Supplementary Information for

Reinvestigation of the ν_3–ν_6 Coriolis Interaction in Trifluoroiodomethane

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Computational results

The optimized equilibrium geometries obtained from *ab initio* calculations are shown in Table S1. Quartic centrifugal distortion constants and Coriolis zeta parameters obtained from harmonic force field calculations are compared with experimental values in Table S2. Ground-state rotational constants, vibration-rotation constants, and fundamental frequencies obtained from cubic force field calculations are compared with experimental values in Table S3. Note that the full cubic and semidiagonal quartic force field was calculated (using the `ANHARM=VPT2` keyword in CFOUR) only when using Hartree-Fock (HF) and Second-Order Møller-Plesset (MP2) methods. In our CCSD calculations, only the cubic force field constants required to calculate vibration-rotation interaction constants were calculated (using the `ANHARM=VIBROT` keyword in CFOUR). In the CCSD(T) calculations, only the harmonic force field was calculated.

Table S1. Optimized equilibrium geometries of CF_3I obtained from *ab initio* calculations. The dihedral angle is constrained to $120°$ (C_{3v} geometry).

	Hartree-Fock			MP2			CCSD			CCSD(T)		
Param.	**3-21G**	**6-311G**	**6-311G****	**3-21G**	**6-311G**	**6-311G****	**3-21G**	**6-311G**	**6-311G****	**3-21G**	**6-311G**	**6-311G****
$r_{\mathrm{CI}}/\mathrm{Å}$	2.1797	2.1361	2.1491	2.2140	2.1492	2.1654	2.2120	2.1573	2.1674	2.2287	2.1640	2.1766
$r_{\mathrm{CF}}/\mathrm{Å}$	1.3407	1.3550	1.3051	1.3667	1.3975	1.3275	1.3646	1.3918	1.3253	1.3684	1.3972	1.3292
$\theta_{\mathrm{ICF}}/\mathrm{deg}$	110.66	111.41	110.57	110.26	111.50	110.34	110.27	111.43	110.48	110.21	111.41	110.40

Table S2. Ground-state quartic centrifugal distortion parameters and Coriolis zeta parameters of $^{12}CF_3I$ calculated from *ab initio* harmonic force fields are compared with experimentally determined values.

	MP2			CCSD			CCSD(T)			
Param.	**3-21G**	**6-311G**	**6-311G****	**3-21G**	**6-311G**	**6-311G****	**3-21G**	**6-311G**	**6-311G****	**Expt.**
D_J/kHz	0.1526	0.1437	0.1588	0.1553	0.1462	0.1580	0.1605	0.1496	0.1641	0.16462(2)[a]
D_{JK}/kHz	0.8294	0.8208	0.8552	0.8450	0.8242	0.8611	0.8529	0.8322	0.8703	0.9925(4)[a]
D_K/kHz	0.3124	0.4240	0.3194	0.3034	0.4087	0.3097	0.3028	0.4161	0.3100	
$\zeta_{66}^{(a)}$	0.1295	0.1288	0.1319	0.1323	0.1313	0.1319	0.1320	0.1327	0.1341	0.13765(9)[b]
$\zeta_{36}^{(b)}$	0.4011	0.4123	0.3996	0.3989	0.4073	0.3945	0.3972	0.4090	0.3963	

[a]Ref. 1.

[b]This work.

References

1. S. W. Walters, D. H. Whiffen, "Rotational spectrum of trifluoroidomethane" *Journal of the Chemical Society, Faraday Transactions 2: Molecular and Chemical Physics* **79**, 941-949 (1983), https://doi.org/10.1039/F29837900941.