

Supplementary Data

Photochemistry of Acetylacetone isolated in parahydrogen matrices upon 266 nm irradiation.

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Table S1 : Harmonic , anharmonic frequencies (cm-1) and harmonic intensities (km/mol) of XYZ (X,Y,Z =C or T) isomers

CCC			CCT		
Anharmonic	Harmonic	IR-Inten	Anharmonic	Harmonic	IR-Inten
-185.8	30.4	0.1	54.8	60.9	3.6
115.8	119.4	1.2	91.6	103.9	0.3
144.0	149.5	0.0	138.2	141.2	2.1
175.2	182.4	0.0	175.3	174.0	3.6
230.1	232.5	3.3	184.7	193.2	1.7
365.9	373.6	7.1	344.4	341.3	0.2
403.6	398.0	2.5	374.1	375.1	5.0
512.1	513.3	11.2	387.2	416.3	80.4
560.7	559.9	0.4	485.3	485.2	15.4
635.1	648.3	12.7	536.1	538.6	4.8
642.9	652.4	0.3	622.0	632.8	12.3
773.8	794.8	31.7	637.3	647.6	0.7
910.6	918.1	36.6	806.0	820.9	24.6
930.7	944.0	2.5	872.1	884.7	76.5
992.1	1008.6	64.9	895.9	914.2	2.7
996.4	1010.5	14.5	973.0	991.6	22.7
1014.0	1035.1	10.2	1018.2	1036.5	1.2
1022.8	1047.4	7.8	1016.4	1038.7	5.7
1178.2	1063.5	1.1	1041.5	1065.7	1.6
1171.3	1194.6	16.1	1159.8	1189.7	5.0
1239.9	1271.2	141.6	1164.0	1197.3	83.8
1298.3	1376.7	83.9	1265.6	1304.1	293.4
1357.3	1391.5	64.3	1349.0	1381.0	49.6
1372.1	1412.3	12.7	1381.4	1411.5	0.1
1421.9	1459.8	130.8	1392.8	1426.3	35.3
1431.2	1471.4	14.3	1436.0	1467.9	13.0
1434.5	1472.4	9.8	1452.2	1477.5	9.6
1429.1	1477.2	6.5	1450.1	1481.8	5.4
1456.0	1491.6	60.7	1465.3	1487.1	10.0
1608.7	1646.1	268.9	1628.2	1673.0	420.1
1624.0	1677.0	372.1	1723.3	1759.6	173.5
2361.6	3006.6	358.4	2909.2	3015.2	22.6
2918.0	3034.3	5.3	2947.1	3025.8	5.2
2928.9	3038.3	17.4	2921.4	3061.6	9.8
2965.1	3088.0	6.5	2940.4	3079.2	11.0
2947.7	3090.2	4.8	2994.0	3135.5	6.8
3035.3	3138.0	9.2	2997.7	3141.2	11.8
3003.2	3143.0	12.1	3058.3	3188.7	6.5
3094.3	3211.8	3.1	3629.7	3817.6	79.0

CTC		
Anharmonic	Harmonic	IR-Inten
56.5	58.5	1.4
83.7	98.7	0.1
95.0	105.2	1.3
170.0	171.7	0.4
226.1	213.6	3.2
347.6	341.6	1.7
395.9	396.8	1.5
486.1	485.2	12.5
469.2	496.3	79.0
535.2	545.8	9.9
593.5	599.4	0.2
623.0	632.3	40.1
819.3	838.5	38.2
831.5	844.6	10.4
932.1	950.1	70.5
967.1	987.1	15.0
1012.6	1029.6	60.5
1015.4	1039.9	3.9
1043.6	1071.4	0.5
1149.3	1180.8	214.7
1199.6	1225.0	41.5
1264.7	1300.5	30.3
1347.5	1383.4	20.4
1370.1	1398.9	24.9
1418.6	1455.5	6.6
1421.8	1461.0	95.2
1430.2	1471.7	17.8
1441.9	1477.9	8.3
1440.8	1492.7	7.9
1588.9	1640.0	580.0
1707.4	1743.4	167.9
2920.5	3027.5	4.2
2923.5	3034.5	16.1
2939.6	3081.1	6.0
2938.2	3081.9	10.3
3019.6	3130.0	15.3
3002.1	3143.5	12.1
3028.7	3176.7	6.1
3606.5	3791.0	43.8

CTT		
Anharmonic	Harmonic	IR-Inten
62.1	63.1	9.0
80.7	102.5	0.1
126.4	131.3	0.1
172.2	174.6	0.2
218.8	215.2	10.7
351.5	344.0	2.3
396.9	397.3	1.0
382.8	404.4	91.2
483.8	480.7	5.5
530.0	531.4	8.0
594.4	601.6	1.3
622.8	633.5	38.6
828.9	840.5	13.4
853.7	873.7	19.8
934.0	949.4	104.6
965.1	982.9	5.4
1007.5	1026.4	11.3
1015.7	1040.4	5.1
1044.1	1071.7	0.5
1148.1	1176.8	138.2
1200.0	1228.7	147.3
1260.6	1297.8	22.1
1350.4	1383.2	19.6
1368.7	1399.1	36.4
1397.6	1433.3	223.3
1416.8	1461.2	23.5
1424.1	1468.1	9.3
1424.5	1476.9	8.0
1450.3	1501.5	7.0
1617.1	1662.8	403.5
1710.9	1745.5	188.6
2913.9	3011.9	31.0
2919.9	3028.5	3.5
2918.0	3058.6	10.5
2939.9	3082.1	9.1
2999.1	3142.9	11.1
3019.5	3159.9	10.3
3042.4	3175.2	4.7
3629.3	3818.6	83.7

TCC		
Anharmonic	Harmonic	IR-Inten
63.3	72.6	3.5
133.6	137.9	0.1
168.6	181.9	2.4
207.2	214.9	2.9
214.3	245.9	1.4
338.6	344.8	1.9
386.9	389.3	3.6
452.9	493.7	67.3
531.0	534.6	18.3
537.7	547.2	2.0
615.6	604.4	2.9
614.4	630.8	5.2
782.1	799.3	5.0
836.3	857.5	16.4
916.0	938.0	19.6
977.8	994.3	32.4
1015.3	1036.4	28.0
1014.0	1040.0	5.6
1040.8	1067.9	1.8
1116.9	1145.1	74.9
1245.6	1278.9	123.6
1282.6	1319.5	45.2
1345.0	1378.6	63.5
1357.1	1394.9	49.6
1394.9	1427.0	47.4
1434.8	1473.7	8.3
1442.3	1482.8	25.7
2095.3	1488.3	6.6
1448.8	1496.2	8.8
1624.3	1669.2	389.3
1684.1	1718.7	237.0
2960.4	3004.5	8.9
2930.4	3036.0	11.2
2924.8	3063.5	7.3
2943.1	3084.9	6.3
2987.2	3134.6	5.5
3000.4	3145.0	6.9
3063.3	3196.8	2.2
3604.9	3803.8	86.2

TCT		
Anharmonic	Harmonic	IR-Inten
63.3	67.7	4.0
142.9	144.6	1.6
151.4	177.9	0.0
191.4	198.9	1.9
196.0	200.8	3.8
332.0	342.6	0.5
333.5	365.7	82.1
379.9	383.4	2.5
534.7	533.5	8.5
533.4	536.9	4.2
589.5	595.5	9.8
619.0	626.6	1.0
795.4	809.8	11.4
843.2	861.8	24.4
910.9	926.4	55.3
986.8	1008.3	41.9
1016.6	1035.5	0.5
1026.1	1047.6	7.1
1041.1	1067.3	1.1
1120.8	1163.0	10.6
1239.0	1277.8	141.3
1266.8	1300.8	172.0
1342.1	1380.3	65.3
1360.2	1394.6	49.7
1384.1	1418.6	28.0
1421.6	1462.3	24.1
1431.5	1475.9	8.4
1443.7	1482.1	8.8
1444.8	1483.8	2.2
1671.7	1708.8	391.4
1686.6	1719.7	111.9
2918.6	3013.3	23.3
2933.4	3042.3	2.8
2918.4	3058.7	10.6
2958.9	3100.2	7.2
3002.9	3138.8	5.2
2998.3	3142.4	12.7
3063.9	3197.6	3.1
3644.3	3832.1	89.1

TTC		
Anharmonic	Harmonic	IR-Inten
97.1	50.0	3.7
236.5	76.6	0.3
179.2	181.0	0.8
237.4	228.3	6.4
213.7	228.8	0.7
323.0	324.1	6.1
410.7	409.5	10.3
479.4	497.5	87.8
528.4	535.0	3.2
546.9	550.1	1.3
586.2	586.2	21.8
575.8	591.8	2.1
775.7	790.2	1.3
846.2	881.7	34.8
885.2	909.5	20.5
1008.5	1018.5	49.3
1010.3	1025.2	1.5
1018.9	1046.5	4.9
1040.2	1065.2	0.2
1193.1	1214.0	220.9
1225.9	1253.0	138.2
1264.3	1295.7	80.8
1347.9	1390.1	34.0
1375.5	1401.9	3.7
1408.5	1444.2	13.4
1428.9	1469.3	3.1
1413.8	1474.0	14.2
1457.7	1487.1	38.0
1446.2	1494.6	1.6
1634.0	1673.9	426.8
1683.3	1709.1	192.1
2928.0	3037.3	5.7
2938.0	3043.0	11.7
2947.7	3086.6	5.3
2957.6	3098.1	7.6
2974.3	3128.0	13.3
2990.0	3140.3	9.9
3073.0	3204.2	2.6
3607.8	3795.6	49.9

TTT		
Anharmonic	Harmonic	IR-Inten
61.6	48.4	0.1
139.5	110.9	0.4
187.1	187.3	0.3
225.9	230.6	0.6
237.8	237.6	0.0
328.3	323.2	6.7
369.8	350.4	90.9
409.8	412.3	1.6
528.7	527.0	4.8
545.9	546.2	9.1
585.5	585.8	30.5
581.4	588.3	4.5
771.0	784.5	1.1
884.9	899.9	53.9
890.5	911.9	19.5
1000.0	1017.0	4.0
1007.1	1024.7	2.4
1023.8	1045.3	6.3
1039.3	1064.7	0.0
1180.2	1210.0	219.6
1215.3	1245.2	90.3
1261.7	1297.4	70.8
1354.0	1387.2	39.4
1358.2	1394.0	125.0
1387.5	1423.7	59.2
1429.6	1470.3	4.1
1435.9	1479.5	14.6
1462.1	1489.9	14.8
1461.0	1500.6	0.2
1652.6	1699.7	426.8
1684.3	1710.6	94.2
2945.8	3017.8	23.4
2936.4	3034.2	7.5
2921.7	3060.1	8.7
2960.1	3094.9	9.0
2997.5	3138.6	10.5
3060.2	3174.8	1.9
3053.4	3198.2	2.1
3648.5	3830.0	88.5