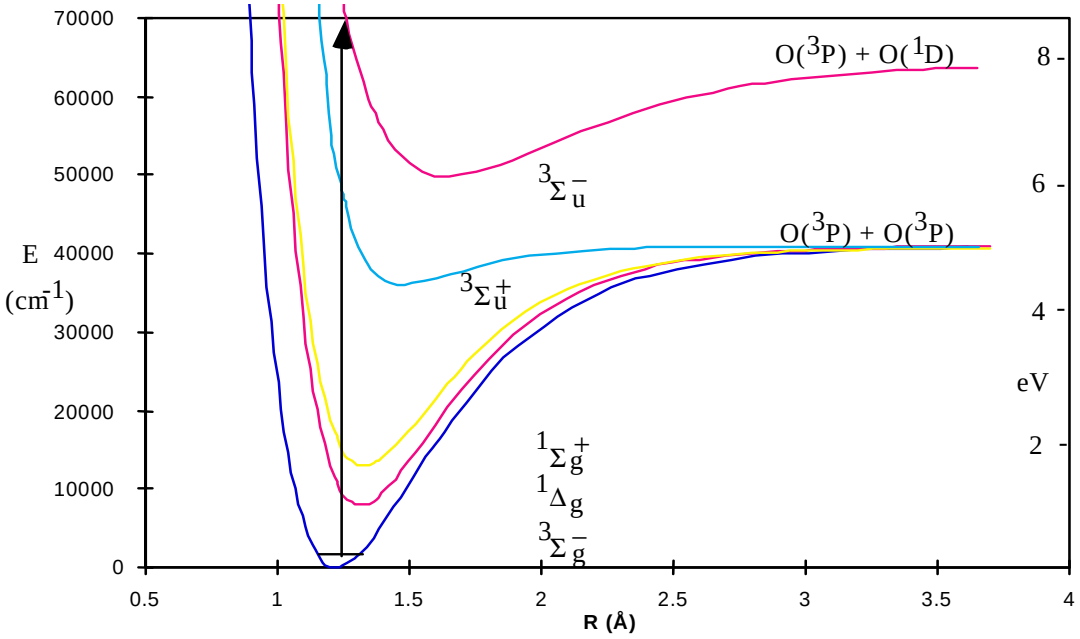

* Configuration diagrams are schematic. No single diagram can represent an open shell system. These diagrams do not take into account electron indistinguishability and orbital degeneracy.