Supporting Information
Phosphines with N-heterocyclic boranyl substituents

M. Kaaz,[a] J. Bender,[a] D. Förster,[a] W. Frey,[b] M. Nieger[c] and D. Gudat[a],

Contents:

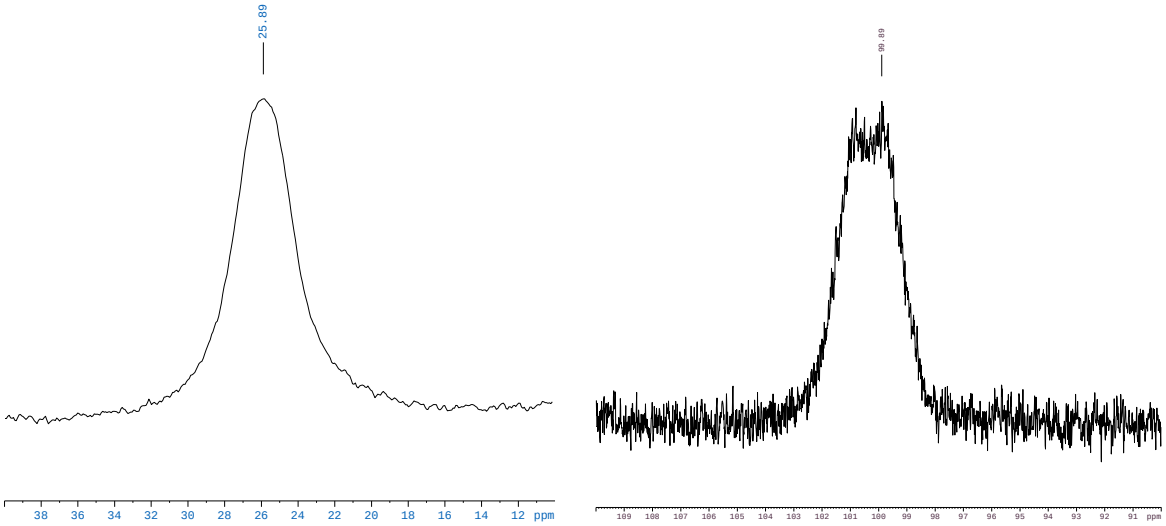

Figure S1 $^{11}B\{^{1}H\}$ (left) and $^{31}P\{^{1}H\}$ NMR spectrum (right) of **4a**

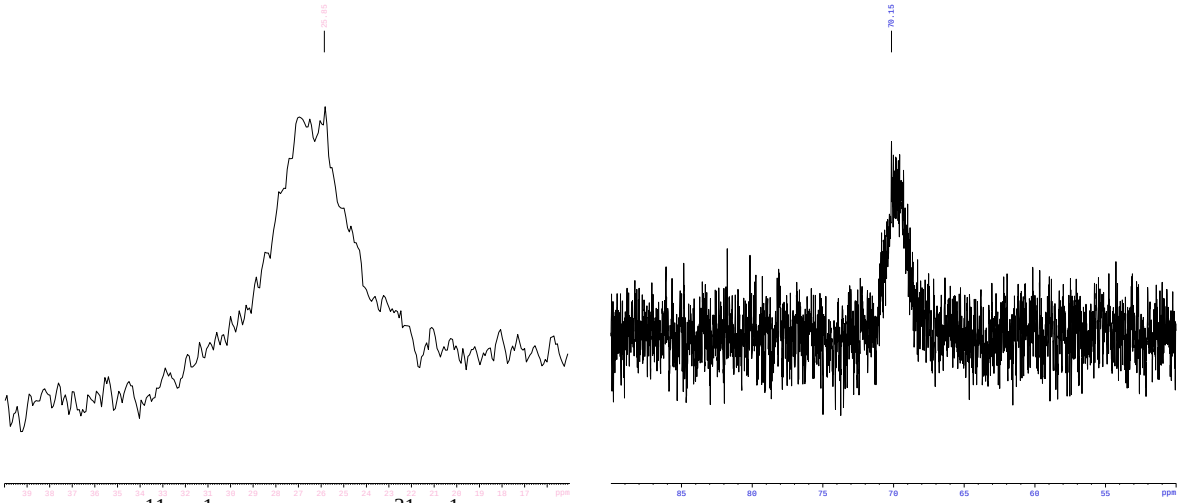

Figure S2 $^{11}B\{^{1}H\}$ (left) and $^{31}P\{^{1}H\}$ NMR spectrum (right) of **4b**

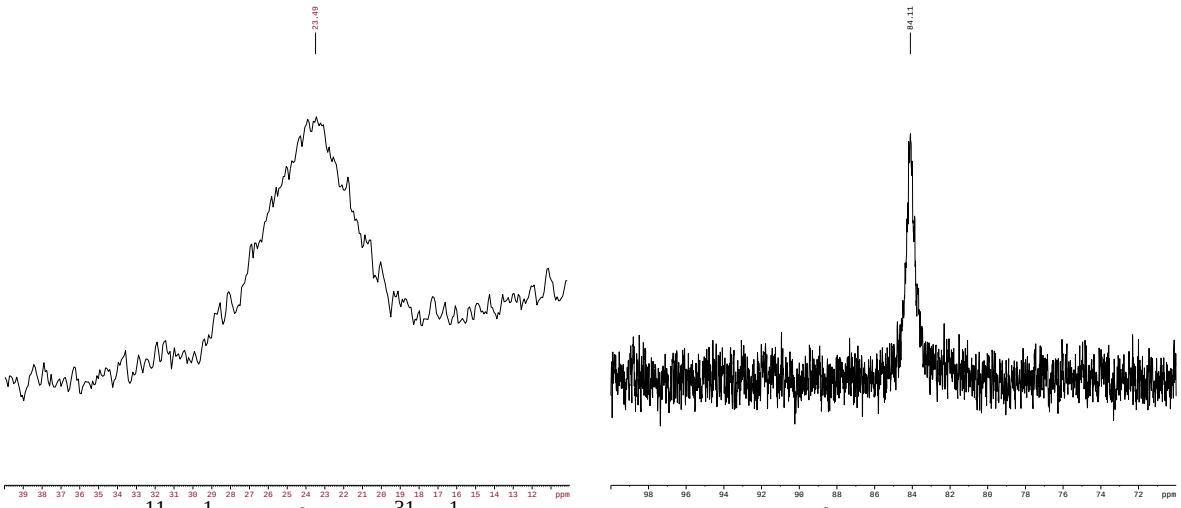

Figure S3 $^{11}B\{^{1}H\}$ (left) and $^{31}P\{^{1}H\}$ NMR spectrum (right) of **4c**

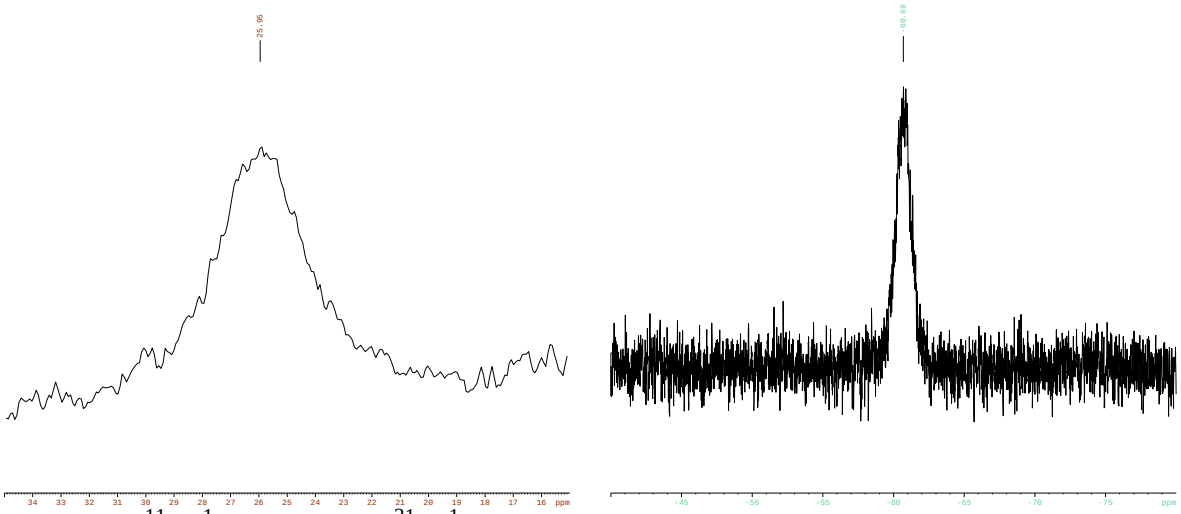

Figure S4 $^{11}B\{^{1}H\}$ (left) and $^{31}P\{^{1}H\}$ NMR spectrum (right) of **4d**

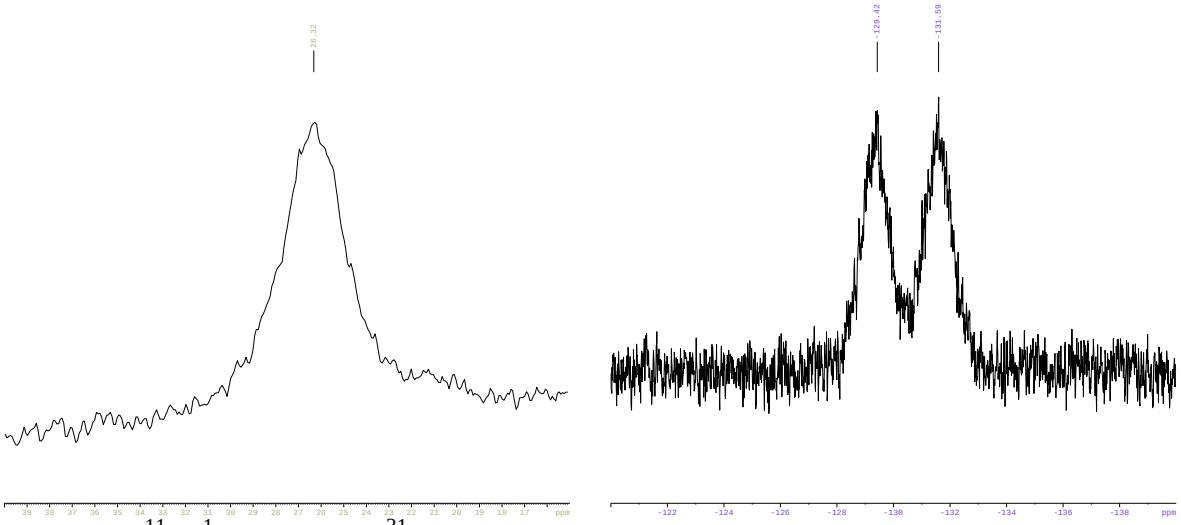

Figure S5 $^{11}B\{^{1}H\}$ (left) and ^{31}P NMR spectrum (right) of **4e**

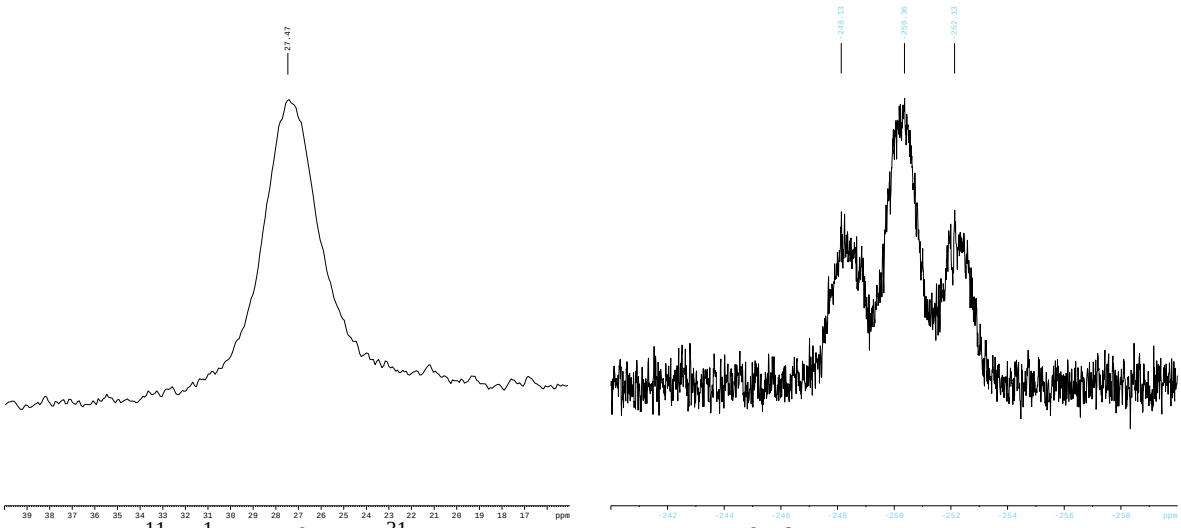

Figure S6 $^{11}B\{^{1}H\}$ (left) and ^{31}P NMR spectrum (right) of **4f**

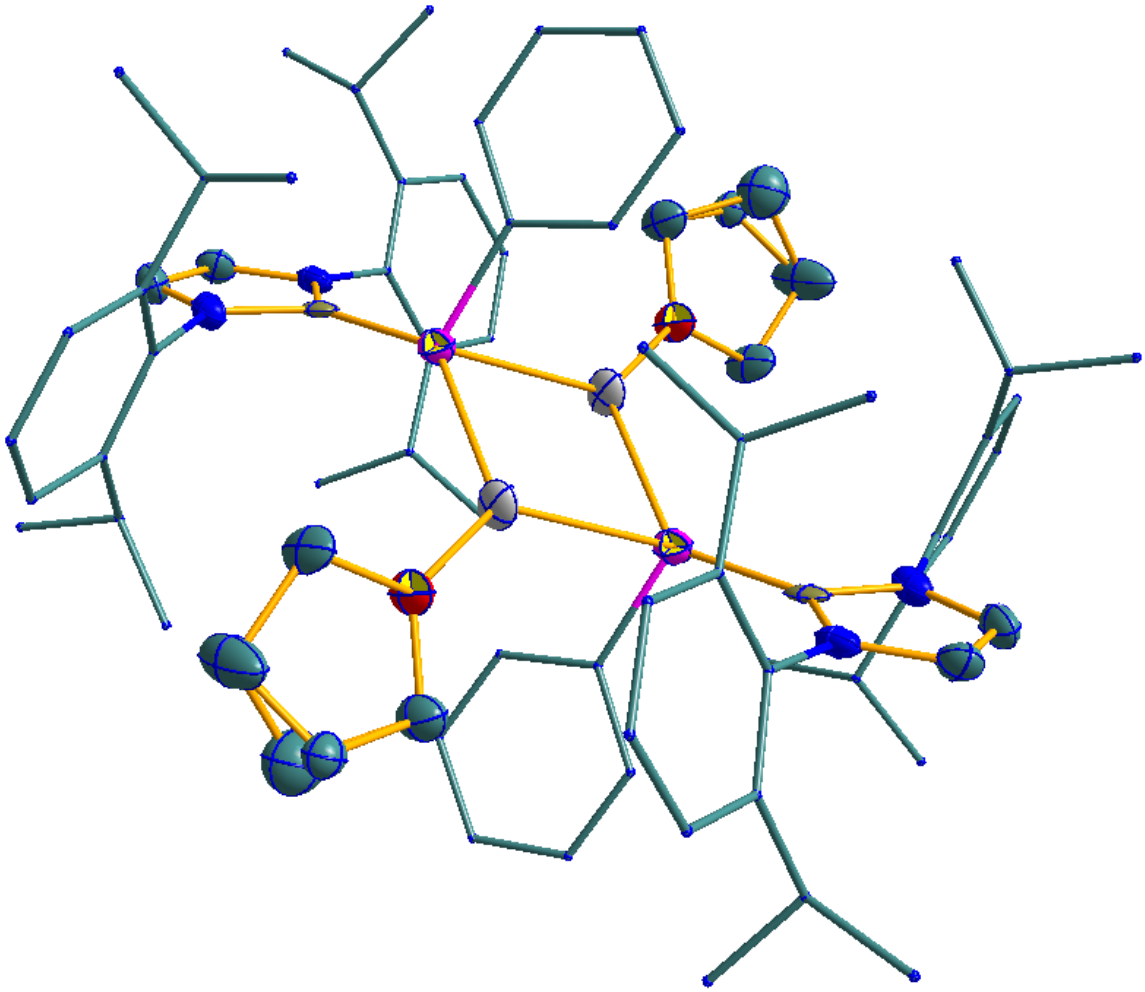

Figure S7 Graphical representation of the molecular structure of **11** in the crystal (triclinic, space group $P\bar{1}$, cell parameters: a = 12.935(2) Å, b = 14.241(3) Å, c = 20.705(4) Å, α = 93.713(8) °, β = 101.431(7) °, γ = 90.891(7) °) measured at 110(2) K. The two coordinating THF molecules are disordered.

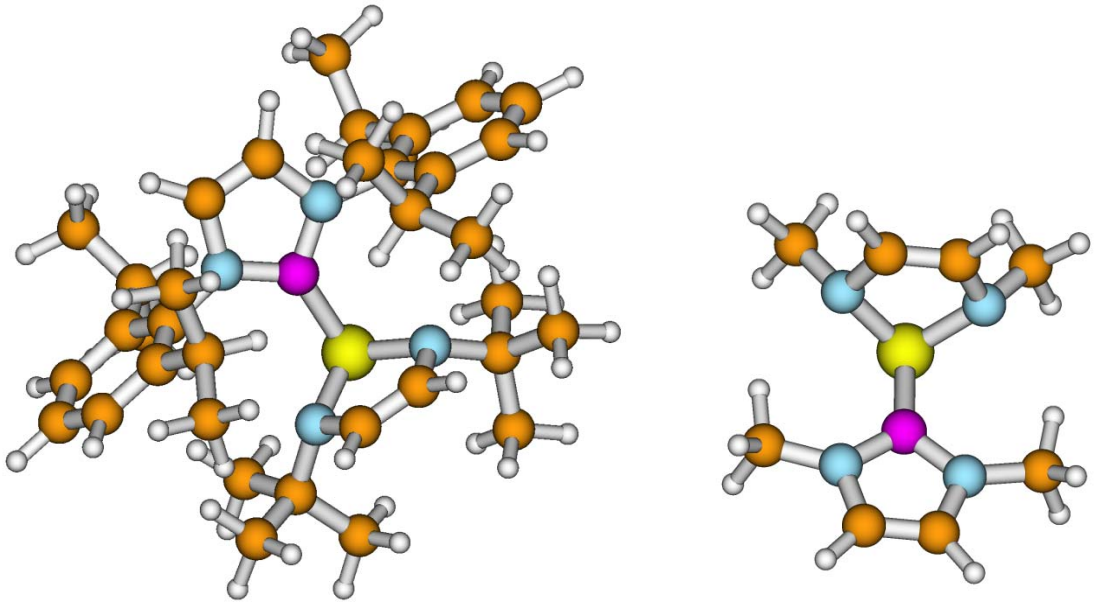

Figure S8 Graphical representation of the computed molecular structures of **4b** (left) and **4'** (right) obtained after energy optimization at the ωB97X-D/cc-pVDZ level.

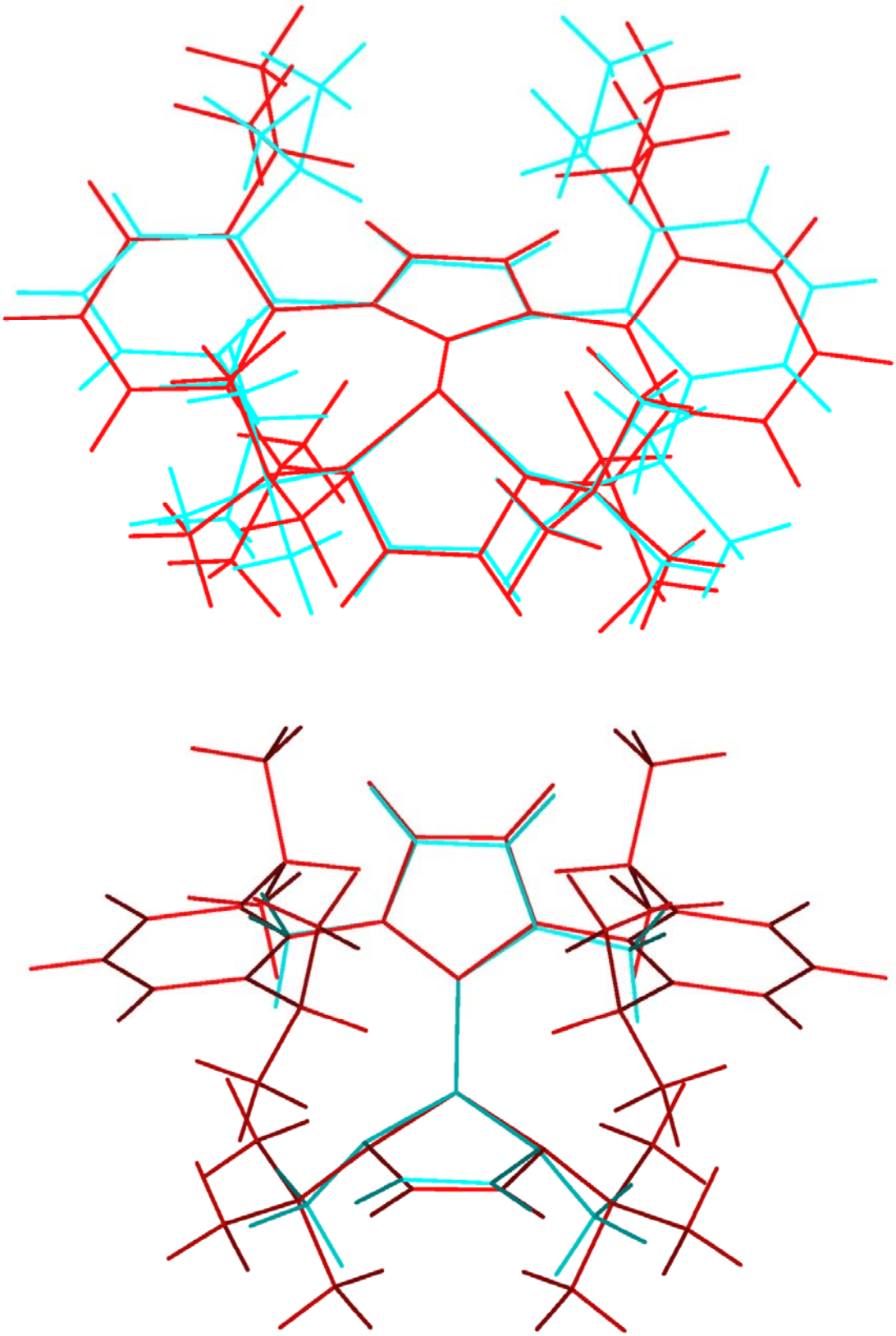

Figure S9 Top: Overlay of the computed (red) and experimentally determined (blue) molecular structures of **4b** (top); bottom: overlay of the computed molecular structures of **4b** (red) and **4'** (blue). Computations were carried out at the ωB97X-D/cc-pVDZ level.

Table S1 Energy, vibrational zero-point energy, and atomic coordinates of the molecular structure of **4b** obtained after energy optimization at the ωB97X-D/cc-pVDZ level.

E(RωB97X-D) = -1990.49216614 A.U. after 1 cycles

Zero-point correction = 0.867381 (Hartree/Particle)

Standard orientation:

Center No.	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-0.000010	0.557012	0.188256
2	15	0	0.000010	-0.818874	-1.193994
3	7	0	1.302568	-1.860452	-0.592163
4	7	0	-1.133588	1.285068	0.690288
5	7	0	1.133587	1.285087	0.690231
6	7	0	-1.302557	-1.860473	-0.592208
7	6	0	-3.172876	0.167892	1.444626
8	6	0	-2.538015	1.065922	0.563037
9	6	0	-3.251892	1.796909	-0.399624
10	6	0	-4.638362	1.618276	-0.468202
11	6	0	-5.284443	0.734571	0.385318
12	6	0	-4.555725	0.016227	1.331207
13	6	0	-0.674736	2.388328	1.414668
14	6	0	0.674752	2.388344	1.414626
15	6	0	2.538012	1.065916	0.563001
16	6	0	3.172863	0.167923	1.444635
17	6	0	4.555716	0.016264	1.331248
18	6	0	5.284447	0.734580	0.385348
19	6	0	4.638374	1.618246	-0.468221
20	6	0	3.251901	1.796865	-0.399681
21	6	0	2.376772	-0.575376	2.508911
22	6	0	2.558316	2.775899	-1.335438
23	6	0	-2.558311	2.775979	-1.335347
24	6	0	-2.376787	-0.575441	2.508880
25	6	0	0.671667	-2.748921	0.314443
26	6	0	-0.671682	-2.748935	0.314410
27	6	0	-2.341385	-2.425766	-1.503062
28	6	0	-1.764248	-3.482895	-2.452108
29	6	0	2.341388	-2.425779	-1.503011
30	6	0	2.949577	-1.280490	-2.312670
31	6	0	-3.452760	-3.052624	-0.652862

32	6	0	-2.949549	-1.280453	-2.312706
33	6	0	3.452749	-3.052639	-0.652794
34	6	0	1.764237	-3.482913	-2.452041
35	1	0	-1.365409	3.081681	1.885291
36	1	0	1.365437	3.081706	1.885219
37	1	0	1.277683	-3.356516	0.986187
38	1	0	-1.277714	-3.356552	0.986121
39	1	0	5.079979	-0.674040	1.993367
40	1	0	6.365827	0.601534	0.317201
41	1	0	5.218358	2.176937	-1.205533
42	1	0	1.474205	2.634026	-1.220378
43	6	0	2.880602	4.222568	-0.940360
44	6	0	2.896963	2.518267	-2.807203
45	6	0	3.012013	-1.895356	2.949292
46	6	0	2.140070	0.315296	3.738013
47	1	0	1.396200	-0.813439	2.070667
48	1	0	-5.218335	2.176988	-1.205508
49	1	0	-6.365820	0.601512	0.317140
50	1	0	-5.079996	-0.674108	1.993289
51	6	0	-2.896755	2.518211	-2.807135
52	6	0	-2.880818	4.222628	-0.940385
53	1	0	-1.474196	2.634249	-1.220158
54	1	0	-1.396223	-0.813507	2.070620
55	6	0	-2.140056	0.315204	3.737996
56	6	0	-3.012040	-1.895421	2.949242
57	1	0	3.735042	-1.667332	-2.979819
58	1	0	2.187179	-0.792213	-2.938692
59	1	0	3.395695	-0.528534	-1.647732
60	1	0	2.565569	-3.953154	-3.043269
61	1	0	1.241097	-4.272082	-1.890870
62	1	0	1.051602	-3.026847	-3.154106
63	1	0	4.261234	-3.408248	-1.309178
64	1	0	3.872080	-2.306111	0.035329
65	1	0	3.098894	-3.919351	-0.074483
66	1	0	-2.565583	-3.953104	-3.043357
67	1	0	-1.051592	-3.026832	-3.154154
68	1	0	-1.241134	-4.272088	-1.890948
69	1	0	-3.735035	-1.667266	-2.979848
70	1	0	-3.395635	-0.528486	-1.647759
71	1	0	-2.187144	-0.792198	-2.938737
72	1	0	-4.261260	-3.408182	-1.309255

73	1	0	-3.098932	-3.919370	-0.074588
74	1	0	-3.872062	-2.306110	0.035293
75	1	0	-2.309771	-2.445123	3.594509
76	1	0	-3.931146	-1.735550	3.536299
77	1	0	-3.261664	-2.538638	2.094530
78	1	0	-1.556437	-0.229434	4.497148
79	1	0	-1.584764	1.227434	3.482660
80	1	0	-3.099885	0.610174	4.193306
81	1	0	2.309740	-2.445043	3.594567
82	1	0	3.261631	-2.538584	2.094588
83	1	0	3.931121	-1.735485	3.536345
84	1	0	1.556449	-0.229315	4.497182
85	1	0	3.099910	0.610257	4.193307
86	1	0	1.584793	1.227532	3.482665
87	1	0	2.323689	3.201714	-3.452688
88	1	0	3.965398	2.684609	-3.018957
89	1	0	2.649859	1.487537	-3.097657
90	1	0	2.343973	4.931404	-1.590337
91	1	0	2.588151	4.426501	0.100442
92	1	0	3.959763	4.427500	-1.033402
93	1	0	-2.344172	4.931493	-1.590316
94	1	0	-3.959987	4.427445	-1.033590
95	1	0	-2.588540	4.426638	0.100452
96	1	0	-2.323554	3.201742	-3.452597
97	1	0	-2.649410	1.487516	-3.097511
98	1	0	-3.965204	2.684321	-3.019001

Table S2: Energy, vibrational zero-point energy, and atomic coordinates of the molecular structure of **4'** obtained after energy optimization at the ωB97X-D/cc-pVDZ level.

E(RwB97XD) = -899.580347466 A.U. after 1 cycles

Zero-point correction = 0.251474 Hartree/Particle

Standard orientation:

Center No.	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-1.022704	0.000000	-0.250937
2	15	0	0.810458	0.000013	-0.911287
3	7	0	-1.868567	1.136935	-0.041978
4	7	0	-1.868556	-1.136942	-0.041966
5	7	0	1.457369	1.295777	0.115496
6	7	0	1.457373	-1.295770	0.115469
7	6	0	-1.585230	2.552539	-0.140957
8	6	0	-1.585207	-2.552544	-0.140932
9	6	0	-3.142800	0.677082	0.277931
10	6	0	-3.142793	-0.677097	0.277937
11	6	0	1.786454	0.670572	1.349895
12	6	0	1.786460	-0.670589	1.349879
13	6	0	2.515396	-2.149575	-0.421853
14	6	0	2.515398	2.149586	-0.421809
15	1	0	-0.499155	2.698532	-0.166740
16	1	0	-2.036232	2.992032	-1.046192
17	1	0	-1.980934	3.087928	0.736624
18	1	0	-0.499131	-2.698528	-0.166705
19	1	0	-1.980913	-3.087930	0.736651
20	1	0	-2.036199	-2.992047	-1.046165
21	1	0	2.748665	-2.938877	0.311157
22	1	0	2.165990	-2.636584	-1.343308
23	1	0	3.451192	-1.601503	-0.645134
24	1	0	2.748610	2.938927	0.311178
25	1	0	3.451219	1.601528	-0.645017
26	1	0	2.166024	2.636544	-1.343302
27	1	0	-3.959243	-1.359761	0.499761
28	1	0	-3.959256	1.359741	0.499746
29	1	0	2.023292	1.298824	2.210884
30	1	0	2.023307	-1.298860	2.210853