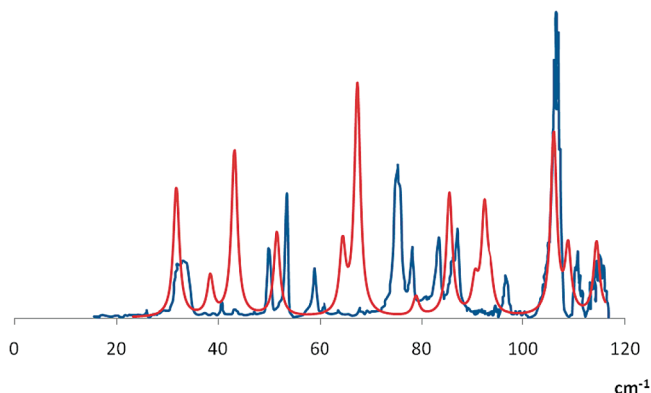


**Carlos Guadarrama-Pérez, Julibeth M. Martínez de la Hoz, and Perla B. Balbuena\***: Theoretical Infrared and Terahertz Spectra of an RDX/Aluminum Complex Page 2284. In Figure 13 we had reported the comparison of our calculated IR and terahertz spectra of the RDX molecule in conformation AAA (three nitro groups in axial positions) adsorbed on a model aluminum substrate ( $\text{Al}_{16}$ ), with the experimental spectrum of RDX crystallized over an Al plate.<sup>1</sup> However, the experimental spectrum was incorrectly extracted from the original reference and it appeared red-shifted. Here we include the corrected Figure 13.



**Figure 13.** Overlap of terahertz and IR spectra of AAA- $\text{Al}_{16}$  (red) and that of experimental RDX crystallized over an Al plate.<sup>1</sup>

Therefore the first two paragraphs of the discussion in section 3.5 are rewritten as follows:

**3.5. AAA- $\text{Al}_{16}$  Complex versus Experimental RDX over Aluminum Surface.** A comparison between the terahertz spectra of RDX experimentally crystallized over an Al plate

and that calculated for the AAA- $\text{Al}_{16}$  model complex is shown in Figure 13. To simulate terahertz experimental observations, the full width at half-maximum of each calculated peak was set to  $3 \text{ cm}^{-1}$ .

The assignments and correspondence among modes are reported in Table 5. Good agreement is found between the experimental and calculated modes. Most assignments reveal coupling of the molecular motions to those of the atoms of the substrate. The corrected Table 5 is included here.

**TABLE 5: Spectral Modes and Assignments for Calculated AAA- $\text{Al}_{16}$  and Experimental RDX Crystallized over an Aluminum Plate<sup>1</sup>**

| calculated (experimental)   | type of motion   |
|---|--|
| 31.8 (33.2)   | out-of-plane Al vibration + OR <sup>a</sup> normal to Al layer plane + NO <sub>2</sub> rocking |
| 38.5 (40.1), 43.2 (42.6), 51.5 (49.8, 53.5), 108.8 (110.7)                      | out-of-plane Al vibration + OR <sup>a</sup> parallel to Al layer plane                         |
| 64.5  | in-plane Al vibration  |
| 67.4, 78.9 (78.2), 85.4 (83.3, 85.8), 92.3 (96.5), 105.9 (106.4), 114.3 (114.0) | out-of-plane Al vibration + NO <sub>2</sub> libration  |

<sup>a</sup> RDX optical rotation.

## References and Notes

(1) Melinger, J. S.; Laman, N.; Grischkowsky, D. The underlying terahertz vibrational spectrum of explosives solids. *Appl. Phys. Lett.* **2008**, *93*, 011102.

10.1021/jp104990g

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