

The new threading system 2-benzyl-5, 6-dimethyl-1*H*-benzo[d]imidazolium - dibenzo-24-crown-8: A model for Monte Carlo calculations incorporating anion for the first time in threaded structures

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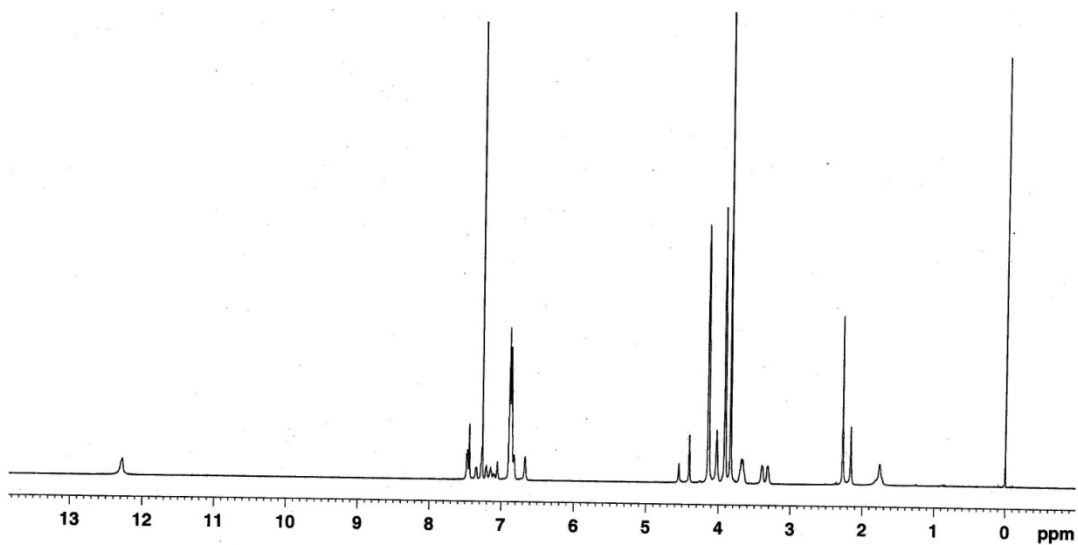
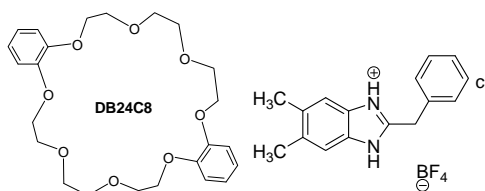
Supporting Information

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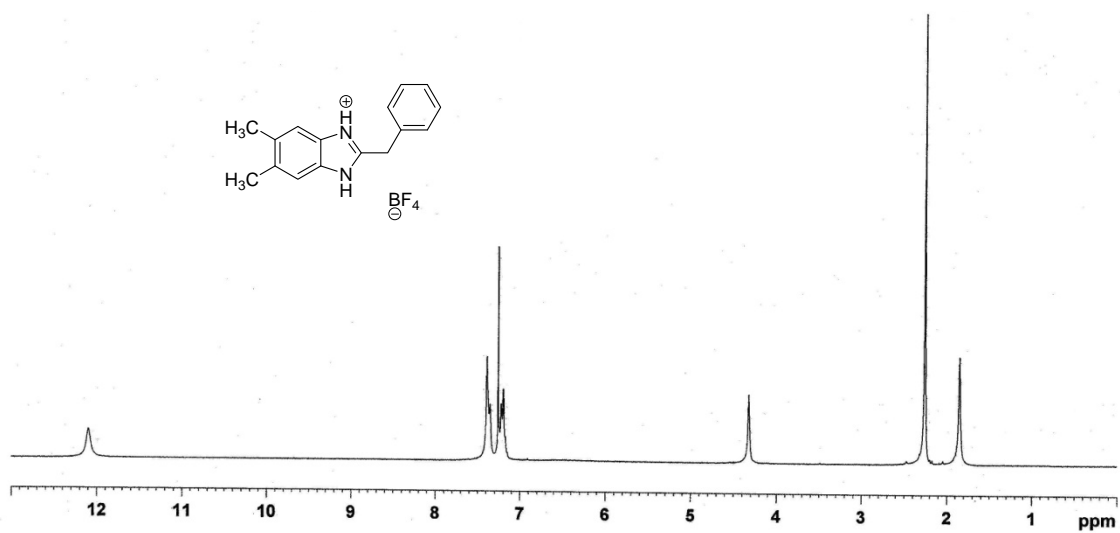
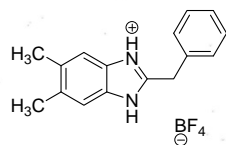
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1. Copies of NMR spectra

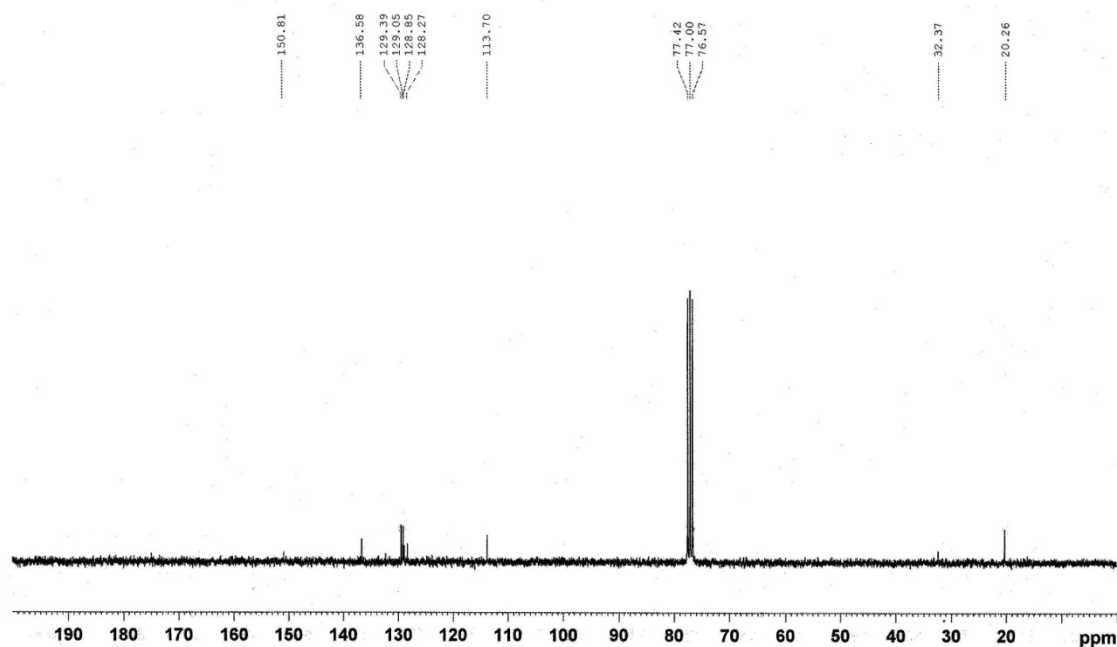
^1H NMR of $[1.\text{BF}_4]\text{DB24C8}$ in CDCl_3



^1H NMR of $1.\text{BF}_4$ salt in CDCl_3



^{13}C NMR of 1.BF₄ salt in CDCl₃



2. Details of DFT calculations

Coordinates of Case A

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	8	0	2.718273	-1.213037	1.705145
2	8	0	1.261355	0.263235	3.747363
3	8	0	-1.594209	0.255084	3.514182
4	8	0	-3.339841	-0.073939	1.073671
5	6	0	3.619219	-1.596906	0.743751
6	6	0	4.136694	-0.701757	-0.208245
7	6	0	5.043297	-1.188812	-1.152769
8	6	0	5.401348	-2.542071	-1.162567
9	6	0	4.851085	-3.423821	-0.236172
10	6	0	3.953291	-2.952470	0.715685
11	6	0	3.351718	-0.430612	2.731007
12	6	0	2.470773	-0.473704	3.980375

13	6	0	0.393622	0.214693	4.886415
14	6	0	-0.902929	0.957320	4.562707
15	6	0	-2.911321	0.796921	3.303782
16	6	0	-3.730910	-0.171716	2.448316
17	8	0	-2.744614	0.192524	-1.515915
18	8	0	-0.510011	1.560484	-3.119460
19	8	0	2.236008	2.041826	-2.240992
20	8	0	3.671440	0.583796	-0.149472
21	6	0	-3.583203	-0.844136	-1.163713
22	6	0	-3.916941	-0.971715	0.201241
23	6	0	-4.788243	-1.997455	0.598126
24	6	0	-5.299556	-2.903567	-0.333003
25	6	0	-4.946810	-2.795558	-1.671335
26	6	0	-4.093470	-1.771886	-2.085163
27	6	0	-2.697647	0.510043	-2.914672
28	6	0	-1.924082	1.808727	-3.144464
29	6	0	0.224353	2.760046	-3.398108
30	6	0	1.707707	2.418928	-3.525406
31	6	0	3.617807	1.656178	-2.359651
32	6	0	4.270024	1.583891	-0.976758
33	1	0	5.488948	-0.553311	-1.909733
34	1	0	6.107254	-2.910167	-1.904700
35	1	0	5.124370	-4.476717	-0.254337
36	1	0	3.518646	-3.636321	1.439616
37	1	0	3.451654	0.605101	2.388389
38	1	0	4.340318	-0.839441	2.976695
39	1	0	2.215785	-1.512029	4.221393
40	1	0	3.004292	-0.019780	4.821942
41	1	0	0.891538	0.686899	5.739947
42	1	0	0.171313	-0.832169	5.120210
43	1	0	-1.529343	0.992981	5.460592
44	1	0	-0.691825	1.974015	4.217636
45	1	0	-2.816137	1.774067	2.821134
46	1	0	-3.410489	0.912743	4.272284
47	1	0	-3.549573	-1.186966	2.820456
48	1	0	-4.791492	0.090726	2.533620
49	1	0	-5.096413	-2.129335	1.629696
50	1	0	-5.973012	-3.694535	-0.010582
51	1	0	-5.340237	-3.503667	-2.396426
52	1	0	-3.842963	-1.734347	-3.139990
53	1	0	-2.199486	-0.301016	-3.458008
54	1	0	-3.719260	0.656282	-3.285119
55	1	0	-2.177242	2.549952	-2.382535
56	1	0	-2.184519	2.201351	-4.133099
57	1	0	-0.128288	3.193744	-4.340748

58	1	0	0.063291	3.471076	-2.582521
59	1	0	2.252830	3.296031	-3.888845
60	1	0	1.841253	1.583096	-4.221740
61	1	0	3.651697	0.687571	-2.867418
62	1	0	4.155542	2.397972	-2.961976
63	1	0	4.097431	2.535094	-0.461818
64	1	0	5.357416	1.459510	-1.040118
65	6	0	-1.728674	5.476086	-0.170905
66	6	0	-2.300239	4.219932	0.015712
67	6	0	-1.505170	3.136814	0.393928
68	6	0	-0.127032	3.297673	0.589810
69	6	0	0.433616	4.570907	0.411974
70	6	0	-0.362125	5.652349	0.027297
71	6	0	0.412503	0.809467	0.532144
72	7	0	-0.169536	-0.202914	1.186151
73	6	0	-0.259291	-1.317564	0.387352
74	6	0	0.269156	-0.946714	-0.843138
75	7	0	0.650755	0.364112	-0.707652
76	6	0	-0.755340	-2.587236	0.638804
77	6	0	-0.708433	-3.495715	-0.439846
78	6	0	-0.165209	-3.113685	-1.706964
79	6	0	0.338926	-1.813792	-1.921276
80	6	0	0.741558	2.167641	1.070513
81	6	0	-1.265897	-4.882024	-0.227615
82	6	0	-0.127395	-4.092576	-2.854020
83	1	0	-1.981917	2.167186	0.525359
84	1	0	0.082829	6.635160	-0.107804
85	1	0	-0.479128	-0.145142	2.158651
86	1	0	1.063976	0.944064	-1.438797
87	1	0	-1.165551	-2.834768	1.607883
88	1	0	0.752368	-1.482565	-2.864869
89	1	0	0.676010	2.100125	2.157367
90	1	0	1.787418	2.328021	0.792483
91	1	0	0.330657	-3.648411	-3.744078
92	1	0	0.465394	-4.972665	-2.583077
93	1	0	-1.142094	-4.400799	-3.122712
94	1	0	-1.635387	-5.013331	0.794707
95	1	0	-2.104965	-5.060758	-0.907681
96	1	0	-0.487842	-5.633132	-0.395847
97	1	0	-3.368188	4.081788	-0.133655
98	1	0	-2.349777	6.319207	-0.463681
99	1	0	1.496464	4.736694	0.577304

Coordinates of Case B

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	8	0	-0.977530	-3.469865	0.130908
2	8	0	-1.979122	-2.530517	2.663004
3	8	0	-1.362136	0.331244	3.005888
4	8	0	-0.392894	2.778492	1.564463
5	6	0	-1.090287	-3.266787	-1.221704
6	6	0	0.097353	-3.360218	-1.973929
7	6	0	0.051790	-3.168486	-3.356894
8	6	0	-1.154752	-2.843621	-3.981804
9	6	0	-2.316772	-2.700790	-3.228427
10	6	0	-2.286029	-2.910232	-1.850233
11	6	0	-2.104369	-4.057772	0.796635
12	6	0	-2.848262	-3.020248	1.634481
13	6	0	-2.663846	-1.638351	3.550197
14	6	0	-1.676418	-0.589624	4.065097
15	6	0	-1.607116	1.689360	3.390810
16	6	0	-1.680483	2.616926	2.177329
17	8	0	1.915147	2.933338	0.242539
18	8	0	4.004999	0.872012	-0.746743
19	8	0	3.647595	-1.991418	-1.225690
20	8	0	1.239666	-3.588581	-1.252444
21	6	0	0.900227	3.768614	-0.170862
22	6	0	-0.335608	3.652678	0.498371
23	6	0	-1.425133	4.421565	0.057996
24	6	0	-1.290735	5.313132	-1.006537
25	6	0	-0.066098	5.451331	-1.642725
26	6	0	1.023814	4.683544	-1.228592
27	6	0	3.197086	3.122900	-0.364473
28	6	0	4.165316	2.030451	0.088410
29	6	0	4.988432	-0.127417	-0.452454
30	6	0	4.849843	-1.247223	-1.481310
31	6	0	3.303150	-2.816761	-2.351439
32	6	0	2.429120	-3.998058	-1.920373
33	1	0	0.935222	-3.242244	-3.979248
34	1	0	-1.187024	-2.678275	-5.055756
35	1	0	-3.250992	-2.413107	-3.704746
36	1	0	-3.200636	-2.748579	-1.285435
37	1	0	-1.689316	-4.821093	1.464718
38	1	0	-2.778686	-4.575746	0.105786
39	1	0	-3.150282	-2.182790	1.006228
40	1	0	-3.731232	-3.478867	2.093227
41	1	0	-3.046276	-2.234047	4.384968
42	1	0	-3.503485	-1.146455	3.052049
43	1	0	-2.102830	-0.077156	4.935188
44	1	0	-0.737400	-1.062956	4.371371
45	1	0	-0.801200	2.002439	4.064568

46	1	0	-2.567602	1.753148	3.916420
47	1	0	-2.381734	2.207209	1.444968
48	1	0	-2.032787	3.590718	2.540599
49	1	0	-2.406902	4.345081	0.516443
50	1	0	-2.148592	5.896934	-1.333165
51	1	0	0.040204	6.149544	-2.469034
52	1	0	1.953616	4.823168	-1.766706
53	1	0	3.116634	3.073761	-1.456774
54	1	0	3.587202	4.097105	-0.048405
55	1	0	3.994400	1.753223	1.129759
56	1	0	5.190527	2.398810	-0.030244
57	1	0	5.989621	0.311612	-0.527421
58	1	0	4.822405	-0.505336	0.560130
59	1	0	5.700078	-1.932503	-1.407009
60	1	0	4.806394	-0.818268	-2.489198
61	1	0	2.782436	-2.179297	-3.070519
62	1	0	4.211813	-3.211087	-2.822197
63	1	0	2.990951	-4.585900	-1.185386
64	1	0	2.215317	-4.671945	-2.758603
65	6	0	4.200681	0.163291	4.185703
66	6	0	3.111632	0.926990	3.773165
67	6	0	2.137591	0.366638	2.945267
68	6	0	2.242459	-0.963623	2.518218
69	6	0	3.335853	-1.726884	2.953360
70	6	0	4.313216	-1.163151	3.776837
71	6	0	0.653988	-0.785924	0.539772
72	7	0	-0.565432	-0.258387	0.380069
73	6	0	-0.682845	0.355393	-0.845193
74	6	0	0.567748	0.250751	-1.439466
75	7	0	1.350043	-0.449999	-0.556395
76	6	0	-1.745405	0.988899	-1.467928
77	6	0	-1.491011	1.538309	-2.742200
78	6	0	-0.201141	1.435522	-3.346716
79	6	0	0.857521	0.778931	-2.688233
80	6	0	1.163333	-1.604343	1.685404
81	6	0	-2.625985	2.240230	-3.442586
82	6	0	0.059831	2.041266	-4.702137
83	1	0	1.292793	0.982953	2.639743
84	1	0	5.154514	-1.765216	4.110763
85	1	0	-1.305809	-0.303212	1.087547
86	1	0	2.323576	-0.712594	-0.699397
87	1	0	-2.711324	1.051286	-0.981859
88	1	0	1.850749	0.683345	-3.103612
89	1	0	0.309208	-1.847336	2.312633
90	1	0	1.525883	-2.526240	1.221343
91	1	0	1.085263	1.849703	-5.034828
92	1	0	-0.613717	1.609899	-5.448563
93	1	0	-0.078446	3.126516	-4.664479
94	1	0	-3.533506	2.251550	-2.829302
95	1	0	-2.358793	3.281061	-3.651830
96	1	0	-2.867255	1.727640	-4.379216
97	1	0	3.011917	1.960387	4.096047

98	1	0	4.955361	0.599886	4.835113
99	1	0	3.428935	-2.770440	2.660706
100	5	0	-4.565840	0.101976	0.577526
101	9	0	-4.481582	-0.608505	-0.418089
102	9	0	-5.353231	-0.385038	1.358302
103	9	0	-3.521933	0.182977	1.086803
104	9	0	-4.939277	1.216303	0.255078
