Rotational and Torsional Properties of Various Monosubstituted Isotopologues of Acetone (CH_3-CO-CH_3) from Explicitly Correlated Ab Initio Methods.

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Table S. Anharmonic fundamentals of the acetone isotopologues ……..2

Table S: Anharmonic fundamentals of the acetone isotopologues (in cm^{-1})[a]

		C_{2v}				C_s			C_1
mode		CH_3-CO-CH_3		CH_3-$C^{18}O$-CH_3	CH_3-^{13}CO-CH_3		$^{13}CH_3$-CO-CH_3	CDH_2-CO-CH_3	CDH_2-CO-CH_3
ν_n		Calc.	Exp.[b]	Calc.	Calc.		Calc.	Calc.	Calc.
1	a_1	3023	3018.5	3022	3023	a'	2972	2974	3023
2		2933	2937	2934	2956		2964	2973	3011
3		1742	1731	1702	1695		1463	1453	2973
4		1417	1435	1445	1451		1432	1263	2941
5		1353	1363.5	1353	1353		1082	1064	2969
6		1061		1054	1061		882	845	2185
7		776	777	770	774		473	467	1722
8		373	385	370	371		128.8	121.3	1451
9	a_2	2972		2972	2972		79,1	75.8	1432
10		1442		1434	1432	a"	3023	3023	1414
11		887		885	886		3013	2939	1358
12		78.6		79.1	79.1		2933	2974	1266
13	b_1	2974	2972	2974	2973		2919	2223	1266
14		1447	1454	1446	1464		1758	1754	1205
15		1086	1090.5	1085	1073		1438	1433	1060
16		473	484	470	464		1447	1414	1035
17		128.9	125.16[c]	128.4	128.8		1358	1358	873
18	b_2	3023	3018.5	3023	3023		1345	1287	771
19		2936	2937	2934	2935		1216	1174	753
20		1444	1410	1439	1438		1056	996	526
21		1361	1363.5	1361	1358		898	863	455
22		1218	1215.5	1216	1192		767	743	357
23		903	891	904	900		527	502	117.5
24		529	530	514	527		370	360	71.5