

Supplementary material

Recoil lineshapes and chemical shifts of C 1s photoemission from gas-phase 10-aminodecane-1-thiol molecules.

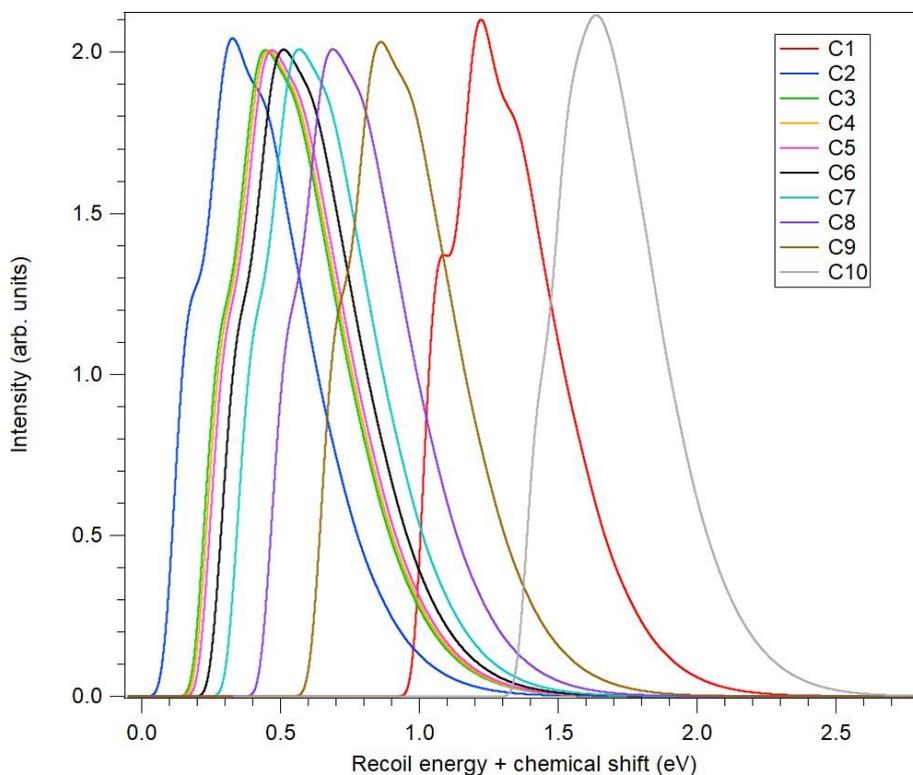


Figure 1. Recoil lineshapes from C 1s photoemission in isotropically oriented gas-phase 10-aminodecane-1-thiol molecules ionized by 10 keV photons. Emission lineshape from each C atom is shown separately and shifted according to the calculated C 1s binding energies (from the molecular orbital energies) relative to the lowest binding energy of C2. The carbon atoms are numbered starting from the amino group towards the thiol end group. Lifetime broadening or Franck-Condon excitations are not included.

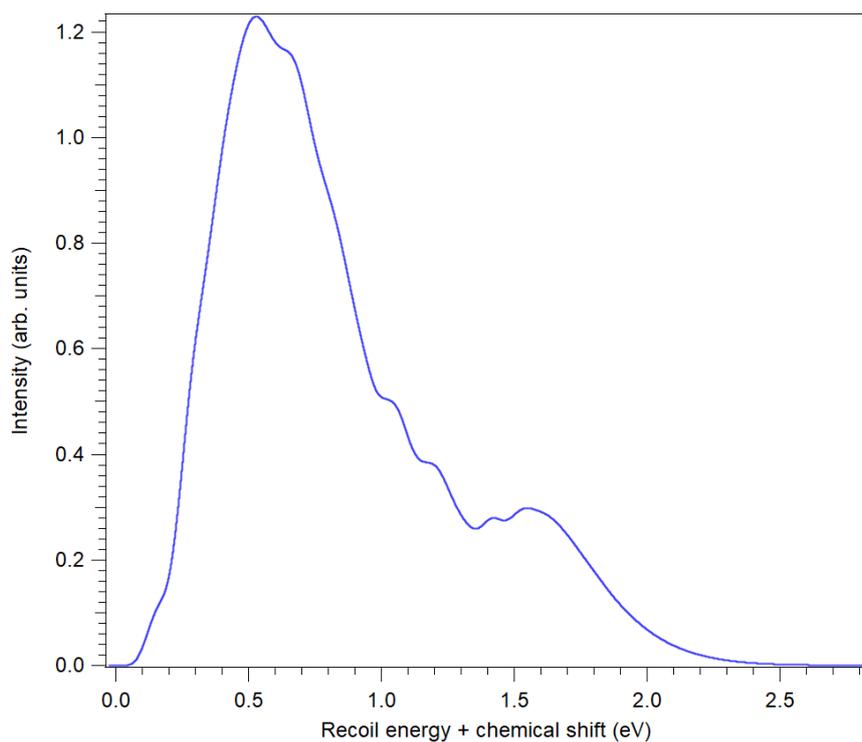


Figure 2. Combined C 1s recoil lineshape of all C atoms in gas-phase 10-aminodecane-1-thiol molecules, as sum of the curves in Figure 1.