Coupled-cluster and many-body perturbation study of energies, struc-tures, and phonon dispersions of solid hydrogen fluoride†

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A linear-scaling electron-correlation method based on a truncated many-body expan-sion of the energies of molecular crystals has been applied to solid hydrogen fluoride. The energies, structures, harmonic and anharmonic frequencies of the infrared- and/or Raman-active vibrations, phonon dispersions, and inelastic neutron scattering (INS) of the solid have been simulated employing an infinite, periodic, one-dimensional zigzag hydrogen-bonded chain model. The Hartree–Fock, second-order Møller–Plesset, and coupled-cluster singles and doubles theories have been combined with the aug-cc-pVDZ and aug-cc-pVTZ basis sets and, in some instances, the counterpoise corrections of the basis-set superposi-tion errors. The computed structural parameters agree with the observed within 0.1–0.2 Å and a few degrees with the observed and the predicted harmonic and anharmonic frequen-cies reproduce the observed semi-quantitatively if a correlated theory is employed. They support the revised infrared and Raman band assignments of librational modes made by Hirata and Iwata and provide more detailed assignments of the observed INS features.