ENERGY LEVEL DESIGNATION FOR DIATOMIC MOLECULES

Notations for rovibronic states of diatomic molecules (e.g. TiO) have the format:

$$Я\ ^{(2S+1)}Э_{\Omega}\ V\ N.$$

- Я is a Latin character. By default Я=X for ground electronic state. Excited electronic states are labelled in alphabetical order corresponding to the value of electronic energy. For example, first excited electronic state is noted as A, the second excited electronic state is noted as B, and so on.

- (2S+1) is electronic multiplet, where S is the electron spin quantum number.

- Э is symmetry of electronic state. For symmetry the Greek characters are used: Σ (L=0), Π (L=1), Δ (L=2), Φ (L=3), … Here L is orbital quantum number.

- Ω is the total electronic angular momentum quantum number: $\vec{\Omega} = \vec{L} + \vec{S}$.

- V is the vibrational quantum number, and N is the rotational quantum number.

Example: A $^3\Pi_2$ 5 40. It is vibration-rotation energy level with vibrational quantum number equal 5 and rotational quantum number equal 40. It belongs to the first excited electronic state of the Π symmetry (it does mean that orbital quantum number L=1). This electronic state is the triplet state. The total electronic angular momentum quantum number is 2.

For the transitions in absorption there are the following selection rules: $\Delta\Omega = 0$, $\Delta J = 0, \pm 1$. In the case of $\Delta J = -1$ one has P branch, in the case of $\Delta J = 0$ one has Q branch and in the case of $\Delta J = 1$ one has R branch.

The possible notation for a transition is $(B\ ^3\Phi \leftarrow X\ ^3\Delta)_2\ 10 \leftarrow 5\ Q(40)$. The construction $Q(40)$ refers to the lower state with the rotational quantum number of 40. This transition is from vibrational state V=5 to vibrational state V=10. Very often the construction $(B\ ^3\Phi \leftarrow X\ ^3\Delta)$ is replaced by a small Greek character, but the precise rules for this are not known to us.

For example, the transition shown above could be designated as β $Q_2(40)$ 10-5 where β was arbitrarily selected for denoting $(B\ ^3\Phi \leftarrow X\ ^3\Delta)$.