IMPROVED DIPOLE MOMENTS FOR ACRYLONITRILE AND PROPIONITRILE

ZBIGNIEW KISIEL, ADAM KRAŚNICKI, *Institute of Physics, Polish Academy of Sciences, Al. Lotników 32/46, 02-668 Warszawa, Poland.*

Previous determinations of the electric dipole moment of acrylonitrile, while in agreement on the total dipole moment, showed an appreciable difference in the value of the smaller μ_b component.[a,b] The value of this component is important for intensity considerations in the THz spectrum of this molecule, which is dominated by *b*-type transitions.[c]

We decided to update the dipole moment determination of acrylonitrile, and also of propionitrile (ethyl cyanide) by making Stark measurements in supersonic expansion. We used the Stark electrode arrangement developed in our laboratory and the program QSTARK for fitting Stark measurements on resolved nuclear quadrupole hyperfine structure.[d] The results for acrylonitrile show a further, significant difference in the value of μ_b, while those for propionitrile, while more precise, are essentially consistent with previous values.[e] The evidence from $ab\ initio$ calculations and from relative intensity measurements supporting the current dipole moment determinations is presented.

---

[a] W.S.Wilcox, J.H.Goldstein, J.W.Simmons, *J.Chem.Phys.*, **22**, 516 (1954)
[b] M.Stolze, D.H.Sutter, *Z.Naturforsch.*, **40a**, 998 (1985)
[c] Z.Kisiel, L.Pszczółkowski, B.J.Drouin, C.S.Brauer, S.Yu, J.C.Pearson, *J. Mol. Spectrosc.* **258**, 26 (2009).
[d] Z.Kisiel, J.Kosarzewski, B.A.Pietrewicz, L.Pszczółkowski, *Chem.Phys.Lett.* **325**, 523 (2000).
[e] H.M.Heise, H.Lutz, H.Dreizler, *Z.Naturforsch.*, **29a**, 1345 (1974)