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Predictions of KRb and RbCs spectra under cold and thermal conditions

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Quantum-mechanical simulations of the excitation spectra of KRb [1] and RbCs [2] from the lowest vibrational level of the lowest triplet and singlet electronic states have been performed using the manifold of potential curves for the Hund's coupling case *a* and the corresponding transition dipole moments (for KRb only, while for RbCs we assumed them to be constant.) Spin-orbit interaction was also neglected. The obtained spectra can be used for a comparison with experimental absorption spectra of KRb and RbCs molecules produced in their vibronic ground state or attached to cold helium droplets.

In addition, we compare the semiclassically simulated spectra with absorption measurements in dense K–Rb [1] and Rb–Cs [3] vapors at high temperatures, which helped us to identify three diffuse bands for KRb as $1\,^3\Sigma^+ \rightarrow 3\,^3\Pi$, $1\,^3\Sigma^+ \rightarrow 4\,^3\Pi$, and $1\,^1\Sigma^+ \rightarrow 4\,^1\Sigma^+$ transitions, while for RbCs the band at 717 nm is identified as the $1\,^1\Sigma^+ \rightarrow 1\,^1\Pi$ transition (*B-X* band) and the diffuse band at 563 nm as the $1\,^1\Sigma^+ \rightarrow 3\,^1\Pi$ transition.

References

[1] R. Beuc, M. Movre, T. Ban, G. Pichler, M. Aymar, O. Dulieu, and W. E. Ernst, J. Phys. B: At. Mol. Opt. Phys. **39** (2006) S1191 – S1201

[2] R. Beuc, M. Movre, B. Horvatić, and G. Pichler, Chem. Phys. Lett. **435** (2007) 236 – 241

[3] R. Beuc, M. Movre, B. Horvatić, M. Čopor, S. Vdović, A. Nevsesyan, T. Varzhapetyan, D. Sarkisyan, and G. Pichler, Appl. Phys B **88** (2007) 111– 115