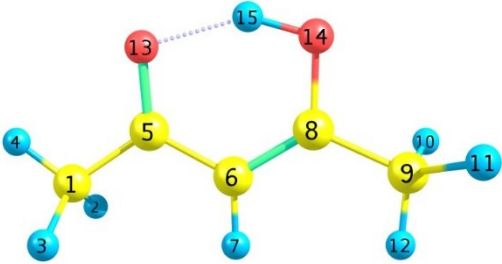


## SUPPLEMENTARY INFORMATION

Optimized geometry parameters for CCC conformer of double deuterated acetylacetone, obtained with B3LYP functional and 6-311++g(3df,3pd) basis set. Distance (R), angle (A) and dihedral angle (D).

Atoms involved	Parameter	Value
CH <sub>3</sub> -C	R(1-5)	1.51
C-C	R(5-6)	1.44
C=O	R(5-13)	1.24
C-H	R(6-7)	1.08
C=C	R(6-8)	1.37
C-CH <sub>3</sub>	R(8-9)	1.49
C-O	R(8-14)	1.32
O··H	R(13-15)	1.61
O-H	R(14-15)	1.00
C-C-CH <sub>3</sub>	A(1-5-6)	118.61
C-C=O	A(6-5-13)	121.57
C-C-H	A(5-6-7)	119.86
HOC-C-CO	A(5-6-8)	120.71
H-C-COH	A(7-6-8)	119.43
C-C-CH <sub>3</sub>	A(6-8-9)	124.25
C-C-OH	A(6-8-14)	121.74
C-O-H	A(8-14-15)	106.00
H-C-CO-C	D(4-1-5-6)	180.00
C-CO-C-H	D(1-5-6-7)	0
C-CO-C-COH	D(1-5-6-8)	180
O=C-C-COH	D(13-5-6-8)	0
OC-C-COH-C	D(5-6-8-9)	180
OC-C-C-OH	D(5-6-8-14)	0
C-COH-C-H	D(6-8-9-12)	0
C-C-O-H	D(6-8-14-15)	0



**R:** distance; **A:** angle; **D:** dihedral angle

Theoretical frequency values (and corresponding intensities: **Int**) of double deuterated acetylacetone (AcAcD<sub>2</sub>) calculated in the harmonic (**Harm**) and anharmonic (**Anharm**) approximations, with B3LYP functional and 6-311++g(3df,3pd) basis set.

CCC			CCT		
Harm	Anharm	Int	Harm	Anharm	Int
3142.9	3003.2	9.6	3141.2	2996.6	12.1
3137.9	2998.7	9.5	3135.9	2995.9	7.6
3090.2	2949.3	4.8	3079.2	2940.1	11.0
3088.0	2954.3	6.5	3061.5	2922.1	9.7
3038.2	2928.5	7.8	3025.8	2946.4	5.4
3034.0	2951.5	2.6	3015.2	2966.0	23.5
2373.8	2297.0	1.3	2779.7	2680.7	50.7
2200.1	1857.1	259.2	2353.6	2276.1	3.1
1663.3	1616.5	262.7	1749.4	1713.2	192.5
1560.3	1515.2	374.1	1653.1	1614.0	427.4
1477.1	1445.9	6.8	1481.6	1451.5	5.6
1476.3	1436.7	86.6	1480.8	1453.3	24.1
1472.3	1433.6	9.1	1477.5	1440.0	9.8
1464.7	1432.6	38.9	1467.5	1436.7	14.9
1418.5	1390.5	27.9	1415.4	1401.1	12.2
1403.5	1368.0	11.3	1382.4	1349.2	27.0
1384.9	1354.1	53.9	1346.0	1313.2	75.1
1303.1	1270.3	125.9	1240.5	1197.1	216.3
1120.2	1076.0	52.3	1090.1	1064.5	6.8
1062.2	1035.5	1.2	1063.2	1037.7	0.6
1047.4	1027.4	34.3	1037.9	1015.7	5.0
1047.1	1020.9	6.6	1008.7	990.4	9.0
1009.4	991.5	9.7	930.4	919.5	28.2
945.7	933.4	24.5	927.0	911.4	14.9
891.9	881.8	16.5	870.5	860.7	58.4
847.7	837.1	0.5	854.5	841.6	16.3
749.7	740.9	38.0	675.0	664.8	8.4
661.0	646.9	0.6	625.9	612.1	13.3
641.5	629.4	14.2	583.8	575.1	5.0
570.5	562.6	16.2	535.9	530.8	0.9
558.4	555.9	0.2	467.1	468.1	15.8
504.7	502.9	10.5	371.4	370.7	4.7
390.6	391.8	2.7	336.9	338.5	0.4
365.7	358.0	7.2	316.6	297.8	42.9
228.1	222.3	3.3	188.6	176.7	2.3
180.5	167.4	0.1	171.4	174.1	3.5
148.4	125.9	0.0	139.0	136.7	2.3
118.2	92.5	1.2	103.8	100.8	0.3
27.9	-92.1	0.1	59.4	56.4	3.8

CTC		
Harm	Anharm	Int
3176.7	3030.2	6.1
3143.4	3002.3	10.6
3081.9	2940.2	10.3
3081.1	2940.5	6.0
3034.5	2935.5	16.1
3027.6	2945.7	4.5
2758.8	2672.1	28.8
2309.9	2227.6	11.8
1734.6	1701.4	169.6
1628.0	1566.1	544.9
1492.7	1451.0	7.5
1477.9	1438.8	8.4
1467.3	1435.8	12.4
1458.7	1418.0	80.3
1411.0	1378.4	48.6
1384.4	1352.1	30.5
1322.2	1288.8	122.2
1289.9	1249.6	15.6
1106.2	1079.6	62.5
1069.9	1043.6	1.6
1039.1	1018.4	2.7
1022.0	999.1	30.0
960.3	934.5	145.0
902.0	886.1	14.2
861.8	848.6	20.5
823.3	808.5	0.8
705.3	699.3	19.9
629.9	618.3	37.8
585.1	588.7	0.3
491.0	492.9	2.2
469.0	471.7	11.7
384.3	381.8	3.3
373.1	350.4	48.2
339.7	345.8	1.7
210.7	228.6	3.1
164.9	160.9	0.2
106.2	91.4	1.3
98.7	109.9	0.1
57.2	59.4	1.5

CTT		
Harm	Anharm	Int
3160.0	3019.8	10.8
3142.9	3001.5	11.4
3082.1	2942.0	9.0
3058.6	2920.6	10.4
3028.5	2946.4	3.6
3012.0	2925.0	32.3
2780.2	2684.0	53.4
2343.8	2264.7	4.3
1732.2	1694.4	171.4
1649.0	1603.3	480.5
1501.6	1448.2	7.4
1476.8	1439.0	8.2
1467.0	1434.9	13.0
1459.7	1427.7	41.3
1405.5	1373.0	46.1
1384.9	1352.7	33.7
1309.9	1275.3	251.1
1290.2	1258.9	17.0
1100.7	1078.2	17.7
1070.4	1043.6	1.2
1039.1	1017.2	3.2
1019.5	994.6	35.0
954.0	936.6	63.6
916.1	901.1	112.5
850.2	837.7	5.1
819.5	812.8	1.2
720.4	707.1	12.0
630.3	621.8	36.3
584.4	579.9	0.3
493.1	489.0	2.8
457.0	456.9	4.7
393.2	390.5	1.1
341.9	345.4	2.2
299.6	290.6	50.5
212.2	210.6	10.8
167.4	162.4	0.1
133.1	112.9	0.1
101.9	101.1	0.1
62.7	56.9	8.9

TCC		
Harm	Anharm	Int
3145.3	3008.2	7.2
3134.5	2995.8	5.5
3084.9	2943.3	6.4
3063.5	2896.6	7.2
3036.1	2964.9	11.4
3005.0	2905.5	8.9
2767.4	2661.9	51.9
2359.2	2279.1	0.7
1716.4	1686.3	232.3
1648.4	1614.0	397.3
1495.6	1486.7	10.1
1486.4	1471.2	11.5
1479.3	1451.2	35.9
1473.6	1433.5	7.7
1421.2	1407.8	33.1
1377.7	1342.4	67.1
1353.7	1319.2	101.3
1234.5	1202.8	67.6
1116.8	1093.3	41.3
1065.4	1039.6	0.8
1038.3	1014.5	4.8
1010.9	990.3	55.2
989.7	970.3	17.8
939.2	903.8	40.5
832.0	818.6	2.7
768.9	750.5	2.4
702.1	687.1	12.6
590.8	585.2	2.8
585.7	574.7	0.0
534.8	527.7	0.0
525.7	521.4	17.3
381.2	380.2	3.5
368.0	347.7	37.8
339.2	334.0	2.5
245.2	220.6	1.6
211.0	204.1	2.9
178.2	163.5	2.8
135.5	128.6	0.2
71.0	56.8	3.4

TCT		
Harm	Anharm	Int
3142.4	3002.5	12.6
3139.1	2999.5	5.6
3100.2	2963.2	7.2
3058.7	2960.2	10.4
3042.2	2947.4	2.9
3013.4	2918.1	24.4
2790.4	2689.2	56.4
2360.9	2282.4	1.3
1717.0	1685.3	174.8
1682.2	1646.3	363.0
1482.0	1453.6	9.1
1480.6	1449.9	11.0
1475.8	1443.0	8.2
1462.1	1424.2	22.0
1418.0	1401.2	23.3
1394.2	1360.3	47.7
1339.8	1303.9	126.1
1232.3	1200.4	117.8
1115.0	1092.3	36.3
1064.8	1039.9	0.1
1045.4	1023.9	5.5
1012.1	993.2	44.4
982.8	964.6	3.4
921.0	908.7	25.3
861.6	853.1	47.1
777.9	764.0	5.1
705.1	693.7	12.1
582.2	580.5	12.4
571.7	561.8	3.4
531.7	526.7	0.5
518.0	514.2	6.7
374.7	375.3	2.9
340.9	337.6	0.6
278.7	275.2	42.2
197.9	193.5	3.7
193.0	178.8	3.7
176.6	161.7	0.0
142.2	141.0	2.0
66.5	61.4	3.9

TTC		
Harm	Anharm	Int
3205.1	3059.5	2.5
3139.6	2999.9	10.4
3097.6	2963.0	7.6
3086.2	2935.2	5.3
3042.8	2924.9	11.8
3036.6	2937.5	5.5
2761.6	2663.7	32.5
2307.3	2228.6	8.1
1706.3	1672.7	194.1
1655.6	1609.4	417.1
1494.8	1445.7	1.5
1486.8	1448.1	46.7
1473.9	1432.8	13.8
1468.6	1428.2	2.7
1420.3	1386.3	23.3
1388.1	1354.2	31.5
1326.5	1298.0	169.8
1272.4	1238.8	16.4
1135.5	1109.7	137.3
1063.8	1037.7	1.3
1044.0	1021.4	2.7
1022.0	1003.0	4.1
997.9	980.1	73.7
910.7	887.2	48.1
824.5	812.7	0.5
772.5	758.1	3.2
731.5	712.8	19.8
584.3	576.5	0.0
578.2	577.3	19.2
540.0	536.9	0.4
483.6	476.8	2.4
395.2	392.9	10.0
369.7	351.9	49.2
321.0	323.8	5.8
230.5	239.1	0.9
226.3	231.0	6.8
173.9	168.1	0.6
82.0	71.5	0.1
49.1	45.6	3.9

TTT		
Harm	Anharm	Int
3198.2	3055.0	2.1
3138.6	2996.9	10.4
3094.9	2960.3	9.0
3060.1	2922.2	8.6
3034.2	2936.7	7.5
3017.8	2904.1	24.4
2788.9	2695.5	57.5
2342.3	2265.3	2.1
1707.9	1671.1	168.0
1677.2	1638.0	398.5
1500.6	1461.8	0.2
1488.5	1458.1	26.7
1479.4	1437.7	14.9
1470.1	1428.7	3.2
1416.9	1400.9	17.3
1386.1	1352.2	34.1
1312.7	1276.9	272.8
1268.4	1234.7	38.9
1123.7	1101.1	28.3
1062.9	1037.4	0.9
1042.6	1021.8	3.1
1020.0	1002.6	3.3
990.8	976.6	99.2
919.2	906.0	51.9
815.9	807.2	3.5
764.8	751.6	1.4
747.7	731.7	13.1
579.6	577.1	26.7
577.8	573.4	1.3
525.7	530.8	11.7
486.6	481.7	2.3
402.7	399.1	2.1
321.8	326.5	6.7
260.0	257.3	49.8
236.6	232.9	0.7
227.3	220.2	0.5
180.3	179.5	0.0
110.3	127.6	0.4
48.3	52.6	0.2

<b>Keto</b>		
<b>Harm</b>	<b>Anharm</b>	<b>Int</b>
3145.4	3000.6	6.2
3145.2	3000.5	8.8
3086.7	2948.7	4.5
3086.5	2948.4	0.1
3030.6	2923.9	0.7
3030.5	2926.9	2.3
2333.5	2255.1	2.1
2230.7	2199.2	0.8
1793.8	1753.0	22.0
1766.2	1735.1	391.2
1474.5	1434.2	17.7
1473.6	1429.9	1.0
1466.5	1427.3	1.3
1466.2	1424.8	29.5
1390.0	1354.2	3.4
1389.8	1356.5	77.2
1230.0	1189.8	27.9
1186.8	1150.0	261.5
1090.8	1082.7	1.8
1082.1	1057.7	8.7
1077.8	1054.2	0.2
1018.2	1000.5	35.3
1008.0	992.8	1.6
942.3	923.1	16.0
797.2	783.0	0.0
795.0	783.4	4.6
758.3	741.1	0.3
740.5	726.1	12.7
627.8	621.5	1.4
520.7	518.8	19.0
492.7	490.6	6.1
479.2	476.2	5.8
358.3	363.7	1.7
318.5	328.3	0.9
162.4	150.8	0.0
161.7	147.4	0.1
142.5	144.1	1.0
56.9	54.4	8.5
46.5	42.7	11.5

Theoretical frequency values (and corresponding intensities: **Int**) of monodeuterated acetylacetonone (AcAcCD) calculated in the harmonic (**Harm**) and anharmonic (**Anharm**) approximations, with B3LYP functional and 6-311++g(3df,3pd) basis set.

CCC			CCT		
Harm	Anharm	Int	Harm	Anharm	Int
3143.0	3004.2	12.2	3817.6	3630.2	79.0
3138.0	2997.3	9.5	3141.2	2997.3	12.1
3090.2	2947.0	4.8	3135.89	2994.3	7.6
3088.0	2958.6	6.5	3079.2	2940.1	11.0
3038.3	2941.3	17.7	3061.6	2922.1	9.8
3034.3	2934.9	5.3	3025.8	2947.2	5.3
3006.5	2351.4	359.2	3015.2	2966.7	22.7
2373.8	2296.2	0.8	2353.6	2272.5	3.1
1665.7	1608.6	355.3	1751.8	1715.3	174.7
1645.8	1603.9	282.7	1667.9	1623.7	415.7
1479.6	1446.9	38.0	1481.9	1458.2	14.5
1477.1	1447.4	6.7	1481.7	1451.8	5.3
1472.3	1429.1	9.6	1477.5	1440.3	9.7
1466.8	1427.8	20.6	1467.6	1438.0	15.6
1437.4	1397.8	179.8	1415.5	1401.4	10.4
1410.9	1365.8	35.2	1382.9	1349.7	37.9
1386.2	1358.9	45.3	1347.2	1314.4	59.0
1372.5	1289.1	72.6	1300.3	1263.1	287.6
1268.4	1232.1	134.8	1195.3	1165.8	71.2
1064.6	1041.4	6.0	1063.2	1038.1	0.5
1062.3	1039.0	0.7	1057.8	1037.2	3.4
1047.1	1024.3	7.9	1038.0	1015.5	4.9
1019.1	1001.4	9.6	1008.8	991.3	10.5
1006.0	986.2	69.9	927.7	910.9	16.4
947.8	933.0	13.6	875.3	863.1	57.7
911.0	907.3	32.4	855.7	841.4	10.6
848.7	838.9	0.9	675.5	666.5	6.2
671.4	671.0	4.4	631.9	620.9	12.0
647.0	635.6	12.5	591.9	582.3	17.1
579.2	575.5	11.3	537.5	532.4	2.7
558.7	557.2	0.0	483.6	482.9	15.6
512.9	511.1	11.2	415.7	383.7	78.0
391.4	398.9	2.5	372.1	369.7	4.8
373.4	362.9	7.1	340.8	340.6	0.3
231.5	227.7	3.3	191.4	178.6	1.5
180.7	174.3	0.0	173.3	173.6	3.6
148.6	146.3	0.0	139.2	137.2	2.1
118.2	126.9	1.2	103.9	100.2	0.3
27.9	-9.1	0.1	60.4	56.9	3.7

CTC		
Harm	Anharm	Int
3790.9	3620.1	43.6
3176.7	3030.1	6.1
3143.4	3002.4	10.6
3081.9	2940.3	10.3
3081.1	2940.6	6.0
3034.5	2938.9	16.2
3027.6	2946.2	4.5
2310.0	2227.2	11.7
1735.8	1700.0	166.3
1634.6	1574.7	571.7
1492.8	1450.9	7.8
1477.9	1440.3	8.4
1467.3	1434.5	12.4
1459.1	1417.2	74.1
1417.1	1381.7	55.6
1385.6	1351.7	42.8
1371.8	1338.7	16.0
1291.7	1252.9	28.2
1189.9	1146.0	229.9
1070.0	1043.4	1.2
1068.7	1040.1	15.5
1039.1	1018.3	2.7
1023.0	1006.2	33.9
948.1	927.1	90.3
864.3	844.9	11.9
827.3	813.3	4.0
707.9	700.1	29.1
631.1	619.5	39.5
588.7	592.0	4.4
499.2	473.8	61.7
489.8	488.2	21.3
480.7	484.7	12.1
396.3	393.4	1.6
340.3	346.5	1.7
212.6	228.0	3.2
166.9	162.6	0.4
106.2	90.4	1.3
98.7	107.1	0.1
57.6	59.6	1.5

CTT		
Harm	Anharm	Int
3818.6	3635.6	83.7
3160.0	3020.4	10.4
3142.9	3001.8	11.5
3082.1	2942.0	9.0
3058.6	2920.7	10.5
3028.5	2947.5	3.6
3012.0	2924.0	31.0
2343.9	2262.6	4.2
1735.9	1699.4	184.6
1659.2	1616.9	399.5
1501.7	1447.3	6.9
1476.8	1441.7	8.1
1467.0	1436.1	13.1
1461.1	1425.1	21.0
1405.5	1372.6	47.6
1385.9	1353.1	56.6
1349.0	1314.0	360.8
1297.5	1261.5	37.1
1208.2	1174.9	28.4
1070.8	1049.0	36.1
1070.4	1043.6	1.2
1039.2	1017.1	3.5
1016.9	996.4	18.8
948.5	931.3	127.9
851.7	840.4	9.5
821.1	808.9	3.3
722.5	709.3	7.7
632.3	625.1	38.0
586.9	582.1	2.4
493.8	490.0	5.8
475.7	477.9	4.9
403.9	389.1	93.4
396.6	394.0	1.1
342.5	347.3	2.2
214.4	221.4	10.6
170.2	166.9	0.4
133.1	113.5	0.1
101.9	108.7	0.1
62.7	56.4	8.9



TCC		
Harm	Anharm	Int
3803.9	3606.8	86.2
3145.3	3006.5	7.3
3134.5	2995.5	5.5
3084.9	2943.3	6.3
3063.5	2898.7	7.3
3036.1	2962.6	11.2
3004.5	29630	8.9
2359.2	2275.5	0.7
1716.9	1682.3	208.7
1656.8	1618.8	442.5
1496.3	1491.8	8.7
1487.6	1472.7	9.2
1479.5	1451.7	38.4
1473.7	1433.3	8.1
1424.4	1402.9	32.2
1378.6	1344.0	40.2
1372.1	1337.2	70.5
1296.2	1264.9	78.7
1199.9	1170.4	122.9
1065.5	1040.4	0.6
1053.5	1029.3	44.6
1038.3	1014.4	4.5
1002.4	987.2	31.7
987.7	968.1	9.6
867.2	854.2	15.6
770.7	751.3	2.5
702.1	685.5	12.9
602.2	591.8	2.5
591.3	575.3	2.6
535.1	527.8	0.4
527.0	523.9	17.5
490.6	469.4	68.3
389.2	387.2	3.6
343.3	338.1	1.8
245.4	219.9	1.4
214.0	208.5	2.9
179.0	164.7	2.5
136.3	128.6	0.1
72.1	59.4	3.5

TCT		
Harm	Anharm	Int
3832.0	3642.2	89.1
3142.4	2999.2	12.6
3139.1	3001.3	5.6
3100.2	2960.4	7.2
3058.8	2918.3	10.6
3042.2	2947.7	2.8
3013.4	2965.2	23.4
2360.9	2276.2	1.2
1718.5	1684.5	114.7
1695.9	1660.6	405.8
1482.1	1451.4	8.6
1481.6	1460.4	6.5
1475.8	1443.4	8.3
1462.1	1424.4	21.3
1418.0	1401.8	22.2
1394.2	1360.4	47.9
1340.4	1304.8	140.4
1288.9	1251.2	148.3
1216.3	1188.2	90.8
1064.8	1040.7	0.1
1061.6	1041.1	7.3
1045.5	1023.0	5.2
1012.2	993.6	45.5
980.8	965.1	9.1
864.9	850.9	40.7
778.5	765.1	4.3
705.2	695.2	12.9
592.9	586.3	9.0
579.4	568.9	11.6
532.1	528.2	1.0
525.8	522.8	8.4
383.4	381.3	2.6
365.3	364.0	80.8
341.6	335.3	0.6
200.1	195.7	3.8
197.0	182.7	1.7
177.1	162.0	0.02
142.5	141.2	1.7
67.2	63.6	4.0

TTC		
Harm	Anharm	Int
3794.8	3610.3	49.7
3205.1	3059.7	2.6
3139.6	3000.7	10.4
3097.6	2963.3	7.6
3086.2	2935.2	5.3
3042.8	2925.4	11.8
3036.6	2937.5	5.5
2307.4	2229.3	7.9
1706.8	1675.4	173.8
1662.4	1617.8	460.3
1494.8	1444.5	1.4
1487.0	1448.9	45.8
1473.9	1431.1	14.2
1468.6	1427.8	2.7
1424.5	1389.7	25.2
1388.9	1355.4	33.8
1372.9	1342.0	25.8
1275.2	1242.2	2.1
1219.1	1199.3	369
1072.7	1062.0	4.3
1063.9	1037.5	1.1
1044.1	1021.9	2.7
1022.4	1004.2	3.8
998.6	984.4	71.2
829.0	816.9	3.1
773.9	759.3	1.9
733.2	714.1	26.6
588.6	578.8	3.9
581.7	581.3	20.9
545.4	541.0	0.8
494.7	466.8	86.6
482.7	474.0	1.2
409.6	405.0	10.1
323.3	326.6	6
230.7	239.5	0.7
228.2	233.2	6.5
175.3	170.0	0.9
82	72.1	0.1
49.7	48.7	3.9

TTT		
Harm	Anharm	Int
3830.0	3651.6	88.4
3198.2	3055.5	2.0
3138.6	2997.0	10.4
3094.9	2960.3	9.0
3060.1	2922.2	8.7
3034.2	2936.7	7.5
3017.8	2956.4	23.5
2342.3	2260.0	2.1
1709.1	1676.5	109.6
1687.8	1648.9	416.0
1500.6	1460.5	0.2
1489.6	1459.8	16.1
1479.5	1438.8	14.4
1470.2	1428.89	3.5
1416.9	1401.2	18.7
1386.9	1352.4	60.5
1348.1	1309.6	343.9
1269.8	1236.0	51.2
1234.8	1206.4	6.0
1075.3	1053.6	99.3
1062.9	1037.9	0.8
1042.7	1021.7	3.5
1020.5	1003.0	2.5
989.9	977.4	73.0
816.4	806.2	4.7
766.6	751.2	1.2
749.0	733.5	9.7
582.1	576.0	5.4
581.0	578.4	26.5
539.7	540.9	11.0
486.9	482.8	3.6
411.9	406.7	1.6
349.9	351.9	91.9
322.3	327.5	6.8
237.2	233.2	0.02
229.6	221.9	06
183.1	182.6	0.5
110.3	128.0	0.4
48.3	52.5	0.2

<b>Keto</b>		
<b>Harm</b>	<b>Anharm</b>	<b>Int</b>
3145.4	3000.8	6.3
3145.3	3000.7	8.7
3107.9	2970.7	4.3
3086.7	2948.7	4.3
3086.5	2948.8	0.2
3030.6	2923.6	0.7
3030.4	2923.7	2.2
2280.4	2211.4	1.3
1795.9	1772.3	21.5
1767.3	1730.49	388.9
1474.5	1430.3	17.7
1473.9	1432.7	1
1466.8	1423.7	2
1466.3	1426.8	27.8
1390.5	1356.8	5.7
1390.0	1357.7	76.2
1326.1	1294.5	19.5
1261.5	1229.0	23.5
1199.3	1164.7	162.6
1173.2	1144.5	98.3
1080.5	1056.6	0.8
1044.6	1020.7	6.1
1024.9	1006.6	26.6
975.9	956.0	4.3
888.8	874.4	17.1
821.7	809.9	4.5
772.5	756.0	2.5
750.1	734.1	9.2
628.0	618.3	1.5
534.6	533.3	22.7
496.7	494.9	3.3
483.1	479.8	6.6
381.7	388.3	1.7
320.5	329.9	0.8
162.5	151.2	0.02
161.7	148.1	0.06
142.9	144.2	1.0
56.9	54.9	8.5
47.0	44.4	11.7

Theoretical frequency values (and corresponding intensities: **Int**) of monodeuterated acetylacetone (AcAcOD) calculated in the harmonic (**Harm**) and anharmonic (**Anharm**) approximations, with B3LYP functional and 6-311++g(3df,3pd) basis set.

CCC			CCT		
Harm	Anharm	Int	Harm	Anharm	Int
3211.8	3083.3	2.9	3188.7	3063.4	6.5
3142.9	3003.3	9.5	3141.2	2996.8	11.7
3137.7	2996.2	9.1	3135.5	2992.9	6.8
3090.2	2947.6	4.8	3079.2	2940.2	11.0
3088.0	2961.8	6.5	3061.5	2922.1	9.7
3038.2	2928.5	7.8	3025.8	2946.9	5.3
3034.0	2946.4	2.5	3015.2	2878.0	23.4
2200.2	1819.3	258.7	2779.7	2680.4	50.7
1673.7	1625.5	273.2	1756.7	1720.1	190.7
1566.5	1517.1	383.6	1659.9	1621.1	429.1
1490.5	1454.2	32.1	1486.8	1464.5	13.1
1477.1	1447.7	6.6	1481.7	1451.8	5.7
1472.3	1424.4	9.3	1477.5	1440.3	9.8
1464.7	1434.0	39.0	1467.8	1437.0	12.7
1434.9	1399.8	63.6	1423.3	1392.0	55.4
1410.9	1373.4	1.7	1410.7	1380.5	2.7
1391.1	1361.4	49.6	1380.9	1348.8	42.9
1304.5	1260.7	119.1	1249.0	1212.6	196.7
1198.4	1170.2	21.0	1192.4	1167.7	48.4
1112.5	1039.3	66.3	1065.7	1039.4	1.6
1063.3	1041.8	2.1	1060.3	1039.5	7.0
1047.3	1025.0	7.0	1038.7	1017.0	5.8
1032.6	1013.7	15.7	995.2	976.8	10.8
991.3	978.9	33.1	931.5	911.5	29.6
938.5	923.3	3.6	914.1	896.6	2.9
901.9	890.5	20.3	876.8	865.8	82.6
801.8	792.9	7.9	819.5	804.6	20.0
746.6	734.1	50.1	642.5	633.7	0.1
642.7	641.1	14.4	626.8	617.7	13.6
631.7	622.3	6.5	536.2	530.6	1.2
558.7	559.0	1.1	468.5	469.6	15.7
505.3	503.3	10.4	374.4	373.9	5.0
397.1	405.3	2.8	337.5	339.7	0.4
365.8	357.9	7.2	316.8	298.4	42.3
228.8	225.7	3.3	190.0	178.1	2.6
182.3	176.3	0.1	172.1	174.8	3.6
149.4	147.7	0.0	141.0	138.1	2.3
119.4	128.0	1.2	103.8	100.8	0.3
28.0	3.4	0.1	59.9	57.6	3.7

CTC		
Harm	Anharm	Int
3176.7	3030.7	6.2
3143.5	3003.2	12.2
3129.9	3008.9	16.2
3081.9	2940.4	10.3
3081.1	2940.7	6.0
3034.5	2941.5	16.1
3027.5	2933.4	4.1
2758.7	2671.7	28.1
1742.1	1705.7	168.5
1634.7	1577.1	556.5
1492.7	1453.1	7.5
1477.9	1437.7	8.3
1469.3	1424.6	11.4
1460.6	1420.0	89.1
1434.1	1395.1	39.1
1393.5	1358.6	19.8
1382.4	1352.4	15.6
1296.7	1261.9	50.7
1187.9	1151.1	137.7
1071.3	1046.3	0.7
1056.1	1030.6	3.0
1039.8	1018.8	3.8
1009.3	986.2	40.6
959.3	940.0	131.7
895.7	864.7	33.8
837.4	825.5	2.7
837.3	826.3	32.3
631.0	619.2	38.4
598.7	605.6	0.0
538.5	537.7	0.1
472.9	479.1	12.2
385.2	383.4	3.2
373.6	351.1	49.1
340.8	349.0	1.6
211.5	229.7	3.1
170.0	167.9	0.3
106.3	91.9	1.3
98.7	110.5	0.1
57.5	59.3	1.5

CTT		
Harm	Anharm	Int
3175.2	3042.8	4.8
3160.0	3018.6	10.7
3142.9	3002.4	11.0
3082.1	2942.1	9.1
3058.6	2920.7	10.4
3028.4	2945.8	3.5
3011.9	2914.5	32.2
2780.2	2683.7	53.4
1741.4	1707.8	175.2
1654.1	1606.9	485.9
1501.6	1448.4	7.4
1476.9	1438.6	8.0
1468.0	1438.7	9.1
1460.5	1420.8	49.8
1421.5	1388.8	102.4
1389.9	1359.7	45.7
1381.2	1350.8	12.7
1293.9	1256.5	40.0
1177.0	1148.9	157.0
1071.8	1044.7	0.4
1055.1	1032.6	60.6
1040.3	1017.4	4.8
989.4	969.9	1.9
956.9	939.4	64.6
909.3	895.5	77.7
872.3	853.8	24.1
839.4	827.6	8.7
631.5	623.5	37.0
601.0	596.8	0.5
528.2	525.2	2.1
461.5	462.4	5.3
394.2	392.0	1.0
343.3	348.7	2.3
300.4	291.5	49.8
213.1	211.5	10.9
171.6	169.3	0.0
133.2	112.8	0.1
101.9	101.4	0.1
63.1	56.8	9.0

TCC		
Harm	Anharm	Int
3196.7	3064.5	2.2
3144.9	3005.2	6.8
3134.5	2995.6	5.5
3084.9	2943.3	6.4
3063.5	2898.1	7.2
3036.0	2961.4	11.4
3005.0	2953.9	8.9
2767.4	2662.4	51.8
1718.4	1686.4	258.3
1661.0	1630.2	347.3
1495.6	1487.4	10.1
1486.7	1469.0	8.0
1482.7	1453.6	24.2
1473.6	1435.3	7.8
1423.0	1402.0	48.9
1390.4	1353.7	93.9
1377.8	1342.9	42.6
1283.5	1257.7	131.4
1213.7	1187.6	7.7
1067.8	1041.7	2.1
1061.0	1039.9	15.2
1040.0	1016.3	6.1
1002.1	982.5	100.2
990.3	971.7	19.0
868.5	845.9	7.0
857.1	834.6	17.4
792.8	775.2	3.0
628.3	615.5	1.6
593.4	587.5	3.2
544.7	537.0	0.0
533.1	529.7	18.1
381.2	381.3	3.4
368.3	348.0	37.7
340.4	335.6	2.6
245.2	220.5	1.6
211.8	204.8	3.0
181.1	167.2	2.9
137.1	129.0	0.1
71.2	57.1	3.3

TCT		
Harm	Anharm	Int
3197.6	3064.0	3.1
3142.4	2999.5	12.7
3138.8	3001.7	5.3
3100.2	2960.3	7.2
3058.7	2918.2	10.4
3042.2	2948.1	2.9
3013.4	2885.1	24.3
2790.4	2689.4	56.4
1718.6	1689.1	208.6
1695.6	1658.8	309.2
1483.2	1465.8	4.1
1482.0	1449.4	9.3
1475.8	1444.9	8.2
1462.2	1423.5	25.0
1418.6	1400.1	29.4
1394.6	1360.5	48.1
1379.5	1342.1	81.3
1284.2	1255.5	140.0
1207.3	1175.7	61.2
1067.3	1042.5	1.1
1058.9	1040.0	12.7
1047.7	1026.7	7.2
1009.2	990.7	42.4
950.9	934.0	6.7
901.5	900.9	65.8
860.4	841.4	20.3
808.7	794.7	13.6
622.5	613.6	0.0
585.8	583.7	13.5
535.1	531.1	1.5
524.4	520.4	6.6
374.8	372.6	2.9
342.1	337.9	0.6
279.0	275.3	41.5
198.6	194.4	3.8
194.5	184.6	4.3
176.6	161.2	0.0
144.2	142.6	2.0
67.0	61.6	3.9

TTC		
Harm	Anharm	Int
3205.1	3060.2	2.6
3139.6	3001.5	9.9
3127.3	3001.7	14.4
3097.6	2963.2	7.6
3086.2	2935.0	5.3
3042.7	2925.4	11.7
3036.6	2937.6	5.6
2761.6	2664.6	31.9
1708.8	1677.6	217.4
1668.2	1628.4	378.5
1494.8	1448.3	1.5
1487.9	1450.0	38.4
1473.9	1432.8	14.0
1469.1	1428.0	3.0
1428.1	1393.3	24.6
1389.8	1356.7	23.3
1382.1	1351.4	23.5
1294.1	1264.0	108.7
1250.8	1221.9	208.9
1065.4	1041.3	0.3
1050.0	1026.9	2.6
1045.9	1023.9	4.9
1024.8	1005.9	4.6
960.7	949.1	128.7
878.3	852.0	30.3
867.0	843.9	5.2
789.1	774.2	2.1
588.4	580.3	0.0
582.4	580.0	20.6
545.6	543.5	0.6
532.4	525.2	0.1
395.5	395.1	10.1
370.4	352.9	50.5
321.6	324.7	5.8
230.8	237.2	0.9
227.3	232.5	6.8
178.9	172.9	0.6
82.4	70.9	0.1
49.1	44.3	3.9

TTT		
Harm	Anharm	Int
3198.2	3056.5	2.1
3174.8	3050.1	2.1
3138.6	2997.1	10.4
3094.9	2960.4	9.0
3060.1	2922.4	8.6
3034.2	2936.8	7.5
3017.8	2906.7	24.3
2788.9	2695.2	57.4
1709.4	1675.6	193.5
1689.7	1641.8	364.1
1500.6	1463.9	0.2
1489.1	1460.5	23.6
1479.5	1440.8	15.1
1470.2	1430.8	4.0
1421.6	1399.3	26.0
1387.2	1354.1	25.0
1371.7	1345.0	77.1
1290.7	1254.6	78.7
1230.2	1201.1	229.1
1064.7	1039.6	0.1
1047.9	1029.3	45.1
1045.2	1022.9	6.0
1022.9	1003.6	0.3
932.1	918.5	3.1
910.8	886.7	23.0
890.4	877.2	74.7
781.8	764.5	1.9
585.7	580.6	1.4
584.7	582.5	30.4
531.3	535.1	10.3
524.9	522.6	1.9
403.1	400.5	2.1
322.6	327.7	6.6
260.9	257.8	49.0
236.8	233.6	1.0
228.3	221.9	0.5
184.3	183.6	0.0
110.9	127.9	0.4
48.4	52.5	0.1

<b>Keto</b>		
<b>Harm</b>	<b>Anharm</b>	<b>Int</b>
3145.4	3000.8	6.3
3145.3	3000.7	8.7
3107.9	2970.7	4.3
3086.7	2948.7	4.3
3086.5	2948.8	0.2
3030.6	2923.6	0.7
3030.4	2923.7	2.2
2280.4	2211.4	1.3
1795.9	1772.3	21.5
1767.3	1730.5	388.9
1474.5	1430.3	17.7
1473.9	1432.7	1.0
1466.8	1423.7	2.0
1466.3	1426.8	27.8
1390.5	1356.8	5.7
1390.0	1357.7	76.2
1326.1	1294.5	19.5
1261.5	1229.0	23.5
1199.3	1164.7	162.6
1173.2	1144.5	98.3
1080.5	1056.6	0.8
1044.6	1020.7	6.1
1024.9	1006.6	26.6
975.9	956.0	4.3
888.8	874.4	17.1
821.7	809.9	4.5
772.5	756.0	2.5
750.1	734.1	9.2
628.0	618.3	1.5
534.6	533.3	22.7
496.7	494.9	3.3
483.1	479.8	6.6
381.7	388.3	1.7
320.5	329.9	0.8
162.5	151.2	0.0
161.7	148.1	0.1
142.9	144.2	1.0
56.9	54.9	8.5
47.0	44.4	11.7