Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information for

Rotational spectroscopy of methyl benzoylformate and methyl mandelate: Structure and internal dynamics of a model reactant and product of enantioselective reduction

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Table S1 Measured transition frequencies of methyl benzoylformate.

J'	K_a'	K_c'	J''	K_a''	K_c''	State	Frequency/MHz	Residual[a]/MHz	J'	K_a'	K_c'	J''	K_a''	K_c''	State	Frequency/MHz	Residual[a]/MHz
7	1	1	6	0	0	E	7860.1659	-0.0020	4	3	2	4	2	3	A	8516.2483	-0.0022
7	1	7	6	0	6	A	7860.2821	0.0017	5	3	3	5	2	4	A	8530.9718	-0.0012
9	3	7	9	2	7	A	7930.0969	0.0006	5	3	2	5	2	4	A	8532.6050	0.0024
8	0	8	7	0	7	E	7956.4291	0.0001	6	3	4	6	2	5	A	8556.4307	-0.0007
8	0	8	7	0	7	A	7956.4529	0.0021	6	3	3	6	2	5	A	8561.3098	0.0007
9	3	6	9	2	7	A	7982.8501	-0.0004	7	3	5	7	2	6	A	8596.3741	0.0009
3	2	2	2	1	1	A	8047.2508	0.0011	7	3	4	7	2	6	A	8608.5232	-0.0004
3	2	1	2	1	1	A	8060.7369	-0.0011	8	3	6	8	2	7	A	8654.7759	0.0002
8	3	6	8	2	6	A	8124.7617	0.0011	8	1	8	7	0	7	E	8661.6969	-0.0028
8	2	7	7	2	6	A	8127.7282	0.0014	8	1	8	7	0	7	A	8661.8024	0.0018
8	2	7	7	2	6	E	8127.8562	-0.0017	6	1	5	5	0	5	E	8694.4538	0.0007
8	3	5	8	2	6	A	8151.3459	-0.0002	6	1	5	5	0	5	A	8694.5918	-0.0008
9	0	9	8	1	8	A	8198.8883	0.0001	9	3	7	9	2	8	A	8735.6924	-0.0005
9	0	9	8	1	8	E	8198.9454	0.0012	9	1	9	8	1	8	E	8762.7404	-0.0051
7	3	5	7	2	5	A	8270.1568	0.0005	9	1	9	8	1	8	A	8762.7608	0.0050
3	2	2	2	1	2	A	8282.1711	0.0004	9	3	6	9	2	8	A	8788.4471	0.0000
7	3	4	7	2	5	A	8282.3070	0.0004	10	3	8	10	2	9	A	8843.1032	-0.0004
3	2	1	2	1	2	A	8295.6595	0.0005	4	2	3	3	1	3	A	9419.2816	-0.0009
8	2	6	7	2	5	A	8331.5270	0.0021	9	1	8	8	1	7	A	9441.3405	0.0001
8	2	6	7	2	5	E	8331.3473	-0.0015	9	1	8	8	1	7	E	9441.2941	-0.0042
11	1	10	10	2	9	A	8341.6678	0.0003	5	2	4	4	1	3	A	9812.5551	-0.0001
11	1	10	10	2	9	E	8342.0042	0.0009	5	2	4	4	1	3	E	9810.7841	-0.0002
6	3	4	6	2	4	A	8371.8686	0.0003	5	2	3	4	1	3	A	9905.9525	0.0012
6	3	3	6	2	4	A	8376.7472	0.0012	5	2	3	4	1	3	E	9906.9142	0.0015
8	1	7	7	1	6	E	8412.2557	-0.0018	5	2	4	4	1	4	A	10595.2149	-0.0026
8	1	7	7	1	6	A	8412.2969	0.0010	5	2	4	4	1	4	E	10593.5083	0.0024
5	3	3	5	2	3	A	8437.5753	-0.0016	6	2	5	5	1	4	A	10637.1744	0.0011
4	3	2	4	2	2	A	8475.9356	-0.0006	6	2	5	5	1	4	E	10636.0945	-0.0012
4	3	1	4	2	2	A	8476.3439	-0.0002									

[a] (Measured transition frequency) – (Fit transition frequency).

Table S2 Measured transition frequencies of methyl mandelate.

J'	K_a'	K_c'	J''	K_a''	K_c''	State	Frequency/MHz	Residual[a]/MHz	J'	K_a'	K_c'	J''	K_a''	K_c''	State	Frequency/MHz	Residual[a]/MHz
4	1	4	3	0	3	A	5196.9733	0.0012	8	0	8	7	1	7	E	8833.7166	-0.0014
4	1	4	3	0	3	E	5196.9435	-0.0011	8	1	8	7	0	7	A	9119.2604	0.0017
5	0	5	4	1	4	A	5253.1875	0.0005	8	1	8	7	0	7	E	9119.7026	-0.0034
5	0	5	4	1	4	E	5253.1213	0.0014	6	2	5	5	1	4	A	9209.9689	0.0021
2	2	1	1	1	0	A	5219.7358	-0.0032	6	2	5	5	1	4	E	9209.8040	-0.0005
2	2	1	1	1	0	E	5216.6898	0.0024	4	3	2	3	2	1	A	9561.4501	-0.0001
2	2	0	1	1	1	A	5339.7549	-0.0016	4	3	2	3	2	1	E	9553.2229	0.0012
2	2	0	1	1	1	E	5342.6063	0.0017	4	3	1	3	2	2	A	9611.9260	-0.0008
5	1	5	4	0	4	A	6165.2663	0.0005	4	3	1	3	2	2	E	9619.8103	0.0041
5	1	5	4	0	4	E	6165.2663	-0.0015	5	2	3	4	1	4	A	9702.4646	0.0063
3	2	2	2	1	1	A	6299.4807	-0.0007	5	2	3	4	1	4	E	9702.4092	-0.0059
3	2	2	2	1	1	E	6298.6146	0.0028	9	0	9	8	1	8	A	9967.6682	0.0007
6	0	6	5	1	5	A	6481.3487	-0.0004	9	0	9	8	1	8	E	9966.5658	-0.0030
6	0	6	5	1	5	E	6481.2132	0.0014	7	2	6	6	1	5	A	10086.2131	0.0021
3	2	1	2	1	2	A	6678.0294	-0.0004	7	2	6	6	1	5	E	10086.0824	-0.0018
5	4	2	5	3	3	A	6731.2718	-0.0012	9	1	9	8	0	8	A	10145.6502	0.0015
5	4	2	5	3	3	E	6723.5701	0.0000	9	1	9	8	0	8	E	10146.6394	-0.0015
6	4	3	6	3	4	A	6724.1992	0.0000	5	3	3	4	2	2	A	10695.8347	0.0002
6	4	3	6	3	4	E	6714.4117	-0.0001	5	3	3	4	2	2	E	10691.1093	0.0007
8	4	5	8	3	6	A	6724.2355	-0.0025	5	3	2	4	2	3	A	10847.6687	-0.0007
8	4	5	8	3	6	E	6716.8538	0.0029	8	2	7	7	1	6	E	10932.5936	-0.0030
6	1	6	5	0	5	A	7132.7007	0.0005	8	2	7	7	1	6	A	10932.6978	0.0028
6	1	6	5	0	5	E	7132.7598	-0.0016	10	0	10	9	1	9	A	11081.7797	0.0012
4	2	3	3	1	2	A	7322.7624	0.0004	10	1	10	9	0	9	A	11189.9467	0.0012
4	2	3	3	1	2	E	7322.3922	0.0019	6	2	4	5	1	5	A	11437.2085	-0.0049
7	0	7	6	1	6	A	7674.3142	0.0004	6	2	4	5	1	5	E	11437.0776	0.0033
7	0	7	6	1	6	E	7674.0417	-0.0001	4	4	0	3	3	1	A	11516.4705	-0.0006
7	1	7	6	0	6	A	8114.9046	0.0015	9	2	8	8	1	7	A	11766.5481	0.0058
7	1	7	6	0	6	E	8115.0852	-0.0034	9	2	8	8	1	7	E	11766.4684	-0.0067
4	2	2	3	1	3	A	8123.2361	-0.0017	6	3	4	5	2	3	A	11774.7555	0.0013
4	2	2	3	1	3	E	8123.3691	0.0020	6	3	3	5	2	4	A	12125.5744	-0.0014
8	1	7	7	2	6	A	8191.0471	0.0062	11	0	11	10	1	10	A	12182.7847	-0.0001
8	1	7	7	2	6	E	8191.0097	-0.0057	11	1	11	10	0	10	A	12247.1461	0.0008
5	2	4	4	1	3	A	8291.4659	-0.0006	5	4	2	4	3	1	A	12706.6799	-0.0006
5	2	4	4	1	3	E	8291.2423	-0.0005	5	4	1	4	3	2	A	12710.4374	-0.0014
3	3	1	2	2	0	A	8391.1103	0.0005	6	4	3	5	3	2	A	13890.7922	-0.0001
3	3	1	2	2	0	E	8379.3879	-0.0011	6	4	2	5	3	3	A	13905.9083	-0.0001
3	3	0	2	2	1	A	8401.0941	-0.0009	6	5	2	5	4	1	A	15828.8540	0.0000
8	0	8	7	1	7	A	8834.2628	0.0008	6	5	1	5	4	2	A	15829.0693	0.0011

[a] (Measured transition frequency) – (Fit transition frequency).

Fig. S1 Molecular graphs of methyl mandelate and methyl benzoylformate, showing bond and ring critical points and the H···O bond paths, at the B3LYP/6-311++G(d,p) level of theory.