

## Supplementary Information

### **An integrated experimental and quantum-chemical investigation on the vibrational spectra of chlorofluoromethane**

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Harmonic intensities predicted at CCSD(T) level of theory and with different basis sets is shown in Table **S.I**. A list of the observed band types for some of the assigned bands is listed in Table **S.II**. Sextic centrifugal-distortion terms computed at CCSD(T) level of theory employing different basis sets are listed in Table **S.III**. Vibration-rotation interaction constants and relevant Coriolis zeta parameters (computed by CFOUR program) are shown in Tables **S.IV-S.VIII** and **S.IX-S.XIII**, respectively.

**Table S.I** Harmonic intensities (km/mol) of CH<sub>2</sub><sup>35</sup>ClF evaluated at the CCSD(T) level of theory and employing different basis sets.

	cc-pCVTZ (fc)	cc-pCVTZ (all)	cc-pVQZ (fc)	aug-cc-pVQZ (fc)	cc-pV5Z (fc)	cc-pV5Z + CV <sup>a</sup>	cc-pV5Z + CV + aug <sup>b</sup>
$\omega_1$	23.23	22.94	19.83	18.24	18.95	18.66	17.06
$\omega_2$	0.05	0.06	0.09	0.17	0.07	0.08	0.15
$\omega_3$	36.58	35.76	33.19	30.95	32.21	31.39	29.16
$\omega_4$	157.74	157.42	159.66	162.70	162.86	162.54	165.57
$\omega_5$	82.41	81.89	85.03	84.97	85.12	84.6	84.54
$\omega_6$	1.33	1.34	1.37	1.43	1.43	1.44	1.50
$\omega_7$	9.51	9.20	6.14	4.46	4.99	4.68	3.01
$\omega_8$	2.65	2.62	2.52	2.46	2.57	2.54	2.47
$\omega_9$	0.77	0.74	0.68	0.52	0.58	0.55	0.38

<sup>a</sup> CV effects evaluated by employing the cc-pCVTZ basis set (see text).

<sup>b</sup> The effects of diffuse function were evaluated by employing the aug-cc-pVQZ basis set (see text).

**Table S.II** Summary of observed band types for some of the assigned bands of CH<sub>2</sub>ClF.

Band	Observed band type	Band	Observed band type
$\nu_6$	mainly <i>b</i>	$\nu_3 + 2\nu_4$	<i>a/b</i>
$\nu_5$	mainly <i>a</i>	$\nu_7 + \nu_5$	<i>c</i>
$\nu_9$	<i>c</i>	$\nu_1 + \nu_9$	<i>c</i>
$\nu_4$	<i>a/b</i>	$\nu_7 + \nu_9$	<i>a/b</i>
$\nu_5 + \nu_6$	<i>a/b</i>	$\nu_4 + \nu_7$	<i>c</i>
$\nu_8$	<i>c</i>	$\nu_1 + \nu_8$	<i>c</i>
$\nu_3$	<i>a/b</i>	$\nu_7 + \nu_8$	<i>a/b</i>
$\nu_2$	mainly <i>b</i>	$\nu_1 + \nu_3$	<i>a/b</i>
$2\nu_5$	<i>a/b</i>	$\nu_3 + \nu_7$	<i>c</i>
$\nu_4 + \nu_5$	<i>a/b</i>	$\nu_2 + \nu_7$	<i>c</i>
$\nu_2 + \nu_6$	<i>a/b</i>	$\nu_6 + \nu_7 + \nu_8$	<i>a/b</i>
$2\nu_9$	<i>c</i>	$\nu_5 + \nu_7 + \nu_9$	<i>a/b</i>
$\nu_3 + \nu_5$	<i>a/b</i>	$\nu_5 + \nu_7 + \nu_8$	<i>a/b</i>
$2\nu_4$	<i>a/b</i>	$\nu_7 + 2\nu_9$	<i>c</i>
$\nu_2 + \nu_5$	<i>a/b</i>	$2\nu_4 + \nu_7$	<i>c</i>
$\nu_8 + \nu_9$	<i>a/b</i>	$\nu_4 + \nu_7 + \nu_8$	<i>a/b</i>
$\nu_4 + \nu_8$	<i>c</i>	$\nu_3 + \nu_7 + \nu_9$	<i>a/b</i>
$\nu_3 + \nu_4$	<i>a/b</i>	$\nu_3 + \nu_4 + \nu_7$	<i>c</i>
$2\nu_8$	<i>a/b</i>	$\nu_7 + 2\nu_8$	<i>c</i>
$2\nu_3$	mainly <i>b</i>	$\nu_3 + \nu_7 + \nu_8$	<i>a/b</i>
$\nu_2 + \nu_3$	<i>a/b</i>	$2\nu_3 + \nu_7$	<i>c</i>
$2\nu_2$	mainly <i>b</i>	$2\nu_1$	mainly <i>a</i>
$\nu_1$	mainly <i>b</i>	$2\nu_2 + \nu_7$	<i>c</i>
$\nu_7$	<i>c</i>	$2\nu_7$	mainly <i>b</i>
$3\nu_4$	<i>a/b</i>		

**Table S.III** Sextic centrifugal-distortion constants (in kHz) of CH<sub>2</sub><sup>35</sup>ClF as computed by anharmonic force fields at the CCSD(T) level of theory employing different basis sets. The experimental data are also reported. <sup>a</sup>

	cc-pVQZ	cc-pVQZ + CV <sup>b</sup>	cc-pVQZ + CV <sup>a</sup> + aug <sup>c</sup>	Expt. <sup>d</sup>
$\Phi_J$	$2.81640 \times 10^{-6}$	$2.82370 \times 10^{-6}$	$2.92310 \times 10^{-6}$	$2.868(45) \times 10^{-6}$
$\Phi_{JK}$	$4.21100 \times 10^{-5}$	$4.20115 \times 10^{-5}$	$4.12793 \times 10^{-5}$	$1.83(29) \times 10^{-5}$
$\Phi_{KJ}$	-0.00280	-0.00281	-0.00278	-0.002746(16)
$\Phi_K$	0.02573	0.02580	0.02510	0.02552(22)
$\phi_J$	$1.07340 \times 10^{-6}$	$1.07550 \times 10^{-6}$	$1.11310 \times 10^{-6}$	$1.055(10) \times 10^{-6}$
$\phi_{JK}$	$1.90462 \times 10^{-5}$	$1.90651 \times 10^{-5}$	$1.95169 \times 10^{-5}$	$4.03(29) \times 10^{-5}$
$\phi_K$	0.00318	0.00318	0.00318	0.00115(27)

<sup>a</sup> All the values (experimental and computed) reported in the Table refer to the Watson's A-reduced Hamiltonian in the  $\Gamma$  representation.

<sup>b</sup> CV effects evaluated by employing the cc-pCVTZ basis set (see text).

<sup>c</sup> The effects of diffuse functions have been evaluated by employing the aug-cc-pVTZ basis set (see text).

<sup>d</sup> Standard deviations in units of the last significant digits are given in parentheses. Data taken from S. Blanco, A. Lesarri, J. C. Lopez, J. L. Alonso and A. Guarnieri, *J. Mol. Spectrosc.* **174**, 397 (1995).

**Table S.IV** Vibration-rotation interaction constants at CCSD(T, fc)/cc-pVTZ

AXIS	MODE	VIB-ROT CONSTANT / (cm-1)			TOTAL
		CORIOLIS	QUADRATIC	ANHARMONIC	
1	6	0.0004788	-0.0037940	-0.0050054	-0.0083205
1	5	0.0017761	-0.0046908	0.0047418	0.0018271
1	9	0.0074374	-0.0000467	-0.0016043	0.0057864
1	4	-0.0041199	-0.0049464	0.0147072	0.0056410
1	8	-0.0004726	-0.0001159	0.0086280	0.0080395
1	3	0.0000313	-0.0002202	0.0041131	0.0039242
1	2	0.0052372	-0.0000082	-0.0007735	0.0044556
1	1	-0.0033659	-0.0007163	0.0081222	0.0040400
1	2	-0.0054505	-0.0000004	0.0076794	0.0022285
2	6	0.0000050	-0.0004584	0.0006957	0.0002423
2	5	0.0000518	-0.0001508	0.0011671	0.0010682
2	9	0.0001558	-0.0000015	0.0003628	0.0005171
2	4	-0.0000741	-0.0000604	0.0005243	0.0003899
2	8	0.0002153	-0.0000005	-0.0002854	-0.0000705
2	3	-0.0000614	-0.0000110	0.0000953	0.0000230
2	2	-0.0001477	-0.0000005	0.0001974	0.0000493
2	1	-0.0000576	-0.0000009	-0.0000383	-0.0000969
2	2	-0.0000646	-0.0000003	-0.0001414	-0.0002063
3	6	0.0001303	-0.0002476	0.0005004	0.0003832
3	5	0.0001356	-0.0000641	0.0010301	0.0011016
3	9	0.0002782	-0.0000071	0.0003510	0.0006221
3	4	-0.0002385	-0.0000274	0.0006445	0.0003786
3	8	-0.0002557	-0.0000146	-0.0000593	-0.0003296
3	3	0.0006196	0.0000000	0.0001638	0.0007834
3	2	-0.0005990	-0.0000011	0.0001475	-0.0004527
3	1	-0.0000240	-0.0000001	-0.0000807	-0.0001048
3	2	-0.0000182	-0.0000003	-0.0001446	-0.0001632

**Table S.V** Vibration-rotation interaction constants obtained at CCSD(T, fc)/aug-cc-pVTZ

AXIS	MODE	VIB-ROT CONSTANT / (cm-1)			TOTAL
		CORIOLIS	QUADRATIC	ANHARMONIC	
1	6	0.0004695	-0.0037541	-0.0048647	-0.0081494
1	5	0.0016787	-0.0045463	0.0047932	0.0019256
1	9	0.0099194	-0.0000424	-0.0016409	0.0082361
1	4	-0.0067809	-0.0050103	0.0149287	0.0031376
1	8	-0.0002530	-0.0001182	0.0087230	0.0083519
1	3	-0.0000101	-0.0002347	0.0044145	0.0041697
1	2	0.0051673	-0.0000083	-0.0008410	0.0043179
1	1	-0.0033153	-0.0006983	0.0079271	0.0039135
1	2	-0.0053477	-0.0000004	0.0073927	0.0020445
2	6	0.0000051	-0.0004615	0.0006914	0.0002350
2	5	0.0000532	-0.0001524	0.0011757	0.0010765
2	9	0.0001988	-0.0000016	0.0003691	0.0005664
2	4	-0.0001258	-0.0000606	0.0005322	0.0003457
2	8	0.0002031	-0.0000005	-0.0003019	-0.0000993
2	3	-0.0000402	-0.0000115	0.0000640	0.0000124
2	2	-0.0001482	-0.0000004	0.0002116	0.0000630
2	1	-0.0000582	-0.0000009	-0.0000353	-0.0000944
2	2	-0.0000650	-0.0000003	-0.0001384	-0.0002038
3	6	0.0001326	-0.0002478	0.0004963	0.0003811
3	5	0.0001468	-0.0000636	0.0010370	0.0011202
3	9	0.0002932	-0.0000067	0.0003547	0.0006413
3	4	-0.0002517	-0.0000287	0.0006573	0.0003769
3	8	-0.0002710	-0.0000150	-0.0000671	-0.0003531
3	3	0.0006126	0.0000000	0.0001453	0.0007579
3	2	-0.0005930	-0.0000013	0.0001579	-0.0004364
3	1	-0.0000237	-0.0000001	-0.0000793	-0.0001031
3	2	-0.0000181	-0.0000003	-0.0001451	-0.0001635

**Table S.VI** Vibration-rotation interaction constants obtained at CCSD(T, fc)/cc-pVQZ

AXIS	MODE	VIB-ROT CONSTANT / (cm-1)			TOTAL
		CORIOLIS	QUADRATIC	ANHARMONIC	
1	6	0.0004795	-0.0038042	-0.0049480	-0.0082727
1	5	0.0017631	-0.0045878	0.0046739	0.0018491
1	9	0.0086496	-0.0000454	-0.0016696	0.0069346
1	4	-0.0054466	-0.0050193	0.0148094	0.0043436
1	8	-0.0003300	-0.0001177	0.0086881	0.0082404
1	3	0.0000112	-0.0002356	0.0043406	0.0041163
1	2	0.0052153	-0.0000096	-0.0007583	0.0044475
1	1	-0.0033605	-0.0007147	0.0080617	0.0039864
1	2	-0.0054308	-0.0000004	0.0075352	0.0021040
2	6	0.0000051	-0.0004623	0.0006892	0.0002319
2	5	0.0000541	-0.0001526	0.0011753	0.0010768
2	9	0.0001774	-0.0000015	0.0003518	0.0005276
2	4	-0.0001001	-0.0000607	0.0005313	0.0003704
2	8	0.0002171	-0.0000005	-0.0002988	-0.0000821
2	3	-0.0000541	-0.0000114	0.0000661	0.0000006
2	2	-0.0001527	-0.0000004	0.0001942	0.0000411
2	1	-0.0000584	-0.0000009	-0.0000421	-0.0001014
2	2	-0.0000654	-0.0000003	-0.0001419	-0.0002075
3	6	0.0001326	-0.0002486	0.0004944	0.0003783
3	5	0.0001455	-0.0000641	0.0010353	0.0011168
3	9	0.0002866	-0.0000070	0.0003415	0.0006211
3	4	-0.0002501	-0.0000285	0.0006535	0.0003749
3	8	-0.0002640	-0.0000149	-0.0000670	-0.0003459
3	3	0.0006365	0.0000000	0.0001447	0.0007812
3	2	-0.0006164	-0.0000012	0.0001440	-0.0004737
3	1	-0.0000242	-0.0000001	-0.0000846	-0.0001090
3	2	-0.0000184	-0.0000003	-0.0001471	-0.0001658



**Table S.VII** Vibration-rotation interaction constants obtained at CCSD(T, fc)/cc-pCVTZ

AXIS	MODE	VIB-ROT CONSTANT / (cm-1)			TOTAL
		CORIOLIS	QUADRATIC	ANHARMONIC	
1	6	0.0004820	-0.0038059	-0.0050175	-0.0083414
1	5	0.0017926	-0.0046918	0.0047211	0.0018220
1	9	0.0076746	-0.0000465	-0.0016467	0.0059815
1	4	-0.0043979	-0.0049598	0.0147922	0.0054346
1	8	-0.0004361	-0.0001165	0.0086470	0.0080944
1	3	0.0000263	-0.0002218	0.0041473	0.0039517
1	2	0.0052576	-0.0000083	-0.0007890	0.0044602
1	1	-0.0033730	-0.0007196	0.0081286	0.0040359
1	2	-0.0054752	-0.0000004	0.0076294	0.0021539
2	6	0.0000050	-0.0004597	0.0006976	0.0002429
2	5	0.0000523	-0.0001512	0.0011688	0.0010699
2	9	0.0001610	-0.0000015	0.0003598	0.0005192
2	4	-0.0000796	-0.0000610	0.0005280	0.0003874
2	8	0.0002167	-0.0000005	-0.0002867	-0.0000705
2	3	-0.0000606	-0.0000110	0.0000901	0.0000186
2	2	-0.0001491	-0.0000005	0.0001972	0.0000476
2	1	-0.0000580	-0.0000009	-0.0000399	-0.0000988
2	2	-0.0000650	-0.0000003	-0.0001421	-0.0002074
3	6	0.0001313	-0.0002480	0.0005013	0.0003846
3	5	0.0001383	-0.0000644	0.0010311	0.0011050
3	9	0.0002799	-0.0000071	0.0003481	0.0006209
3	4	-0.0002421	-0.0000277	0.0006493	0.0003795
3	8	-0.0002572	-0.0000147	-0.0000594	-0.0003313
3	3	0.0006222	0.0000000	0.0001602	0.0007825
3	2	-0.0006014	-0.0000012	0.0001473	-0.0004553
3	1	-0.0000243	-0.0000001	-0.0000824	-0.0001068
3	2	-0.0000184	-0.0000003	-0.0001463	-0.0001651

**Table S.VIII** Vibration-rotation interaction constants obtained at CCSD(T, all)/cc-pCVTZ

AXIS	MODE	VIB-ROT CONSTANT / (cm-1)			TOTAL
		CORIOLIS	QUADRATIC	ANHARMONIC	
1	6	0.0004849	-0.0038202	-0.0050261	-0.0083614
1	5	0.0018123	-0.0047074	0.0047336	0.0018385
1	9	0.0076875	-0.0000464	-0.0016744	0.0059667
1	4	-0.0044184	-0.0049704	0.0148545	0.0054657
1	8	-0.0004285	-0.0001172	0.0086699	0.0081242
1	3	0.0000259	-0.0002231	0.0041600	0.0039628
1	2	0.0052757	-0.0000084	-0.0007951	0.0044722
1	1	-0.0033811	-0.0007229	0.0081578	0.0040538
1	2	-0.0055013	-0.0000004	0.0076577	0.0021560
2	6	0.0000050	-0.0004608	0.0006984	0.0002426
2	5	0.0000527	-0.0001515	0.0011716	0.0010728
2	9	0.0001617	-0.0000015	0.0003601	0.0005203
2	4	-0.0000803	-0.0000613	0.0005310	0.0003894
2	8	0.0002193	-0.0000005	-0.0002875	-0.0000687
2	3	-0.0000613	-0.0000111	0.0000888	0.0000164
2	2	-0.0001509	-0.0000005	0.0001971	0.0000457
2	1	-0.0000582	-0.0000009	-0.0000398	-0.0000989
2	2	-0.0000653	-0.0000003	-0.0001410	-0.0002066
3	6	0.0001317	-0.0002485	0.0005018	0.0003851
3	5	0.0001394	-0.0000647	0.0010335	0.0011083
3	9	0.0002802	-0.0000071	0.0003483	0.0006214
3	4	-0.0002436	-0.0000278	0.0006526	0.0003813
3	8	-0.0002574	-0.0000148	-0.0000596	-0.0003318
3	3	0.0006269	0.0000000	0.0001594	0.0007863
3	2	-0.0006059	-0.0000012	0.0001471	-0.0004600
3	1	-0.0000244	-0.0000001	-0.0000824	-0.0001070
3	2	-0.0000185	-0.0000003	-0.0001456	-0.0001645

**Table S.IX** Relevant Coriolis zeta parameters calculated at CCSD(T, fc)/cc-pVTZ

AXIS IXYZ = 1			AXIS IXYZ = 2			AXIS IXYZ = 3		
Mode	Mode		Mode	Mode		Mode	Mode	
9	6	-0.1514069691	9	6	0.0273250867	5	6	0.4179692900
9	5	0.2230344525	9	5	0.2794872128	3	6	0.5181496698
4	9	0.2712049037	4	9	-0.2694461085	3	5	-0.7390610873
8	6	-0.0762665744	8	6	-0.1294131901	8	9	0.7638030029
8	5	0.0848954585	8	5	0.1361463837	3	6	-0.1201681467
8	4	-0.1824742238	8	4	0.1752049031	3	5	0.0267860316
3	9	0.0283308217	3	9	-0.3464402926	3	4	0.0777610100
3	8	0.0099013600	3	8	-0.2640890117	2	6	-0.0509073344
2	9	-0.0181092187	2	9	-0.3225510683	2	5	0.0056433779
2	8	-0.1006972682	2	8	0.4509035457	2	4	-0.0469441478
1	9	-0.7817592984	1	9	-0.4377085744	2	3	-0.8183557206
1	8	-0.4395112754	1	8	0.6957255389	1	6	0.0334270204
7	6	-0.0034796050	7	6	0.0458482609	1	5	-0.0010706045
7	5	0.0560361492	7	5	0.0102919601	1	4	0.0714910001
7	4	-0.0197255993	7	4	0.1054910912	1	3	0.5424829577
7	3	0.1000507755	7	3	0.8469777030	1	2	0.1198172549
7	2	-0.9886181678	7	2	0.0426188754	7	9	-0.1986545460
7	1	0.0528686981	7	1	0.0012510264	7	8	0.4733885638

**Table S.X** Relevant Coriolis zeta parameters calculated at CCSD(T, fc)/aug-cc-pVTZ

AXIS IXYZ = 1			AXIS IXYZ = 2			AXIS IXYZ = 3		
Mode	Mode		Mode	Mode		Mode	Mode	
9	6	-0.1528675542	9	6	0.0242628742	5	6	0.4233679620
9	5	0.2214384874	9	5	0.2862297406	3	6	0.5138817217
4	9	0.2767024628	4	9	-0.2758206528	3	5	-0.7375321409
8	6	-0.0725934001	8	6	-0.1308509178	8	9	0.7657170872
8	5	0.0773187406	8	5	0.1312629794	3	6	-0.1291451966
8	4	-0.1758188458	8	4	0.1640180639	3	5	0.0344661712
3	9	0.0293129050	3	9	-0.3639243460	3	4	0.0796180605
3	8	0.0041720091	3	8	-0.2258283692	2	6	-0.0492446553
2	9	-0.0223907061	2	9	-0.2861349274	2	5	0.0078214882
2	8	-0.1053307206	2	8	0.4707934689	2	4	-0.0594464382
1	9	-0.7918607973	1	9	-0.4246691735	2	3	-0.8192577491
1	8	-0.4221517365	1	8	0.7066206180	1	6	0.0324795340
7	6	-0.0039057486	7	6	0.0446202333	1	5	0.0021701468
7	5	0.0551435041	7	5	0.0155825545	1	4	0.0772008500
7	4	-0.0312265008	7	4	0.1131661385	1	3	0.5441700214
7	3	0.0421708963	7	3	0.8488970737	1	2	0.0904548966
7	2	-0.9922748819	7	2	-0.0096849169	7	9	-0.1839905543
7	1	0.0519604102	9	1	0.0015568157	7	8	0.4764689173

**Table S.XI** Relevant Coriolis zeta parameters calculated at CCSD(T, fc)/cc-pVQZ

AXIS IXYZ = 1			AXIS IXYZ = 2			AXIS IXYZ = 3		
Mode	Mode		Mode	Mode		Mode	Mode	
9	6	-0.1523582252	9	6	0.0258718945	5	6	0.4220794245
9	5	0.2216543495	9	5	0.2828275982	3	6	0.5158489911
4	9	0.2745104559	4	9	-0.2733509095	3	5	-0.7372986603
8	6	-0.0749743928	8	6	-0.1307334939	8	9	0.7643064026
8	5	0.0812914966	8	5	0.1346404129	3	6	-0.1250846536
8	4	-0.1802420111	8	4	0.1701567017	3	5	0.0316604904
3	9	0.0288463341	3	9	-0.3523853019	3	4	0.0819636767
3	8	0.0077561118	3	8	-0.2496319306	2	6	-0.0517108913
2	9	-0.0209719554	2	9	-0.3082573013	2	5	0.0096661177
2	8	-0.1041173827	2	8	0.4598787165	2	4	-0.0539834126
1	9	-0.7853361787	1	9	-0.4332234507	2	3	-0.8177440302
1	8	-0.4327252161	1	8	0.6990753885	1	6	0.0329084396
7	6	-0.0041335237	7	6	0.0449893329	1	5	-0.0002133760
7	5	0.0560619665	7	5	0.0120988196	1	4	0.0761233489
7	4	-0.0275748142	7	4	0.1115555038	1	3	0.5436044222
7	3	0.0778943995	7	3	0.8476996209	1	2	0.1095552873
7	2	-0.9902283948	7	2	0.0217610583	7	9	-0.1926672020
7	1	0.0532165965	7	1	0.0021379529	7	8	0.4749165699

**Table S.XII** Relevant Coriolis zeta parameters calculated at CCSD(T, fc)/cc-pCVTZ

AXIS IXYZ = 1			AXIS IXYZ = 2			AXIS IXYZ = 3		
Mode	Mode		Mode	Mode		Mode	Mode	
9	6	-0.1519127158	9	6	0.0273775545	5	6	0.4187393940
9	5	0.2234971643	9	5	0.2797096924	3	6	0.5183266366
4	9	0.2716606084	4	9	-0.2702501506	3	5	-0.7384716648
8	6	-0.0762010349	8	6	-0.1295107449	8	9	0.7632578686
8	5	0.0845753846	8	5	0.1354833467	3	6	-0.1201718144
8	4	-0.1819989538	8	4	0.1745326450	3	5	0.0264792936
3	9	0.0288627901	3	9	-0.3488467356	3	4	0.0790819075
3	8	0.0097793936	3	8	-0.2620459144	2	6	-0.0509065479
2	9	-0.0184061297	2	9	-0.3202293990	2	5	0.0068130822
2	8	-0.1014068835	2	8	0.4533595496	2	4	-0.0469969131
1	9	-0.7823473294	1	9	-0.4366248271	2	3	-0.8177475924
1	8	-0.4379479092	1	8	0.6958599555	1	6	0.0334443981
7	6	-0.0035931776	7	6	0.0456561938	1	5	-0.0014918574
7	5	0.0559141598	7	5	0.0099031857	1	4	0.0716123884
7	4	-0.0209889316	7	4	0.1052964726	1	3	0.5436065057
7	3	0.0957444490	7	3	0.8467859110	1	2	0.1180813356
7	2	-0.9889789407	7	2	0.0383891847	7	9	-0.1977867380
7	1	0.0528522616	7	1	0.0014972922	7	8	0.4745614757

**Table S.XIII** Relevant Coriolis zeta parameters calculated at CCSD(T, all)/cc-pCVTZ

AXIS IXYZ = 1			AXIS IXYZ = 2			AXIS IXYZ = 3		
Mode	Mode		Mode	Mode		Mode	Mode	
9	6\	-0.1557218487	9	6	0.0238718992	5	6	0.4270403845
9	5	0.2189683849	9	5	0.2820708108	3	6	0.5265259266
4	9	0.2722044541	4	9	-0.2775022446	3	5	-0.7256333453
8	6	-0.0745636550	8	6	-0.1301663489	8	9	0.7634495264
8	5	0.0771304780	8	5	0.1299150666	3	6	-0.1309898369
8	4	-0.1751511567	8	4	0.1655759167	3	5	0.0334028087
3	9	0.0283600830	3	9	-0.3534188807	3	4	0.0876970420
3	8	0.0081039254	3	8	-0.2533247799	2	6	-0.0588529244
2	9	-0.0168120696	2	9	-0.3064836144	2	5	0.0103171365
2	8	-0.1025811465	2	8	0.4592187853	2	4	-0.0574488758
1	9	-0.7912621831	1	9	-0.4277341604	2	3	-0.8175356827
1	8	-0.4272486498	1	8	0.7036383270	1	6	0.0342735538
7	6	-0.0045121938	7	6	0.0463548448	1	5	0.0025393397
7	5	0.0574686036	7	5	0.0172685327	1	4	0.0800502339
7	4	-0.0348406814	7	4	0.1165733344	1	3	0.5400308824
7	3	0.0916513752	7	3	0.8432360830	1	2	0.1159342750
7	2	-0.9890593500	7	2	0.0314119748	7	9	-0.1902866423
7	1	0.0450924686	7	1	0.0008221168	7	8	0.4818064735