

# SPECTRA OF ALKALI DIMERS ADSORBED ON THE HELIUM NANO CRIOSTAT

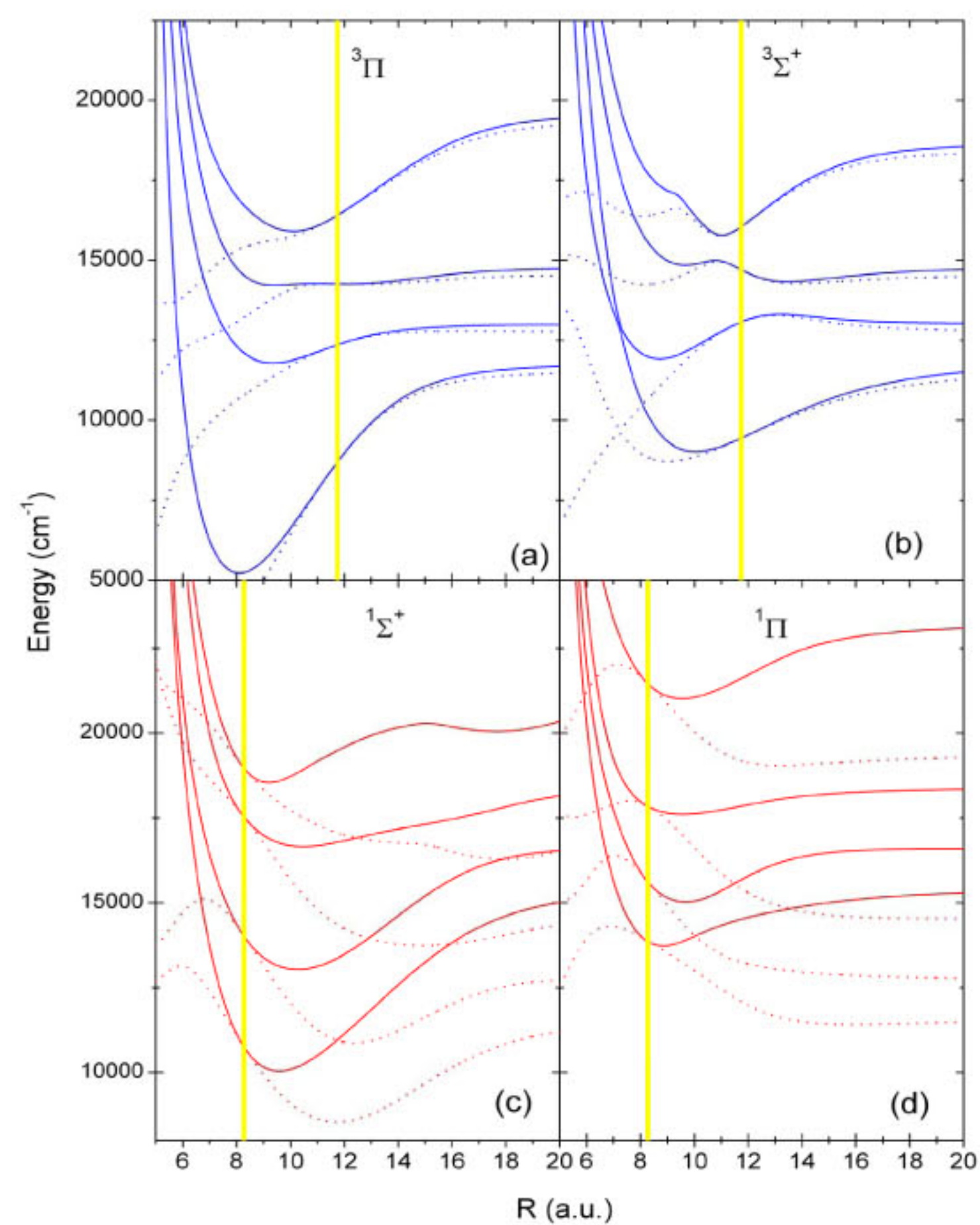
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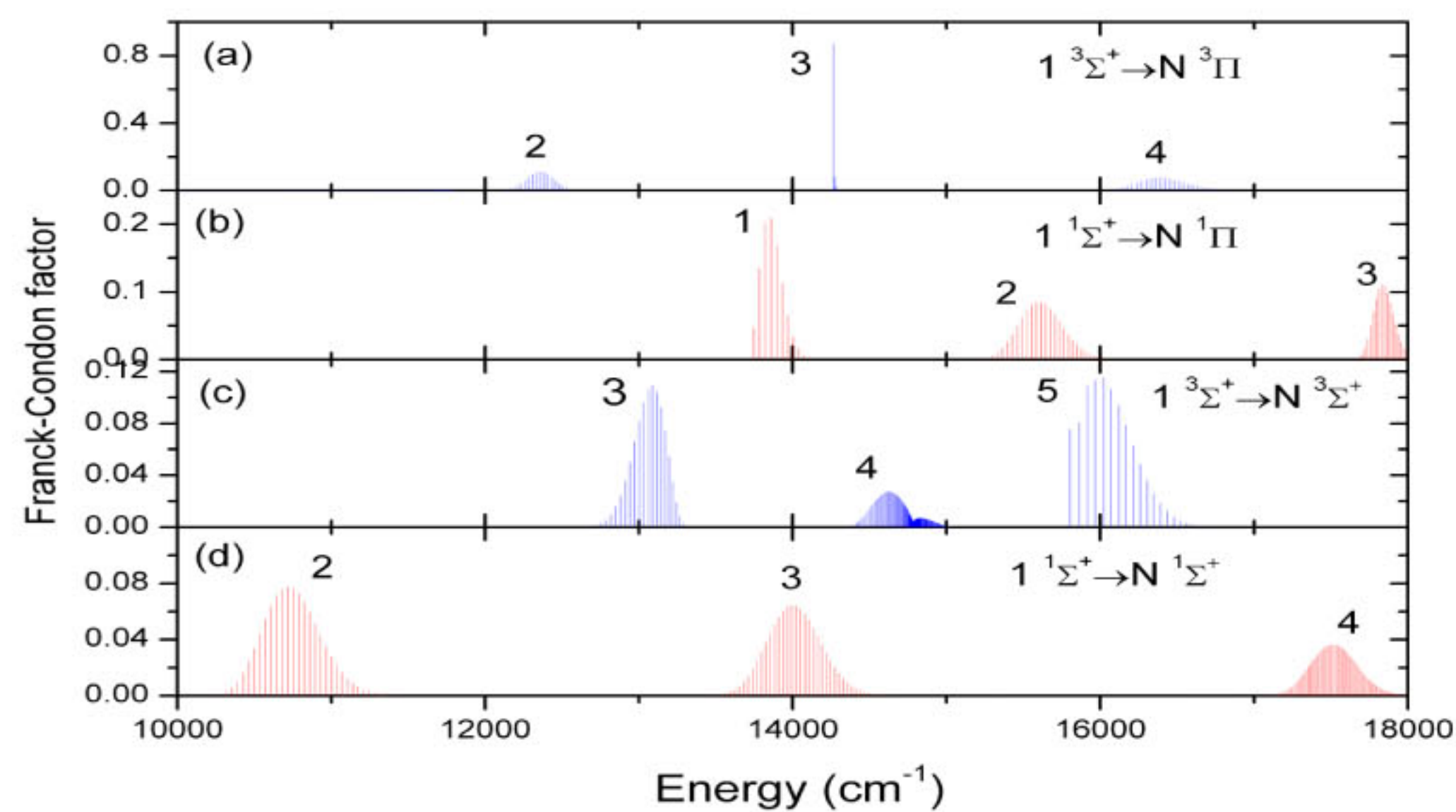
Cold nanodroplets (or clusters) of about  $10^4$  helium atoms have been shown to provide a weakly interacting, low temperature environment of 0.37 K (nano cryostat) for the formation and spectroscopy of molecules. Alkali metal atoms picked up by a beam of helium nanodroplets, remain on the helium surface where they „skate“ around and form molecules in cold collisions. After the formation of molecules with a certain large binding energy, this energy is released into the surrounding helium cluster and causes evaporation of helium atoms, one helium atom for every  $5 \text{ cm}^{-1}$  of energy. As a result, helium droplets loaded with weakly bound molecules are observed at larger abundance downstream in the helium cluster beam than droplets loaded with strongly bound molecules.

Due to the low temperature of the helium environment, only the lowest vibrational state is populated in each case. This enables easy quantum simulation of absorption spectra if the relevant potential curves are available. Few additional approximations lead to analytical formulas [1,2] which are suitable for the analysis of the experimental spectra. Our spectral simulations were performed by using the set of potential curves calculated in Hund's case (a). The direct comparison with experimental observation was made for  $\text{Cs}_2$  molecule [3]. Recently, this method was applied for heteronuclear alkali molecules KRB [4] and RbCs [5] stabilized on the cold helium droplet. The results will be shown and discussed.

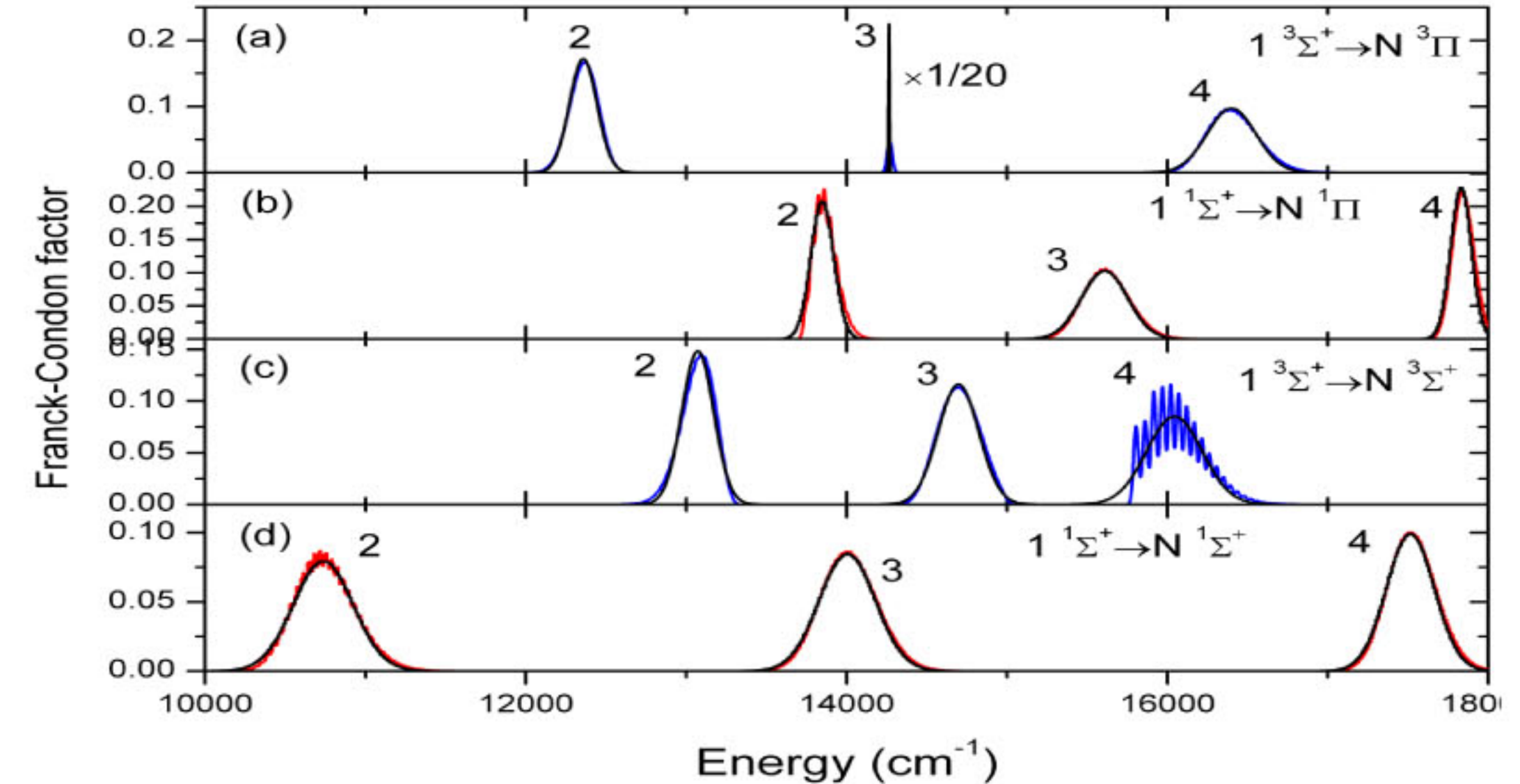
1. Gislason E A 1973 *J. Chem. Phys.* **58** 3702
2. Hüpper B and Eckhardt B 1998 *Phys. Rev. A* **57** 1536
3. Ernst W E, Huber R, Jiang S, Beuc R, Movre M and Pichler G 2006 *J. Chem. Phys.* **124** 024313
4. Beuc R, Movre M, Ban T, Pichler G, Aymar M, Dulieu O and Ernst W E, *J. Phys. B*, accepted
5. Beuc R, Movre M, Vdovic S, Pichler G, Nevseyan A, Varzhapetyan T and Sarkisyan D, *J. Phys. B*, in preparation



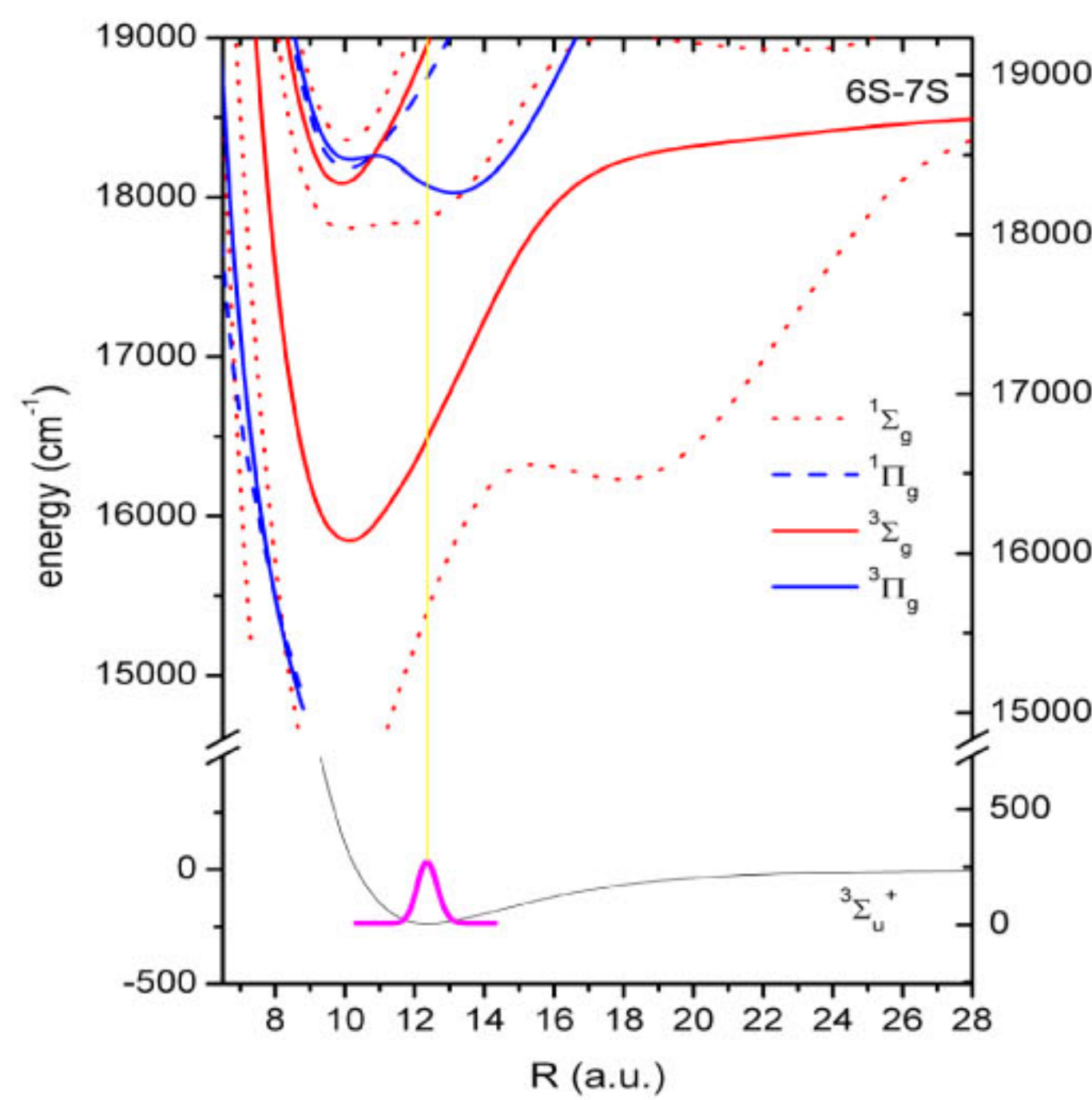
Potential curves (full lines) from reference of **RbCs** molecule: (a)  $^3\Pi$ , (b)  $^1\Pi$ , (c)  $^3\Sigma^+$ , (d)  $^1\Sigma^+$ . The corresponding difference potentials (broken lines) are also shown.



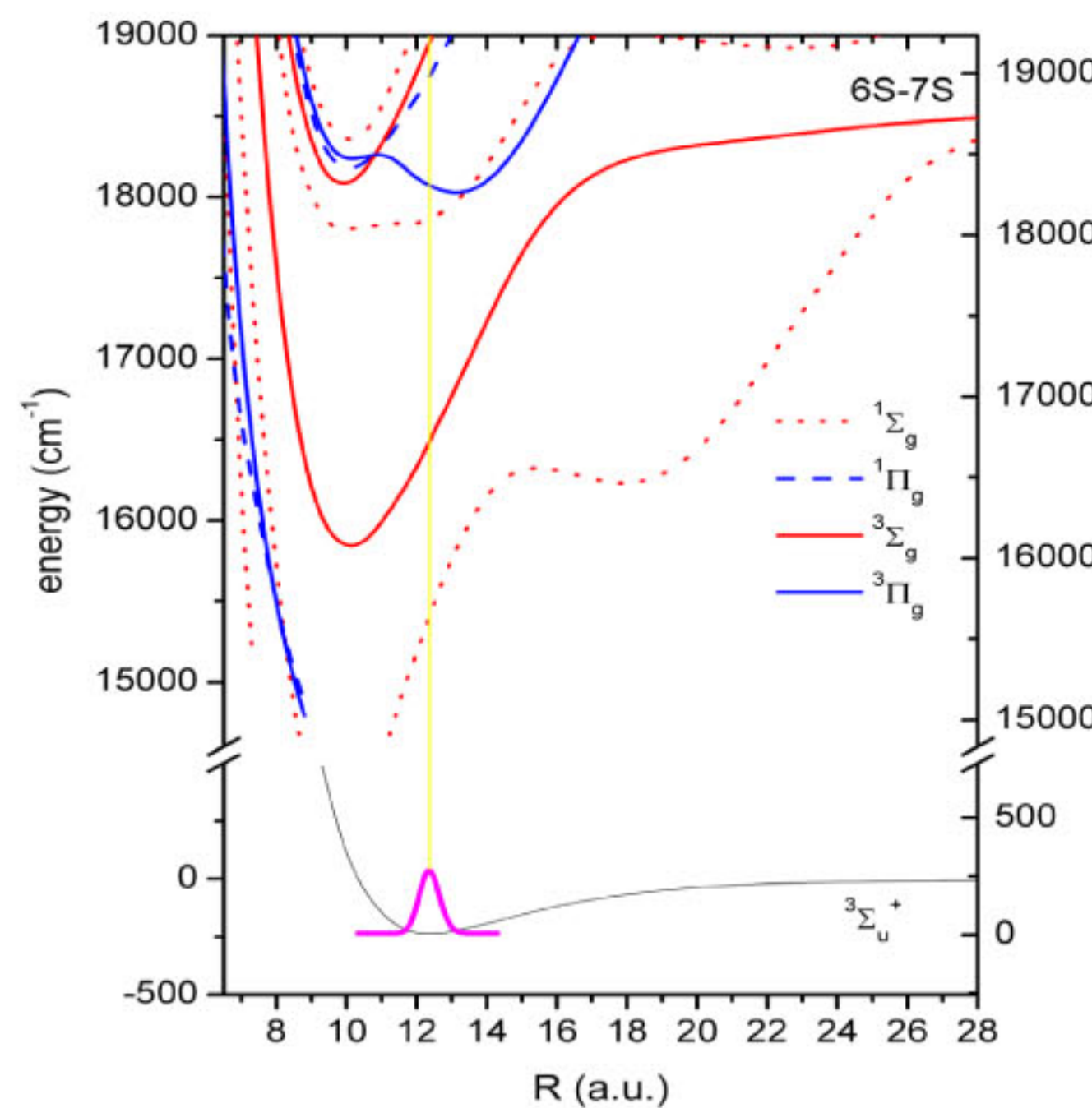
Computed Franck-Condon factors for the transitions starting from the lowest vibrational level: (a)  $1\ ^3\Sigma^+ \rightarrow N\ ^3\Pi$  ( $N=1,2,3,4$ ), (b)  $1\ ^1\Sigma^+ \rightarrow N\ ^1\Pi$  ( $N=1,2,3,4$ ), (c)  $1\ ^3\Sigma^+ \rightarrow N\ ^3\Sigma^+$  ( $N=2,3,4,5$ ), (d)  $1\ ^1\Sigma^+ \rightarrow N\ ^1\Sigma^+$  ( $N=2,3,4,5$ ). Line positions within the bands are represented by vertical bars.



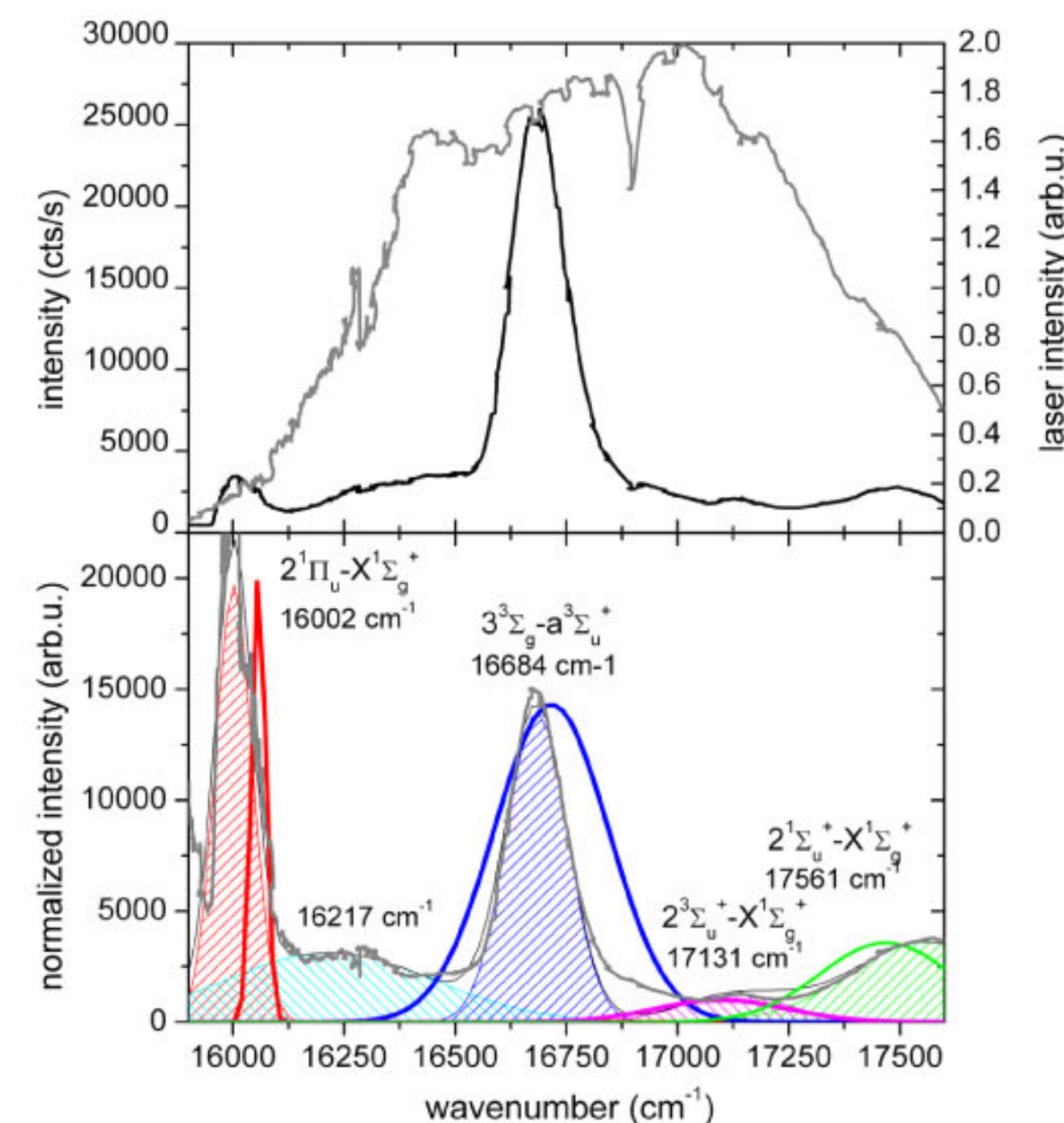
Franck-Condon factors calculated in reflection approximation (black lines) compared with the quantum-mechanical band shapes (gray lines) obtained from equation (3) using Gaussian line shape function of width  $w=30 \text{ cm}^{-1}$  centered at the calculated vibrational frequency  $\nu_g$  for transitions shown in figure 2.



**Cs<sub>2</sub>** potential energy curves from (Hund's case a), relevant to the observed transitions. The ground state wavefunction (here for  $3\Sigma_g^+$ ) is shown with a vertical line extending to the excited state potentials such as to indicate the described calculation procedures. Potentials accessible through weakly allowed transitions are shown with dashed lines.



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Spectrum of cesium molecules on helium droplets in the Rh6G dye laser regime. The upper panel shows the observed spectrum and the simultaneously recorded relative laser intensity. The normalized spectrum and Gaussian fits to the band maxima as well as the positions of the bands are depicted in the lower panel. In addition, calculated bands are indicated by lines. The assignments refer to Table II. The prominent feature in the center is believed to be due to the  $3\Sigma_g^+ - 3\Sigma_g^+$  transition.

If we neglect the  $J$ -dependence of the matrix elements and put  $J'=J''=0$  to obtain:

$$k(\nu) = \frac{8\pi^3}{3c} N \sum_{v'} \left| \langle \phi_0 | D(R) | \phi_{v'} \rangle \right|^2 g(\nu - \nu_{v'}),$$

where  $\phi_{v',J',\Lambda'} \equiv \phi_0$  is the lowest rovibrational wave function ( $v''=0, J''=0, \Lambda''=0$ ).

The small vibrational spacings in the bands of the heavy alkali diatomics are usually not resolved in any spectrum because of the helium induced line broadening. In order to get coarse-grained spectrum, we replace the summation over  $v'$  with an integral over (quasicontinuum) energy  $E$  and recalling that unit normalized bound state wave function can be turned into

energy-normalized wave function,  $\phi(E) = \left( \frac{\partial E}{\partial v} \right)^{1/2} \phi_v$ , we get

$$k(\nu) = \frac{8\pi^3}{3c} N \left| \langle \phi_0 | D(R) | \phi(E) \rangle \right|^2.$$

Now, all unresolved structure in the spectrum due to the discrete nature of the bound states is effectively smoothed down.

If excited potential  $V_e(R)$  is steep around  $R_0$ , the Franck-Condon factor is well described by the following relation (reflection approximation):

$$\langle \phi_0 | D(R) | \phi(E) \rangle = \frac{1}{\sqrt{|V'_e|}} D(R_0) \phi_0(R_0),$$

where  $R_0$  is the turning point in excited state potential for a given energy  $E$ .

Writing the ground state wave function, the energy of the lowest vibrational level, and the transition energy as:

$$\phi_0(R) = \frac{1}{\pi^{1/4} \sigma^{1/2}} e^{-\frac{(R-R_0)^2}{2\sigma^2}},$$

$$E_g = V_g + \frac{1}{2} \hbar \omega,$$

$$\hbar \nu = V_e - E_g + V'_e(R_0 - R_0),$$

where  $\sigma^2 = \hbar / \mu \omega$ , equation for the absorption coefficient can be brought to the form:

$$k(\nu) = \frac{8\pi^3}{3c} N \frac{V_0 D(R)^2}{w} \sqrt{\frac{2}{w}} e^{-\frac{(E_0 - \hbar \nu)^2}{w^2}}$$

where  $E_0 = V_e - E_g = \hbar \nu_0$ , and  $w = |2V'_e \sigma|$ .

Here we also assumed that  $D$  and  $v$  are slowly varying function of  $R$ . In our model, the widths and the peak intensities of the absorption bands are determined from a few quantities ( $V_g$ ,  $V'_g$ ,  $V_e$ ,  $V'_e$ ,  $v$ , and  $D$ ) evaluated at  $R_0$ .

Among various approximations supposed, the most critical one is the steepness of the excited potential which allows the reflection approximation to be used.