Pacheco and Schöne Reply: In response to the preceding Comment [1], as stated in our Letter [2], the adiabatic approximation relies on the different time scales characteristic of nuclear and electronic motion. This allows one to write the wave function of the system as a direct product of a nuclear wave function $\Theta_k(\vec{R})$ and an electronic wave function $\psi_n(\vec{r};\vec{R})$ which depends parametrically on the nuclear coordinates $(\vec{R})$. Consistently with such an approximation, the electronic transitions can be assumed to take place "instantaneously." One can write for the transition amplitude for a photon excitation from the electronic ground state 0 to an electronic state n

$$A_{0,n}(\vec{R}) = \int d\vec{r}\,\psi_n^*(\vec{r};\vec{R})\hat{D}_e\psi_0(\vec{r};\vec{R})\,.$$

At zero temperature, the quantal nature of the nuclei manifests itself, within such an approximation, via the well-known Franck-Condon factors, F_{k_0,k_n}, which are directly related to the overlap of the nuclear wave functions

$$F_{k_0,k_n} = \left| \int d\vec{R}\,\Theta_{k_n}^*(\vec{R})\Theta_{k_0}(\vec{R}) \right|^2 = \left| \int S_{k_0,k_n}(\vec{R})d\vec{R} \right|^2 .$$

At finite temperature, one has to take into account not only quantal effects but also thermal effects, which will become dominant at sufficiently high temperatures. The case of Na_8 has been explicitly studied in Ref. [3], where it has been found that for $T > 50$ K thermal effects were already dominant. Similar conclusions have been obtained for the (lighter) lithium clusters [4] where it was found that the quantized nuclear motion of the lithium atoms leads to a renormalization of the vibrational temperature without any major modifications on their physical behavior.

In [2] we considered three temperature values: $T = 0$, for which the photoabsorption was computed *at the equilibrium configuration of the cluster*, therefore including *no* quantal or thermal effects; $T = 100$ and 300 K, for which the thermal limit has been utilized, in view of the results of Ref. [3]. At the heart of this limit is the expression for the transition strength between the lowest electronic state of the cluster (at a specific set of nuclear coordinates $\vec{R}$) and an excited electronic state n compatible with the selection rules. Assuming that the cluster is in thermal equilibrium at a vibrational temperature T $(\beta = 1/K_B T)$, we may write for the transition strength

$$T(\beta;0 \rightarrow n) = \int d\vec{R} \sum |A_{0,n}(\vec{R})|^2 \times \left\{ \sum_{k_0,k_n} \frac{1}{Z}\exp[-\beta E_{k_0}]\,|S_{k_0,k_n}(\vec{R})|^2 \right\},$$

where Z is the usual partition function, and E_{k_0} are the vibrational eigenstates of the nuclear Hamiltonian in the electronic ground state. In this way, the quantal treatment of the nuclear motion provides a contribution to the absorption probability, via the sum over the (thermally accessible) nuclear vibrational states. At $T = 0$ we obtain the usual expression involving the Franck-Condon factors. As the temperature increases, the number of thermally accessible states increases significantly, with a corresponding increase of the number of incoherent contributions to the double sum in braces above. The classical (high-T) limit reads [3,5]

$$T(\beta;0 \rightarrow n) = \int d\vec{R}\,\frac{1}{Z_{\mathrm{CL}}}\,e^{-\beta E(\vec{R})} \left| \sum_n A_{0,n}(\vec{R}) \right|^2,$$

$$Z_{\mathrm{CL}} = \int d\vec{R}\,e^{-\beta E(\vec{R})},$$

where $E(\vec{R})$ is the lowest electronic energy of the cluster for a given set of nuclear coordinates $\vec{R}$. Equation (1) in [2] can be obtained along a similar (though more lengthy) limiting procedure, carried out for the photo cross section of the cluster. In this way, the treatment undertaken in [2] is consistent with both the adiabatic approximation and the classical treatment of the nuclear motion, which is legitimate in view of the results of Ref. [3].

In what concerns the temperature and the renormalization factor used for comparison with experiment, they are well documented in the literature—see Ref. [6] and references therein, in particular Ref. [17]. At any rate, the main goal of our paper was to put in evidence that a proper treatment of the absorption in the thermally excited clusters cannot be simply seen as a superposition of that process occurring in a few isomers of the same cluster—sometimes referred to in the literature as isomerization. It is, instead, directly linked to the increasing availability of phase space opened up by temperature (which means one must include, besides the local minima, the full topologic structure of the potential energy surface) leading, as shown in [2], to sizable changes as one moves across a structural phase transition, such as melting.

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