Electronic Supplementary Information

Conformational equilibria and interaction preference in complex of

isoprene-maleic anhydride

Tianyue Gao, Juncheng Lei, Siyu Zou, Chenxu Wang, Xuefang Xu,* and Qian Gou*

Contents:

Table S1. The measured transition frequencies of isomer I with quantum numbers and difference to calculated frequencies Δv in the least squares fit.

Table S2. The measured transition frequencies of isomer II with quantum numbers and difference to calculated frequencies Δv in the least squares fit.

Table S3. Comparison of theoretical (with different methods) and experimental spectroscopic constants of isomersI and II.

 Table S4. CP-B2PLYP-D3(BJ)/def2-TZVP calculated geometries of isomer I.

Table S5. CP-B2PLYP-D3(BJ)/def2-TZVP calculated geometries of isomer II.

Table S6. Intensities (in arbitrary units) of isomers I and II for several selected μ_c -type transitions.

Table S7. SAPT analysis (all values in kJ mol⁻¹).

Table S8. Stabilization energy contributions (E⁽²⁾≥ 0.40 kJ mol⁻¹) for isomers I and II of ISO-MA.

Tran	sitions		
J' Ka' Kc'	<i>J" K</i> a" <i>K</i> c"	v/MHz	Δv/MHz
5 0 5	4 0 4	6755.3681	0.0009
5 1 5	4 1 4	6732.2758	0.0006
5 1 4	4 1 3	7451.2625	0.0006
6 0 6	5 0 5	8034.1955	0.0001
6 1 6	5 1 5	8025.8731	0.0008
6 1 5	5 1 4	8723.1197	-0.0003
7 0 7	6 0 6	9317.8273	-0.0087
7 1 7	6 1 6	9315.0775	0.0027
7 1 6	6 1 5	9975.5716	0.0010
8 0 8	7 0 7	10603.4651	0.0004
8 1 8	7 1 7	10602.5959	-0.0001
8 1 7	7 1 6	11239.1927	0.0001
909	8 0 8	11889.7999	0.0002
9 1 9	8 1 8	11889.5376	0.0012
3 1 2	2 0 2	5408.2937	-0.0009
3 2 2	2 1 2	5939.2868	-0.0003
3 2 1	2 1 1	5651.0802	0.0008
3 3 1	2 2 1	6518.0685	0.0029
3 3 0	2 2 0	6470.2680	0.0001
4 1 3	3 0 3	7300.4731	-0.0020
4 2 3	3 1 3	7677.8386	0.0003
4 2 2	3 1 2	7250.6856	0.0002
4 3 2	3 2 2	8084.0694	-0.0027
4 3 1	3 2 1	7898.8744	-0.0005
4 4 1	3 3 1	8798.7030	0.0006
4 4 0	3 3 0	8787.7491	-0.0080
5 1 4	4 0 4	9267.4349	-0.0014
524	4 1 4	9482.8022	0.0005
5 2 3	4 1 3	8976.9898	0.0018
5 3 3	4 2 3	9715.5997	0.0021
5 3 2	4 2 2	9336.7563	0.0008
5 4 2	4 3 2	10314.4195	0.0000
5 4 1	4 3 1	10248.0424	0.0002
5 5 1	4 4 1	11093.5960	0.0003
5 5 0	4 4 0	11091.5913	0.0003
6 1 5	5 0 5	11235.1887	-0.0005
6 2 5	5 1 5	11335.7617	-0.0005
624	514	10844.8427	0.0007

Table S1. The measured transition frequencies of isomer I with quantum numbers and difference to calculated

 frequencies Δv in the least squares fit.

6	3	4	5	2	4	11420.3041	0.0010
6	3	3	5	2	3	10866.1333	0.0006
6	4	3	5	3	3	11864.8197	0.0014
6	4	2	5	3	2	11657.7924	-0.0007
6	5	2	5	4	2	12591.6875	-0.0002
6	5	1	5	4	1	12575.2407	-0.0008
6	6	1	5	5	1	13391.7681	-0.0010
6	6	0	5	5	0	13391.4428	0.0013
7	1	6	6	0	6	13176.5649	0.0004
7	2	6	6	1	6	13217.3583	-0.0011
7	2	5	6	1	5	12822.5691	0.0006
7	3	5	6	2	5	13195.1120	0.0030
7	3	4	6	2	4	12534.5243	-0.0008
7	4	4	6	3	4	13469.8126	0.0009
7	4	3	6	3	3	13046.7801	0.0005
7	5	3	6	4	3	14100.0007	0.0004
7	5	2	6	4	2	14028.9154	0.0024
7	6	2	6	5	2	14885.7182	-0.0001
7	6	1	6	5	1	14882.3566	0.0002
7	7	1	6	6	1	15690.4400	0.0012
7	7	0	6	6	0	15690.3900	0.0012
8	1	7	7	0	7	15097.9283	0.0072
8	2	7	7	1	7	15113.0129	-0.0084
8	2	6	7	1	6	14828.7100	-0.0019
8	3	6	7	2	6	15027.0452	0.0000
8	3	5	7	2	5	14361.7584	0.0000
8	4	5	7	3	5	15143.3214	-0.0001
8	4	4	7	3	4	14502.9516	-0.0003
8	5	4	7	4	4	15634.0467	0.0000
8	5	3	7	4	3	15427.7612	-0.0007
8	6	3	7	5	3	16379.6373	-0.0021
8	6	2	7	5	2	16361.3794	0.0005
8	7	2	7	6	2	17183.8333	-0.0018
8	7	1	7	6	1	17183.2206	-0.0005
8	8	1	7	7	1	17989.0605	-0.0023
8	8	0	7	7	0	17989.0605	0.0049
9	2	7	8	1	7	16807 5098	0.0026
a	ר ג	7	8	- 2	7	16897 8777	-0 0009
٥	2	6	2 2	- 2	6	16321 5182	-0 0010
9	с л	6	0	2 2	6	16800 2002	-0.0019
9	4	C E	o o	5	U E	16000 9564	0.0007
9	4 F	5 E	ð n	3 ∧	5	17212 0240	-0.0007
9	э г	5	ō	4	د	16701 0471	0.0014
9	5	4	ŏ	4	4	10/81.84/1	0.0010

9	6	4	8	5	4	17879.2215	0.0003
9	6	3	8	5	3	17810.7984	-0.0008
9	7	3	8	6	3	18674.8140	-0.0009
9	7	2	8	6	2	18670.8342	-0.0012

Tran	Transitions		
J' Ka' Kc'	J" Ka" Kc"	v/MHz	Δv/MHz
4 0 4	3 0 3	5139.8940	-0.0027
4 1 4	3 1 3	5035.4844	-0.0033
4 1 3	3 1 2	5575.2082	0.0002
4 2 3	3 2 2	5337.8483	0.0002
4 2 2	3 2 1	5555.7719	-0.0004
4 3 2	3 3 1	5401.9456	-0.0007
4 3 1	3 3 0	5419.8782	0.0004
5 0 5	4 0 4	6331.7258	0.0016
5 1 5	4 1 4	6262.8832	0.0001
5 1 4	4 1 3	6900.3388	-0.0001
5 2 4	4 2 3	6640.3046	-0.0013
523	4 2 2	7003.7954	0.0008
5 3 3	4 3 2	6759.1725	0.0009
5 4 2	4 4 1	6754.8867	0.0011
5 4 1	4 4 0	6757.2432	-0.0015
6 0 6	5 0 5	7518.0504	-0.0002
6 1 6	5 1 5	7479.4362	-0.0001
6 1 5	5 1 4	8171.9560	-0.0009
6 2 5	524	7923.3722	-0.0001
6 2 4	5 2 3	8431.9690	0.0010
6 3 3	532	8254.4004	0.0000
6 3 4	5 3 3	8110.8022	-0.0009
6 4 3	5 4 2	8121.7624	-0.0003
6 4 2	5 4 1	8132.0870	0.0014
7 0 7	6 0 6	8708.0365	-0.0004
7 1 7	6 1 6	8688.5123	-0.0013
7 1 6	6 1 5	9389.4682	-0.0011
726	6 2 5	9186.1961	-0.0019
7 2 5	6 2 4	9821.6521	-0.0015
7 3 5	6 3 4	9450.3910	-0.0028
7 3 4	6 3 3	9723.7274	-0.0013
744	6 4 3	9493.0030	0.0020
7 4 3	6 4 2	9525.7907	0.0006
7 5 3	6 5 2	9469.1375	0.0056
7 5 2	6 5 1	9470.5453	0.0032
8 0 8	7 0 7	9902.2907	-0.0013
8 1 8	7 1 7	9893.0566	0.0031
8 1 7	7 1 6	10571.8297	0.0000

Table S2. The measured transition frequencies of isomer II with quantum numbers and difference to calculatedfrequencies Δv in the least squares fit.

8 2 7 7 2 6 10430.0849 -0.0005 8 3 6 7 2 5 11159.9243 -0.0015 8 3 5 7 3 4 11203.1132 0.0006 8 4 5 7 4 4 10864.6286 -0.0025 8 4 4 7 4 3 10947.9023 -0.0007 8 5 3 7 5 2 10847.7906 0.0024 9 0 9 8 0 8 1092.2991 0.0028 9 1 9 8 1 7 11744.4794 0.00017 9 2 7 8 2 6 12436.8436 -0.0028 10 110 9 9 1 8 12297.7205 -0.004 10 110 9 9 1 8 12297.205 -0.0021 11 110 10 1 9 1 9 12295.8845				
8 2 6 7 2 5 11159.9243 -0.0015 8 3 5 7 3 5 10772.3754 -0.0005 8 4 5 7 4 4 10864.6286 -0.0025 8 4 4 7 4 3 10947.9023 -0.0007 8 5 4 7 5 3 10842.3154 0.0004 9 0 9 8 0 8 1099.2891 0.0028 9 1 9 8 1 7 11744.4794 0.0004 9 2 7 8 2 6 12436.8436 -0.0007 9 1 8 8 2 7 11658.1903 0.0017 9 2 7 8 2 6 12436.8436 -0.0028 10 10 10 9 9 1 8 12297.205 -0.0004 10 11 10 9 1 9 1 1	8 2 7	7 2 6	10430.0849	-0.0005
8 3 6 7 3 5 10772.3754 -0.0005 8 3 5 7 3 4 11203.1132 0.0006 8 4 5 7 4 4 10947.9023 -0.0027 8 5 3 7 5 2 10842.3154 0.0004 8 5 3 7 5 2 10847.906 0.0024 9 0 9 8 0 8 1099.2891 0.0028 9 1 9 8 1 8 1095.1038 -0.0071 9 2 8 8 2 7 11658.1903 0.0017 9 2 7 8 2 6 12436.8436 -0.0028 10 0 10 9 9 1 8 1292.1088 0.0007 11 110 9 9 1 8 1292.1088 0.0001 12 8 9 2 7 13652.864 0.0007	8 2 6	7 2 5	11159.9243	-0.0015
8 3 5 7 3 4 11203.1132 0.0006 8 4 5 7 4 4 10864.6286 -0.0025 8 4 4 7 5 3 10947.9023 -0.0007 8 5 4 7 5 2 10847.906 0.0024 9 0 9 8 0 8 1095.1038 -0.0007 9 1 9 8 1 7 11744.4794 0.0004 9 2 8 8 2 7 11658.1903 0.0017 9 2 7 8 2 6 12436.8436 -0.0028 10 0 10 9 9 1 8 12927.7205 -0.0044 10 110 9 9 1 8 12922.1088 0.0007 11 111 10 110 13496.0517 0.0018 111 11 111 10 110 13496.0517 0.0012 <td< td=""><td>8 3 6</td><td>7 3 5</td><td>10772.3754</td><td>-0.0005</td></td<>	8 3 6	7 3 5	10772.3754	-0.0005
8 4 5 7 4 4 10864.6286 -0.0025 8 5 4 7 5 3 10947.9023 -0.0007 8 5 3 7 5 2 10847.7906 0.0024 9 0 9 8 0 8 11095.1038 -0.0007 9 1 9 8 1 7 11744.4794 0.0004 9 2 8 8 2 7 11658.1903 0.0017 9 2 8 8 2 7 11658.1903 0.0004 10 0 10 9 9 1 8 1297.7205 -0.0004 10 1 9 9 1 8 1292.1088 0.0007 11 10 10 10 1 10 100 100000 11 11 11 10 10 19 14107.6317 0.0001 13 1 2 2 1 2 289.4546 0.0	8 3 5	7 3 4	11203.1132	0.0006
8 4 4 7 4 3 10947.9023 -0.0007 8 5 4 7 5 3 10842.3154 0.0004 8 5 3 7 5 2 10847.7966 0.0024 9 0 9 8 0 8 11099.2891 0.0028 9 1 9 8 1 8 1095.1038 -0.0007 9 1 8 8 1 7 11744.4794 0.0004 9 2 7 8 2 6 12436.8436 -0.0008 10 110 9 1 9 12297.7205 -0.004 10 110 9 1 8 1292.1088 0.0007 11 111 10 10 1407.6317 0.0018 10 1 9 2 8 12874.5880 0.0001 13 1 10 10 1407.6317 0.001 14 1 10 10 19 1410	8 4 5	7 4 4	10864.6286	-0.0025
8 5 4 7 5 3 10842.3154 0.0004 8 5 3 7 5 2 10847.7906 0.0024 9 1 9 8 0 8 11099.2891 0.0028 9 1 9 8 1 8 11095.1038 -0.0007 9 1 8 8 1 7 11744.4794 0.0004 9 2 7 8 2 6 12436.8436 -0.0008 10 0.10 9 1 9 12297.7205 -0.0004 10 1 9 1 8 1292.1088 0.0007 10 1 9 1 8 12297.7205 -0.0021 11 110 10 0 10 13496.0517 0.0017 11 011 10 10 1407.6317 0.0012 3 1 2 2 1 2 5002.0230 0.0012 3 1 2 1 1 <td>8 4 4</td> <td>7 4 3</td> <td>10947.9023</td> <td>-0.0007</td>	8 4 4	7 4 3	10947.9023	-0.0007
8 5 3 7 5 2 10847.7906 0.0024 9 0 9 8 0 8 11099.2891 0.0028 9 1 8 8 1 7 11744.4794 0.0004 9 2 8 8 1 7 11744.4794 0.0004 9 2 7 8 2 6 12436.8436 -0.0008 10 0 10 9 9 9 12297.7205 -0.0004 10 1 9 9 1 8 1292.1088 0.0005 10 2 8 9 2 7 13652.8064 0.0007 11 0 11 10 10 13496.8328 -0.0021 11 111 10 19 14107.6317 0.001 3 1 2 0 2 5002.0230 0.001 3 1 2 1 1 5605.1029 0.0006 3 3 0 2	8 5 4	7 5 3	10842.3154	0.0004
9 0 9 8 0 8 11092.891 0.0028 9 1 9 8 1 8 1005.1038 -0.0007 9 1 8 8 1 7 11744.4794 0.0004 9 2 8 8 2 7 11658.1903 0.0017 9 2 7 8 2 6 12436.8436 -0.0008 10 110 9 9 1 9 12297.7205 -0.0004 10 1 9 9 1 8 1292.1088 0.0005 10 2 9 9 2 8 1292.108 0.0001 10 1 9 9 2 8 12874.5880 0.0001 10 1 10 0 10 13496.6327 0.0018 11 111 10 10 1407.6317 0.0001 3 2 1 2 5002.0230 0.0012 3 3 0 2	8 5 3	7 5 2	10847.7906	0.0024
9 1 9 8 1 8 1095.1038 -0.0007 9 1 8 8 1 7 11744.4794 0.0004 9 2 8 8 2 7 11658.1903 0.0017 9 2 7 8 2 6 12436.8436 -0.0008 10 0 10 9 9 9 12297.7205 -0.0004 10 1 9 9 1 8 12292.1088 0.0005 10 2 9 9 2 8 12874.5880 0.0007 11 0 10 10 19 14107.6317 0.001 11 11 10 19 14107.6317 0.001 3 1 2 2 1 2 5002.0230 0.001 3 1 2 2 1 2 5002.0230 0.001 3 3 0 3 6656.6616 0.0099 4 2 2 1 0.015	9 0 9	8 0 8	11099.2891	0.0028
9 1 8 8 1 7 11744.4794 0.0004 9 2 8 8 2 7 11658.1903 0.0017 9 2 7 8 2 6 12436.8436 -0.0008 10 0 10 9 0 9 12297.7205 -0.0004 10 1 10 9 1 9 12295.8845 -0.0028 10 1 9 9 1 8 12292.1088 0.0007 11 0 10 10 0 10 13496.8328 -0.0021 11 11 10 10 19 14107.6317 0.001 3 1 2 2 1 2 5002.0230 0.0012 3 1 2 2 1 2 5899.4546 0.0012 3 2 1 2 1 1 5605.1029 0.0006 3 3 1 2 2 1 6819.6586 -0.0018	9 1 9	8 1 8	11095.1038	-0.0007
9 2 8 8 2 7 11658.1903 0.0017 9 2 7 8 2 6 12436.8436 -0.0008 10 0 10 9 0 9 12297.7205 -0.0044 10 1 10 9 1 9 12295.8845 -0.0028 10 1 9 9 2 8 12222.1088 0.0007 11 0 11 10 0.10 13496.8328 -0.0021 11 111 10 10 19 14107.6317 0.001 3 1 2 2 0 2 5002.0230 0.001 3 1 2 2 1 2 5002.0230 0.0012 3 3 1 2 2 1 5605.1029 0.0006 3 3 1 2 2 1 6566.6616 0.0019 4 1 3 0 3 7 42.041 0.0015 4	9 1 8	8 1 7	11744.4794	0.0004
9 2 7 8 2 6 12436,8436 -0.0008 10 0 10 9 0 9 12297,7205 -0.0004 10 1 10 9 1 9 12295,8845 -0.0028 10 2 9 9 2 8 12221,088 0.0007 11 0 11 10 0 10 13496,8328 -0.0021 11 11 10 10 19 14107,6317 0.001 3 1 2 2 0 2 589,4546 0.0012 3 1 2 2 1 1 5605,1029 0.0006 3 3 1 2 2 1 1 5605,1029 0.0006 3 3 1 2 2 1 1 6819,6586 -0.0018 3 3 0 3 1 3 0 3 6656,6616 0.0009 4 1 3 1 3 1	928	8 2 7	11658.1903	0.0017
10 0 10 9 0 9 12297.7205 -0.0004 10 1 10 9 1 9 12295.8845 -0.0028 10 1 9 9 1 8 12292.1088 0.0005 10 2 9 9 2 8 12874.5880 0.0007 11 0 10 0 10 13496.8328 -0.021 11 11 10 10 19 14107.6317 0.001 3 1 2 2 1 2 5002.0230 0.0001 3 2 2 1 2 5605.1029 0.0006 3 3 1 2 2 1 6819.6586 -0.0018 3 3 0 2 2 0 6796.8568 -0.0019 4 1 3 0 3 1 3 0.0025 0.0025 4 2 3 1 2 2 0 6796.8568 -0.0019	927	8 2 6	12436.8436	-0.0008
10 1 1 9 1 9 12295.8845 -0.0028 10 1 9 9 1 8 12221.088 0.0005 10 2 9 9 2 8 12874.5880 0.0007 11 0 1 10 10 13496.8328 -0.021 11 1 10 10 19 14107.6317 0.001 3 1 2 2 0 2 5002.0230 0.0001 3 2 2 1 2 5605.1029 0.0006 3 3 1 2 2 1 6819.6586 -0.0018 3 3 0 2 2 0 6796.8568 -0.0019 4 1 3 0 3 1 2 0 6796.8568 -0.0019 4 1 3 1 3 1 3 0.022 0.0025 0.0025 4 2 3 1 2 6951.0832 0.0025	10 010	9 0 9	12297.7205	-0.0004
10 1 9 9 1 8 1292.1088 0.0005 10 2 9 9 2 8 12874.5880 0.0007 11 0 1 10 0 10 13496.8328 -0.021 11 1 10 1 10 1 10 13496.8328 -0.0021 11 1 10 1 10 1 10 13496.8328 -0.0021 11 1 10 1 10 1 10 13496.8328 -0.0021 3 1 2 2 0 2 5002.0230 0.0001 3 1 2 1 1 5605.1029 0.0006 3 3 1 2 2 1 6819.6586 -0.018 3 3 0 2 2 0 6796.8568 -0.0019 4 1 3 3 1 2 6951.0832 0.0025 4 3 1 3 2 1 8100.	10 110	9 1 9	12295.8845	-0.0028
10 2 9 9 2 8 12874.5880 0.0000 10 2 8 9 2 7 13652.8064 0.0007 11 0 11 10 0 10 13496.8328 -0.021 11 1 11 10 1 10 13496.0517 0.0018 11 1 10 1 9 2 5002.0230 0.0001 3 1 2 2 1 1 5605.1029 0.0006 3 3 1 2 2 1 6505.616 0.0012 3 3 1 2 2 0 6796.8568 -0.018 3 3 0 2 2 0 6796.8568 -0.0019 4 1 3 3 1 3 742.7041 0.0015 4 2 3 1 3 2 1 8100.468 -0.0000 4 1 3 3 1 9264.0556 -0.0020	10 1 9	9 1 8	12922.1088	0.0005
10 2 8 9 2 7 13652.8064 0.0007 11 0 11 10 0 10 13496.8328 -0.021 11 1 1 10 1 10 13496.0517 0.0018 11 1 10 1 9 14107.6317 0.0001 3 1 2 2 0 2 5002.0230 0.0001 3 2 2 1 2 5899.4546 0.0012 3 3 1 2 2 1 6819.6586 -0.0018 3 3 1 2 2 1 6819.6586 -0.0019 4 1 3 3 0 3 6656.6616 0.0009 4 2 3 1 3 7442.7041 0.0015 4 2 2 3 1 3 0 9261.2965 0.0003 4 4 1 3 3 1 9264.0556 -0.0020 4 <td< td=""><td>10 2 9</td><td>9 2 8</td><td>12874.5880</td><td>0.0000</td></td<>	10 2 9	9 2 8	12874.5880	0.0000
11 0 11 10 0 10 13496.8328 -0.021 11 1 11 10 10 10 19 14107.6317 0.001 3 1 2 2 0 2 5002.0230 0.0001 3 2 2 2 1 2 5899.4546 0.0012 3 2 1 2 1 1 5605.1029 0.0006 3 3 1 2 2 1 6819.6586 -0.0018 3 3 0 2 2 0 6796.8568 -0.0019 4 1 3 3 1 3 6556.6616 0.0009 4 2 3 1 3 7442.7041 0.0015 4 2 2 3 1 3 0.0025 0.0025 4 3 1 3 2 2 8202.9735 -0.0005 4 4 1 3 3 1 9264.0556 -0.0020 4 4 <t< td=""><td>10 2 8</td><td>927</td><td>13652.8064</td><td>0.0007</td></t<>	10 2 8	927	13652.8064	0.0007
11 111 10 10 140 13496.0517 0.0018 11 10 10 19 14107.6317 0.0001 3 1 2 2 0 2 5002.0230 0.0001 3 2 2 2 1 2 5899.4546 0.012 3 2 1 2 1 1 5605.1029 0.0006 3 3 1 2 2 1 6819.6586 -0.018 3 3 0 2 2 0 6796.8568 -0.0019 4 1 3 3 1 3 6656.6616 0.0009 4 2 3 3 1 3 7442.7041 0.0015 4 2 2 3 2 1 8100.0468 -0.0020 4 3 1 3 2 1 8100.0468 -0.0020 4 4 0 4 4 0 4 0.0013 5 1 4	11 011	10 010	13496.8328	-0.0021
11 10 19 14107.6317 0.001 3 1 2 2 1 2 5002.0230 0.0001 3 2 2 1 2 5899.4546 0.0012 3 2 1 2 1 1 5605.1029 0.0006 3 3 1 2 2 1 6819.6586 -0.018 4 1 3 0 2 2 0 6796.8568 -0.0019 4 1 3 3 0 3 6656.6616 0.0009 4 2 3 1 3 7442.7041 0.0015 4 2 2 3 1 2 6951.0832 0.0025 4 3 1 3 2 1 8100.0468 -0.0000 4 4 0 4 8417.1044 0.0015 0.0013 5 1 4 0 4 8417.1044 0.0013 5 3 3 4 1 3	11 111	10 1 10	13496.0517	0.0018
31222025002.02300.00013212125899.45460.00123212115605.10290.00063312216819.6586-0.0018413302206796.8568-0.0019413302206796.8568-0.00194233136656.66160.00094233137442.70410.00154223228202.9735-0.00054313218100.0468-0.00004413309261.29650.00035144048417.10440.00155234138379.6670-0.00025334239624.29890.001353243110598.66440.001354143111716.8477-0.002155044011716.5730-0.003861550510257.3325-0.0030	11 110	10 19	14107.6317	0.0001
3 2 2 1 2 1 2 5899.4546 0.0012 3 2 1 2 1 1 5605.1029 0.0006 3 3 1 2 2 1 6819.6586 -0.0018 3 3 0 2 2 0 6796.8568 -0.0019 4 1 3 3 0 3 6656.6616 0.0009 4 2 3 3 1 3 7442.7041 0.0015 4 3 2 3 1 2 6951.0832 0.0025 4 3 1 3 2 1 8100.0468 -0.0000 4 4 1 3 3 1 9264.0556 -0.0020 4 4 0 3 3 0 9261.2965 0.0003 5 1 4 4 1 3 8379.6670 -0.0002 5 3 2 4 1 3 8379.6670 -0.0003	3 1 2	2 0 2	5002.0230	0.0001
3 2 1 2 1 1 5605.1029 0.0006 3 3 1 2 2 1 6819.6586 -0.0018 3 3 0 2 2 0 6796.8568 -0.0019 4 1 3 3 0 3 6656.6616 0.0009 4 2 3 3 1 3 7442.7041 0.0015 4 2 2 3 1 2 6951.0832 0.0025 4 3 2 3 2 1 8100.0468 -0.0000 4 3 1 3 2 1 8100.0468 -0.0020 4 4 0 3 3 0 9264.0556 -0.0020 5 1 4 4 0 4 8417.1044 0.0015 5 2 3 4 1 3 8379.6670 -0.0020 5 3 2 4 1 3 8379.6670 -0.00013	3 2 2	2 1 2	5899.4546	0.0012
3 3 1 2 2 1 6819.6586 -0.0018 3 3 0 2 2 0 6796.8568 -0.0019 4 1 3 3 0 3 6656.6616 0.0009 4 2 3 3 1 3 7442.7041 0.0015 4 2 2 3 1 2 6951.0832 0.0025 4 3 2 3 2 2 8202.9735 -0.0005 4 3 1 3 2 1 8100.0468 -0.0020 4 4 1 3 3 1 9264.0556 -0.0020 4 4 0 3 3 0 9261.2965 0.0003 5 1 4 4 1 4 9047.5219 0.0011 5 2 3 4 1 3 8379.6670 -0.0022 5 3 2 2 3 9624.2989 0.0013 5	3 2 1	2 1 1	5605.1029	0.0006
3 3 0 2 2 0 6796.8568 -0.0019 4 1 3 3 0 3 6656.6616 0.0009 4 2 3 3 1 3 7442.7041 0.0015 4 2 2 3 1 2 6951.0832 0.0025 4 3 2 3 1 2 6951.0832 0.0005 4 3 1 3 2 1 8100.0468 -0.0000 4 4 1 3 3 1 9264.0556 -0.0020 4 4 0 3 3 0 9261.2965 0.0003 5 1 4 4 0 4 8417.1044 0.0015 5 2 3 4 1 3 8379.6670 -0.0002 5 3 2 4 2 3 9624.2989 0.0013 5 3 2 4 2 2 9362.9918 0.0003	3 3 1	2 2 1	6819.6586	-0.0018
4 1 3 3 0 3 6655.6616 0.0009 4 2 3 3 1 3 7442.7041 0.0015 4 2 2 3 1 2 6951.0832 0.0025 4 3 2 3 1 2 6951.0832 0.0005 4 3 1 3 2 1 8202.9735 -0.0005 4 3 1 3 2 1 8100.0468 -0.0020 4 4 1 3 3 1 9264.0556 -0.0020 4 4 0 3 3 0 9261.2965 0.0013 5 1 4 0 4 8417.1044 0.0015 0.0011 5 2 3 4 1 3 8379.6670 -0.0002 5 3 3 4 2 3 9624.2989 0.0013 5 3 2 10616.9965 -0.0004 0.0003 0.0034 0.0013	3 3 0	2 2 0	6796.8568	-0.0019
4 2 3 3 1 3 7442.7041 0.0015 4 2 2 3 1 2 6951.0832 0.0025 4 3 2 3 2 2 8202.9735 -0.0005 4 3 1 3 2 1 8100.0468 -0.0020 4 4 1 3 3 1 9264.0556 -0.0020 4 4 0 3 3 0 9261.2965 0.0003 5 1 4 0 4 8417.1044 0.0015 5 2 4 4 1 4 9047.5219 0.0011 5 2 3 4 2 3 9624.2989 0.0013 5 3 2 4 3 2 10616.9965 -0.0004 5 4 2 4 3 1 10598.6644 0.0013 5 5 1 4 4 1 11716.8477 -0.0021 5	4 1 3	3 0 3	6656.6616	0.0009
4 2 2 3 1 2 6951.0832 0.0025 4 3 2 3 2 2 8202.9735 -0.0005 4 3 1 3 2 1 8100.0468 -0.0020 4 4 1 3 3 1 9264.0556 -0.0020 4 4 0 3 3 0 9261.2965 0.0003 5 1 4 0 3 3 0 9261.2965 0.0003 5 1 4 4 0 4 8417.1044 0.0015 5 2 4 4 1 4 9047.5219 0.0011 5 2 3 4 2 3 9624.2989 0.0033 5 3 2 4 3 2 10616.9965 -0.0004 5 4 2 4 3 1 10598.6644 0.0013 5 5 1 4 4 1 11716.8477 -0.0021	4 2 3	3 1 3	7442.7041	0.0015
4 3 2 3 2 2 8202.9735 -0.0005 4 3 1 3 2 1 8100.0468 -0.0020 4 4 1 3 3 1 9264.0556 -0.0020 4 4 0 3 3 0 9261.2965 0.0003 5 1 4 0 4 8417.1044 0.0015 5 2 4 4 1 4 9047.5219 0.0011 5 2 3 4 1 3 8379.6670 -0.0022 5 3 3 4 2 3 9624.2989 0.0013 5 3 2 4 2 2 9362.9918 0.0003 5 4 2 4 3 2 10616.9965 -0.0004 5 4 1 4 3 1 10598.6644 0.0013 5 5 1 4 4 1 11716.8477 -0.0021 5	4 2 2	3 1 2	6951.0832	0.0025
4 3 1 3 2 1 8100.0468 -0.0000 4 4 1 3 3 1 9264.0556 -0.0020 4 4 0 3 3 0 9261.2965 0.0003 5 1 4 0 4 4 0.0015 0.0015 5 2 4 4 1 4 9047.5219 0.0011 5 2 3 4 1 3 8379.6670 -0.0022 5 3 3 4 2 3 9624.2989 0.0013 5 3 2 4 2 3 9624.2989 0.0003 5 3 2 4 3 2 10616.9965 -0.0004 5 4 1 4 3 1 10598.6644 0.0013 5 5 1 4 4 0 11716.5730 -0.0021 5 5 0 4 4 0 11716.5730 -0.0030	4 3 2	3 2 2	8202.9735	-0.0005
4 4 1 3 3 1 9264.0556 -0.0020 4 4 0 3 3 0 9261.2965 0.0003 5 1 4 4 0 4 8417.1044 0.0015 5 2 4 4 1 4 9047.5219 0.0011 5 2 3 4 1 3 8379.6670 -0.0002 5 3 3 4 2 3 9624.2989 0.0013 5 3 2 4 2 2 9362.9918 0.0003 5 3 2 4 2 2 9362.9918 0.0013 5 4 2 4 3 2 10616.9965 -0.0004 5 4 1 4 3 1 10598.6644 0.0013 5 5 0 4 4 0 11716.5730 -0.0038 6 1 5 5 0 5 10257.3325 -0.0030 <td>4 3 1</td> <td>3 2 1</td> <td>8100.0468</td> <td>-0.0000</td>	4 3 1	3 2 1	8100.0468	-0.0000
4 4 0 3 3 0 9261.2965 0.0003 5 1 4 4 0 4 8417.1044 0.0015 5 2 4 4 1 4 9047.5219 0.0011 5 2 3 4 1 3 8379.6670 -0.0002 5 3 3 4 2 3 9624.2989 0.0013 5 3 2 4 2 2 9362.9918 0.0003 5 3 2 4 3 2 10616.9965 -0.0004 5 4 1 4 3 1 10598.6644 0.0013 5 5 1 4 4 1 11716.8477 -0.0021 5 5 0 4 4 0 11716.5730 -0.0038 6 1 5 5 0 5 10257.3325 -0.0030	4 4 1	3 3 1	9264.0556	-0.0020
5 1 4 4 0 4 8417.1044 0.0015 5 2 4 4 1 4 9047.5219 0.0011 5 2 3 4 1 3 8379.6670 -0.0002 5 3 3 4 2 3 9624.2989 0.0013 5 3 2 4 2 2 9362.9918 0.0003 5 4 2 4 3 2 10616.9965 -0.0004 5 4 1 4 3 1 10598.6644 0.0013 5 5 1 4 4 1 11716.8477 -0.0021 5 5 0 4 4 0 11716.5730 -0.0038 6 1 5 5 0 5 10257.3325 -0.0030	4 4 0	3 3 0	9261.2965	0.0003
5 2 4 4 1 4 9047.5219 0.0011 5 2 3 4 1 3 8379.6670 -0.0002 5 3 3 4 2 3 9624.2989 0.0013 5 3 2 4 2 2 9362.9918 0.0003 5 4 2 2 9362.9918 0.0013 5 4 2 4 3 2 10616.9965 -0.0004 5 4 1 1598.6644 0.0013 -0.0021 -0.0021 -0.0021 5 5 0 4 4 1 11716.8477 -0.0021 5 5 0 4 4 0 11716.5730 -0.0038 6 1 5 5 0 5 10257.3325 -0.0030	5 1 4	4 0 4	8417.1044	0.0015
5 2 3 4 1 3 8379.6670 -0.0002 5 3 3 4 2 3 9624.2989 0.0013 5 3 2 4 2 2 9362.9918 0.0003 5 4 2 2 9362.9918 0.0003 5 4 2 4 3 2 10616.9965 -0.0004 5 4 1 10598.6644 0.0013 -0.0021 5 5 1 4 4 1 11716.8477 -0.0021 5 5 0 4 4 0 11716.5730 -0.0038 6 1 5 5 0 5 0 5 10257.3325 -0.0030	5 2 4	4 1 4	9047.5219	0.0011
5 3 3 4 2 3 9624.2989 0.0013 5 3 2 4 2 2 9362.9918 0.0003 5 4 2 4 3 2 10616.9965 -0.0004 5 4 1 4 3 1 10598.6644 0.0013 5 5 1 4 4 1 11716.8477 -0.0021 5 5 0 4 4 0 11716.5730 -0.0038 6 1 5 5 0 5 0 5 10257.3325 -0.0030	5 2 3	4 1 3	8379.6670	-0.0002
5 3 2 4 2 2 9362.9918 0.0003 5 4 2 4 3 2 10616.9965 -0.0004 5 4 1 4 3 1 10598.6644 0.0013 5 5 1 4 4 1 11716.8477 -0.0021 5 5 0 4 4 0 11716.5730 -0.0038 6 1 5 5 0 5 0 5 0.0030	5 3 3	4 2 3	9624.2989	0.0013
5 4 2 4 3 2 10616.9965 -0.0004 5 4 1 4 3 1 10598.6644 0.0013 5 5 1 4 4 1 11716.8477 -0.0021 5 5 0 4 4 0 11716.5730 -0.0038 6 1 5 5 0 5 0 5 10257.3325 -0.0030	5 3 2	4 2 2	9362.9918	0.0003
5 4 1 4 3 1 10598.6644 0.0013 5 5 1 4 4 1 11716.8477 -0.0021 5 5 0 4 4 0 11716.5730 -0.0038 6 1 5 5 0 5 0 5 -0.0030	5 4 2	4 3 2	10616.9965	-0.0004
5 5 1 4 4 1 11716.8477 -0.0021 5 5 0 4 4 0 11716.5730 -0.0038 6 1 5 5 0 5 10257.3325 -0.0030	5 4 1	4 3 1	10598.6644	0.0013
5 5 0 4 4 0 11716.5730 -0.0038 6 1 5 5 0 5 10257.3325 -0.0030	5 5 1	4 4 1	11716.8477	-0.0021
6 1 5 0 5 10257.3325 -0.0030	5 5 0	4 4 0	11716.5730	-0.0038
	6 1 5	5 0 5	10257.3325	-0.0030
			10237.3323	0.0050

6	2	5	5	1	5	10708.0112	0.0011
6	2	4	5	1	4	9911.2952	-0.0011
6	3	4	5	2	4	11094.7940	-0.0007
6	3	3	5	2	3	10613.5974	0.0002
6	4	3	5	3	3	11979.5877	-0.0004
6	4	2	5	3	2	11912.0332	0.0014
6	5	2	5	4	2	13064.5484	-0.0001
6	5	1	5	4	1	13062.1780	0.0002
6	6	0	5	5	0	14170.5427	0.0079
7	1	6	6	0	6	12128.7558	0.0015
7	2	6	6	1	6	12414.7679	-0.0037
7	2	5	6	1	5	11560.9911	-0.0019
7	3	5	6	2	5	12621.8180	0.0016
7	3	4	6	2	4	11905.3570	-0.0009
7	4	4	6	3	4	13361.7877	0.0018
7	4	3	6	3	3	13183.4244	0.0028
7	5	3	6	4	3	14411.9171	-0.0006
7	5	2	6	4	2	14400.6317	-0.0025
7	6	2	6	5	2	15517.8841	-0.0004
7	6	1	6	5	1	15517.6250	0.0000
7	7	0	6	6	0	16624.2322	-0.0021

	Isomers	A [MHz]	B [MHz]	C [MHz]
	I	1149.541060	830.244541	643.462812
Exp.	П	1227.008821	739.493310	600.064693
	I	1144.1 (-0.5%) ^a	838.8(1.0%)	646.3 (0.4%)
CP-B2PLYP-D3(BJ)/def2-12VP	П	1217.4 (-0.8%)	752.8(1.8%)	604.4 (0.7%)
B2PLYP-D3(BJ)/def2-TZVP	I	1144.2 (-0.5%)	855.3 (3.0%)	656.2 (2.0%)
	П	1217.4 (-0.8%)	766.8 (3.7%)	612.71 (2.1%)
	I	1143.8 (-0.5%)	851.3 (2.5%)	652.9 (1.5%)
CP-B3LYP-D3(BJ)/def2-12VP	П	1214.0 (-1.3%)	768.1 (3.9%)	611.3 (1.9%)
	I	1143.2 (-0.6%)	857.3 (3.3%)	656.2 (2.0%)
B3LYP-D3(BJ)/def2-12VP	П	1213.9 (-1.1%)	773.6 (4.6%)	614.6 (2.4%)
	I	1152.1 (0.2%)	857.7 (3.3%)	656.2 (2.0%)
CP-MP2/def2-TZVP	П	1225.2 (0.1%)	771.3 (4.3%)	616.6 (2.8%)
	I	1158.3 (3.1%)	890.6 (9.1%)	682.6 (9.4%)
MP2/def2-TZVP	П	1227.9 (0.1%)	802.3 (8.5%)	636.2 (6.0%)

 Table S3. Comparison of theoretical (with different methods) and experimental spectroscopic constants of isomers

 I and II.

^a The error with respect to experiment is indicated as percentage between parentheses.

 Table S4. CP-B2PLYP-D3(BJ)/def2-TZVP calculated geometries of isomer I.

Bond len	gths (Å)	Valence angles (°)		Dihedral angles (°)		
0201	2.267					
0302	2.266	030201	161.2			
C4O3	1.192	C4O3O2	31.3	C4O3O2O1	-5.5	
C501	1.192	C50102	31.2	C50102C4	2.3	
C6C4	1.484	C6C4O3	130.1	C6C4O3O2	179.4	
C7C6	1.331	C7C6C4	108.2	C7C6C4O3	-178.8	
H8C7	1.077	H8C7C6	129.7	H8C7C6C4	-179.9	
H9C6	1.077	H9C6C4	122.0	H9C6C4O3	1.3	
C10C5	3.413	C10C5C7	92.6	C10C5C7C6	-96.3	
C11C7	3.468	C11C7C6	90.3	C11C7C6C4	-79.4	
C12C11	1.462	C12C11C10	125.5	C12C11C10C5	82.3	
C13C12	1.502	C13C12C11	118.9	013C12C11C10	4.3	
C14C12	1.341	C14C12C11	119.4	C14C13C11C10	-175.3	
H15C10	1.081	H15C10C11	121.1	H15C10C11C12	179.1	
H16C10	1.081	H16C10C11	122.1	H16C10C11C12	-0.4	
H17C11	1.086	H17C11C12	115.6	H17C11C12C14	3.9	
H18C13	1.091	H18C13C12	111.4	H18C13C12C14	121.6	
H19C13	1.092	H19C13C12	110.6	H19C13C12C14	-119.2	
H20C13	1.088	H20C13C12	110.8	H20C13C12C14	1.3	
H21C14	1.083	H21C14C12	121.1	H21C14C12C11	-1.3	
H22C14	1.081	H22C14C12	121.6	H22C14C12C11	179.1	



Table S5. CP-B2PLYP-D3	3(BJ)/def2-TZVP c	alculated geometries of	isomer II.
------------------------	-------------------	-------------------------	------------

Bond lengths (Å)		Valence ang	gles (°)	Dihedral angle	es (°)
0201	2.265				
0302	2.267	030201	161.2		
C4O3	1.193	C4O3O2	31.2	C4O3O2O1	1.0
C501	1.193	C50102	31.2	C5O1O2C4	-0.9
C6C4	1.484	C6C4O3	130.0	C6C4O3O2	179.2
C7C5	1.485	C7C5O1	130.0	C7C5O1O2	-180.0
H8C6	1.078	H8C6C7	129.7	H8C6C7C5	179.8
H9C7	1.077	H9C7C5	122.1	H9C7C5O1	-0.03
C10H9	3.365	C10H9C7	89.4	C10H9C7C5	-68.0
C11C7	3.381	C11C7C6	96.6	C11C7C6C4	-89.6
C12C11	1.501	C12C11C10	121.6	C12C11C10H9	-83.7
C13C11	1.461	C13C11C10	119.7	O13C12C10H9	95.5
C14C13	1.337	C14C13C11	125.4	C14C13C11C10	-176.8
H15C10	1.082	H15C10C11	121.3	H15C10C11C13	-0.2
H16C10	1.082	H16C10C11	121.5	H16C10C11C13	179.9
H17C13	1.085	H17C13C11	115.7	H17C13C11C10	2.2
H18C12	1.088	H18C12C11	111.0	H18C12C11C10	-1.0
H19C12	1.092	H19C12C11	111.0	H19C12C11C10	-121.6
H20C12	1.093	H20C12C11	111.0	H20C12C11C10	119.6
H21C14	1.081	H21C14C13	121.0	H21C14C13C11	178.8
H22C14	1.082	H22C14C13	122.2	H22C14C13C11	-1.1



Transitions	Isomers	Frequencies	Intensities
$3_{30} \leftarrow 2_{20}$	I	6470.2680	0.0093
	Ш	6796.8591	0.0036
a / 2	I	7898.8750	0.0107
4 ₃₁ ← 3 ₂₁	П	8100.0479	0.004
F / 4	I	9336.7572	0.0225
$5_{32} \leftarrow 4_{23}$	П	9362.9912	0.0067
5 _{3 3} ← 4 _{2 3}	I	9715.5975	0.0227
	П	9624.2973	0.0083
F / A	I	10248.0416	0.0107
5 41 ⊂ 4 31	П	10598.6617	0.0033
F / A	l	10314.4195	0.0079
5 ₄₂ ← 4 ₃₂	П	10616.9940	0.0024
	I	11864.8182	0.0115
043 ← 533	П	11979.5889	0.0035
с <u>/</u> Г	I	12575.2411	0.009
6 _{5 1} ← 5 _{4 1}	Ш	13062.1782	0.0028

Table S6. Intensities (in arbitrary units) of isomers I and II for several selected μ_c -type transitions.

 Table S7.
 SAPT analysis (all values in kJ mol⁻¹).

	Electrostatic	Induction	Dispersion	Exchange	Total
ISO-MA- I	-19.4 (33.2%) ª	-5.2 (8.8%)	-33.9 (58.0%)	35.1	-23.4
iso-ma- II	-19.4 (34.0%)	-4.9 (8.6%)	-32.7 (57.4%)	34.6	-22.4
(Dibenzofuran) ₂	-29.5(25.2%)	-6.7(5.7%)	-80.9(69.1%)	65.6	-51.5
(Benzene) ₂	-9.2(20.8%)	-2.6(5.8%)	-32.47(73.4%)	33.5	-27.7

^a Percentage contribution to total attracting energy.

Isomer I		
Donor NBO	Acceptor NBO	E ⁽²⁾ [kJ mol ⁻¹]
from ISO to MA		
BD (2) C1 - C2	RY*(3) C16	0.75
BD (2) C1 - C2	BD*(2) C14 - O15	1.59
BD (2) C1 - C2	BD*(2) C16 – C17	3.09
BD (2) C5 - C6	BD*(2) C16 - C17	1.17
BD (2) C5 - C6	BD*(2) C19 - O20	1.80
from MA to ISO		
BD (2) C16 - C17	BD*(2) C5 - C6	1.46
BD (2) C19 - O20	BD*(2) C5 - C6	0.71
LP (2) O21	BD*(1) C10 - H13	0.46
Isomer II		
Donor NBO	Acceptor NBO	E ⁽²⁾ [kJ mol ⁻¹]
from ISO to MA		
BD (2) C1 - C2	RY*(3) C16	0.67
BD (2) C1 - C2	BD*(2) C16 – C17	3.47
BD (1) C5 - C6	RY*(8) C19	0.50
BD (2) C5 - C6	BD*(2) C14 - O15	0.54
BD (2) C5 - C6	BD*(2) C16 - C17	0.54
BD (2) C5 - C6	BD*(2) C19 - O20	2.38
from MA to ISO		
BD (2) C16 - C17	BD*(2) C1 - C2	0.92
BD (2) C19 - O20	BD*(2) C5 - C6	0.54

Table S8. Stabilization energy contributions ($E^{(2)} \ge 0.40 \text{ kJ mol}^{-1}$) for isomers I and II of ISO-MA.



Isomer I



Isomer II