Supplementary Material (ESI) for New Journal of Chemistry

A tautomeric equilibrium between functionalized 2-formylphenylboronic acids and corresponding 1,3-dihydro-1,3-dihydroxybenzo[c][2,1]oxaboroles

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Electronic Supplementary Information

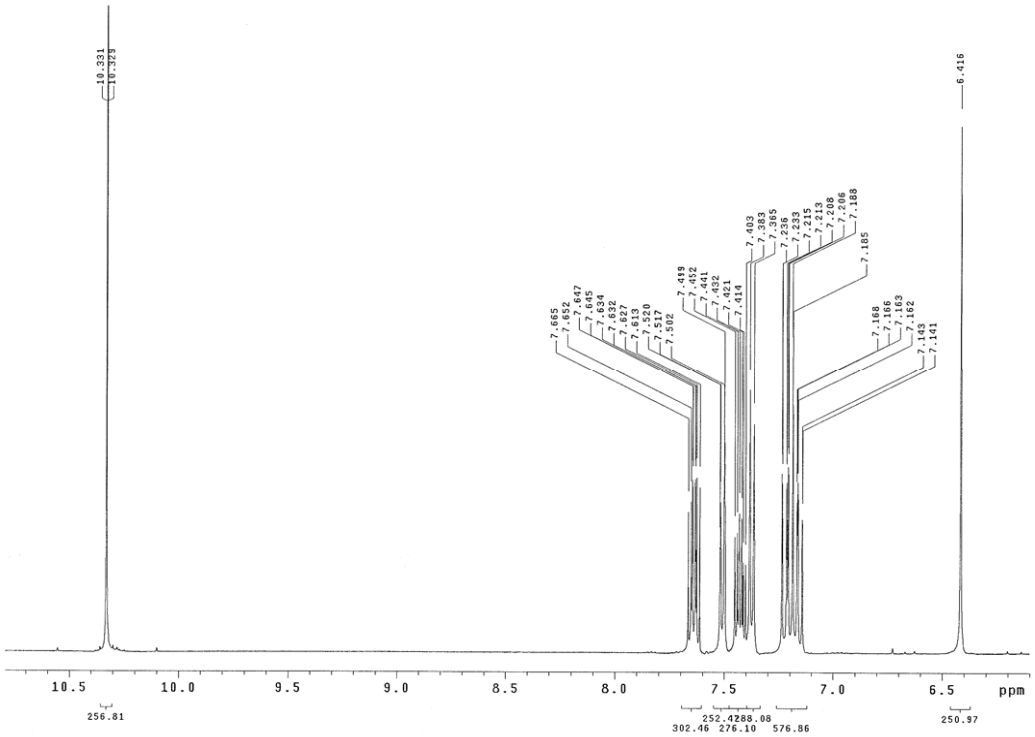


Figure 1. The ^{1}H NMR spectrum of **1**.

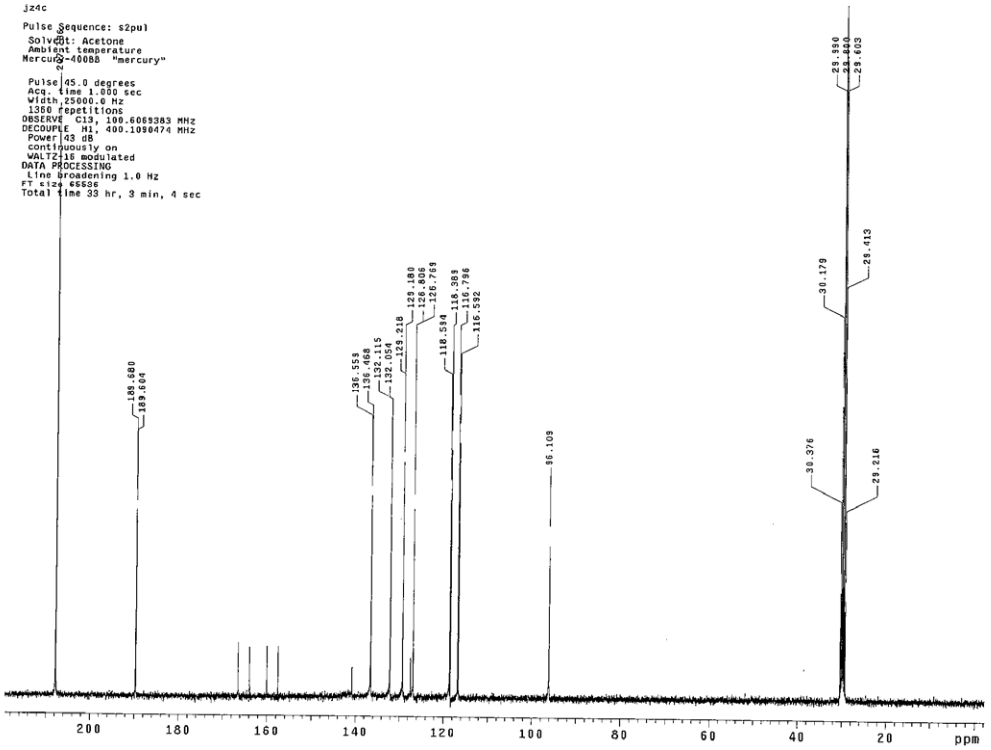


Figure 2. The ^{13}C{^{1}H} NMR spectrum of **1**.

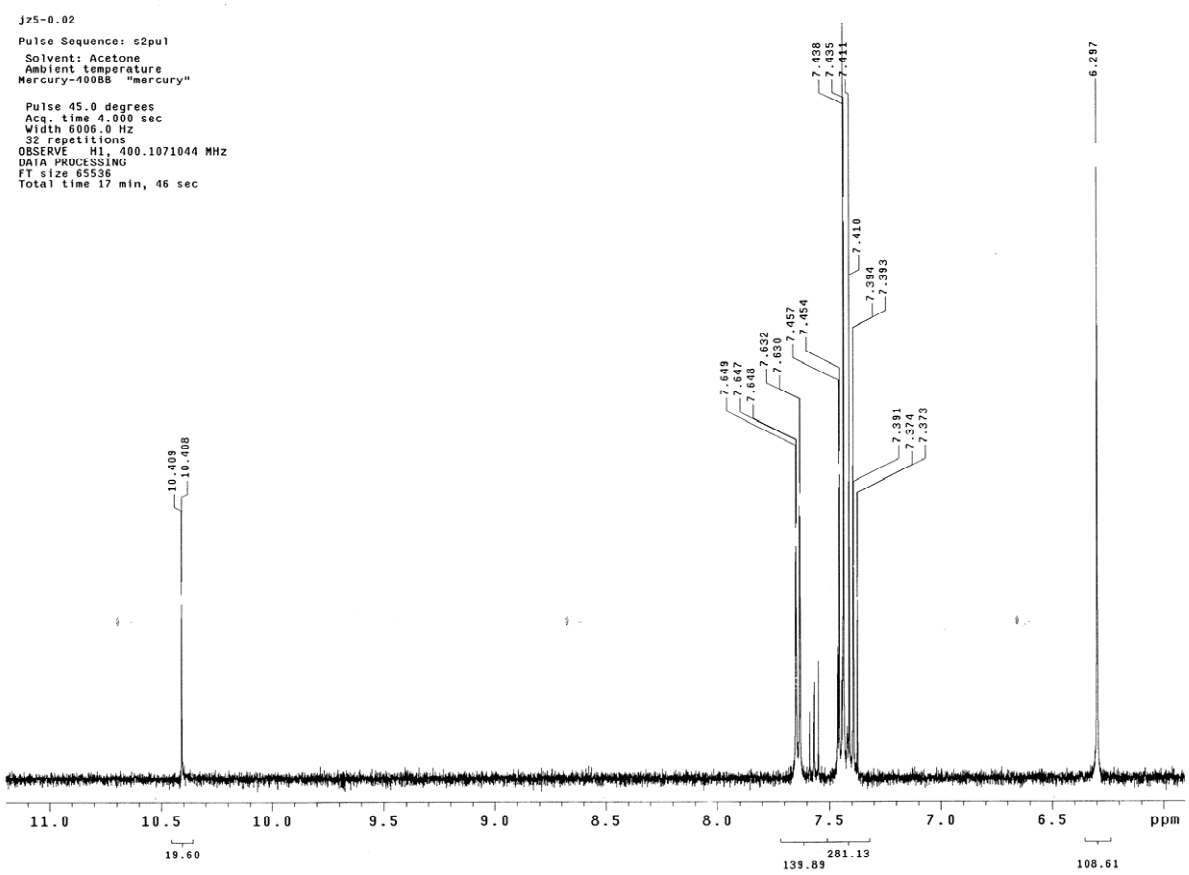


Figure 3. The ^{1}H NMR spectrum of **2**.

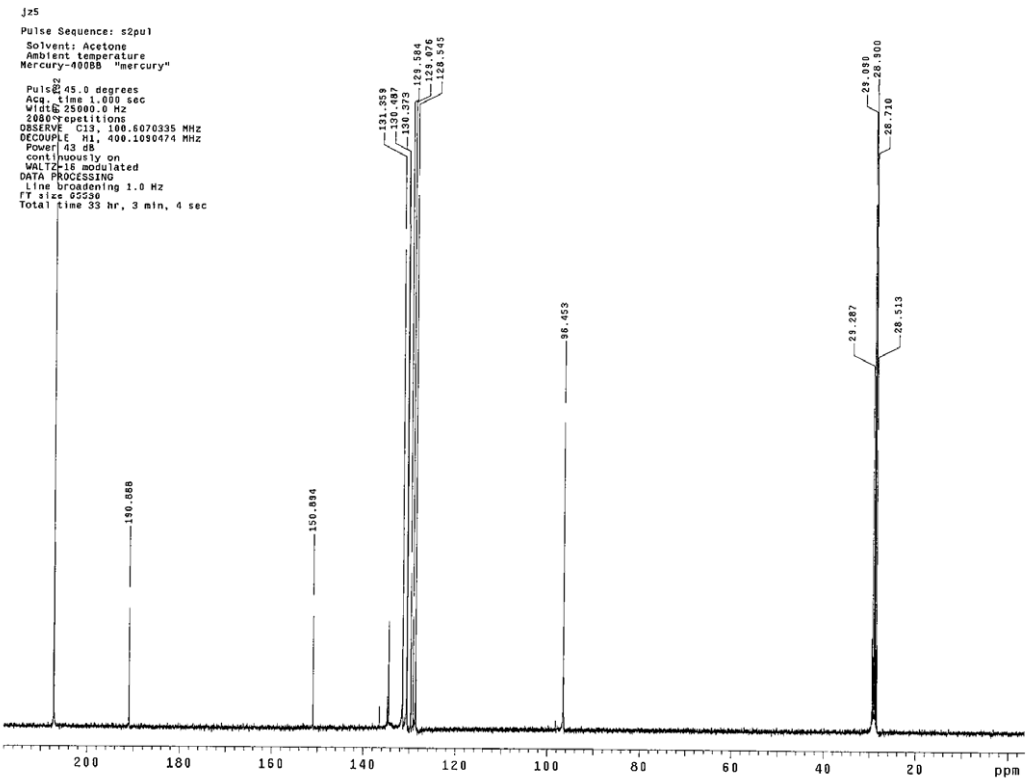


Figure 4. The $^{13}C\{^{1}H\}$ NMR spectrum of **2**.

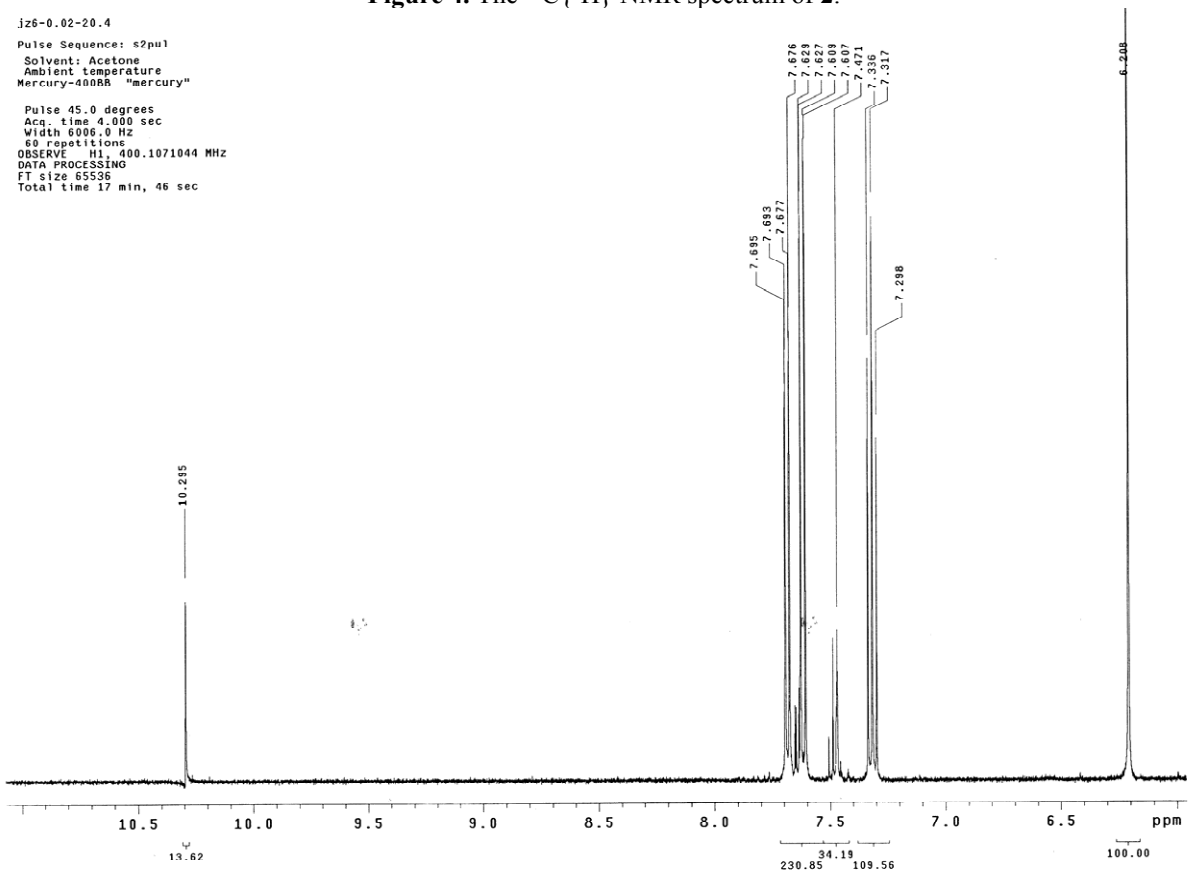


Figure 5. The ^{1}H NMR spectrum of **3**.

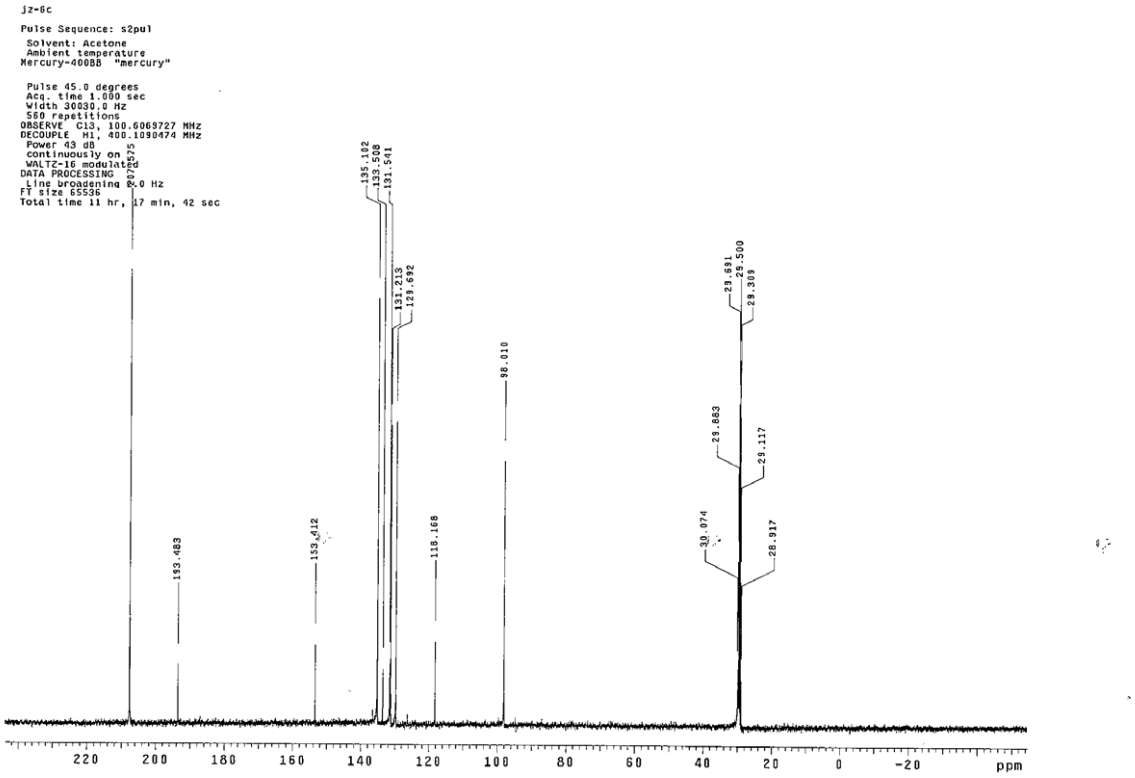


Figure 6. The $^{13}C\{^{1}H\}$ NMR spectrum of **3**.

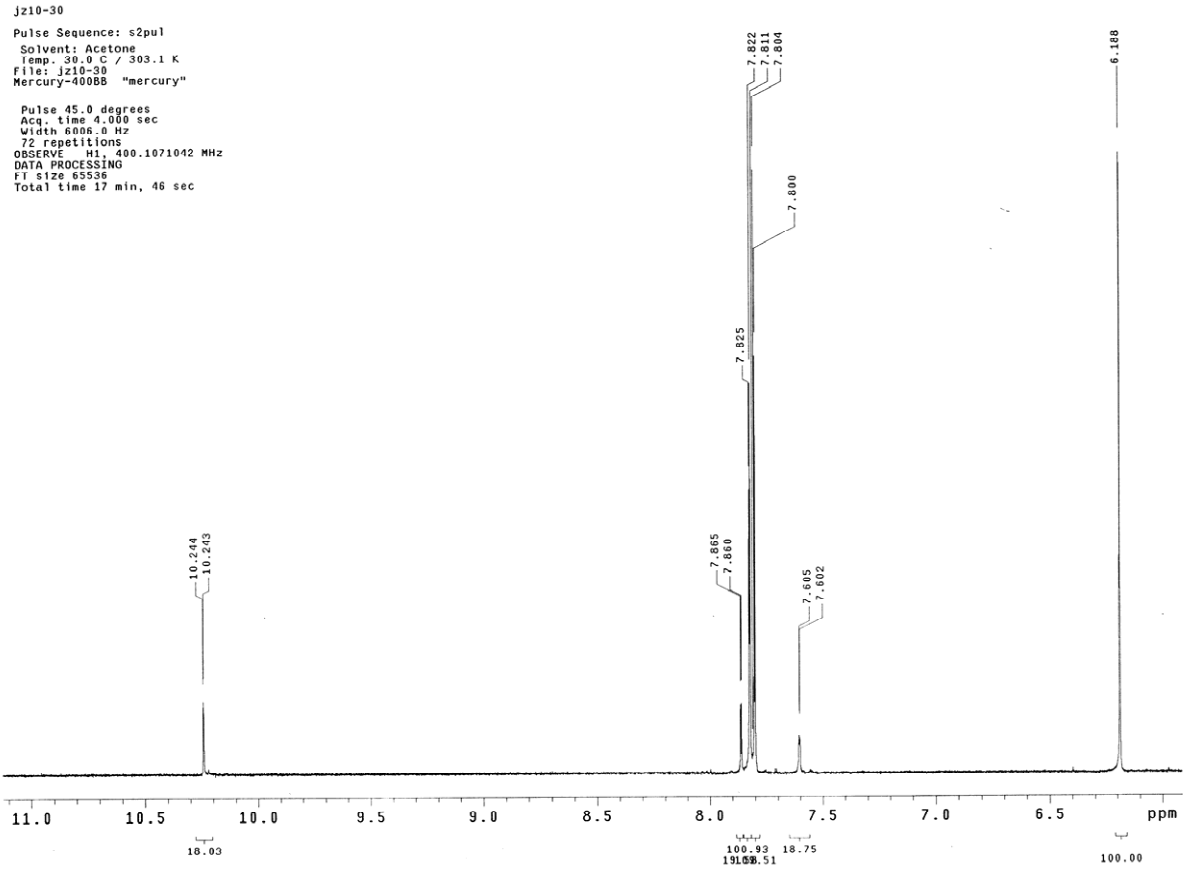


Figure 7. The ^{1}H NMR spectrum **5**.

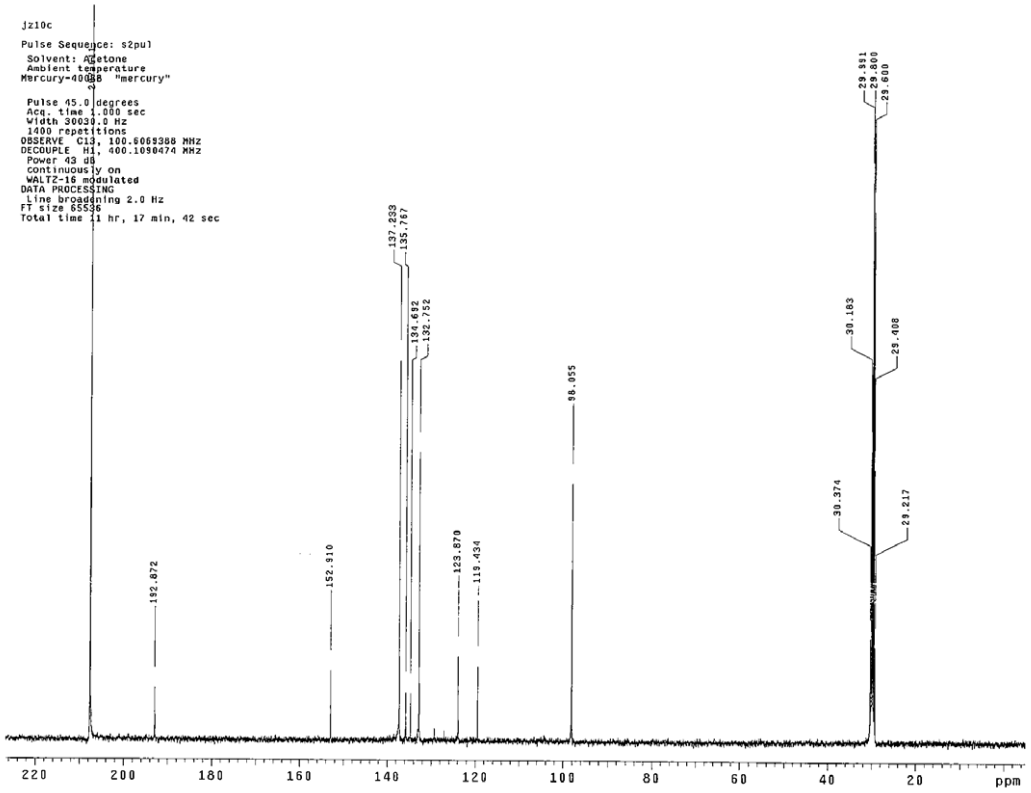


Figure 8. The $^{13}C\{^{1}H\}$ NMR spectrum of **5**.

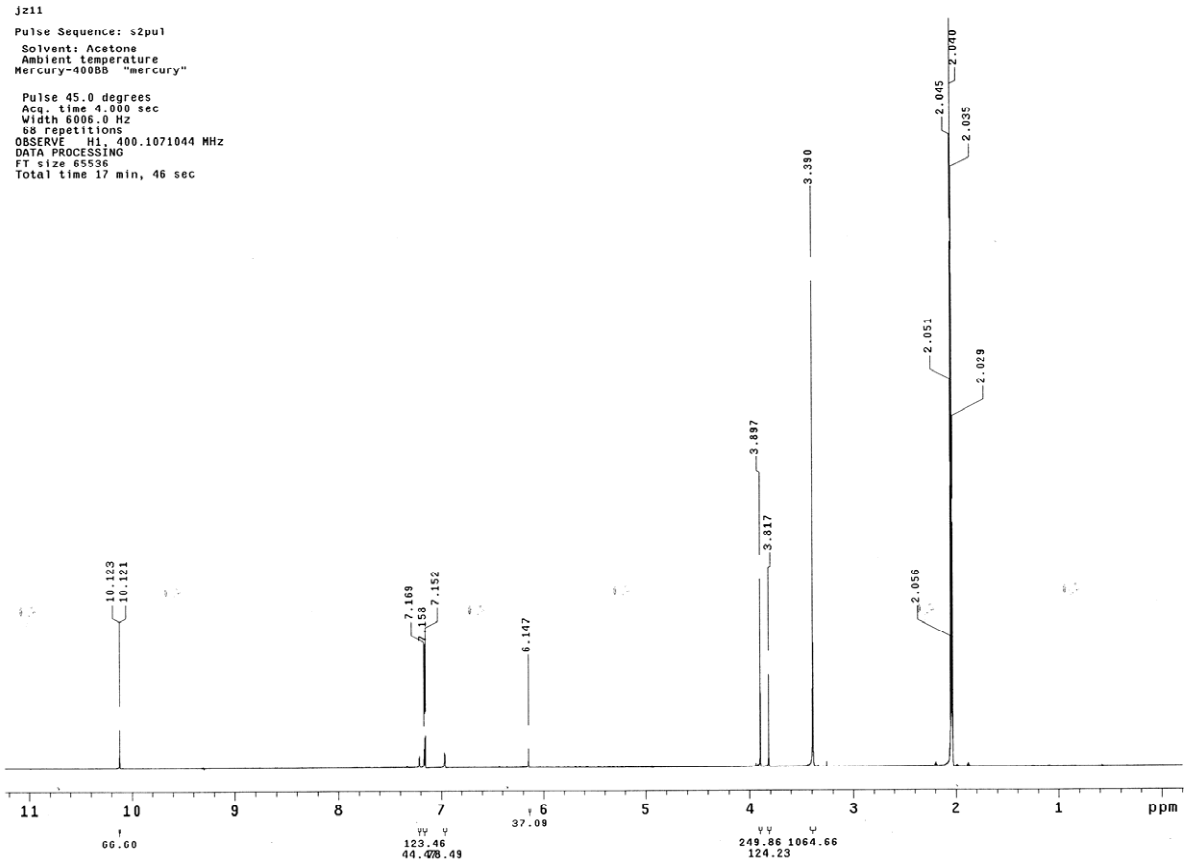


Figure 9. The ^{1}H NMR spectrum of **6**.

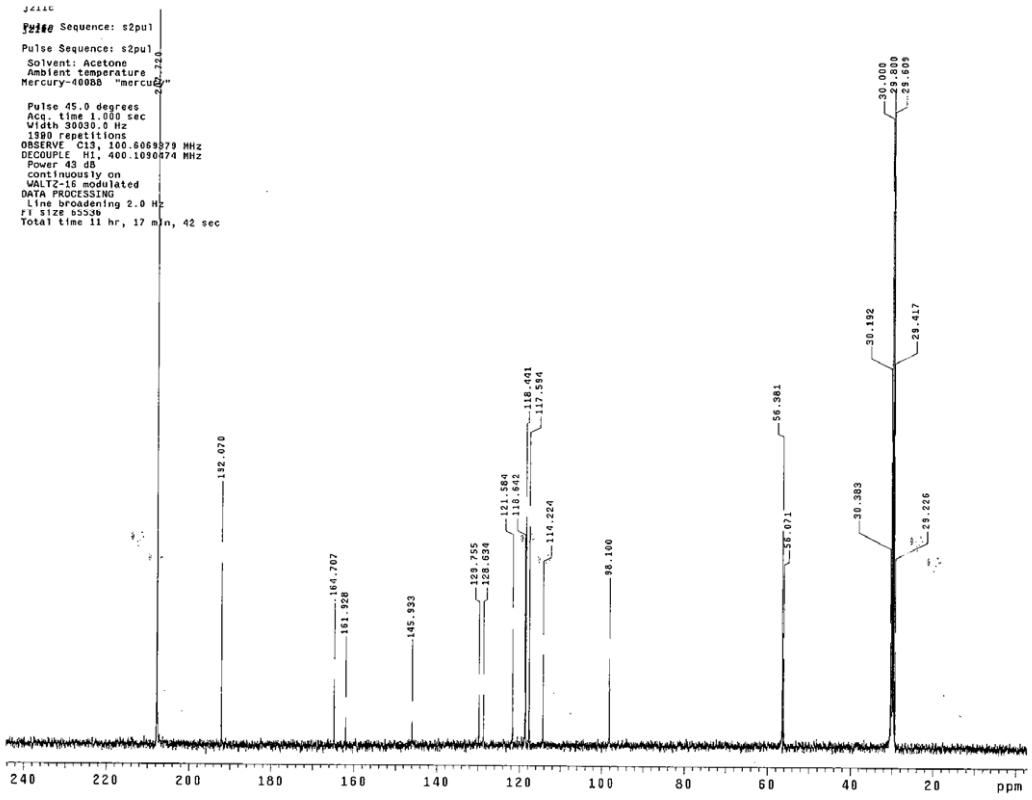


Figure 10. The $^{13}C\{^{1}H\}$ NMR spectrum of **6**.

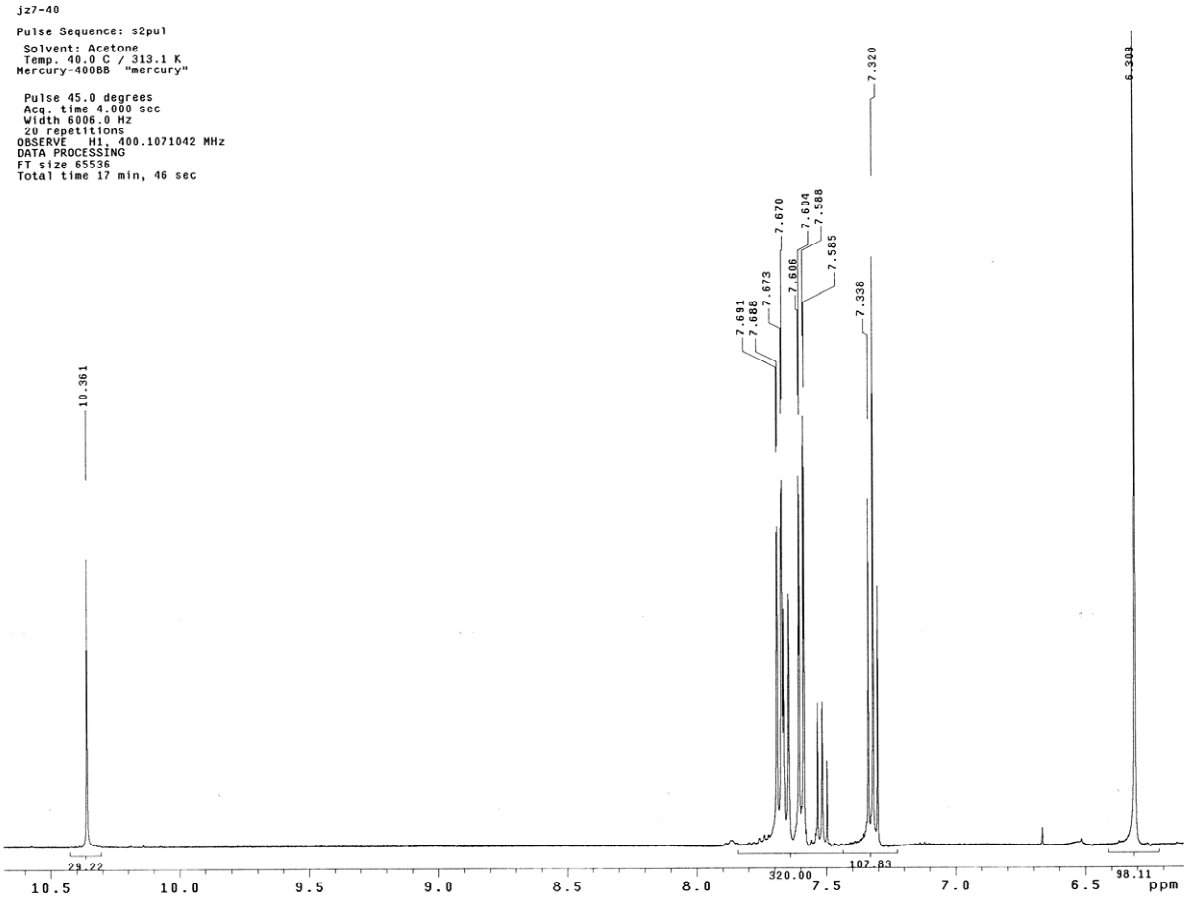


Figure 11. The ^{1}H NMR spectrum **7**.

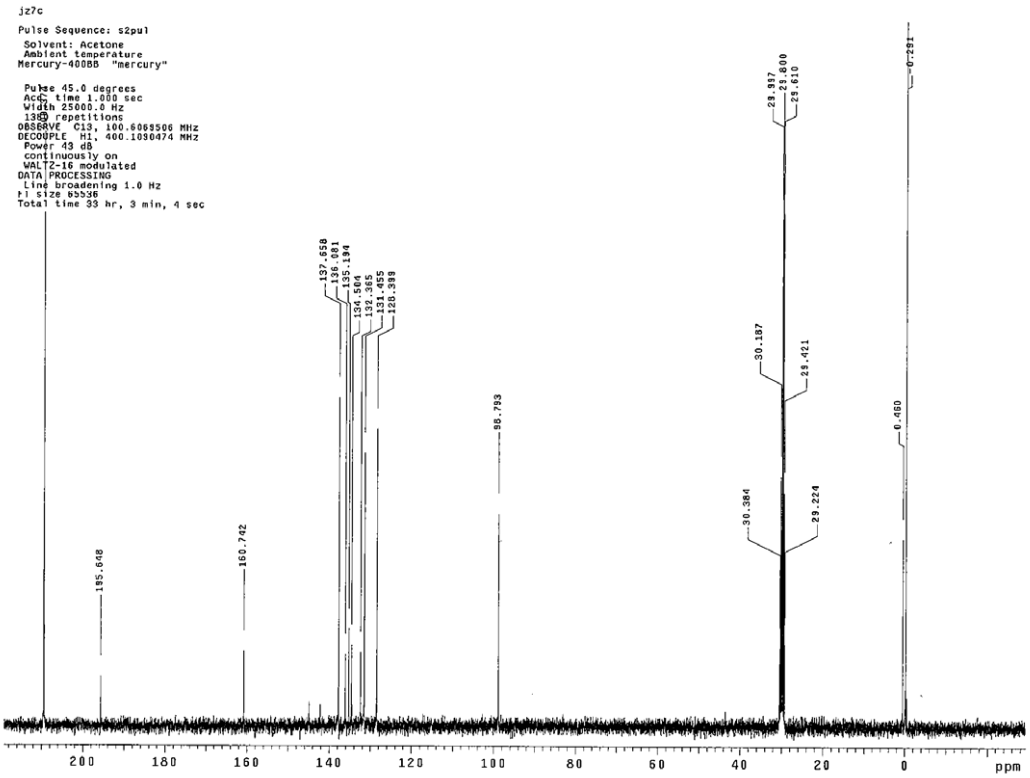


Figure 12. The $^{13}C\{^{1}H\}$ NMR spectrum of **7**.

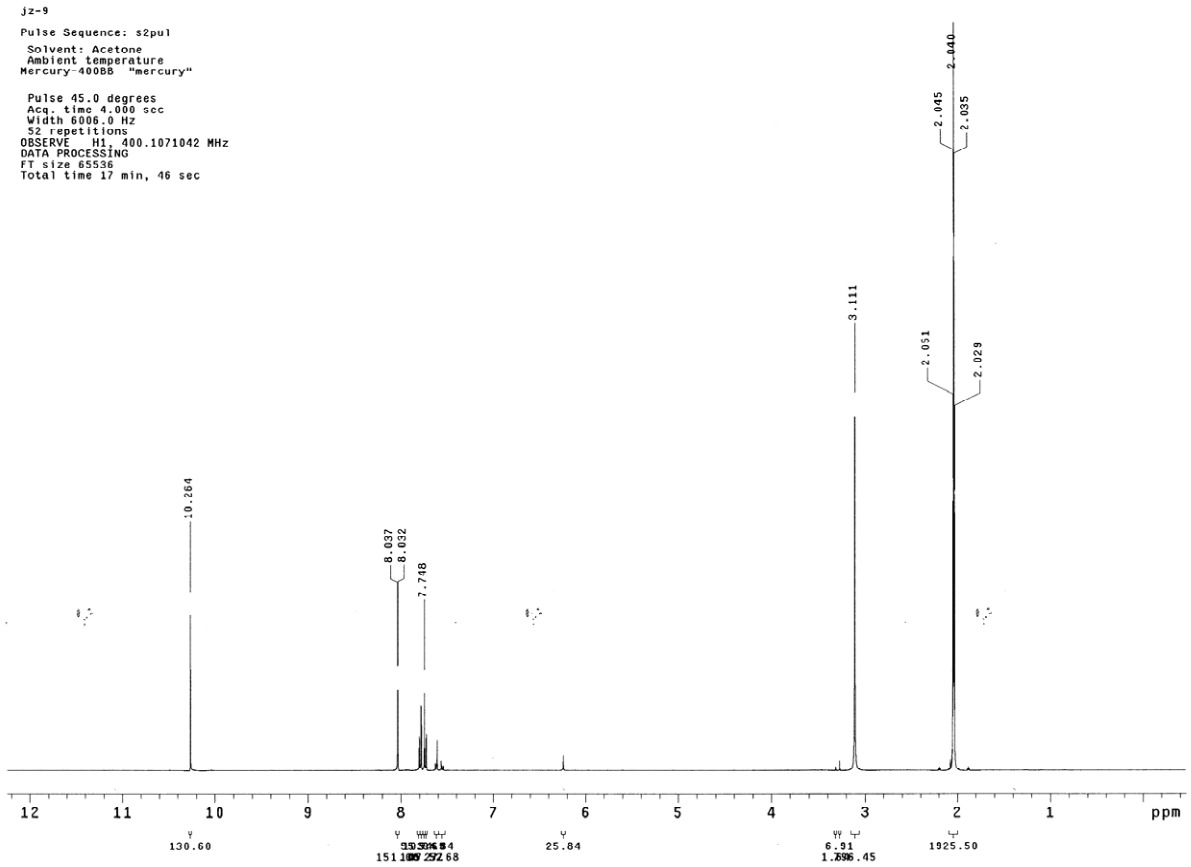


Figure 13. The ^{1}H NMR spectrum **8**.

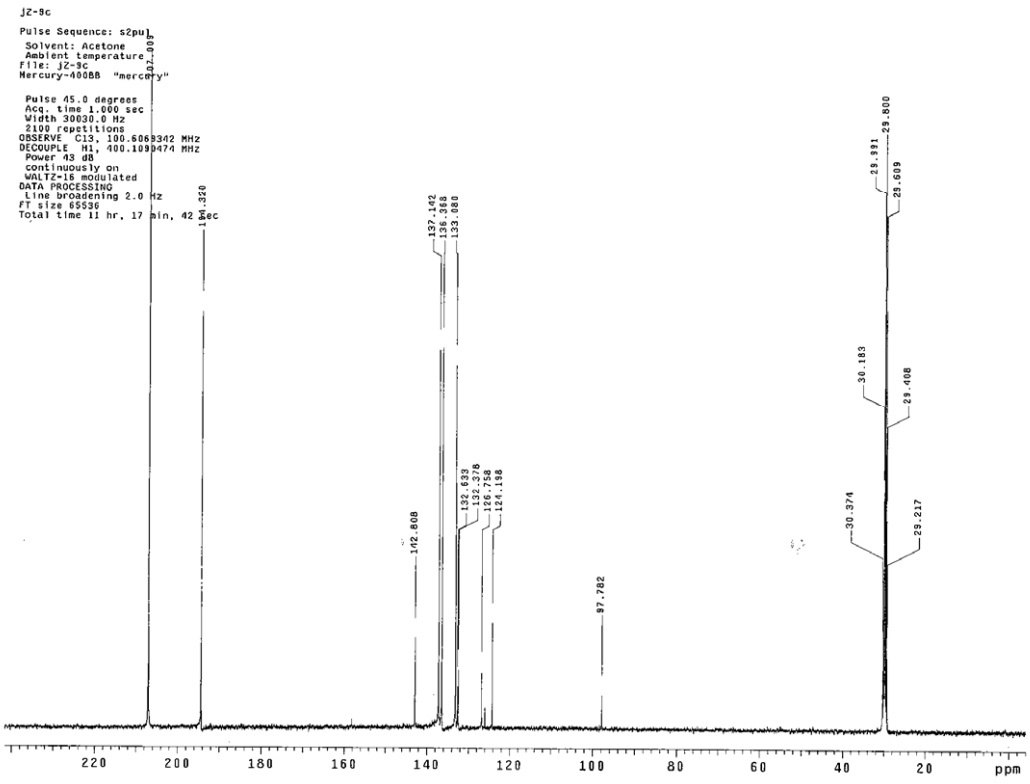


Figure 14. The $^{13}C\{^{1}H\}$ NMR spectrum of **8**.

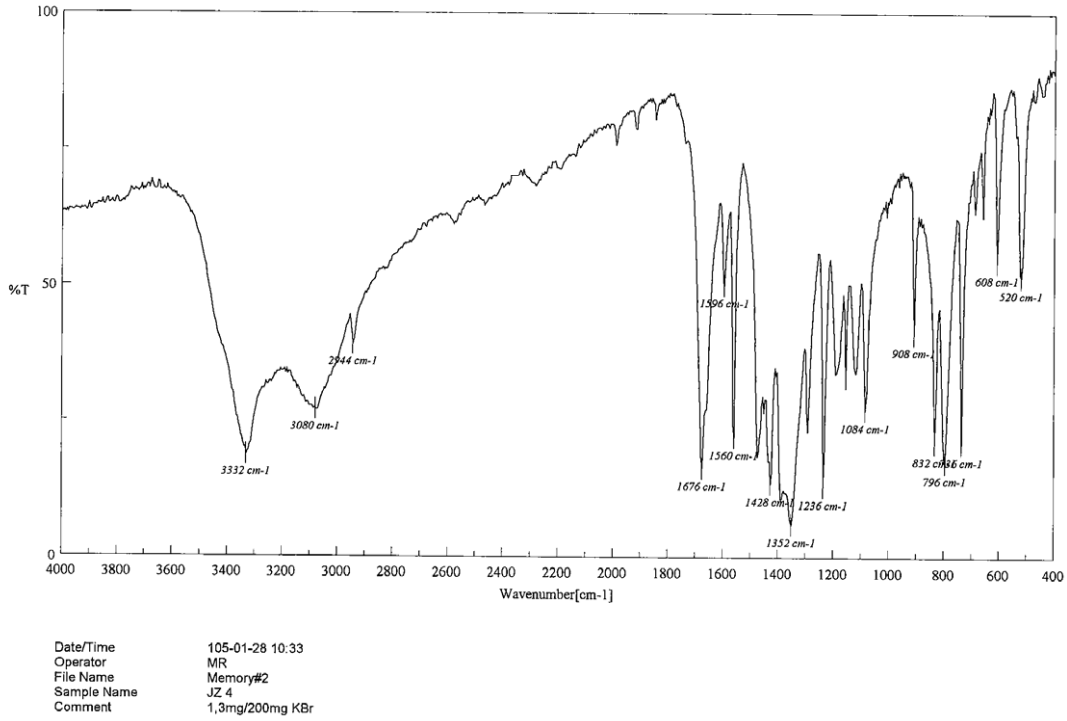


Figure 15. The IR spectrum of **1**.

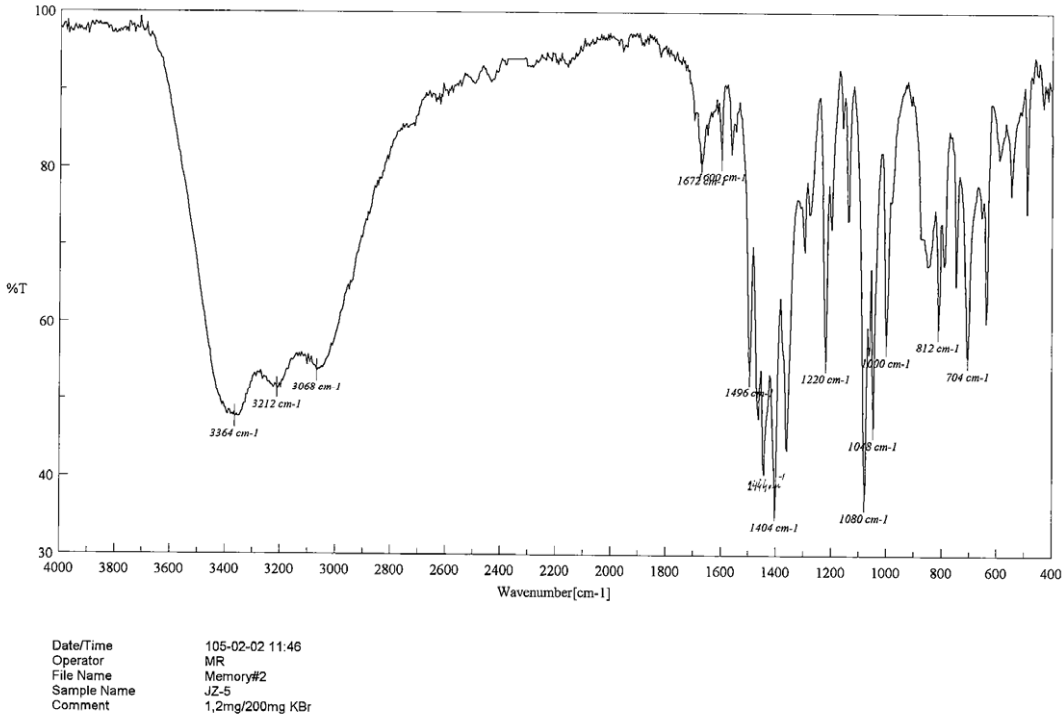


Figure 16. The IR spectrum of **2**.

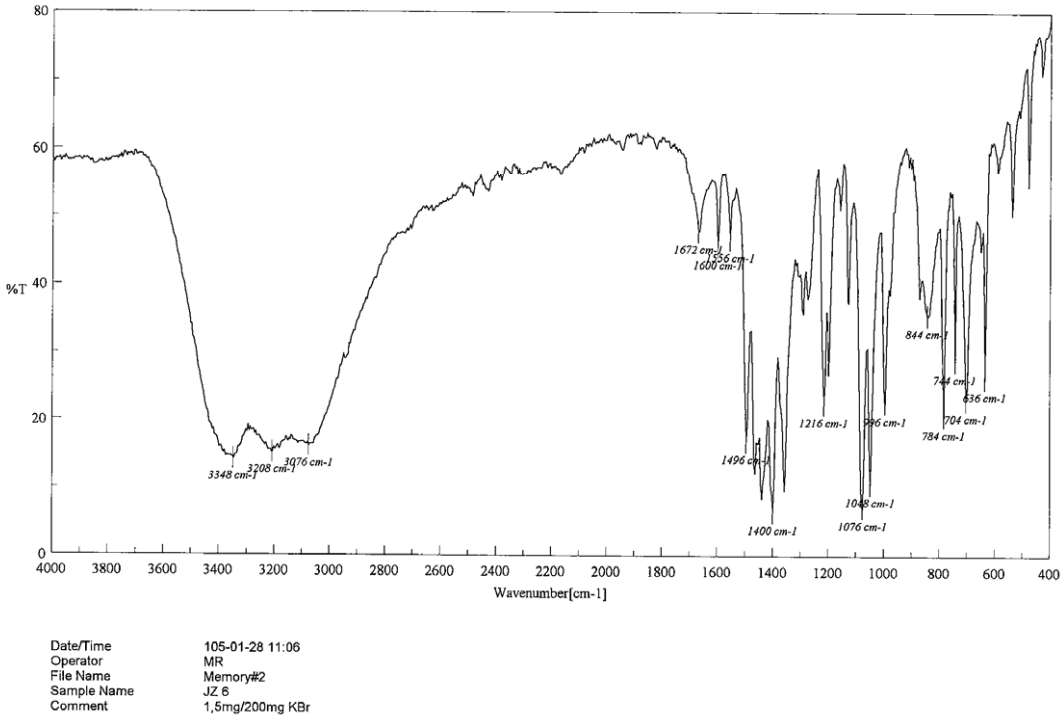


Figure 17. The IR spectrum of **3**.

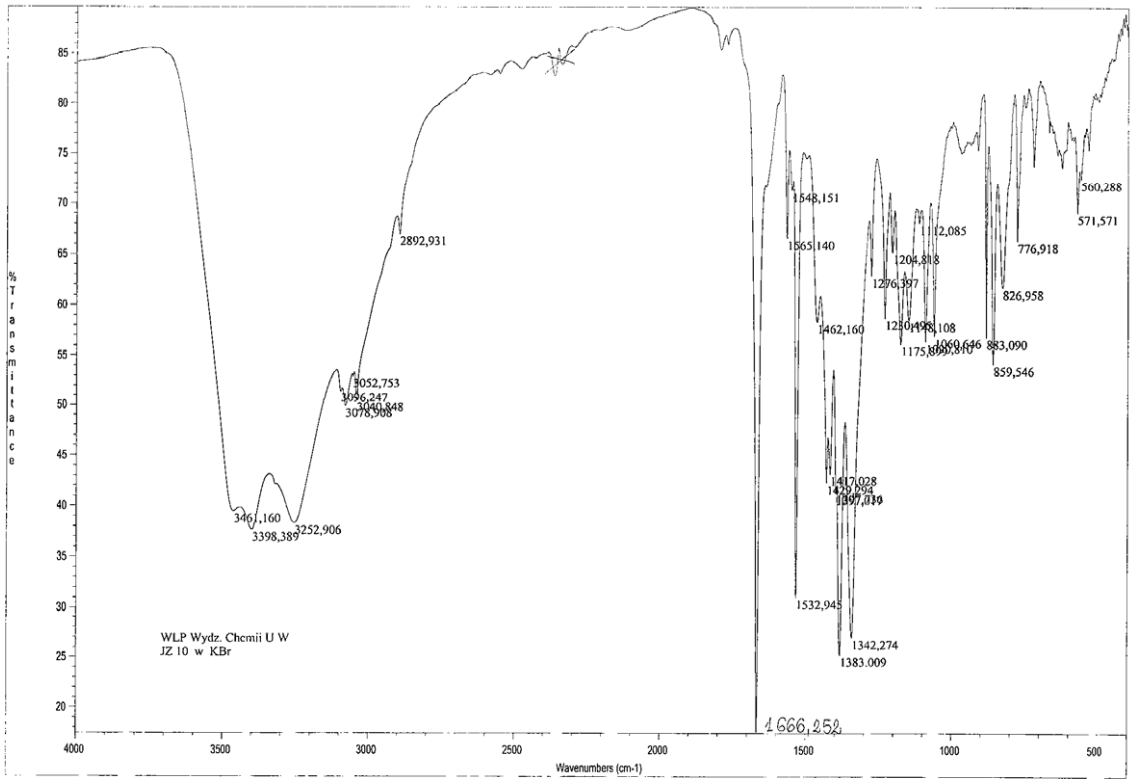


Figure 18. The IR spectrum of **5**.

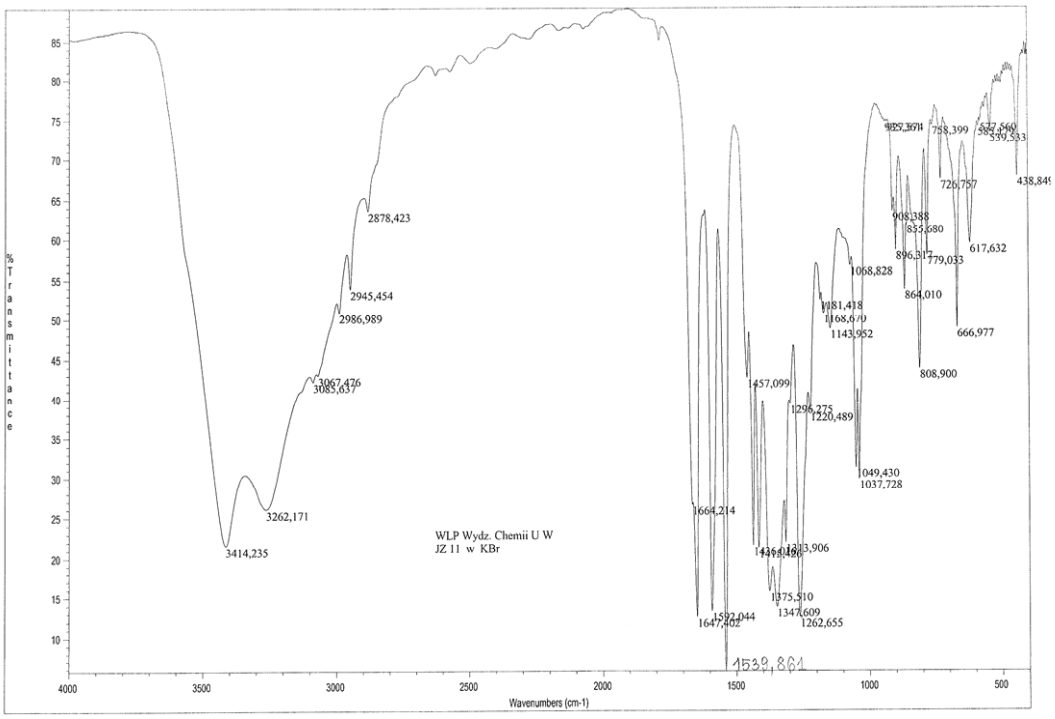


Figure 19. The IR spectrum of **6**.

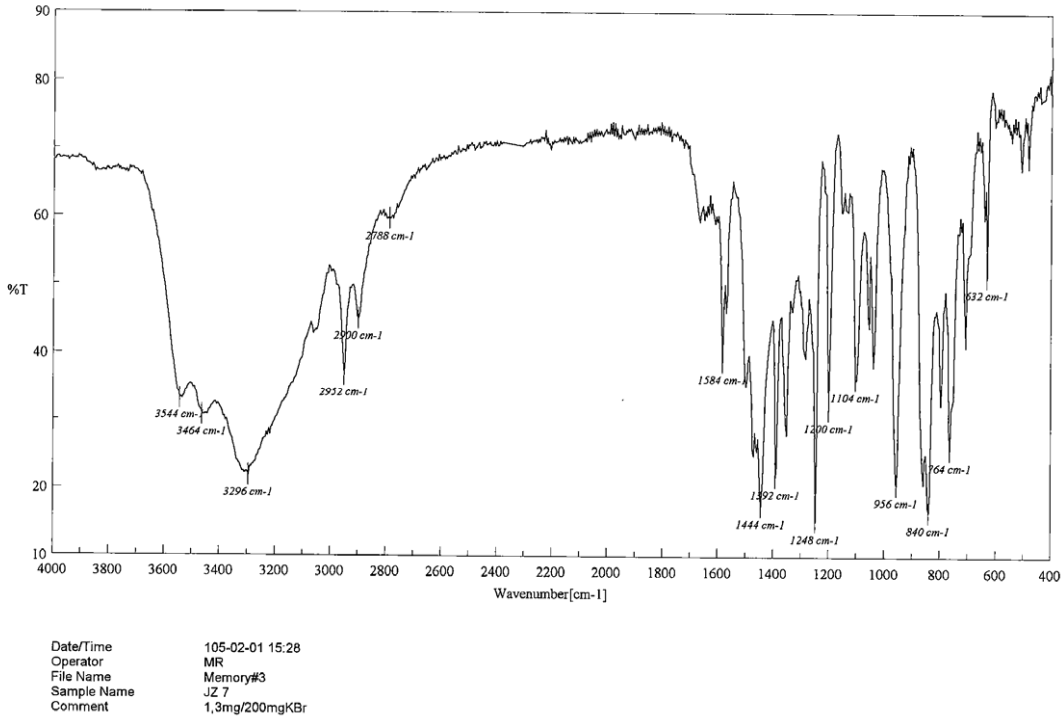


Figure 20. The IR spectrum of **7**.

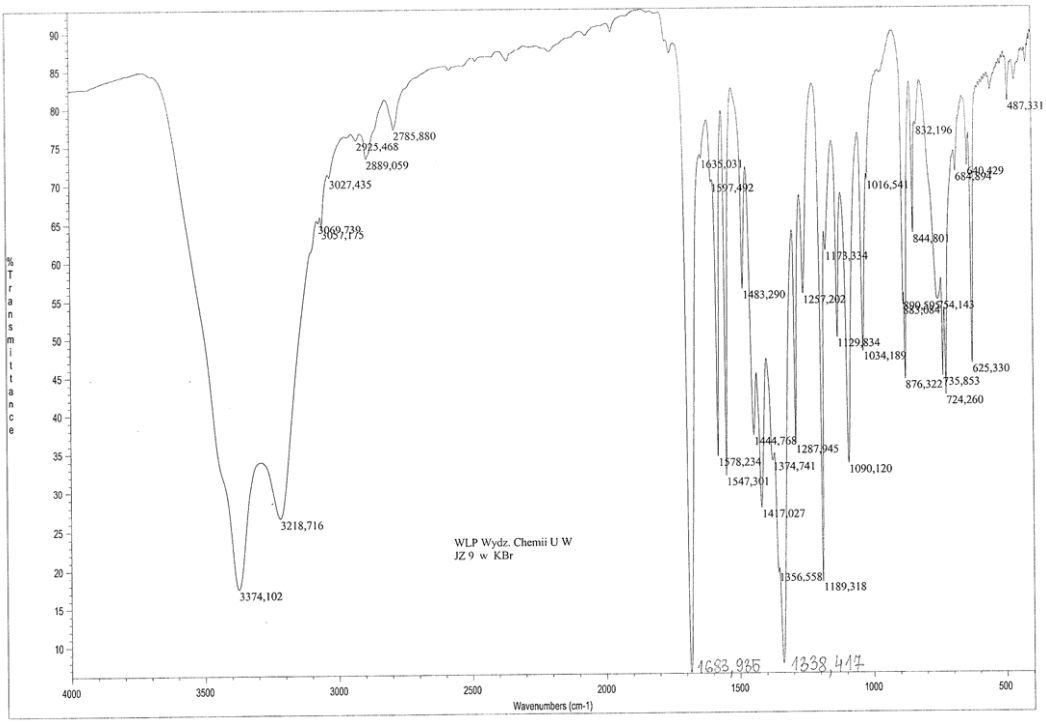


Figure 21. The IR spectrum of **8**.

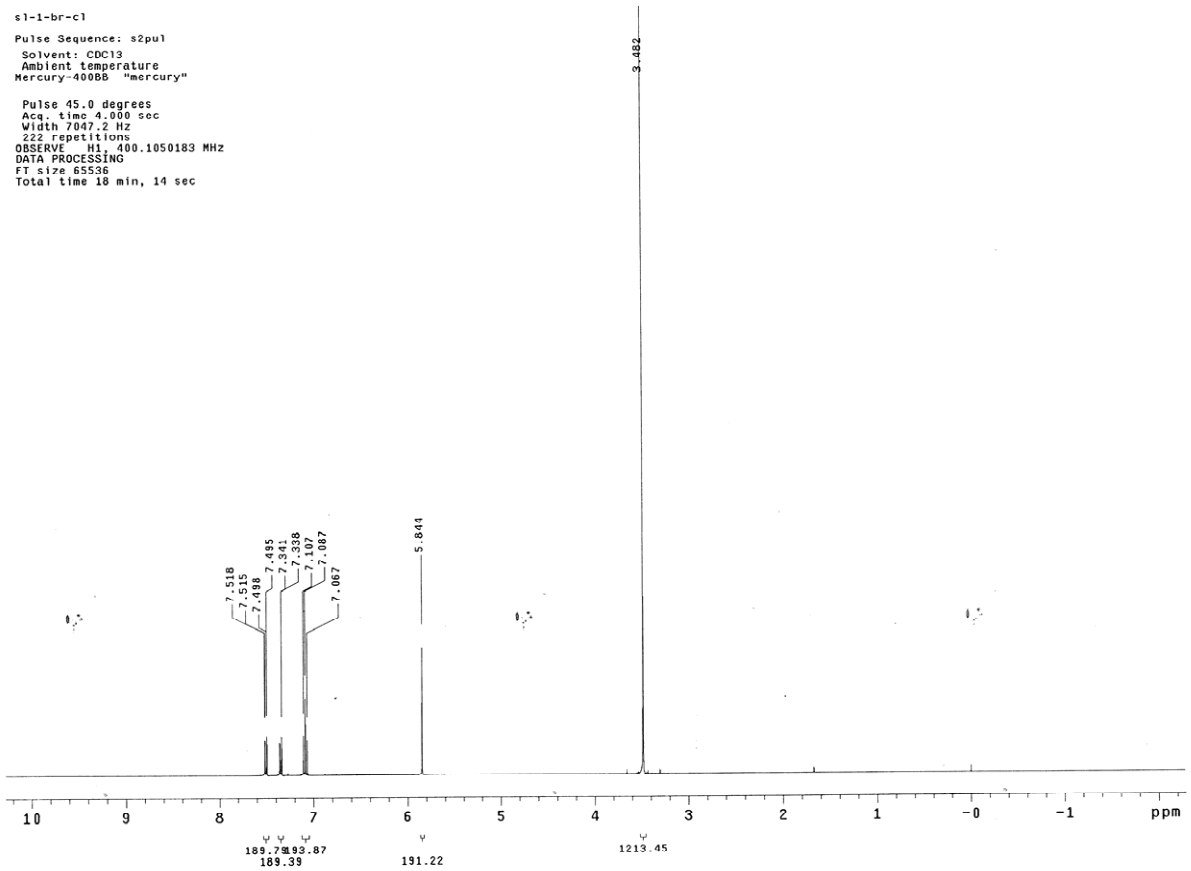


Figure 22. The ^{1}H NMR spectrum of 1-bromo-3-chloro-2-(dimethoxymethyl)benzene.

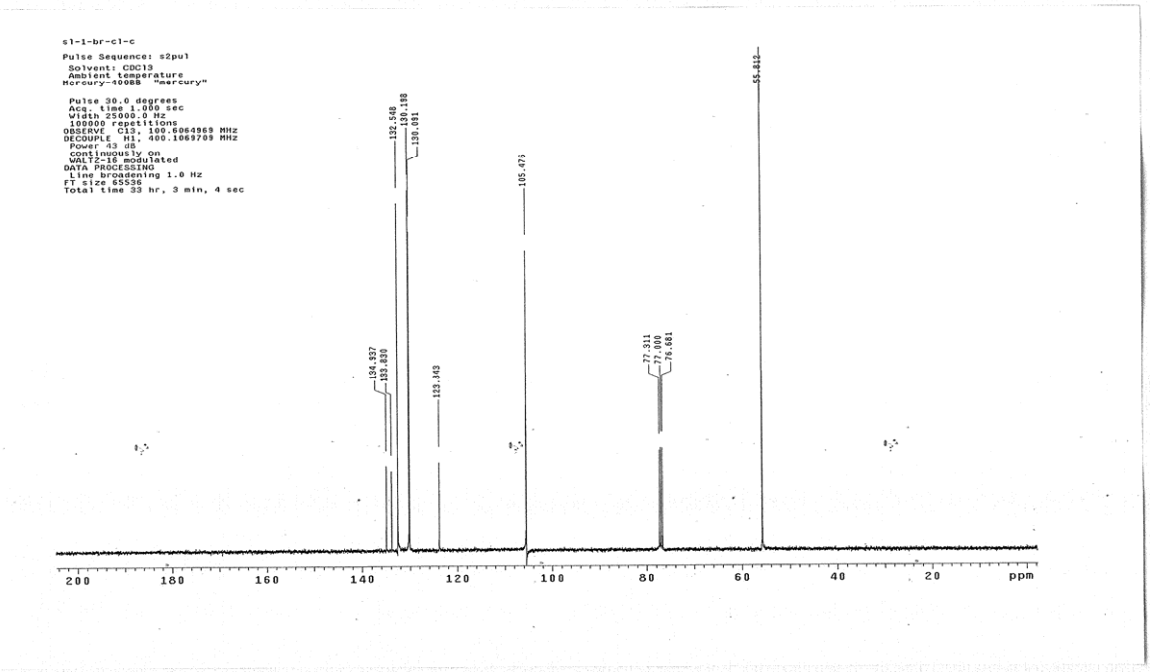


Figure 23. The $^{13}C\{^{1}H\}$ NMR spectrum of 1-bromo-3-chloro-2-(dimethoxymethyl)benzene.

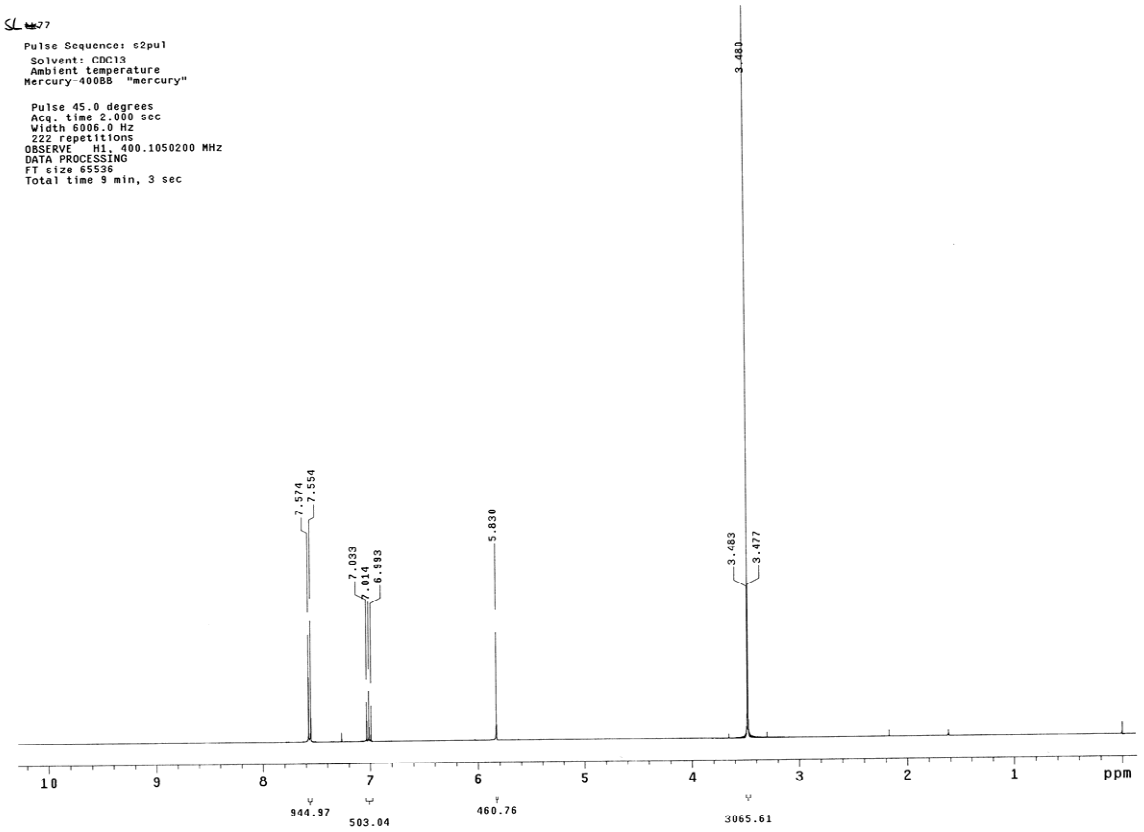


Figure 24. The $^{13}C\{^{1}H\}$ NMR spectrum of 1,3-dibromo-2-(dimethoxymethyl)benzene.

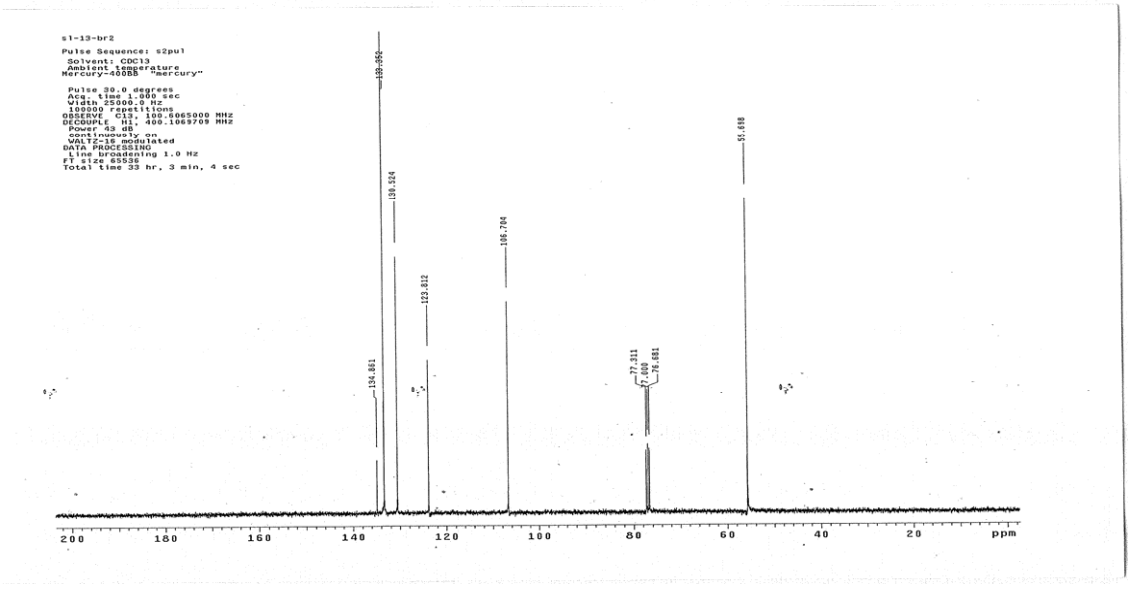


Figure 25. The $^{13}C\{^{1}H\}$ NMR spectrum of 1,3-dibromo-2-(dimethoxymethyl)benzene.

Table 1. Equilibrium constants K_{cycl} for compounds **1–3**, **5–8** at variable temperature.

1		**2**		**3**		**5**	
T/K	K_{cycl}	T/K	K_{cycl}	T/K	K_{cycl}	T/K	K_{cycl}
293	1.09	293.5	5.54	293.5	7.34	295.5	5.55
303	0.94	303	4.74	303	6.22	303	4.94
313	0.82	313	4.11	313	5.18	313	4.29
321	0.74	321	3.55	321	4.57	321	3.74

6		**7**		**8**	
T/K	K_{cycl}	T/K	K_{cycl}	T/K	K_{cycl}
295.5	0.49	293.5	5.21	293	0.21
303	0.46	303	4.21	303	0.19
313	0.41	313	3.31	313	0.17
321	0.37	321	2.82	321	0.16

Table 2. Calculated geometries of 2-formylphenylboronic acid.

form	**I** (planar)				**II**				**I**-(twisted)			
	B3LYP	MP2			B3LYP	MP2			B3LYP	MP2		
		6-31G*	6-31+G*	aug-cc-pVDZ		6-31G*	6-31+G*	aug-cc-pVDZ		6-31G*	6-31+G*	aug-cc-pVDZ
Bond Lengths												
O(1)–B(1)	1.375	1.380	1.383	1.390	1.357	1.363	1.365	1.371	1.363	1.369	1.371	1.378
O(2)–B(1)	1.351	1.359	1.362	1.366	1.382	1.387	1.391	1.396	1.372	1.379	1.381	1.387
C(1)–B(1)	1.594	1.594	1.594	1.597	1.556	1.557	1.557	1.565	1.587	1.584	1.584	1.589
O(3)–C(7)	1.219	1.234	1.236	1.235	1.396	1.398	1.402	1.405	1.214	1.231	1.234	1.232
C(1)–C(2)	1.425	1.424	1.426	1.432	1.401	1.401	1.404	1.413	1.411	1.409	1.411	1.419
Bond Angles												
O(1)–B(1)–O(2)	117.99	117.90	117.63	118.36	122.53	122.81	122.77	123.00	118.27	118.52	118.66	118.60
O(1)–B(1)–C(1)	115.09	114.46	114.66	114.78	128.74	128.06	128.21	127.93	118.10	117.68	117.52	117.81
O(2)–B(1)–C(1)	126.92	127.64	127.71	126.86	108.73	109.13	109.01	109.07	122.98	123.08	123.17	122.93
O(3)–C(7)–C(2)	128.53	128.51	128.21	128.38	114.96	113.88	114.09	114.00	123.89	123.11	122.77	122.81
C(7)–C(2)–C(1)	126.36	126.34	126.49	126.37	110.71	110.96	111.03	110.93	119.63	118.54	118.66	118.38
C(2)–C(1)–B(1)	128.33	128.98	128.90	128.45	104.51	104.12	104.18	104.09	122.62	122.17	121.64	121.81
Torsion angles												
C(2)-C(1)-B(1)-O(2)	-0.11	0.06	-2.32	-0.01	0.93	1.07	1.48	1.04	-95.57	-94.15	-103.05	-94.75
C(1)-C(2)-C(7)-O(3)	-0.04	-0.02	4.21	-0.03	-124.53	-123.69	-123.36	-123.27	3.22	3.22	5.76	2.51
HBond geometry												
H...O(3)	1.690	1.720	1.728	1.682								
O(2)...O(3)	2.634	2.671	2.675	2.641								
O(2)-H(2)...O(3)	160.68	161.58	159.91	164.03								

Table 3. Calculated geometries of **1**.

	I (planar)				**II**				**I**-(twisted)			
	B3LYP	MP2			B3LYP	MP2			B3LYP	MP2		
		6-31G*	6-31+G*	aug-cc-pVDZ		6-31G*	6-31+G*	aug-cc-pVDZ		6-31G*	6-31+G*	aug-cc-pVDZ
Bond Lengths												
O(1)–B(1)	1.375	1.380	1.382	1.390	1.356	1.362	1.364	1.370	1.362	1.368	1.371	1.378
O(2)–B(1)	1.349	1.357	1.362	1.364	1.379	1.386	1.389	1.395	1.371	1.378	1.380	1.387
C(1)–B(1)	1.599	1.597	1.596	1.600	1.559	1.559	1.560	1.568	1.590	1.586	1.586	1.591
O(3)–C(7)	1.221	1.235	1.237	1.237	1.393	1.396	1.398	1.402	1.215	1.232	1.235	1.234
C(1)–C(2)	1.429	1.427	1.428	1.436	1.402	1.402	1.405	1.414	1.412	1.410	1.412	1.419
F(1)–C(3)	1.357	1.362	1.371	1.371	1.353	1.355	1.364	1.364	1.355	1.360	1.369	1.369
Bond Angles												
O(1)–B(1)–O(2)	118.10	117.95	117.88	118.37	122.93	123.08	123.13	123.33	118.51	118.73	118.89	118.77
O(1)–B(1)–C(1)	114.75	114.18	114.31	114.46	128.31	127.74	127.83	127.56	117.82	117.41	117.23	117.51
O(2)–B(1)–C(1)	127.15	127.88	127.80	127.17	108.76	109.18	109.04	109.11	122.86	123.04	123.12	122.89
O(3)–C(7)–C(2)	127.19	127.10	126.20	126.93	115.19	114.05	114.23	114.10	122.23	121.72	121.16	121.23
C(7)–C(2)–C(1)	126.58	126.84	126.45	126.60	111.33	111.75	111.74	111.59	119.53	119.07	118.91	118.44
C(2)–C(1)–B(1)	127.97	128.58	128.36	128.21	104.03	103.53	103.63	103.58	121.77	121.42	120.95	121.05
Torsion angles												
C(2)-C(1)-B(1)-O(2)	0.06	0.21	13.86	0.08	0.98	1.49	1.83	1.15	-96.06	-94.94	-103.96	-96.24
C(1)-C(2)-C(7)-O(3)	-0.14	-0.25	-16.59	-0.01	-121.60	-119.57	-119.48	-119.89	3.58	3.56	7.68	3.07
HBond geometry												
H...O(3)	1.669	1.707	1.736	1.666								
O(2)...O(3)	2.614	2.658	2.669	2.625								
O(2)-H(2)...O(3)	160.65	161.31	156.81	163.72								

Table 4. Calculated geometries of **2**.

	I (planar)				**II**				**I**-(twisted)			
	B3LYP	MP2			B3LYP	MP2			B3LYP	MP2		
		6-31G*	6-31+G*	aug-cc-pVDZ		6-31G*	6-31+G*	aug-cc-pVDZ		6-31G*	6-31+G*	aug-cc-pVDZ
Bond Lengths												
O(1)–B(1)	1.376	1.378	1.381	1.390	1.356	1.362	1.364	1.370	1.363	1.369	1.372	1.379
O(2)–B(1)	1.348	1.359	1.363	1.364	1.378	1.384	1.388	1.394	1.372	1.379	1.381	1.388
C(1)–B(1)	1.604	1.596	1.595	1.603	1.558	1.559	1.560	1.568	1.591	1.587	1.587	1.592
O(3)–C(7)	1.221	1.234	1.236	1.236	1.393	1.396	1.399	1.402	1.215	1.232	1.235	1.234
C(1)–C(2)	1.432	1.424	1.425	1.437	1.403	1.403	1.404	1.414	1.413	1.411	1.413	1.420
Cl(1)–C(3)	1.769	1.750	1.748	1.762	1.757	1.738	1.738	1.749	1.763	1.746	1.745	1.757
Bond Angles												
O(1)–B(1)–O(2)	117.76	118.21	117.97	118.18	123.02	123.28	123.22	123.45	118.44	118.71	118.77	118.72
O(1)–B(1)–C(1)	114.49	114.10	114.26	114.27	128.26	127.62	127.77	127.48	117.69	117.27	117.14	117.37
O(2)–B(1)–C(1)	127.75	127.61	127.70	127.53	108.72	109.10	109.01	109.08	122.80	122.89	123.03	122.80
O(3)–C(7)–C(2)	127.44	126.03	125.50	126.85	115.16	114.03	113.94	114.06	121.95	121.36	121.06	121.01
C(7)–C(2)–C(1)	124.69	123.44	123.25	124.52	110.80	111.12	111.27	111.25	117.43	116.66	116.72	116.62
C(2)–C(1)–B(1)	128.76	128.51	128.27	128.62	104.38	103.94	103.91	103.78	121.78	121.56	121.04	121.02
Torsion angles												
C(2)-C(1)-B(1)-O(2)	-0.36	-24.71	-24.03	-11.46	1.21	1.53	2.31	1.28	-97.60	-98.37	-105.45	-97.70
C(1)-C(2)-C(7)-O(3)	0.40	27.60	34.09	16.45	-120.26	-118.38	-118.04	-118.79	4.07	5.03	6.40	3.67
HBond geometry												
H...O(3)	1.654	1.749	1.775	1.669								
O(2)...O(3)	2.596	2.654	2.674	2.616								

O(2)-H(2)...O(3)	159.76	151.64	150.31	160.50

Table 5. Calculated gas-phase electronic energies E, E_0, E_{298}, enthalpies H and free enthalpies G (in hartree units) of 2-formylphenylboronic acid, **1** and **2**. ΔE, ΔE_0, ΔE_{298}, enthalpies ΔH and free enthalpies ΔG values are given in kJ mol^{-1}.

compound-form	MP2/aug-cc-pVDZ			hartree			kJ mol^{-1}				
	E(electron),	Zpc	E_0	E_{298}	H_{298}	G_{298}	ΔE(elec)	ΔE_0	ΔE	ΔH	ΔG
FPB-**I** (planar)	-520.234189	0.134864	-520.099325	-520.089928	-520.088984	-520.134291	0.00	0.00	0.00	0.00	0.00
FPB-**II**	-520.228100	0.136277	-520.091824	-520.082946	-520.082002	-520.125729	15.99	19.69	18.33	18.33	22.48
FPB-**I** (twisted)	-520.226919	0.133397	-520.093522	-520.083493	-520.082548	-520.129359	19.09	15.24	16.90	16.90	12.95
1-I (planar)	-619.288895	0.126811	-619.162083	-619.151789	-619.150845	-619.198488	0.00	0.00	0.00	0.00	0.00
1-II	-619.284687	0.128278	-619.156409	-619.146664	-619.145720	-619.191559	11.05	14.90	13.46	13.46	18.19
1-I (twisted)	-619.283121	0.125400	-619.157721	-619.146849	-619.145905	-619.194713	15.16	11.45	12.97	12.97	9.91
2-I (planar)	-979.295034	0.124948	-979.170086	-979.159278	-979.158334	-979.207906	0.00	0.00	0.00	0.00	0.00
2-II	-979.294514	0.126630	-979.167884	-979.157734	-979.156790	-979.203879	1.37	5.78	4.05	4.05	10.57
2-I (twisted)	-979.291738	0.123770	-979.167968	-979.156713	-979.155769	-979.205755	8.65	5.56	6.73	6.73	5.65
	MP2/6-31+G*										
FPB-**I** (planar)	-520.074054	0.134558	-519.939496	-519.929701	-519.928757	-519.975912	0.00	0.00	0.00	0.00	0.00
FPB-**II**	-520.069203	0.136602	-519.932601	-519.923602	-519.922658	-519.966622	12.74	18.10	16.01	16.01	24.39
FPB-**I** (twisted)	-520.068441	0.133365	-519.935076	-519.924893	-519.923949	-519.971003	14.74	11.60	12.62	12.62	12.89
1-I (planar)	-619.098521	0.126468	-618.972054	-618.961457	-618.960512	-619.008911	0.00	0.00	0.00	0.00	0.00
1-II	-619.094751	0.128153	-618.966597	-618.956636	-618.955692	-619.001949	9.90	14.33	12.66	12.65	18.28
1-I (twisted)	-619.094217	0.125073	-618.969144	-618.958054	-618.957110	-619.006283	11.30	7.64	8.93	8.93	6.90
2-I (planar)	-979.102167	0.125678	-978.976490	-978.965729	-978.964785	-979.013820	0.00	0.00	0.00	0.00	0.00
2-II	-979.102607	0.127139	-978.975467	-978.965278	-978.964334	-979.011491	-1.16	2.69	1.18	1.18	6.11
2-I (twisted)	-979.099441	0.124182	-978.975259	-978.963951	-978.963007	-979.013158	7.16	3.23	4.67	4.67	1.74
	MP2/6-31G*										
FPB-**I** (planar)	-520.037100	0.135762	-519.901338	-519.891781	-519.890837	-519.936844	0.00	0.00	0.00	0.00	0.00
FPB-**II**	-520.030850	0.137729	-519.893120	-519.884258	-519.883314	-519.927044	16.41	21.58	19.75	19.75	25.73
FPB-**I** (twisted)	-520.029890	0.134414	-519.895475	-519.885395	-519.884450	-519.931567	18.93	15.39	16.77	16.77	13.85
1-I (planar)	-619.053502	0.127550	-618.925952	-618.915483	-618.914538	-618.963139	0.00	0.00	0.00	0.00	0.00

1-II	-619.047631	0.129508	-618.918123	-618.908363	-618.907419	-618.953306	15.41	20.56	18.69	18.69	25.82
1-I (twisted)	-619.047338	0.126323	-618.921015	-618.910083	-618.909139	-618.958224	16.18	12.96	14.18	14.18	12.90
2-I (planar)	-979.063199	0.126143	-978.937057	-978.926272	-978.925328	-978.974371	0.00	0.00	0.00	0.00	0.00
2-II	-979.062252	0.127981	-978.934271	-978.924148	-978.923203	-978.970255	2.49	7.31	5.58	5.58	10.81
2-I (twisted)	-979.059771	0.124787	-978.934984	-978.923697	-978.922753	-978.972935	9.00	5.44	6.76	6.76	3.77

Table 5 (continued). Calculated gas-phase electronic energies E, E_0, E_{298}, enthalpies H and free enthalpies G (in hartree units) of 2-formylphenylboronic acid, **1** and **2**. ΔE, ΔE_0, ΔE_{298}, enthalpies ΔH and free enthalpies ΔG values are given in kJ mol^{-1}.

	B3LYP/6-311+G**			hartree					kJ mol^{-1}		
	E(electron)	zpc	E_0	E_{298}	H_{298}	G_{298}	ΔE(elec)	ΔE_0	ΔE	ΔH	ΔG
FPB-**I** (planar)	-521.757604	0.135061	-521.622543	-521.613239	-521.612295	-521.657433	0.00	0.00	0.00	0.00	0.00
FPB-**II**	-521.747356	0.136637	-521.610720	-521.601986	-521.601041	-521.644484	26.91	31.04	29.54	29.55	34.00
FPB-**I** (twisted)	-521.748734	0.133635	-521.615099	-521.605166	-521.604222	-521.650847	23.29	19.54	21.20	21.20	17.29
1-I (planar)	-621.022105	0.126845	-620.895261	-620.885070	-620.884126	-620.931462	0.00	0.00	0.00	0.00	0.00
1-II	-621.013277	0.128425	-620.884852	-620.875232	-620.874288	-620.919865	23.18	27.33	25.83	25.83	30.45
1-I (twisted)	-621.014620	0.125479	-620.889142	-620.878352	-620.877408	-620.926029	19.65	16.07	17.64	17.64	14.26
2-I (planar)	-981.372186	0.125215	-981.246970	-981.236254	-981.235310	-981.285031	0.00	0.00	0.00	0.00	0.00
2-II	-981.367528	0.126912	-981.240616	-981.230598	-981.229654	-981.276493	12.23	16.68	14.85	14.85	22.42
2-I (twisted)	-981.367215	0.124054	-981.243162	-981.232018	-981.231073	-981.280811	13.05	10.00	11.12	11.12	11.08

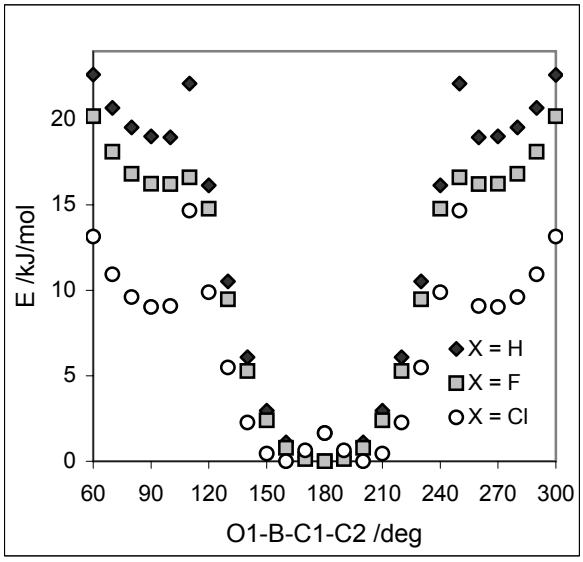
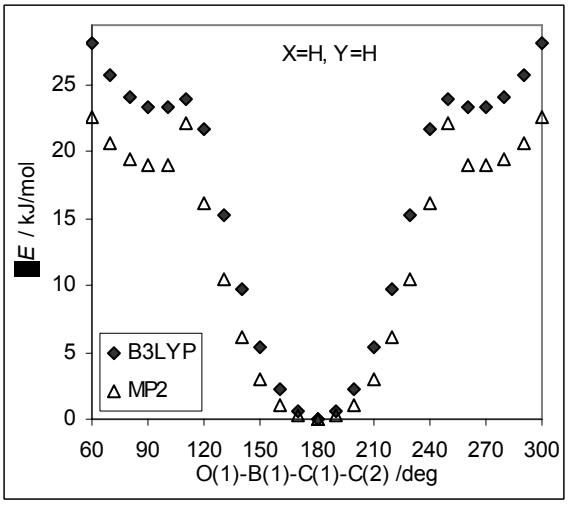
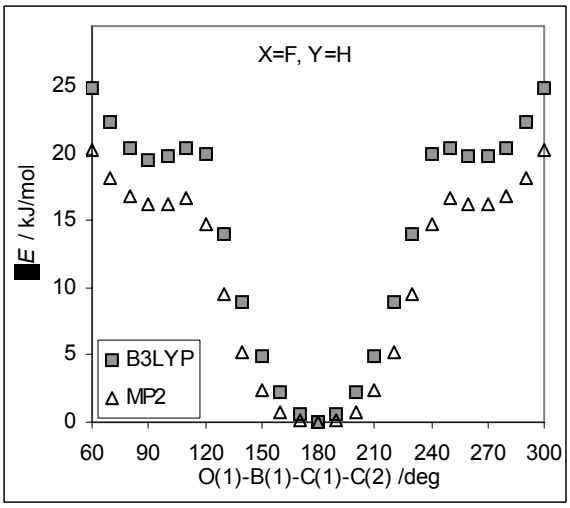


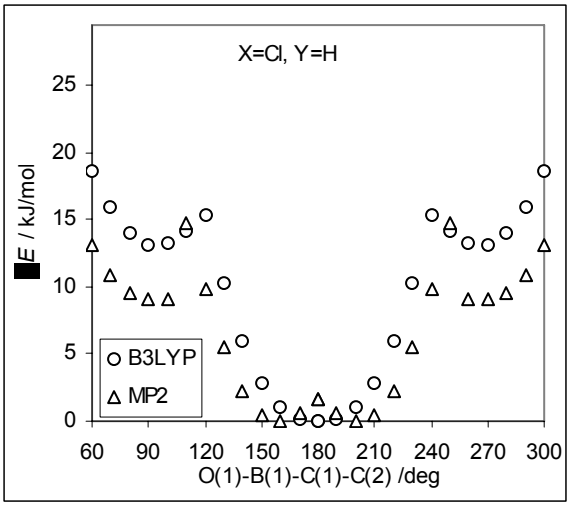
Figure 26. Dependence of calculated (MP2/6-31G*) relative electronic energy, kJ mol^{-1}, of open forms **I** on a O(1)–B–C(1)–C(2) torsion angle in 2-formylphenylboronic acid and its analogues **1** and **2**.



a)



b)



c)

Figure 27. Relationship between the relative electronic energy, Δ*E*, of open form **I** and a O(1)–B(1)–C(1)–C(2) torsion angle in (a) 2-formylphenylboronic acid and its analogues (b) **1** and (c) **2**.

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Table 6. Atomic coordinates of optimized structures of 2-formylphenylboronic acid and its analogues **1** and **2**.

2-formylphenylboronic acid

B3LYP/6-311+G** form **I**

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.425256
C	1.213431	0.000000	2.134387
C	2.437970	-0.000855	1.479555
C	2.454103	-0.000679	0.088986
C	1.255521	-0.000137	-0.625060
B	-1.250802	-0.001124	-0.988718
C	-1.189230	0.000326	2.300640
H	1.186722	0.000790	3.219270
H	3.362236	-0.001121	2.045430
H	3.398034	-0.000735	-0.445049
H	1.285525	-0.000159	-1.707246
H	-0.938624	0.000014	3.378227
O	-2.366511	0.001239	1.982648
O	-0.935893	-0.000254	-2.327529
H	-1.732103	-0.002599	-2.869667
O	-2.557349	-0.004390	-0.644694
H	-2.695318	-0.002351	0.325195

B3LYP/6-311+G** form **II**

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.400761
C	1.181686	0.000000	2.134768
C	2.389222	-0.003022	1.435024
C	2.406676	-0.006870	0.035653
C	1.215092	-0.003985	-0.688380
B	-1.506139	0.024180	-0.389952
C	-1.420910	0.006082	1.937887
H	1.169699	0.006124	3.219299
H	3.326083	-0.002468	1.981259
H	3.357515	-0.010800	-0.485653
H	1.234494	-0.004634	-1.772795
H	-1.674353	-0.907059	2.480678
O	-1.713877	1.049897	2.817240
O	-2.063080	0.020559	-1.627527
H	-3.026171	0.042757	-1.607751
O	-2.263072	0.057464	0.765329
H	-1.421304	1.879902	2.420606

B3LYP/6-311+G** form **I**-twisted

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.411055
C	1.195920	0.000000	2.137520
C	2.418527	-0.005553	1.474601
C	2.436806	-0.006842	0.081120
C	1.241742	-0.000439	-0.643005
B	-1.335838	0.033474	-0.855329
C	-1.282530	-0.005288	2.140384
H	1.161543	0.004648	3.222768
H	3.346356	-0.006635	2.034665
H	3.384348	-0.005990	-0.446620
H	1.286237	0.011583	-1.727356
H	-1.205932	0.045513	3.245573
O	-2.368037	-0.066396	1.600326
O	-1.802716	1.244946	-1.269148
H	-2.610480	1.164263	-1.789363
O	-1.933177	-1.097460	-1.352133
H	-1.586870	-1.917108	-0.990438

Supplementary Material (ESI) for New Journal of Chemistry

2-formylphenylboronic acid

MP2/aug-cc-pVDZ form **I**

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.432106
C	1.218620	0.000000	2.155096
C	2.457425	0.000002	1.497449
C	2.479410	-0.000194	0.092745
C	1.270392	-0.000166	-0.628553
B	-1.250465	0.000437	-0.992804
C	-1.196316	-0.000117	2.313041
H	1.185838	0.000028	3.249909
H	3.388393	0.000027	2.071302
H	3.433407	-0.000308	-0.443123
H	1.303070	-0.000274	-1.720960
H	-0.946328	-0.000580	3.397934
O	-2.388286	0.000197	1.988002
O	-0.921919	0.000409	-2.343602
H	-1.733660	0.000783	-2.871863
O	-2.571374	0.000793	-0.646572
H	-2.676166	0.000874	0.331106

MP2/aug-cc-pVDZ form **II**

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.412766
C	1.188350	0.000000	2.160300
C	2.407666	-0.002069	1.454640
C	2.426039	-0.004959	0.041465
C	1.225338	-0.001681	-0.694277
B	-1.518230	0.021401	-0.381009
C	-1.417973	0.017471	1.955048
H	1.172459	0.007080	3.254705
H	3.353488	-0.002318	2.005158
H	3.386997	-0.007663	-0.482002
H	1.248187	-0.001349	-1.788442
H	-1.682156	-0.885445	2.524202
O	-1.686978	1.094094	2.816891
O	-2.072855	0.012849	-1.635139
H	-3.040493	0.032537	-1.596166
O	-2.281383	0.056113	0.787764
H	-1.347074	1.896281	2.389880

MP2/aug-cc-pVDZ form **I**-twisted

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.418727
C	1.196359	0.000000	2.164406
C	2.432844	-0.005805	1.496602
C	2.459517	-0.006817	0.089358
C	1.255233	-0.001646	-0.645562
B	-1.350091	0.013414	-0.837335
C	-1.304902	0.003562	2.123558
H	1.154224	0.005993	3.259230
H	3.367589	-0.006954	2.064571
H	3.418590	-0.005954	-0.437703
H	1.302700	0.009120	-1.739892
H	-1.268864	0.044107	3.236850
O	-2.384423	-0.038794	1.530503
O	-1.830667	1.232967	-1.262654
H	-2.641331	1.117361	-1.780693
O	-1.951707	-1.141200	-1.316684
H	-1.551339	-1.938959	-0.948760

Compound **1**

B3LYP/6-311+G** form **I**

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.429181
C	1.241764	0.000000	2.088667
C	2.460899	0.000773	1.437585
C	2.451828	0.001015	0.049356
C	1.242868	0.000484	-0.646210
B	-1.260856	-0.001085	-0.984097
C	-1.186402	-0.000608	2.309679
F	1.272005	-0.000545	3.444853
H	3.376103	0.001039	2.015823
H	3.389960	0.001559	-0.493990
H	1.255393	0.000440	-1.727870
H	-0.956533	-0.002611	3.384219
O	-2.358974	0.001212	1.968343
O	-0.946296	-0.002728	-2.322474
H	-1.742708	-0.003799	-2.864413
O	-2.564479	-0.001054	-0.637815
H	-2.695943	0.000479	0.333946

B3LYP/6-311+G** form **II**

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.401981
C	1.204519	0.000000	2.086372
C	2.410757	0.018794	1.399549
C	2.404613	0.028422	0.001973
C	1.202994	0.016087	-0.706151
B	-1.512209	-0.035618	-0.377900
C	-1.415270	-0.013738	1.954653
F	1.220880	-0.025022	3.439211
H	3.337892	0.020773	1.959876
H	3.350071	0.040547	-0.528195
H	1.206176	0.014016	-1.789930
H	-1.638049	-0.911023	2.534167
O	-1.737584	1.056480	2.785306
O	-2.069163	-0.070139	-1.613372
H	-3.032366	-0.091125	-1.595129
O	-2.259387	-0.030825	0.781354
H	-1.464287	1.878683	2.360285

B3LYP/6-311+G** form **I**-twisted

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.412210
C	1.221129	0.000000	2.090130
C	2.440221	-0.003790	1.435852
C	2.433892	-0.004714	0.043634
C	1.229037	-0.000818	-0.663804
B	-1.351187	0.027646	-0.837003
C	-1.284836	-0.002087	2.140000
F	1.220662	0.000789	3.445426
H	3.358760	-0.005050	2.008875
H	3.376187	-0.003288	-0.492617
H	1.255983	0.010337	-1.747970
H	-1.236147	0.055132	3.239828
O	-2.354528	-0.068055	1.566642
O	-1.817542	1.238411	-1.251499
H	-2.628684	1.159354	-1.766652
O	-1.942981	-1.106044	-1.332141
H	-1.597697	-1.925668	-0.969472

Compound **1**

MP2/aug-cc-pVDZ form **I**

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.435793
C	1.245965	0.000000	2.105938
C	2.480621	0.000108	1.455495
C	2.478125	0.000092	0.053380
C	1.258294	-0.000019	-0.648745
B	-1.257397	-0.000463	-0.989919
C	-1.193841	0.000294	2.322483
F	1.269812	-0.000060	3.476289
H	3.400927	0.000156	2.043935
H	3.426566	0.000135	-0.491301
H	1.273597	-0.000144	-1.740623
H	-0.966494	0.000017	3.404489
O	-2.380200	0.000747	1.971804
O	-0.927035	-0.002091	-2.340152
H	-1.738632	-0.002018	-2.868693
O	-2.577123	0.000549	-0.645676
H	-2.679023	0.001142	0.332841

MP2/aug-cc-pVDZ form **II**

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.413592
C	1.210158	0.000000	2.110709
C	2.429698	0.016963	1.422132
C	2.425068	0.027142	0.010229
C	1.214827	0.015623	-0.710075
B	-1.523336	-0.034663	-0.367983
C	-1.411574	0.008326	1.972056
F	1.217877	-0.026256	3.474008
H	3.364721	0.017164	1.988406
H	3.381331	0.038629	-0.520949
H	1.222862	0.013709	-1.803667
H	-1.648441	-0.871981	2.585218
O	-1.702691	1.119737	2.775814
O	-2.079623	-0.072513	-1.619376
H	-3.047331	-0.091686	-1.580560
O	-2.276953	-0.025396	0.805723
H	-1.391800	1.909635	2.306346

MP2/aug-cc-pVDZ form **I**-twisted

C	-0.356785	-0.581530	0.000701
C	0.512358	0.540498	-0.005172
C	1.902764	0.343137	-0.006452
C	2.478360	-0.929795	0.001373
C	1.619339	-2.042960	0.007868
C	0.219504	-1.868112	0.006176
B	-1.936904	-0.395778	-0.015217
C	-0.086901	1.899149	-0.013632
F	2.729641	1.434213	-0.013581
H	3.565767	-1.035431	0.001209
H	2.046647	-3.050006	0.009580
H	-0.425488	-2.752489	0.000319
H	0.600388	2.766928	-0.070664
O	-1.308872	2.059667	0.040953
O	-2.569127	-0.427529	-1.239008
H	-3.527577	-0.335711	-1.130494
O	-2.709613	-0.419795	1.136215
H	-2.172929	-0.383383	1.937912

Compound **2**

B3LYP/6-311+G** form **I**

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.431595
C	1.244697	0.000000	2.103510
C	2.456503	-0.000372	1.425780
C	2.448136	-0.000452	0.039039
C	1.239900	-0.000065	-0.651822
B	-1.250527	0.000841	-1.004010
C	-1.217667	0.000585	2.274330
Cl	1.371100	-0.000492	3.867844
H	3.383698	-0.000640	1.983606
H	3.386747	-0.000678	-0.503704
H	1.247809	0.000354	-1.733353
H	-1.026055	0.007242	3.354434
O	-2.379375	-0.005593	1.899820
O	-0.911455	0.007319	-2.337232
H	-1.699641	0.006895	-2.891032
O	-2.561554	-0.005020	-0.689613
H	-2.709955	-0.008589	0.279531

B3LYP/6-311+G** form **II**

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.402764
C	1.201526	0.000000	2.101515
C	2.405994	0.023054	1.399582
C	2.402111	0.037909	0.002984
C	1.201990	0.020970	-0.706143
B	-1.507881	-0.057928	-0.386958
C	-1.423153	-0.013597	1.943258
Cl	1.233363	-0.054881	3.857537
H	3.340652	0.023453	1.946479
H	3.349041	0.054069	-0.524668
H	1.204751	0.017394	-1.790125
H	-1.640410	-0.900609	2.540546
O	-1.761479	1.071977	2.747149
O	-2.055296	-0.107462	-1.626295
H	-3.018190	-0.143126	-1.614885
O	-2.260959	-0.059354	0.767111
H	-1.492758	1.886957	2.305559

B3LYP/6-311+G** form **I**-twisted

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.412817
C	1.220148	0.000000	2.104509
C	2.433637	-0.004359	1.427621
C	2.428886	-0.004644	0.036019
C	1.225142	-0.001265	-0.669427
B	-1.352174	0.029357	-0.838043
C	-1.313327	0.005078	2.094480
Cl	1.271530	-0.003396	3.866946
H	3.362237	-0.006510	1.983591
H	3.372585	-0.003008	-0.498050
H	1.247474	0.009377	-1.753855
H	-1.313683	0.073322	3.193151
O	-2.358440	-0.063996	1.477730
O	-1.814012	1.242796	-1.252641
H	-2.620318	1.165647	-1.775411
O	-1.928783	-1.101969	-1.358676
H	-1.585222	-1.924273	-1.000619

Compound **2**

MP2/aug-cc-pVDZ form **I**

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.436551
C	1.246698	0.000000	2.122314
C	2.475173	-0.001592	1.444450
C	2.473944	0.009641	0.043402
C	1.254808	0.013057	-0.656061
B	-1.252524	-0.001102	-1.000547
C	-1.226848	0.038506	2.280685
Cl	1.345429	-0.040452	3.881348
H	3.406186	-0.012674	2.016144
H	3.423022	0.014524	-0.500647
H	1.265446	0.027663	-1.747901
H	-1.057252	0.316069	3.337112
O	-2.383778	-0.205427	1.918994
O	-0.920259	0.218860	-2.332207
H	-1.723431	0.185561	-2.872612
O	-2.563176	-0.217063	-0.690884
H	-2.670978	-0.329023	0.279352

MP2/aug-cc-pVDZ form **II**

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.413869
C	1.206816	0.000000	2.126859
C	2.425436	0.025178	1.423738
C	2.422981	0.041396	0.012832
C	1.214401	0.023736	-0.709936
B	-1.521436	-0.056958	-0.373422
C	-1.415964	0.004354	1.964418
Cl	1.215400	-0.052897	3.875142
H	3.366316	0.024967	1.980387
H	3.380503	0.059870	-0.516404
H	1.222925	0.021241	-1.803755
H	-1.644999	-0.868089	2.592366
O	-1.721985	1.127438	2.746294
O	-2.070490	-0.108676	-1.627381
H	-3.038016	-0.143392	-1.593635
O	-2.278068	-0.055966	0.796976
H	-1.404279	1.910703	2.270076

MP2/aug-cc-pVDZ form **I**-twisted

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.420494
C	1.220254	0.000000	2.129586
C	2.449522	-0.001047	1.450487
C	2.453224	-0.000040	0.045467
C	1.239153	0.000999	-0.671116
B	-1.364673	0.015570	-0.820600
C	-1.329255	0.003487	2.086758
Cl	1.248864	-0.003299	3.886504
H	3.382640	-0.002064	2.019249
H	3.408270	0.003976	-0.488535
H	1.265130	0.011666	-1.765568
H	-1.359263	0.066870	3.192069
O	-2.370923	-0.061459	1.428054
O	-1.844517	1.241806	-1.229314
H	-2.652953	1.134259	-1.752371
O	-1.941680	-1.133939	-1.342015
H	-1.541279	-1.938075	-0.988384