# HIGHLY ACCURATE QUANTUM-CHEMICAL CALCULATIONS FOR THE INTERSTELLAR MOLECULES $C_3$ AND l-$C_3H^+$

PETER BOTSCHWINA, BENJAMIN SCHRÖDER, CHRISTOPHER STEIN, PETER SEBALD, RAINER OSWALD, *Institute of Physical Chemistry, Georg-August-Universität Göttingen, Göttingen, Germany*.

Composite potential energy surfaces with coupled-cluster contributions up to CCSDTQP were constructed for $C_3$ and l-$C_3H^+$ and used in the calculation of spectroscopic properties. The use of very large AO basis sets and the consideration of higher-order correlation beyond CCSD(T) is of utmost importance for $C_3$ in order to arrive at quantitative spectroscopic data. The first detection of l-$C_3H^+$ in the interstellar medium was reported by Pety et al.,[a] who attributed 9 radio lines observed in the horsehead photodissociation region to that species. That assignment was questioned by the recent theoretical work of Huang et al.[b] However, our more accurate calculations are well in support of the original assignment. The calculated ground-state rotational constant is $B_0 = 11248$ MHz, only $0.03\%$ off from the radio astronomical value of $11244.9512 \pm 0.0015$ MHz. The ratio of centrifugal distortion constants $D_0$(exp.)/$D_e$(theor.) of 1.8 is quite large, but reasonable in comparison with $C_3O$[c] and $C_3$.

---

[a] J. Pety, P. Gratier, V. Guzmán, E. Roueff, M. Gerin et al., *Astron. Astrophys.* **2012**, *A68*, 1-8.

[b] X. Huang, R. C. Fortenberry, T. J. Lee, *Astrophys. J. Lett.* **2013**, *768:L25*, 1-5.

[c] P. Botschwina, R. Oswald, *J. Chem. Phys.* **2008**, *129*, 044305.