ROTATIONAL AND SPIN-ORBIT PREDISSOCIATION OF THE Ne·XH ($\tilde{X}\,^2\Pi$, X=O,S) VAN DER WAALS COMPLEXES

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The rotational and spin-orbit predissociation dynamics of Ne·XH ($\tilde{X}\,^2\Pi$, X=O,S) complexes is investigated theoretically using the stabilization method of Mandelshtam *et al.*[a] using *ab initio* potential surfaces to describe the Ne·XH interactions.[b,c] The calculations show large variations in the lifetimes of the Ne·XH complexes within narrow ranges of energy. In particular, we found a strong dependence of the lifetime on the parity of the state and the projection of the angular momentum onto the internuclear axis. Comparisons with available experimental data are made and the results of this purely *ab inito* treatment are found to be in good agreement with the experimental resonance energies and lifetimes.

[a] V. A. Mandelshtam, H. S. Taylor, V. Ryaboy and N. Moiseyev, *Phys. Rev. A* **50** 2764 (1994)
[b] S. M. Cyblulski, R. R. Toczylowski, H.-S. Lee and A. B. McCoy, *J. Chem. Phys.*, **113**, 5736 (2000)
[c] H.-S. Lee, A. B. McCoy, R. R. Toczylowski and S. M. Cyblulski, *J. Chem. Phys.*, **113**, 9549 (2000)