P5385: TOWARD 0.1% UNCERTAINTY FOR CO_2 THEORETICAL IR INTENSITIES

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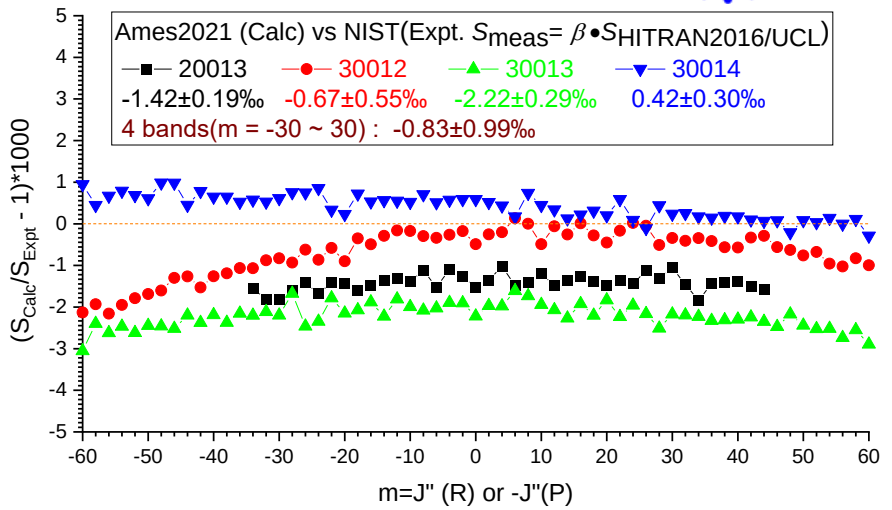
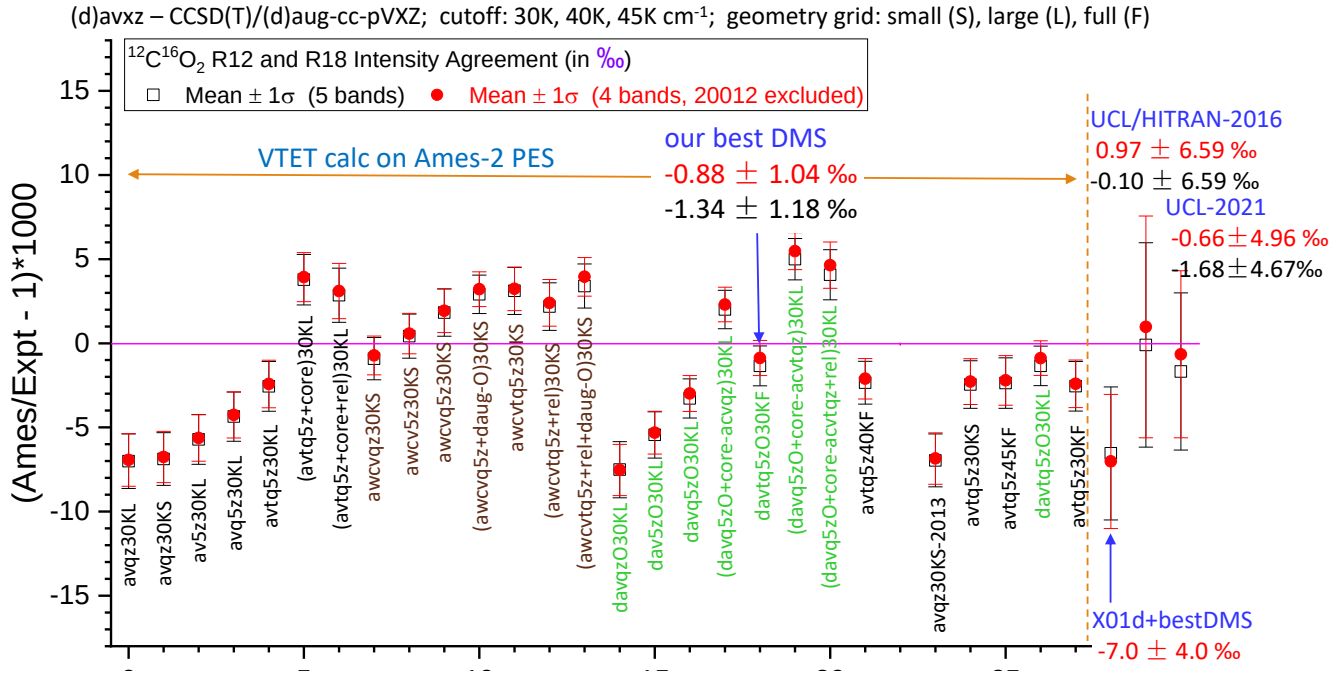
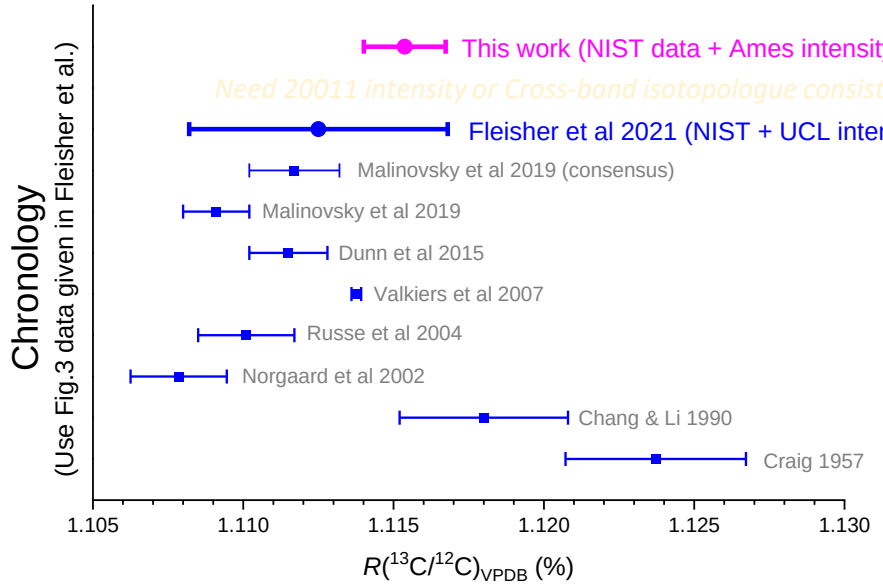
- Best experimental CO_2 IR intensities (NIST) have uncertainties 0.6-0.9‰, but old theoretical intensities (Ames & UCL) had 0.5~1.0%, one order of magnitude worse.
- New Ames IR intensity computed with CCSD(T)/davtq5zO DMS + Ames-2 PES:
  (1) unprecedented agreement for 4 bands = -0.83±0.99‰, close to experiment.
  (2) similar uncertainty expected for other isotopologues and higher energies
  (3) $R(^{13}C/^{12}C)_{VPDB}$ = 0.0011154±14 vs 0.0011125±43 (original NIST+UCL, 2021)
- 0.1% or smaller uncertainty probably requires more accurate PES (and DMS).







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