Electronic Supplementary Material (ESI) for Dalton Transactions

Supporting Information

Aryl Pyrazaboles: A New Class of Tunable and Highly Fluorescent Materials

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Contents

1. X-ray crystallographic analysis

Single crystal X-ray structural studies of **2, 5**, and **7** were performed on a CCD Agilent Technologies (Oxford Diffraction) SUPER NOVA diffractometer. Data were collected at 150(2) K using graphite-monochromated Mo Kα radiation (λ_α = 0.71073 Å). The strategy for the Data collection was evaluated by using the CrysAlisPro CCD software. The data were collected by the standard 'phi-omega scan techniques, and were scaled and reduced using CrysAlisPro RED software. The structures were solved by direct methods using SHELXS-97, and refined by full matrix least-squares with SHELXL-97, refining on F^2. The crystal, and refinement data are summarized in Table 1. The CCDC numbers **928340, 928339**, and **950019** contain the supplementary crystallographic data for **2, 5,** and **7** respectively. These data can be obtained free of charge via www.ccdc.cam.ac.uk (or from the Cambridge Crystallographic Data Centre, 12 union Road, Cambridge CB21 EZ, UK; Fax: (+44) 1223-336-033; or deposit@ccdc.cam.ac.uk).

Table S1. Crystal data and structure refinement parameters.

Pyrazaboles	**2**	**5**	**7**
Empirical formula	$C_{34}H_{50}B_2N_4$	$C_{13.50}H_{14.50}B_{0.50}N$	$C_{23}H_{27}B_2N_2$
Crystal size	0.23 x 0.16 x 0.14 mm	0.23 x 0.18 x 0.14 mm	0.23 x 0.18 x 0.13 mm
Crystal system	Triclinic	Triclinic	Monoclinic
Space group	*P* -1	*P* -1	*P 21/c*
Formula weight	536.40	196.17	342.28
***T*,K**	150(2) K	150(2)	150(2)
***θ* range for data collection/°**	3.25 to 25.00 deg.	2.94 to 25.00	3.01 to 25.00
***a* (Å)**	9.9014(14)	8.9617(7)	12.8407(4)
***b* (Å)**	12.1457(14)	9.4626(9)	10.3162(3)
***c* (Å)**	15.3957(19)	14.4845(14)	15.3851(5)

***α*/°**	76.110(10)	79.710(8)	90
***β*/°**	87.689(11)	82.667(8)	99.994(3)
***γ*/°**	71.391(12)	66.359(9)	90
Z	2	4	4
***F*(000)**	584	420	736
V (A°)^3	1702.0(4)	1104.98(17)	2007.10(11)
$D_{calc,}$ Mg m^{-3}	1.047	1.179	1.133
Collected refins	12606	7326	15671
Unique refins	5999 [R(int) = 0.1143]	3877 [R(int) = 0.0512]	3527 [R(int) = 0.0307]
Data/restrains/param iters	5999 / 0 / 366	3877 / 0 / 293	3527 / 0 / 237
Goodness-of-fit on F^2	0.973	1.073	1.068
Final R indices [I>2σ(l)] [6]	R_1 = 0.0970, wR_2 = 0.2679	R_1 = 0.0932, wR_2 = 0.2647	R1 = 0.0487, wR2= 0.1320
R indices (all data)	R_1 = 0.1990, wR_2 = 0.3760	R_1 = 0.1269, wR_2 = 0.3149	R1 = 0.0547, wR2 = 0.1371

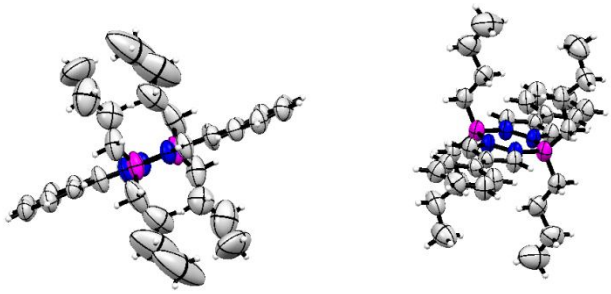

Fig. S1 Crystal structure of **2** shows two molecules in asymmetric unit (50% probability for thermal ellipsoids).

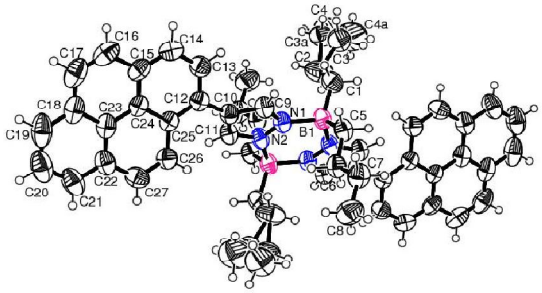

Fig. S2 Crystal structure of **5** (50% probability for thermal ellipsoids).

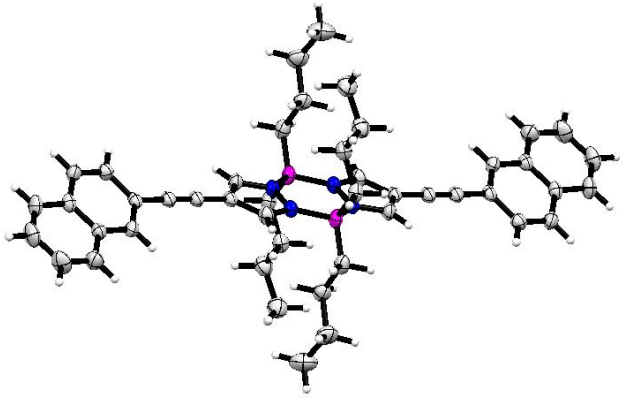

Fig. S3 Crystal structure of **7** (50% probability for thermal ellipsoids).

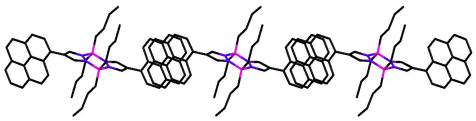

Fig. S4 Crystal packing of pyrazabole **5** view along *b*-axis.

Table S2. Selected bond lengths and angles of pyrazabole 2.

pyrazabole 2			
Bond lengths (Å)		**Bond angles °**	
B(1)-N(2)	1.572(8)	N(2)-B(1)-N(1)#1	104.5(4)
B(1)-N(1)#1	1.591(7)	N(2)-B(1)-C(5)	112.4(6)
B(2)-N(4)#2	1.587(6)	N(1)#1-B(1)-C(5)	109.0(5)
B(2)-N(3)	1.589(5)	N(4)#2-B(2)-N(3)	104.7(3)
B(1)-C(1)	1.544(11)	N(4)#2-B(2)-C(22)	109.2(4)
B(1)-C(5)	1.617(13)	N(3)-B(2)-C(22)	110.4(3)
B(2)-C(22)	1.597(7)	N(3)-B(2)-C(18)	109.9(4)
B(2)-C(18)	1.612(7)	C(22)-B(2)-C(18)	112.1(4)

Table S3. Selected bond lengths and angles of pyrazabole 5.

pyrazabole 5			
Bond lengths (Å)		**Bond angles °**	
B(1)-N(1)	1.598(4)	N(2)#1-B(1)-N(1)	105.0(3)
B(1)-N(2)	1.578(5)	N(2)#1-B(1)-C(5)	110.6(3)
B(1)-C(5)	1.608(5)	N(1)-B(1)-C(5)	109.6(3)
B(1)-C(1)	1.611(5)	N(2)#1-B(1)-C(1)	108.6(3)
N(1)-C(9)	1.338(4)	N(1)-B(1)-C(1)	111.1(3)
N(1)-N(2)	1.345(3)	C(5)-B(1)-C(1)	111.6(3)
N(2)-C(11)	1.337(4)	C(9)-N(1)-N(2)	108.7(2)

Table S4. Selected bond lengths and angles of pyrazabole 7.

pyrazabole 7			
Bond lengths (Å)		**Bond angles °**	
B(1)-N(1)	1.588(2)	N(1)-B(1)-N(2)#1	104.60(14)
B(1)-N(2)#1	1.588(2)	N(1)-B(1)-C(16)	110.40(15)
B(1)-C(16)	1.608(3)	N(1)-B(1)-C(5)	109.6(3)
B(1)-C(20)	1.609(3)	N(1)-B(1)-C(20)	110.07(15)
N(1)-C(1)	1.338(2)	C(3)-N(2)-B(1)#1	123.91(14)
N(1)-N(2)	1.3549(19)	N(1)-N(2)-B(1)#1	127.23(13)
N(2)-C(3)	1.333(2)	C(1)-N(1)-N(2)	107.89(14)

2. The fluorescence quantum yields (ϕ_F) :

The fluorescence quantum yields (ϕ_F) were calculated by the steady-state comparative method using 2-amino pyridine (ϕ_{st} = 0.60, 0.1M H_2SO_4) for compounds **3** and **6,** and 9, 10-diphenylanthracence (ϕ_{st} = 0.90, ethanol) as a standard for compounds **4, 5, 8,** and **9**.

$$\phi_F = \phi_{st} \times S_u/S_{st} \times A_{st} / A_u \times n^2_{Du}/n^2_{Dst} \quad \text{..... (Eq. 1)}$$

Where ϕ_F is the emission quantum yield of the sample, ϕst is the emission quantum yield of the standard, A_{st} and A_u represent the absorbance of the standard and sample at the excitation wavelength, respectively, while Sst and Su are the integrated emission band areas of the standard and sample, respectively, and n_{Dst} and n_{Du} the solvent refractive index of the standard and sample, u and st refer to the unknown and standard, respectively.

3. Concentration dependent study:

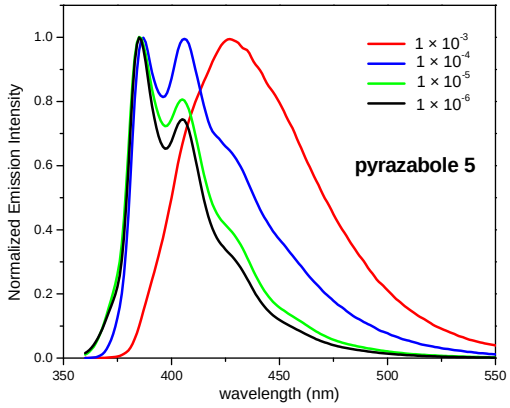

Fig. S5 Effect of concentration on the fluorescence emission spectrum of pyrazabole **5** in dichloromethane.

To evaluate the aggregation induced effect in pyrazabole **5**, the emission spectra were recorded at different concentrations; we examined the concentration effect with respect to fluorescence spectra in dichloromethane, by increasing the concentration from 10^{-6} M to 10^{-3} M. The PL spectra (Figure S5) shows decreased fluorescence intensity from 10^{-6} M to 10^{-3} M, and another important observation was that, the shoulder band located at 428 nm progressively intensifies with increasing concentration, while at higher concentration it becomes prominent, and fluorescence bands located at 395 nm and 415 nm disappear. The peaks at 395 nm and 415 nm (at 1.0×10^{-6} M) concentration are assigned to the monomer emission of the pyrene moiety,[1] whereas the peak at 428 nm (at 1.0×10^{-3} M) associated with the emission of pyrene excimers.[2]

4. Copies of NMR and Mass spectra of new compounds.

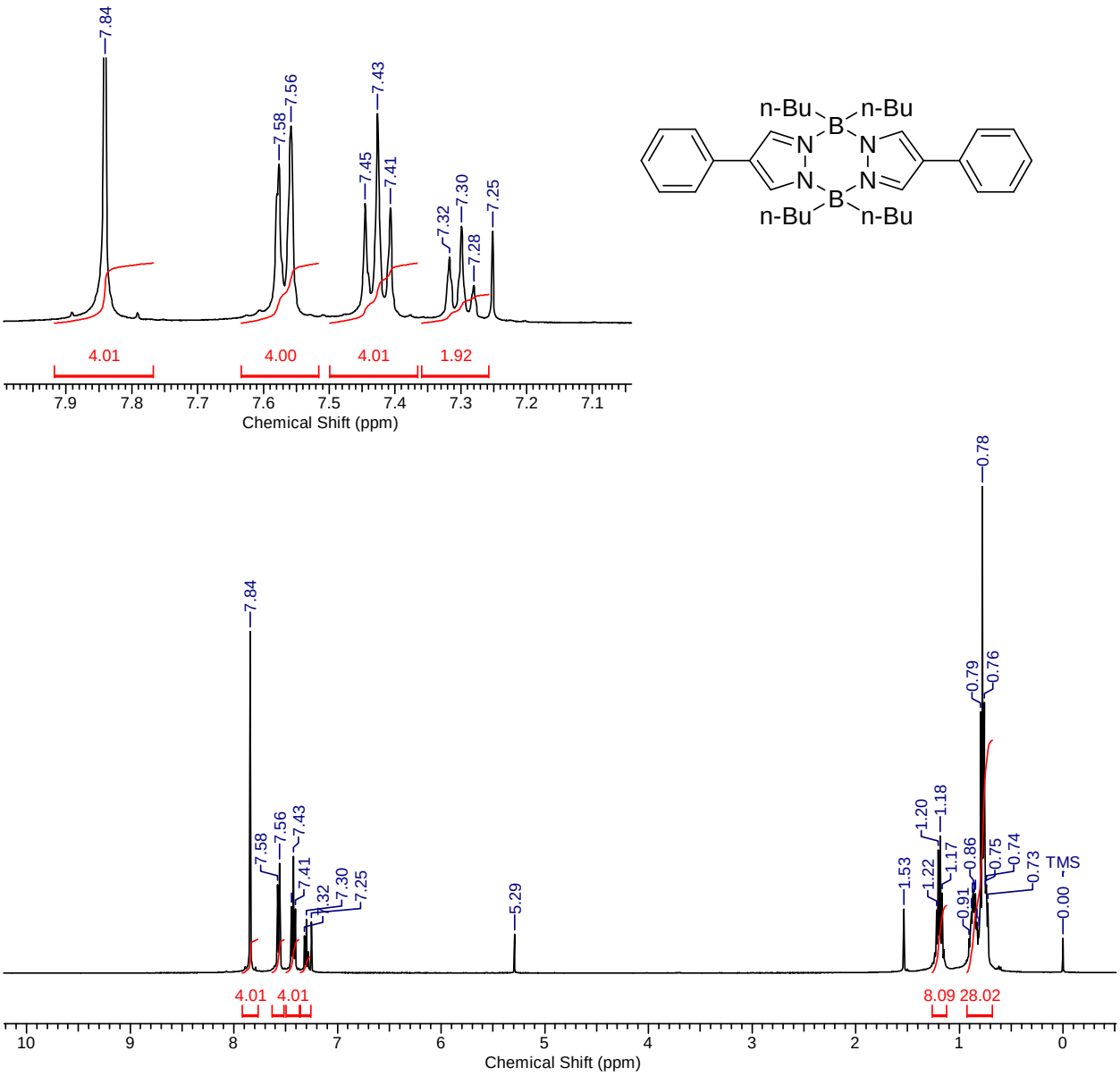

Fig. S6 ^{1}H-NMR spectrum of pyrazabole **2**.

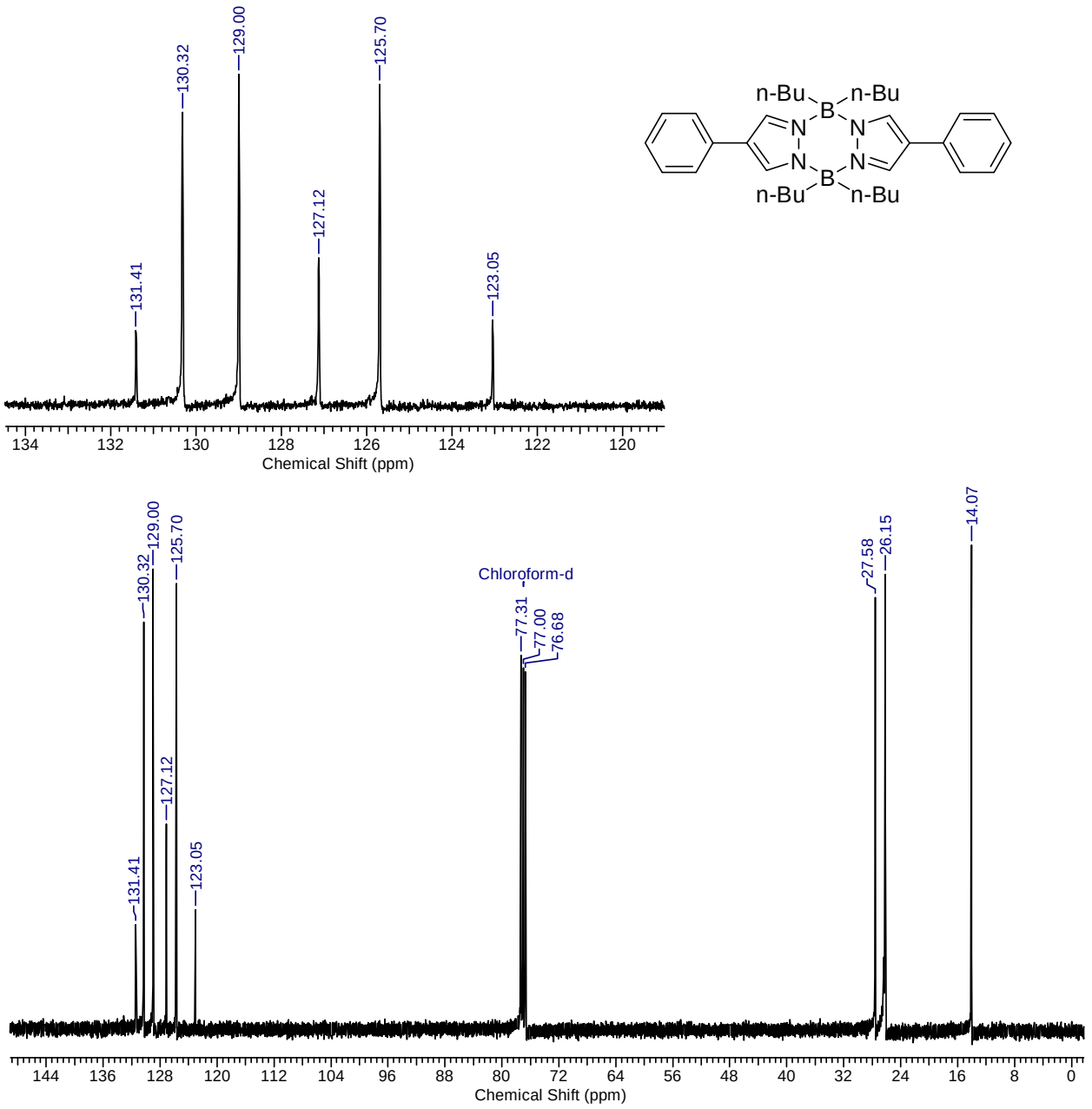

Fig. S7 ^{13}C-NMR spectrum of pyrazabole **2**.

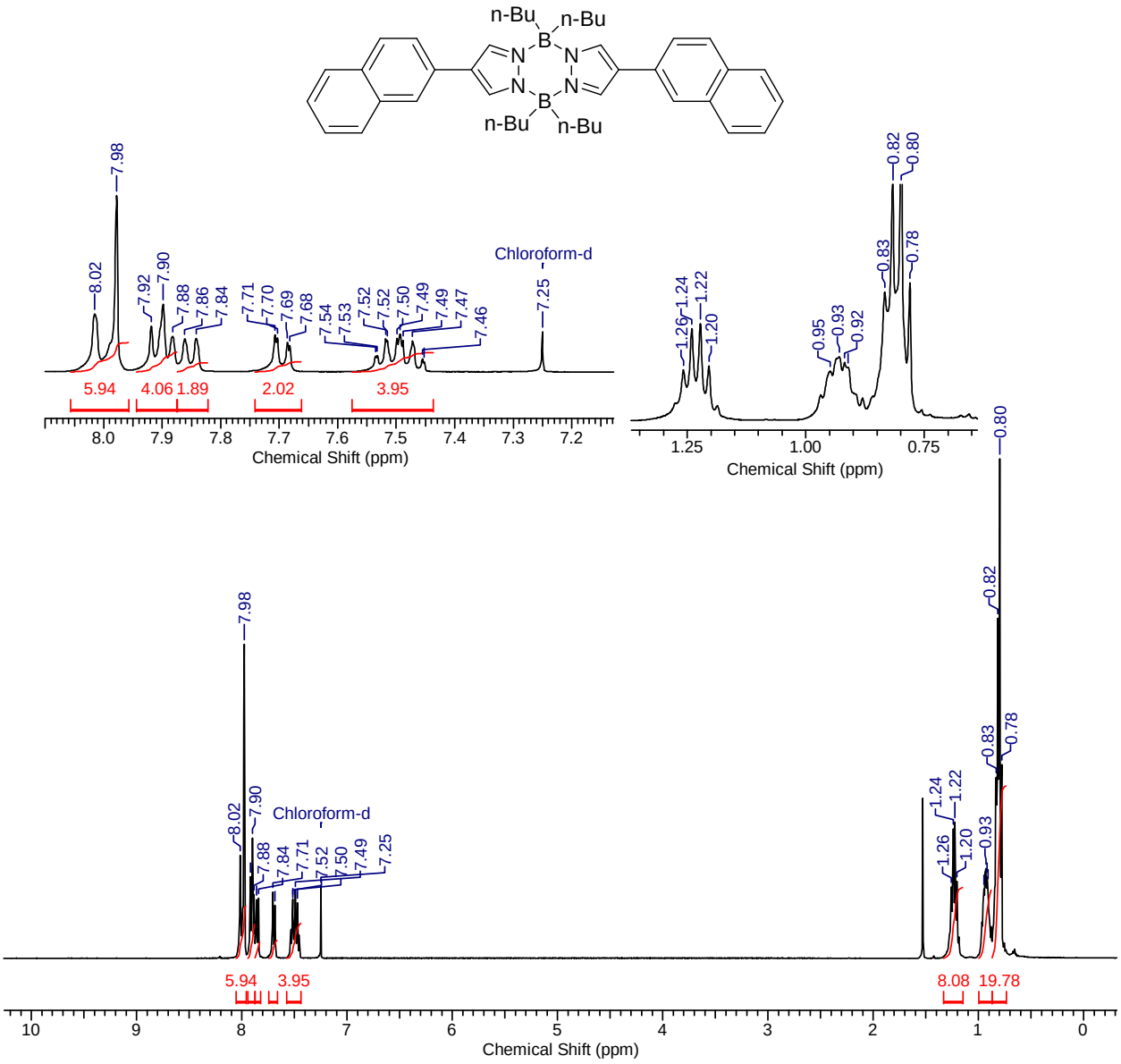

Fig. S8 ^{1}H-NMR spectrum of pyrazabole **3**.

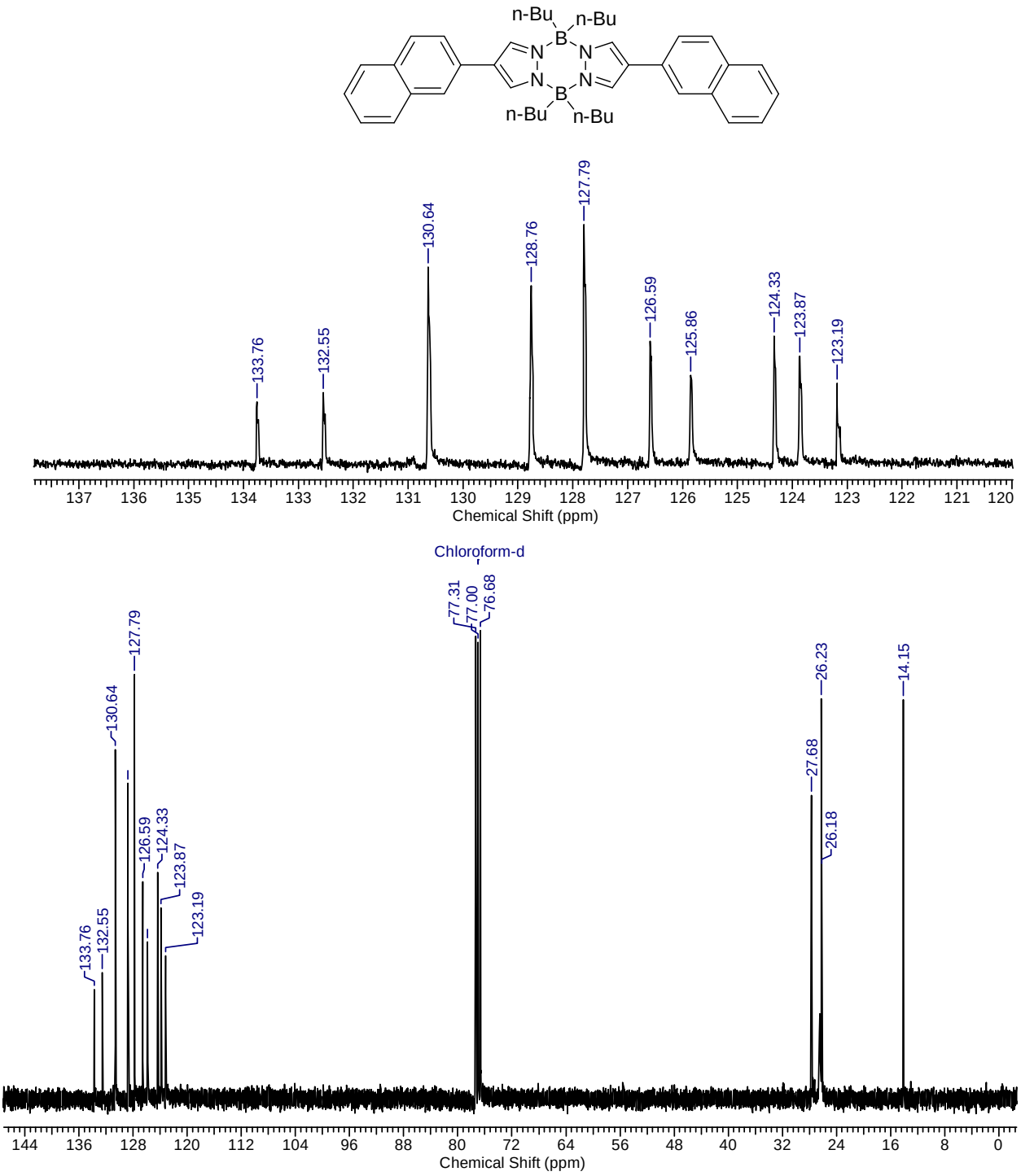

Fig. S9 ^{13}C-NMR spectrum of pyrazabole **3**.

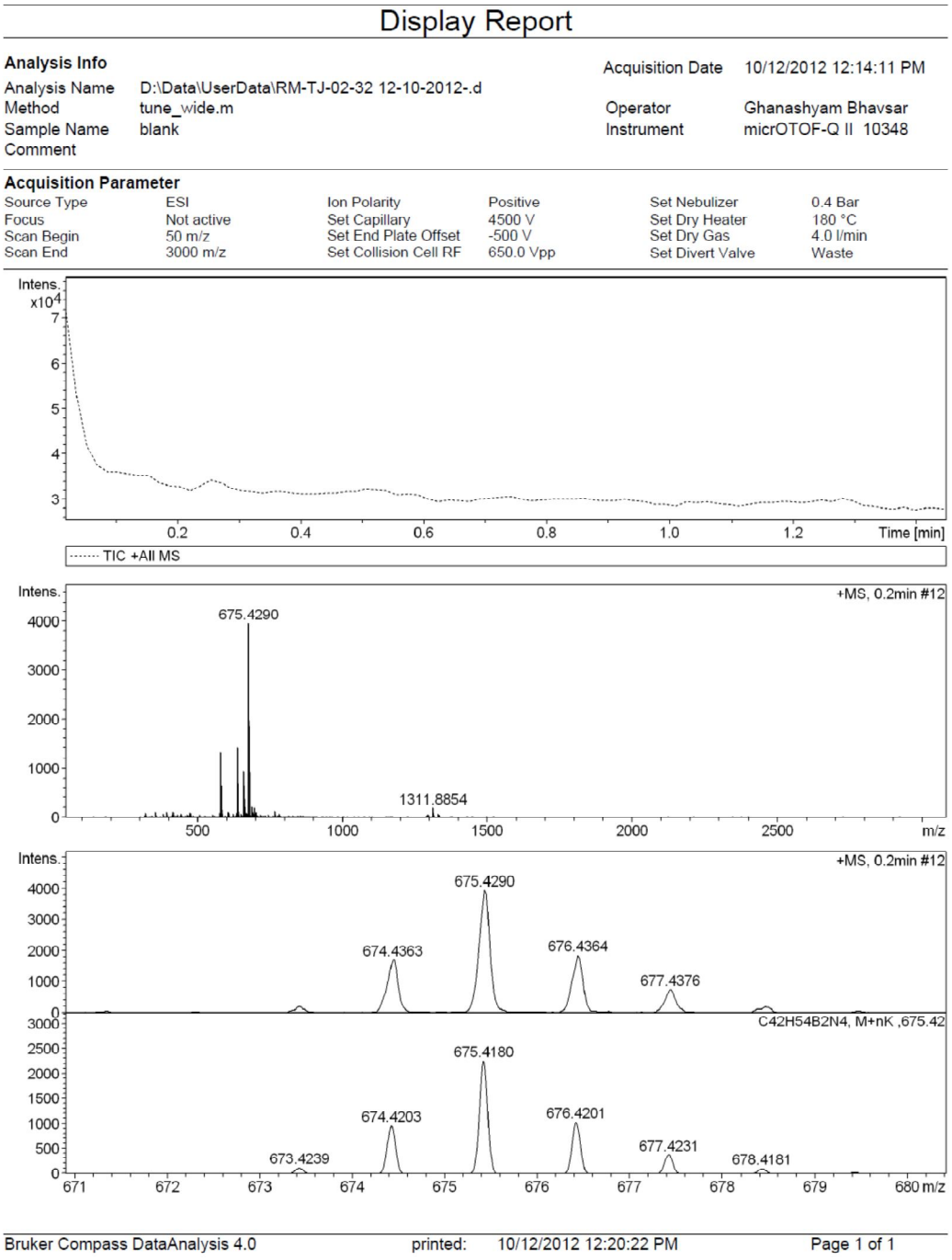

Fig. S10 HRMS spectrum of pyrazabole **3**.

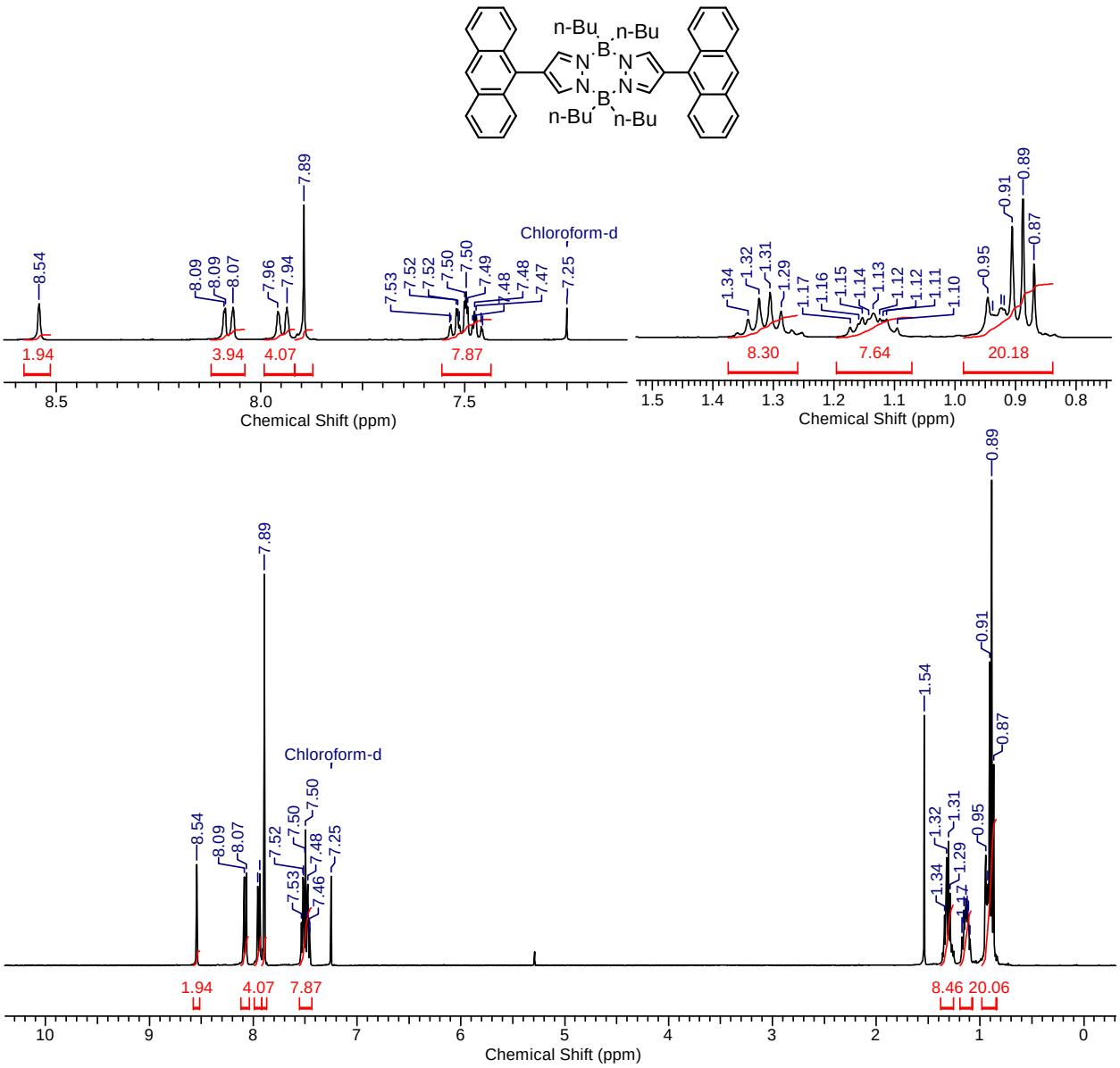

Fig. S11 ^{1}H-NMR spectrum of pyrazabole **4**.

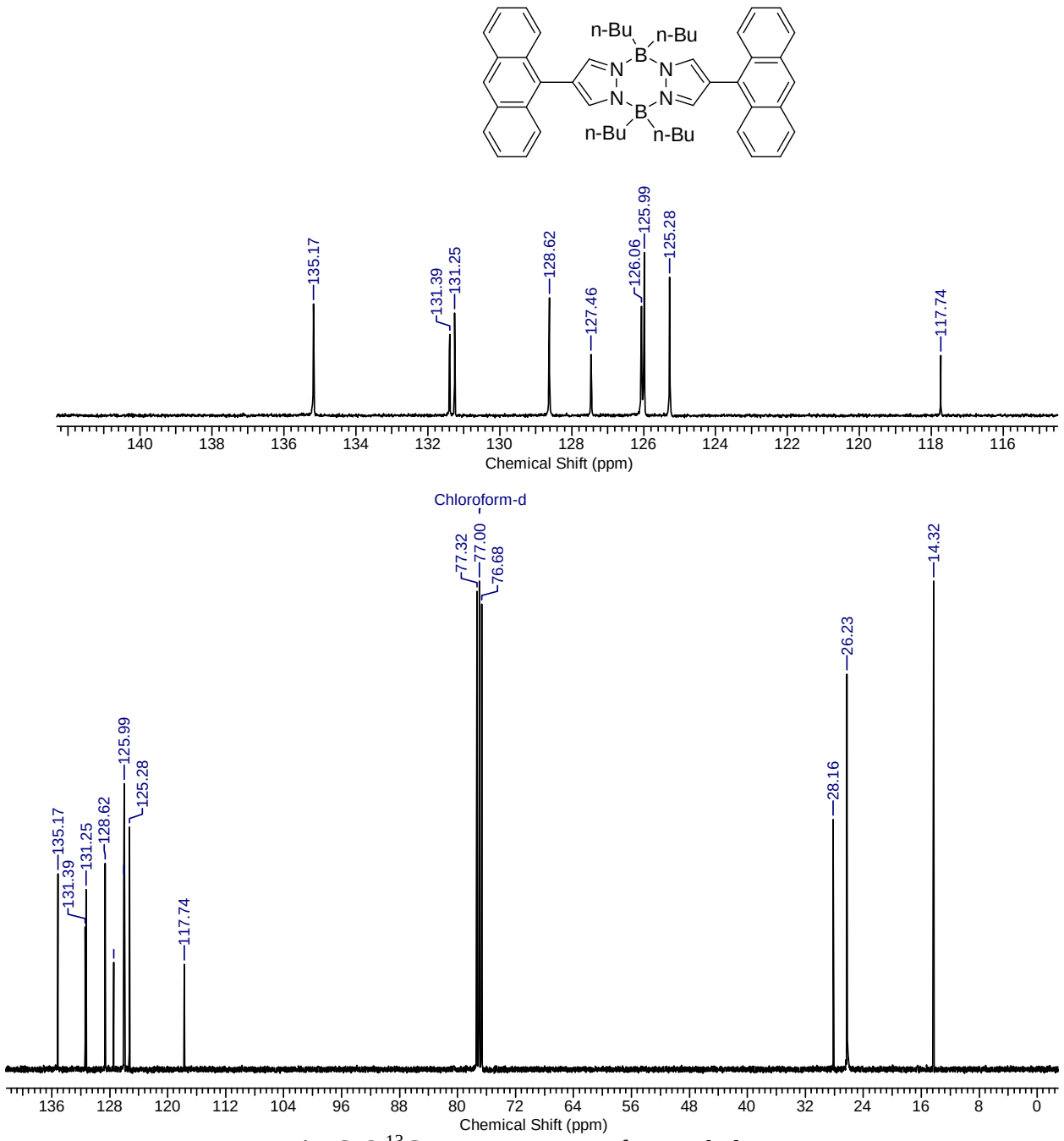

Fig. S12 ^{13}C-NMR spectrum of pyrazabole **4**.

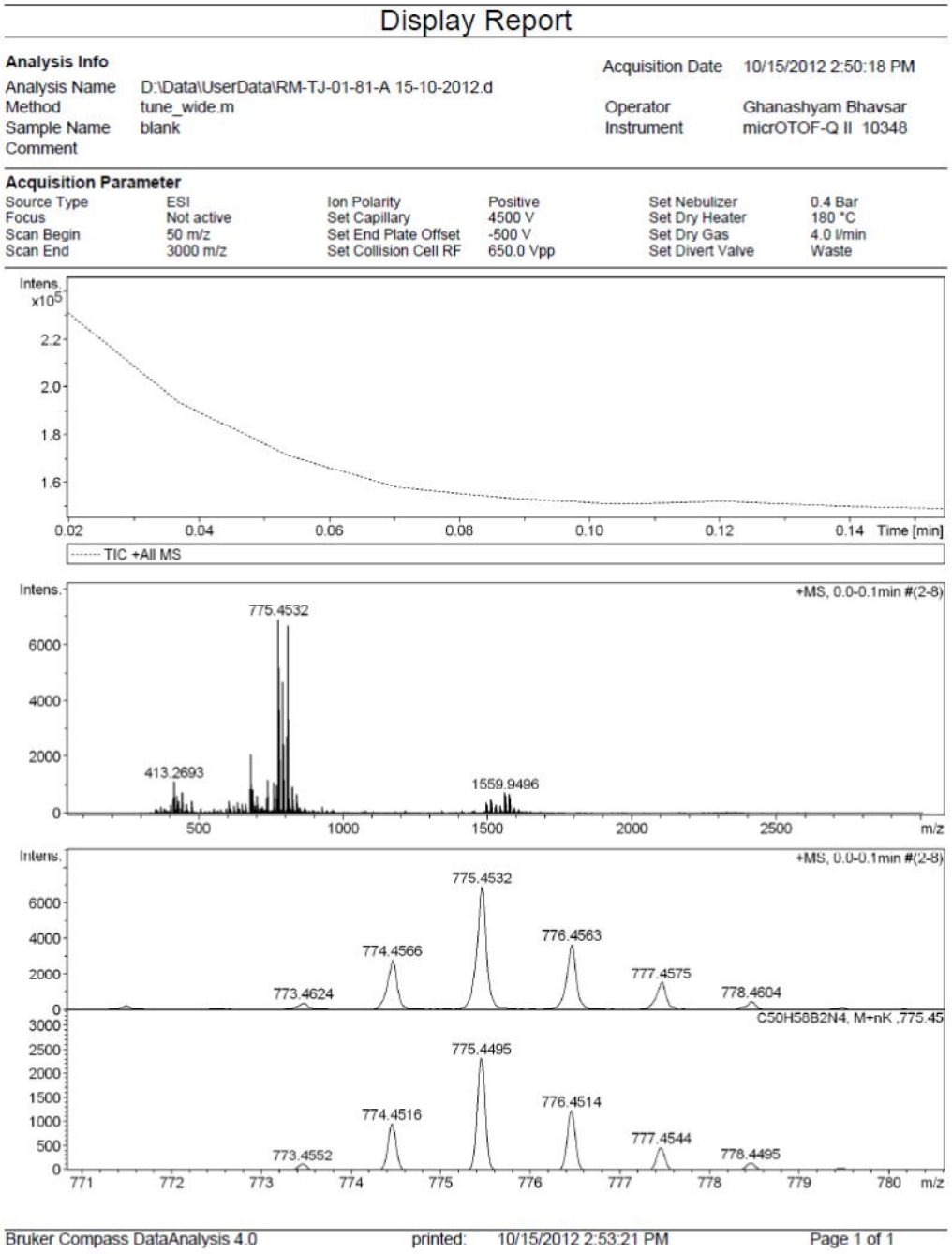

Fig. S13 HRMS spectrum of pyrazabole **4**.

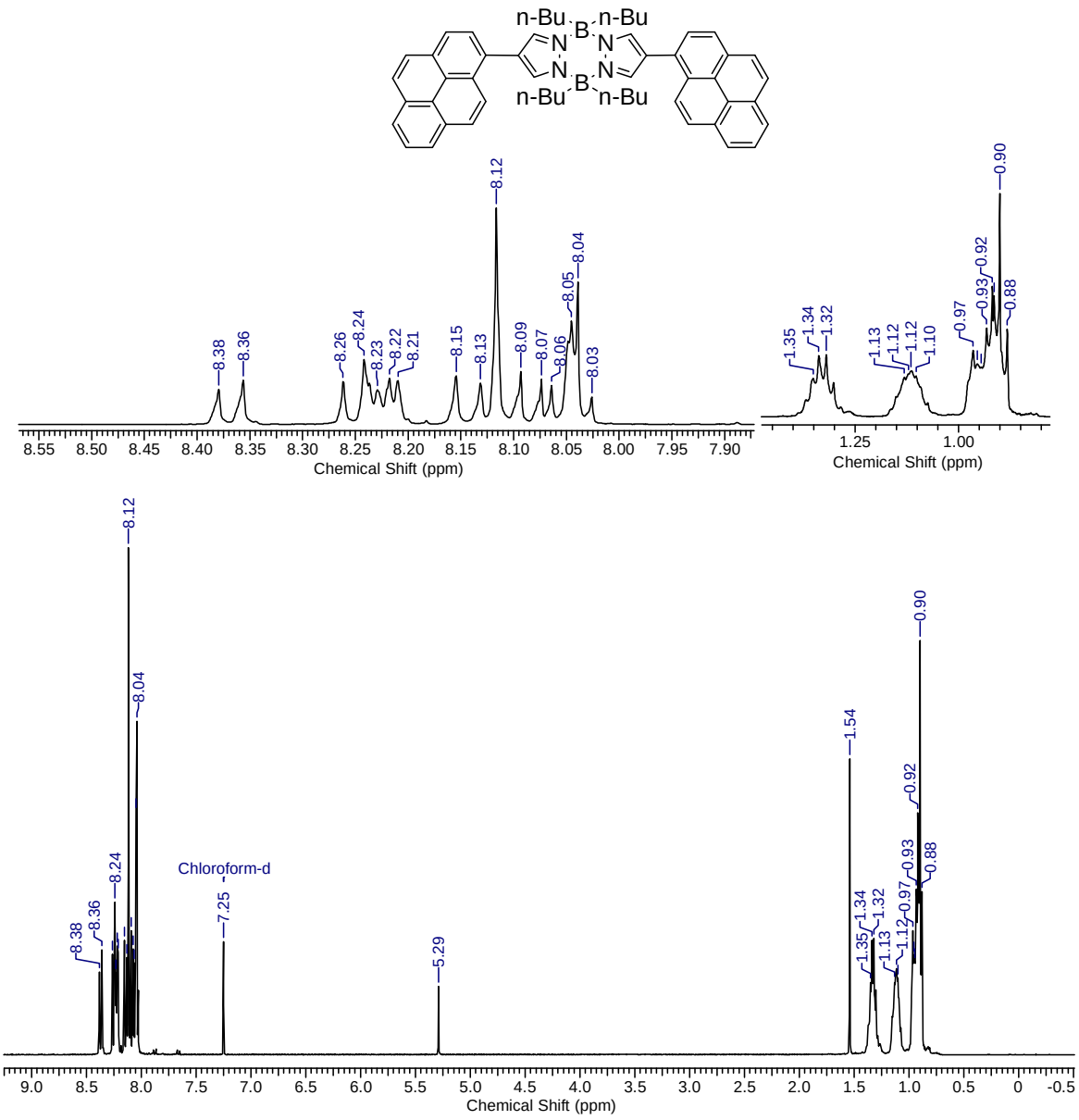

Fig. S14 ^{1}H-NMR spectrum of pyrazabole **5**.

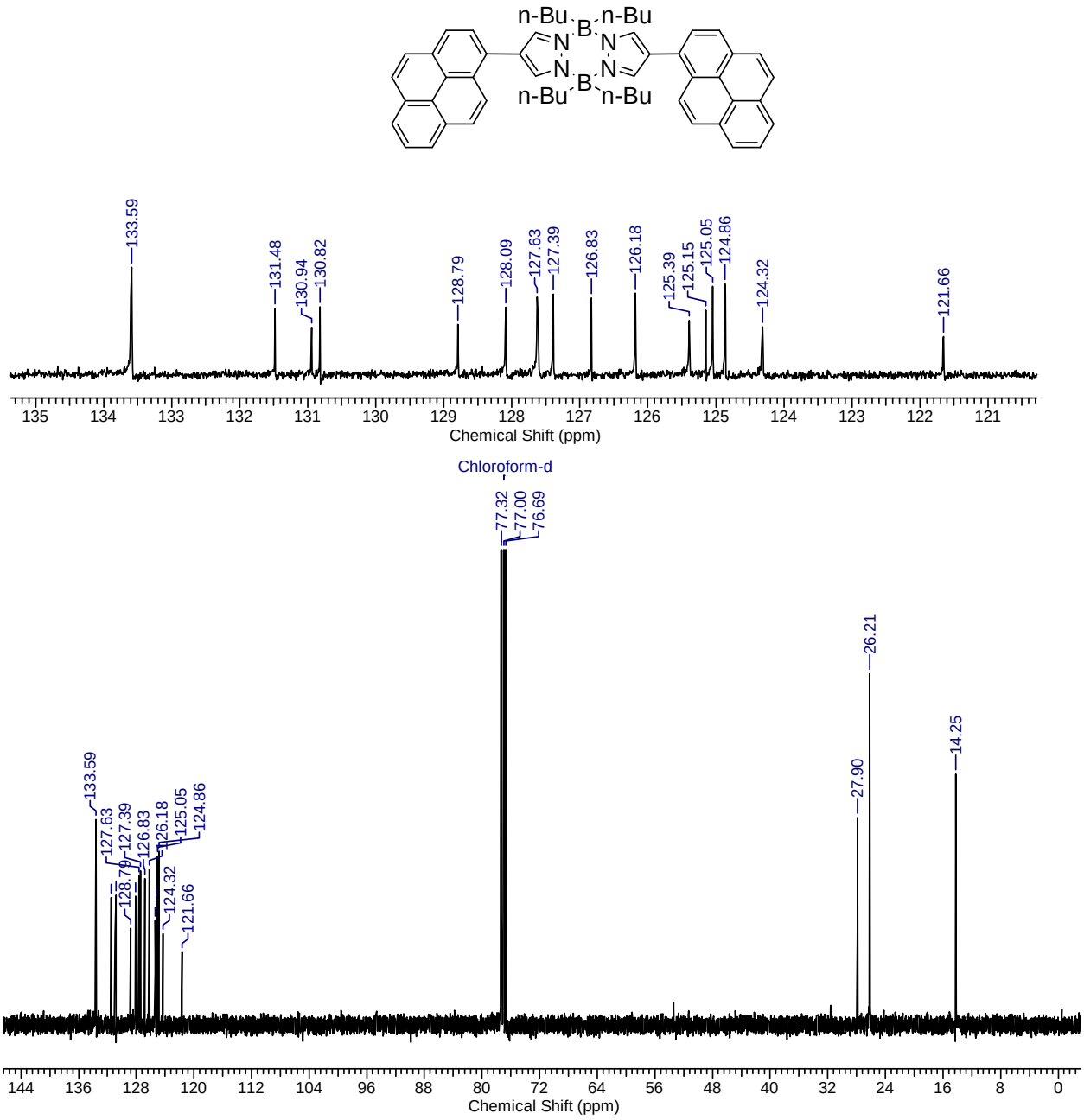

Fig. S15 ^{13}C-NMR spectrum of pyrazabole **5**.

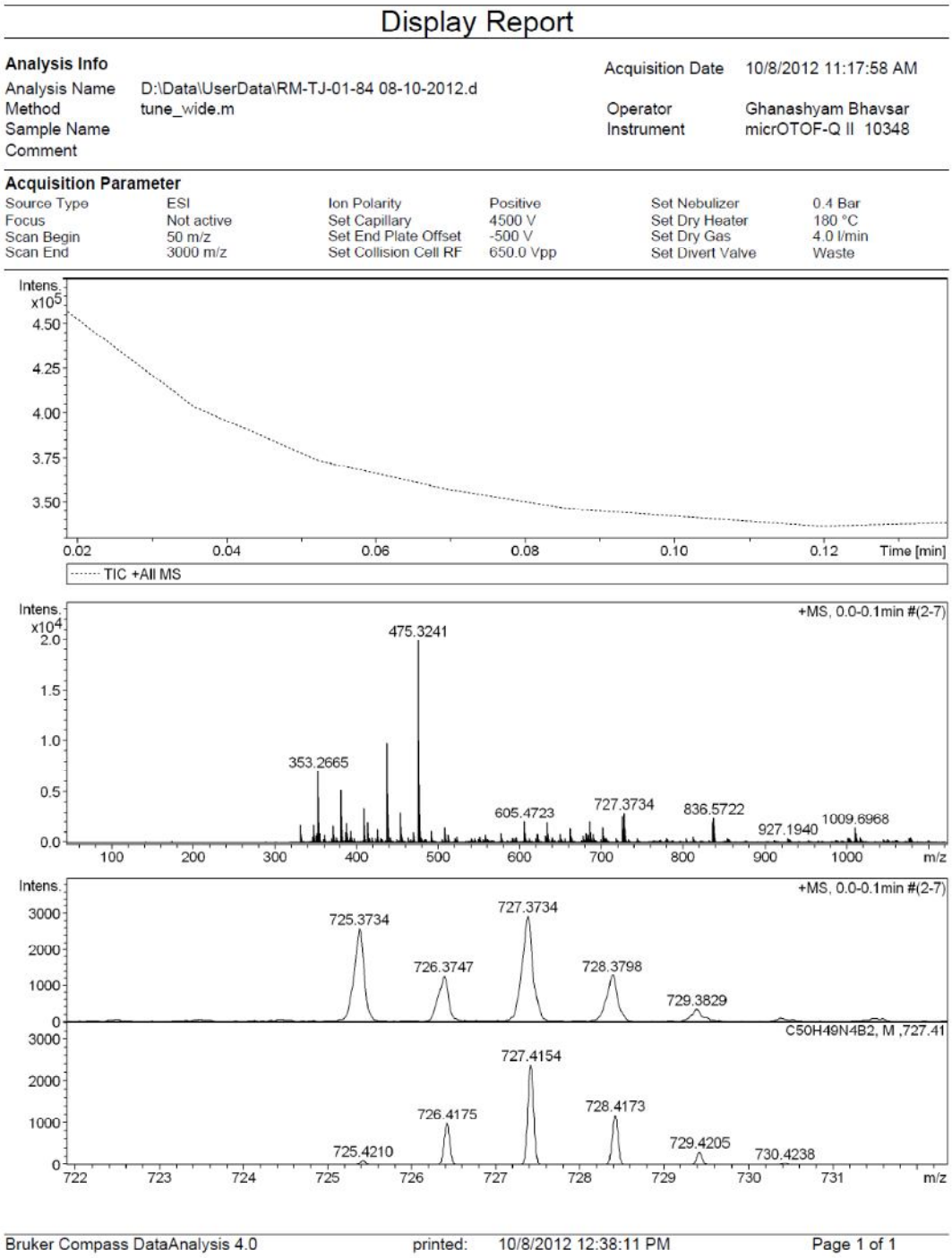

Fig. S16 HRMS spectrum of pyrazabole **5**.

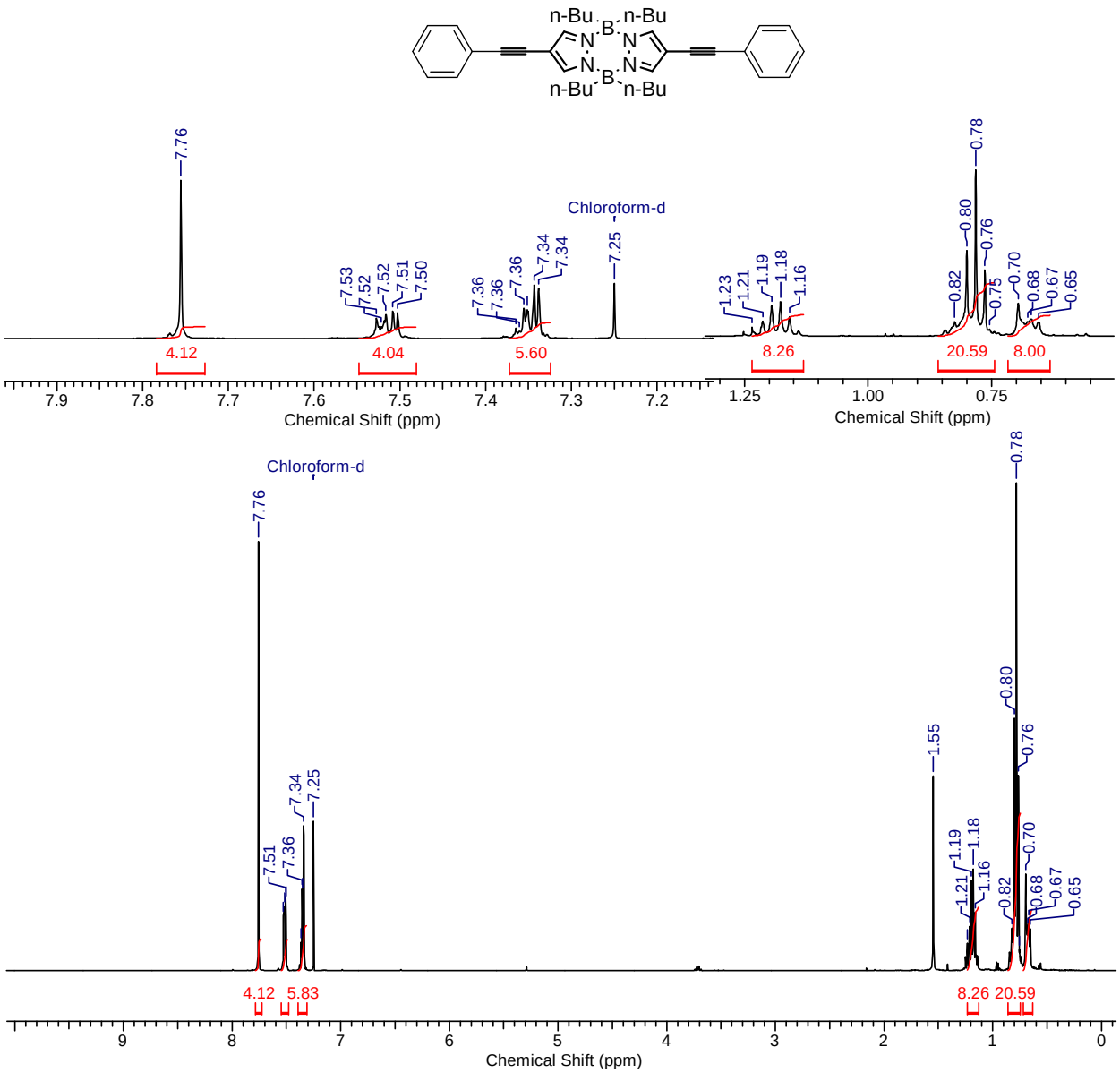

Fig. S17 ^{1}H-NMR spectrum of pyrazabole **6**.

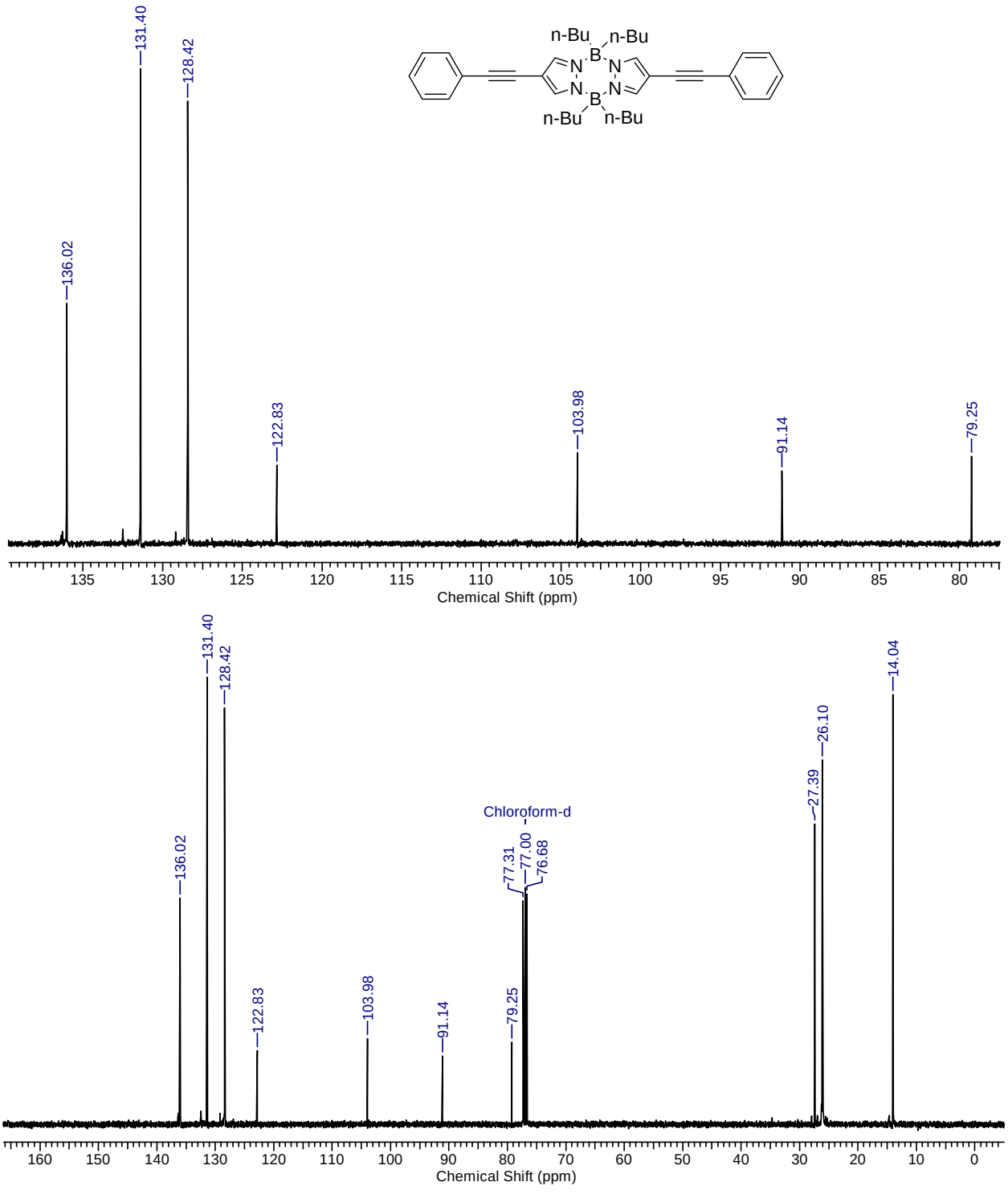

Fig. S18 ^{13}C-NMR spectrum of pyrazabole **6**.

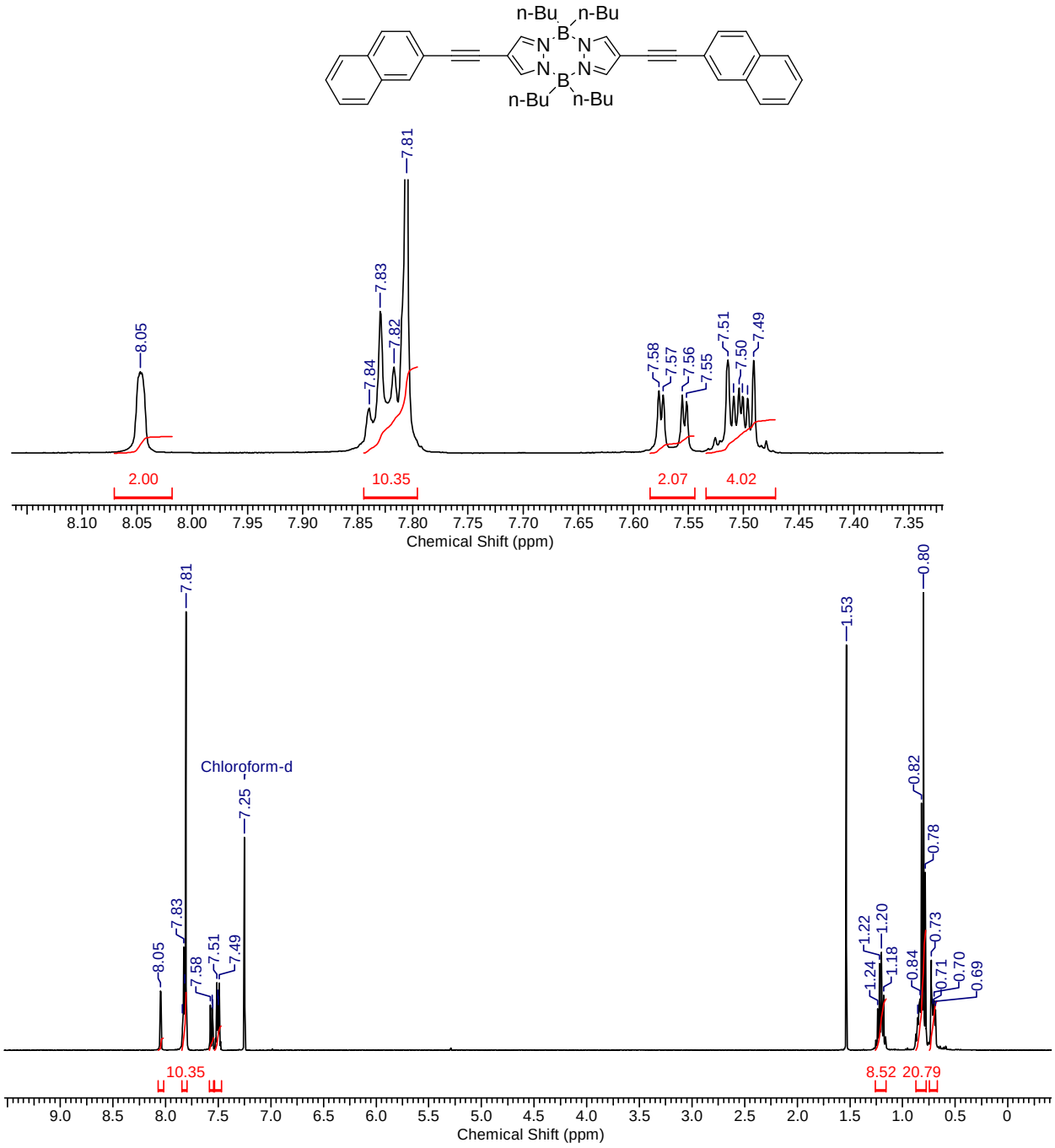

Fig. S19 ^{1}H-NMR spectrum of pyrazabole **7**.

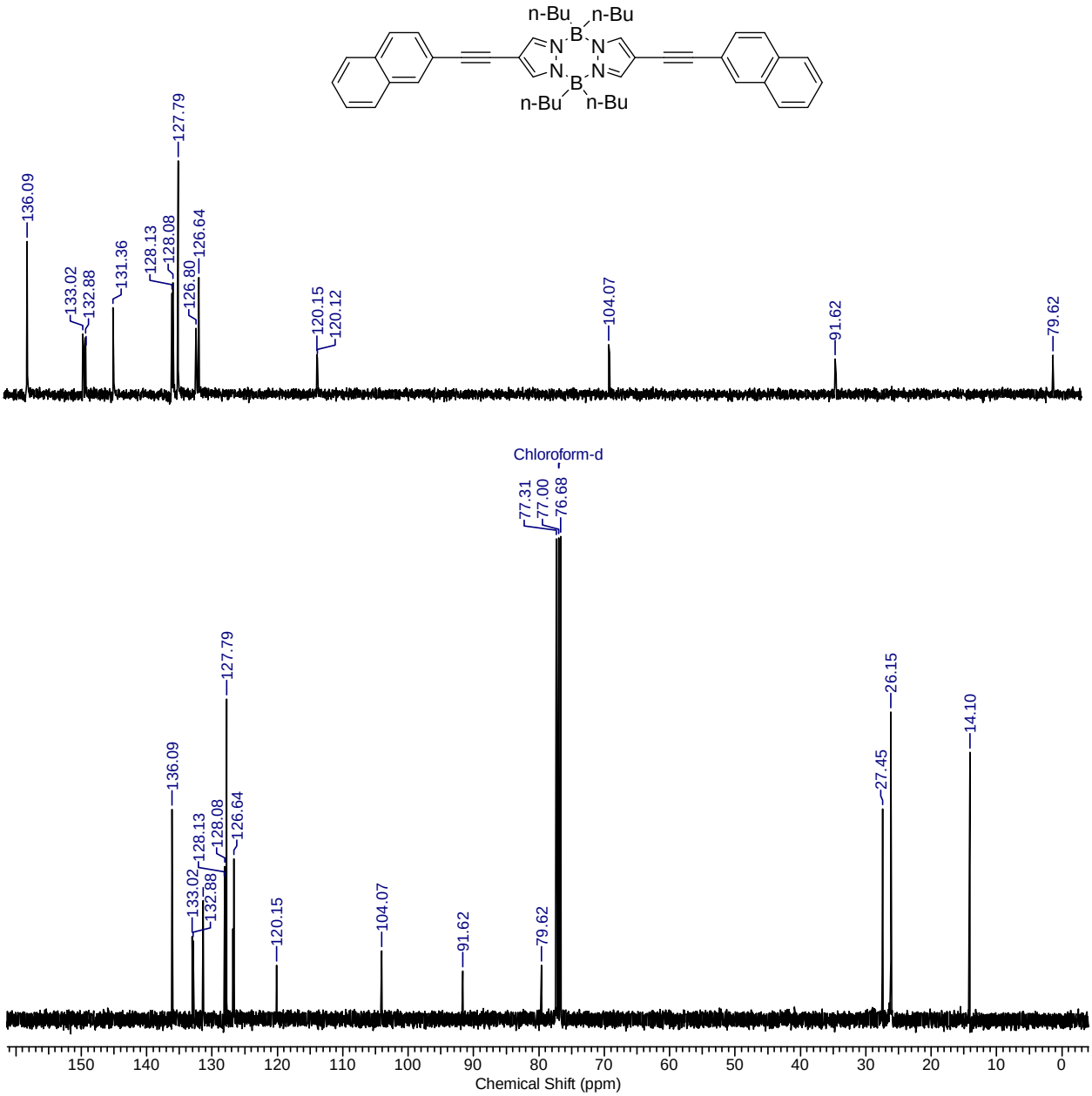

Fig. S20 ^{13}C-NMR spectrum of pyrazabole **7**.

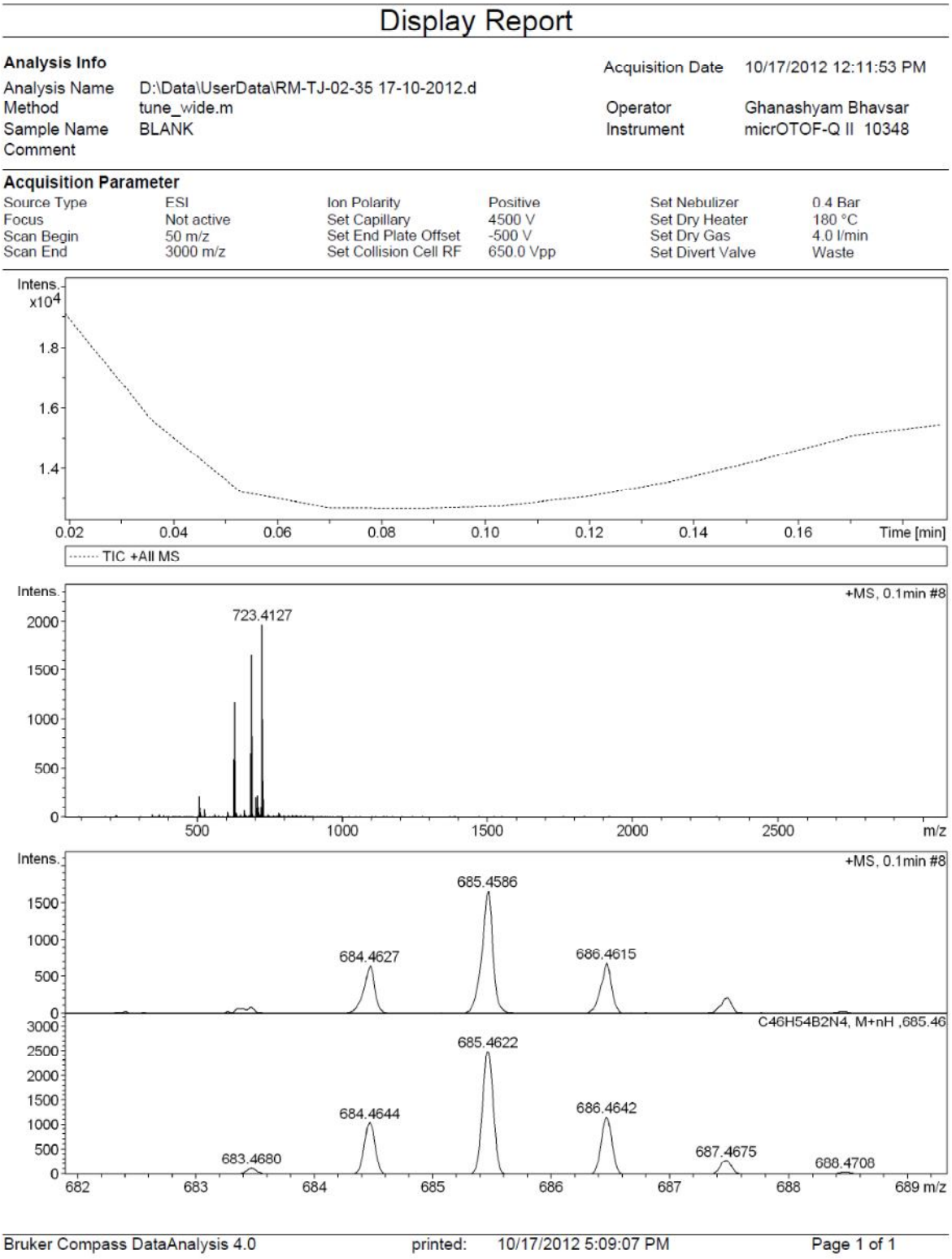

Fig. S21 HRMS spectrum of pyrazabole **7**.

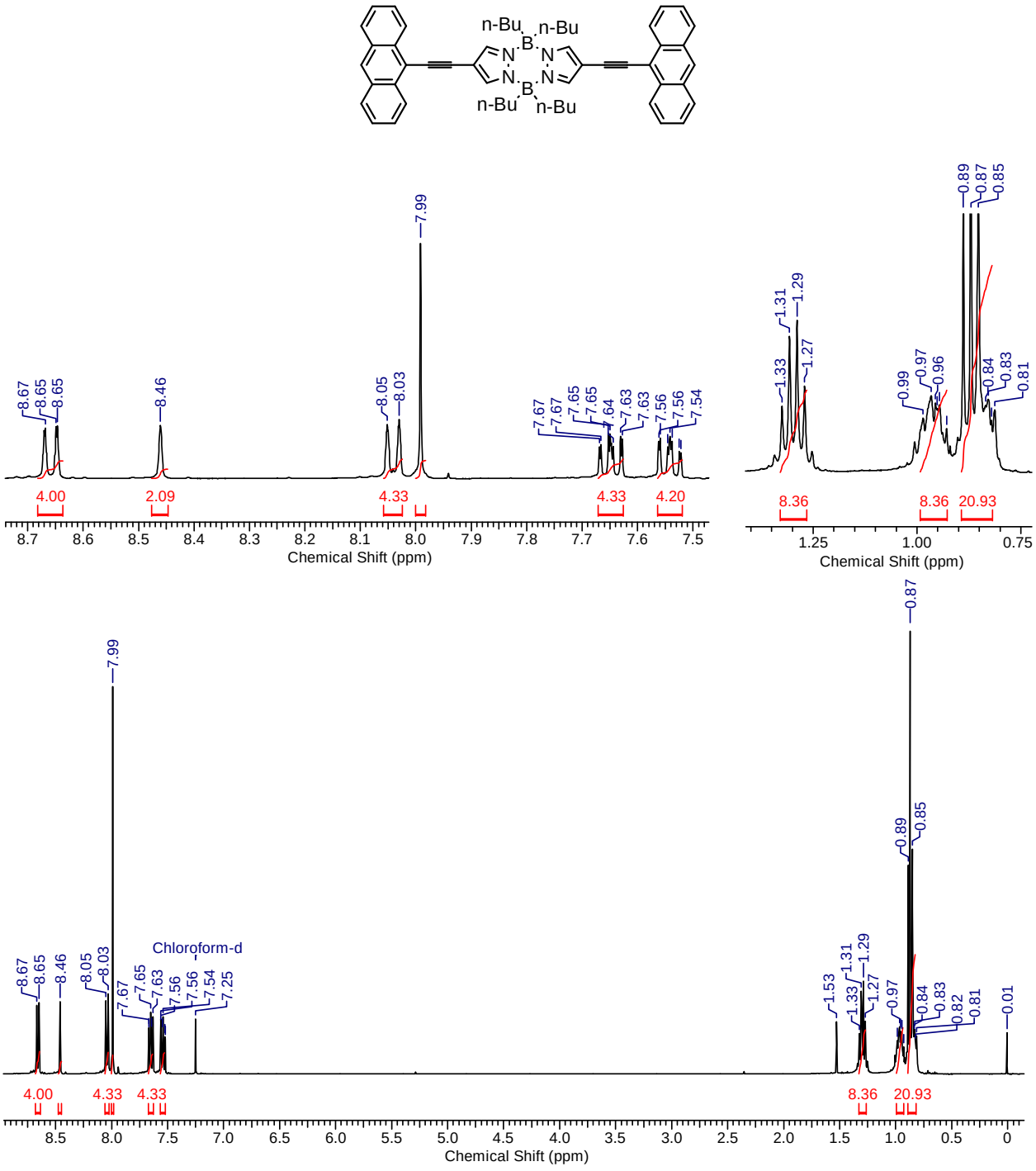

Fig. S22 ^{1}H-NMR spectrum of pyrazabole **8**.

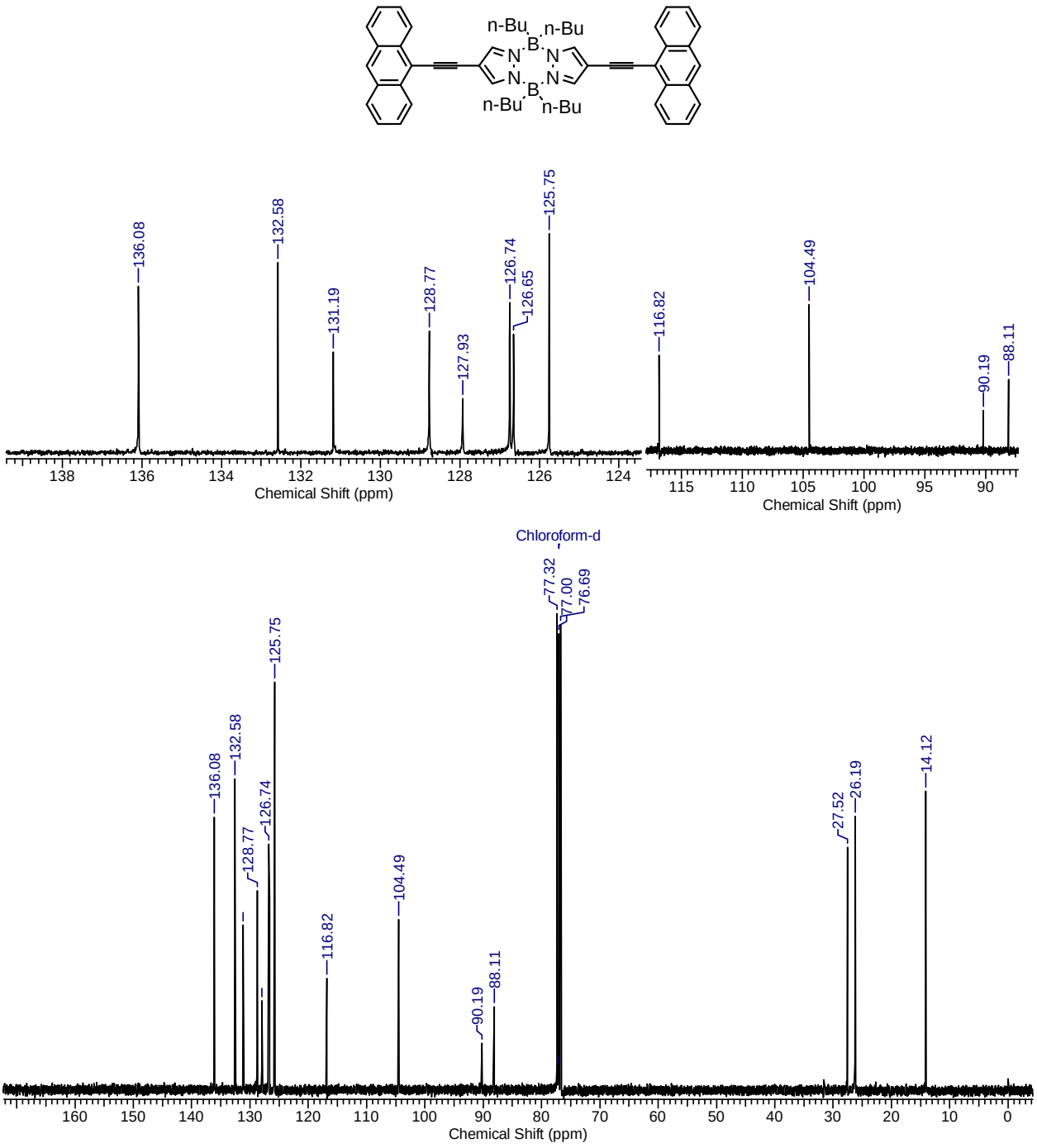

Fig. S23 ^{13}C-NMR spectrum of pyrazabole **8**.

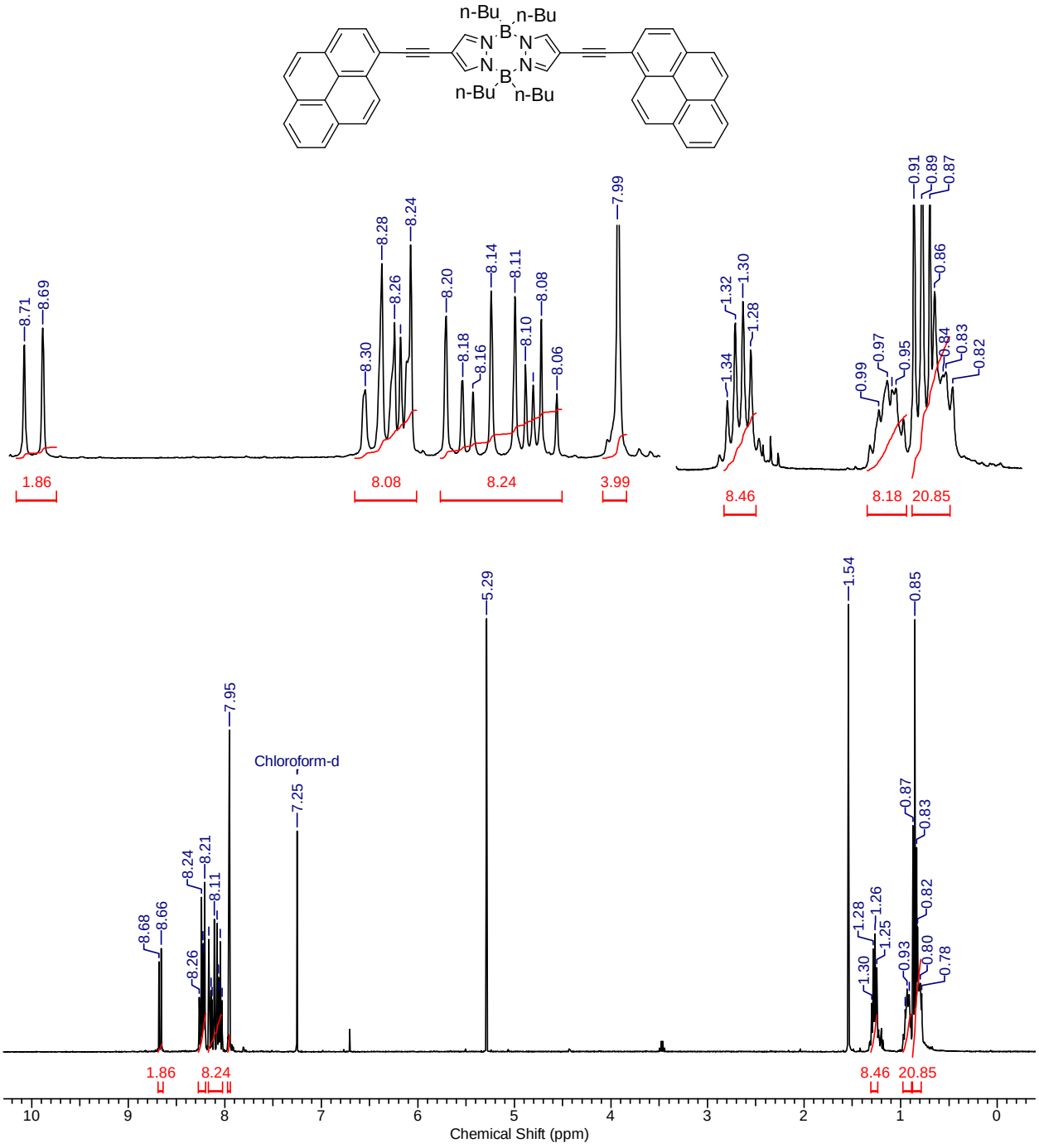

Fig. S24 ^{1}H-NMR spectrum of pyrazabole **9**.

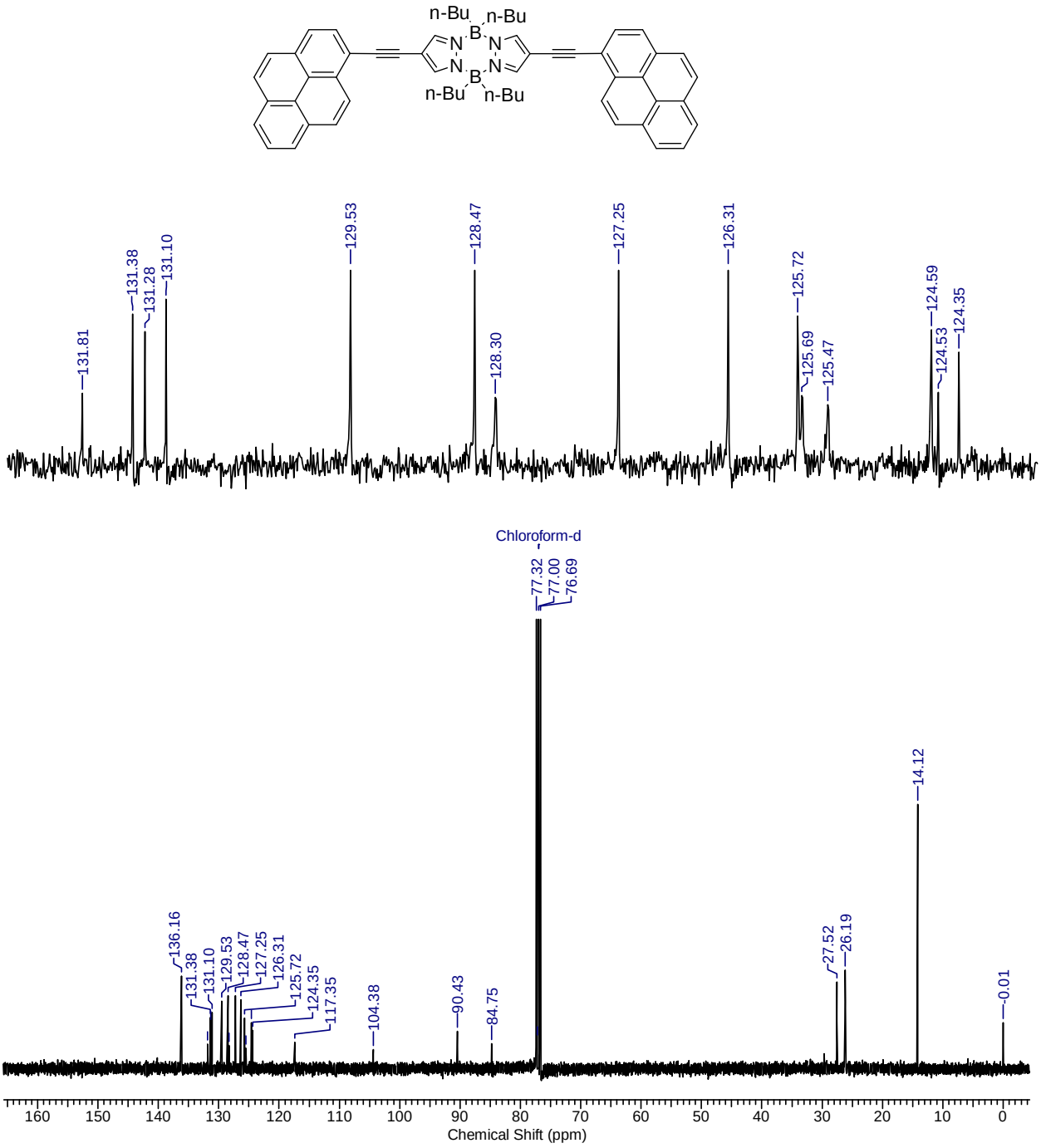

Fig. S25 ^{13}C-NMR spectrum of pyrazabole **9**.

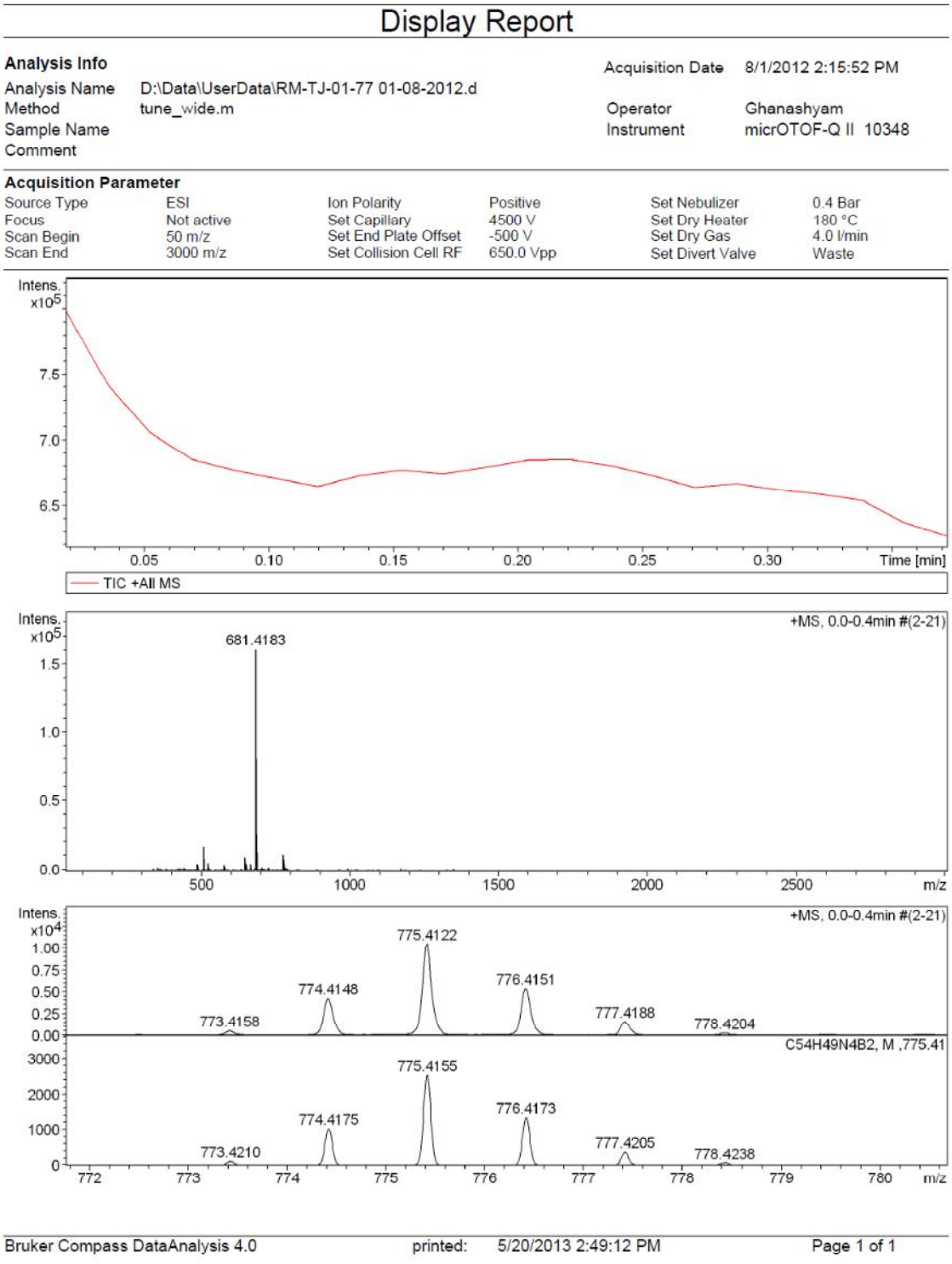

Fig. S26 HRMS spectrum of pyrazabole **9**.

DFT Calculations.

Pyrazabole 2:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.265933	-0.008431	0.678395
2	7	0	1.265922	0.008366	-0.678430
3	6	0	2.542754	0.014409	-1.098226
4	1	0	2.761994	0.005975	-2.155217
5	6	0	3.409327	-0.000210	-0.000037
6	6	0	2.542772	-0.014904	1.098165
7	1	0	2.762052	-0.006543	2.155147
8	6	0	-0.007258	-1.337575	2.572497
9	1	0	0.872054	-1.290993	3.236870
10	1	0	-0.867334	-1.262635	3.255742
11	6	0	0.007016	1.344370	2.569310
12	1	0	-0.872239	1.299452	3.233866
13	1	0	0.867099	1.270925	3.252702
14	6	0	-0.024333	-2.709083	1.881406
15	1	0	0.815998	-2.770197	1.176514
16	1	0	-0.933931	-2.803726	1.270040
17	5	0	-0.000163	0.002304	1.639791
18	6	0	0.058240	-3.918660	2.830341
19	1	0	0.974252	-3.840424	3.434476
20	6	0	0.024234	2.714276	1.875047
21	1	0	-0.816472	2.774066	1.170487
22	1	0	0.933532	2.807155	1.262962
23	6	0	1.150956	4.090414	3.750882
24	1	0	1.259129	3.238572	4.431577
25	1	0	1.057632	4.993258	4.365795
26	1	0	2.081692	4.175501	3.175185
27	6	0	-0.057250	3.926037	2.821295
28	1	0	-0.167087	4.838538	2.218596
29	1	0	-0.972834	3.849459	3.426288
30	7	0	-1.266264	-0.010679	-0.678360
31	7	0	-1.266254	0.010690	0.678375
32	6	0	-2.543085	0.018355	1.098158
33	1	0	-2.762283	0.013460	2.155175
34	6	0	-3.409669	-0.000032	0.000030
35	6	0	-2.543106	-0.018434	-1.098113
36	1	0	-2.762317	-0.013659	-2.155127
37	6	0	-0.007227	1.337960	-2.572234
38	1	0	-0.867354	1.263263	-3.255438
39	1	0	0.872036	1.291428	-3.236675
40	6	0	0.006854	-1.343990	-2.569588
41	1	0	0.866995	-1.270583	-3.252906

42	1	0	-0.872356	-1.298769	-3.234195
43	6	0	-0.024092	2.709321	-1.880851
44	1	0	-0.933598	2.803922	-1.269342
45	1	0	0.816341	2.770192	-1.176060
46	5	0	-0.000193	-0.002121	-1.639803
47	6	0	0.058480	3.919092	-2.829536
48	1	0	0.974419	3.840904	-3.433788
49	6	0	0.023761	-2.714018	-1.875555
50	1	0	0.933049	-2.807211	-1.263496
51	1	0	-0.816946	-2.773730	-1.170994
52	6	0	-0.058057	-3.925611	-2.821988
53	1	0	-0.168072	-4.838168	-2.219408
54	1	0	0.167944	-4.832458	2.229591
55	6	0	-1.149221	-4.081379	3.761194
56	1	0	-1.257029	-3.228163	4.440222
57	1	0	-2.080396	-4.167847	3.186406
58	1	0	-1.055221	-4.982943	4.377877
59	1	0	0.168328	4.832755	-2.228605
60	1	0	-0.973668	-3.848725	-3.426903
61	6	0	1.150040	-4.090133	-3.751702
62	1	0	1.258296	-3.238242	-4.432317
63	1	0	2.080819	-4.175453	-3.176105
64	1	0	1.056488	-4.992902	-4.366687
65	6	0	-1.149063	4.082108	-3.760232
66	1	0	-1.257011	3.229038	-4.439422
67	1	0	-2.080170	4.168539	-3.185331
68	1	0	-1.055049	4.983789	-4.376742
69	6	0	-4.879984	-0.000072	0.000026
70	6	0	-5.600255	0.547652	1.074726
71	6	0	-5.600200	-0.547845	-1.074678
72	6	0	-6.993747	0.542940	1.076652
73	1	0	-5.063995	0.998139	1.905654
74	6	0	-6.993695	-0.543217	-1.076630
75	1	0	-5.063898	-0.998308	-1.905594
76	6	0	-7.697438	-0.000159	0.000002
77	1	0	-7.530757	0.973440	1.917665
78	1	0	-7.530658	-0.973754	-1.917654
79	1	0	-8.783887	-0.000190	-0.000007
80	6	0	4.879641	-0.000301	-0.000048
81	6	0	5.599889	0.544543	-1.076226
82	6	0	5.599841	-0.545239	1.076108
83	6	0	6.993382	0.539762	-1.078172
84	1	0	5.063583	0.992844	-1.908308
85	6	0	6.993342	-0.540645	1.078019
86	1	0	5.063504	-0.993477	1.908203
87	6	0	7.697068	-0.000489	-0.000083
88	1	0	7.530409	0.968014	-1.920320
89	1	0	7.530326	-0.968972	1.920155
90	1	0	8.783518	-0.000562	-0.000104

Total Energy (HF) = - 1594.591318 Hartree

Pyrazabole 3:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.200527	0.223300	-0.759046
2	7	0	1.322825	-0.008147	0.572449
3	6	0	2.632006	-0.060430	0.871420
4	1	0	2.946038	-0.212390	1.892992
5	6	0	3.396447	0.140491	-0.283255
6	6	0	2.434366	0.315599	-1.283861
7	1	0	2.557312	0.477441	-2.343985
8	6	0	-0.238400	1.783283	-2.333320
9	1	0	0.575194	1.837805	-3.076173
10	1	0	-1.157555	1.790359	-2.939247
11	6	0	-0.221859	-0.873350	-2.698453
12	1	0	-1.155268	-0.746457	-3.272345
13	1	0	0.576590	-0.699694	-3.436323
14	6	0	-0.192043	3.049400	-1.464909
15	1	0	0.713527	3.029681	-0.843184
16	1	0	-1.037269	3.046851	-0.760924
17	5	0	-0.146088	0.329268	-1.596610
18	6	0	-0.208252	4.375340	-2.247593
19	1	0	0.637796	4.388557	-2.950519
20	6	0	-0.148945	-2.324486	-2.200929
21	1	0	-0.925334	-2.485223	-1.440471
22	1	0	0.809682	-2.492783	-1.688387
23	6	0	0.810515	-3.436009	-4.328942
24	1	0	0.877735	-2.500323	-4.895454
25	1	0	0.656938	-4.246671	-5.050945
26	1	0	1.782133	-3.601746	-3.845917
27	6	0	-0.318909	-3.396366	-3.292677
28	1	0	-0.392131	-4.382084	-2.812036
29	1	0	-1.278279	-3.236975	-3.806760
30	7	0	-1.198772	-0.023399	0.799994
31	7	0	-1.320581	0.172696	-0.537166
32	6	0	-2.629449	0.219802	-0.837612
33	1	0	-2.942508	0.390702	-1.856465
34	6	0	-3.394650	0.052589	0.321976
35	6	0	-2.432964	-0.094590	1.327535
36	1	0	-2.556146	-0.266870	2.385956
37	6	0	0.223129	-1.601489	2.373223
38	1	0	-0.585614	-1.635079	3.119541
39	1	0	1.147302	-1.628878	2.974637
40	6	0	0.241318	1.054468	2.735769
41	1	0	1.164822	0.900632	3.314995
42	1	0	-0.568267	0.904987	3.469903
43	6	0	0.169725	-2.868039	1.506122

44	1	0	-0.767546	-2.885488	0.930794
45	1	0	0.975999	-2.829074	0.760871
46	5	0	0.148451	-0.147494	1.634769
47	6	0	0.294647	-4.192294	2.281959
48	1	0	1.226978	-4.181254	2.865637
49	6	0	0.187337	2.506879	2.239611
50	1	0	1.019873	2.692860	1.545131
51	1	0	-0.729095	2.654976	1.652115
52	6	0	0.226118	3.575297	3.347991
53	1	0	0.046623	4.560693	2.895524
54	1	0	-0.032904	5.202632	-1.545584
55	6	0	-1.507981	4.645715	-3.014575
56	1	0	-1.691234	3.888633	-3.785346
57	1	0	-2.371797	4.645612	-2.337343
58	1	0	-1.477814	5.621666	-3.513134
59	1	0	0.396987	-5.016044	1.561584
60	1	0	-0.608429	3.403616	4.043792
61	6	0	1.540233	3.625832	4.136081
62	1	0	1.728690	2.689980	4.673977
63	1	0	2.393282	3.802181	3.468190
64	1	0	1.526537	4.433834	4.876936
65	6	0	-0.883658	-4.497063	3.214248
66	1	0	-0.986291	-3.743372	4.003233
67	1	0	-1.829008	-4.524892	2.657185
68	1	0	-0.759074	-5.469911	3.704199
69	6	0	4.859408	0.165410	-0.417702
70	6	0	5.677323	-0.508171	0.473861
71	6	0	5.466774	0.894190	-1.482319
72	6	0	7.090230	-0.483619	0.355811
73	1	0	5.237621	-1.092178	1.279039
74	6	0	6.831800	0.930527	-1.628997
75	1	0	4.836289	1.445533	-2.174289
76	6	0	7.937984	-1.170785	1.267127
77	6	0	7.686525	0.249495	-0.721207
78	1	0	7.276772	1.495359	-2.444845
79	6	0	9.306457	-1.131755	1.123286
80	1	0	7.485753	-1.729540	2.083246
81	6	0	9.100885	0.270326	-0.841459
82	6	0	9.894665	-0.403949	0.059389
83	1	0	9.942633	-1.660886	1.827626
84	1	0	9.548190	0.829565	-1.659976
85	1	0	10.976163	-0.381290	-0.042817
86	6	0	-4.857838	0.033530	0.454434
87	6	0	-5.672408	-0.314070	-0.610160
88	6	0	-5.469274	0.376585	1.696118
89	6	0	-7.085604	-0.329064	-0.495473
90	1	0	-5.229617	-0.604857	-1.559926
91	6	0	-6.834890	0.363380	1.841901
92	1	0	-4.841737	0.671992	2.532323
93	6	0	-7.929334	-0.682725	-1.583748
94	6	0	-7.686051	0.014564	0.759139
95	1	0	-7.283228	0.631994	2.795556

96	6	0	-9.298329	-0.692322	-1.440014
97	1	0	-7.473445	-0.945918	-2.535402
98	6	0	-9.100871	-0.004601	0.874537
99	6	0	-9.890784	-0.349522	-0.199443
100	1	0	-9.931623	-0.963732	-2.280291
101	1	0	-9.551782	0.258507	1.828627
102	1	0	-10.972657	-0.361077	-0.099279

Total Energy (HF) = - 1901.8795999 Hartree

Pyrazabole 4:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.294170	0.053526	0.636606
2	7	0	1.284094	-0.199773	-0.696492
3	6	0	2.558678	-0.313265	-1.111491
4	1	0	2.777771	-0.513358	-2.149643
5	6	0	3.430801	-0.131346	-0.035056
6	6	0	2.574973	0.097490	1.045410
7	1	0	2.809967	0.286982	2.082057
8	6	0	-0.000450	-0.848758	2.759807
9	1	0	0.878456	-0.692335	3.407274
10	1	0	-0.859716	-0.620604	3.409061
11	6	0	0.091528	1.778237	2.232741
12	1	0	-0.772670	1.887276	2.909060
13	1	0	0.965868	1.815415	2.900632
14	6	0	-0.048339	-2.328946	2.353237
15	1	0	0.805016	-2.551741	1.697871
16	1	0	-0.946898	-2.519433	1.747743
17	5	0	0.036611	0.281622	1.582344
18	6	0	-0.026280	-3.326833	3.526213
19	1	0	0.872711	-3.147345	4.133816
20	6	0	0.124403	2.985177	1.284290
21	1	0	-0.750927	2.948179	0.620555
22	1	0	1.000128	2.913846	0.621844
23	6	0	1.416457	4.644220	2.785847
24	1	0	1.534434	3.943563	3.619907
25	1	0	1.399743	5.656307	3.206920
26	1	0	2.311735	4.561676	2.155657
27	6	0	0.145470	4.360135	1.976777
28	1	0	0.029821	5.142089	1.212956
29	1	0	-0.731125	4.445763	2.635538
30	7	0	-1.246241	-0.119150	-0.691169
31	7	0	-1.236091	0.135604	0.641635
32	6	0	-2.510682	0.249168	1.056616

33	1	0	-2.729884	0.449800	2.094615
34	6	0	-3.382849	0.065623	-0.019478
35	6	0	-2.527076	-0.164118	-1.099777
36	1	0	-2.762182	-0.354862	-2.136159
37	6	0	0.045669	0.784549	-2.813907
38	1	0	-0.835703	0.629069	-3.457712
39	1	0	0.901988	0.562363	-3.471823
40	6	0	-0.042600	-1.841893	-2.289332
41	1	0	0.820711	-1.948690	-2.967106
42	1	0	-0.917752	-1.878723	-2.956176
43	6	0	0.105486	2.266490	-2.418145
44	1	0	-0.755784	2.517747	-1.781959
45	1	0	0.996333	2.452266	-1.800359
46	5	0	0.011424	-0.345962	-1.637067
47	6	0	0.129649	3.226240	-3.616951
48	1	0	-0.762912	3.052678	-4.235289
49	1	0	0.990898	2.982535	-4.255777
50	6	0	-0.072871	-3.051136	-1.343677
51	1	0	0.804026	-3.015272	-0.681894
52	1	0	-0.947216	-2.982082	-0.679129
53	6	0	-1.367876	-4.707136	-2.846103
54	1	0	-1.489537	-4.003794	-3.677351
55	1	0	-1.351175	-5.717744	-3.270711
56	1	0	-2.261142	-4.627946	-2.212652
57	6	0	-0.094570	-4.424069	-2.040305
58	1	0	0.024597	-5.208553	-1.279589
59	1	0	0.779961	-4.506507	-2.702189
60	1	0	0.077046	-4.344297	3.123375
61	6	0	-4.867622	0.099552	-0.016222
62	6	0	-5.598326	-1.111766	-0.069325
63	6	0	-5.544135	1.341838	0.039033
64	6	0	-4.967230	-2.396897	-0.107402
65	6	0	-7.043197	-1.072354	-0.073115
66	6	0	-6.989334	1.365997	0.046008
67	6	0	-4.856762	2.597635	0.076677
68	6	0	-5.704681	-3.550920	-0.160807
69	1	0	-3.884065	-2.448514	-0.087581
70	6	0	-7.773981	-2.300147	-0.132772
71	6	0	-7.696604	0.161828	-0.012869
72	6	0	-7.665031	2.624893	0.107102
73	1	0	-3.772417	2.600653	0.055876
74	6	0	-5.542300	3.783118	0.131850
75	6	0	-7.128035	-3.505947	-0.178203
76	1	0	-5.200207	-4.513073	-0.186983
77	1	0	-8.860346	-2.251960	-0.139177
78	1	0	-8.784545	0.185876	-0.011807
79	6	0	-6.966251	3.800928	0.151339
80	1	0	-8.752451	2.624881	0.115650
81	1	0	-4.995775	4.721979	0.158215
82	1	0	-7.695082	-4.431670	-0.222824
83	1	0	-7.491748	4.750817	0.197124
84	6	0	4.915545	-0.166396	-0.038287

85	6	0	5.647269	1.044225	0.016570
86	6	0	5.590999	-1.409188	-0.095338
87	6	0	5.017274	2.329823	0.056979
88	6	0	7.092113	1.003592	0.019902
89	6	0	7.036174	-1.434541	-0.102827
90	6	0	4.902555	-2.664356	-0.134205
91	6	0	5.755709	3.483132	0.112189
92	1	0	3.934141	2.382402	0.037597
93	6	0	7.823947	2.230671	0.081361
94	6	0	7.744463	-0.231043	-0.042476
95	6	0	7.710794	-2.693919	-0.165842
96	1	0	3.818221	-2.666542	-0.112709
97	6	0	5.587077	-3.850344	-0.191059
98	6	0	7.179032	3.436935	0.129053
99	1	0	5.252062	4.445662	0.140263
100	1	0	8.910273	2.181556	0.087387
101	1	0	8.832384	-0.255998	-0.043922
102	6	0	7.011002	-3.869310	-0.211253
103	1	0	8.798211	-2.694807	-0.174800
104	1	0	5.039723	-4.788698	-0.218094
105	1	0	7.746864	4.362107	0.175112
106	1	0	7.535690	-4.819581	-0.258415
107	6	0	0.193906	4.703405	-3.214808
108	1	0	-0.673092	4.986368	-2.604723
109	1	0	1.094183	4.914173	-2.623962
110	1	0	0.211193	5.360189	-4.092541
111	6	0	-1.266023	-3.275797	4.426578
112	1	0	-1.372048	-2.302679	4.918874
113	1	0	-2.181034	-3.455812	3.847587
114	1	0	-1.215631	-4.038204	5.212755

Total Energy (HF) = - 2209.1426502 Hartree

Pyrazabole 5:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.250399	0.299999	-1.593853
2	7	0	-1.133681	0.330625	-0.818017
3	7	0	-1.336395	0.117969	0.507536
4	1	0	-0.052947	1.958101	-3.066478
5	6	0	0.187984	-0.794981	-2.804683
6	1	0	1.162447	-0.784744	-3.320300
7	1	0	-0.514740	-0.406118	-3.560268
8	6	0	-2.320004	0.607708	-1.385080
9	1	0	-2.382294	0.805032	-2.444689

10	6	0	-3.332990	0.579799	-0.421069
11	6	0	-2.649295	0.265792	0.758979
12	6	0	-0.636875	-1.757156	2.230861
13	1	0	-1.609966	-1.610583	2.726147
14	6	0	-0.189027	-2.253534	-2.510103
15	1	0	-1.162063	-2.293814	-1.997902
16	1	0	0.537888	-2.696951	-1.814525
17	6	0	-0.262836	-3.119078	-3.778102
18	1	0	-0.989435	-2.671502	-4.471807
19	1	0	0.707116	-3.081863	-4.294758
20	6	0	-0.644890	-4.579301	-3.516633
21	1	0	-1.617172	-4.651063	-3.012903
22	1	0	-0.712408	-5.149878	-4.450524
23	1	0	0.095510	-5.076095	-2.877957
24	1	0	-3.023030	0.157743	1.765564
25	6	0	0.189111	2.254285	2.510472
26	1	0	1.162258	2.294469	1.998479
27	1	0	-0.537622	2.697712	1.814725
28	6	0	0.262714	3.119914	3.778424
29	1	0	0.989217	2.672419	4.472283
30	1	0	-0.707317	3.082732	4.294935
31	6	0	0.644784	4.580121	3.516861
32	1	0	1.617121	4.651834	3.013224
33	1	0	0.712204	5.150799	4.450697
34	1	0	-0.095549	5.076841	2.878050
35	1	0	3.022903	-0.157331	-1.765248
36	6	0	0.636895	1.757934	-2.230422
37	1	0	1.609950	1.611275	-2.725749
38	6	0	0.731883	3.036031	-1.369943
39	1	0	1.221845	2.820035	-0.409351
40	5	0	-0.250435	-0.299222	1.594242
41	7	0	1.133642	-0.329836	0.818418
42	7	0	1.336318	-0.117319	-0.507162
43	1	0	0.052938	-1.957230	3.066964
44	6	0	-0.188023	0.795771	2.805047
45	1	0	-1.162511	0.785564	3.320621
46	1	0	0.514669	0.406845	3.560625
47	6	0	2.319959	-0.606974	1.385460
48	1	0	2.382271	-0.804155	2.445095
49	6	0	3.332904	-0.579318	0.421395
50	6	0	2.649195	-0.265301	-0.758646
51	6	0	-0.731708	-3.035304	1.370443
52	1	0	-1.388998	-3.756796	1.879336
53	1	0	-1.221488	-2.819359	0.409738
54	6	0	0.607050	-3.742621	1.106532
55	1	0	1.241916	-3.125770	0.458198
56	1	0	1.149320	-3.841600	2.058909
57	6	0	0.438579	-5.131956	0.482655
58	1	0	1.407856	-5.609705	0.296239
59	1	0	-0.136674	-5.792626	1.143483
60	1	0	-0.094959	-5.077917	-0.473334
61	6	0	-0.606855	3.743300	-1.105780

62	1	0	-1.149276	3.842252	-2.058073
63	1	0	-1.241597	3.126431	-0.457342
64	6	0	-0.438374	5.132657	-0.481954
65	1	0	0.136739	5.793348	-1.142884
66	1	0	-1.407665	5.610341	-0.295429
67	1	0	0.095289	5.078696	0.473965
68	1	0	1.389067	3.757569	-1.878915
69	6	0	-4.760133	0.894735	-0.625216
70	6	0	-5.807388	0.090019	-0.104631
71	6	0	-5.084384	2.042577	-1.365413
72	6	0	-7.166200	0.492548	-0.312994
73	6	0	-5.571837	-1.138899	0.606084
74	6	0	-6.401089	2.425070	-1.584212
75	1	0	-4.277455	2.659995	-1.750327
76	6	0	-8.238475	-0.287871	0.219574
77	6	0	-7.462791	1.674770	-1.058138
78	6	0	-6.595475	-1.882825	1.109448
79	1	0	-4.551780	-1.487435	0.721749
80	1	0	-6.616441	3.325892	-2.153520
81	6	0	-7.963819	-1.483262	0.949942
82	6	0	-9.594100	0.120571	0.021561
83	6	0	-8.834077	2.059083	-1.244066
84	1	0	-6.386158	-2.810526	1.636739
85	6	0	-9.031907	-2.233153	1.468774
86	6	0	-10.629249	-0.660413	0.560059
87	6	0	-9.852411	1.319487	-0.726429
88	1	0	-9.041993	2.962979	-1.811538
89	6	0	-10.349261	-1.822990	1.276029
90	1	0	-8.818581	-3.143388	2.023869
91	1	0	-11.659594	-0.347109	0.410281
92	1	0	-10.885700	1.624259	-0.873679
93	1	0	-11.164129	-2.414377	1.684658
94	6	0	4.759997	-0.894473	0.625517
95	6	0	5.807388	-0.090183	0.104545
96	6	0	5.084069	-2.042157	1.366045
97	6	0	7.166126	-0.493009	0.312820
98	6	0	5.572059	1.138592	-0.606493
99	6	0	6.400704	-2.424905	1.584794
100	1	0	4.277041	-2.659264	1.751251
101	6	0	8.238525	0.286935	-0.220198
102	6	0	7.462524	-1.675062	1.058306
103	6	0	6.595816	1.882074	-1.110273
104	1	0	4.552083	1.487399	-0.722054
105	1	0	6.615905	-3.325591	2.154375
106	6	0	7.964075	1.482163	-0.950909
107	6	0	9.594071	-0.121829	-0.022302
108	6	0	8.833733	-2.059692	1.244126
109	1	0	6.386667	2.809683	-1.637791
110	6	0	9.032280	2.231569	-1.470201
111	6	0	10.629342	0.658671	-0.561268
112	6	0	9.852182	-1.320561	0.726050
113	1	0	9.041497	-2.963452	1.811870

114	6	0	10.349552	1.821086	-1.277577
115	1	0	8.819110	3.141680	-2.025560
116	1	0	11.659624	0.345118	-0.411585
117	1	0	10.885412	-1.625574	0.873213
118	1	0	11.164511	2.412097	-1.686569

Total Energy (HF) = - 2361.6287035 Hartree

Pyrazabole 6:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.267342	0.001219	0.679752
2	7	0	1.267301	-0.001061	-0.679856
3	6	0	2.540023	-0.001686	-1.103544
4	1	0	2.770444	-0.003599	-2.157665
5	6	0	3.406110	0.000075	-0.000122
6	6	0	2.540087	0.001852	1.103357
7	1	0	2.770595	0.003760	2.157458
8	6	0	0.002037	-1.339768	2.571763
9	1	0	0.878491	-1.285761	3.239048
10	1	0	-0.860796	-1.273065	3.252298
11	6	0	-0.001867	1.343264	2.570237
12	1	0	-0.878211	1.290031	3.237728
13	1	0	0.861060	1.277322	3.250722
14	6	0	-0.000288	-2.710853	1.879355
15	1	0	0.844476	-2.765052	1.179130
16	1	0	-0.905841	-2.812919	1.263261
17	5	0	0.000012	0.001225	1.642723
18	6	0	0.087213	-3.919781	2.828633
19	1	0	0.998954	-3.833742	3.437918
20	6	0	0.000364	2.713566	1.876271
21	1	0	-0.844594	2.767001	1.176220
22	1	0	0.905749	2.814871	1.259806
23	6	0	1.125423	4.098284	3.746600
24	1	0	1.245391	3.247478	4.426664
25	1	0	1.027358	5.000018	4.362289
26	1	0	2.051950	4.192191	3.165514
27	6	0	-0.086797	3.923582	2.824195
28	1	0	-0.208368	4.835186	2.222577
29	1	0	-0.998228	3.838168	3.434033
30	7	0	-1.267435	0.000024	-0.679711
31	7	0	-1.267394	0.000118	0.679899
32	6	0	-2.540115	0.000192	1.103587
33	1	0	-2.770534	0.000055	2.157711

34	6	0	-3.406202	0.000056	0.000165
35	6	0	-2.540178	-0.000055	-1.103317
36	1	0	-2.770687	0.000082	-2.157419
37	6	0	0.001782	1.339929	-2.571709
38	1	0	-0.861125	1.273228	-3.252148
39	1	0	0.878163	1.285944	-3.239093
40	6	0	-0.002106	-1.343102	-2.570208
41	1	0	0.860745	-1.277148	-3.250791
42	1	0	-0.878525	-1.289855	-3.237598
43	6	0	-0.000478	2.711003	-1.879275
44	1	0	-0.905967	2.813054	-1.263083
45	1	0	0.844358	2.765185	-1.179136
46	5	0	-0.000108	-0.001075	-1.642681
47	6	0	0.086925	3.919950	-2.828534
48	1	0	0.998586	3.833912	-3.437940
49	6	0	0.000208	-2.713418	-1.876272
50	1	0	0.905659	-2.814725	-1.259903
51	1	0	-0.844678	-2.766887	-1.176137
52	6	0	-0.087026	-3.923410	-2.824220
53	1	0	-0.208463	-4.835038	-2.222611
54	1	0	0.208399	-4.832093	2.228011
55	6	0	-1.124558	-4.093274	3.751858
56	1	0	-1.244074	-3.241661	4.430991
57	1	0	-2.051395	-4.187748	3.171358
58	1	0	-1.026281	-4.994305	4.368542
59	1	0	0.208204	4.832246	-2.227907
60	1	0	-0.998550	-3.838020	-3.433921
61	6	0	1.125065	-4.098011	-3.746812
62	1	0	1.244878	-3.247175	-4.426865
63	1	0	2.051686	-4.191884	-3.165871
64	1	0	1.026958	-4.999732	-4.362515
65	6	0	-1.124964	4.093492	-3.751595
66	1	0	-1.244594	3.241897	-4.430731
67	1	0	-2.051720	4.187976	-3.170968
68	1	0	-1.026749	4.994533	-4.368275
69	6	0	-4.819990	0.000051	0.000155
70	6	0	-6.035490	-0.000069	0.000110
71	6	0	4.819898	0.000077	-0.000120
72	6	0	6.035397	-0.000056	-0.000098
73	6	0	-7.460837	-0.000142	0.000045
74	6	0	-8.177156	-0.001930	1.213670
75	6	0	-8.177040	0.001567	-1.213656
76	6	0	-9.569216	-0.001998	1.208412
77	6	0	-9.569094	0.001484	-1.208520
78	1	0	-7.629725	0.002983	-2.151255
79	6	0	-10.270229	-0.000289	-0.000085
80	1	0	-10.109223	0.002828	-2.151418
81	6	0	7.460745	-0.000134	-0.000089
82	6	0	8.177014	-0.002745	-1.213742
83	6	0	8.176997	0.002394	1.213581
84	6	0	9.569074	-0.002807	-1.208540
85	6	0	9.569051	0.002302	1.208389

86	1	0	7.629720	0.004442	2.151202
87	6	0	10.270137	-0.000287	-0.000073
88	1	0	10.109218	0.004282	2.151264
89	1	0	11.356623	-0.000343	-0.000037
90	1	0	10.109245	-0.004847	-2.151412
91	1	0	7.629740	-0.004735	-2.151365
92	1	0	-7.629920	-0.003292	2.151317
93	1	0	-10.109424	-0.003399	2.151263
94	1	0	-11.356715	-0.000341	-0.000165

Total Energy (HF) = -1746.9003387 Hartree

Pyrazabole 7:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.221962	-0.746301	0.135838
2	7	0	-0.729829	-0.111667	1.232868
3	5	0	-0.599149	-0.758302	-1.328367
4	6	0	-2.356943	-1.372310	0.481662
5	1	0	-2.916523	-1.940356	-0.245373
6	6	0	-2.624914	-1.149158	1.840470
7	6	0	-1.557377	-0.343029	2.262587
8	1	0	-1.353625	0.070533	3.237981
9	6	0	-3.712170	-1.623392	2.609262
10	6	0	-4.641364	-2.025188	3.282548
11	6	0	-5.732981	-2.503474	4.062322
12	6	0	-6.744505	-3.311649	3.454935
13	1	0	-6.661134	-3.546266	2.398447
14	6	0	-7.799957	-3.781514	4.194924
15	1	0	-8.563945	-4.395392	3.723837
16	6	0	-7.920986	-3.482114	5.579917
17	6	0	-9.000828	-3.955828	6.369473
18	1	0	-9.764003	-4.570221	5.897492
19	6	0	-9.084569	-3.645745	7.708973
20	1	0	-9.916370	-4.014992	8.302572
21	6	0	-8.088817	-2.844729	8.320696
22	1	0	-8.165862	-2.606740	9.378090
23	6	0	-7.028857	-2.369438	7.582581
24	1	0	-6.263029	-1.754785	8.049620
25	6	0	-6.912538	-2.671635	6.197784
26	6	0	-5.832453	-2.197941	5.414013
27	1	0	-5.067654	-1.584631	5.882249
28	6	0	-0.242833	-2.286047	-1.774804

29	1	0	-1.192096	-2.839081	-1.867141
30	1	0	0.149649	-2.254622	-2.804697
31	6	0	0.719353	-3.111395	-0.908866
32	1	0	0.329007	-3.183421	0.116824
33	1	0	1.685435	-2.592882	-0.824633
34	6	0	0.965541	-4.529882	-1.443558
35	1	0	0.002807	-5.054591	-1.529384
36	1	0	1.364759	-4.464915	-2.466254
37	6	0	1.920433	-5.354193	-0.574026
38	1	0	2.901926	-4.870577	-0.494372
39	1	0	2.076458	-6.357595	-0.987457
40	1	0	1.528862	-5.471032	0.444172
41	6	0	-1.638261	-0.082319	-2.388160
42	1	0	-1.179765	-0.134998	-3.389474
43	1	0	-2.520326	-0.739677	-2.461960
44	6	0	-2.119933	1.355132	-2.145538
45	1	0	-1.257138	2.034920	-2.093372
46	1	0	-2.612433	1.422521	-1.164434
47	6	0	-3.089258	1.869093	-3.220090
48	1	0	-2.599947	1.812473	-4.203373
49	1	0	-3.955707	1.194088	-3.275950
50	6	0	-3.573187	3.301644	-2.972511
51	1	0	-4.099336	3.382293	-2.013152
52	1	0	-4.261129	3.635564	-3.758193
53	1	0	-2.732020	4.005400	-2.945257
54	7	0	1.221962	0.746301	-0.135838
55	7	0	0.729829	0.111667	-1.232868
56	5	0	0.599149	0.758302	1.328367
57	6	0	2.356943	1.372310	-0.481662
58	1	0	2.916523	1.940356	0.245373
59	6	0	2.624914	1.149158	-1.840470
60	6	0	1.557377	0.343029	-2.262587
61	1	0	1.353625	-0.070533	-3.237981
62	6	0	3.712170	1.623392	-2.609262
63	6	0	4.641364	2.025188	-3.282548
64	6	0	5.732981	2.503474	-4.062322
65	6	0	6.744505	3.311649	-3.454935
66	1	0	6.661134	3.546266	-2.398447
67	6	0	7.799957	3.781514	-4.194924
68	1	0	8.563945	4.395392	-3.723837
69	6	0	7.920986	3.482114	-5.579917
70	6	0	9.000828	3.955828	-6.369473
71	1	0	9.764003	4.570221	-5.897492
72	6	0	9.084569	3.645745	-7.708973
73	1	0	9.916370	4.014992	-8.302572
74	6	0	8.088817	2.844729	-8.320696
75	1	0	8.165862	2.606740	-9.378090
76	6	0	7.028857	2.369438	-7.582581
77	1	0	6.263029	1.754785	-8.049620
78	6	0	6.912538	2.671635	-6.197784
79	6	0	5.832453	2.197941	-5.414013
80	1	0	5.067654	1.584631	-5.882249

81	6	0	0.242833	2.286047	1.774804
82	1	0	1.192096	2.839081	1.867141
83	1	0	-0.149649	2.254622	2.804697
84	6	0	-0.719353	3.111395	0.908866
85	1	0	-0.329007	3.183421	-0.116824
86	1	0	-1.685435	2.592882	0.824633
87	6	0	-0.965541	4.529882	1.443558
88	1	0	-0.002807	5.054591	1.529384
89	1	0	-1.364759	4.464915	2.466254
90	6	0	-1.920433	5.354193	0.574026
91	1	0	-2.901926	4.870577	0.494372
92	1	0	-2.076458	6.357595	0.987457
93	1	0	-1.528862	5.471032	-0.444172
94	6	0	1.638261	0.082319	2.388160
95	1	0	1.179765	0.134998	3.389474
96	1	0	2.520326	0.739677	2.461960
97	6	0	2.119933	-1.355132	2.145538
98	1	0	1.257138	-2.034920	2.093372
99	1	0	2.612433	-1.422521	1.164434
100	6	0	3.089258	-1.869093	3.220090
101	1	0	2.599947	-1.812473	4.203373
102	1	0	3.955707	-1.194088	3.275950
103	6	0	3.573187	-3.301644	2.972511
104	1	0	4.099336	-3.382293	2.013152
105	1	0	4.261129	-3.635564	3.758193
106	1	0	2.732020	-4.005400	2.945257

Total Energy (HF) = - 2054.1940969 Hartree

Pyrazabole 8:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.274429	-0.591072	-0.304916
2	7	0	-1.259035	0.617380	0.317454
3	6	0	-2.526809	1.006707	0.518328
4	1	0	-2.744670	1.942758	1.008804
5	6	0	-3.405741	0.035017	0.016451
6	6	0	-2.551631	-0.954352	-0.493801
7	1	0	-2.793411	-1.885664	-0.982128
8	6	0	-0.030355	-2.913094	-0.091784
9	1	0	-0.906091	-3.455717	-0.479886
10	1	0	0.831751	-3.478826	-0.482894
11	6	0	-0.028643	-1.575821	-2.416025
12	1	0	0.837034	-2.193718	-2.707720
13	1	0	-0.903384	-2.185729	-2.689560

14	6	0	-0.015896	-2.999843	1.441963
15	1	0	-0.904950	-2.497393	1.850740
16	1	0	0.846635	-2.439810	1.828701
17	5	0	-0.018457	-1.439393	-0.790134
18	6	0	0.045997	-4.429155	2.011053
19	1	0	0.938587	-4.935960	1.615737
20	6	0	-0.018889	-0.292640	-3.259978
21	1	0	0.846193	0.322050	-2.975173
22	1	0	-0.906340	0.313295	-3.024700
23	6	0	-1.214117	-1.192350	-5.366949
24	1	0	-1.358879	-2.200466	-4.962538
25	1	0	-1.140275	-1.283163	-6.456942
26	1	0	-2.118319	-0.611896	-5.142694
27	6	0	0.031973	-0.516877	-4.782461
28	1	0	0.173845	0.453926	-5.277628
29	1	0	0.920520	-1.116525	-5.028528
30	7	0	1.274445	0.591464	0.305125
31	7	0	1.259040	-0.616882	-0.317445
32	6	0	2.526805	-1.006200	-0.518361
33	1	0	2.744646	-1.942198	-1.008947
34	6	0	3.405758	-0.034610	-0.016313
35	6	0	2.551652	0.954689	0.494099
36	1	0	2.793426	1.885938	0.982548
37	6	0	0.030477	2.913543	0.091915
38	1	0	0.906186	3.456137	0.480116
39	1	0	-0.831657	3.479292	0.482939
40	6	0	0.028536	1.576236	2.416141
41	1	0	-0.837140	2.194159	2.707781
42	1	0	0.903279	2.186103	2.689762
43	6	0	0.016189	3.000309	-1.441833
44	1	0	0.905285	2.497860	-1.850520
45	1	0	-0.846302	2.440285	-1.828670
46	5	0	0.018464	1.439836	0.790246
47	6	0	-0.045634	4.429628	-2.010915
48	1	0	-0.938266	4.936434	-1.615690
49	6	0	0.018667	0.293025	3.260047
50	1	0	-0.846408	-0.321628	2.975138
51	1	0	0.906121	-0.312927	3.024822
52	6	0	1.213725	1.192615	5.367162
53	1	0	1.358572	2.200727	4.962767
54	1	0	1.139767	1.283430	6.457148
55	1	0	2.117927	0.612123	5.143006
56	6	0	-0.032329	0.517199	4.782534
57	1	0	-0.174268	-0.453622	5.277647
58	1	0	-0.920882	1.116858	5.028545
59	1	0	-0.187028	4.370208	-3.099104
60	1	0	0.187508	-4.369725	3.099227
61	6	0	-4.819215	0.048806	0.023664
62	6	0	-6.036598	0.059767	0.029898
63	6	0	4.819213	-0.048522	-0.023516
64	6	0	6.036598	-0.059721	-0.029836
65	6	0	-7.458399	0.071749	0.037770

66	6	0	-8.175676	-1.153151	-0.057546
67	6	0	-8.154110	1.308347	0.141138
68	6	0	-7.521426	-2.417183	-0.158328
69	6	0	-9.617143	-1.129139	-0.049770
70	6	0	-9.595775	1.308175	0.150271
71	6	0	-7.477837	2.561345	0.233953
72	6	0	-8.240717	-3.581485	-0.248754
73	1	0	-6.436613	-2.439301	-0.160095
74	6	0	-10.329450	-2.365151	-0.146735
75	6	0	-10.286783	0.095156	0.054278
76	6	0	-10.286302	2.555835	0.255339
77	1	0	-6.392851	2.565348	0.223007
78	6	0	-8.176619	3.737417	0.332474
79	6	0	-9.664092	-3.558057	-0.243897
80	1	0	-7.721913	-4.533305	-0.323863
81	1	0	-11.416370	-2.334910	-0.140796
82	1	0	-11.374774	0.104183	0.060645
83	6	0	-9.600156	3.737547	0.344384
84	1	0	-11.373571	2.543628	0.262126
85	1	0	-7.641317	4.680550	0.401184
86	1	0	-10.217329	-4.490315	-0.316598
87	1	0	-10.136990	4.678843	0.423362
88	6	0	7.458376	-0.071950	-0.037804
89	6	0	8.153801	-1.307952	-0.150025
90	6	0	8.175950	1.152076	0.066240
91	6	0	7.477256	-2.560104	-0.251802
92	6	0	9.595465	-1.308044	-0.159207
93	6	0	9.617412	1.127772	0.058228
94	6	0	7.522019	2.415510	0.176124
95	6	0	8.175765	-3.735602	-0.358768
96	1	0	6.392271	-2.563951	-0.240882
97	6	0	10.285707	-2.555076	-0.273225
98	6	0	10.286760	-0.095903	-0.054587
99	6	0	10.330018	2.362888	0.164010
100	1	0	6.437211	2.437877	0.178136
101	6	0	8.241591	3.578964	0.274863
102	6	0	9.599300	-3.735968	-0.370713
103	1	0	7.640247	-4.678094	-0.434237
104	1	0	11.372979	-2.543060	-0.279963
105	1	0	11.374748	-0.105137	-0.061063
106	6	0	9.664959	3.555229	0.269756
107	1	0	11.416931	2.332426	0.157805
108	1	0	7.723020	4.530343	0.356845
109	1	0	10.135921	-4.676793	-0.456451
110	1	0	10.218425	4.486807	0.349113
111	6	0	1.192988	5.285163	-1.720124
112	1	0	1.334717	5.445657	-0.645405
113	1	0	2.101869	4.806758	-2.107445
114	1	0	1.111620	6.271698	-2.191260
115	6	0	-1.192653	-5.284698	1.720404
116	1	0	-2.101492	-4.806297	2.107832
117	1	0	-1.334507	-5.445191	0.645701

118	1	0	-1.111224	-6.271233	2.191530

Total Energy (HF) = - 2361.4638146 Hartree

Pyrazabole 9:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.141463	-0.871945	0.200369
2	7	0	-1.359914	0.469923	0.182747
3	6	0	-2.684175	0.683604	0.181969
4	1	0	-3.079838	1.687274	0.173698
5	6	0	-3.361979	-0.544597	0.200393
6	6	0	-2.329377	-1.494316	0.211284
7	1	0	-2.387328	-2.571588	0.223058
8	6	0	0.420649	-2.538551	1.529536
9	1	0	-0.336984	-3.338535	1.481903
10	1	0	1.381182	-3.070993	1.453303
11	6	0	0.397770	-2.540567	-1.151744
12	1	0	1.366076	-3.066528	-1.104950
13	1	0	-0.350595	-3.344298	-1.074621
14	6	0	0.323487	-1.856191	2.902076
15	1	0	-0.630388	-1.315419	2.970712
16	1	0	1.108117	-1.090556	2.993221
17	5	0	0.262814	-1.621380	0.189324
18	6	0	0.423393	-2.808377	4.108137
19	1	0	-0.362165	-3.574027	4.027780
20	6	0	0.276333	-1.861756	-2.524092
21	1	0	1.019091	-1.055540	-2.597313
22	1	0	-0.705053	-1.372423	-2.610711
23	6	0	-0.623264	-3.868634	-3.881738
24	1	0	-0.644143	-4.552718	-3.025970
25	1	0	-0.461203	-4.473307	-4.781669
26	1	0	-1.617016	-3.410009	-3.964628
27	6	0	0.465219	-2.799604	-3.730942
28	1	0	0.496042	-2.193836	-4.647366
29	1	0	1.447627	-3.288658	-3.656411
30	7	0	1.141539	0.872456	0.200842
31	7	0	1.359973	-0.469402	0.182112
32	6	0	2.684230	-0.683096	0.180897
33	1	0	3.079870	-1.686769	0.171858
34	6	0	3.362053	0.545077	0.200107
35	6	0	2.329462	1.494805	0.211980
36	1	0	2.387437	2.572067	0.224570
37	6	0	-0.397747	2.541008	-1.151306

38	1	0	0.350658	3.344713	-1.074273
39	1	0	-1.366048	3.066976	-1.104516
40	6	0	-0.420526	2.539201	1.529931
41	1	0	-1.381044	3.071657	1.453609
42	1	0	0.337096	3.339182	1.482144
43	6	0	-0.276411	1.862067	-2.523595
44	1	0	0.704957	1.372700	-2.610245
45	1	0	-1.019205	1.055871	-2.596694
46	5	0	-0.262743	1.621897	0.189844
47	6	0	-0.465343	2.799798	-3.730526
48	1	0	-1.447744	3.288865	-3.656006
49	6	0	-0.323354	1.857157	2.902630
50	1	0	-1.108005	1.091574	2.994004
51	1	0	0.630504	1.316374	2.971360
52	6	0	-0.423181	2.809679	4.108444
53	1	0	-0.202803	2.243819	5.024411
54	1	0	0.203196	-2.242242	5.023977
55	6	0	1.785707	-3.493445	4.267361
56	1	0	2.021633	-4.137335	3.412570
57	1	0	2.590835	-2.752879	4.357337
58	1	0	1.810185	-4.120055	5.166595
59	1	0	-0.496201	2.193943	-4.646892
60	1	0	0.362298	3.575378	4.027765
61	6	0	-1.785533	3.494666	4.267692
62	1	0	-2.021670	4.138282	3.412753
63	1	0	-2.590577	2.754053	4.358035
64	1	0	-1.809907	4.121543	5.166743
65	6	0	0.623140	3.868812	-3.881451
66	1	0	0.644012	4.553002	-3.025768
67	1	0	1.616893	3.410176	-3.964279
68	1	0	0.461084	4.473373	-4.781458
69	6	0	4.756314	0.776388	0.211118
70	6	0	5.955183	0.984708	0.224816
71	6	0	-4.756233	-0.775965	0.211542
72	6	0	-5.955079	-0.984401	0.225397
73	6	0	7.350402	1.258148	0.257886
74	6	0	8.306925	0.265732	-0.094516
75	6	0	7.791291	2.537807	0.650615
76	6	0	9.695990	0.590239	-0.036830
77	6	0	7.926184	-1.053783	-0.509403
78	6	0	9.140981	2.848042	0.704246
79	1	0	7.049860	3.284779	0.916357
80	6	0	10.672899	-0.391312	-0.386154
81	6	0	10.117019	1.894116	0.367831
82	6	0	8.859254	-1.988485	-0.843775
83	1	0	6.868214	-1.291889	-0.552820
84	1	0	9.454969	3.842226	1.012146
85	6	0	10.263658	-1.696397	-0.795275
86	6	0	12.064237	-0.071100	-0.328489
87	6	0	11.520826	2.186595	0.416926
88	1	0	8.549198	-2.982511	-1.157100
89	6	0	11.242009	-2.645266	-1.135362

90	6	0	13.005711	-1.053010	-0.677438
91	6	0	12.451457	1.248790	0.085008
92	1	0	11.828732	3.182081	0.727437
93	6	0	12.596684	-2.324445	-1.076031
94	1	0	10.929428	-3.638825	-1.447258
95	1	0	14.064462	-0.809444	-0.633795
96	1	0	13.511584	1.486639	0.127313
97	1	0	13.339891	-3.070954	-1.342571
98	6	0	-7.350268	-1.258001	0.258646
99	6	0	-8.306957	-0.265980	-0.094404
100	6	0	-7.790940	-2.537469	0.652237
101	6	0	-9.695968	-0.590675	-0.036458
102	6	0	-7.926436	1.053310	-0.510197
103	6	0	-9.140579	-2.847891	0.706114
104	1	0	-7.049380	-3.284145	0.918451
105	6	0	-10.673043	0.390480	-0.386426
106	6	0	-10.116777	-1.894344	0.369099
107	6	0	-8.859667	1.987631	-0.845190
108	1	0	-6.868505	1.291561	-0.553790
109	1	0	-9.454395	-3.841921	1.014689
110	6	0	-10.264022	1.695347	-0.796458
111	6	0	-12.064330	0.070085	-0.328498
112	6	0	-11.520535	-2.187012	0.418445
113	1	0	-8.549779	2.981491	-1.159204
114	6	0	-11.242535	2.643823	-1.137178
115	6	0	-13.005970	1.051603	-0.678097
116	6	0	-12.451327	-1.249582	0.085917
117	1	0	-11.828271	-3.182334	0.729649
118	6	0	-12.597157	2.322827	-1.077585
119	1	0	-10.930123	3.637216	-1.449772
120	1	0	-14.064681	0.807900	-0.634251
121	1	0	-13.511415	-1.487569	0.128425
122	1	0	-13.340491	3.069032	-1.344620

Total Energy (HF) = - 2513.9504758 Hartree

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[1] A. G. Crawford, A. D. Dwyer, Z. Liu, A. Steffen, A. Beeby, L.-O. Palsson, D. J. Tozer and T. B. Marder, *J. Am. Chem. Soc.*, 2011, **133**, 13349.

[2] (a)Z. Zhao, S. Chen, J. W. Y. Lam, Z. Wang, P. Lu, M. Faisal, H. H. Y. Sung, I. D. Williams, Y. Ma, H. S. Kwok and B. Z. Tang, *J. Mater. Chem.*, 2011, **21**, 7210.