10.6: Inversion Symmetry

One more quantum number, that relating to the inversion (i) symmetry operator can be used in atomic cases because the total potential energy V is unchanged when **all** of the electrons have their position vectors subjected to inversion (i.e., $i\mathbf{r} = \mathbf{-r}$). This quantum number is straightforward to determine. Because each L, S, M_L, M_S, H state discussed previously consists of a few (or, in the case of configuration interaction several) symmetry adapted combinations of Slater determinant functions, the effect of the inversion operator on such a wavefunction Ψ can be determined by:

i. applying i to each orbital occupied in Ψ thereby generating a ± 1 factor for each orbital (+1 for s, d, g, i, etc orbitals; -1 for p, f, h, j, etc orbitals),
ii. multiplying these ± 1 factors to produce an overall sign for the character of Ψ under $\hat{i}$.

When this overall sign is positive, the function Ψ is termed "even" and its term symbol is appended with an "e" superscript (e.g., the ${}^3P$ level of the O atom, which has $1s^2 2s^2 2p^4$ occupancy is labeled ${}^3P^e$); if the sign is negative Ψ is called "odd" and the term symbol is so amended (e.g., the ${}^3P$ level of $1s^2 2s^1 2p^1$ B^+ ion is labeled ${}^3P_o$).