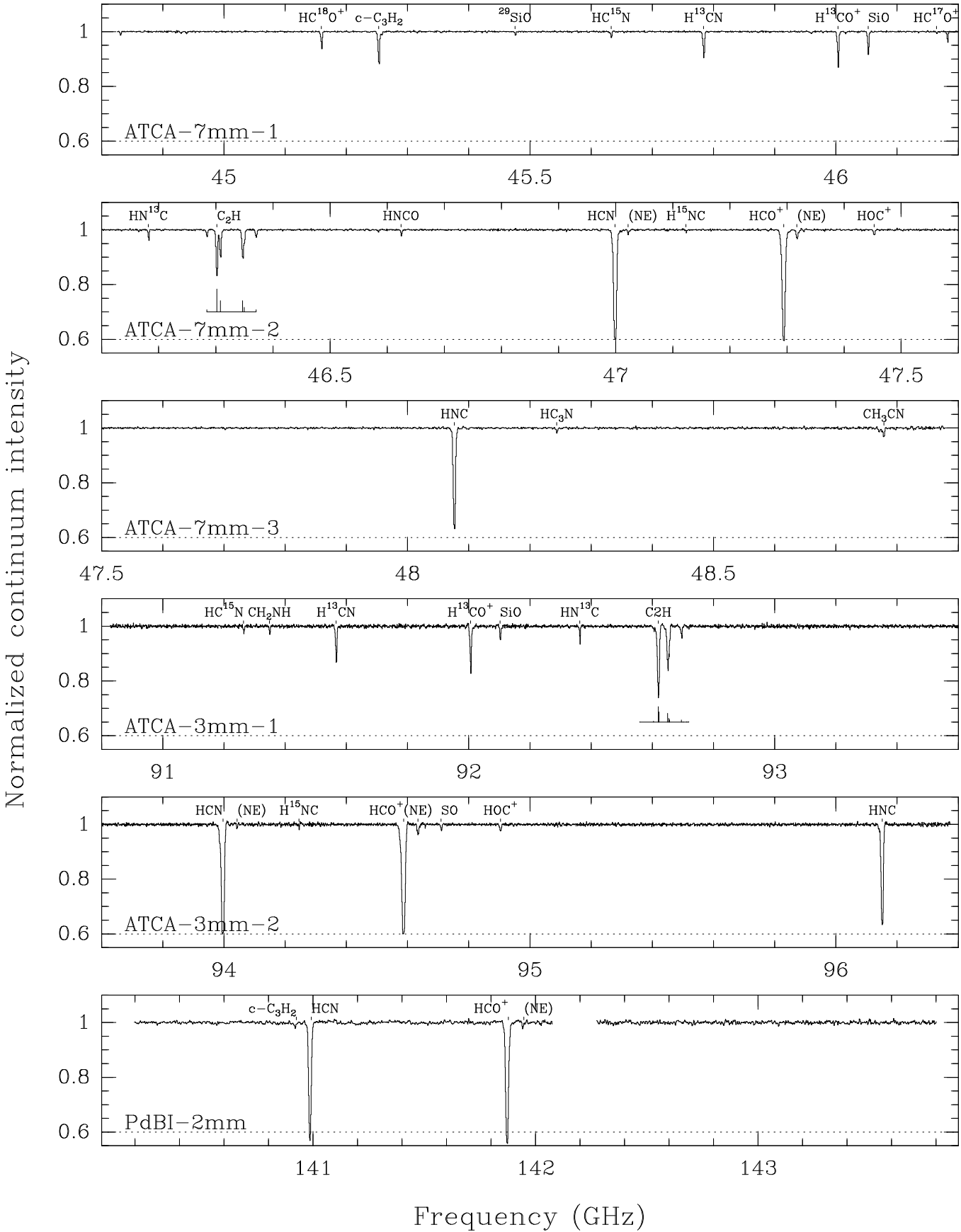1. spectra and fit results