

Table S1: Fit $\varepsilon = \text{obs} - \text{calc}$ (cm^{-1}) of Observed Anharmonic (ν_{obsd}) and "Observed" Harmonic (ω_{obsd}) Frequencies from Scaled QC Force Fields for 1,1-Difluorocyclopropane- d_0

Sym.	Mode		dtz+	dcct	mtz+	mcct	dtz+		dcct		mtz+		mcct	
		ν_{obsd}^a	ε	ε	ε	ε	ω_{obsd}^a	ε	ω_{obsd}^a	ε	ω_{obsd}^a	ε	ω_{obsd}^a	ε
A ₁	$\nu \omega_1$	3038	2.5	2.5	1.9	2.0	3158.1	2.8	3158.3	3.0	3155.0	0.4	3157.1	2.1
	$\nu \omega_2$	1488 ^c	3.3	2.3	-0.2	-1.9	1545.8	17.0	1544.5	13.1	1544.9	10.0	1514.8^b	-20.3
	$\nu \omega_3$	1351	0.3	1.0	1.6	2.5	1384.5	-7.0	1385.4	-6.2	1386.4	-5.2	1387.2	-1.9
	$\nu \omega_4$	1007	0.8	2.0	-8.1	-4.4	1035.1	4.6	1034.1	5.1	1035.3	-7.0	1036.1	-2.5
	$\nu \omega_5$	952	-2.7	-1.6	-1.6	-0.1	979.7	1.1	978.9	2.4	981.5	3.8	980.5	3.8
	$\nu \omega_6$	702 ^c	-3.0	-3.7	0.3	-1.0	718.7	-3.4	715.3	-6.9	716.3	-2.6	716.9	-3.3
	$\nu \omega_7$	468	-0.3	-0.4	0.4	0.4	471.9	0.1	472.4	0.1	471.5	0.6	472.1	0.6
A ₂	$\nu \omega_8$	3114	4.3	4.3	3.9	3.6	3260.1	5.8	3260.0	6.5	3257.4	4.5	3256.4	4.3
	$\nu \omega_9$	1153	2.3	-2.1	2.3	-6.0	1185.7	14.0	1185.2	7.2	1184.6	5.0	1184.0	-0.8
	$\nu \omega_{10}$	882^d	0.0	3.1	1.7	8.2	896.0	1.2	903.4	9.7	896.3	1.2	902.3	15.6
	$\nu \omega_{11}$	335	1.4	1.0	1.6	0.7	340.4	2.7	341.3	2.2	337.7	1.8	337.8	0.7
B ₁	$\nu \omega_{12}$	3035	0.5	0.5	1.1	1.0	3156.3	1.8	3156.3	1.8	3154.1	1.5	3154.9	1.8
	$\nu \omega_{13}$	1409	-3.4	-3.9	-5.1	-5.7	1447.1	3.8	1448.1	2.3	1446.7	1.6	1449.0	0.2
	$\nu \omega_{14}$	1075 ^c	-4.3	-5.4	-4.9	-6.3	1110.8	1.4	1109.4	-0.1	1112.2	0.4	1112.6	-0.3
	$\nu \omega_{15}$	1032	-0.8	-0.2	3.4	2.4	1056.7	1.4	1057.8	2.8	1060.1	6.4	1058.3	3.5
	$\nu \omega_{16}$	534	-0.9	-1.0	-0.4	-0.5	539.6	-0.2	540.5	-0.4	540.2	0.3	540.8	0.3
B ₂	$\nu \omega_{17}$	3120	-0.3	-0.3	0.1	0.4	3265.1	-0.4	3264.9	0.0	3263.0	-0.3	3261.9	0.0
	$\nu \omega_{18}$	1283	3.7	-0.4	0.5	-5.6	1312.9	5.8	1314.1	3.9	1315.1	5.9	1316.5	-0.1
	$\nu \omega_{19}$	935	-5.7	-0.7	-4.1	2.2	956.0	-6.8	955.7	-1.4	957.3	-3.7	957.0	1.8
	$\nu \omega_{20}$	750	-0.8	-1.5	-2.0	-1.7	759.9	-1.6	758.6	-2.0	758.2	-3.0	755.8	-3.2
	$\nu \omega_{21}$	350	-0.8	-0.6	-0.8	-0.6	347.9	-0.5	348.9	-0.1	347.4	-0.9	348.9	-0.4
	ΣWSE^e		1.30	0.96	1.73	1.47		4.78		3.17		3.00		0.83

^a In bold, data not used in the 15-parameter scale factor refinements.

^b Datum not used, due to anomalous Δ value (see text and Table 1). ^c Fermi resonance correction applied.

^d No experimental value for ν_{10} and therefore for ω_{10} was available. The value of 882.0 is that estimated from the dtz+ scaled force field.

^e Sum of weighted squares of errors.