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Title:Electric dipole moments of acrylonitrile and of propionitrile measured in supersonic expansion

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Publisher:Academic Press Inc., 6277 Sea Harbor Drive, Orlando, FL 32887-4900, United States Abstract:New determinations of the ground-state electric dipole moments of acrylonitrile and propionitrile have been made from Stark effect measurements at conditions of supersonic expansion. The measurements were made on selected Stark lobes of fully resolved hyperfine components of several lowest-J rotational transitions. The results are ua = 3.821(3) D, ub = 0.687(8) D, utot = 3.882(3) D for acrylonitrile, and ua = 3.816(3) D, ub = 1.235(1) D, utot = 4.011(3) D for propionitrile. The new value of ub for acrylonitrile is appreciably different from those reported previously and it has been substantiated by both ab initio calculations and relative intensity measurements. The new dipole moment implies a considerable revision in the calculated intensities of the strongest THz-region rotational transitions of acrylonitrile, to 59% of previous values.

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