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Supplementary Material

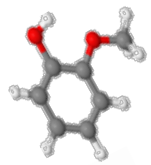
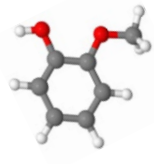
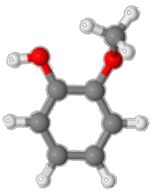
Switching On/Off the Intramolecular Hydrogen Bonding of 2-Methoxyphenol Conformers: An NMR Study

Frederick Backler[A] and Feng Wang[A,B]

[A]Centre for Translational Atomaterials, Department of Chemistry and Biotechnology, Faculty of Science, Engineering and Technology, Swinburne University of Technology, Melbourne, Vic. 3122, Australia.

[B]Corresponding author. Email: fwang@swin.edu.au

Table S1. Rotamer notation of 2-MP in literature.

Structure	Caminati et al[30]	Fujimaki et al[17]	Wilke et al[31]	Cesari et al [9]	This work
	(0.0)	I	Down/ up	Cisoid (C1)	AntiSyn (AS)
	(180,0)	III	Down/ down	Transoid (C2)	AntiAnti (AA)
	(180,110)	V[A]		C3(C4)	AntiGauche (AG)

[A]This local minimum structure of 2-MP is not shown in Fujimaki, Fujii [17].

Table S2: Coordinates of the stable rotamers of 2-MP in their ground electronic states using the B3LYP/6-311++G** model.

AS (2-MP)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.171960	2.845005	0.000000
2	8	0	-0.628619	1.669170	0.000000
3	6	0	-0.000000	0.446743	0.000000
4	6	0	1.373821	0.234605	0.000000
5	6	0	-0.884985	-0.647540	0.000000
6	6	0	1.872089	-1.073053	0.000000
7	6	0	0.997702	-2.153552	0.000000
8	6	0	-0.382663	-1.940910	0.000000
9	8	0	-2.232279	-0.438607	0.000000
10	1	0	-0.523662	3.682407	0.000000
11	1	0	0.801045	2.893170	0.894686
12	1	0	0.801045	2.893170	-0.894686
13	1	0	2.060006	1.071495	0.000000
14	1	0	2.943528	-1.233731	0.000000
15	1	0	1.382177	-3.166634	0.000000
16	1	0	-1.081934	-2.768475	0.000000
17	1	0	-2.382568	0.516315	0.000000

AG (2-MP)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.605870	-0.463665	0.533451
2	8	0	1.647439	-0.768191	-0.487686
3	6	0	0.341760	-0.447894	-0.214723
4	6	0	-0.599768	-1.471561	-0.141599
5	6	0	-0.086594	0.885799	-0.090624
6	6	0	-1.950915	-1.194193	0.061488
7	6	0	-2.367719	0.126424	0.200849
8	6	0	-1.435937	1.160493	0.126582
9	8	0	0.857438	1.873609	-0.202025
10	1	0	2.357957	-0.993252	1.460084
11	1	0	3.565073	-0.819305	0.158708
12	1	0	2.659465	0.610268	0.721521
13	1	0	-0.246631	-2.489585	-0.257710
14	1	0	-2.668094	-2.004664	0.112410
15	1	0	-3.413486	0.359274	0.363618
16	1	0	-1.757949	2.193789	0.223872
17	1	0	0.429867	2.733563	-0.133693

AA (2-MP)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

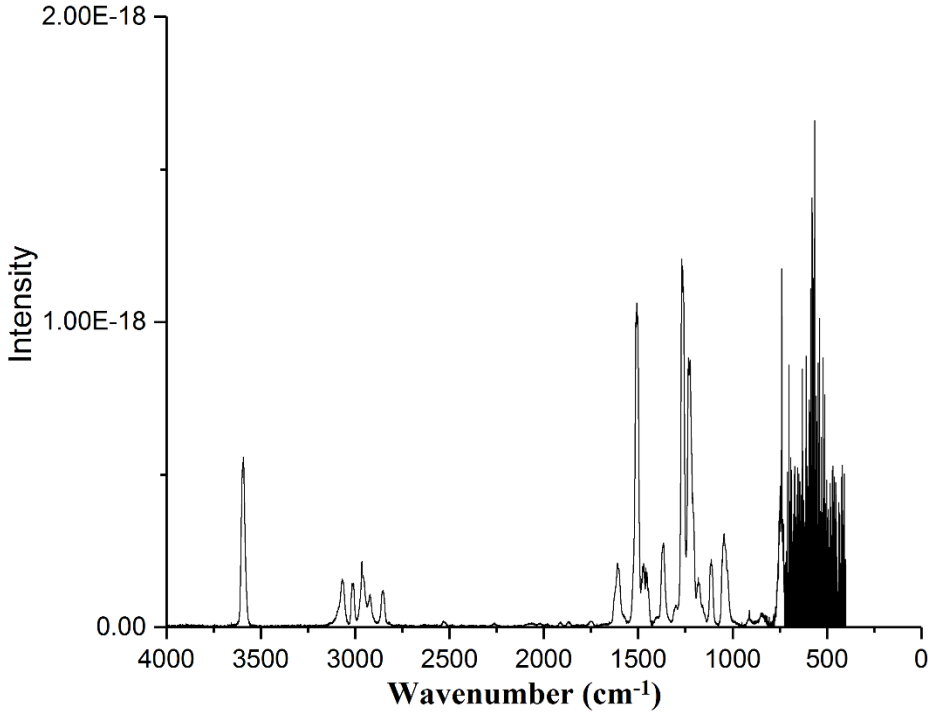
1	6	0	0.327041	2.842161	0.000000
2	8	0	-0.546606	1.723070	0.000000
3	6	0	0.000000	0.476422	0.000000
4	6	0	1.365907	0.198734	0.000000
5	6	0	-0.917786	-0.595711	0.000000
6	6	0	1.826224	-1.122416	0.000000
7	6	0	0.921495	-2.173985	0.000000
8	6	0	-0.449748	-1.903685	0.000000
9	8	0	-2.247432	-0.278769	0.000000
10	1	0	0.960039	2.856899	0.894318
11	1	0	0.960039	2.856899	-0.894318
12	1	0	-0.317267	3.719825	0.000000
13	1	0	2.082114	1.009336	0.000000
14	1	0	2.892600	-1.314488	0.000000
15	1	0	1.267029	-3.200800	0.000000
16	1	0	-1.166532	-2.720264	0.000000
17	1	0	-2.764519	-1.090921	0.000000

Table S3 Full calculated IR spectra of AS and GA of 2-MP with respect to AA (gas phase)

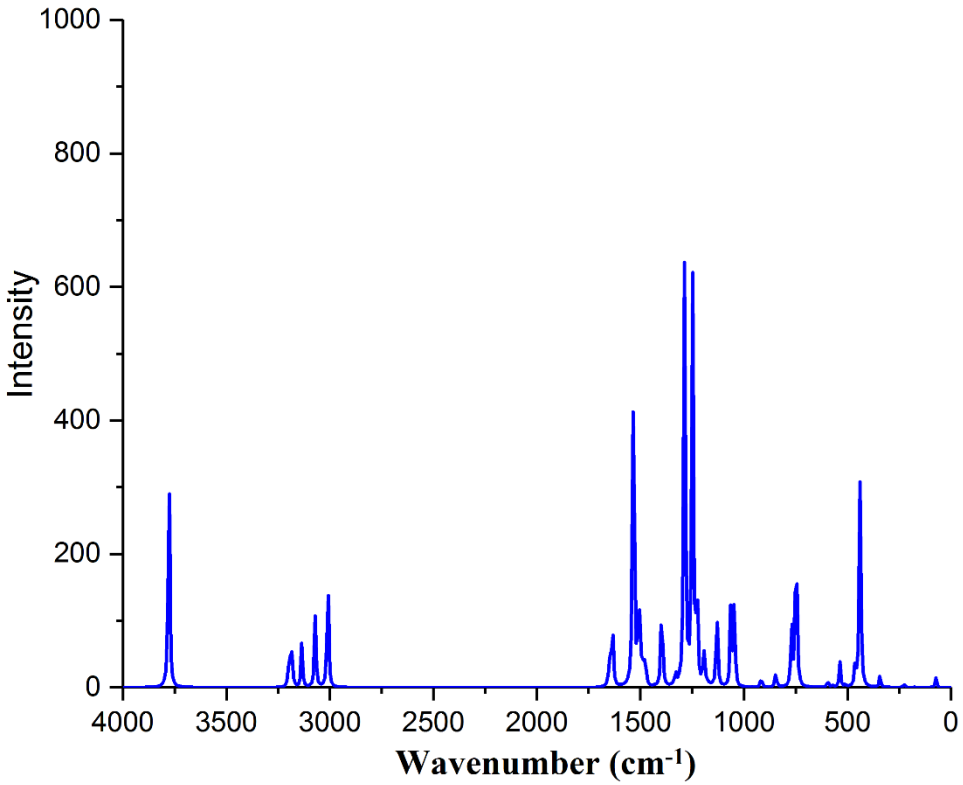
ASυ	I	AGυυ	I	AAυ	I	Δυ(AS-AA)	Δυ(AG-AA)
84.6238	314.4279	72.6262	236.6024	78.3028	227.5506	-11.9976	-6.321
168.2157	0.054547	177.0744	6.119012	136.4426	63.48296	8.8587	-31.7731
229.3674	102.3442	222.5513	20.73829	166.8878	50.41255	-6.8161	-62.4796
235.5582	359.0892	232.002	8.006239	238.5181	76.26614	-3.5562	2.9599
254.8395	1092.387	304.116	1.402316	298.259	417.057	49.2765	43.4195
312.7551	149.7068	343.0949	56.90237	316.8249	858.9487	30.3398	4.0698
343.0539	43.81601	438.7105	890.5119	359.3891	63.3694	95.6566	16.3352
463.4094	18.16973	461.6698	93.35904	439.4656	59.80843	-1.7396	-23.9438
506.5464	6.784111	509.424	9.203217	487.106	68.88116	2.8776	-19.4404
533.162	35.08106	536.3862	81.48725	556.4179	54.20072	3.2242	23.2559
569.0905	0.042061	571.4324	7.468002	578.0343	10.61407	2.3419	8.9438
597.5858	31.75238	595.5874	22.96832	600.3047	16.48646	-1.9984	2.7189
737.6709	3.556366	733.8794	1.610155	739.3301	9.647441	-3.7915	1.6592
741.3116	488.0109	747.7866	447.4847	751.0328	264.9774	6.475	9.7212
769.0158	74.93584	769.5286	143.5466	762.198	209.4983	0.5128	-6.8178
830.4984	0.113846	845.614	32.85537	845.9737	37.75851	15.1156	15.4753
846.7486	74.35627	845.6386	0.588758	855.071	99.74858	-1.11	8.3224
898.4801	21.32344	916.185	22.2769	934.816	11.73583	17.7049	36.3359
944.2126	0.081122	959.875	0.736057	968.8818	0.685568	15.6624	24.6692
1054.215	103.8001	1046.605	141.4461	1028.032	222.2096	-7.6096	-26.1831
1070.14	98.03728	1062.612	142.1139	1059.582	67.6319	-7.5278	-10.5575
1124.845	456.2151	1130.526	135.3368	1110.679	214.7347	5.6807	-14.1661
1166.957	2.085024	1169.635	1.750425	1169.893	9.506207	2.6784	2.936
1181.492	99.02081	1180.361	7.570775	1176.325	69.44821	-1.1303	-5.1665
1186.12	171.9512	1193.939	55.52126	1182.347	111.701	7.8192	-3.7731
1207.334	53.9269	1227.168	169.4514	1204.27	124.0335	19.8344	-3.0632
1261.807	493.269	1248.637	575.0963	1251.951	284.5833	-13.17	-9.8561
1295.797	514.8227	1286.312	665.0352	1289.276	473.5744	-9.485	-6.5212
1328.135	54.02289	1330.453	16.76416	1310.746	215.5535	2.3173	-17.3892
1379.438	178.2235	1396.803	123.3386	1357.974	130.7581	17.3652	-21.4637
1472.884	10.15657	1476.895	37.81284	1468.073	14.016	4.0106	-4.8111
1487.349	77.18651	1490.608	25.81051	1485.538	83.87644	3.2588	-1.811
1491.346	23.43086	1497.147	7.594035	1488.842	7.022784	5.8004	-2.5047
1504.418	89.70123	1506.861	113.4801	1509.423	25.94311	2.4425	5.0048
1546.835	367.8496	1533.142	465.4125	1537.405	293.3192	-13.6923	-9.4301
1630.304	94.78508	1635.18	86.19711	1632.558	35.36667	4.876	2.2541
1645.102	52.6158	1650.277	30.2012	1638.518	39.28632	5.1746	-6.5845
3000.305	75.66918	3010.18	68.23039	3012.302	89.55576	9.8751	11.9973
3057.439	52.42962	3070.806	43.49523	3090.639	37.569	13.367	33.1997
3132.469	26.71337	3135.721	24.0464	3130.304	26.56757	3.2526	-2.1645
3145.87	19.096	3170.771	0.752517	3144.241	17.12632	24.9014	-1.6288
3173.35	6.258879	3183.785	16.65335	3172.711	4.299209	10.435	-0.6392
3190.006	21.45216	3193.946	15.72666	3184.591	16.48916	3.9398	-5.4148
3205.474	7.046064	3201.72	5.872977	3195.465	10.60838	-3.7542	-10.0093

3834.71	65.99254	3777.938	109.3241	3834.83	67.21626	-56.7714	0.1207

Figure S1 Experiment measurement of IR of 2-MP in gas phase and calculated IR for AS conformer of 2-MP in gas phase.



(a) Measured FTIR [10]



(b) The calculated IR.

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