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Addition/Correction

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Correction and Addition to "Vibrational Anharmonicities and Reactivity of Tetrafluoroethylene"

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Due to a misunderstanding in the proof corrections, many calculated anharmonicities in Table 2 cannot be distinguished from the spectroscopic ones. This table is therefore reproduced here once more.

In the meantime, we were able to calculate at the same level (MP2/cc-pVTZ) as the anharmonicities the Fermi resonance terms (interaction matrix elements between the levels) that were derived from the spectra in the original paper. We compare

Table 2. Anharmonic Constants x_{ij} (cm^{-1}) of $^{12}C_2F_4$[a]

	1	2	3	4	5	6
1	(−7.83)					
2	−3.1	−3.8				
	(−3.04)	(−0.62)				
3			+0.05			
	(−1.93)	(−0.22)	(+0.03)			
4	−1.5	−0.7, −0.3	+0.9	+0.8		
	(−1.14)	(−0.24)	(−0.22)	(−0.03)		
5			−1.5	−3.2		
	(−8.85)	(+8.49)	(−1.86)	(−0.69)	(−2.06)	
6	−5.0	−10.85, −8.7	+2.0	−1.1		−0.95
	(−4.54)	(−13.35)	(−0.07)	(−0.82)	(+10.88)	(−0.002)
7	−4.6, −3.8	−9.5, −10.1	−1.4	+0.3		−0.7
	(−3.27)	(−9.18)	(−0.44)	(+0.24)	(−2.16)	(−0.78)
8	−18.5 to −19.65	−1.32	+0.4	−1.05, −0.7		−4.9, −2.3
	(−18.27)	(−3.08)	(+0.24)	(−0.75)	(−4.73)	(+0.10)
9	−3.3	−2.0		−0.9	+0.2	−2.75
	(−3.78)	(−4.02)	(−1.72)	(−0.85)	(−11.89)	(−2.52)
10	−1.04	+0.9, +1.0	−1.75	−1.3	−1.2, **−1.5**	−0.1
	(−1.27)	(−0.39)	(−0.26)	(−0.03)	(−2.86)	(−0.16)
11	−4.6	−1.5	−2.3	−0.7, −0.25	+4.9	−1.4
	(−4.56)	(−3.32)	(−1.44)	(−0.52)	(−6.14)	(−0.98)
12	−0.4	+0.6	+0.85	+0.25		
	(+0.13)	(+0.04)	(+0.05)	(−0.10)	(−3.81)	(−0.36)
	7	8	9	10	11	12
7	+4.1					
	(+2.38)					
8	−1.6, −1.5	+0.05				
	(−1.24)	(+2.04)				
9	−2.0					
	(−2.03)	(−3.82)	(−2.68)			
10	+0.3	−0.7	−1.2 to −1.5	+1.25		
	(+0.39)	(−0.40)	(−1.50)	(+0.99)		
11	−1.15	−0.7		−0.7	−1.6, −0.45	
	(−0.81)	(−0.13)	(−6.48)	(+0.96)	(−1.74)	
12	−0.25	+0.5		−0.2		+0.33
	(−0.08)	(+1.02)	(−3.17)	(+0.48)	(−3.81)	(+0.12)

[a]Experimental values are shown without parentheses. In parentheses: values calculated at the MP2/cc-pVTZ level. Where two values or a range are given for the experimental data, it may indicate (a) a dependence of the effective x_{ij} on the involved levels due to perturbations (Fermi resonances, section 4.4) or (b) an uncertainty due to error limits (e.g., where broad bands are involved) or an uncertain assignment. A preferred value is indicated by boldface type. For further details on the derivation of each x_{ij} and some isotopic data, see the Supporting Information of the original paper.

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Table A. Fermi Interaction Terms (cm^{-1})

	interacting levels	calculated	experimental[a]
FR1	$\nu_3/2\nu_7$	15.4	16.4
FR2	$\nu_5/\nu_2 + \nu_6$	−15.5	≈11
FR3	$\nu_1/\nu_5 + \nu_6$	0.9	≤2.5
FR4	$\nu_2/2\nu_3$	−4.5	small
FR5	$\nu_3/2\nu_{10}$	−3.8	small
FR6	$\nu_3/2\nu_4$	−2.9	small

[a]Magnitudes.

the two sets briefly (Table A). The large FR1 is confirmed and FR2 is even larger than the preliminary experimental value (possibly because our model did not include the other interactions). The other interactions are small, in particular FR3, as also concluded from the spectra.

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