

**Are Lithium and Sodium Salts of *N*-(2-Hydroxyphenyl)-
salicylaldimine Aromatic Metalla-hetero[10]annulenes? An
Answer Tried by Spatial Magnetic Properties (Through Space
NMR Shieldings – TSNMRS) †**

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Supplementary Information (ESI)

Coordinates and absolute energies (a.u.) at the B3LYP/6-311G** level of theory of all studied
compounds **1–9**:

1

E= -707.3803313 a.u.

1	6	0	1.780083	-0.236465	0.104093
2	6	0	2.561121	0.891953	-0.215184
3	6	0	3.948841	0.767448	-0.269111
4	6	0	4.555321	-0.456965	-0.015648
5	6	0	3.783698	-1.576844	0.296367
6	6	0	2.400946	-1.461226	0.363363
7	7	0	0.384932	-0.057260	0.160887
8	8	0	2.022517	2.112423	-0.477191
9	1	0	4.529958	1.646573	-0.518807
10	1	0	5.635130	-0.536196	-0.060427
11	1	0	4.256383	-2.528492	0.505887
12	1	0	1.795440	-2.314590	0.645924
13	6	0	-0.567668	-0.933847	-0.126474
14	6	0	-1.920464	-0.576707	-0.063192
15	6	0	-2.277508	0.807194	0.257260
16	6	0	-3.680828	1.113414	0.259982
17	6	0	-4.617809	0.156428	-0.023207
18	6	0	-4.256702	-1.184211	-0.337464
19	6	0	-2.935128	-1.532352	-0.358470
20	8	0	-1.396095	1.685236	0.513487
21	1	0	1.062240	2.063159	-0.569740
22	1	0	-0.064025	0.860780	0.450851

23	1	0	-0.272150	-1.934000	-0.433598
24	1	0	-3.959468	2.133111	0.497162
25	1	0	-5.669632	0.424279	-0.009015
26	1	0	-5.026047	-1.913039	-0.559843
27	1	0	-2.637151	-2.548970	-0.598854

2

E= -714.4059832 a.u.

1	6	0	-1.820341	-0.401140	-0.000232
2	6	0	-2.458584	0.890414	0.000040
3	6	0	-3.876043	0.875346	0.000277
4	6	0	-4.582589	-0.314500	0.000240
5	6	0	-3.928192	-1.557922	-0.000077
6	6	0	-2.543675	-1.596520	-0.000330
7	7	0	-0.430753	-0.305170	-0.000343
8	8	0	-1.753048	1.975993	0.000125
9	1	0	-4.387143	1.831048	0.000449
10	1	0	-5.667270	-0.286257	0.000428
11	1	0	-4.499453	-2.477968	-0.000174
12	1	0	-2.023893	-2.549188	-0.000669
13	6	0	0.579810	-1.138330	0.000140
14	6	0	1.923164	-0.659671	0.000037
15	6	0	2.230942	0.759866	-0.000154
16	6	0	3.605847	1.114670	-0.000094
17	6	0	4.600906	0.160328	0.000073
18	6	0	4.297020	-1.215711	0.000217
19	6	0	2.978116	-1.605448	0.000209
20	8	0	1.306524	1.668463	-0.000312
21	3	0	-0.149297	2.698460	0.000414
22	1	0	-0.105814	0.670853	-0.000811
23	1	0	0.384088	-2.206808	0.000843
24	1	0	3.843600	2.172120	-0.000230
25	1	0	5.638960	0.476407	0.000073
26	1	0	5.090867	-1.952174	0.000322
27	1	0	2.723133	-2.661166	0.000348

3

E= -869.1605773 a.u.

1	6	0	-1.812376	-0.580948	-0.000153
2	6	0	-2.526042	0.672409	0.000038
3	6	0	-3.944240	0.565744	0.000237
4	6	0	-4.579404	-0.662514	0.000173
5	6	0	-3.850972	-1.864155	-0.000097
6	6	0	-2.466395	-1.815854	-0.000288
7	7	0	-0.424074	-0.423344	-0.000302
8	8	0	-1.893944	1.794130	0.000059
9	1	0	-4.511655	1.489615	0.000381
10	1	0	-5.664154	-0.699132	0.000319
11	1	0	-4.363883	-2.818041	-0.000204
12	1	0	-1.893648	-2.737776	-0.000550

13	6	0	0.582804	-1.264097	0.000065
14	6	0	1.939342	-0.834913	0.000006
15	6	0	2.294960	0.573747	-0.000301
16	6	0	3.687039	0.876143	-0.000253
17	6	0	4.645456	-0.113393	0.000076
18	6	0	4.291675	-1.478894	0.000383
19	6	0	2.959414	-1.819297	0.000341
20	8	0	1.402261	1.503113	-0.000633
21	11	0	-0.147365	2.965104	0.000431
22	1	0	-0.118417	0.559457	-0.000642
23	1	0	0.363088	-2.327822	0.000485
24	1	0	3.965099	1.924196	-0.000505
25	1	0	5.694867	0.163844	0.000089
26	1	0	5.058336	-2.243693	0.000644
27	1	0	2.665795	-2.865192	0.000583

4

E= -387.0642823 a.u.

1	6	0	2.342505	0.705245	0.057449
2	6	0	2.342458	-0.705168	-0.057337
3	6	0	1.255551	-1.616560	-0.012508
4	6	0	-0.000027	-1.233458	0.458450
5	6	0	-1.255534	-1.616548	-0.012500
6	6	0	-2.342510	-0.705168	-0.057263
7	6	0	-2.342463	0.705229	0.057429
8	6	0	-1.255532	1.616569	0.012342
9	6	0	0.000033	1.233312	-0.458507
10	6	0	1.255511	1.616546	0.012471
11	1	0	3.323588	1.143886	0.247715
12	1	0	3.323545	-1.143808	-0.247686
13	1	0	1.394282	-2.597311	-0.471972
14	1	0	0.000018	-0.331498	1.062258
15	1	0	-1.394221	-2.597261	-0.472043
16	1	0	-3.323597	-1.143811	-0.247557
17	1	0	-3.323537	1.143894	0.247748
18	1	0	-1.394171	2.597478	0.471485
19	1	0	0.000026	0.331067	-1.061924
20	1	0	1.394113	2.597372	0.471820

5

E= -399.7769764 a.u.

1	6	0	2.019584	-0.680598	0.000041
2	6	0	2.082154	0.679087	0.000201
3	6	0	0.890319	1.455867	-0.000042
4	6	0	-0.309489	0.795066	-0.000263
5	6	0	-0.297007	-0.669492	-0.000129
6	8	0	0.860935	-1.363604	-0.000154
7	7	0	-1.469934	-1.221740	0.000122
8	6	0	-2.334217	-0.123244	0.000156
9	6	0	-1.703918	1.100747	-0.000013
10	1	0	2.872453	-1.343375	0.000041

11	1	0	3.056129	1.149451	0.000544
12	1	0	0.950401	2.538808	-0.000133
13	1	0	-3.400258	-0.306165	0.000277
14	1	0	-2.161229	2.077696	-0.000067

6

E= -574.5984776 a.u.

1	6	0	-0.799704	-0.576286	0.000034
2	6	0	-1.646361	0.544087	0.000035
3	6	0	-1.083605	1.852950	0.000005
4	6	0	0.266475	2.042928	-0.000020
5	6	0	2.557402	1.077269	-0.000021
6	6	0	3.390864	-0.018305	0.000035
7	6	0	2.858251	-1.325171	0.000040
8	6	0	1.495866	-1.514895	-0.000010
9	6	0	0.619544	-0.403736	-0.000034
10	6	0	1.150409	0.921290	-0.000041
11	8	0	-1.280637	-1.819846	-0.000058
12	6	0	-3.081564	0.354046	0.000071
13	1	0	-1.759668	2.702219	-0.000004
14	1	0	0.687006	3.041776	-0.000057
15	1	0	2.970868	2.079968	-0.000071
16	1	0	4.466156	0.121524	0.000064
17	1	0	3.526260	-2.178576	0.000101
18	1	0	1.070990	-2.510246	-0.000030
19	8	0	-3.639883	-0.743626	-0.000014
20	1	0	-2.268781	-1.748517	-0.000033
21	1	0	-3.694129	1.274564	0.000035

7

E= -400.0164788 a.u.

1	6	0	-1.493595	-0.967850	-0.148870
2	6	0	-2.561017	-0.166497	-0.039211
3	1	0	-1.627770	-2.031721	-0.292452
4	1	0	-3.563327	-0.558541	-0.141965
5	1	0	3.034948	-1.399975	0.275281
6	1	0	3.479804	0.999683	0.057590
7	7	0	-0.175477	-0.503855	-0.092065
8	8	0	-2.558446	1.177577	0.176875
9	6	0	0.922087	-1.257767	0.093309
10	6	0	2.194032	-0.735853	0.130977
11	6	0	2.425511	0.671141	0.000819
12	8	0	1.541521	1.525172	-0.166715
13	1	0	-1.688048	1.474325	0.469263
14	1	0	0.055366	0.486001	-0.242324
15	1	0	0.750655	-2.323827	0.215636

8

E= -407.035221 a.u.

1	6	0	-1.549791	-1.181477	0.000021
2	6	0	-2.398354	-0.095263	-0.000091
3	1	0	-1.858780	-2.215441	0.000331
4	1	0	-3.476515	-0.290105	0.000370
5	1	0	3.098634	-1.215148	0.000475
6	1	0	3.156914	1.182492	0.000234
7	7	0	-0.205776	-0.847594	-0.000357
8	8	0	-1.996595	1.130960	0.000174
9	6	0	0.961131	-1.458815	0.000103
10	6	0	2.151569	-0.693165	0.000102
11	6	0	2.170952	0.700140	-0.000097
12	8	0	1.145970	1.474628	-0.000298
13	3	0	-0.529830	2.125934	0.000675
14	1	0	-0.078385	0.164697	-0.000783
15	1	0	0.980015	-2.544366	0.000610

9

E= -561.7905283 a.u.

1	6	0	-1.238627	-1.671932	-0.000174
2	6	0	-2.301026	-0.793461	-0.000108
3	1	0	-1.330205	-2.747755	0.000025
4	1	0	-3.306458	-1.238435	0.000306
5	1	0	3.362113	-1.118942	0.000698
6	1	0	3.197383	1.275868	0.000150
7	7	0	0.024786	-1.094997	-0.000375
8	8	0	-2.196030	0.486330	0.000146
9	6	0	1.260083	-1.557537	0.000071
10	6	0	2.371114	-0.685480	0.000032
11	6	0	2.256515	0.704730	-0.000716
12	8	0	1.164925	1.370237	-0.000568
13	11	0	-0.848209	2.124917	0.000930
14	1	0	0.001762	-0.074715	-0.000665
15	1	0	1.392683	-2.635586	0.000632