

2 Quality checks implemented in processing chain

QC philosophy: sequential QC along the processing chain of each spectrum, the processing of the spectrum stops if one QC test fails (e.g. FFT and all subsequent steps are omitted if DC variation of IFG is found too big ... no output spectrum is generated, just the error flag state in the log file listing the QC status for each spectrum)

Tests:

0: formal test: is the submitted OPUS file compatible with COCCON and the functional extent of the preprocessor? No flag is generated, program execution is stopped altogether. Requirements: (I) RES = 0.5 cm⁻¹ (II) NSS even (III) interferogram is double sided

All subsequent tests modify the flagging state. The total flagging state of each spectrum is mapped on a single integer number. A spectrum passing all tests has flag content 00000000 (8 zeroes). Each test modifies a certain position in this integer, QC_i adds 1 in position i if QC_i fails in the primary channel, adds 3 if QC_i fails in the second channel.

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QC1: minimum DC value relative to available ADC range (requested: 0.05)

QC2: maximum variability of DC in interferogram (requested: 0.1. Note: the assumed operation scheme is coaddition of 5 FWD and 5 BWD scans – allows for 50% intensity variation in a single scan)

QC3: compares the centerburst amplitudes of FWD and BWD interferograms (requested: agreement within 0.05)

QC4: is the centerburst location centered in the interferogram (otherwise, a double-sided FFT becomes impossible)?

QC5: check relative amplitude of out-of band artefacts (requested: primary channel: 0.005 (~ 950 - 4350 cm⁻¹) / secondary channel: 0.01 (~6270 - 15700))

QC6: check slope, curvature, and change of curvature of phase spectrum

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QC7: check spectral calibration based on cross-correlation of spectral structure wrt a reference spectrum. Is the zero-shifted result maximal (rejects shifts beyond $0.5 \times \text{FFT grid width} \sim 0.12 \text{ cm}^{-1}$)?

QC8: compare spectra derived from forward and backward scans. After allowing for an overall ordinate scaling factor for adjustment, the summed difference between the spectra should amount less than 0.005 (secondary channel: 0.01).