Corrigendum to "Conformational analysis and vibrational study of sulfanilamide" [Vib. Spectrosc. 58 (2012) 12–18]

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Corrigendum

Corrigendum to "Conformational analysis and vibrational study of sulfanilamide" [Vib. Spectrosc. 58 (2012) 12–18]

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After the above paper was published, we found an incorrect statement in the text on p. 14, a few errors in Table 4, and a wrong version of Fig. 3. They should be corrected as follows:

1. On p. 14, middle section of the right hand column, this sentence starting with "While the NC stretching mode. . ." should be removed from the text and replaced with the following sentence: "While the OSCC torsion mode is observed at 563 and 564 cm^{-1} in IR and Raman spectra, respectively, and is calculated as 524 and 526 cm^{-1} for conformers I and II, respectively, this mode cannot be observed in the calculated spectra of conformers III and IV."
2. In Table 4, the calculated "DFT (harmonic)" vibrational frequencies (cm^{-1}) for "ν_{21}, ν_{SO_2} sym" mode in columns 6–9 should be corrected as 1155, 1155, 1157, and 1157, respectively. The corresponding scale factor of the calculated SO_2 stretching frequencies should be 1.023 (instead of 1.033) in footnote "b" under the table.
3. On p. 16, the simulated spectral plots presented in Fig. 3 (inserted there from a previous revision of the work by the editor's mistake) should be replaced by the final version shown below (in accordance with the data of Table 4).

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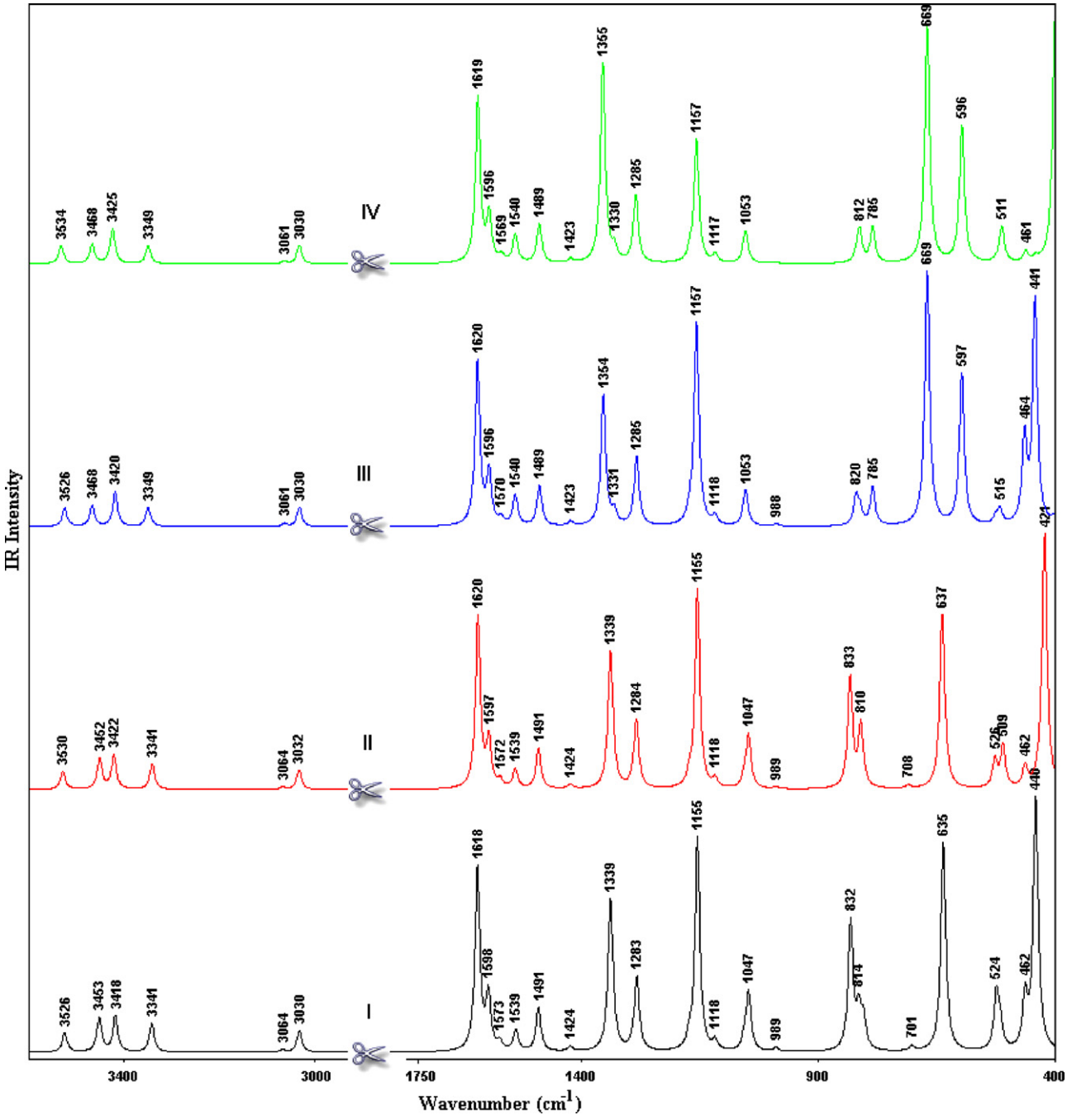

Fig. 3. Scaled theoretical IR spectra of global minimum conformer (I), second (II), third (III) and fourth (IV) lowest energy conformers, from bottom to top, respectively.