

Electronic Supplementary Information

Ruthenium, osmium and rhodium complexes of 1, 4-diaryl 1, 4-diazabutadiene: radical versus non-radical states

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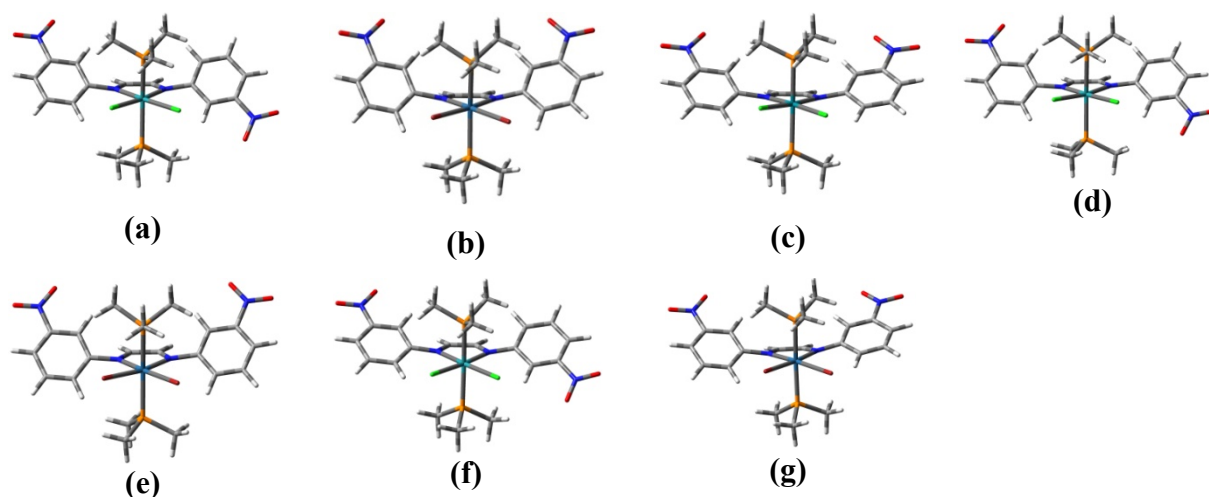


Fig. S1 Gas phase optimized geometries of (a) 1^{Me} , (b) 2^{Me} , (c) 3^{Me} , (d) $[1^{\text{Me}}]^+$, (e) $[2^{\text{Me}}]^+$, (f) $[1^{\text{Me}}]^-$, (g) $[2^{\text{Me}}]^-$.

Table S1 EPR measurement parameters

complexes	Conditions	Temp (K)	Mod. Amp. (G)	B ₀ Field (mT)	B ₀ Sweep (mT)	Frequency (GHz)	Sweep Time (s)
3	Solid	298	0.2	336.83	299.89	9.445855	30
		248	0.2	336.83	299.89	9.446124	30
		198	0.2	336.83	299.89	9.446289	30
		153	0.2	336.83	299.89	9.446391	30
	CH ₂ Cl ₂ solution	293	0.18	339.89	199.74	9.442533	30
	CH ₂ Cl ₂ solution	273	0.18	339.89	199.74	9.442577	30
	CH ₂ Cl ₂ solution	233	0.18	339.89	199.74	9.442538	30
	CH ₂ Cl ₂ -frozen glass	193	0.18	339.89	199.74	9.442520	30
	CH ₂ Cl ₂ -frozen glass	173	0.18	339.89	199.74	9.442743	30
	CH ₂ Cl ₂ -frozen glass	153	0.18	339.89	199.74	9.443524	30
	CH ₂ Cl ₂ -frozen glass	133	0.18	339.89	199.74	9.443648	30
	CH ₂ Cl ₂ -frozen glass	113	0.18	339.89	199.74	9.443525	30
$[1]^+$	CH ₂ Cl ₂ -toluene frozen glass	110	0.1	326.82	499.64	9.674012	30
$[1]^-$			0.3	336.83	499.64	9.44804	30
$[2]^+$			0.18	322.36	399.48	9.470513	30
$[2]^-$			0.1	324.87	499.64	9.443613	30

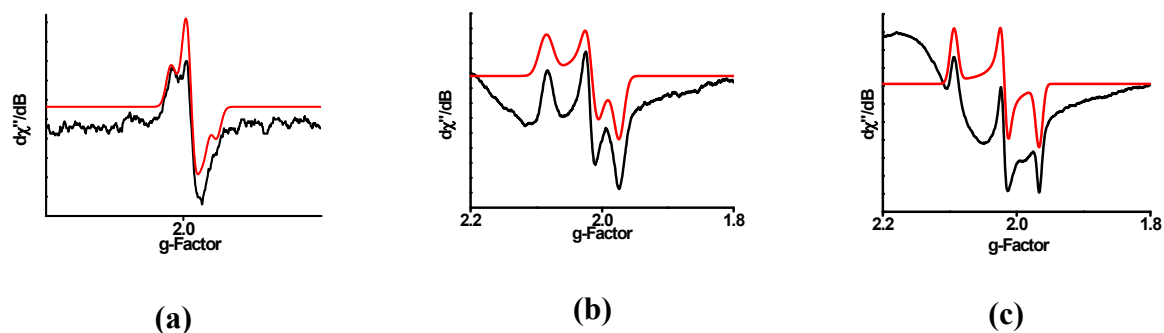


Fig. S2 EPR spectra of **3** in (a) CH₂Cl₂ solution (0.04 mM) at 293 K (b) frozen glass at 173 K and (c) frozen glass at 133 K (black = experimental, red = simulated).

Table S2 Optimized coordinates of **1**^{Me}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.244007	1.708392	-0.492513
2	6	0	2.697372	0.437492	-0.743294
3	6	0	3.554313	-0.659514	-0.882222
4	6	0	4.926958	-0.450436	-0.791778
5	6	0	5.488914	0.800592	-0.534748
6	6	0	4.625945	1.884665	-0.385308
7	1	0	2.582073	2.557457	-0.351979
8	1	0	3.169222	-1.650783	-1.049869
9	1	0	6.564058	0.907588	-0.457776
10	7	0	1.279076	0.282234	-0.860805
11	6	0	0.670523	1.160124	-1.650107
12	1	0	1.236460	1.850362	-2.271091
13	6	0	-0.738567	1.175057	-1.624718

14	1	0	-1.309757	1.869289	-2.236124
15	7	0	-1.337498	0.319296	-0.804230
16	6	0	-2.748943	0.487417	-0.652467
17	6	0	-3.282762	1.775097	-0.502885
18	6	0	-3.613992	-0.618185	-0.641927
19	6	0	-4.661283	1.928508	-0.369510
20	1	0	-2.647247	2.651058	-0.460680
21	6	0	-4.991993	-0.433857	-0.514708
22	1	0	-3.200492	-1.613408	-0.709318
23	6	0	-5.536565	0.843028	-0.376153
24	1	0	-5.646488	-1.300217	-0.511527
25	1	0	-6.602240	1.003962	-0.267082
26	44	0	-0.018176	-0.986109	0.142281
27	17	0	1.757244	-2.423440	1.100890
28	17	0	-1.753159	-2.323831	1.332172
29	7	0	-5.202097	3.289053	-0.205241
30	8	0	-4.402158	4.228183	-0.187330
31	8	0	-6.422418	3.412284	-0.096441
32	15	0	-0.075830	-2.733961	-1.587231
33	15	0	0.007786	0.166527	2.279817
34	6	0	-1.293119	-2.513604	-2.968260
35	1	0	-1.211664	-3.338359	-3.686073
36	1	0	-2.314754	-2.490626	-2.579911
37	1	0	-1.104910	-1.571878	-3.494760
38	6	0	1.475790	-3.041449	-2.543157
39	1	0	1.814594	-2.129115	-3.043529

40	1	0	1.297925	-3.812354	-3.302171
41	1	0	2.260686	-3.391868	-1.867710
42	6	0	0.348783	-0.902125	3.735916
43	1	0	0.275682	-0.309178	4.655317
44	1	0	-0.378662	-1.717051	3.753678
45	1	0	1.346089	-1.337523	3.644671
46	6	0	-1.575766	0.993404	2.744997
47	1	0	-2.383221	0.257377	2.703807
48	1	0	-1.804255	1.806553	2.049405
49	1	0	-1.510363	1.405748	3.758820
50	6	0	-0.463386	-4.416225	-0.953838
51	1	0	-1.466070	-4.430701	-0.521719
52	1	0	-0.387661	-5.151776	-1.763284
53	1	0	0.247890	-4.657192	-0.159128
54	6	0	1.234177	1.534861	2.498041
55	1	0	1.160592	1.960838	3.505760
56	1	0	1.050683	2.331108	1.769126
57	1	0	2.247793	1.151415	2.349899
58	7	0	5.824211	-1.606752	-0.984978
59	8	0	7.024864	-1.439567	-0.763361
60	8	0	5.324272	-2.665157	-1.365179
61	1	0	5.028316	2.872254	-0.179755

Table S2 Optimized coordinates of **2^{Me}**

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

1	6	0	3.164469	1.640245	-0.682376	
2	6	0	2.700038	0.318733	-0.712639	
3	6	0	3.622215	-0.733253	-0.615525	
4	6	0	4.988182	-0.465602	-0.501453	
5	6	0	5.463646	0.845148	-0.468869	
6	6	0	4.532139	1.878595	-0.560525	
7	1	0	2.481754	2.479283	-0.731134	
8	1	0	3.268942	-1.752638	-0.620825	
9	1	0	5.687776	-1.292999	-0.430326	
10	1	0	6.518714	1.071211	-0.373115	
11	7	0	1.292325	0.077563	-0.864689	
12	6	0	0.707336	0.787755	-1.842046	
13	1	0	1.297650	1.347169	-2.560902	
14	6	0	-0.688709	0.817052	-1.825668	
15	1	0	-1.274498	1.391779	-2.536006	
16	7	0	-1.276698	0.135766	-0.830299	
17	6	0	-2.680210	0.397010	-0.672591	
18	6	0	-3.119613	1.723381	-0.593298	
19	6	0	-3.619907	-0.643040	-0.623912	
20	6	0	-4.484097	1.980645	-0.467167	
21	1	0	-2.420289	2.550383	-0.611625	

22	6	0	-4.981621	-0.356562	-0.507314
23	1	0	-3.283934	-1.668306	-0.668710
24	6	0	-5.433225	0.960346	-0.422580
25	1	0	-5.696535	-1.173071	-0.472995
26	1	0	-6.484699	1.200725	-0.322462
27	7	0	-4.928422	3.381707	-0.371611
28	8	0	-4.065395	4.262440	-0.401272
29	8	0	-6.137034	3.594401	-0.266903
30	7	0	5.000112	3.275300	-0.519120
31	8	0	6.211377	3.471103	-0.413116
32	8	0	4.152982	4.168540	-0.592751
33	15	0	-0.063119	-2.886922	-1.295640
34	15	0	0.054263	0.359082	2.283454
35	6	0	-1.209937	-2.700637	-2.737539
36	1	0	-1.110164	-3.556564	-3.414626
37	1	0	-2.246326	-2.644662	-2.394603
38	1	0	-0.982101	-1.785070	-3.292242
39	6	0	1.527243	-3.264383	-2.157792
40	1	0	1.900443	-2.380352	-2.683229
41	1	0	1.378379	-4.071999	-2.883635
42	1	0	2.268528	-3.583796	-1.420619
43	6	0	0.263447	-0.522736	3.885796
44	1	0	0.182866	0.198438	4.707323
45	1	0	-0.509009	-1.288754	3.981456
46	1	0	1.238820	-1.012255	3.912891
47	6	0	-1.452331	1.379004	2.596404

48	1	0	-2.328585	0.725904	2.634726
49	1	0	-1.592632	2.112613	1.797612
50	1	0	-1.357170	1.912270	3.549251
51	6	0	-0.527769	-4.530105	-0.614171
52	1	0	-1.552409	-4.500304	-0.237340
53	1	0	-0.433726	-5.297230	-1.391389
54	1	0	0.133377	-4.762477	0.224889
55	6	0	1.401326	1.621213	2.376928
56	1	0	1.355848	2.152443	3.334704
57	1	0	1.307694	2.353213	1.569183
58	1	0	2.373396	1.127118	2.291353
59	76	0	-0.012027	-1.024511	0.285316
60	35	0	-1.905462	-2.267444	1.658734
61	35	0	1.777632	-2.531969	1.521687

Table S3 Optimized coordinates of **3^{Me}**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.362078	1.554999	-0.713354
2	6	0	2.797808	0.269790	-0.586966
3	6	0	3.667579	-0.815135	-0.356875
4	6	0	5.046388	-0.624604	-0.286630
5	6	0	5.610634	0.641527	-0.438528
6	6	0	4.742632	1.710493	-0.646737

7	1	0	2.747562	2.436768	-0.835626
8	1	0	3.248963	-1.799666	-0.211719
9	1	0	5.690640	-1.481183	-0.112317
10	1	0	6.678503	0.811446	-0.390009
11	7	0	1.405200	0.088441	-0.708361
12	6	0	0.739155	0.918939	-1.534979
13	1	0	1.290357	1.542565	-2.234544
14	6	0	-0.647717	0.962484	-1.519240
15	1	0	-1.177588	1.608013	-2.215686
16	7	0	-1.341765	0.177395	-0.674342
17	6	0	-2.734185	0.370756	-0.590278
18	6	0	-3.277885	1.665210	-0.691459
19	6	0	-3.620071	-0.713660	-0.431302
20	6	0	-4.658455	1.834124	-0.660814
21	1	0	-2.646593	2.540669	-0.772073
22	6	0	-4.998513	-0.510614	-0.398900
23	1	0	-3.217093	-1.709267	-0.311972
24	6	0	-5.542794	0.767821	-0.518513
25	1	0	-5.657909	-1.364962	-0.279138
26	1	0	-6.609792	0.948293	-0.496399
27	17	0	1.604253	-2.521913	1.516430
28	17	0	-1.707631	-2.228633	1.700119
29	7	0	-5.198478	3.200655	-0.767008
30	8	0	-4.395025	4.127667	-0.874621
31	8	0	-6.420945	3.334120	-0.743148
32	7	0	5.299955	3.067485	-0.782140

33	8	0	6.522487	3.190242	-0.723913
34	8	0	4.510572	3.998356	-0.946764
35	15	0	-0.080622	-2.788741	-1.295515
36	15	0	0.041709	0.421508	2.296937
37	6	0	-1.154547	-2.439530	-2.756152
38	1	0	-1.102542	-3.261292	-3.479050
39	1	0	-2.192508	-2.308028	-2.440330
40	1	0	-0.824548	-1.515815	-3.240345
41	6	0	1.538506	-3.185004	-2.081420
42	1	0	1.970336	-2.286354	-2.529164
43	1	0	1.408995	-3.948604	-2.856358
44	1	0	2.220226	-3.562263	-1.315474
45	6	0	0.493290	-0.393718	3.878003
46	1	0	0.408073	0.317700	4.707114
47	1	0	-0.178617	-1.240636	4.035581
48	1	0	1.513306	-0.777725	3.813805
49	6	0	-1.580184	1.212860	2.657354
50	1	0	-2.335916	0.431046	2.764611
51	1	0	-1.871224	1.870251	1.834354
52	1	0	-1.520076	1.799721	3.580619
53	6	0	-0.656649	-4.423165	-0.685803
54	1	0	-1.679847	-4.341450	-0.313465
55	1	0	-0.604364	-5.171503	-1.484632
56	1	0	-0.019396	-4.719539	0.151275
57	6	0	1.195974	1.855018	2.187655
58	1	0	1.131536	2.466664	3.094344

59	1	0	0.941296	2.475150	1.323219
60	1	0	2.222691	1.499898	2.067420
61	45	0	-0.003791	-1.076477	0.415614

Table S4 Optimized coordinates of [1^{Me}]⁺

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.273276	1.772264	-0.575789
2	6	0	2.707109	0.494175	-0.746622
3	6	0	3.542266	-0.616747	-0.892891
4	6	0	4.918471	-0.418924	-0.894176
5	6	0	5.502336	0.834624	-0.723594
6	6	0	4.658516	1.935126	-0.560265
7	1	0	2.633068	2.635714	-0.422102
8	1	0	3.150168	-1.612762	-1.014344
9	1	0	6.581405	0.934780	-0.716821
10	7	0	1.281181	0.344797	-0.793670
11	6	0	0.628520	1.223090	-1.513259
12	1	0	1.151462	1.956767	-2.122803
13	6	0	-0.799440	1.192536	-1.484356
14	1	0	-1.380152	1.897477	-2.075259
15	7	0	-1.381087	0.289140	-0.736294
16	6	0	-2.809745	0.367401	-0.637171
17	6	0	-3.400576	1.614335	-0.395275

18	6	0	-3.618380	-0.769793	-0.786726
19	6	0	-4.787284	1.696418	-0.319234
20	1	0	-2.810742	2.508315	-0.232832
21	6	0	-5.006929	-0.651678	-0.723884
22	1	0	-3.165862	-1.736925	-0.952796
23	6	0	-5.610503	0.585091	-0.484162
24	1	0	-5.624767	-1.534679	-0.853104
25	1	0	-6.686837	0.692611	-0.416921
26	44	0	-0.013889	-1.024018	0.263080
27	17	0	1.728023	-2.320329	1.185340
28	17	0	-1.750585	-2.185573	1.360739
29	7	0	-5.392866	3.018121	-0.040787
30	8	0	-4.624484	3.966351	0.126343
31	8	0	-6.616939	3.079634	0.005147
32	15	0	-0.080880	-2.721304	-1.583882
33	15	0	0.092665	0.254940	2.373909
34	6	0	-0.959574	-2.229359	-3.134827
35	1	0	-0.906234	-3.041882	-3.868267
36	1	0	-2.012138	-2.005033	-2.943597
37	1	0	-0.491004	-1.341857	-3.573292
38	6	0	1.542232	-3.290258	-2.245439
39	1	0	2.052661	-2.480933	-2.775512
40	1	0	1.374056	-4.110459	-2.952176
41	1	0	2.182666	-3.649832	-1.436106
42	6	0	0.181518	-0.813881	3.865380
43	1	0	0.209325	-0.183721	4.761303

44	1	0	-0.691912	-1.468440	3.905240
45	1	0	1.080360	-1.433449	3.825750
46	6	0	-1.355690	1.342567	2.705784
47	1	0	-2.274824	0.751423	2.663925
48	1	0	-1.416520	2.146010	1.965615
49	1	0	-1.268483	1.793215	3.700743
50	6	0	-0.885219	-4.299129	-1.089648
51	1	0	-1.927354	-4.135676	-0.806470
52	1	0	-0.838305	-5.013994	-1.918516
53	1	0	-0.362706	-4.713593	-0.222606
54	6	0	1.539873	1.376738	2.571152
55	1	0	1.542182	1.809795	3.577714
56	1	0	1.501211	2.192349	1.843319
57	1	0	2.466876	0.815138	2.425489
58	7	0	5.789797	-1.601683	-1.088493
59	8	0	7.000849	-1.430206	-0.992850
60	8	0	5.238740	-2.673741	-1.336799
61	1	0	5.081896	2.923892	-0.413633

Table S5 Optimized coordinates of $[2^{\text{Me}}]^+$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.270897	1.640340	-0.639648
2	6	0	2.738128	0.347280	-0.722897

3	6	0	3.602433	-0.755011	-0.774392
4	6	0	4.984628	-0.562676	-0.759114
5	6	0	5.529890	0.719642	-0.671027
6	6	0	4.652543	1.799470	-0.609582
7	1	0	2.641760	2.519025	-0.570352
8	1	0	3.202146	-1.754676	-0.836709
9	1	0	5.643065	-1.424059	-0.811938
10	1	0	6.600313	0.887166	-0.646033
11	7	0	1.304820	0.196524	-0.788420
12	6	0	0.692552	1.010806	-1.631047
13	1	0	1.254776	1.651463	-2.303256
14	6	0	-0.719720	1.011669	-1.606146
15	1	0	-1.308527	1.638695	-2.268338
16	7	0	-1.298129	0.199556	-0.738737
17	6	0	-2.734413	0.307120	-0.657919
18	6	0	-3.296229	1.578126	-0.497818
19	6	0	-3.568131	-0.815030	-0.765140
20	6	0	-4.682056	1.697771	-0.445519
21	1	0	-2.685743	2.465945	-0.387079
22	6	0	-4.954404	-0.660899	-0.730327
23	1	0	-3.140472	-1.800503	-0.881274
24	6	0	-5.530605	0.600172	-0.563210
25	1	0	-5.591558	-1.534447	-0.825953
26	1	0	-6.604734	0.737297	-0.519613
27	7	0	-5.257969	3.047026	-0.249093
28	8	0	-4.468721	3.984297	-0.124172

29	8	0	-6.480812	3.140047	-0.222386
30	7	0	5.193415	3.173043	-0.497806
31	8	0	6.413423	3.299770	-0.492106
32	8	0	4.380368	4.094623	-0.416175
33	15	0	-0.098852	-2.841096	-1.281195
34	15	0	0.138551	0.501089	2.351578
35	6	0	-0.922923	-2.417701	-2.879918
36	1	0	-0.874557	-3.274972	-3.560218
37	1	0	-1.971393	-2.148241	-2.735712
38	1	0	-0.411664	-1.573791	-3.354613
39	6	0	1.509118	-3.506122	-1.893329
40	1	0	2.051829	-2.744123	-2.460187
41	1	0	1.313958	-4.354564	-2.558057
42	1	0	2.124553	-3.847476	-1.057212
43	6	0	0.264883	-0.353426	3.974579
44	1	0	0.246487	0.397065	4.772316
45	1	0	-0.571342	-1.043587	4.103456
46	1	0	1.198041	-0.918085	4.029073
47	6	0	-1.315949	1.609358	2.569927
48	1	0	-2.232752	1.016617	2.627218
49	1	0	-1.397390	2.311972	1.735836
50	1	0	-1.207108	2.185031	3.495613
51	6	0	-0.954065	-4.365092	-0.713007
52	1	0	-2.000291	-4.163947	-0.472634
53	1	0	-0.900521	-5.128838	-1.496215
54	1	0	-0.464987	-4.736689	0.192089

55	6	0	1.566176	1.662359	2.399607
56	1	0	1.558879	2.211524	3.347556
57	1	0	1.510642	2.387905	1.583651
58	1	0	2.506540	1.109779	2.321336
59	76	0	0.007342	-0.999995	0.385298
60	35	0	-1.870185	-2.065859	1.701127
61	35	0	1.809309	-2.348734	1.530324

Table S6 Optimized coordinates of [1^{Me}]⁻

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.312289	1.683576	-0.646199
2	6	0	2.731374	0.391640	-0.689423
3	6	0	3.604226	-0.716566	-0.670094
4	6	0	4.978399	-0.503901	-0.642865
5	6	0	5.559948	0.769652	-0.602221
6	6	0	4.696949	1.863008	-0.605717
7	1	0	2.664437	2.553772	-0.610079
8	1	0	3.204990	-1.719477	-0.651283
9	1	0	6.636382	0.880311	-0.569472
10	7	0	1.343620	0.216838	-0.772940
11	6	0	0.666334	1.144706	-1.490049
12	1	0	1.203948	1.840011	-2.133409
13	6	0	-0.715854	1.176138	-1.448761

14	1	0	-1.255211	1.885179	-2.074608
15	7	0	-1.388161	0.287317	-0.678769
16	6	0	-2.767407	0.477182	-0.554831
17	6	0	-3.354894	1.761227	-0.643785
18	6	0	-3.633909	-0.620201	-0.336687
19	6	0	-4.740281	1.901833	-0.560478
20	1	0	-2.747565	2.651095	-0.742886
21	6	0	-5.014043	-0.445378	-0.250727
22	1	0	-3.199540	-1.602232	-0.199713
23	6	0	-5.599849	0.817260	-0.369973
24	1	0	-5.645347	-1.314581	-0.084408
25	1	0	-6.670227	0.968165	-0.309401
26	44	0	-0.009562	-1.114180	0.226799
27	17	0	1.749920	-2.656268	1.154442
28	17	0	-1.707208	-2.554339	1.453427
29	7	0	-5.314426	3.249419	-0.658771
30	8	0	-4.548697	4.206512	-0.820625
31	8	0	-6.543146	3.369122	-0.577806
32	15	0	-0.117370	-2.631124	-1.628205
33	15	0	0.054284	0.092752	2.295328
34	6	0	-1.428946	-2.331797	-2.908816
35	1	0	-1.382865	-3.082236	-3.708740
36	1	0	-2.417571	-2.370289	-2.441432
37	1	0	-1.299876	-1.335263	-3.344126
38	6	0	1.382678	-2.779408	-2.707645
39	1	0	1.650396	-1.800501	-3.118161

40	1	0	1.203348	-3.478358	-3.534928
41	1	0	2.222724	-3.146309	-2.110747
42	6	0	0.440433	-0.915339	3.791401
43	1	0	0.397077	-0.299455	4.699136
44	1	0	-0.284933	-1.731464	3.851027
45	1	0	1.432712	-1.359763	3.679189
46	6	0	-1.526884	0.913865	2.800903
47	1	0	-2.317483	0.157616	2.822247
48	1	0	-1.804777	1.682484	2.072833
49	1	0	-1.435196	1.376438	3.792253
50	6	0	-0.411775	-4.396951	-1.181676
51	1	0	-1.366071	-4.481836	-0.655204
52	1	0	-0.408481	-5.035919	-2.074178
53	1	0	0.375858	-4.708000	-0.489054
54	6	0	1.260832	1.491931	2.466695
55	1	0	1.192533	1.959138	3.457703
56	1	0	1.062235	2.249628	1.701396
57	1	0	2.277627	1.115594	2.318219
58	7	0	5.869805	-1.674076	-0.682968
59	8	0	7.072495	-1.491327	-0.449080
60	8	0	5.386543	-2.772513	-0.959683
61	1	0	5.103957	2.870619	-0.563654

Table S7 Optimized coordinates of [2^{Me}]⁻

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

1	6	0	3.288485	1.584191	-0.886089
2	6	0	2.723147	0.322735	-0.574891
3	6	0	3.608377	-0.687268	-0.132491
4	6	0	4.981220	-0.463651	-0.045495
5	6	0	5.545572	0.768215	-0.385570
6	6	0	4.667089	1.773331	-0.797122
7	1	0	2.668095	2.426680	-1.159522
8	1	0	3.196696	-1.644014	0.161176
9	1	0	5.623799	-1.272496	0.293529
10	1	0	6.610395	0.955552	-0.330287
11	7	0	1.350221	0.082762	-0.708343
12	6	0	0.694700	0.872116	-1.614109
13	1	0	1.250430	1.432930	-2.360623
14	6	0	-0.676675	0.912771	-1.583992
15	1	0	-1.238671	1.505090	-2.302387
16	7	0	-1.332826	0.150287	-0.662323
17	6	0	-2.712241	0.392694	-0.548153
18	6	0	-3.221453	1.705713	-0.631514
19	6	0	-3.639550	-0.661543	-0.394334
20	6	0	-4.598538	1.924313	-0.574001
21	1	0	-2.554521	2.554418	-0.715556
22	6	0	-5.010490	-0.412245	-0.332954
23	1	0	-3.270310	-1.673701	-0.312477
24	6	0	-5.519306	0.884305	-0.424486

25	1	0	-5.694153	-1.248864	-0.214193
26	1	0	-6.580755	1.093585	-0.382340
27	7	0	-5.095790	3.302072	-0.661169
28	8	0	-4.275811	4.216983	-0.794680
29	8	0	-6.317716	3.486746	-0.599158
30	7	0	5.214301	3.094892	-1.132745
31	8	0	6.435999	3.263312	-1.033698
32	8	0	4.434969	3.980022	-1.501811
33	15	0	-0.070248	-2.750067	-1.356550
34	15	0	0.054196	0.271828	2.333916
35	6	0	-1.179453	-2.425830	-2.809122
36	1	0	-1.080037	-3.215881	-3.564213
37	1	0	-2.221724	-2.378334	-2.479048
38	1	0	-0.922672	-1.462715	-3.261079
39	6	0	1.548491	-3.034684	-2.210524
40	1	0	1.913760	-2.093886	-2.634135
41	1	0	1.452156	-3.779830	-3.010490
42	1	0	2.274908	-3.386735	-1.472310
43	6	0	0.357653	-0.559043	3.954511
44	1	0	0.294410	0.167168	4.774783
45	1	0	-0.388511	-1.347064	4.088057
46	1	0	1.343914	-1.029721	3.943586
47	6	0	-1.484629	1.232986	2.705585
48	1	0	-2.320725	0.532964	2.794515
49	1	0	-1.702104	1.929153	1.890015
50	1	0	-1.378962	1.798985	3.639714

51	6	0	-0.550662	-4.472270	-0.896793
52	1	0	-1.571879	-4.474843	-0.505924
53	1	0	-0.475051	-5.142952	-1.762029
54	1	0	0.111388	-4.812361	-0.095280
55	6	0	1.334329	1.613506	2.371013
56	1	0	1.265039	2.195026	3.298988
57	1	0	1.201009	2.287080	1.518443
58	1	0	2.332079	1.169740	2.300442
59	76	0	-0.028012	-1.131457	0.398327
60	35	0	-1.915654	-2.462978	1.778323
61	35	0	1.647564	-2.859784	1.614145
