Electronic Supplementary Material (ESI) for Dalton Transactions.

Expansion of the scope of N→B-Ladder boranes: New Substituents and alternative substrates

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1. Supporting Information

1.1. Supplementary Analytical data

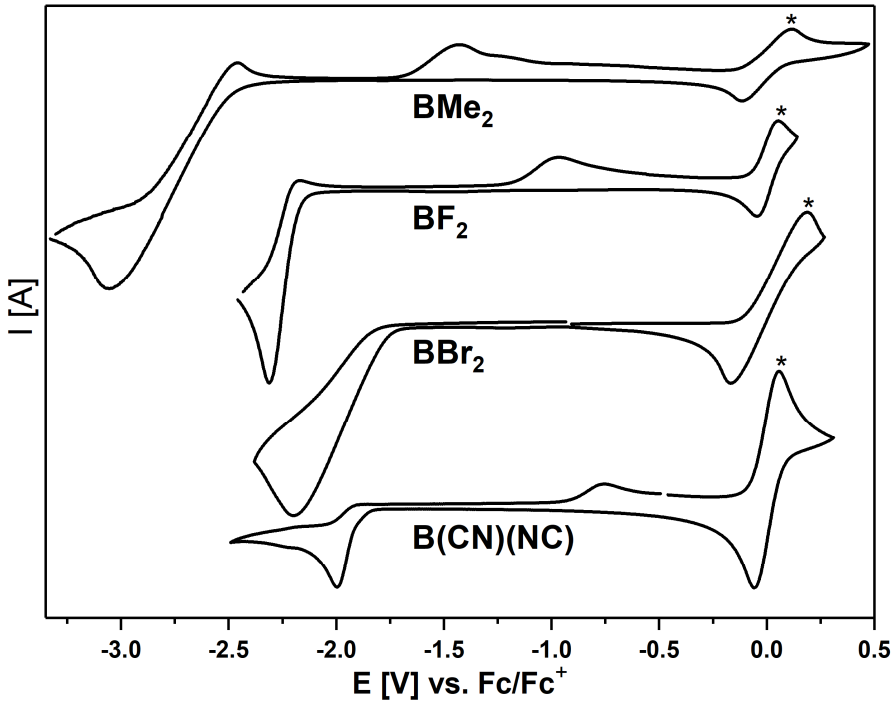


Figure S 1. Cyclic voltammetry scans of **BMe_2**, **BF_2**, **BBr_2**, and **B(CN)(NC)**. * internal standard Ferrocene.

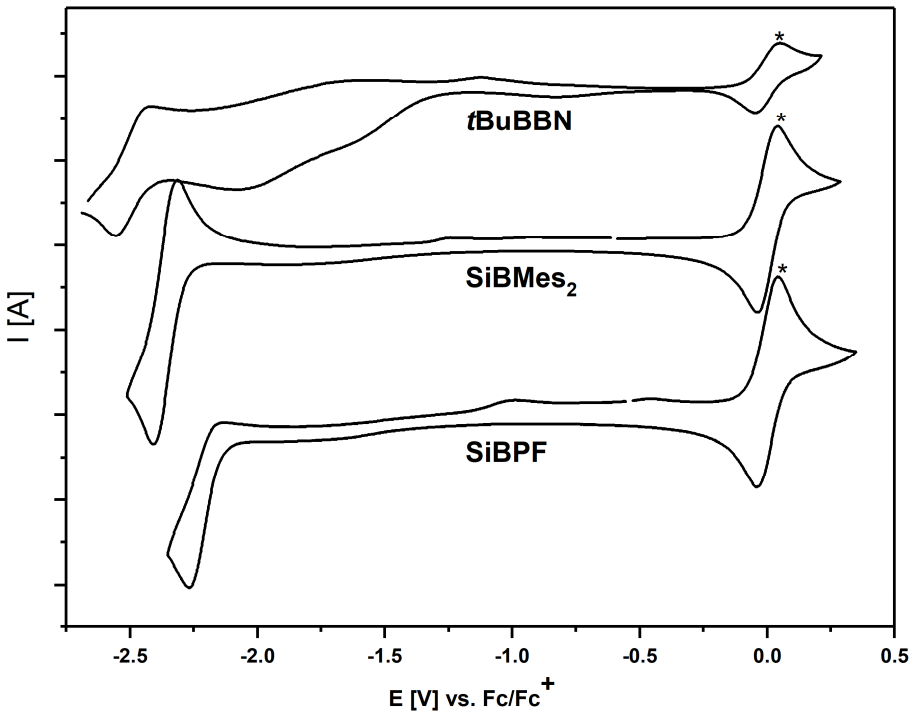


Figure S 2. Cyclic voltammetry scans of ***t*BuBBN**, **SiBMes$_2$, SiBPF**. * internal standard Ferrocene.

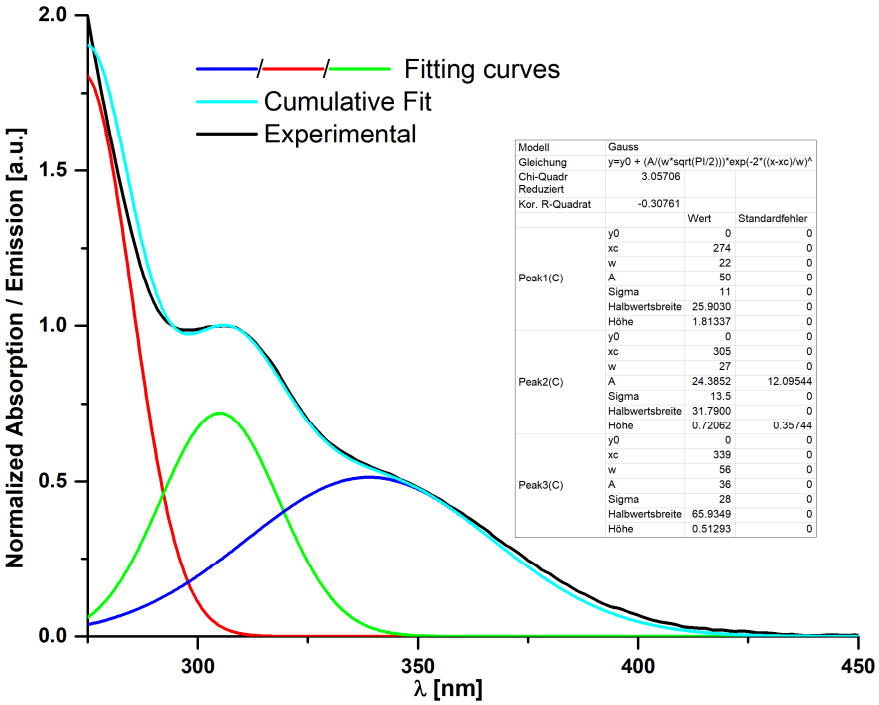


Figure S 3. Gaussian deconvolution of the UV-vis absorption spectrum ***t*BuBBN**.

2. DFT-calculations

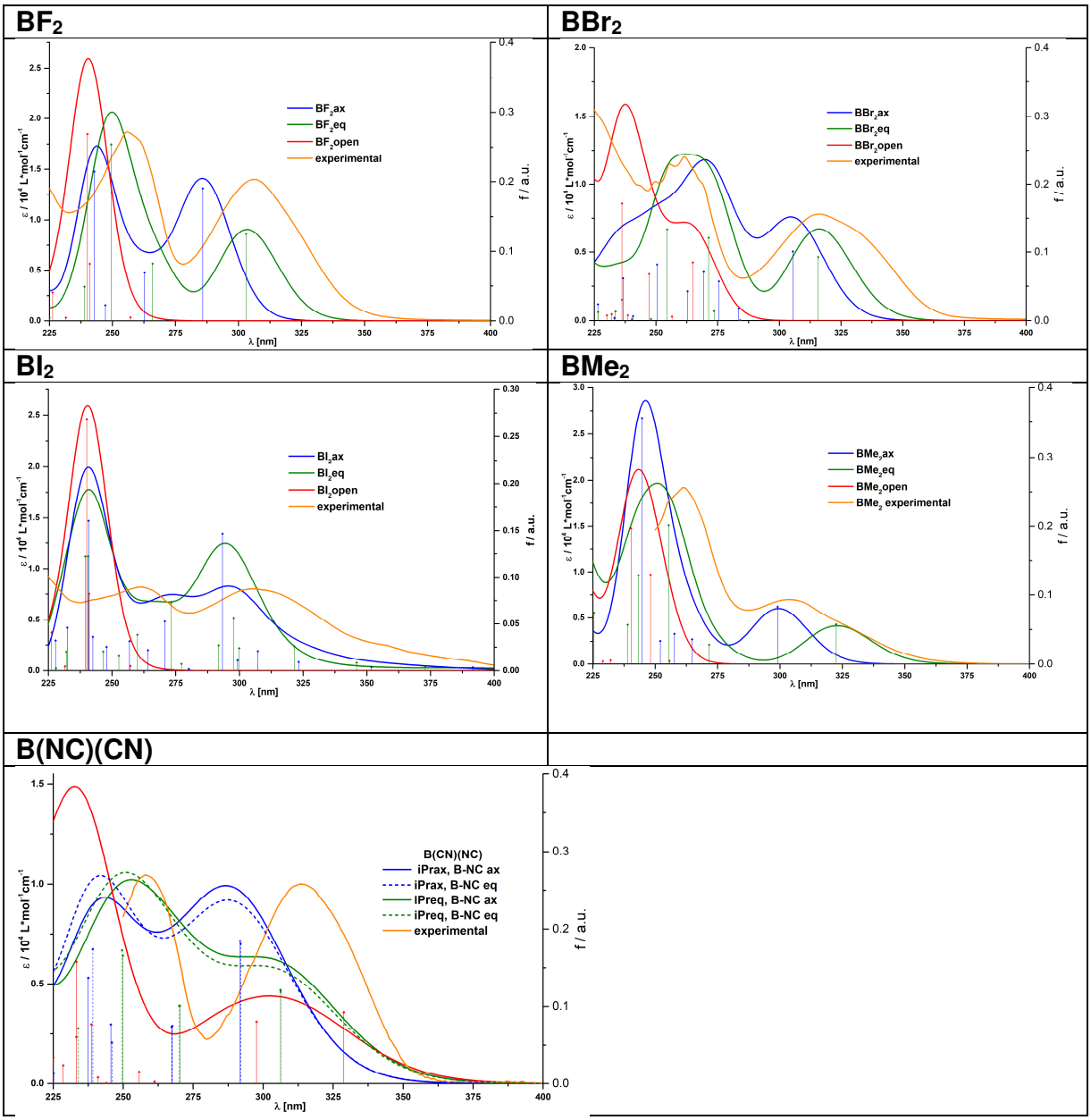


Figure S4. Calculated and Experimental UV-vis absorption spectra for alkyl-boranes.

Spectra simulated with a half-width at half height of 0.62 eV (5000 cm^{-1}).

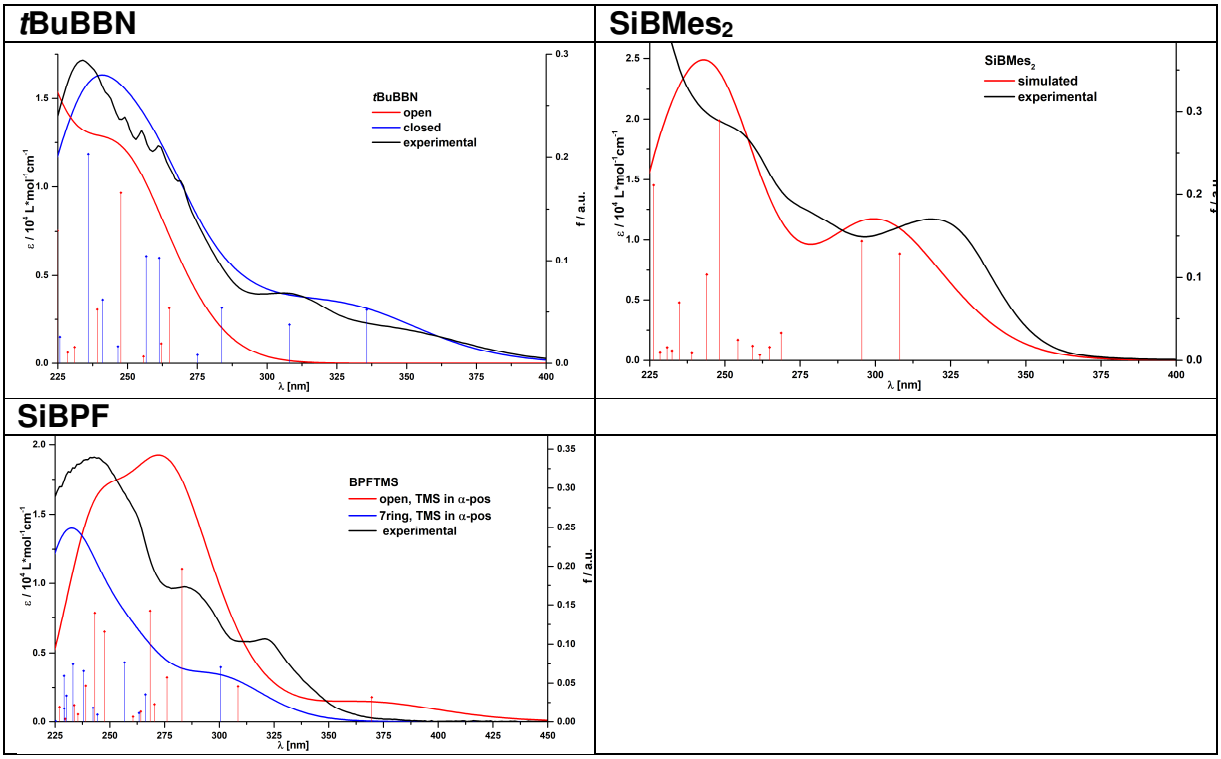
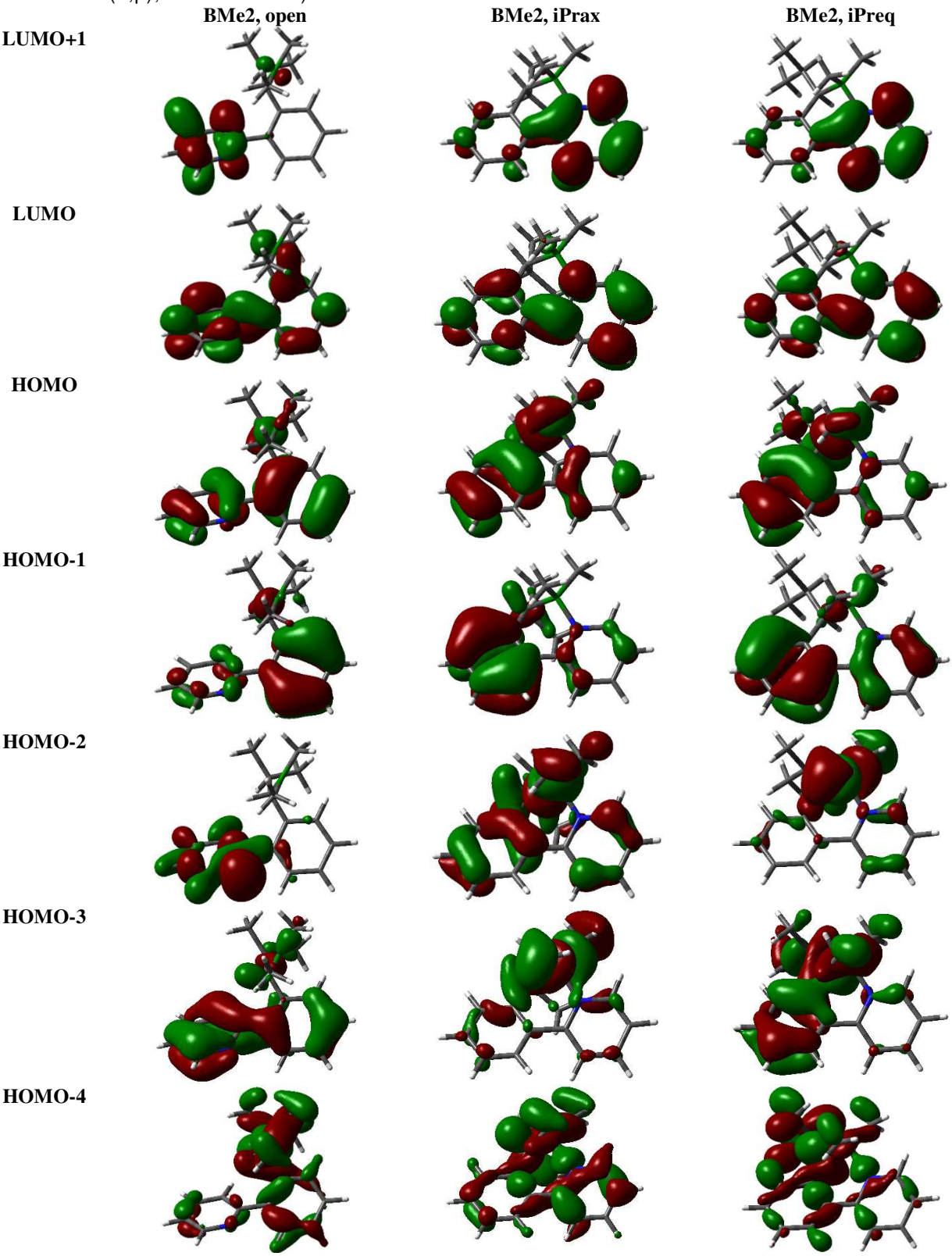


Figure S5. Calculated and Experimental UV-vis absorption spectra for vinyl-boranes.

Spectra simulated with a half-width at half height of 0.62 eV (5000 cm^{-1}).

Table S1. Frontier orbital plots of borylated compounds depending on their conformation. (M06-2X/6-311+G(d,p); Isovalue: 0.02)



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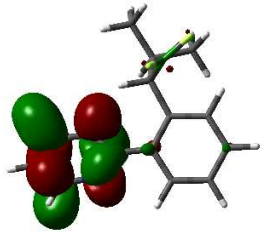
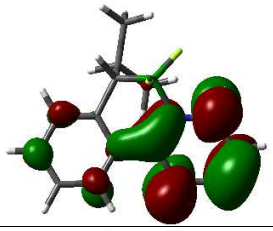
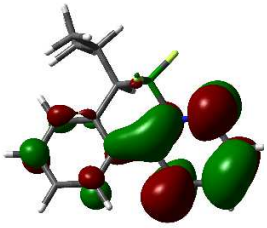
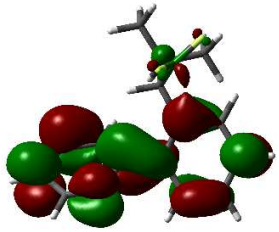
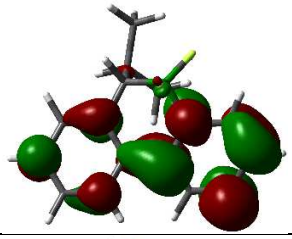
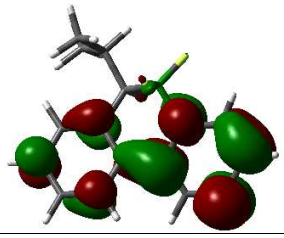
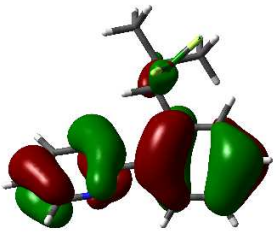
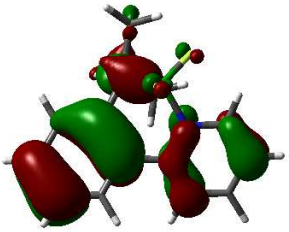
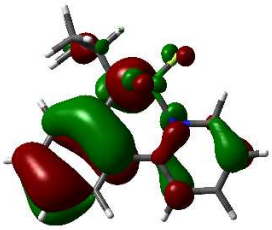
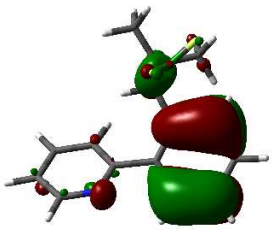
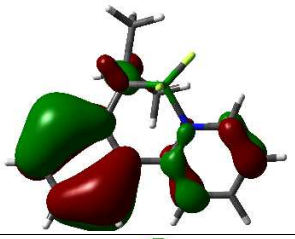
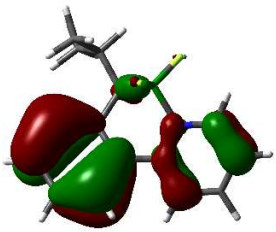
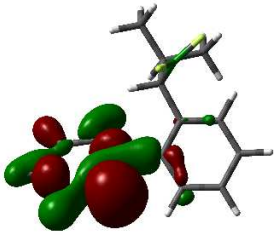
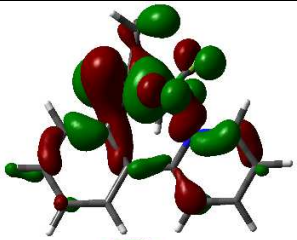
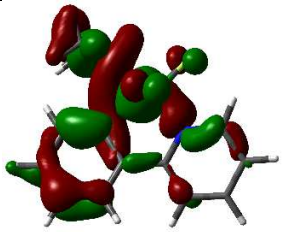
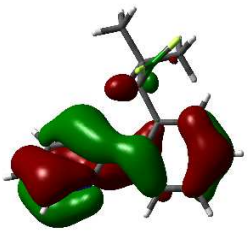
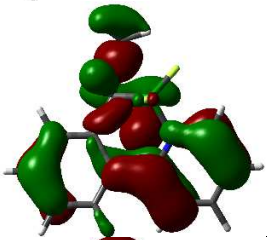
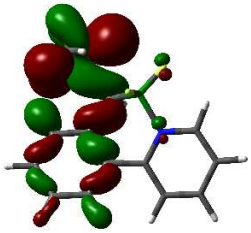
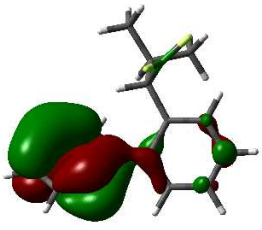
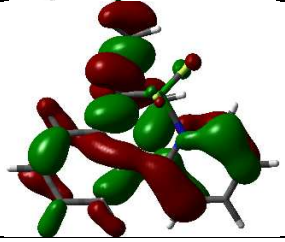
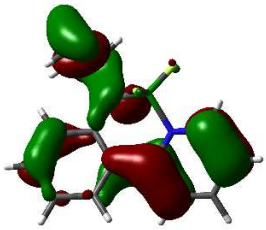
LUMO+1			
LUMO			
HOMO			
HOMO-1			
HOMO-2			
HOMO-3			
HOMO-4			

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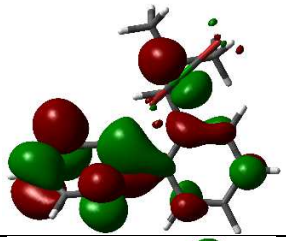
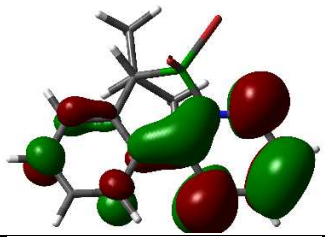
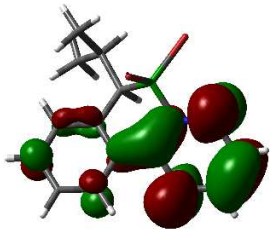
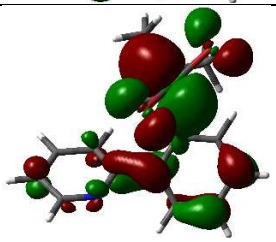
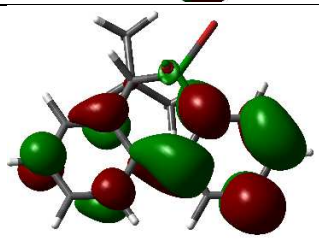
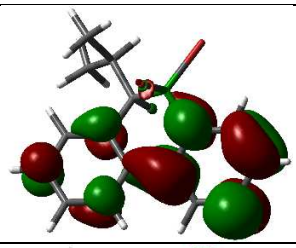
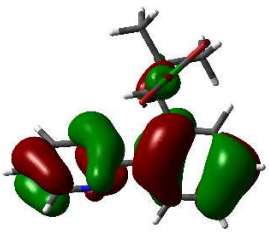
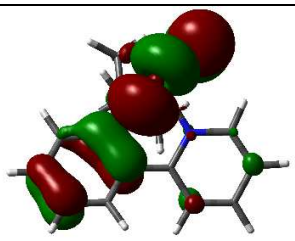
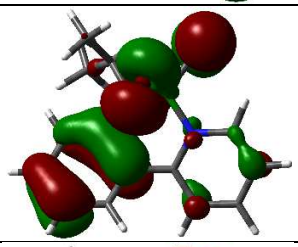
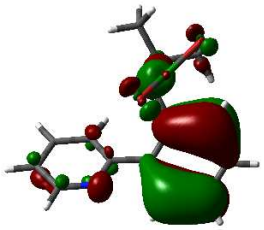
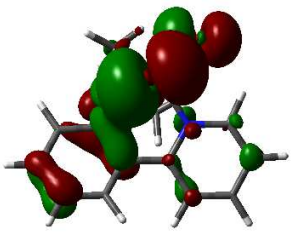
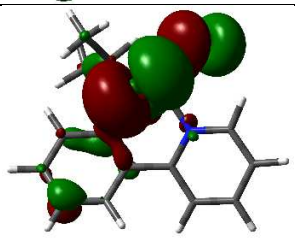
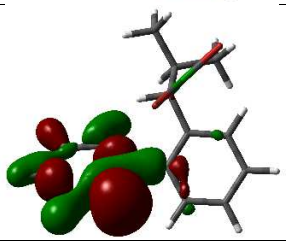
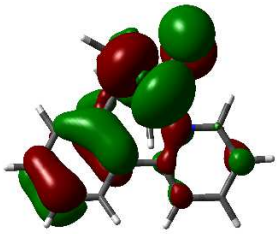
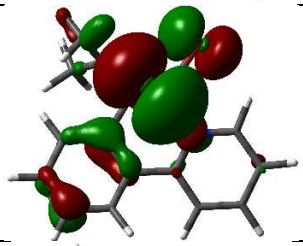
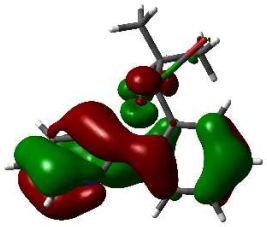
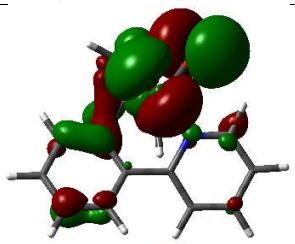
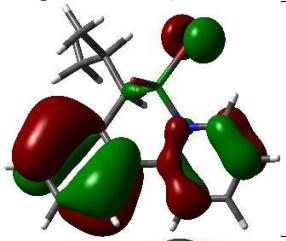
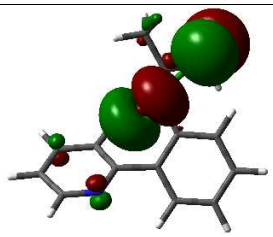
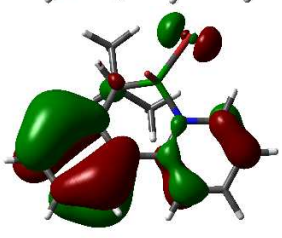
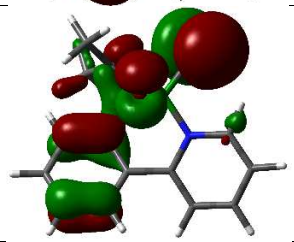
LUMO+1			
LUMO			
HOMO			
HOMO-1			
HOMO-2			
HOMO-3			
HOMO-4			

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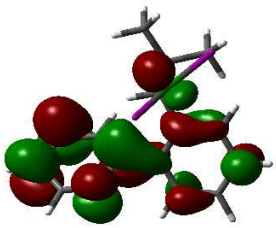
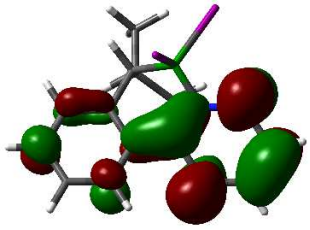
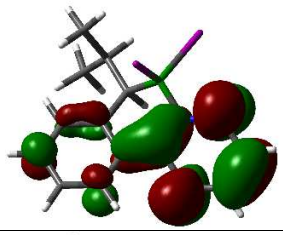
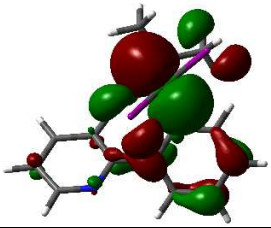
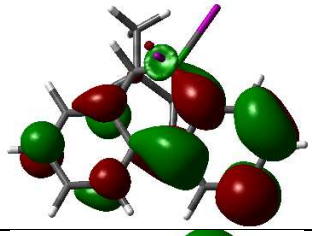
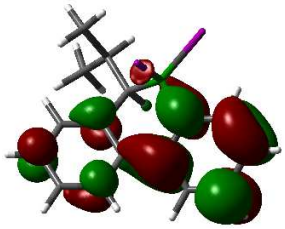
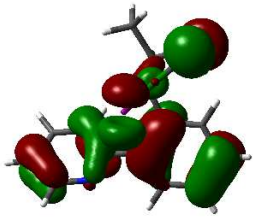
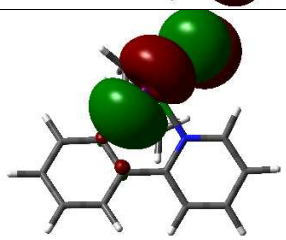
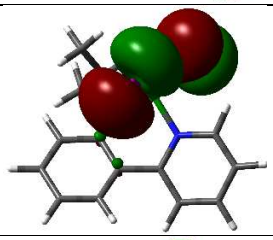
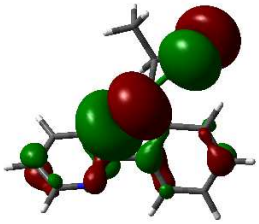
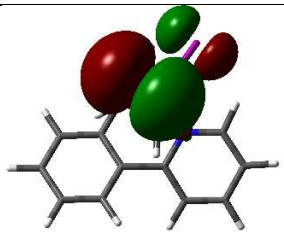
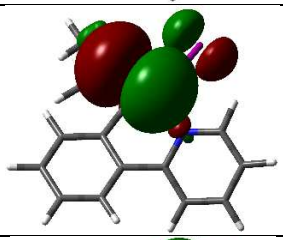
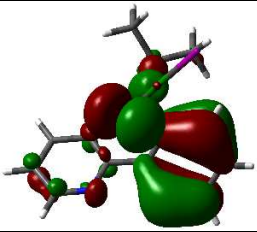
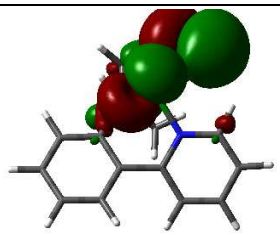
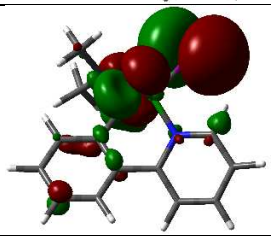
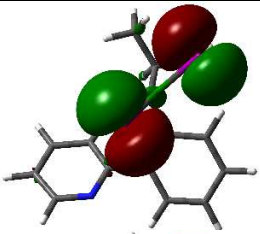
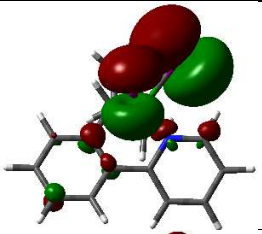
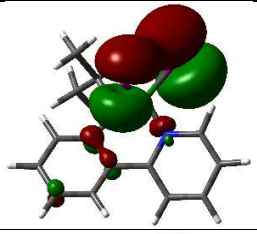
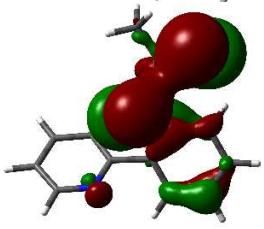
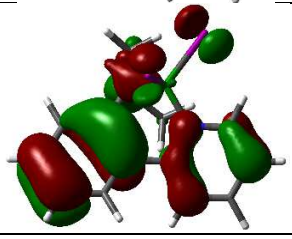
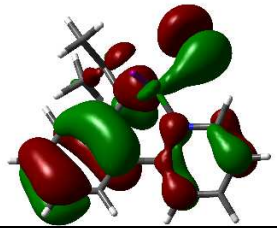
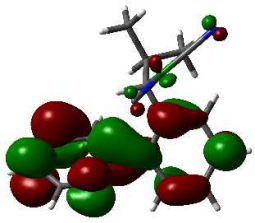
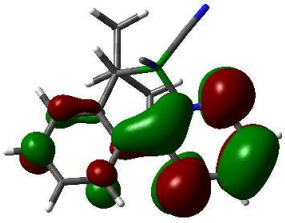
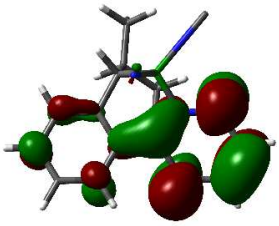
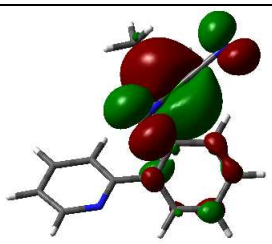
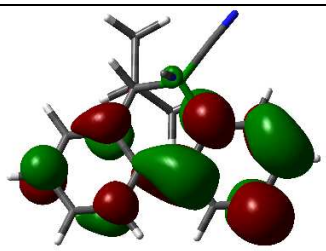
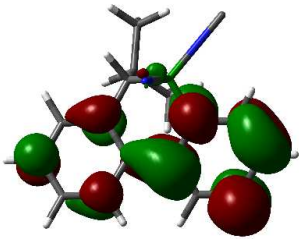
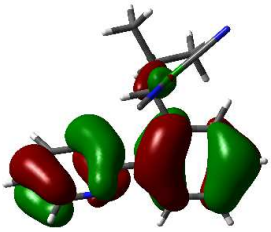
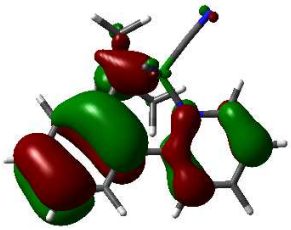
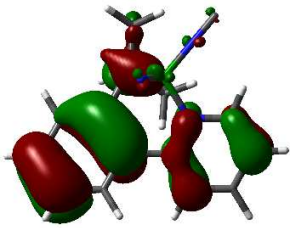
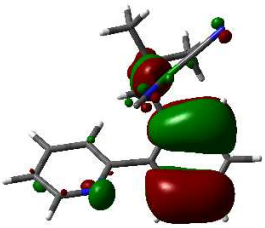
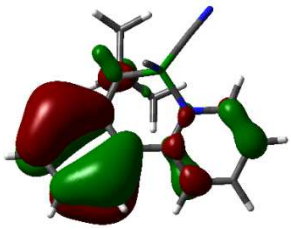
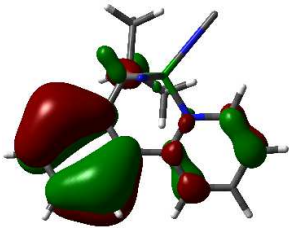
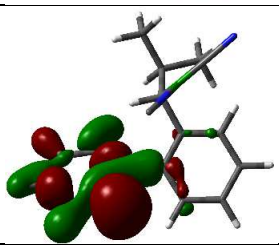
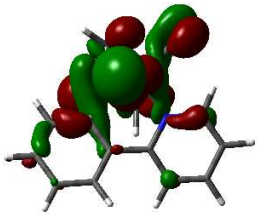
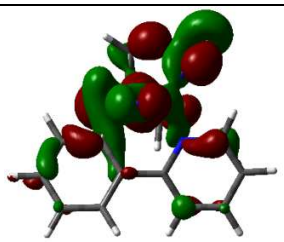
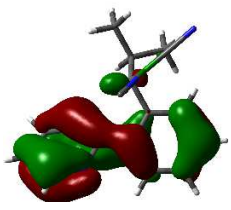
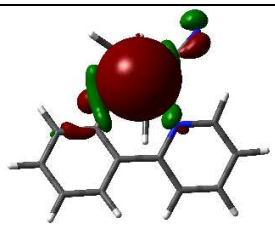
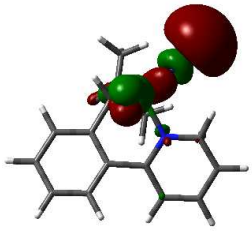
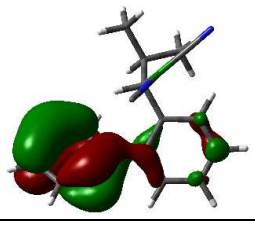
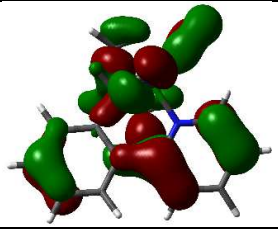
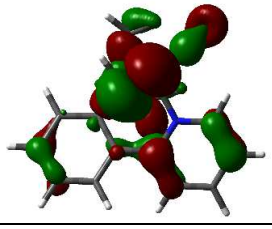
LUMO+1			
LUMO			
HOMO			
HOMO-1			
HOMO-2			
HOMO-3			
HOMO-4			

	B(CN)(NC), open	B(CN)(NC), B-NCax, iPrax	B(CN)(NC), B-NCeq, iPrax
LUMO+1			
LUMO			
HOMO			
HOMO-1			
HOMO-2			
HOMO-3			
HOMO-4			

2.1. TD-DFT calculations

2.1.1. Simulated UV/Vis spectra

Table S2. Calculated Frontier orbital levels and lowest excited states (ES1 and ES2) of the investigated ladder-boranes. Frontier orbital levels give in eV.

		Calculated[a]							
Borane	Conf.	HOMO–1	HOMO	LUMO	LUMO+1	$ES1$ [eV]	f	$ES2$ [eV]	f
BMe_2	**^{i}Pr$_{ax}$**	**-8.25**	**-7.66**	**-1.24**	**-0.72**	**4.15**	**0.0829**	**4.68**	**0.0361**
	^{i}Pr$_{eq}$	**-8.18**	**-7.38**	**-1.23**	**-0.69**	**3.84**	**0.0574**	**4.56**	**0.0284**
	open	**-8.08**	**-7.77**	**-0.42**	**-0.05**	**4.85**	**0.0046**	**5.00**	**0.1296**
BF_2	**^{i}Pr$_{ax}$**	**-8.43**	**-8.04**	**-1.46**	**-0.90**	**4.34**	**0.1905**	**4.72**	**0.0691**
	^{i}Pr$_{eq}$	**-8.38**	**-7.84**	**-1.46**	**-0.89**	**4.09**	**0.1250**	**4.66**	**0.0824**
	open	**-8.31**	**-7.98**	**-0.56**	**-0.13**	**4.82**	**0.0048**	**5.14**	**0.0821**
BBr_2	**^{i}Pr$_{ax}$**	**-8.64**	**-8.24**	**-1.85**	**-1.17**	**4.06**	**0.1006**	**4.37**	**0.0172**
	^{i}Pr$_{eq}$	**-8.18**	**-7.89**	**-1.79**	**-1.08**	**3.93**	**0.0926**	**4.36**	**0.0006**
	open	**-8.27**	**-7.98**	**-0.96**	**-0.35**	**4.68**	**0.0847**	**4.83**	**0.0057**
BI_2	**iPr$_{ax}$**	**-7.45**	**-7.00**	**-1.95**	**-1.19**	**3.17**	**0.0034**	**3.52**	**0.0036**
	iPr$_{eq}$	**-7.47**	**-7.13**	**-1.93**	**-1.17**	**3.33**	**0.0040**	**3.58**	**0.0083**
	open	**-8.07**	**-7.96**	**-1.22**	**-0.41**	**4.82**	**0.0048**	**5.14**	**0.0821**
B(CN)(NC) B-NCax	**iPr$_{ax}$**	**-8.76**	**-8.42**	**-1.95**	**-1.30**	**4.26**	**0.1939**	**4.64**	**0.0780**
	iPr$_{eq}$	**-8.72**	**-8.25**	**-1.95**	**-1.29**	**4.05**	**0.1266**	**4.59**	**0.1094**
B(CN)(NC) B-NCeq	**iPr$_{ax}$**	**-8.76**	**-8.41**	**-1.94**	**-1.30**	**4.25**	**0.1807**	**4.64**	**0.0738**
	iPr$_{eq}$	**-8.72**	**-8.24**	**-1.93**	**-1.28**	**4.05**	**0.1185**	**4.59**	**0.1007**
	open	**-8.61**	**-8.23**	**-2.22**	**-0.66**	**3.96**	**0.0737**	**4.35**	**0.0592**
$B(CN)_2$	**iPr$_{ax}$**	**-8.79**	**-8.45**	**-1.98**	**-1.34**	**4.25**	**0.1845**	**4.63**	**0.0749**
	iPr$_{eq}$	**-8.75**	**-8.28**	**-1.97**	**-1.33**	**4.05**	**0.1210**	**4.59**	**0.1007**
	open	**-8.75**	**-8.31**	**-2.47**	**-0.72**	**3.77**	**0.0927**	**4.17**	**0.0804**
Vinyl-boranes									
tBuBBN	**closed**	**-7.52**	**-7.18**	**-1.36**	**-0.70**	**3.69**	**0.0522**	**4.03**	**0.0377**
	open	**-8.07**	**-7.69**	**-0.55**	**-0.30**	**4.68**	**0.0537**	**4.73**	**0.0193**
$SiBMes_2$	**open**	**-7.44**	**-7.41**	**-0.92**	**-0.49**	**4.02**	**0.1287**	**4.20**	**0.1438**
SiBPF	**closed**	**-8.27**	**-7.92**	**-1.71**	**-1.14**	**4.12**	**0.0706**	**4.66**	**0.0354**
	open	**-8.25**	**-7.96**	**-2.34**	**-0.76**	**3.35**	**0.0319**	**4.02**	**0.0458**

[a] Geometry optimizations performed at the M06-2X / 6-31G(d,p) level of theory; electronic transition calculated by time-dependent DFT at the M06-2X / 6-311+G(d,p) level. [b] Shoulder band; maximum derived via Gaussian fit.

2.1.2. List of Computed optical transitions of Alkyl-boranes

BBr2, iPrax

	E		Osc. Strength f	Mayor Contribs	Minor Contribs
	eV	nm			
1	4.06	305	0.1006	HOMO->LUMO (86%)	H-2->LUMO (3%), H-1->LUMO (7%)
2	4.37	283	0.0172	H-1->LUMO (89%)	HOMO->LUMO (8%)
3	4.50	276	0.0570	H-2->LUMO (87%)	H-3->LUMO (2%), HOMO->LUMO (2%)
4	4.60	269	0.0706	H-4->LUMO (68%), HOMO->L+1 (11%)	H-3->LUMO (2%), H-2->L+1 (4%), H-1->L+1 (2%)
5	4.72	263	0.0426	H-3->LUMO (88%)	H-4->LUMO (3%)
6	4.95	250	0.0817	H-4->LUMO (12%), HOMO->L+1 (73%)	H-4->L+1 (5%), H-2->LUMO (2%)
7	5.15	241	0.0063	H-5->LUMO (70%), H-1->L+1 (18%)	H-2->L+1 (3%)
8	5.24	237	0.0613	H-5->LUMO (17%), H-4->L+1 (11%), H-2->L+1 (13%), H-1->L+1 (32%)	H-7->LUMO (3%), H-3->L+1 (4%), HOMO->L+1 (9%)
9	5.32	233	0.0036	H-2->L+1 (55%), H-1->L+1 (36%)	
10	5.47	226	0.0242	H-3->L+1 (61%), H-2->L+1 (10%)	H-7->LUMO (3%), H-4->LUMO (4%), H-1->L+1 (2%), HOMO->L+3 (5%)
11	5.52	225	0.0157	H-4->L+1 (52%), H-3->L+1 (19%)	H-6->LUMO (4%), H-5->LUMO (2%), H-4->LUMO (4%), H-3->LUMO (2%), H-2->L+1 (5%), H-1->L+1 (2%), HOMO->L+3 (2%)
12	5.85	212	0.0176	H-6->LUMO (50%), H-5->L+1 (17%), H-4->L+1 (16%)	H-9->LUMO (2%), H-7->LUMO (2%), H-3->L+1 (3%)
13	5.92	209	0.0655	H-7->LUMO (22%), H-5->L+1 (19%), HOMO->L+3 (17%)	H-11->LUMO (2%), H-6->LUMO (4%), H-4->L+1 (6%), H-3->L+1 (6%), H-2->L+1 (2%), H-2->L+3 (3%), H-1->L+3 (5%)
14	5.98	207	0.0146	H-7->LUMO (38%), H-6->LUMO (10%), H-5->L+1 (20%)	H-5->LUMO (2%), H-4->LUMO (2%), H-2->L+1 (3%), HOMO->L+3 (6%)
15	6.08	204	0.1346	H-6->LUMO (18%), H-5->L+1 (33%), HOMO->L+3 (20%)	H-9->LUMO (2%), H-7->LUMO (5%), HOMO->L+2 (5%)

BBr2, iPreq

1	3.93	316	0.0926	HOMO->LUMO (87%)	H-1->LUMO (7%)
2	4.36	284	0.0006	H-1->LUMO (89%)	HOMO->LUMO (8%)
3	4.53	274	0.0137	H-2->LUMO (87%)	HOMO->L+1 (7%)
4	4.57	271	0.1208	H-3->LUMO (72%), HOMO->L+1 (10%)	H-4->LUMO (2%)
5	4.87	255	0.1335	H-3->LUMO (16%), HOMO->L+1 (67%)	H-4->LUMO (5%), H-3->L+1 (2%), H-2->LUMO (6%)
6	5.00	248	0.0022	H-4->LUMO (73%)	H-3->L+1 (9%), HOMO->L+1 (4%)
7	5.16	240	0.0020	H-5->LUMO (54%), H-1->L+1 (39%)	
8	5.25	236	0.0305	H-5->LUMO (29%), H-1->L+1 (47%)	H-4->LUMO (4%), H-3->L+1 (4%), HOMO->L+1 (4%)
9	5.31	234	0.0131	H-3->L+1 (14%), H-2->L+1 (62%)	H-7->LUMO (2%), H-5->LUMO (6%), H-1->L+1 (6%)
10	5.47	227	0.0124	H-3->L+1 (37%), H-2->L+1 (28%)	H-7->LUMO (2%), H-5->LUMO (4%), H-4->LUMO (9%), H-4->L+1 (2%), H-3->LUMO (3%), HOMO->L+4 (5%)
11	5.66	219	0.0462	H-4->L+1 (44%), H-3->L+1 (21%), HOMO->L+4 (10%)	H-9->LUMO (3%), H-7->LUMO (4%), H-3->L+4 (3%)
12	5.91	210	0.0273	H-7->LUMO (41%), H-6->LUMO (16%), H-5->L+1 (17%)	H-10->LUMO (2%), H-3->L+1 (2%), HOMO->L+4 (4%)
13	5.92	209	0.0016	H-6->LUMO (52%), H-5->L+1 (28%)	H-11->LUMO (2%), H-4->L+1 (3%)
14	5.96	208	0.1002	H-4->L+1 (42%), HOMO->L+4 (28%)	H-9->LUMO (2%), H-7->LUMO (4%), H-5->L+1 (3%), H-3->L+1 (4%), H-1->L+4 (3%)
15	6.05	205	0.0444	H-8->LUMO (51%)	H-13->LUMO (3%), H-9->LUMO (7%), H-7->LUMO (3%), H-5->L+1 (7%), HOMO->L+2 (4%), HOMO->L+4 (6%)

BBr2, open

	E eV	nm	Osc. Strength f	Mayor Contribs	Minor Contribs
1	4.68	265	0.0847	H-1->LUMO (33%), HOMO->LUMO (49%)	H-5->LUMO (7%)
2	4.83	256	0.0057	H-2->L+1 (62%), H-2->L+2 (12%)	H-2->LUMO (7%), H-2->L+3 (3%), H-1->L+1 (4%)
3	5.02	247	0.0675	H-1->LUMO (38%), HOMO->LUMO (29%)	H-2->L+1 (2%), H-1->L+1 (4%), H-1->L+12 (3%), HOMO->L+2 (2%), HOMO->L+5 (8%), HOMO->L+6 (2%)
4	5.20	239	0.0078	H-4->LUMO (72%)	H-5->LUMO (7%), H-4->L+1 (7%), H-3->LUMO (2%)
5	5.25	236	0.1715	H-5->LUMO (12%), HOMO->L+1 (58%)	H-3->L+1 (5%), H-2->LUMO (2%), HOMO->L+5 (2%)
6	5.34	232	0.0094	H-2->LUMO (15%), H-2->L+2 (44%)	H-5->LUMO (6%), H-2->L+1 (6%), H-2->L+3 (4%), H-2->L+5 (3%), H-2->L+12 (3%), HOMO->L+1 (2%), HOMO->L+2 (4%)
7	5.39	230	0.0075	H-5->LUMO (19%), HOMO->LUMO (12%), HOMO->L+2 (21%)	H-5->L+1 (3%), H-4->LUMO (5%), H-3->LUMO (4%), H-3->L+1 (3%), H-2->LUMO (2%), H-2->L+2 (5%), H-1->L+1 (7%), HOMO->L+1 (4%), HOMO->L+3 (2%)
8	5.70	218	0.1613	H-5->LUMO (23%), HOMO->L+1 (17%), HOMO->L+2 (26%)	H-4->LUMO (3%), H-3->LUMO (2%), H-3->L+1 (3%), H-1->LUMO (8%), H-1->L+1 (3%)
9	5.82	213	0.0364	H-1->LUMO (11%), H-1->L+1 (27%), HOMO->L+5 (16%)	H-3->L+1 (3%), H-1->L+2 (6%), HOMO->LUMO (4%), HOMO->L+1 (6%), HOMO->L+2 (7%), HOMO->L+4 (2%), HOMO->L+6 (4%)
10	6.08	204	0.0515	H-7->LUMO (20%), H-6->LUMO (26%), H-3->LUMO (23%)	H-7->L+1 (3%), H-5->LUMO (3%), H-1->L+1 (7%), H-1->L+5 (3%)
11	6.16	201	0.0896	H-7->LUMO (15%), H-6->LUMO (16%), H-1->L+5 (17%)	H-6->L+1 (2%), H-3->LUMO (7%), H-3->L+1 (5%), H-1->L+1 (5%), H-1->L+2 (4%), H-1->L+6 (4%), HOMO->L+2 (8%)
12	6.21	200	0.1609	H-1->L+1 (33%), HOMO->L+5 (26%)	H-3->LUMO (9%), H-1->LUMO (3%), H-1->L+5 (3%), HOMO->L+4 (3%), HOMO->L+6 (8%)
13	6.28	197	0.0306	HOMO->L+2 (10%), HOMO->L+3 (54%)	H-3->L+1 (3%), H-3->L+3 (2%), H-1->L+5 (5%), H-1->L+6 (2%), HOMO->L+1 (2%), HOMO->L+7 (3%)
14	6.36	195	0.1451	H-3->LUMO (27%), H-1->L+2 (14%), H-1->L+5 (13%)	H-9->LUMO (5%), H-7->LUMO (2%), H-6->LUMO (4%), H-5->LUMO (2%), H-1->L+3 (3%), H-1->L+6 (3%), HOMO->L+3 (7%), HOMO->L+12 (5%)
15	6.45	192	0.0153	H-3->L+1 (12%), H-1->L+2 (22%), HOMO->L+3 (10%)	H-3->L+2 (4%), H-1->L+4 (4%), H-1->L+5 (8%), HOMO->L+1 (2%), HOMO->L+2 (7%), HOMO->L+4 (5%), HOMO->L+5 (2%), HOMO->L+6 (2%)

BI2, iPrax

	E eV	nm	Osc. Strength f	Mayor Contribs	Minor Contribs
1	3.17	392	0.0034	HOMO->LUMO (97%)	
2	3.52	352	0.0036	H-1->LUMO (96%)	
3	3.84	323	0.0090	H-2->LUMO (91%)	H-4->LUMO (4%)
4	4.04	307	0.0208	H-3->LUMO (15%), HOMO->L+1 (79%)	H-4->LUMO (3%)
5	4.14	299	0.0109	H-3->LUMO (80%), HOMO->L+1 (14%)	
6	4.23	293	0.1467	H-4->LUMO (83%)	H-2->LUMO (4%), HOMO->L+1 (4%)
7	4.43	280	0.0016	H-1->L+1 (92%)	H-5->LUMO (3%)
8	4.58	271	0.0525	H-5->LUMO (63%), H-2->L+1 (10%)	H-4->L+1 (7%), H-4->L+3 (3%), H-1->L+1 (5%)
9	4.69	264	0.0219	H-5->LUMO (10%), H-2->L+1 (75%)	H-6->LUMO (7%)
10	4.83	257	0.0314	H-6->LUMO (69%), H-3->L+1 (14%)	H-4->L+1 (3%), H-2->L+1 (8%)
11	5.00	248	0.0253	H-6->LUMO (10%), H-3->L+1 (71%)	H-5->LUMO (3%), H-4->L+1 (6%)
12	5.11	242	0.0360	H-4->L+1 (16%), HOMO->L+3 (28%), HOMO->L+7 (18%), HOMO->L+10 (11%)	H-5->LUMO (3%), HOMO->L+9 (3%), HOMO->L+13 (3%)
13	5.15	241	0.1604	H-4->L+1 (46%), HOMO->L+3 (11%)	H-7->LUMO (3%), H-6->LUMO (9%), H-5->L+1 (8%), H-3->L+1 (4%), HOMO->L+7 (4%)
14	5.33	232	0.0458	HOMO->L+3 (32%), HOMO->L+7 (10%), HOMO->L+10 (10%)	H-7->LUMO (3%), H-5->LUMO (3%), H-5->L+1 (3%), H-3->L+1 (2%), HOMO->L+2 (4%), HOMO->L+5 (7%), HOMO->L+6 (3%), HOMO->L+13 (2%)
15	5.44	228	0.0322	H-7->LUMO (20%), H-5->L+1 (22%), HOMO->L+2 (15%)	H-6->L+1 (4%), H-5->LUMO (3%), H-4->L+1 (6%), H-4->L+3 (5%), HOMO->L+3 (4%), HOMO->L+5 (3%)

BI2, iPreq

	E		Osc. Strength f	Mayor Contribs	Minor Contribs
1	3.33	373	0.0040	HOMO->LUMO (97%)	
2	3.58	346	0.0083	H-1->LUMO (95%)	H-2->LUMO (3%)
3	3.86	322	0.0261	H-4->LUMO (17%), H-2->LUMO (76%)	H-1->LUMO (3%)
4	4.13	300	0.0240	H-3->LUMO (56%), HOMO->L+1 (37%)	H-4->LUMO (3%)
5	4.16	298	0.0564	H-4->LUMO (56%), H-3->LUMO (18%), H-2->LUMO (12%)	HOMO->L+1 (6%)
6	4.25	292	0.0270	H-4->LUMO (16%), H-3->LUMO (22%), HOMO->L+1 (54%)	H-2->LUMO (3%)
7	4.47	277	0.0070	H-1->L+1 (88%)	H-5->LUMO (7%)
8	4.54	273	0.0727	H-5->LUMO (60%), H-2->L+1 (14%)	H-4->L+1 (5%), H-4->L+3 (2%), H-1->L+1 (9%)
9	4.77	260	0.0383	H-5->LUMO (18%), H-2->L+1 (63%)	H-6->LUMO (8%), H-5->L+1 (3%), H-4->L+1 (3%)
10	4.91	253	0.0162	H-6->LUMO (56%), H-3->L+1 (16%), H-2->L+1 (13%)	H-4->L+1 (8%)
11	5.03	247	0.0205	H-4->L+1 (21%), H-3->L+1 (64%)	H-6->LUMO (2%), H-2->L+1 (4%)
12	5.15	241	0.1223	H-6->LUMO (20%), H-4->L+1 (37%), HOMO->L+3 (13%)	H-3->L+1 (7%), HOMO->L+7 (5%), HOMO->L+11 (2%)
13	5.18	239	0.1221	H-4->L+1 (12%), HOMO->L+3 (37%)	H-6->LUMO (8%), H-5->L+1 (2%), H-3->L+1 (5%), HOMO->L+7 (9%), HOMO->L+9 (3%), HOMO->L+10 (3%), HOMO->L+11 (5%)
14	5.34	232	0.0202	H-5->L+1 (47%)	H-9->LUMO (3%), H-8->LUMO (5%), H-7->LUMO (6%), H-5->LUMO (4%), H-4->L+1 (3%), H-4->L+3 (7%), H-1->L+3 (2%)
15	5.44	228	0.0024	H-1->L+3 (46%), H-1->L+7 (15%), H-1->L+11 (12%)	H-5->L+1 (3%), H-1->L+9 (5%), H-1->L+13 (3%)

BI2, open

	E		Osc. Strength f	Mayor Contribs	Minor Contribs
	eV	nm			
1	4.82	257	0.0048	H-2->LUMO (52%), H-2->L+1 (28%)	H-2->L+2 (4%), H-1->LUMO (5%)
2	5.14	241	0.0821	H-1->LUMO (35%), HOMO->LUMO (25%), HOMO->L+3 (19%)	H-3->L+3 (2%), H-1->L+1 (2%), H-1->L+8 (3%)
3	5.16	240	0.2684	H-1->LUMO (15%), HOMO->LUMO (57%)	H-2->L+1 (2%), HOMO->L+1 (7%), HOMO->L+3 (4%)
4	5.36	232	0.0044	H-2->LUMO (28%), H-2->L+1 (33%)	H-2->L+2 (8%), H-2->L+8 (5%), H-2->L+9 (2%), H-1->L+1 (2%), HOMO->L+1 (9%)
5	5.48	226	0.0406	H-3->LUMO (10%), HOMO->LUMO (11%), HOMO->L+1 (43%)	H-4->LUMO (3%), H-2->LUMO (3%), H-2->L+1 (7%), HOMO->L+2 (5%), HOMO->L+3 (4%)
6	6.13	202	0.3726	H-1->LUMO (29%), HOMO->L+3 (40%)	H-1->L+3 (9%), HOMO->L+1 (5%), HOMO->L+4 (2%)
7	6.24	199	0.0614	H-3->LUMO (23%), H-1->L+3 (25%), HOMO->L+1 (11%)	H-1->LUMO (7%), HOMO->L+2 (4%), HOMO->L+3 (8%), HOMO->L+5 (4%), HOMO->L+8 (3%)
8	6.29	197	0.0659	H-1->L+3 (21%), HOMO->L+1 (12%), HOMO->L+2 (42%)	H-3->L+2 (3%), HOMO->L+8 (4%), HOMO->L+10 (3%)
9	6.38	194	0.0096	H-3->LUMO (19%), H-1->L+1 (16%), HOMO->L+2 (17%)	H-3->L+1 (3%), H-1->LUMO (3%), H-1->L+3 (4%), HOMO->L+1 (4%), HOMO->L+4 (4%), HOMO->L+5 (9%), HOMO->L+7 (2%), HOMO->L+8 (4%), HOMO->L+9 (2%)
10	6.47	192	0.0308	H-3->LUMO (15%), H-1->L+1 (63%)	H-2->L+1 (2%), H-1->L+4 (3%), HOMO->L+4 (3%)
11	6.53	190	0.0888	HOMO->L+2 (11%), HOMO->L+4 (43%)	H-4->L+1 (3%), H-3->LUMO (2%), H-1->L+2 (2%), H-1->L+3 (8%), H-1->L+5 (3%), HOMO->L+5 (6%)
12	6.62	187	0.0136	H-1->L+2 (13%), H-1->L+4 (48%), H-1->L+5 (14%)	H-1->L+7 (3%), HOMO->L+4 (4%), HOMO->L+5 (2%)
13	6.70	185	0.2775	H-3->L+1 (24%), H-1->L+3 (15%), HOMO->L+8 (15%)	H-4->LUMO (8%), H-4->L+1 (6%), HOMO->L+4 (7%), HOMO->L+5 (4%), HOMO->L+6 (2%)
14	6.71	185	0.0223	H-4->LUMO (17%), H-3->L+1 (14%), HOMO->L+4 (18%), HOMO->L+8 (15%)	H-3->LUMO (2%), H-3->L+2 (5%), HOMO->L+1 (3%), HOMO->L+2 (3%), HOMO->L+3 (3%), HOMO->L+5 (3%)
15	6.82	182	0.0199	H-1->L+2 (24%), HOMO->L+5 (18%), HOMO->L+6 (14%)	H-1->L+5 (3%), H-1->L+8 (7%), H-1->L+9 (4%), HOMO->L+8 (3%)

BF2, iPrax

	E eV	nm	Osc. Strength f	Mayor Contribs	Minor Contribs
1	4.34	286	0.1905	HOMO->LUMO (93%)	
2	4.72	263	0.0691	H-1->LUMO (63%), HOMO->L+1 (22%)	HOMO->L+4 (5%)
3	5.02	247	0.0229	H-2->LUMO (81%)	H-1->L+1 (3%), HOMO->L+1 (3%)
4	5.11	243	0.2148	H-1->LUMO (18%), H-1->L+1 (12%), HOMO->L+1 (57%)	H-2->LUMO (7%)
5	5.58	222	0.0332	H-1->L+1 (59%), HOMO->L+1 (10%)	H-3->LUMO (3%), H-1->LUMO (9%), HOMO->L+4 (7%)
6	5.80	214	0.0107	H-2->L+1 (80%)	HOMO->L+4 (6%)
7	6.02	206	0.1071	H-1->L+1 (21%), HOMO->L+4 (38%)	H-6->L+1 (2%), H-4->LUMO (7%), H-3->LUMO (6%), H-2->L+1 (6%), H-1->L+4 (3%)
8	6.21	200	0.0291	H-4->LUMO (11%), H-3->LUMO (21%), HOMO->L+2 (34%)	H-6->L+1 (3%), H-1->LUMO (2%), HOMO->L+3 (4%), HOMO->L+4 (8%)
9	6.26	198	0.0271	H-3->LUMO (21%), HOMO->L+2 (37%), HOMO->L+3 (10%)	H-6->L+1 (2%), H-4->LUMO (3%), H-1->LUMO (2%), H-1->L+4 (7%)
10	6.29	197	0.0039	H-6->LUMO (15%), H-4->LUMO (41%), H-3->LUMO (12%)	H-10->LUMO (4%), H-9->LUMO (2%), H-8->LUMO (7%), H-4->L+1 (3%), H-1->L+4 (3%)
11	6.33	196	0.1833	H-1->L+4 (45%), HOMO->L+4 (16%), HOMO->L+9 (11%)	H-4->LUMO (4%), H-3->L+1 (3%), HOMO->L+8 (3%)
12	6.49	191	0.0057	H-1->L+2 (44%), H-1->L+3 (19%), HOMO->L+3 (19%)	HOMO->L+5 (6%)
13	6.62	187	0.0858	H-6->LUMO (35%)	H-10->LUMO (4%), H-6->L+1 (2%), H-5->LUMO (2%), H-4->LUMO (8%), H-3->LUMO (9%), H-3->L+1 (8%), H-2->L+4 (8%)
14	6.68	186	0.0044	H-1->L+3 (20%), HOMO->L+2 (12%), HOMO->L+3 (36%)	H-2->L+4 (4%), H-1->L+2 (8%), HOMO->L+4 (2%), HOMO->L+5 (8%)
15	6.69	185	0.0181	H-2->L+4 (59%)	H-6->LUMO (7%), H-4->L+1 (4%), H-3->L+1 (2%), H-1->L+4 (3%)

BF2, iPreq

	E eV	nm	Osc. Strength f	Mayor Contribs	Minor Contribs
1	4.09	303	0.1250	HOMO->LUMO (94%)	
2	4.66	266	0.0824	H-1->LUMO (57%), HOMO->L+1 (31%)	HOMO->L+4 (2%)
3	4.97	250	0.2540	H-1->LUMO (31%), HOMO->L+1 (57%)	H-1->L+1 (7%)
4	5.19	239	0.0489	H-2->LUMO (66%), H-1->L+1 (12%)	HOMO->L+4 (4%)
5	5.51	225	0.0040	H-2->LUMO (16%), H-1->L+1 (63%)	H-4->LUMO (2%), H-1->LUMO (2%), HOMO->L+1 (6%)
6	5.87	211	0.0968	H-2->L+1 (24%), HOMO->L+4 (28%), HOMO->L+5 (10%)	H-4->LUMO (3%), H-2->LUMO (5%), H-1->LUMO (4%), H-1->L+1 (4%), H-1->L+4 (2%)
7	6.06	205	0.0027	H-3->LUMO (12%), HOMO->L+2 (56%), HOMO->L+3 (10%)	H-1->L+2 (2%), HOMO->L+5 (4%)
8	6.07	204	0.0014	H-3->LUMO (54%), HOMO->L+2 (14%)	H-9->LUMO (3%), H-8->LUMO (2%), H-4->LUMO (5%), HOMO->L+3 (2%), HOMO->L+5 (2%)
9	6.13	202	0.0662	H-2->L+1 (47%), HOMO->L+4 (14%)	H-6->L+1 (2%), H-5->LUMO (2%), H-4->LUMO (4%), H-3->LUMO (6%), H-1->L+1 (7%), HOMO->L+5 (4%)
10	6.20	200	0.0636	H-5->LUMO (15%), H-4->LUMO (27%), HOMO->L+4 (17%)	H-6->LUMO (3%), H-6->L+1 (6%), H-4->L+1 (4%), H-3->LUMO (3%), H-2->L+1 (2%), H-1->LUMO (2%), H-1->L+1 (2%), H-1->L+4 (3%), HOMO->L+9 (2%)
11	6.24	199	0.0678	H-1->L+4 (25%), HOMO->L+8 (14%), HOMO->L+9 (10%)	H-5->LUMO (4%), H-4->LUMO (4%), H-2->L+1 (8%), H-1->L+5 (9%), HOMO->L+1 (2%), HOMO->L+4 (4%), HOMO->L+6 (4%)
12	6.42	193	0.0088	H-1->L+2 (34%), HOMO->L+3 (33%)	H-1->L+3 (7%), HOMO->L+2 (4%), HOMO->L+5 (7%), HOMO->L+6 (5%)
13	6.55	189	0.0175	H-1->L+2 (15%), HOMO->L+3 (24%), HOMO->L+6 (15%)	H-6->LUMO (4%), H-1->L+3 (8%), H-1->L+4 (3%), H-1->L+5 (4%), HOMO->L+4 (4%), HOMO->L+5 (7%)
14	6.60	188	0.0093	H-6->LUMO (13%), H-1->L+2 (12%), H-1->L+3 (10%), HOMO->L+5 (16%)	H-4->LUMO (4%), H-4->L+1 (3%), H-1->L+4 (4%), HOMO->L+2 (9%), HOMO->L+3 (5%), HOMO->L+4 (7%), HOMO->L+8 (3%)
15	6.64	187	0.0709	H-6->LUMO (23%), HOMO->L+5 (16%)	H-10->LUMO (2%), H-6->L+1 (2%), H-5->LUMO (5%), H-5->L+1 (4%), H-4->LUMO (8%), H-4->L+1 (8%), H-1->L+4 (2%), HOMO->L+2 (2%), HOMO->L+4 (4%)

BF2, open

	E eV	nm	Osc. Strength f	Mayor Contribs	Minor Contribs
1	4.82	257	0.0048	H-2->LUMO (52%), H-2->L+1 (28%)	H-2->L+2 (4%), H-1->LUMO (5%)
2	5.14	241	0.0821	H-1->LUMO (35%), HOMO->LUMO (25%), HOMO->L+3 (19%)	H-3->L+3 (2%), H-1->L+1 (2%), H-1->L+8 (3%)
3	5.16	240	0.2684	H-1->LUMO (15%), HOMO->LUMO (57%)	H-2->L+1 (2%), HOMO->L+1 (7%), HOMO->L+3 (4%)
4	5.36	232	0.0044	H-2->LUMO (28%), H-2->L+1 (33%)	H-2->L+2 (8%), H-2->L+8 (5%), H-2->L+9 (2%), H-1->L+1 (2%), HOMO->L+1 (9%)
5	5.48	226	0.0406	H-3->LUMO (10%), HOMO->LUMO (11%), HOMO->L+1 (43%)	H-4->LUMO (3%), H-2->LUMO (3%), H-2->L+1 (7%), HOMO->L+2 (5%), HOMO->L+3 (4%)
6	6.13	202	0.3726	H-1->LUMO (29%), HOMO->L+3 (40%)	H-1->L+3 (9%), HOMO->L+1 (5%), HOMO->L+4 (2%)
7	6.24	199	0.0614	H-3->LUMO (23%), H-1->L+3 (25%), HOMO->L+1 (11%)	H-1->LUMO (7%), HOMO->L+2 (4%), HOMO->L+3 (8%), HOMO->L+5 (4%), HOMO->L+8 (3%)
8	6.29	197	0.0659	H-1->L+3 (21%), HOMO->L+1 (12%), HOMO->L+2 (42%)	H-3->L+2 (3%), HOMO->L+8 (4%), HOMO->L+10 (3%)
9	6.38	194	0.0096	H-3->LUMO (19%), H-1->L+1 (16%), HOMO->L+2 (17%)	H-3->L+1 (3%), H-1->LUMO (3%), H-1->L+3 (4%), HOMO->L+1 (4%), HOMO->L+4 (4%), HOMO->L+5 (9%), HOMO->L+7 (2%), HOMO->L+8 (4%), HOMO->L+9 (2%)
10	6.47	192	0.0308	H-3->LUMO (15%), H-1->L+1 (63%)	H-2->L+1 (2%), H-1->L+4 (3%), HOMO->L+4 (3%)
11	6.53	190	0.0888	HOMO->L+2 (11%), HOMO->L+4 (43%)	H-4->L+1 (3%), H-3->LUMO (2%), H-1->L+2 (2%), H-1->L+3 (8%), H-1->L+5 (3%), HOMO->L+5 (6%)
12	6.62	187	0.0136	H-1->L+2 (13%), H-1->L+4 (48%), H-1->L+5 (14%)	H-1->L+7 (3%), HOMO->L+4 (4%), HOMO->L+5 (2%)
13	6.70	185	0.2775	H-3->L+1 (24%), H-1->L+3 (15%), HOMO->L+8 (15%)	H-4->LUMO (8%), H-4->L+1 (6%), HOMO->L+4 (7%), HOMO->L+5 (4%), HOMO->L+6 (2%)
14	6.71	185	0.0223	H-4->LUMO (17%), H-3->L+1 (14%), HOMO->L+4 (18%), HOMO->L+8 (15%)	H-3->LUMO (2%), H-3->L+2 (5%), HOMO->L+1 (3%), HOMO->L+2 (3%), HOMO->L+3 (3%), HOMO->L+5 (3%)
15	6.82	182	0.0199	H-1->L+2 (24%), HOMO->L+5 (18%), HOMO->L+6 (14%)	H-1->L+5 (3%), H-1->L+8 (7%), H-1->L+9 (4%), HOMO->L+8 (3%)

BMe2, open

	E eV	nm	Osc. Strength f	Mayor Contribs	Minor Contribs
1	4.85	256	0.0046	H-2->LUMO (44%), H-2->L+1 (32%)	H-2->L+2 (9%), H-1->LUMO (4%)
2	5.00	248	0.1296	H-1->LUMO (15%), HOMO->LUMO (58%)	H-1->L+4 (4%), HOMO->L+7 (6%)
3	5.16	240	0.1970	H-1->LUMO (37%), HOMO->LUMO (26%)	H-2->L+1 (2%), HOMO->L+1 (7%), HOMO->L+2 (4%), HOMO->L+4 (4%), HOMO->L+6 (2%), HOMO->L+7 (4%)
4	5.34	232	0.0058	H-2->LUMO (18%), H-2->L+1 (11%), HOMO->L+1 (23%)	H-3->L+1 (3%), H-2->L+2 (6%), H-2->L+7 (4%), H-1->L+1 (4%), H-1->L+2 (2%), HOMO->L+2 (5%), HOMO->L+4 (3%)
5	5.41	229	0.0040	H-2->LUMO (16%), H-2->L+1 (14%), HOMO->L+1 (18%)	H-3->LUMO (3%), H-2->L+2 (8%), H-2->L+4 (2%), H-2->L+7 (5%), HOMO->L+2 (3%), HOMO->L+4 (6%)
6	5.68	218	0.1442	HOMO->L+4 (24%)	H-4->LUMO (7%), H-4->L+1 (2%), H-4->L+4 (4%), H-4->L+7 (4%), H-3->LUMO (3%), H-1->LUMO (4%), H-1->L+1 (5%), H-1->L+7 (2%), HOMO->LUMO (5%), HOMO->L+2 (2%), HOMO->L+5 (3%), HOMO->L+6 (4%), HOMO->L+7 (5%), HOMO->L+15 (2%)
7	6.06	205	0.1804	H-1->LUMO (22%), HOMO->L+7 (10%)	H-3->LUMO (8%), H-1->L+1 (5%), H-1->L+2 (5%), H-1->L+7 (9%), HOMO->L+1 (7%), HOMO->L+2 (7%), HOMO->L+3 (2%), HOMO->L+4 (7%), HOMO->L+6 (4%)
8	6.11	203	0.0061	H-5->LUMO (17%), H-5->L+4 (13%), H-5->L+7 (12%)	H-6->LUMO (4%), H-6->L+4 (4%), H-6->L+7 (3%), H-5->L+1 (5%), H-5->L+5 (3%), H-5->L+15 (6%), H-3->LUMO (5%)
9	6.15	202	0.0096	HOMO->L+1 (28%), HOMO->L+2 (35%)	H-3->LUMO (5%), HOMO->L+3 (2%), HOMO->L+4 (3%), HOMO->L+5 (5%), HOMO->L+6 (4%), HOMO->L+8 (2%)
10	6.20	200	0.0643	H-1->L+4 (21%), H-1->L+7 (11%), HOMO->L+7 (16%)	H-3->LUMO (4%), H-1->LUMO (8%), H-1->L+2 (2%), H-1->L+3 (7%), H-1->L+6 (8%), HOMO->L+2 (5%), HOMO->L+15 (3%)
11	6.30	197	0.0350	H-1->L+1 (35%), HOMO->L+3 (17%)	H-4->LUMO (2%), H-3->L+1 (4%), H-1->L+5 (3%), H-1->L+6 (3%), H-1->L+7 (3%), HOMO->L+1 (3%), HOMO->L+2 (8%), HOMO->L+7 (2%)
12	6.33	196	0.0015	H-3->LUMO (14%), H-1->L+1 (12%), HOMO->L+4 (18%)	H-6->LUMO (3%), H-4->LUMO (8%), H-3->L+1 (3%), H-1->L+4 (2%), H-1->L+7 (4%), HOMO->L+1 (3%), HOMO->L+2 (2%), HOMO->L+3 (3%), HOMO->L+5 (4%)
13	6.40	194	0.0521	H-1->L+1 (11%), H-1->L+2 (18%), HOMO->L+3 (26%), HOMO->L+7 (14%)	H-3->LUMO (6%), H-1->L+4 (4%), HOMO->L+4 (7%)
14	6.43	193	0.1238	H-3->LUMO (12%), H-1->L+4 (33%), HOMO->L+7 (12%)	H-6->L+1 (3%), H-4->LUMO (2%), H-1->L+1 (6%), HOMO->L+2 (7%), HOMO->L+4 (3%), HOMO->L+5 (3%)
15	6.48	191	0.0253	H-1->L+2 (25%), HOMO->L+3 (17%)	H-4->LUMO (3%), H-3->LUMO (4%), H-3->L+1 (2%), H-1->L+3 (8%), H-1->L+4 (6%), H-1->L+5 (3%), H-1->L+6 (7%), HOMO->L+6 (4%), HOMO->L+7 (3%)

BMe2, iPreq

	E eV	nm	Osc. Strength f	Mayor Contribs	Minor Contribs
1	3.84	323	0.0574	HOMO->LUMO (96%)	
2	4.56	272	0.0284	H-1->LUMO (19%), HOMO->L+1 (70%)	
3	4.85	255	0.2015	H-1->LUMO (66%), HOMO->L+1 (18%)	H-2->LUMO (5%), H-1->L+1 (3%), HOMO->L+5 (2%)
4	5.10	243	0.1286	H-2->LUMO (87%)	HOMO->L+1 (6%)
5	5.19	239	0.0568	H-3->LUMO (49%), H-1->L+1 (17%)	H-6->LUMO (3%), HOMO->L+5 (6%), HOMO->L+6 (5%)
6	5.50	225	0.0739	H-3->LUMO (22%), H-1->L+1 (58%)	H-3->L+1 (3%), H-2->L+1 (5%)
7	5.68	218	0.0002	H-4->LUMO (41%), H-2->L+1 (21%)	H-7->LUMO (2%), H-6->LUMO (3%), H-5->LUMO (6%), H-1->L+1 (6%), HOMO->L+2 (4%)
8	5.71	217	0.0098	HOMO->L+2 (68%), HOMO->L+4 (12%)	H-4->LUMO (3%), HOMO->L+3 (5%)
9	5.74	216	0.0173	H-4->LUMO (18%), H-2->L+1 (64%)	H-5->LUMO (6%), H-1->L+1 (3%)
10	5.76	215	0.1785	H-3->LUMO (18%), HOMO->L+5 (37%), HOMO->L+6 (18%)	H-3->L+1 (3%), H-1->LUMO (5%), HOMO->L+7 (3%), HOMO->L+9 (3%)
11	6.00	207	0.0554	HOMO->L+3 (18%), HOMO->L+5 (15%), HOMO->L+10 (23%)	H-3->L+1 (5%), H-1->L+5 (7%), H-1->L+6 (4%), HOMO->L+4 (3%), HOMO->L+6 (2%), HOMO->L+8 (3%), HOMO->L+9 (6%)
12	6.11	203	0.0435	H-3->L+1 (19%), HOMO->L+3 (44%), HOMO->L+6 (11%)	H-6->LUMO (2%), HOMO->L+2 (5%), HOMO->L+4 (4%), HOMO->L+10 (3%)
13	6.15	202	0.0051	H-3->L+1 (38%), HOMO->L+4 (26%)	H-6->LUMO (6%), H-1->L+2 (3%), HOMO->L+2 (8%), HOMO->L+3 (3%), HOMO->L+7 (2%), HOMO->L+8 (3%)
14	6.21	200	0.0336	H-6->LUMO (33%), HOMO->L+4 (12%)	H-8->L+1 (3%), H-7->LUMO (5%), H-1->LUMO (2%), H-1->L+1 (4%), H-1->L+2 (3%), H-1->L+5 (5%), H-1->L+6 (3%), HOMO->L+3 (3%), HOMO->L+10 (5%)
15	6.25	198	0.0041	H-6->LUMO (11%), H-3->L+1 (21%), HOMO->L+4 (18%), HOMO->L+10 (11%)	H-7->LUMO (2%), H-6->L+1 (2%), H-4->L+1 (2%), H-1->L+1 (3%), H-1->L+2 (5%), HOMO->L+3 (7%)

BMe2, iPrax

	E eV	nm	Osc. Strength f	Mayor Contribs	Minor Contribs
1	4.15	299	0.0829	HOMO->LUMO (95%)	
2	4.68	265	0.0361	H-1->LUMO (32%), HOMO->L+1 (47%)	H-2->LUMO (8%)
3	4.81	258	0.0440	H-3->LUMO (11%), H-2->LUMO (63%), H-1->LUMO (12%)	
4	4.92	252	0.0339	H-3->LUMO (62%), H-1->LUMO (17%)	H-1->L+1 (5%), HOMO->L+1 (7%)
5	5.07	245	0.3560	H-3->LUMO (20%), H-2->LUMO (19%), H-1->LUMO (19%), HOMO->L+1 (36%)	H-1->L+1 (3%)
6	5.52	225	0.0035	H-3->L+1 (43%), H-2->L+1 (38%)	H-1->L+1 (9%)
7	5.60	221	0.0076	H-3->L+1 (39%), H-2->L+1 (45%)	H-1->L+1 (2%), HOMO->L+5 (2%)
8	5.62	220	0.0315	H-1->LUMO (10%), H-1->L+1 (53%)	H-3->L+1 (8%), H-2->L+1 (6%), HOMO->L+1 (3%), HOMO->L+4 (4%), HOMO->L+5 (4%)
9	5.76	215	0.0049	H-4->LUMO (71%)	H-8->LUMO (6%), H-6->LUMO (3%), H-5->LUMO (5%), H-3->L+1 (2%)
10	5.90	210	0.1300	H-1->L+1 (14%), HOMO->L+2 (16%), HOMO->L+4 (29%), HOMO->L+5 (16%)	H-2->L+1 (5%), H-1->LUMO (2%), HOMO->L+6 (5%)
11	6.02	206	0.0280	HOMO->L+2 (58%), HOMO->L+3 (12%), HOMO->L+5 (10%)	H-2->L+2 (2%), H-1->L+1 (3%), HOMO->L+6 (2%)
12	6.23	199	0.0114	H-5->LUMO (52%)	H-9->L+1 (3%), H-7->L+1 (3%), H-6->LUMO (7%), H-4->LUMO (4%), H-4->L+1 (5%), H-1->LUMO (2%), H-1->L+1 (5%), H-1->L+4 (2%), H-1->L+5 (2%)
13	6.25	198	0.0990	H-1->L+4 (15%), H-1->L+5 (17%), HOMO->L+10 (18%)	H-2->L+4 (6%), H-2->L+5 (5%), H-1->L+6 (3%), HOMO->L+4 (3%), HOMO->L+5 (2%), HOMO->L+9 (6%), HOMO->L+11 (3%)
14	6.32	196	0.0084	H-1->L+2 (13%), HOMO->L+2 (10%), HOMO->L+3 (40%), HOMO->L+4 (10%)	H-2->L+4 (2%), H-1->L+3 (5%), HOMO->L+5 (5%)
15	6.35	195	0.0511	H-2->L+4 (18%), H-2->L+5 (20%)	H-7->LUMO (3%), H-5->LUMO (2%), H-4->L+1 (7%), H-3->L+4 (4%), H-3->L+5 (4%), H-2->L+6 (6%), H-1->L+4 (5%), H-1->L+5 (6%), HOMO->L+5 (2%)

BCN2, iPrax

	E eV	nm	Osc. Strength f	Mayor Contribs	Minor Contribs
1	4.25	292	0.1845	HOMO->LUMO (94%)	
2	4.63	268	0.0749	H-1->LUMO (72%), HOMO->L+1 (14%)	HOMO->L+3 (5%)
3	5.05	246	0.0768	H-2->LUMO (11%), H-1->LUMO (10%), H-1->L+1 (13%), HOMO->L+1 (57%)	
4	5.22	238	0.1371	H-2->LUMO (76%), HOMO->L+1 (13%)	H-1->LUMO (2%)
5	5.51	225	0.0137	H-1->L+1 (61%)	H-6->LUMO (3%), H-2->LUMO (3%), H-1->LUMO (9%), HOMO->L+1 (7%), HOMO->L+3 (8%)
6	5.94	209	0.0445	H-6->LUMO (13%), H-2->L+1 (20%), H-1->L+1 (16%), HOMO->L+3 (25%)	H-9->L+1 (2%), H-5->LUMO (2%), H-3->LUMO (5%), H-1->L+3 (3%)
7	6.05	205	0.0083	H-6->LUMO (19%), H-2->L+1 (53%)	H-7->LUMO (2%), H-5->LUMO (3%), H-5->L+1 (2%), H-3->LUMO (6%), H-1->L+1 (2%)
8	6.08	204	0.0321	H-7->LUMO (14%), H-5->LUMO (14%), H-4->LUMO (12%), H-2->L+1 (15%), HOMO->L+3 (11%)	H-11->LUMO (3%), H-3->LUMO (6%), H-1->L+3 (6%)
9	6.14	202	0.0789	H-7->LUMO (13%), H-4->LUMO (30%), HOMO->L+3 (16%)	H-11->LUMO (4%), H-6->LUMO (3%), H-5->LUMO (3%), H-3->LUMO (5%), H-1->LUMO (3%), HOMO->L+1 (4%)
10	6.30	197	0.0986	H-5->LUMO (19%), H-1->L+3 (28%), HOMO->L+3 (15%)	H-7->LUMO (4%), H-6->LUMO (9%), HOMO->L+7 (5%), HOMO->L+8 (3%)
11	6.32	196	0.0186	H-6->LUMO (27%), H-3->LUMO (46%)	H-1->L+3 (6%)
12	6.39	194	0.1624	H-5->LUMO (31%), H-3->LUMO (12%), H-1->L+3 (20%)	H-7->LUMO (3%), H-4->LUMO (2%), H-4->L+1 (3%), HOMO->L+2 (3%), HOMO->L+3 (3%), HOMO->L+7 (4%), HOMO->L+8 (3%)
13	6.40	194	0.0064	HOMO->L+2 (71%), HOMO->L+4 (14%)	H-1->L+2 (3%)
14	6.44	193	0.0069	H-7->LUMO (30%), H-4->LUMO (39%)	H-11->LUMO (4%), H-9->LUMO (3%), H-5->LUMO (5%), H-3->LUMO (8%)
15	6.64	187	0.0081	H-1->L+2 (32%), H-1->L+4 (15%)	H-10->L+15 (2%), H-2->L+3 (4%), H-2->L+15 (4%), HOMO->L+4 (9%)

BCN2, iPreq

	E eV	nm	Osc. Strength f	Mayor Contribs	Minor Contribs
1	4.05	306	0.1210	HOMO->LUMO (95%)	
2	4.59	270	0.1007	H-1->LUMO (71%), HOMO->L+1 (18%)	HOMO->L+3 (3%)
3	4.96	250	0.1653	H-1->LUMO (16%), H-1->L+1 (10%), HOMO->L+1 (69%)	
4	5.32	233	0.0603	H-2->LUMO (35%), H-1->L+1 (31%)	H-6->LUMO (6%), H-1->LUMO (4%), HOMO->L+1 (4%), HOMO->L+3 (8%)
5	5.54	224	0.0277	H-2->LUMO (47%), H-1->L+1 (42%)	HOMO->L+1 (3%)
6	5.91	210	0.0746	H-6->LUMO (14%), H-1->L+1 (12%), HOMO->L+3 (27%)	H-4->LUMO (3%), H-3->LUMO (6%), H-2->LUMO (9%), H-2->L+1 (5%), H-1->L+3 (3%), HOMO->L+5 (4%)
7	5.95	208	0.0255	H-3->LUMO (45%)	H-7->LUMO (9%), H-6->LUMO (3%), H-4->LUMO (9%), H-1->L+3 (3%), HOMO->L+3 (9%)
8	6.10	203	0.0281	H-6->LUMO (45%), H-3->LUMO (11%)	H-7->LUMO (3%), H-5->L+1 (2%), H-1->LUMO (3%), HOMO->L+3 (8%)
9	6.21	200	0.0568	H-1->L+3 (15%), HOMO->L+2 (40%)	H-2->L+1 (3%), HOMO->L+3 (8%), HOMO->L+4 (5%), HOMO->L+5 (9%), HOMO->L+7 (6%)
10	6.25	198	0.0220	H-7->LUMO (11%), H-4->LUMO (32%), H-3->LUMO (13%)	H-8->LUMO (6%), H-2->L+1 (5%), H-1->L+3 (3%), HOMO->L+2 (7%), HOMO->L+3 (2%)
11	6.26	198	0.0754	H-2->L+1 (25%), HOMO->L+2 (20%), HOMO->L+3 (14%)	H-4->LUMO (4%), H-1->L+2 (2%), H-1->L+3 (7%), HOMO->L+4 (6%), HOMO->L+8 (3%)
12	6.31	196	0.0349	H-4->LUMO (12%), H-2->L+1 (40%)	H-3->LUMO (3%), H-1->L+3 (9%), HOMO->L+2 (3%), HOMO->L+5 (3%), HOMO->L+7 (4%), HOMO->L+8 (6%)
13	6.39	194	0.0444	H-5->LUMO (66%)	H-9->LUMO (5%), H-6->L+1 (3%), H-4->LUMO (3%), H-2->L+1 (4%), HOMO->L+3 (2%)
14	6.50	191	0.0182	H-7->LUMO (39%), H-4->LUMO (25%)	H-14->LUMO (4%), H-10->LUMO (3%), H-8->LUMO (3%), H-6->LUMO (5%), H-5->LUMO (3%), H-2->LUMO (3%)
15	6.59	188	0.0113	H-1->L+2 (50%), H-1->L+4 (13%), HOMO->L+4 (20%)	HOMO->L+6 (5%)

BCN2, open

	E eV	nm	Osc. Strength f	Mayor Contribs	Minor Contribs
1	3.77	329	0.0927	H-1->LUMO (21%), HOMO->LUMO (71%)	H-5->LUMO (4%)
2	4.17	298	0.0804	H-1->LUMO (66%), HOMO->LUMO (24%)	H-5->LUMO (2%), H-3->LUMO (2%)
3	4.75	261	0.0025	H-2->LUMO (22%), H-2->L+1 (48%), H-2->L+2 (13%)	H-1->L+1 (4%)
4	4.85	256	0.0157	H-5->LUMO (65%)	H-13->LUMO (3%), H-11->LUMO (3%), H-8->LUMO (4%), H-1->LUMO (6%)
5	5.08	244	0.0005	H-8->LUMO (65%)	H-11->LUMO (4%), H-9->LUMO (9%), H-7->LUMO (4%)
6	5.14	241	0.0080	H-2->LUMO (48%), H-2->L+2 (33%)	H-2->L+4 (5%), H-1->L+2 (2%), HOMO->L+2 (2%)
7	5.20	239	0.0770	H-3->LUMO (61%), HOMO->L+1 (20%)	H-7->LUMO (2%), H-3->L+1 (3%), HOMO->L+2 (3%)
8	5.31	233	0.1576	H-3->LUMO (21%), HOMO->L+1 (38%), HOMO->L+2 (13%)	H-4->LUMO (2%), H-4->L+2 (2%), H-2->L+2 (2%), H-1->L+1 (4%)
9	5.42	229	0.0240	H-1->L+1 (30%), HOMO->L+3 (10%), HOMO->L+4 (21%)	H-3->LUMO (4%), H-2->LUMO (5%), H-2->L+2 (4%), H-1->LUMO (2%), H-1->L+2 (2%), HOMO->L+1 (2%)
10	5.51	225	0.0343	H-2->LUMO (17%), H-2->L+1 (25%), H-2->L+2 (12%), HOMO->L+2 (11%)	H-3->LUMO (2%), H-2->L+9 (2%), HOMO->L+1 (7%), HOMO->L+3 (3%)
11	5.59	222	0.0984	HOMO->L+1 (23%), HOMO->L+2 (29%)	H-4->LUMO (4%), H-4->L+1 (2%), H-3->L+1 (8%), H-2->L+1 (4%), H-2->L+2 (7%), HOMO->L+4 (9%)
12	5.73	216	0.0339	H-7->LUMO (20%), H-6->LUMO (30%), H-4->LUMO (13%)	H-18->LUMO (2%), H-15->LUMO (3%), H-11->LUMO (4%), H-9->LUMO (4%), H-5->LUMO (4%)
13	5.98	207	0.0126	H-4->LUMO (73%)	H-6->LUMO (7%), H-5->LUMO (5%), HOMO->L+2 (6%)
14	6.11	203	0.0566	H-10->LUMO (11%), H-7->LUMO (40%), H-6->LUMO (19%)	H-16->LUMO (2%), H-14->LUMO (3%), H-8->LUMO (4%), H-3->LUMO (3%), H-1->L+1 (4%)
15	6.22	199	0.0985	H-10->LUMO (27%)	H-16->LUMO (7%), H-13->LUMO (5%), H-12->LUMO (4%), H-9->LUMO (6%), H-7->LUMO (3%), H-6->LUMO (9%), H-5->LUMO (2%), H-1->L+1 (9%), HOMO->L+3 (2%), HOMO->L+4 (3%)

B(CN)(NC), iPrax, B-NCeq

	E eV	nm	Osc. Strength f	Mayor Contribs	Minor Contribs
1	4.25	292	0.1807	HOMO->LUMO (94%)	
2	4.64	267	0.0738	H-1->LUMO (71%), HOMO->L+1 (15%)	HOMO->L+3 (5%)
3	5.04	246	0.0530	H-2->LUMO (19%), H-1->L+1 (12%), HOMO->L+1 (49%)	H-1->LUMO (9%)
4	5.18	239	0.1737	H-2->LUMO (67%), HOMO->L+1 (20%)	H-1->LUMO (3%)
5	5.51	225	0.0163	H-1->L+1 (61%)	H-6->LUMO (2%), H-2->LUMO (3%), H-1->LUMO (9%), HOMO->L+1 (7%), HOMO->L+3 (8%)
6	5.93	209	0.0374	H-2->L+1 (35%), H-1->L+1 (14%), HOMO->L+3 (22%)	H-8->LUMO (2%), H-6->LUMO (6%), H-4->LUMO (2%), H-1->L+3 (2%)
7	6.04	205	0.0305	H-6->LUMO (10%), H-2->L+1 (51%)	H-8->LUMO (6%), H-3->LUMO (5%), H-1->L+1 (7%), HOMO->L+3 (7%)
8	6.07	204	0.0167	H-7->LUMO (26%), H-6->LUMO (10%), H-5->LUMO (20%)	H-18->LUMO (2%), H-10->LUMO (5%), H-4->LUMO (4%), H-3->LUMO (6%), H-2->L+1 (2%), H-1->L+3 (4%), HOMO->L+3 (4%)
9	6.13	202	0.0856	H-5->LUMO (17%), H-4->LUMO (17%), HOMO->L+3 (19%)	H-10->LUMO (3%), H-7->LUMO (7%), H-6->LUMO (9%), H-1->LUMO (3%), H-1->L+3 (2%), HOMO->L+1 (4%)
10	6.26	198	0.0456	H-3->LUMO (45%), H-1->L+3 (14%)	H-8->LUMO (4%), H-6->LUMO (7%), H-5->LUMO (4%), H-4->LUMO (3%), HOMO->L+3 (7%), HOMO->L+8 (2%)
11	6.31	196	0.0129	H-8->LUMO (12%), H-6->LUMO (15%), H-4->LUMO (46%)	H-3->LUMO (6%), HOMO->L+3 (3%)
12	6.36	195	0.1934	H-3->LUMO (16%), H-1->L+3 (39%), HOMO->L+8 (11%)	H-4->LUMO (5%), HOMO->L+2 (3%), HOMO->L+3 (6%), HOMO->L+7 (2%)
13	6.39	194	0.0091	HOMO->L+2 (70%), HOMO->L+4 (13%)	H-1->L+2 (3%)
14	6.43	193	0.0306	H-7->LUMO (34%), H-5->LUMO (40%)	H-10->LUMO (3%), H-3->LUMO (6%)
15	6.56	189	0.0029	H-8->LUMO (46%)	H-9->LUMO (2%), H-6->LUMO (7%), H-6->L+1 (3%), H-5->L+1 (2%), H-4->LUMO (7%), H-3->LUMO (5%), H-3->L+1 (4%), H-2->LUMO (2%)

B(CN)(NC), iPreq, B-NCeq

	E eV	nm	Osc. Strength f	Mayor Contribs	Minor Contribs
1	4.05	306	0.1185	HOMO->LUMO (95%)	
2	4.59	270	0.1007	H-1->LUMO (70%), HOMO->L+1 (19%)	HOMO->L+3 (3%)
3	4.97	250	0.1721	H-1->LUMO (17%), H-1->L+1 (10%), HOMO->L+1 (68%)	
4	5.30	234	0.0716	H-2->LUMO (41%), H-1->L+1 (25%)	H-7->LUMO (4%), H-1->LUMO (3%), HOMO->L+1 (4%), HOMO->L+3 (7%)
5	5.53	224	0.0215	H-2->LUMO (39%), H-1->L+1 (47%)	HOMO->L+1 (3%)
6	5.91	210	0.0925	H-7->LUMO (11%), H-1->L+1 (12%), HOMO->L+3 (32%)	H-2->LUMO (9%), H-2->L+1 (7%), H-1->L+3 (4%), H-1->L+8 (3%), HOMO->L+5 (4%)
7	5.97	208	0.0095	H-4->LUMO (52%)	H-12->LUMO (2%), H-8->LUMO (8%), H-6->LUMO (6%), H-5->LUMO (6%), H-3->LUMO (3%), HOMO->L+3 (3%)
8	6.10	203	0.0319	H-7->LUMO (46%), H-4->LUMO (10%)	H-11->L+1 (3%), H-6->LUMO (2%), H-5->L+1 (4%), H-1->LUMO (4%), HOMO->L+3 (8%)
9	6.21	200	0.0245	HOMO->L+2 (56%)	H-1->L+3 (8%), HOMO->L+3 (6%), HOMO->L+4 (6%), HOMO->L+5 (9%), HOMO->L+8 (3%)
10	6.25	198	0.0799	H-5->LUMO (11%), H-1->L+3 (15%), HOMO->L+2 (12%), HOMO->L+3 (11%)	H-10->LUMO (2%), H-8->LUMO (3%), H-7->L+1 (2%), H-6->LUMO (3%), H-4->LUMO (6%), H-3->LUMO (3%), H-2->L+1 (2%), HOMO->L+4 (7%), HOMO->L+8 (9%)
11	6.26	198	0.0425	H-6->LUMO (11%), H-3->LUMO (24%), H-2->L+1 (25%)	H-10->LUMO (2%), H-7->LUMO (6%), H-5->LUMO (4%), H-4->LUMO (5%), H-1->L+3 (2%), HOMO->L+3 (4%)
12	6.29	197	0.0040	H-3->LUMO (26%), H-2->L+1 (43%)	H-1->L+3 (5%), HOMO->L+2 (2%), HOMO->L+8 (4%)
13	6.34	196	0.0980	H-8->LUMO (11%), H-5->LUMO (31%), H-3->LUMO (17%)	H-4->LUMO (4%), H-1->L+3 (5%), HOMO->L+3 (3%), HOMO->L+5 (2%), HOMO->L+8 (8%)
14	6.44	192	0.0008	H-6->LUMO (41%), H-5->LUMO (17%), H-3->LUMO (13%)	H-14->LUMO (3%), H-10->LUMO (5%), H-9->LUMO (3%), H-2->LUMO (2%), H-2->L+1 (2%)
15	6.58	188	0.0074	H-1->L+2 (49%), H-1->L+4 (12%), HOMO->L+4 (18%)	HOMO->L+6 (5%)

B(CN)(NC), iPreq, B-NCax

	E eV	nm	Osc. Strength f	Mayor Contribs	Minor Contribs
1	4.05	306	0.1266	HOMO->LUMO (95%)	
2	4.59	270	0.1094	H-1->LUMO (73%), HOMO->L+1 (16%)	HOMO->L+3 (3%)
3	4.97	250	0.1654	H-1->LUMO (15%), HOMO->L+1 (71%)	H-1->L+1 (9%)
4	5.29	234	0.0543	H-3->LUMO (18%), H-2->LUMO (29%), H-1->L+1 (23%)	H-6->LUMO (2%), H-1->LUMO (3%), HOMO->L+1 (2%), HOMO->L+3 (7%)
5	5.51	225	0.0143	H-3->LUMO (18%), H-2->LUMO (18%), H-1->L+1 (49%)	HOMO->L+1 (4%)
6	5.87	211	0.0254	H-3->LUMO (47%), H-2->LUMO (28%)	H-7->LUMO (2%), H-4->LUMO (2%), H-1->L+1 (3%), HOMO->L+3 (4%)
7	5.92	209	0.0563	H-5->LUMO (10%), H-4->LUMO (17%), H-2->LUMO (12%), HOMO->L+3 (21%)	H-6->LUMO (8%), H-2->L+1 (3%), H-1->L+1 (9%), HOMO->L+5 (2%)
8	5.96	208	0.0445	H-4->LUMO (32%), HOMO->L+3 (16%)	H-6->LUMO (8%), H-5->LUMO (3%), H-3->LUMO (7%), H-2->LUMO (7%), H-1->LUMO (2%), H-1->L+3 (3%)
9	6.11	203	0.0078	H-7->LUMO (14%), H-5->LUMO (22%), H-4->LUMO (16%)	H-10->L+1 (3%), H-8->LUMO (4%), H-6->LUMO (8%), H-5->L+1 (3%), H-4->L+1 (2%), H-1->LUMO (3%), H-1->L+1 (2%), HOMO->L+3 (3%)
10	6.22	199	0.0303	HOMO->L+2 (58%), HOMO->L+5 (10%)	H-1->L+3 (8%), HOMO->L+4 (9%), HOMO->L+7 (2%), HOMO->L+8 (2%)
11	6.25	198	0.1301	H-2->L+1 (12%), H-1->L+3 (16%), HOMO->L+2 (10%), HOMO->L+3 (27%), HOMO->L+8 (11%)	H-3->L+1 (9%), HOMO->L+4 (2%)
12	6.29	197	0.0136	H-3->L+1 (24%), H-2->L+1 (33%), H-1->L+3 (11%)	HOMO->L+2 (4%), HOMO->L+5 (2%), HOMO->L+8 (8%)
13	6.38	194	0.0385	H-10->LUMO (11%), H-7->LUMO (39%), H-6->LUMO (16%), H-4->LUMO (11%)	H-17->LUMO (2%), H-5->LUMO (3%), H-3->LUMO (2%)
14	6.49	191	0.0103	H-6->LUMO (31%), H-5->LUMO (30%)	H-12->LUMO (5%), H-10->LUMO (3%), H-9->LUMO (9%), H-8->LUMO (2%), H-5->L+1 (3%), H-3->L+1 (3%)
15	6.58	188	0.0127	H-1->L+2 (49%), H-1->L+4 (12%), HOMO->L+4 (21%)	HOMO->L+6 (5%)

B(CN)(NC), iPrax, B-NCax

	E eV	nm	Osc. Strength f	Mayor Contribs	Minor Contribs
1	4.26	291	0.1939	HOMO->LUMO (94%)	
2	4.64	267	0.0780	H-1->LUMO (73%), HOMO->L+1 (13%)	HOMO->L+3 (5%)
3	5.06	245	0.0593	H-2->LUMO (17%), H-1->L+1 (13%), HOMO->L+1 (52%)	H-5->LUMO (2%), H-1->LUMO (8%)
4	5.17	240	0.1368	H-2->LUMO (64%), HOMO->L+1 (17%)	H-3->LUMO (7%), H-1->LUMO (3%)
5	5.51	225	0.0165	H-1->L+1 (60%)	H-5->LUMO (2%), H-1->LUMO (9%), HOMO->L+1 (8%), HOMO->L+3 (8%)
6	5.83	213	0.0140	H-3->LUMO (78%), H-2->LUMO (10%)	H-8->LUMO (3%), H-1->L+1 (2%)
7	5.96	208	0.0421	H-2->L+1 (33%), H-1->L+1 (12%), HOMO->L+3 (24%)	H-10->L+1 (2%), H-5->LUMO (6%), H-4->LUMO (5%), H-2->LUMO (2%), H-1->L+3 (2%)
8	6.02	206	0.0131	H-6->LUMO (11%), H-5->LUMO (13%), H-2->L+1 (39%)	H-8->L+1 (3%), H-4->LUMO (8%), H-3->L+1 (7%), H-1->L+1 (6%), HOMO->L+3 (2%)
9	6.12	203	0.0788	H-4->LUMO (16%), H-2->L+1 (12%), HOMO->L+3 (26%)	H-6->LUMO (6%), H-5->LUMO (7%), H-1->LUMO (4%), H-1->L+3 (8%), H-1->L+8 (2%), HOMO->L+1 (4%)
10	6.18	201	0.0069	H-6->LUMO (39%), H-4->LUMO (17%)	H-18->LUMO (3%), H-12->LUMO (6%), H-9->LUMO (4%), H-8->LUMO (4%), H-7->LUMO (5%), H-3->LUMO (5%)
11	6.33	196	0.1702	H-1->L+3 (47%), HOMO->L+3 (17%)	H-10->LUMO (2%), H-8->LUMO (3%), H-5->LUMO (3%), H-4->L+1 (3%), HOMO->L+7 (5%), HOMO->L+8 (8%)
12	6.40	194	0.0111	HOMO->L+2 (70%), HOMO->L+4 (13%)	H-1->L+2 (3%)
13	6.43	193	0.0706	H-8->LUMO (13%), H-5->LUMO (27%), H-4->LUMO (29%)	H-9->LUMO (4%), H-1->L+3 (5%), HOMO->L+2 (3%)
14	6.53	190	0.0409	H-7->LUMO (26%), H-3->L+1 (46%)	H-10->LUMO (5%), H-8->L+1 (3%), H-6->LUMO (2%), H-4->LUMO (2%), H-2->L+1 (6%)
15	6.59	188	0.0038	H-7->LUMO (40%), H-3->L+1 (28%)	H-10->LUMO (8%), H-8->LUMO (5%), H-2->L+1 (4%)

B(CN)NC), open

	E eV	nm	Osc. Strength f	Mayor Contribs	Minor Contribs
1	3.96	313	0.0737	H-1->LUMO (28%), HOMO->LUMO (62%)	H-5->LUMO (4%)
2	4.35	285	0.0592	H-1->LUMO (59%), HOMO->LUMO (32%)	H-3->LUMO (2%)
3	4.81	258	0.0020	H-2->L+1 (58%), H-2->L+2 (18%)	H-2->LUMO (7%), H-1->L+1 (4%)
4	5.06	245	0.0131	H-5->LUMO (64%)	H-13->LUMO (5%), H-1->LUMO (4%), H-1->L+1 (2%), HOMO->L+4 (3%)
5	5.24	237	0.1670	H-2->LUMO (12%), HOMO->L+1 (43%), HOMO->L+2 (13%)	H-4->L+2 (3%), H-3->L+1 (3%), H-2->L+1 (4%), H-2->L+2 (7%)
6	5.26	236	0.0688	H-2->LUMO (23%), H-2->L+2 (35%), HOMO->L+1 (20%)	H-3->LUMO (3%), H-2->L+3 (4%)
7	5.37	231	0.0141	H-10->LUMO (11%), H-1->L+1 (25%), HOMO->L+4 (23%)	H-8->LUMO (3%), H-6->LUMO (5%), H-3->LUMO (4%), H-3->L+4 (3%), H-1->LUMO (3%), H-1->L+11 (2%), HOMO->L+2 (2%)
8	5.39	230	0.0143	H-10->LUMO (19%), H-6->LUMO (28%), H-3->LUMO (17%)	H-12->LUMO (3%), H-11->LUMO (3%), H-9->LUMO (2%), H-7->LUMO (3%), H-1->L+1 (6%), HOMO->L+4 (3%)
9	5.49	226	0.0074	H-10->LUMO (10%), H-3->LUMO (53%)	H-5->LUMO (4%), H-2->LUMO (5%), H-1->L+1 (5%), HOMO->L+1 (3%), HOMO->L+4 (5%)
10	5.57	223	0.0906	H-2->LUMO (15%), HOMO->L+1 (19%), HOMO->L+2 (36%)	H-4->L+1 (2%), H-3->L+1 (5%), H-2->L+1 (5%), HOMO->L+4 (2%)
11	5.61	221	0.0063	H-6->LUMO (20%), H-2->LUMO (13%)	H-12->LUMO (2%), H-11->LUMO (3%), H-10->LUMO (8%), H-7->LUMO (2%), H-3->LUMO (8%), H-2->L+1 (8%), H-2->L+2 (8%), HOMO->L+1 (2%), HOMO->L+2 (6%), HOMO->L+4 (3%)
12	5.63	220	0.0173	H-10->LUMO (10%), H-6->LUMO (22%), H-2->LUMO (21%)	H-12->LUMO (2%), H-11->LUMO (2%), H-7->LUMO (7%), H-3->L+1 (2%), H-2->L+1 (7%), H-2->L+2 (6%), HOMO->L+1 (3%), HOMO->L+2 (2%), HOMO->L+4 (2%)
13	6.12	203	0.1423	H-8->LUMO (12%), H-4->LUMO (34%)	H-9->LUMO (3%), H-7->LUMO (9%), H-6->LUMO (3%), H-1->L+1 (6%), H-1->L+4 (9%), HOMO->L+4 (6%)
14	6.20	200	0.1829	H-4->LUMO (37%), H-1->L+1 (23%), HOMO->L+2 (12%), HOMO->L+4 (15%)	H-1->L+4 (3%)
15	6.24	199	0.0263	H-8->LUMO (11%), H-7->LUMO (15%), H-4->LUMO (17%), H-1->L+1 (16%), HOMO->L+4 (13%)	H-9->LUMO (4%), H-6->LUMO (9%), H-5->LUMO (4%)

2.1.3. List of Computed optical transitions of vinyl-boranes

*t*BuBBN, closed

	E eV	nm	Osc. Strength f	Mayor Contribs	Minor Contribs
1	3.69	336	0.0522	HOMO->LUMO (92%)	H-2->LUMO (2%), H-1->LUMO (3%)
2	4.03	308	0.0377	H-2->LUMO (10%), H-1->LUMO (81%)	HOMO->LUMO (5%)
3	4.37	284	0.0540	H-2->LUMO (76%), H-1->LUMO (11%)	H-3->LUMO (2%), HOMO->L+1 (3%)
4	4.51	275	0.0082	H-3->LUMO (11%), HOMO->L+1 (72%)	H-4->LUMO (3%), H-2->LUMO (3%), H-2->L+1 (2%)
5	4.74	261	0.1028	H-3->LUMO (40%), H-1->L+1 (23%), HOMO->L+1 (19%)	H-4->LUMO (3%), H-2->L+1 (4%)
6	4.83	257	0.1044	H-3->LUMO (33%), H-1->L+1 (49%)	H-4->LUMO (6%)
7	5.03	247	0.0166	H-4->LUMO (52%), H-1->L+1 (18%)	H-5->LUMO (5%), H-3->L+1 (2%), H-2->L+1 (3%), HOMO->L+4 (3%)
8	5.14	241	0.0620	H-2->L+1 (53%)	H-8->LUMO (2%), H-6->LUMO (2%), H-4->LUMO (9%), H-3->LUMO (3%), H-3->L+1 (4%), H-1->L+1 (3%), HOMO->L+4 (6%), HOMO->L+5 (4%)
9	5.26	236	0.2029	H-4->LUMO (12%), H-2->L+1 (20%), HOMO->L+4 (20%), HOMO->L+5 (12%)	H-6->LUMO (3%), H-5->LUMO (3%), H-4->L+1 (2%), H-3->LUMO (2%), H-1->L+1 (4%), HOMO->L+6 (5%)
10	5.49	226	0.0258	H-6->LUMO (11%), H-5->LUMO (32%), HOMO->L+4 (14%)	H-4->LUMO (3%), H-4->L+1 (5%), H-2->L+4 (3%), HOMO->L+2 (5%), HOMO->L+5 (5%)
11	5.55	223	0.0101	H-3->L+1 (75%)	H-2->L+1 (7%), HOMO->L+2 (5%), HOMO->L+5 (3%)
12	5.57	223	0.0291	HOMO->L+2 (55%), HOMO->L+5 (10%)	H-3->L+1 (8%), H-1->L+5 (3%), HOMO->L+7 (6%)
13	5.71	217	0.0533	H-5->LUMO (11%), H-1->L+4 (19%), H-1->L+5 (12%)	H-2->L+4 (5%), H-2->L+5 (6%), H-1->L+2 (3%), H-1->L+3 (3%), H-1->L+6 (4%), HOMO->L+2 (5%), HOMO->L+4 (4%), HOMO->L+5 (4%)
14	5.77	215	0.0169	H-5->LUMO (21%), H-1->L+2 (11%)	H-4->L+1 (5%), H-3->L+5 (2%), H-1->L+4 (3%), H-1->L+7 (3%), H-1->L+10 (3%), HOMO->L+2 (5%), HOMO->L+3 (4%), HOMO->L+7 (6%), HOMO->L+8 (4%), HOMO->L+10 (9%)
15	5.80	214	0.0032	H-5->LUMO (13%), H-1->L+2 (32%), HOMO->L+3 (20%)	H-6->LUMO (4%), H-4->L+1 (4%), H-1->L+4 (4%)

*t*BuBBN, open

	E eV	nm	Osc. Strength f	Mayor Contribs	Minor Contribs
1	4.68	265	0.0537	H-2->LUMO (15%), HOMO->LUMO (32%)	H-4->L+1 (2%), H-3->LUMO (7%), H-3->L+1 (4%), H-2->L+1 (7%), H-1->LUMO (8%), HOMO->L+1 (7%)
2	4.73	262	0.0193	H-2->LUMO (34%), H-2->L+1 (15%), HOMO->LUMO (22%)	H-3->LUMO (2%), H-1->LUMO (6%)
3	4.85	256	0.0066	H-5->L+1 (20%), H-4->LUMO (15%), H-4->L+1 (19%)	H-5->LUMO (9%), H-5->L+3 (8%), H-4->L+3 (9%), H-1->L+1 (4%)
4	5.01	248	0.1656	HOMO->LUMO (25%), HOMO->L+1 (53%)	H-1->LUMO (5%)
5	5.18	239	0.0525	H-1->LUMO (15%), H-1->L+1 (27%), HOMO->L+7 (13%)	H-5->LUMO (4%), H-4->LUMO (3%), H-4->L+1 (3%), H-1->L+3 (2%), H-1->L+14 (2%), HOMO->L+3 (3%), HOMO->L+8 (4%)
6	5.37	231	0.0159	H-1->LUMO (11%), HOMO->L+3 (20%)	H-5->LUMO (8%), H-5->L+3 (5%), H-4->L+3 (9%), H-3->L+1 (3%), H-1->L+1 (4%), H-1->L+3 (4%), HOMO->LUMO (7%), HOMO->L+1 (5%), HOMO->L+4 (3%)
7	5.42	229	0.0105	H-5->L+3 (16%), H-4->LUMO (13%), H-4->L+3 (15%), HOMO->L+3 (10%)	H-5->LUMO (7%), H-1->LUMO (4%), HOMO->LUMO (3%), HOMO->L+1 (2%), HOMO->L+4 (2%), HOMO->L+7 (2%)
8	5.51	225	0.1292	H-3->LUMO (29%), HOMO->L+1 (14%), HOMO->L+3 (17%)	H-4->LUMO (4%), H-3->L+1 (4%), H-2->LUMO (7%), H-1->LUMO (2%), HOMO->L+4 (3%)
9	5.68	218	0.0680	H-3->LUMO (24%), H-2->LUMO (13%), H-1->LUMO (29%)	H-1->L+1 (3%), HOMO->L+1 (7%), HOMO->L+3 (7%), HOMO->L+4 (2%)
10	5.84	212	0.0460	H-5->LUMO (10%), H-4->LUMO (14%), H-1->L+1 (30%)	H-6->LUMO (3%), H-5->L+1 (5%), H-4->L+1 (7%), H-2->LUMO (2%), H-1->LUMO (5%), H-1->L+7 (3%)
11	5.96	208	0.1872	H-3->L+1 (21%), H-2->L+1 (32%)	H-4->LUMO (2%), H-4->L+1 (2%), H-2->LUMO (2%), H-1->L+1 (6%), HOMO->L+7 (7%)
12	6.03	205	0.1446	H-2->L+1 (11%), HOMO->L+2 (20%), HOMO->L+7 (14%)	H-5->LUMO (2%), H-4->L+1 (3%), H-3->L+1 (6%), H-2->LUMO (4%), H-1->LUMO (6%), H-1->L+1 (3%), HOMO->L+3 (7%), HOMO->L+5 (3%), HOMO->L+8 (2%)
13	6.12	203	0.0404	HOMO->L+2 (46%), HOMO->L+6 (13%)	H-1->L+1 (2%), H-1->L+4 (2%), HOMO->L+3 (7%), HOMO->L+4 (5%), HOMO->L+7 (3%), HOMO->L+8 (5%)
14	6.23	199	0.0288	H-6->LUMO (17%), H-1->L+3 (10%)	H-8->LUMO (2%), H-8->L+3 (4%), H-6->L+1 (9%), H-5->LUMO (2%), H-3->LUMO (3%), H-3->L+1 (3%), H-2->LUMO (3%), H-2->L+1 (7%), H-1->L+7 (3%), HOMO->L+1 (3%), HOMO->L+3 (9%), HOMO->L+4 (8%)
15	6.26	198	0.0581	H-1->L+1 (10%), H-1->L+3 (13%), H-1->L+7 (22%)	H-1->L+4 (9%), H-1->L+5 (3%), H-1->L+8 (5%), H-1->L+9 (2%), HOMO->L+3 (3%), HOMO->L+5 (2%), HOMO->L+13 (5%), HOMO->L+14 (4%)

SiBPF, closed

	E eV	E nm	Osc. Strength f	Mayor Contribs	Minor Contribs
1	4.12	301	0.0706	HOMO->LUMO (86%)	HOMO->L+1 (5%)
2	4.66	266	0.0354	H-4->LUMO (10%), H-1->LUMO (51%), HOMO->L+1 (11%)	H-5->LUMO (5%), H-3->LUMO (2%), H-2->LUMO (8%)
3	4.71	263	0.0113	H-1->LUMO (35%), HOMO->L+1 (33%)	H-4->LUMO (8%), H-2->LUMO (2%), HOMO->LUMO (8%)
4	4.83	257	0.0768	H-4->LUMO (13%), H-2->LUMO (26%), HOMO->L+1 (35%)	H-5->LUMO (4%), H-3->LUMO (3%), H-1->LUMO (4%)
5	5.07	244	0.0093	H-4->LUMO (20%), H-2->LUMO (56%)	H-5->LUMO (4%), H-3->LUMO (4%), HOMO->L+3 (3%)
6	5.12	242	0.0182	H-1->L+1 (36%)	H-4->LUMO (5%), H-1->LUMO (3%), H-1->L+2 (3%), H-1->L+3 (5%), H-1->L+7 (2%), HOMO->L+2 (6%), HOMO->L+3 (9%)
7	5.21	238	0.0656	H-4->L+1 (19%), H-2->L+1 (15%)	H-9->LUMO (3%), H-6->LUMO (4%), H-5->L+1 (3%), H-4->L+3 (2%), H-3->L+1 (4%), HOMO->L+1 (2%), HOMO->L+2 (3%), HOMO->L+3 (7%), HOMO->L+7 (6%)
8	5.32	233	0.0745	H-2->L+1 (10%), H-1->L+1 (16%), HOMO->L+3 (14%)	H-5->LUMO (3%), H-4->LUMO (7%), H-2->L+3 (4%), H-2->L+7 (4%), H-2->L+12 (3%), H-1->L+16 (4%), HOMO->L+2 (7%)
9	5.39	230	0.0339	H-5->LUMO (34%), H-4->LUMO (15%)	H-10->LUMO (4%), H-6->LUMO (4%), H-3->LUMO (2%), H-3->L+5 (4%), H-3->L+6 (3%), H-2->L+1 (4%)
10	5.41	229	0.0173	H-5->LUMO (11%), H-3->LUMO (10%), H-3->L+5 (15%)	H-5->L+9 (3%), H-5->L+10 (3%), H-4->L+9 (3%), H-4->L+10 (3%), H-3->L+1 (3%), H-3->L+2 (8%), H-3->L+3 (4%), H-3->L+6 (9%)
11	5.41	229	0.0593	H-1->L+1 (15%), HOMO->L+3 (11%)	H-5->L+1 (3%), H-4->L+1 (5%), H-2->L+2 (2%), H-2->L+3 (4%), H-2->L+7 (7%), H-2->L+12 (5%), H-1->L+16 (4%), HOMO->L+1 (4%), HOMO->L+2 (7%), HOMO->L+7 (2%)
12	5.50	225	0.0007	H-4->LUMO (11%), H-3->LUMO (65%)	H-3->L+2 (4%), H-3->L+5 (3%), H-3->L+6 (2%)
13	5.58	222	0.0205	H-2->L+1 (17%), H-1->L+3 (12%)	H-5->LUMO (3%), H-4->L+1 (8%), H-2->L+5 (2%), H-2->L+8 (3%), H-2->L+11 (2%), H-1->L+1 (7%), H-1->L+2 (4%), HOMO->L+2 (4%), HOMO->L+6 (5%), HOMO->L+7 (4%)
14	5.59	222	0.0197	H-5->LUMO (13%), H-2->L+1 (11%)	H-10->LUMO (7%), H-6->L+1 (2%), H-4->L+1 (4%), H-4->L+2 (3%), H-4->L+3 (5%), HOMO->L+1 (5%), HOMO->L+6 (3%), HOMO->L+7 (9%)
15	5.64	220	0.0472	H-6->LUMO (19%), H-2->L+1 (10%)	H-9->LUMO (5%), H-7->LUMO (5%), H-5->LUMO (7%), H-4->L+1 (3%), H-2->L+2 (4%), H-1->L+1 (7%), H-1->L+2 (5%), H-1->L+3 (9%)

SiBPF, open

	E eV	nm	Osc. Strength f	Mayor Contribs	Minor Contribs
1	3.35	370	0.0319	H-1->LUMO (19%), HOMO->LUMO (69%)	H-10->LUMO (2%)
2	4.02	309	0.0458	H-1->LUMO (65%), HOMO->LUMO (23%)	H-3->LUMO (5%)
3	4.38	283	0.1967	H-3->LUMO (43%), H-2->LUMO (36%)	H-4->LUMO (8%), H-1->LUMO (5%)
4	4.49	276	0.0573	H-3->LUMO (24%), H-2->LUMO (58%)	H-5->LUMO (4%), H-4->LUMO (5%)
5	4.59	270	0.0228	H-5->LUMO (79%)	H-4->LUMO (7%)
6	4.62	268	0.1423	H-6->LUMO (83%)	H-10->LUMO (2%)
7	4.69	264	0.0132	H-10->LUMO (20%), H-8->LUMO (23%), H-7->LUMO (15%)	H-11->LUMO (8%), H-2->LUMO (3%), H-1->LUMO (4%)
8	4.76	261	0.0065	H-4->LUMO (11%), H-4->L+1 (28%), H-4->L+8 (12%), H-3->L+1 (11%)	H-4->L+2 (3%), H-4->L+7 (2%), H-3->L+8 (5%), H-1->L+1 (5%)
9	5.01	248	0.1157	HOMO->L+1 (60%)	H-1->L+1 (4%), H-1->L+3 (2%), HOMO->L+2 (4%), HOMO->L+4 (3%), HOMO->L+10 (3%)
10	5.10	243	0.1396	H-1->L+1 (40%), HOMO->L+1 (17%)	H-4->LUMO (5%), H-1->L+3 (2%), HOMO->L+3 (2%), HOMO->L+4 (2%), HOMO->L+7 (2%), HOMO->L+10 (4%)
11	5.19	239	0.0465	H-8->LUMO (51%), H-7->LUMO (17%)	H-12->LUMO (5%), H-10->LUMO (6%), H-4->LUMO (3%)
12	5.27	235	0.0097	H-7->LUMO (31%), H-4->LUMO (18%)	H-11->LUMO (2%), H-10->LUMO (9%), H-4->L+1 (6%), H-3->LUMO (7%)
13	5.30	234	0.0217	H-10->LUMO (11%), H-7->LUMO (14%), H-4->L+1 (10%)	H-12->LUMO (2%), H-11->LUMO (2%), H-8->LUMO (7%), H-4->LUMO (8%), H-4->L+3 (4%), H-4->L+4 (3%), H-3->L+1 (5%), HOMO->L+4 (2%)
14	5.40	230	0.0037	H-2->L+3 (15%), H-2->L+4 (13%)	H-3->L+10 (2%), H-3->L+12 (2%), H-2->L+2 (2%), H-2->L+7 (6%), H-2->L+12 (2%), H-1->L+8 (4%), H-1->L+10 (3%), HOMO->L+3 (6%), HOMO->L+10 (3%), HOMO->L+12 (4%)
15	5.46	227	0.0193	H-7->LUMO (12%), HOMO->L+3 (14%), HOMO->L+8 (17%)	H-7->L+1 (5%), H-4->LUMO (2%), H-1->L+4 (4%), H-1->L+7 (4%), HOMO->L+1 (3%), HOMO->L+2 (3%), HOMO->L+6 (4%)

SiBMes2 closed

	E		Osc.	Mayor Contribs	Minor Contribs
	eV	nm	Strength f		
1	4.02	308	0.1287	H-1->LUMO (27%), HOMO->LUMO (39%)	H-7->LUMO (7%), H-1->L+1 (4%), HOMO->L+1 (8%)
2	4.20	296	0.1438	H-1->LUMO (47%), HOMO->LUMO (31%)	H-1->L+1 (3%), HOMO->L+1 (4%)
3	4.61	269	0.0330	H-3->LUMO (18%), H-2->LUMO (44%), H-1->L+1 (11%)	H-2->L+1 (2%)
4	4.68	265	0.0161	H-4->LUMO (10%), H-3->LUMO (23%), H-2->LUMO (22%), H-2->L+1 (11%)	H-2->L+4 (2%), H-1->L+1 (7%)
5	4.74	262	0.0068	H-6->L+1 (15%), H-3->LUMO (14%), H-3->L+1 (11%)	H-10->L+1 (2%), H-9->L+1 (6%), H-9->L+2 (2%), H-8->L+1 (2%), H-7->LUMO (5%), H-6->LUMO (3%), H-6->L+2 (6%), H-2->L+1 (2%), H-1->L+1 (4%)
6	4.78	259	0.0175	H-4->LUMO (45%)	H-4->L+1 (8%), H-4->L+2 (4%), H-4->L+4 (4%), H-3->LUMO (5%), H-3->L+1 (4%)
7	4.88	254	0.0247	H-6->L+1 (11%), H-5->LUMO (10%), H-1->L+1 (16%)	H-7->LUMO (2%), H-6->LUMO (9%), H-5->L+4 (4%), H-4->L+1 (8%), H-3->L+1 (6%), H-1->L+4 (3%), HOMO->L+1 (5%)
8	5.00	248	0.2890	H-7->LUMO (13%), H-5->LUMO (37%)	H-7->L+1 (3%), H-5->L+1 (6%), H-3->LUMO (2%), H-1->LUMO (3%), HOMO->L+1 (5%), HOMO->L+4 (5%)
9	5.08	244	0.1035	H-7->LUMO (29%)	H-11->LUMO (3%), H-6->LUMO (5%), H-5->LUMO (8%), H-5->L+1 (5%), H-3->LUMO (3%), H-3->L+1 (4%), H-1->L+1 (6%), H-1->L+4 (5%), HOMO->L+2 (3%), HOMO->L+4 (3%)
10	5.19	239	0.0099	H-6->L+2 (11%), H-1->L+2 (14%)	H-9->L+2 (4%), H-6->LUMO (7%), H-5->L+1 (3%), H-3->L+2 (5%), H-2->L+2 (3%), H-1->LUMO (3%), H-1->L+4 (4%), HOMO->LUMO (3%), HOMO->L+1 (7%), HOMO->L+4 (3%)
11	5.28	235	0.0695	H-6->LUMO (12%), H-5->L+2 (10%)	H-12->LUMO (2%), H-11->L+2 (2%), H-10->L+2 (3%), H-9->LUMO (3%), H-6->L+2 (7%), H-5->L+1 (6%), H-5->L+4 (2%), H-3->L+2 (3%), H-2->L+1 (5%), H-1->L+2 (8%), HOMO->L+2 (5%)
12	5.33	232	0.0120	HOMO->LUMO (14%), HOMO->L+1 (21%)	H-7->LUMO (7%), H-7->L+1 (5%), H-7->L+2 (3%), H-6->LUMO (4%), H-6->L+2 (4%), HOMO->L+2 (2%), HOMO->L+4 (5%)
13	5.37	231	0.0159	H-2->LUMO (19%)	H-3->LUMO (5%), H-2->L+1 (2%), H-2->L+4 (3%), HOMO->L+2 (4%), HOMO->L+8 (2%), HOMO->L+10 (8%), HOMO->L+12 (2%), HOMO->L+14 (2%)
14	5.43	228	0.0105	H-4->LUMO (21%)	H-4->L+4 (4%), H-3->LUMO (8%), H-3->L+10 (3%), H-2->L+8 (3%), H-1->L+10 (5%), HOMO->L+2 (4%), HOMO->L+13 (3%), HOMO->L+15 (2%)
15	5.48	226	0.2114	H-5->LUMO (16%), H-1->L+4 (21%)	H-11->LUMO (4%), H-7->LUMO (3%), H-5->L+2 (9%), H-3->L+1 (3%), H-3->L+4 (6%), HOMO->L+1 (4%), HOMO->L+4 (3%)

2.2. NMR and MS-Data

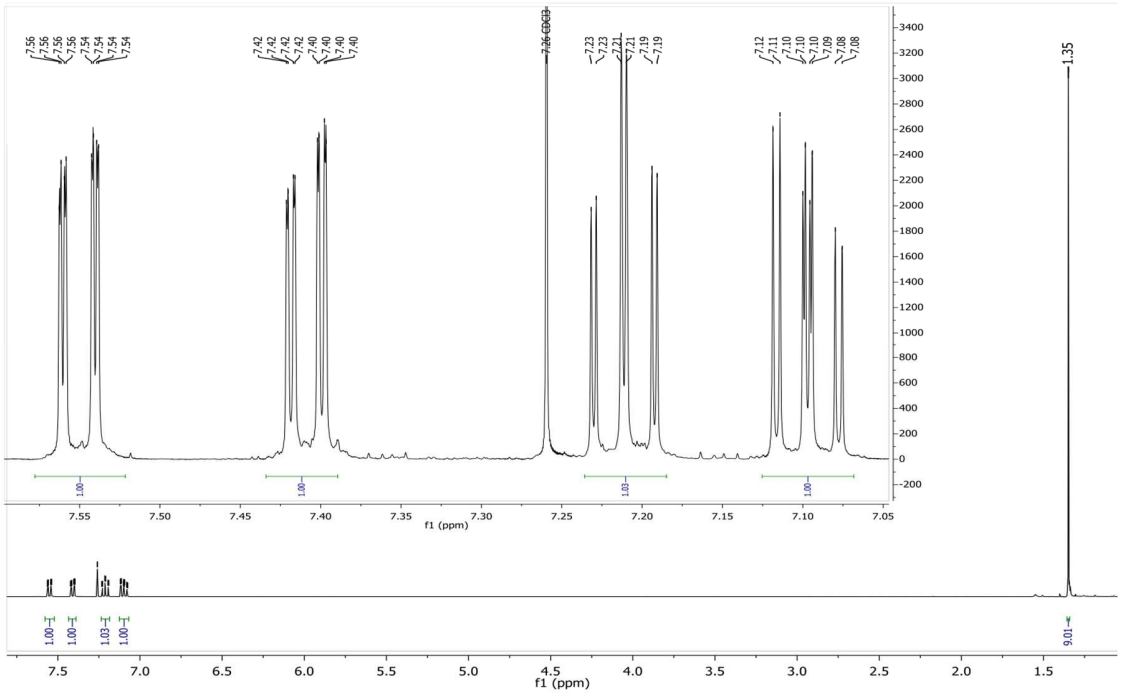


Figure S6. ^{1}H NMR-spectrum of **Br*t*Bu** in $CDCl_3$.

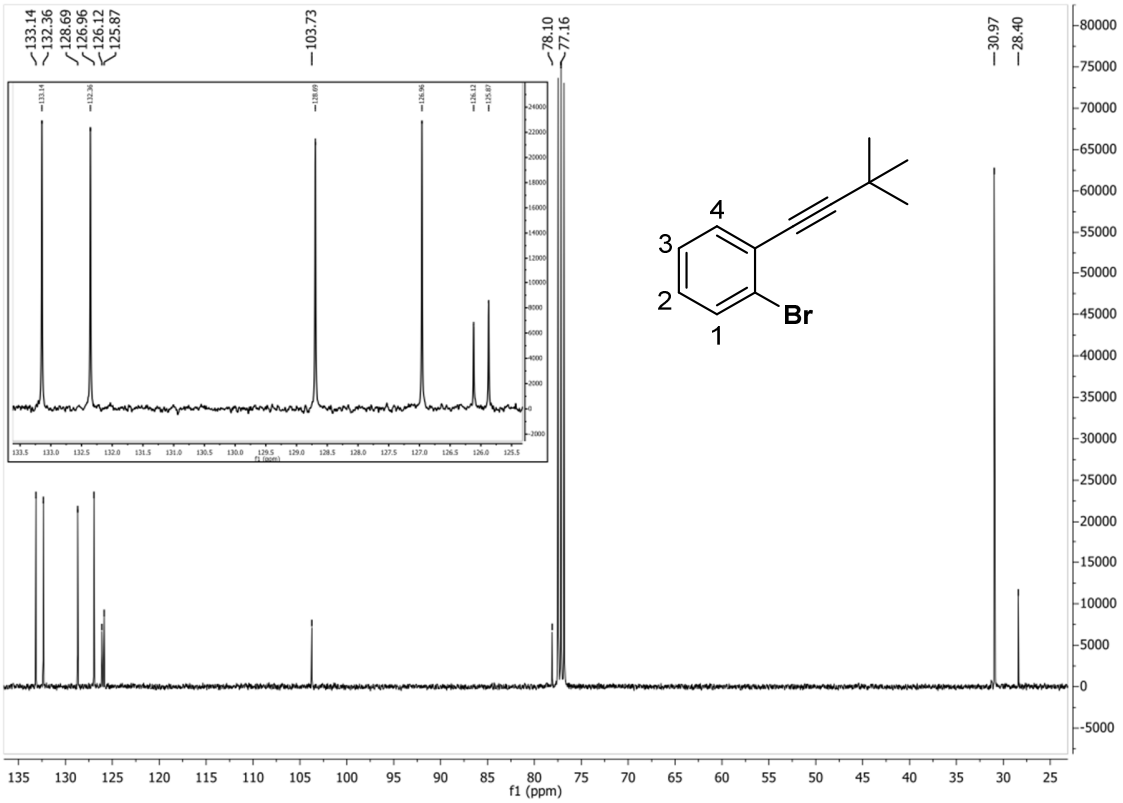


Figure S7. ^{13}C NMR-spectrum of **Br*t*Bu** in $CDCl_3$.

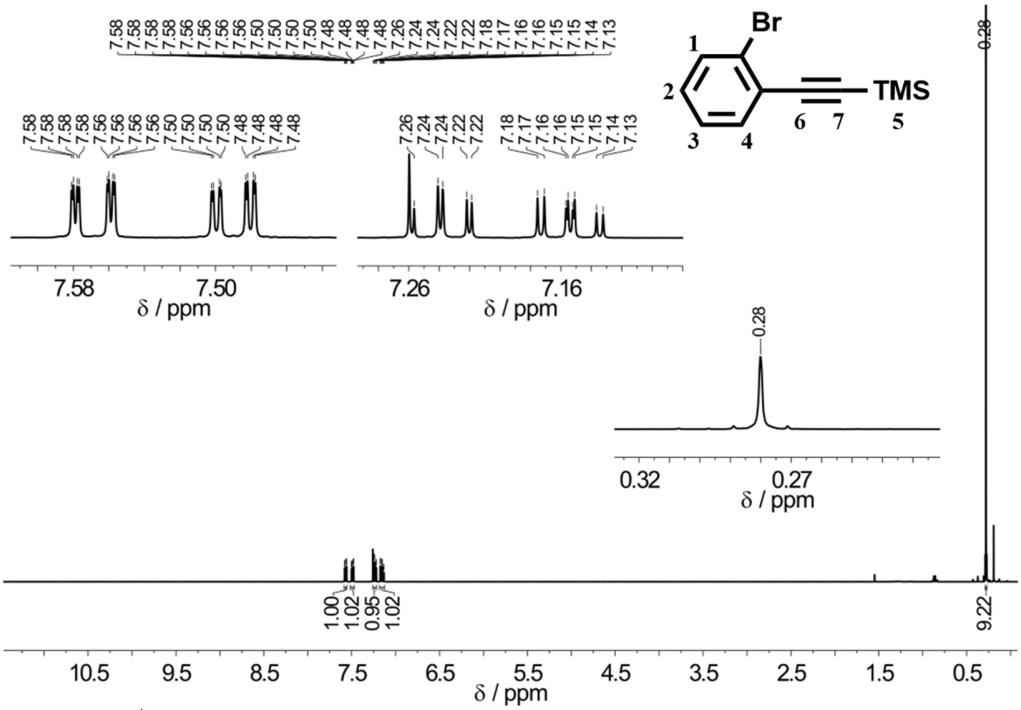


Figure S8. ^{1}H NMR-spectrum of **BrTMS** in $CDCl_3$ (*).

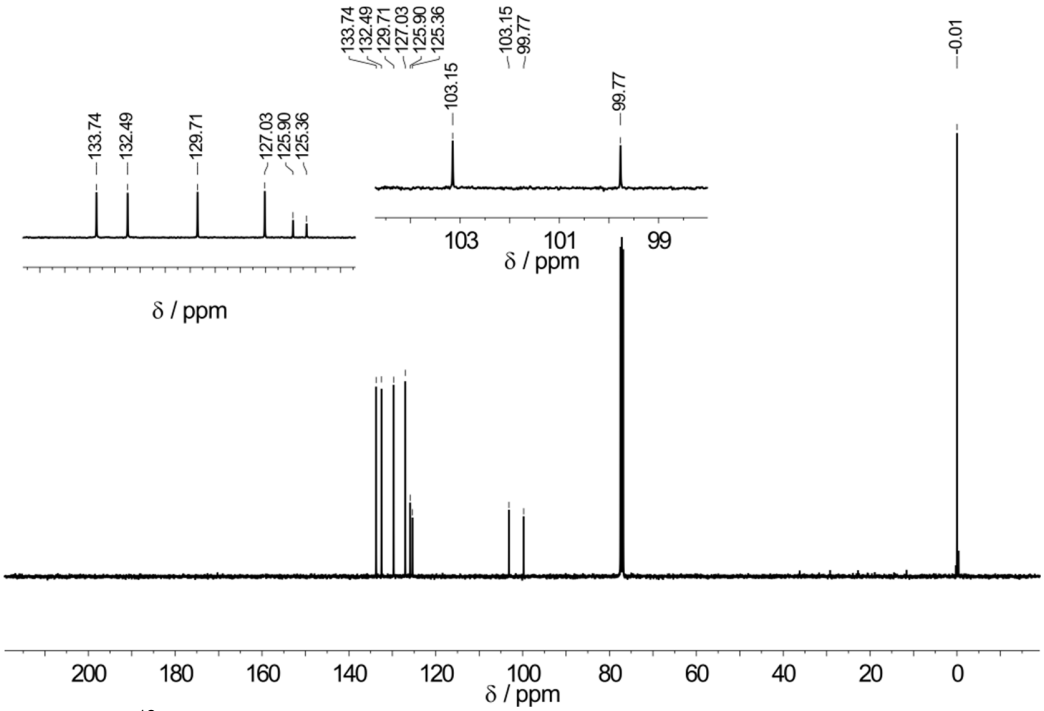


Figure S9. ^{13}C NMR-spectrum of **BrTMS** in $CDCl_3$ (*).

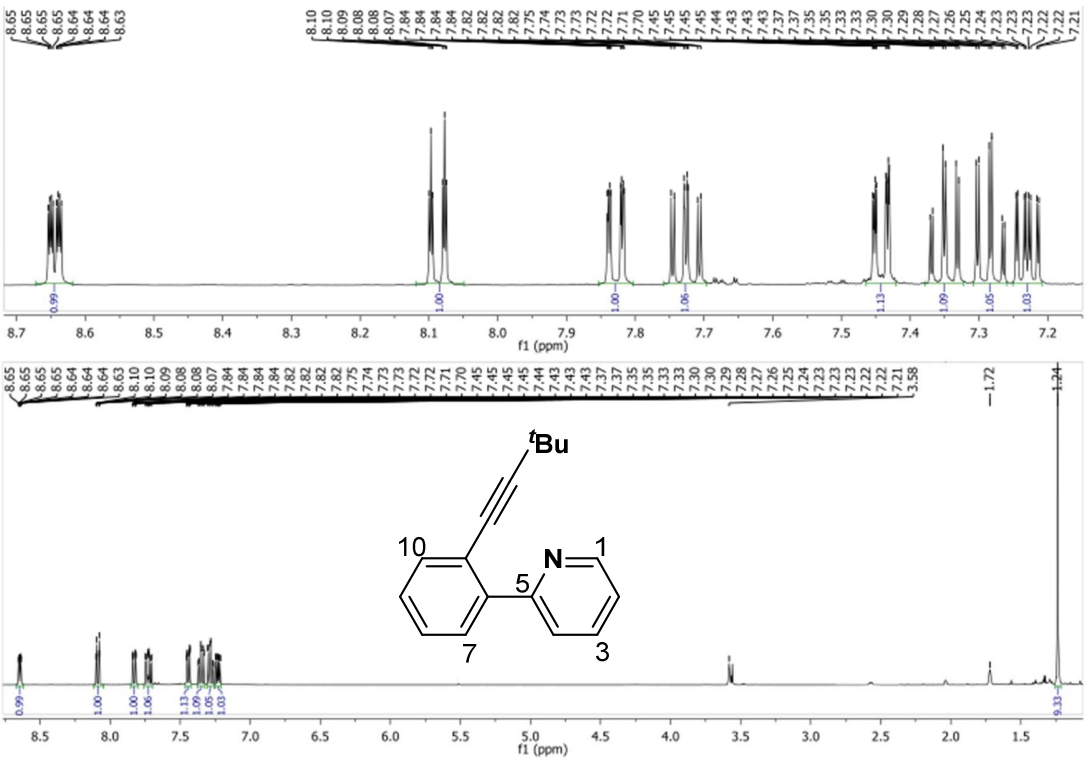


Figure S10. ^{1}H NMR-spectrum of **2a** in THF-d_8.

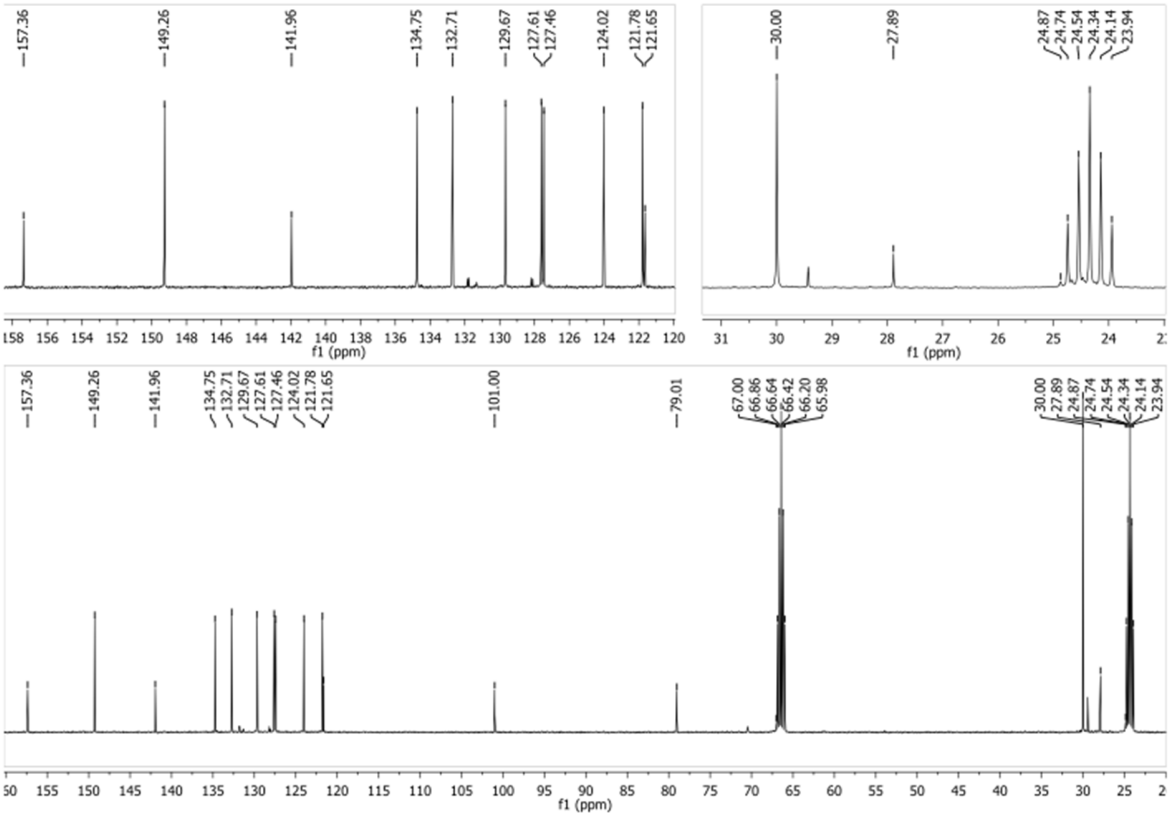


Figure S11. ^{13}C NMR-spectrum of **2a** in THF-d_8.

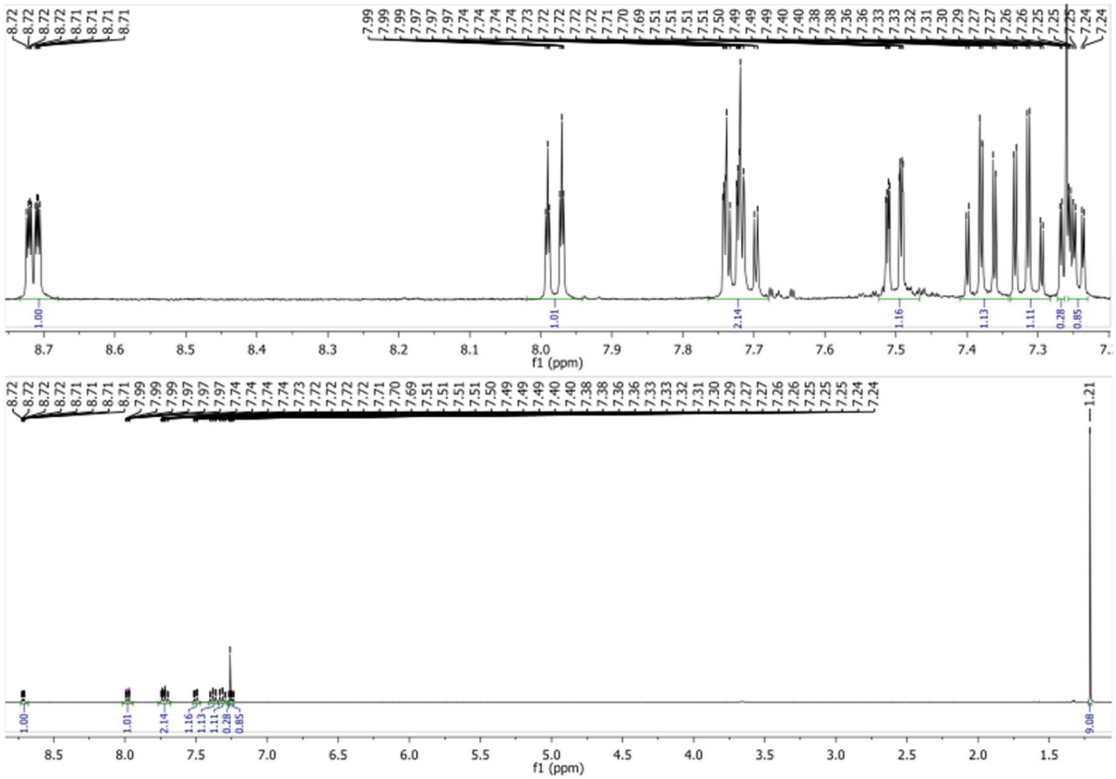


Figure S12. ^{1}H NMR-spectrum of **2a** in $CDCl_3$.

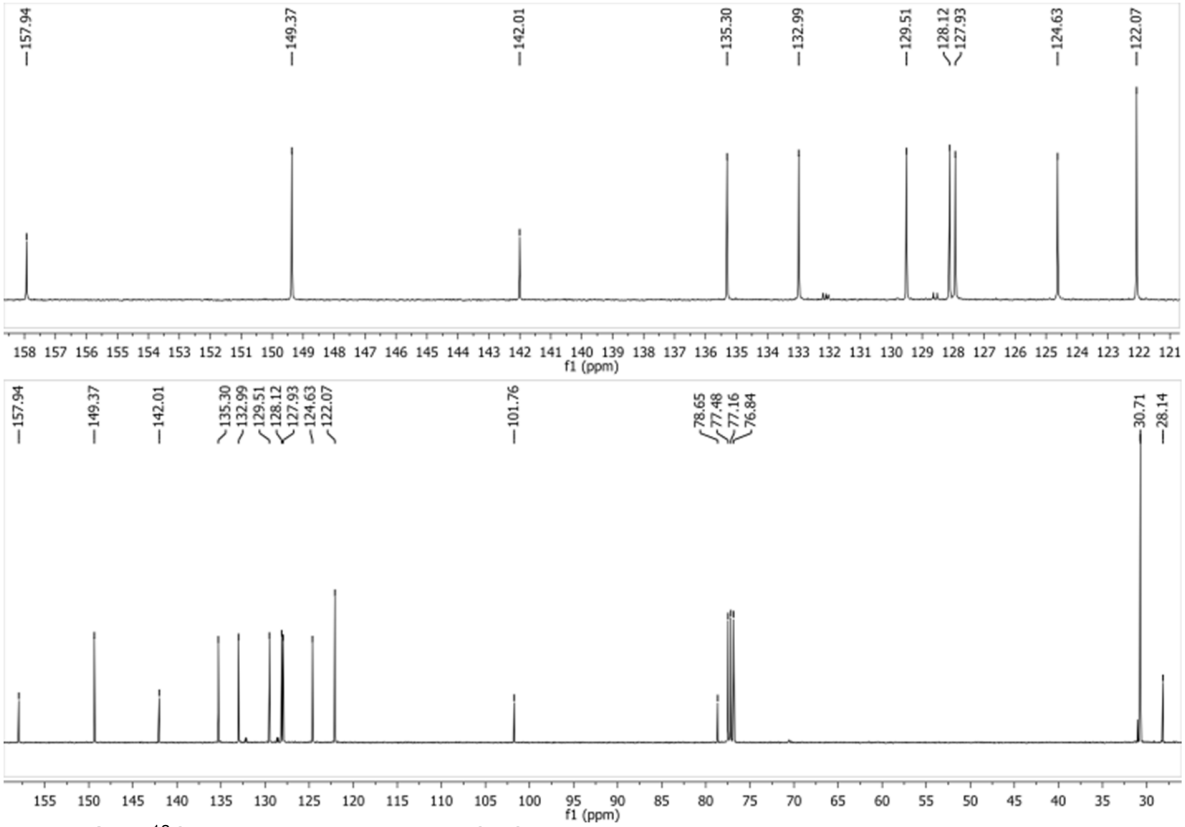


Figure S13. ^{13}C NMR-spectrum of **2a** in $CDCl_3$.

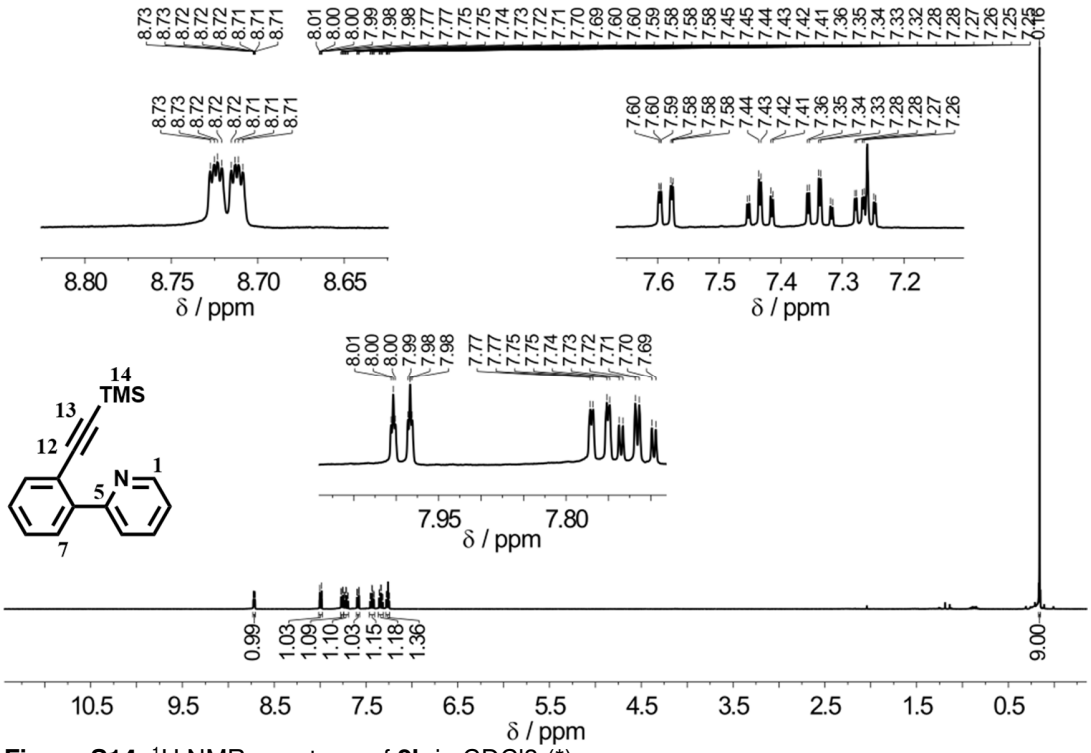


Figure S14. ^{1}H NMR-spectrum of **2b** in CDCl3 (*).

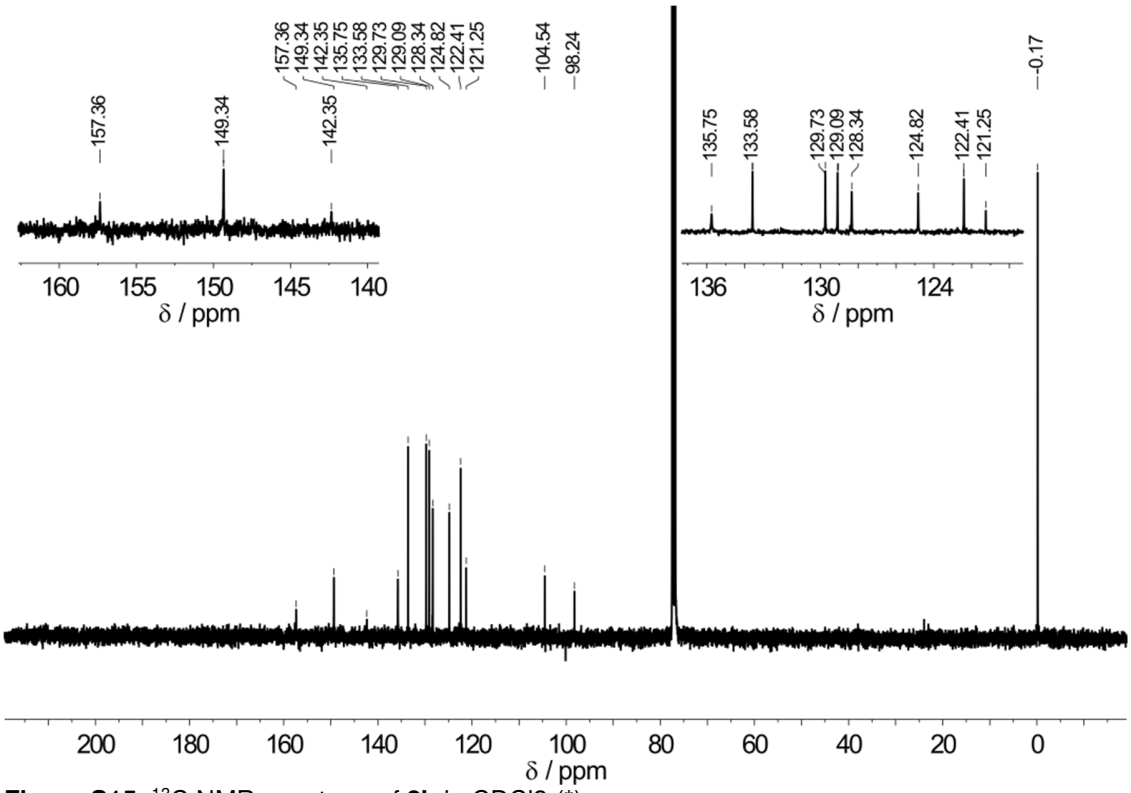


Figure S15. ^{13}C NMR-spectrum of **2b** in CDCl3 (*).

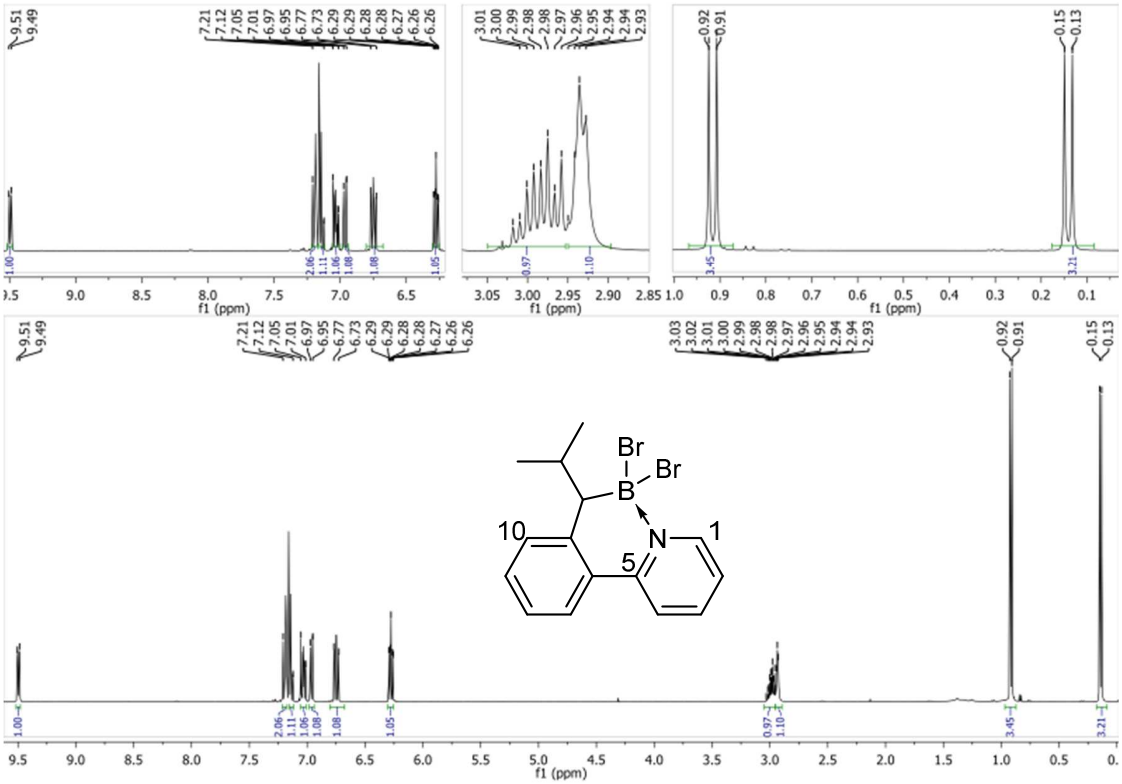


Figure S16. ^{1}H NMR-spectrum of **BBr_2** in C_6D_6.

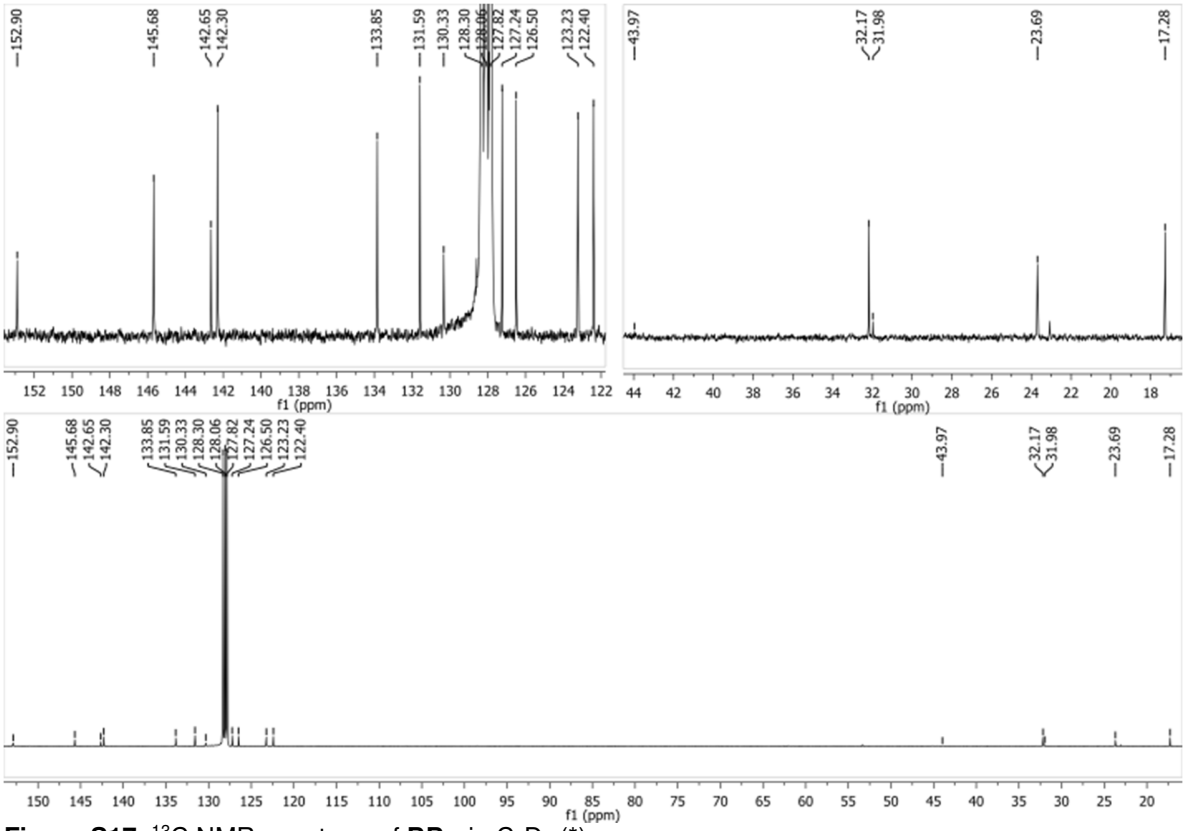


Figure S17. ^{13}C NMR-spectrum of **BBr_2** in C_6D_6 (*).

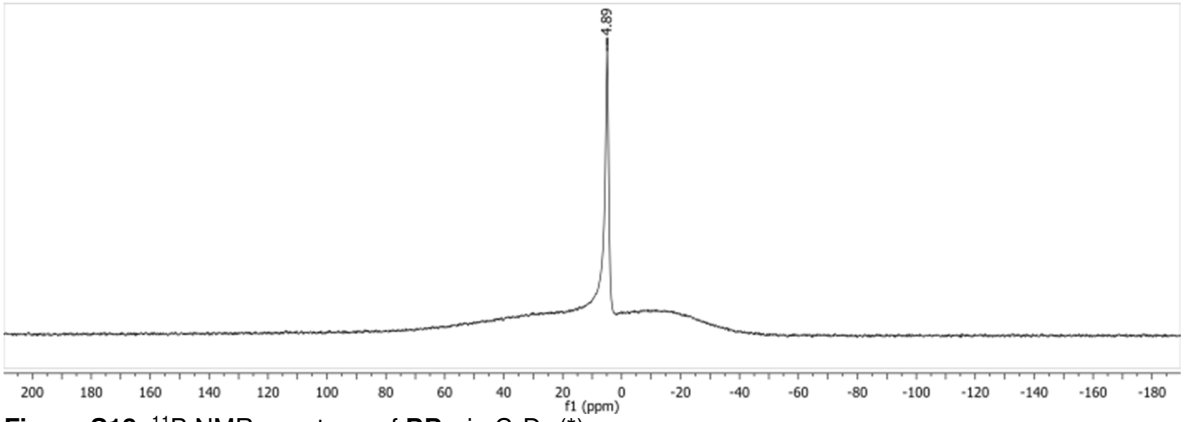


Figure S18. ^{11}B NMR-spectrum of **BBr_2** in C_6D_6 (*).

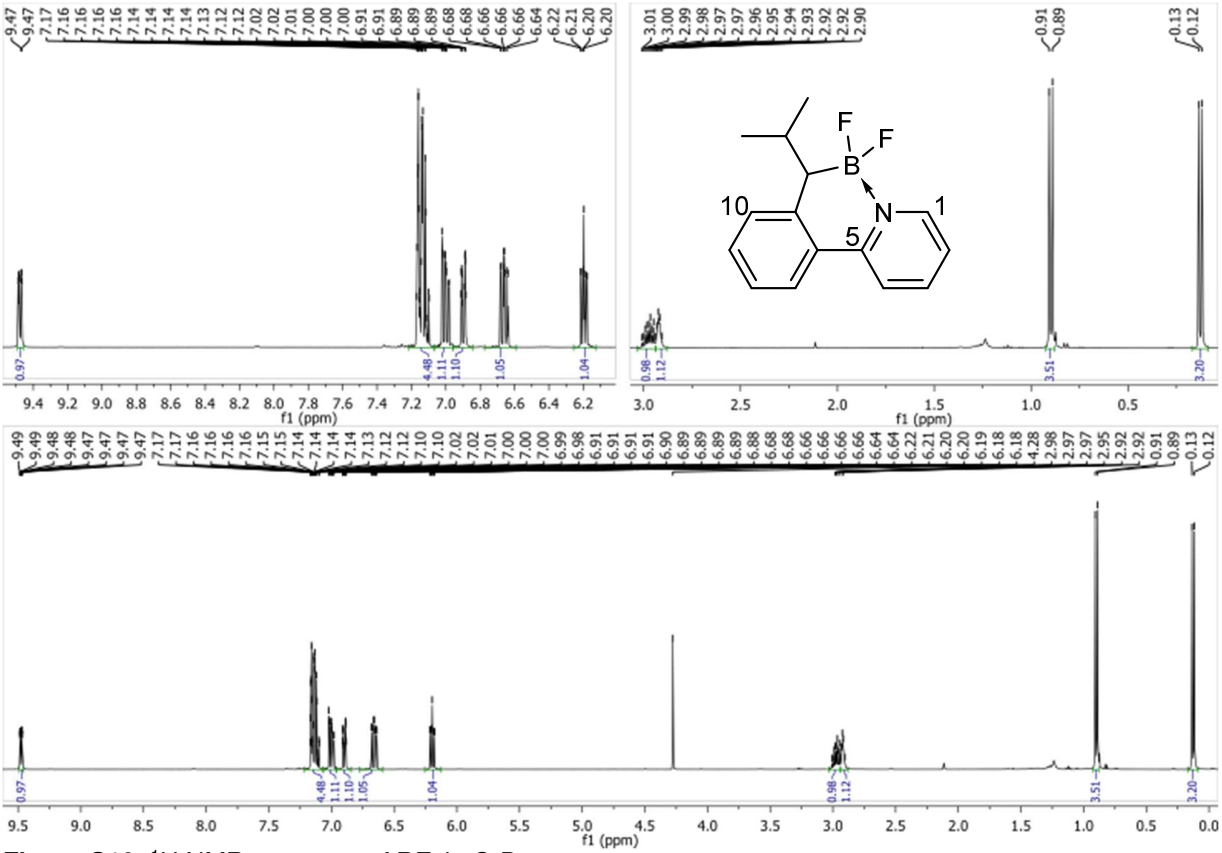


Figure S19. ^{1}H NMR-spectrum of **BF_2** in C_6D_6.

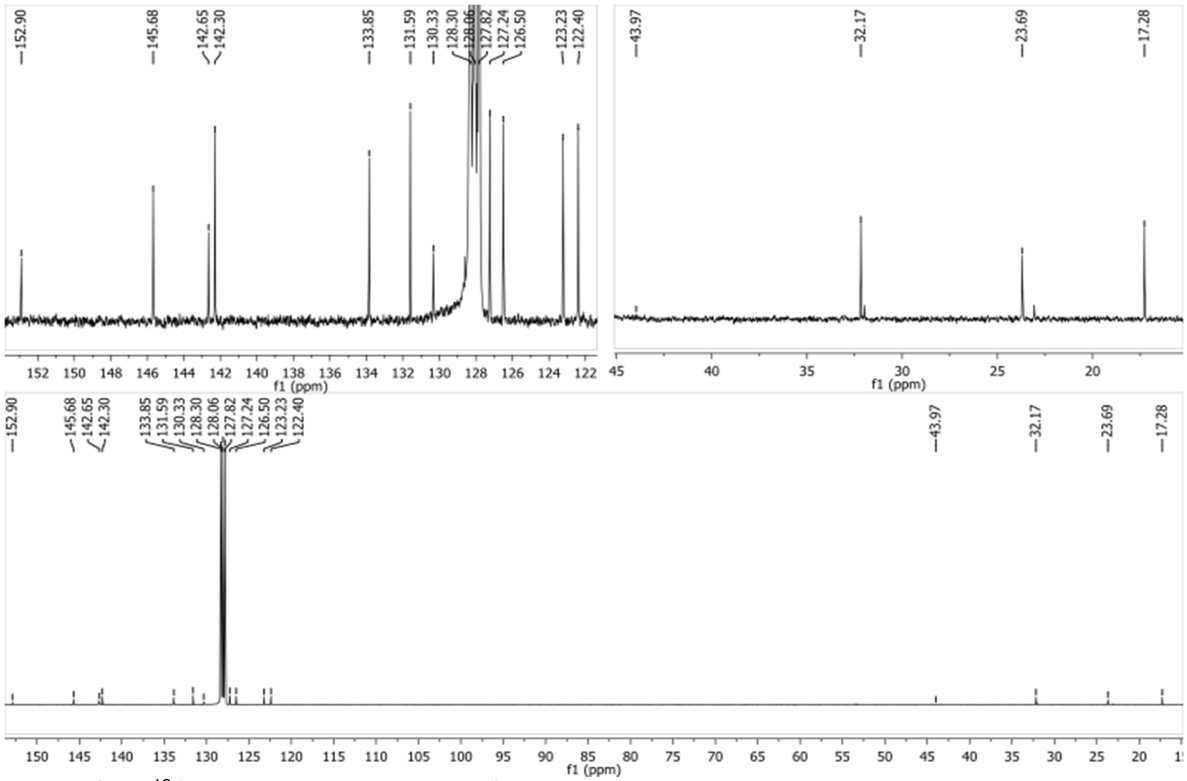


Figure S20. ^{13}C NMR-spectrum of **BF_2** in C_6D_6.

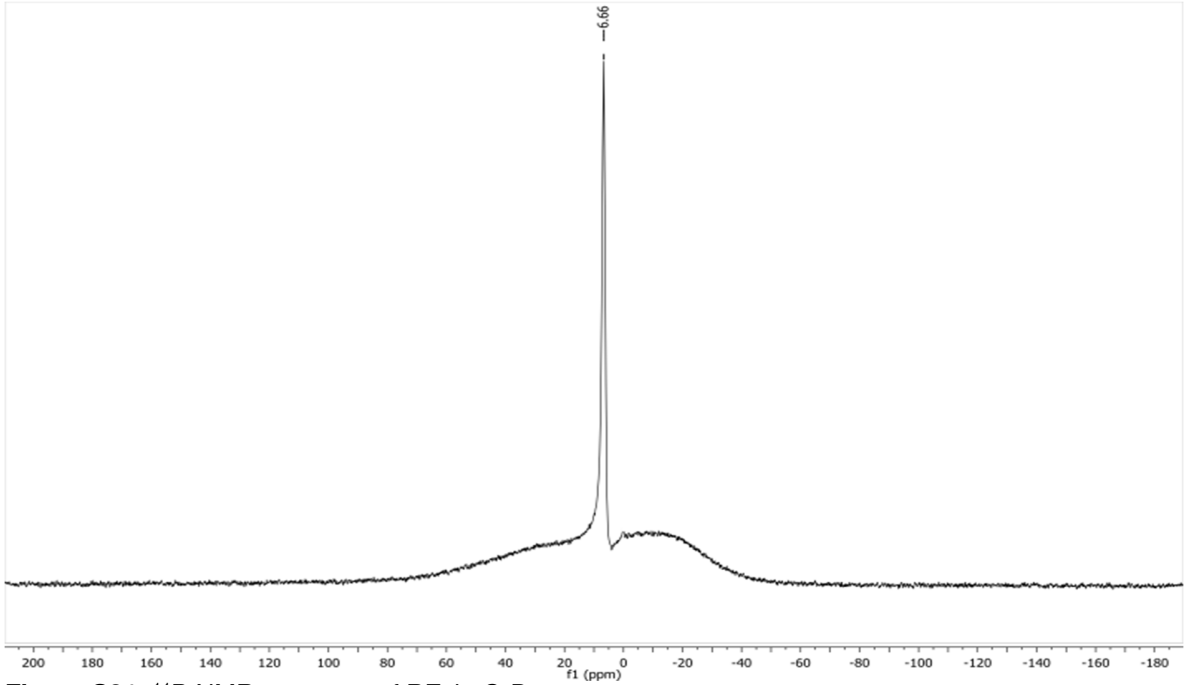


Figure S21. ^{11}B NMR-spectrum of **BF_2** in C_6D_6.

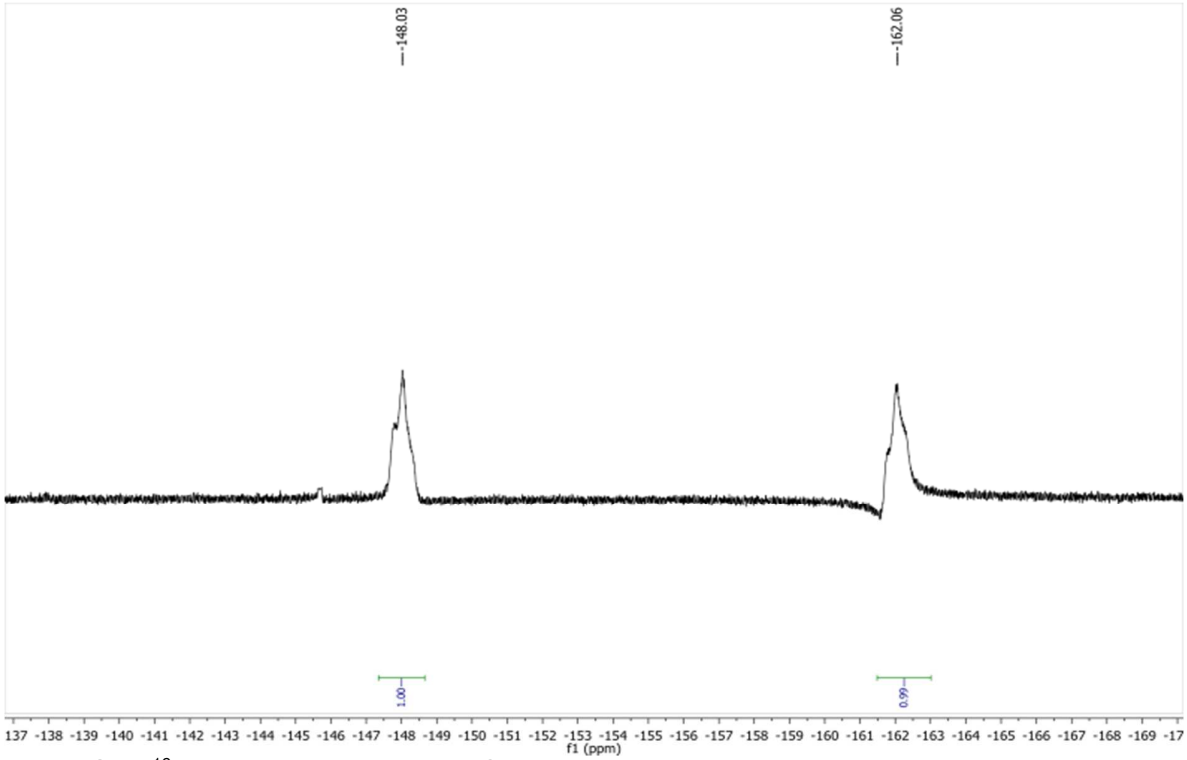


Figure S22. ^{19}F NMR-spectrum of **BF_2** in C_6D_6.

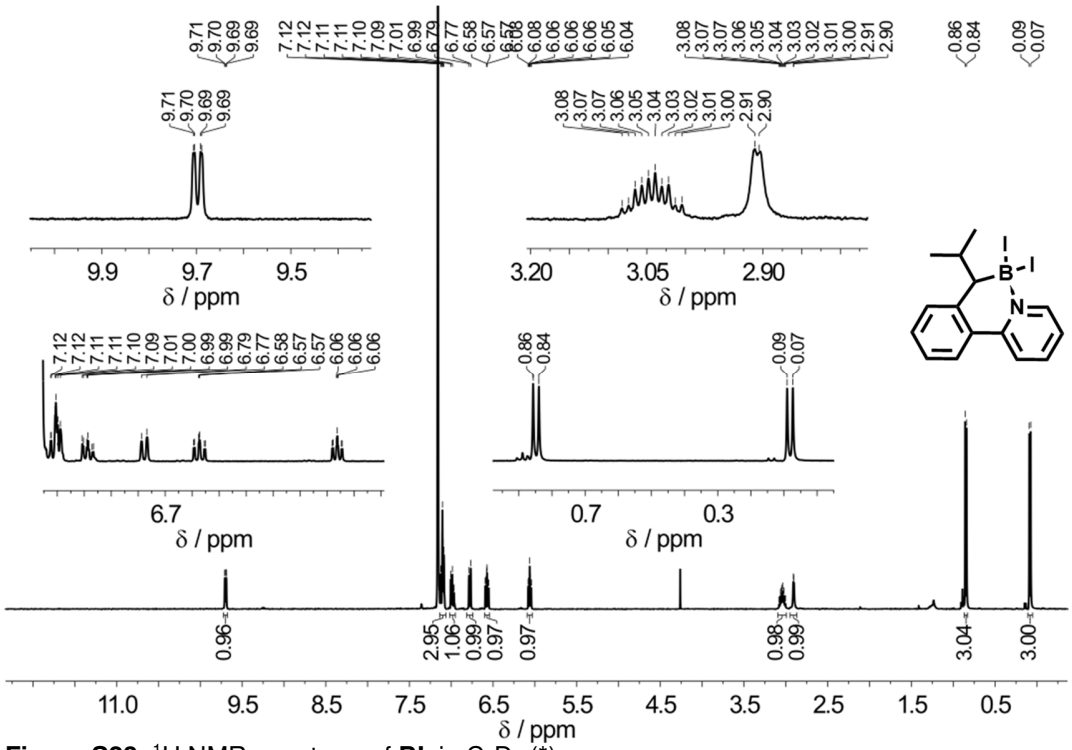


Figure S23. ^{1}H NMR-spectrum of **BI_2** in C_6D_6 (*).

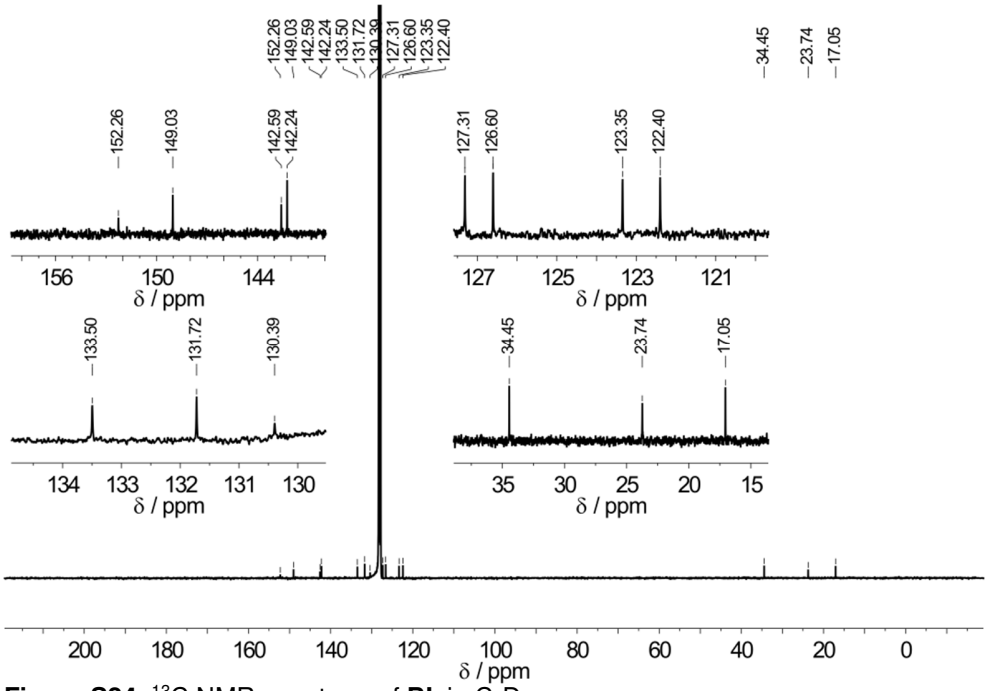


Figure S24. ^{13}C NMR-spectrum of **BI_2** in C_6D_6.

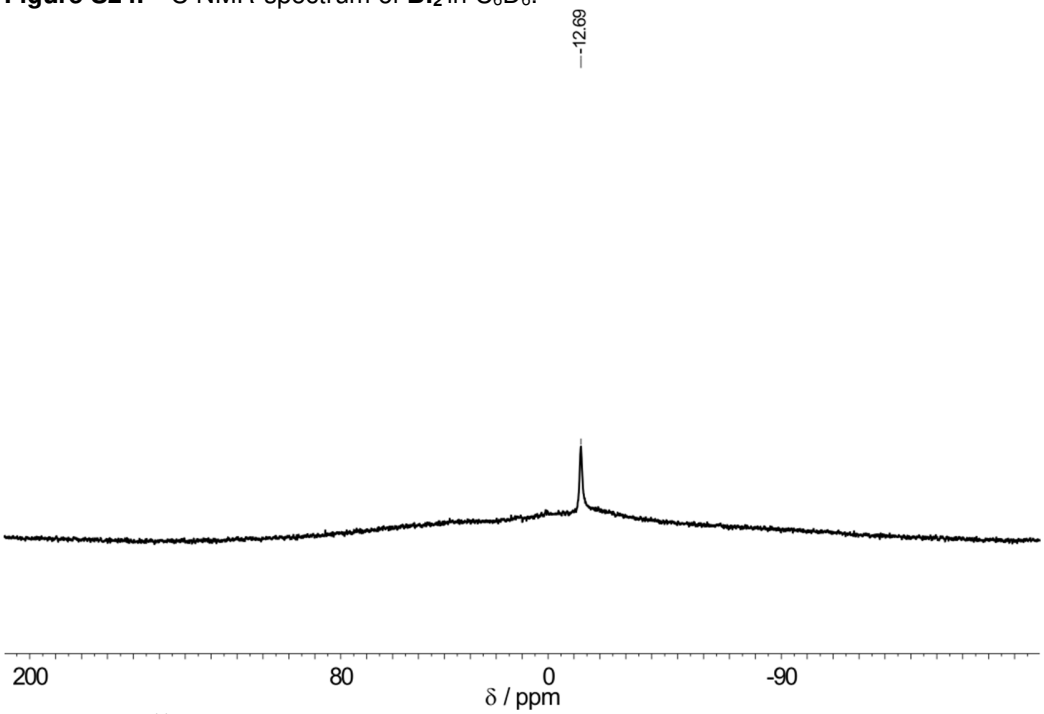


Figure S25. ^{11}B NMR-spectrum of **BI_2** in C_6D_6.

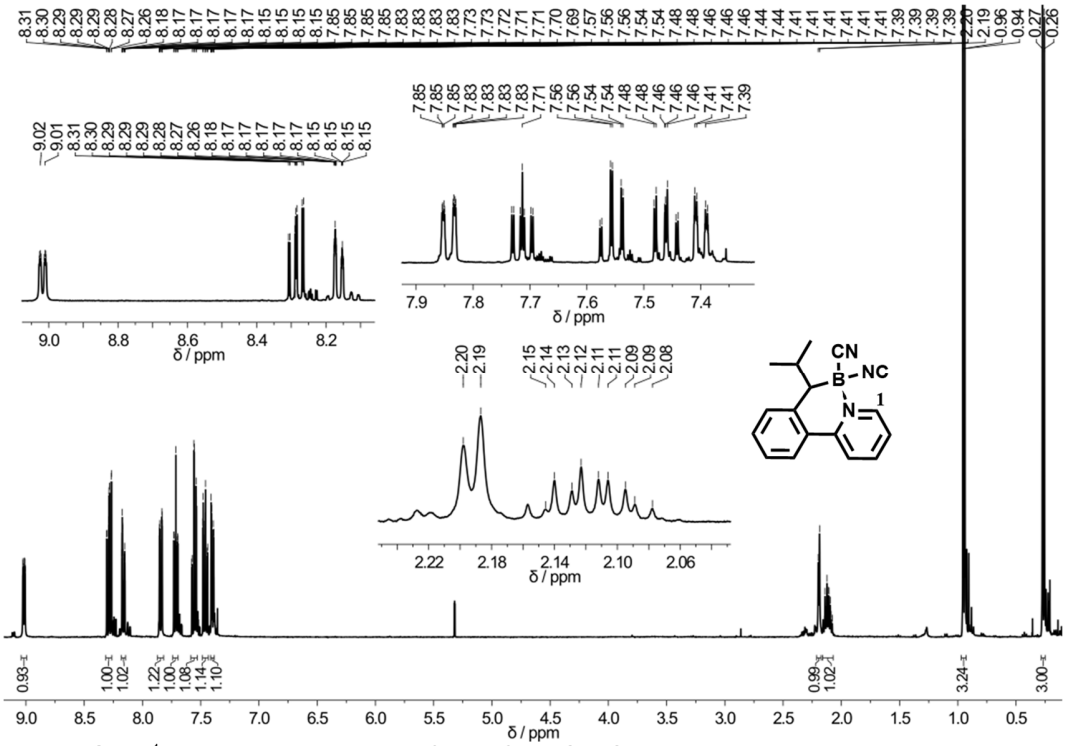


Figure S26. ^{1}H NMR-spectrum of **B(CN)(NC)** in CD_2Cl_2 (*).

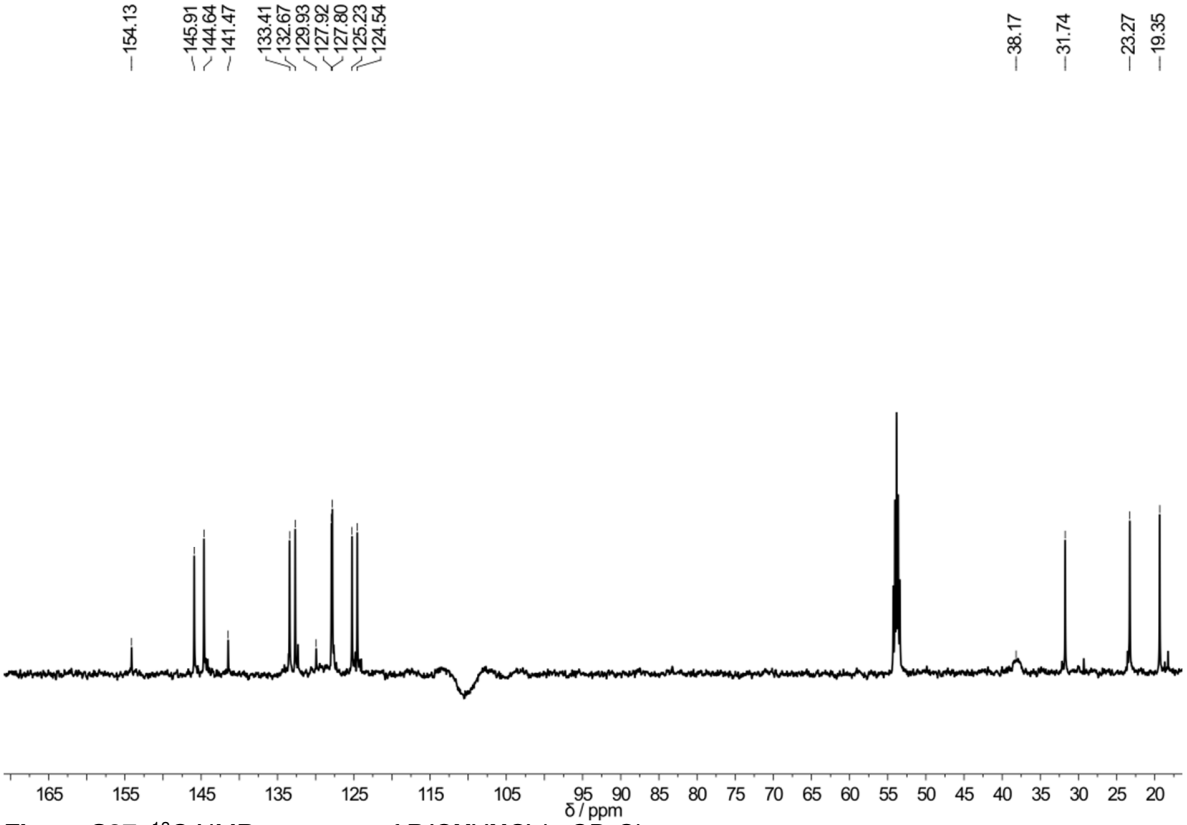


Figure S27. ^{13}C NMR-spectrum of **B(CN)(NC)** in CD_2Cl_2.

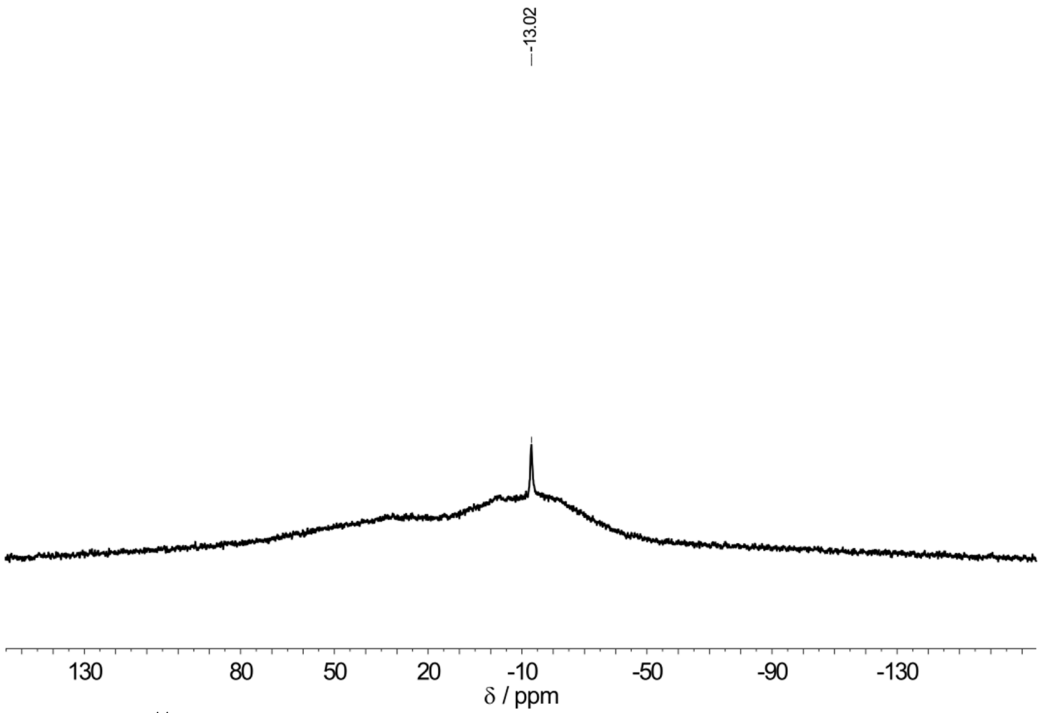
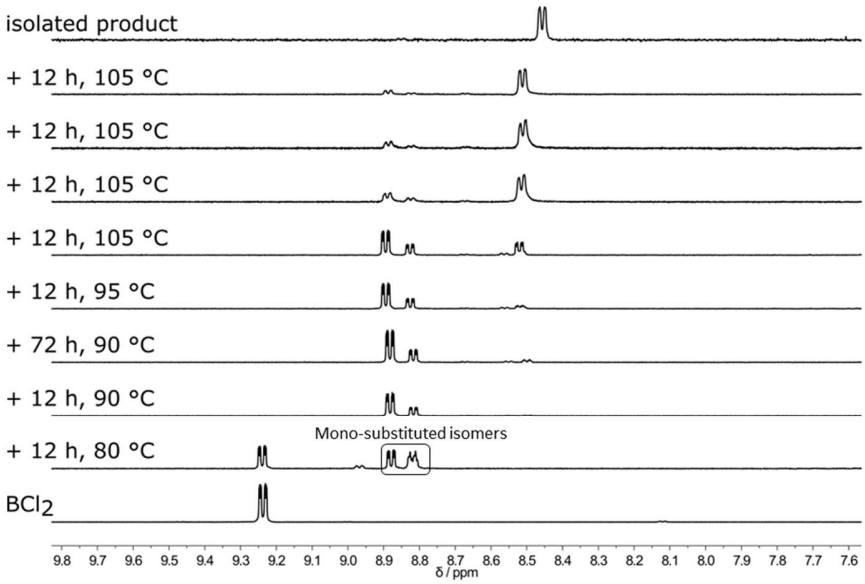
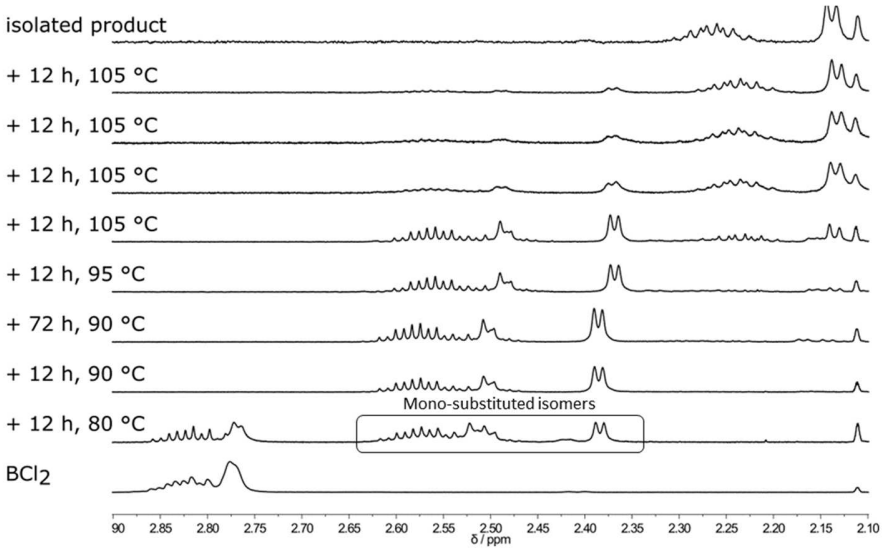


Figure S28. ^{11}B NMR-spectrum of **B(CN)(NC)** in C_6D_6.



Aromatic region of ^{1}H-NMR controls during the reaction between BCl_2 and TMS-CN in C_6D_6.



Aliphatic region of ^{1}H-NMR controls during the reaction between BCl_2 and TMS-CN in C_6D_6.

Figure S29. Monitoring of the formation of **B(CN)(NC)** in C_6D_6 (*).

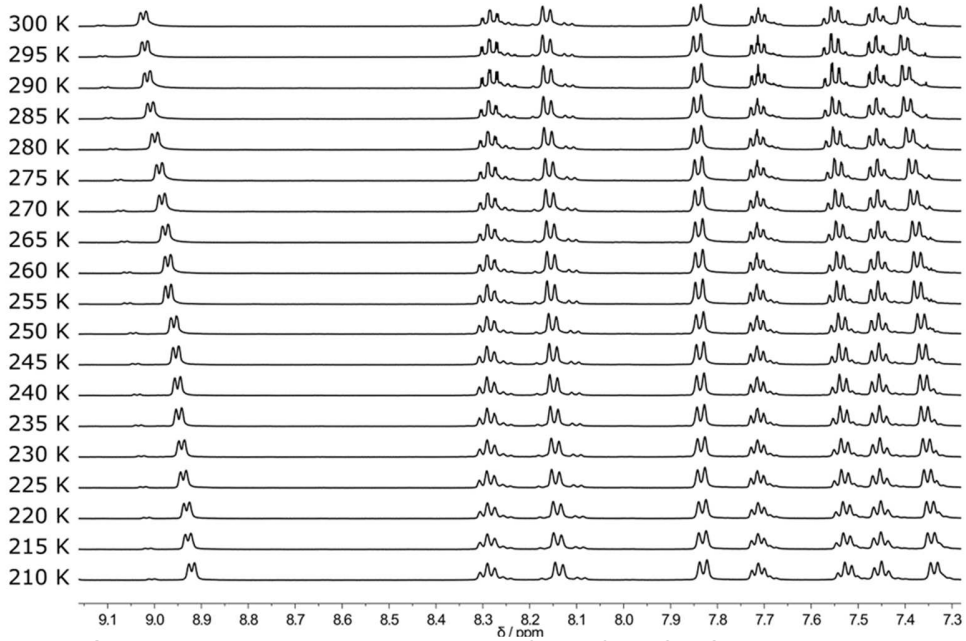


Figure S30. Variable temperature NMR of **B(CN)(NC)** in CD_2Cl_2 (*).

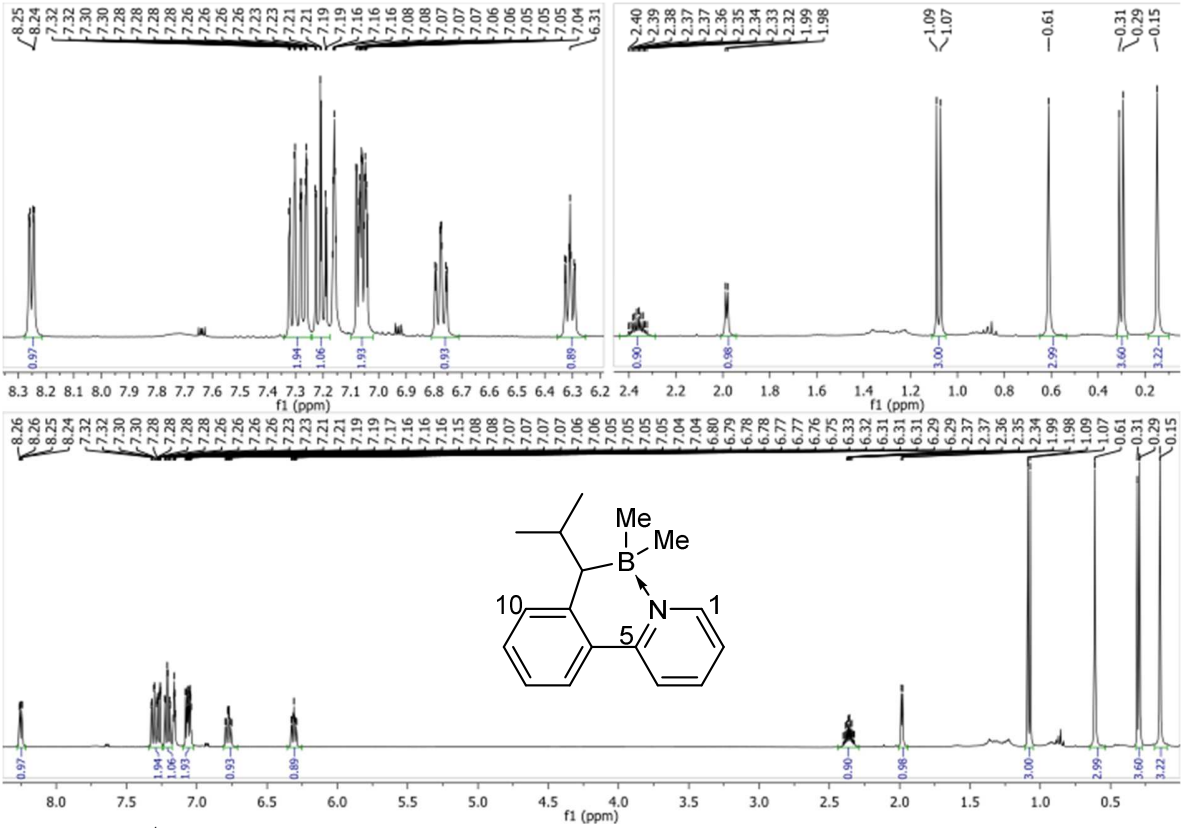


Figure S31. ^{1}H NMR-spectrum of **BMe_2** in C_6D_6 (*).

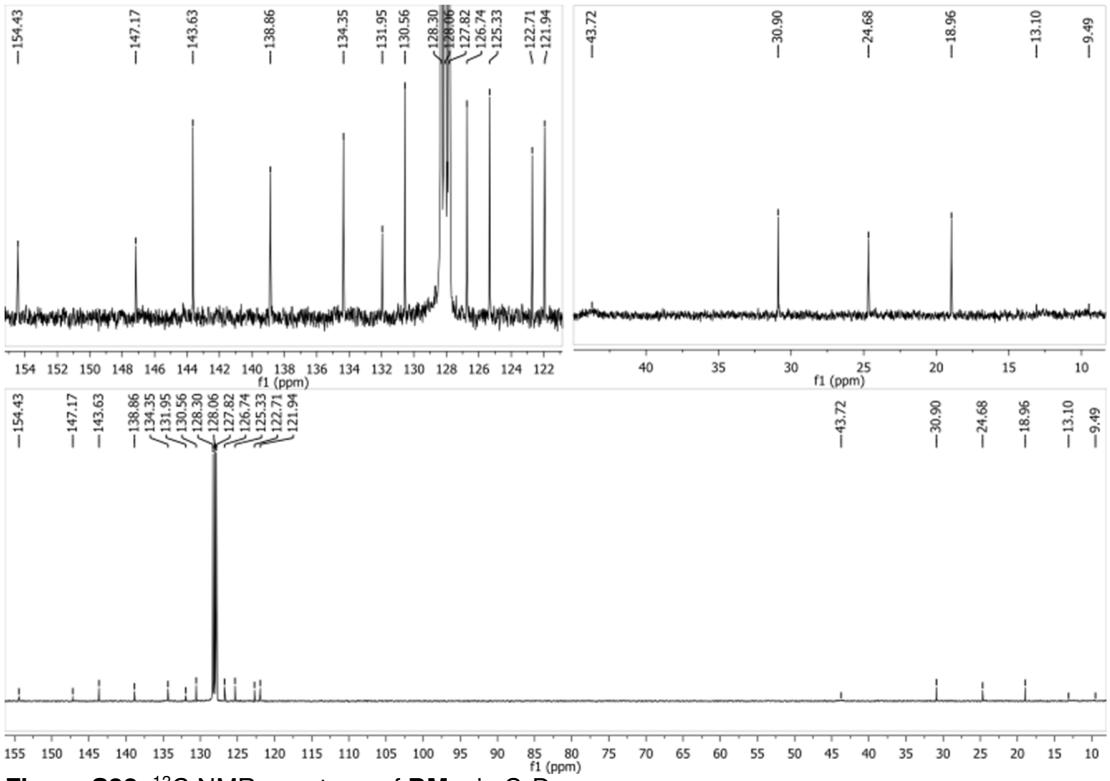


Figure S32. ^{13}C NMR-spectrum of **BMe_2** in C_6D_6.

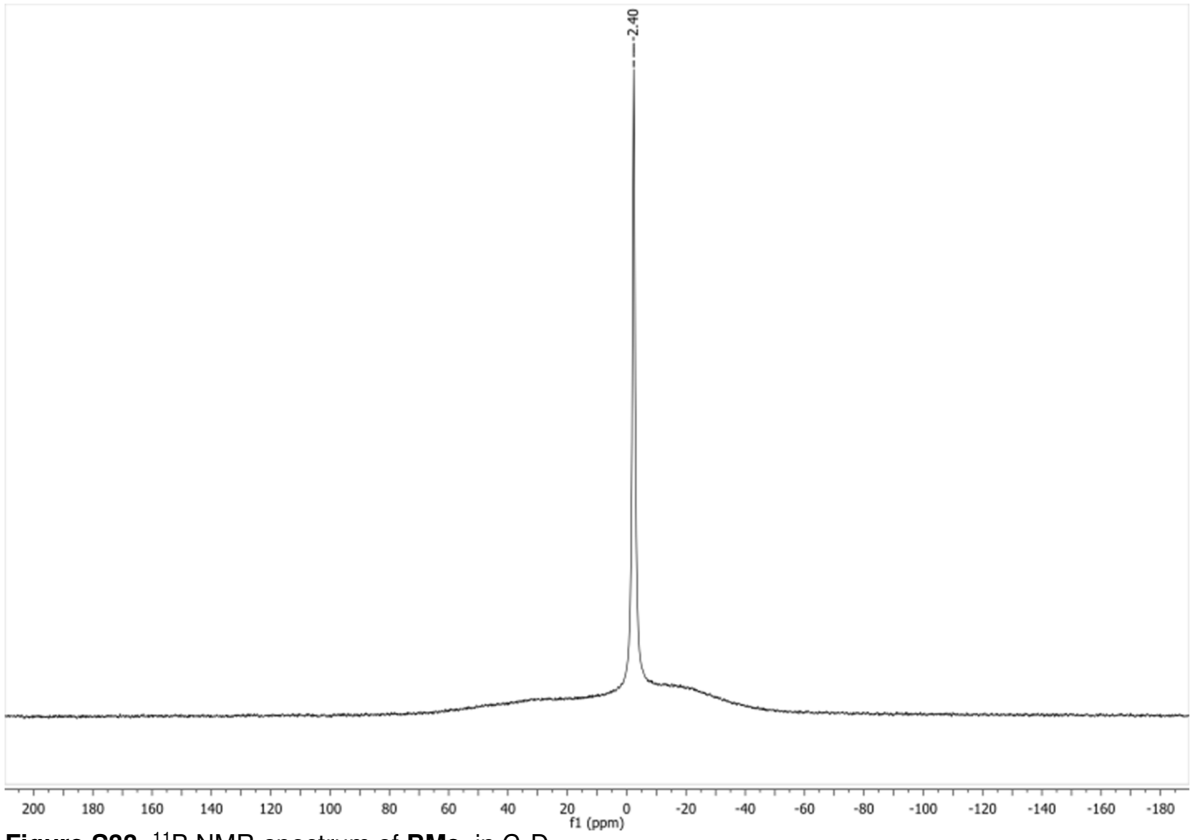


Figure S33. ^{11}B NMR-spectrum of **BMe_2** in C_6D_6.

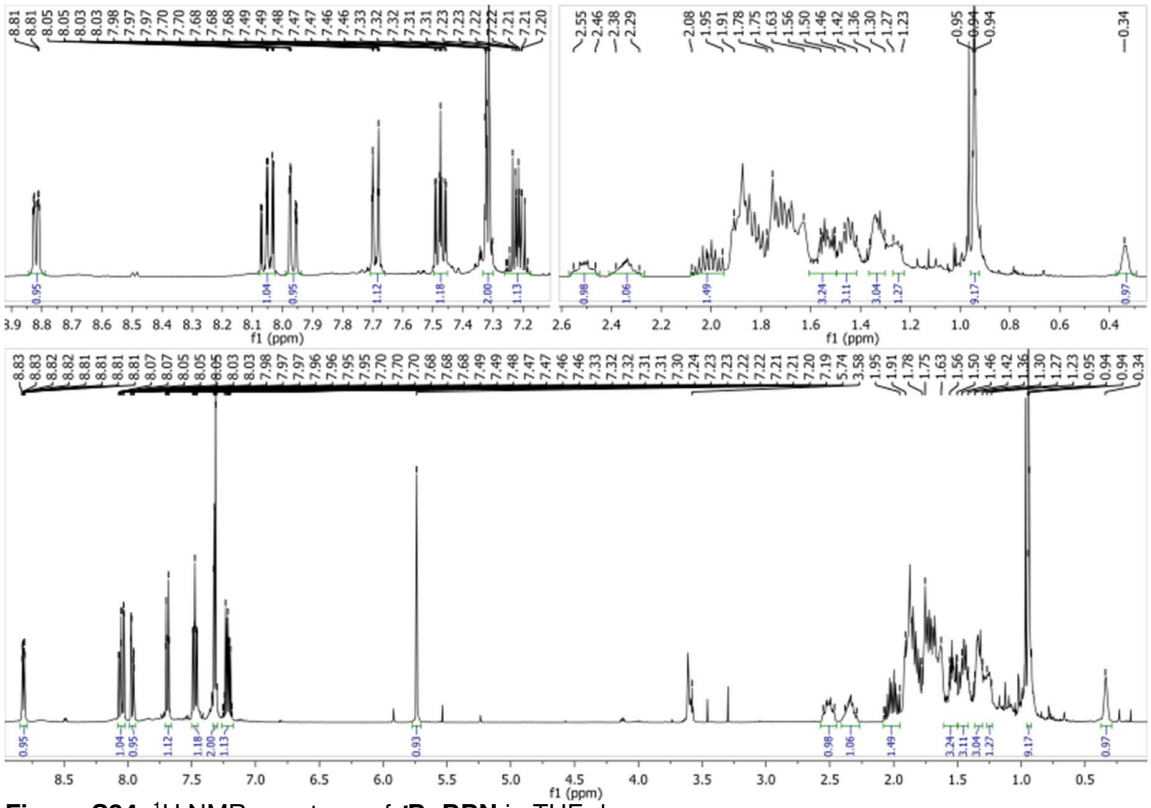


Figure S34. ^{1}H NMR-spectrum of ***t*BuBBN** in THF-d_8.

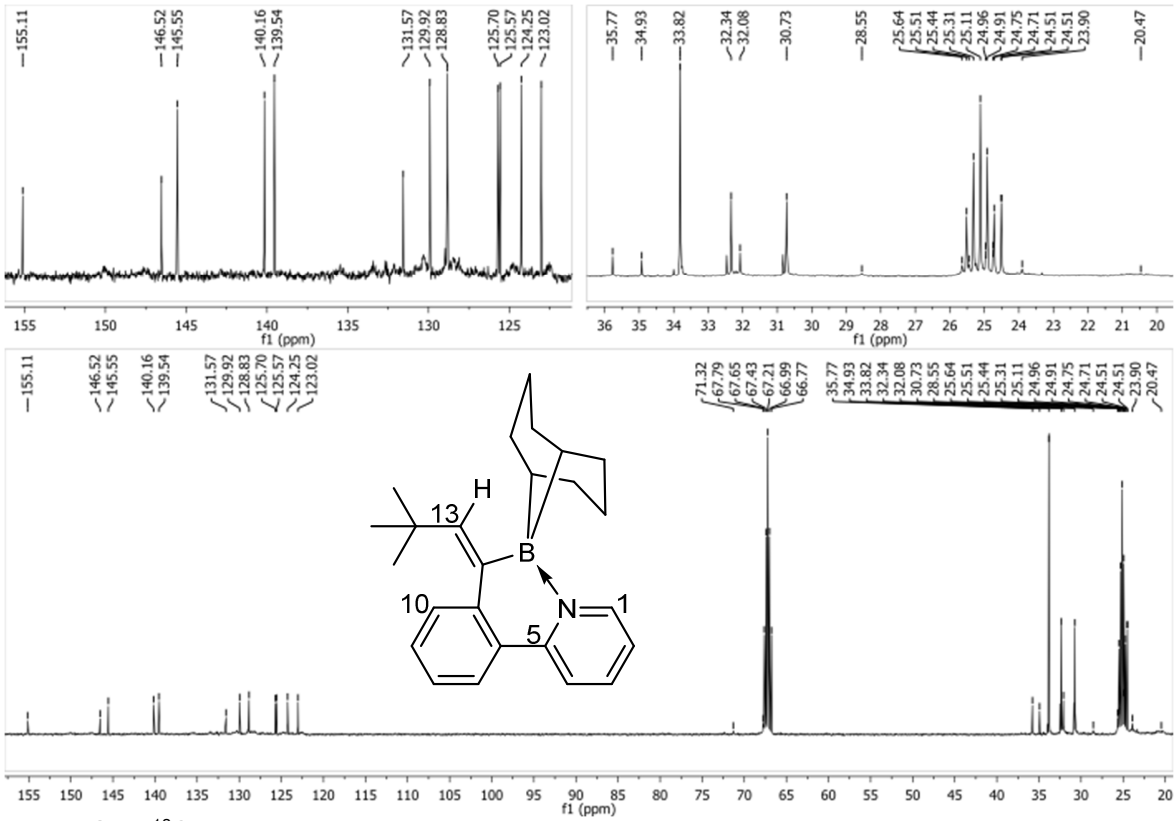


Figure S35. ^{13}C NMR-spectrum of ***t*BuBBN** in THF-d_8.

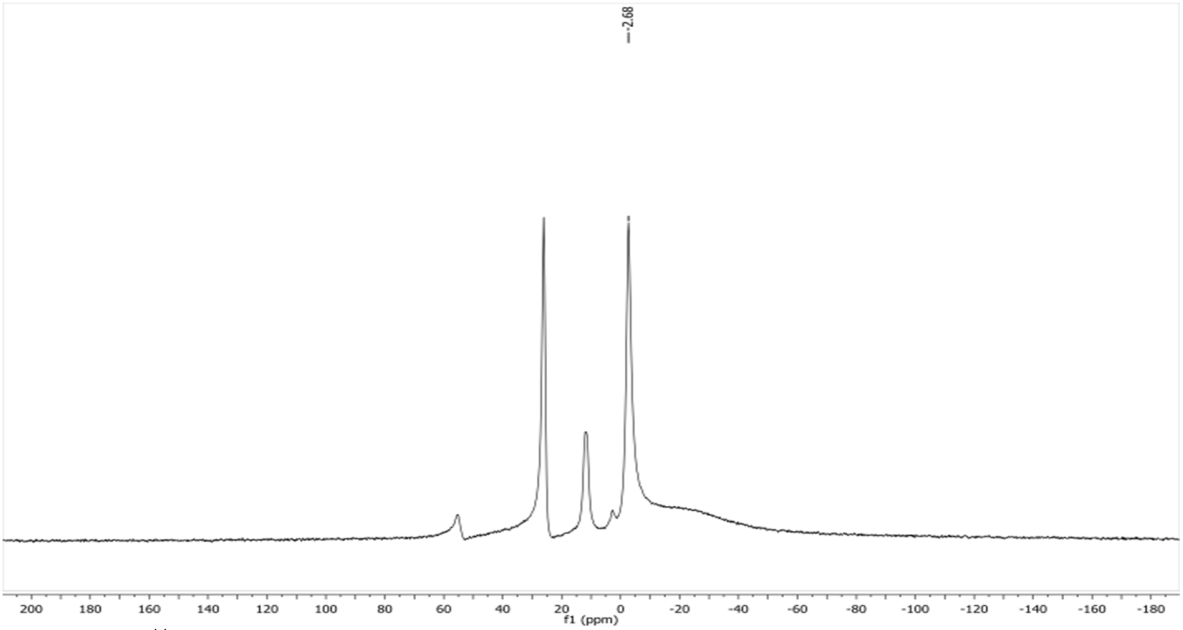


Figure S36. ^{11}B NMR-spectrum of ***t*BuBBN** in THF-d_8.

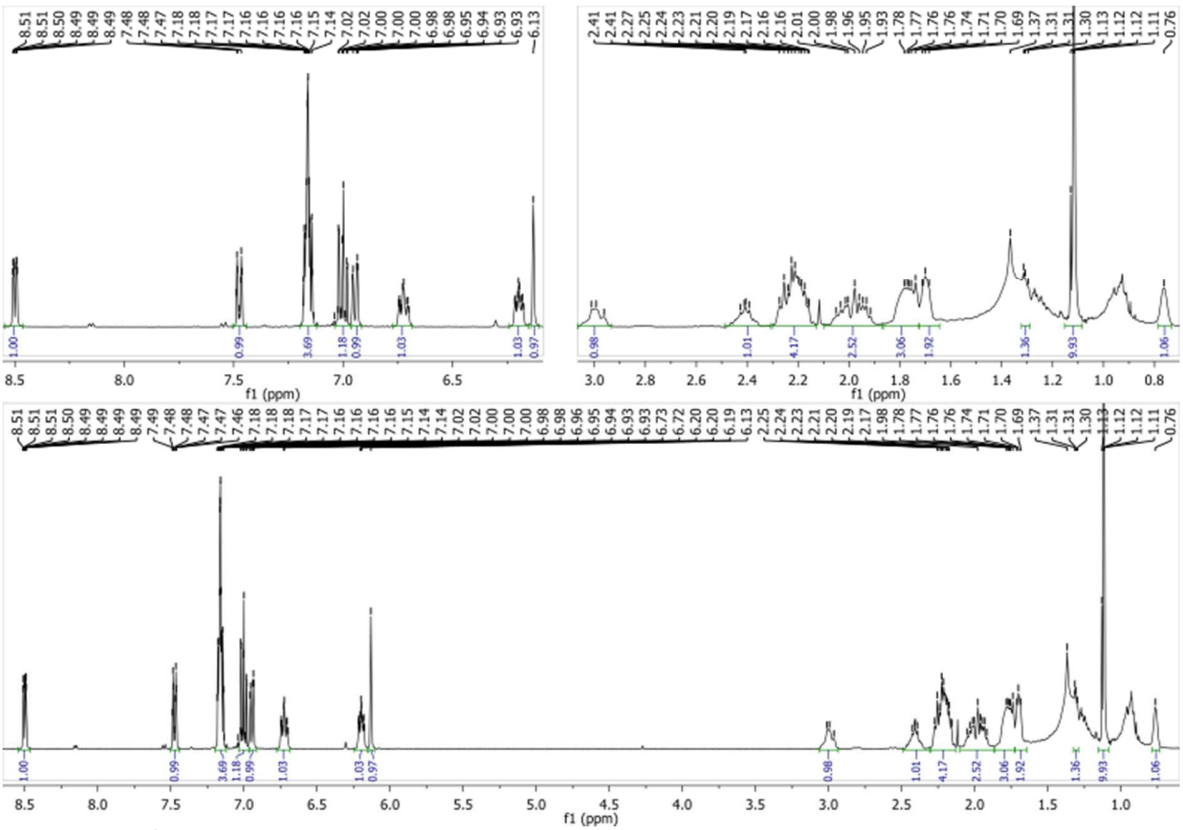


Figure S37. ^{1}H NMR-spectrum of ***t*BuBBN** in C_6D_6.

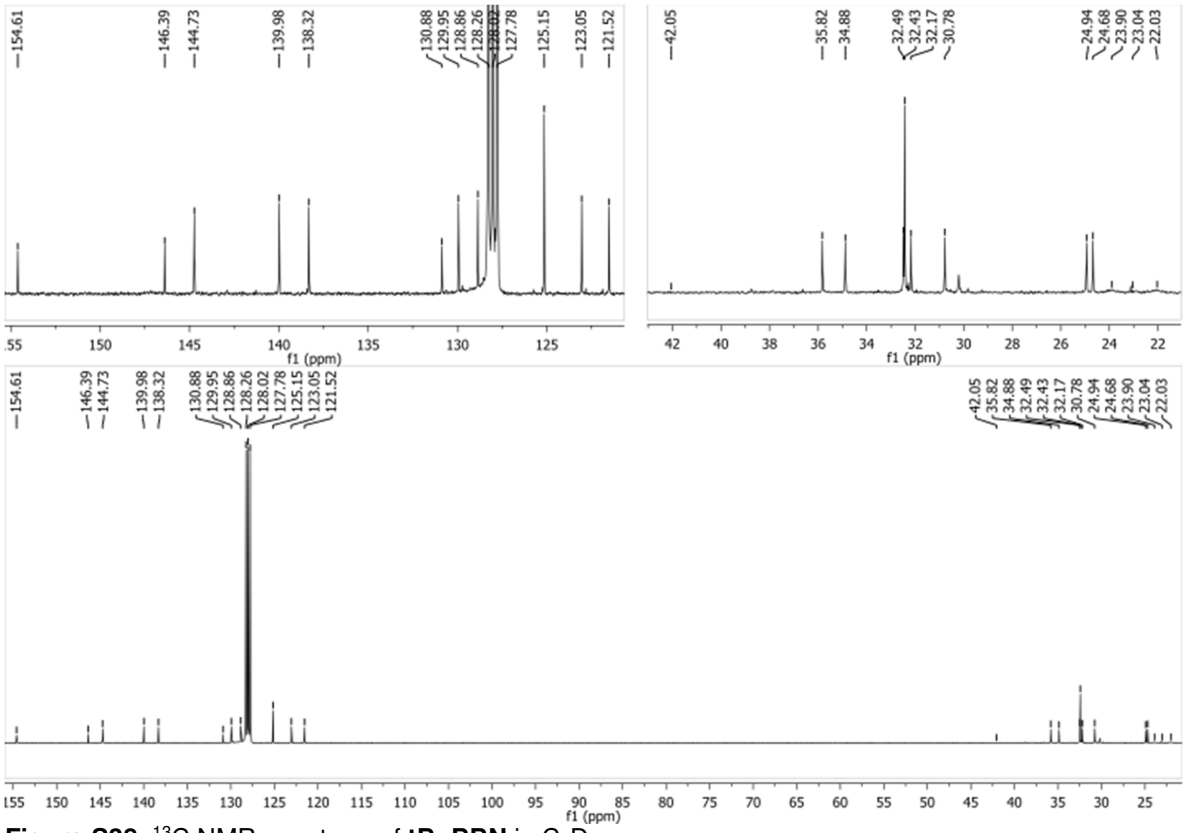


Figure S38. ^{13}C NMR-spectrum of **tBuBBN** in C_6D_6.

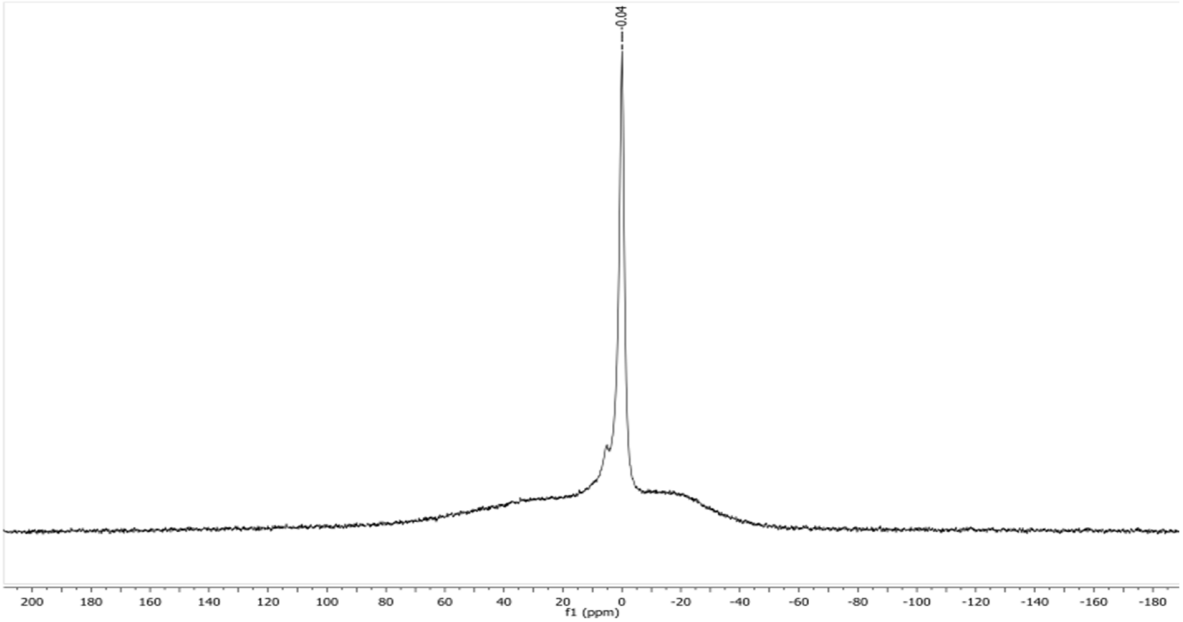


Figure S39. ^{11}B NMR-spectrum of **tBuBBN** in C_6D_6.

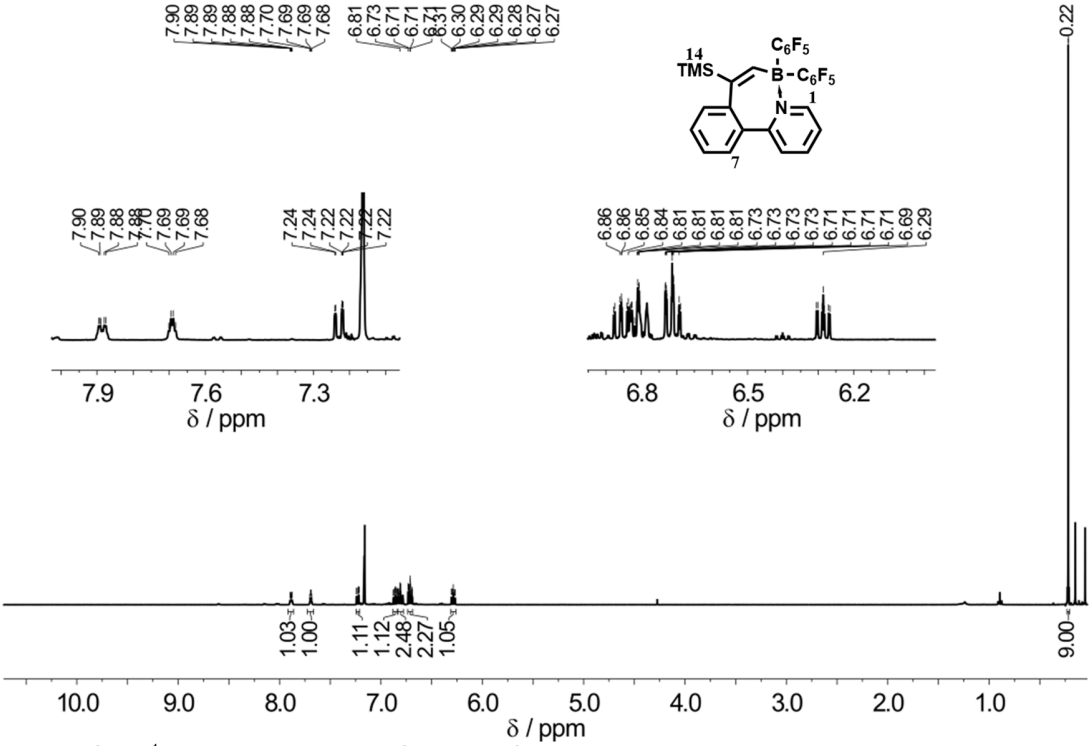


Figure S40. ^{1}H NMR-spectrum of **SiBPF** in C_6D_6.

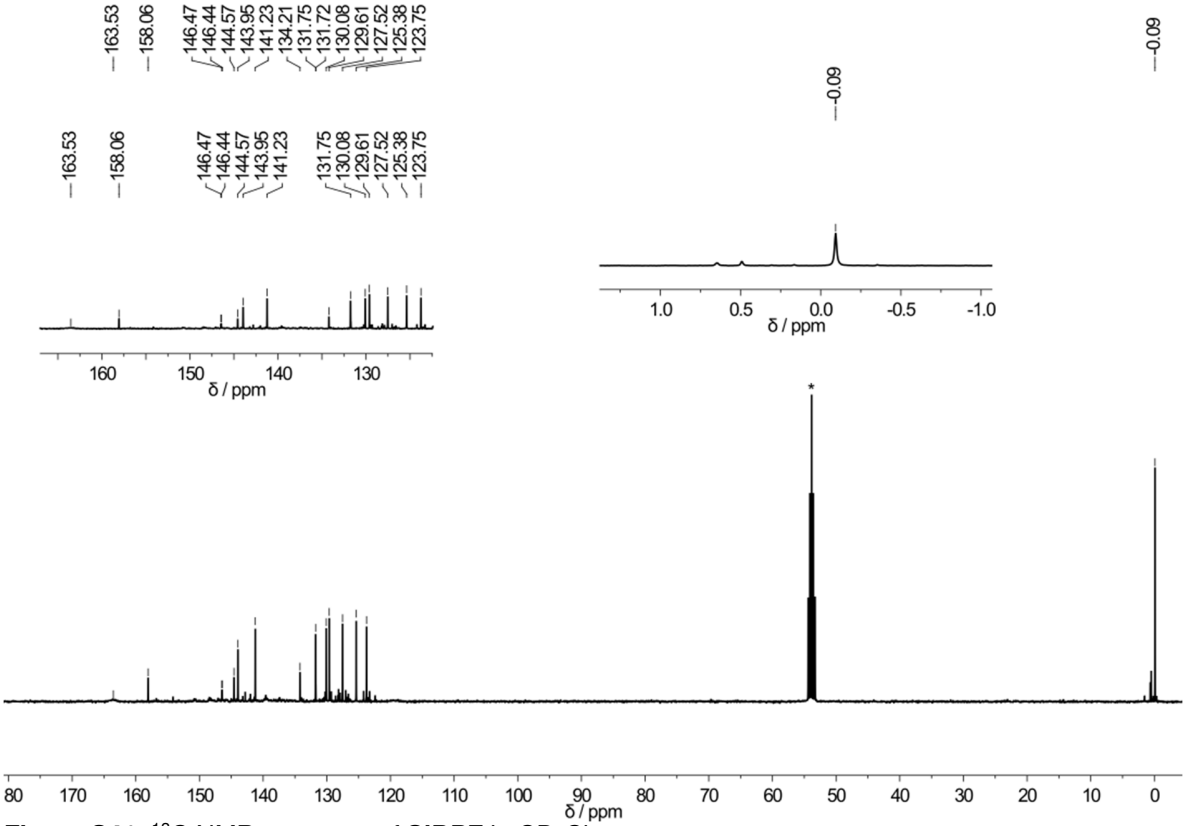


Figure S41. ^{13}C NMR-spectrum of **SiBPF** in CD_2Cl_2.

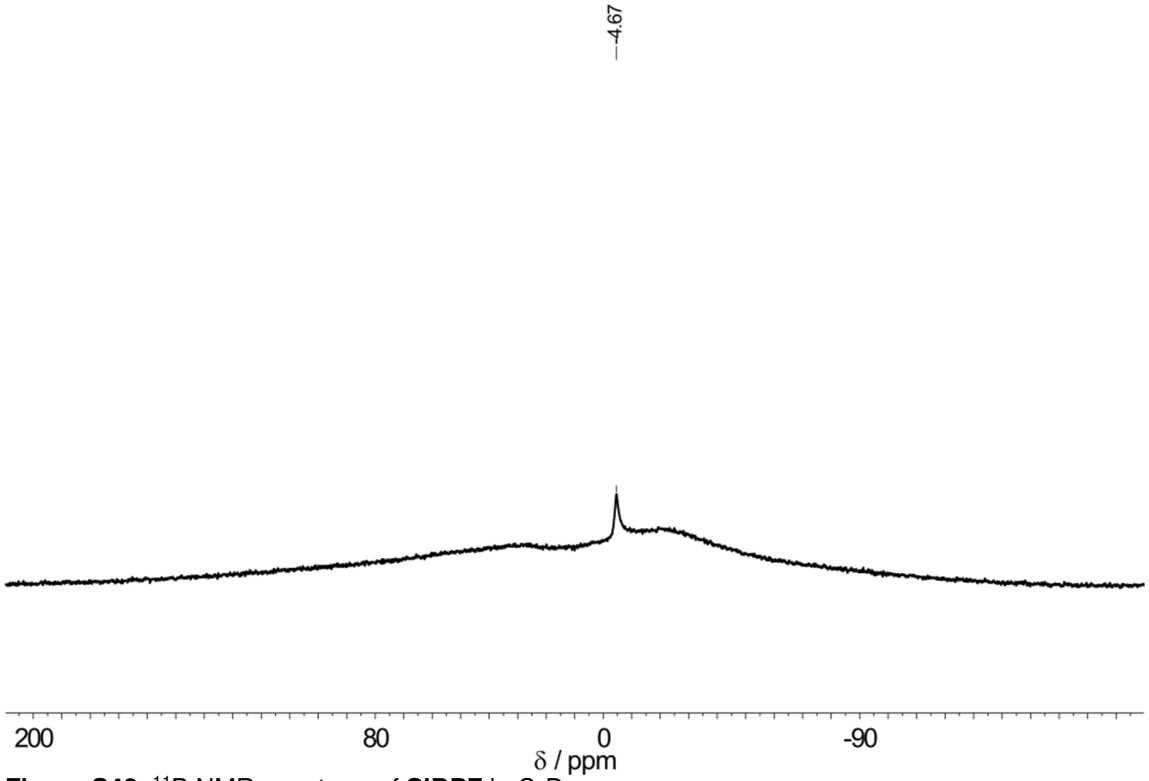


Figure S42. ^{11}B NMR-spectrum of **SiBPF** in C_6D_6.

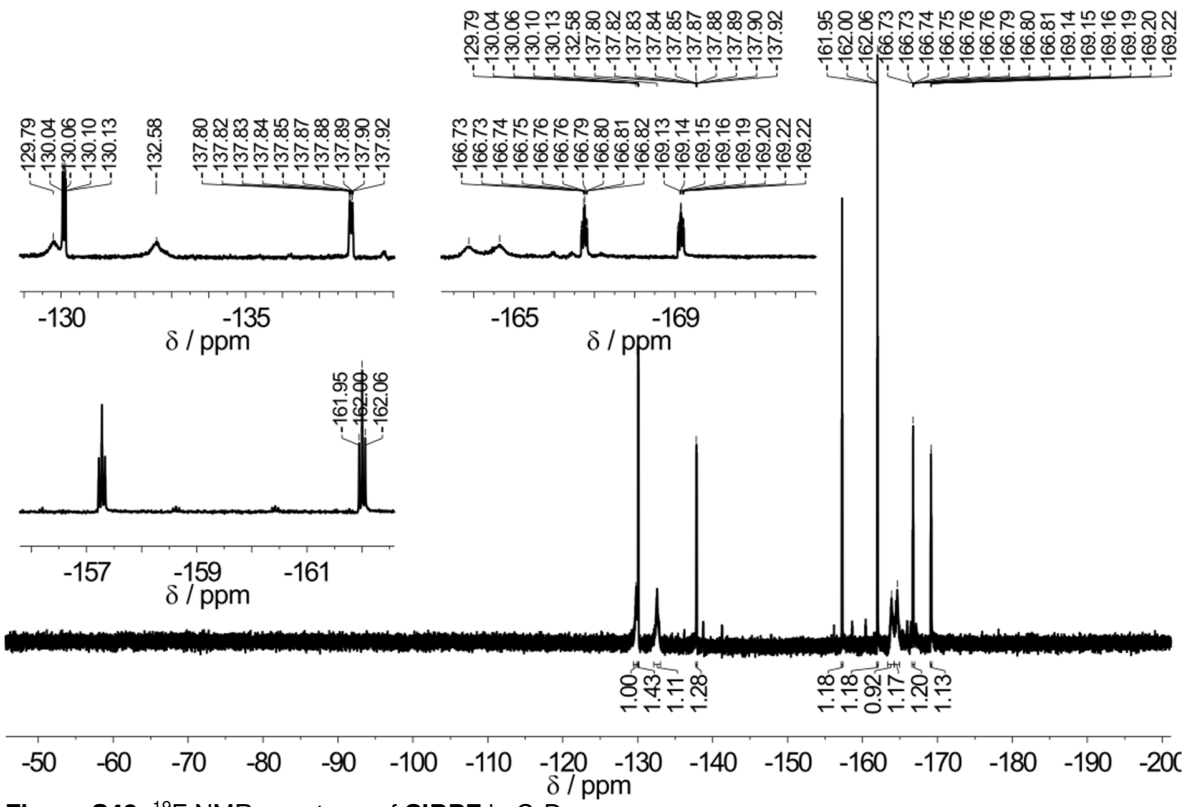


Figure S43. ^{19}F NMR-spectrum of **SiBPF** in C_6D_6.

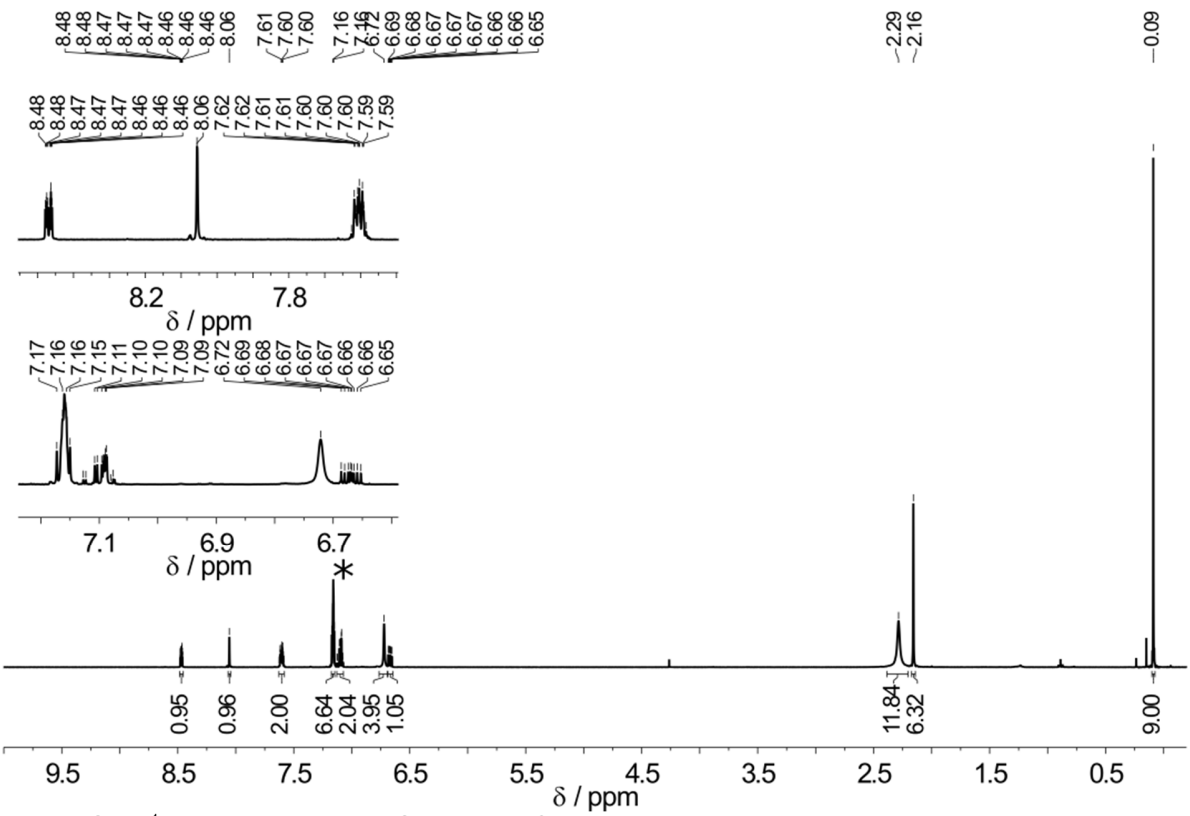


Figure S44. ^{1}H NMR-spectrum of **SiBMes$_2$** in C_6D_6 (*).
*Signal is superimposed by solvent peak

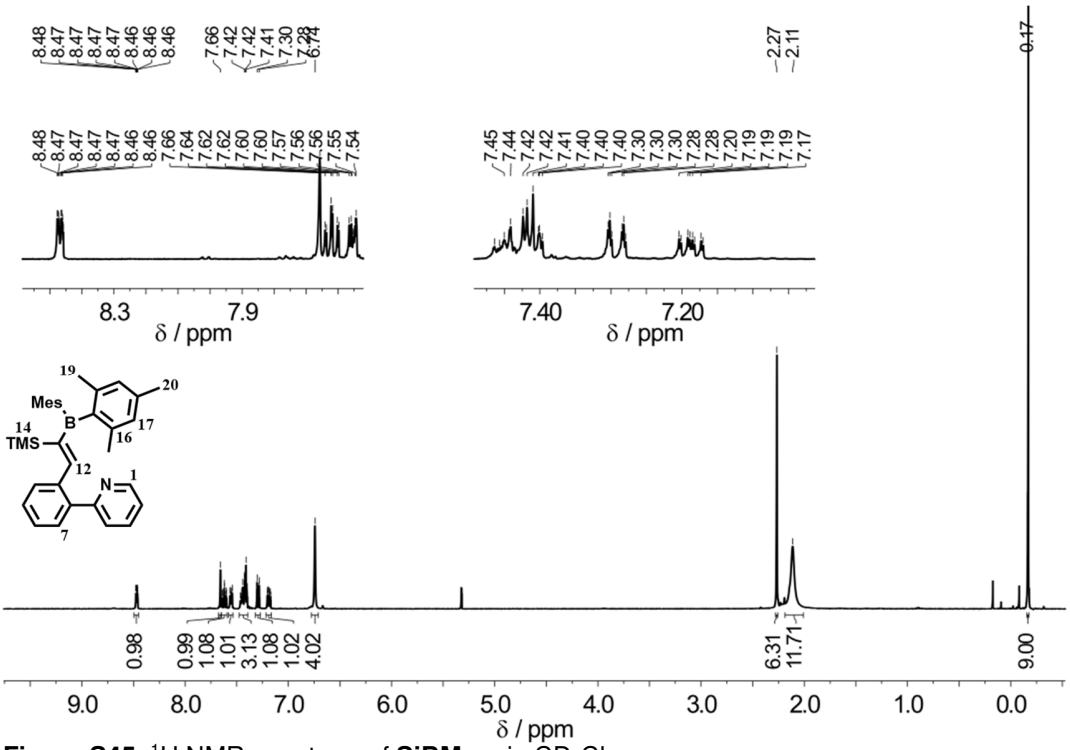


Figure S45. ^{1}H NMR-spectrum of **SiBMes$_2$** in CD_2Cl_2.

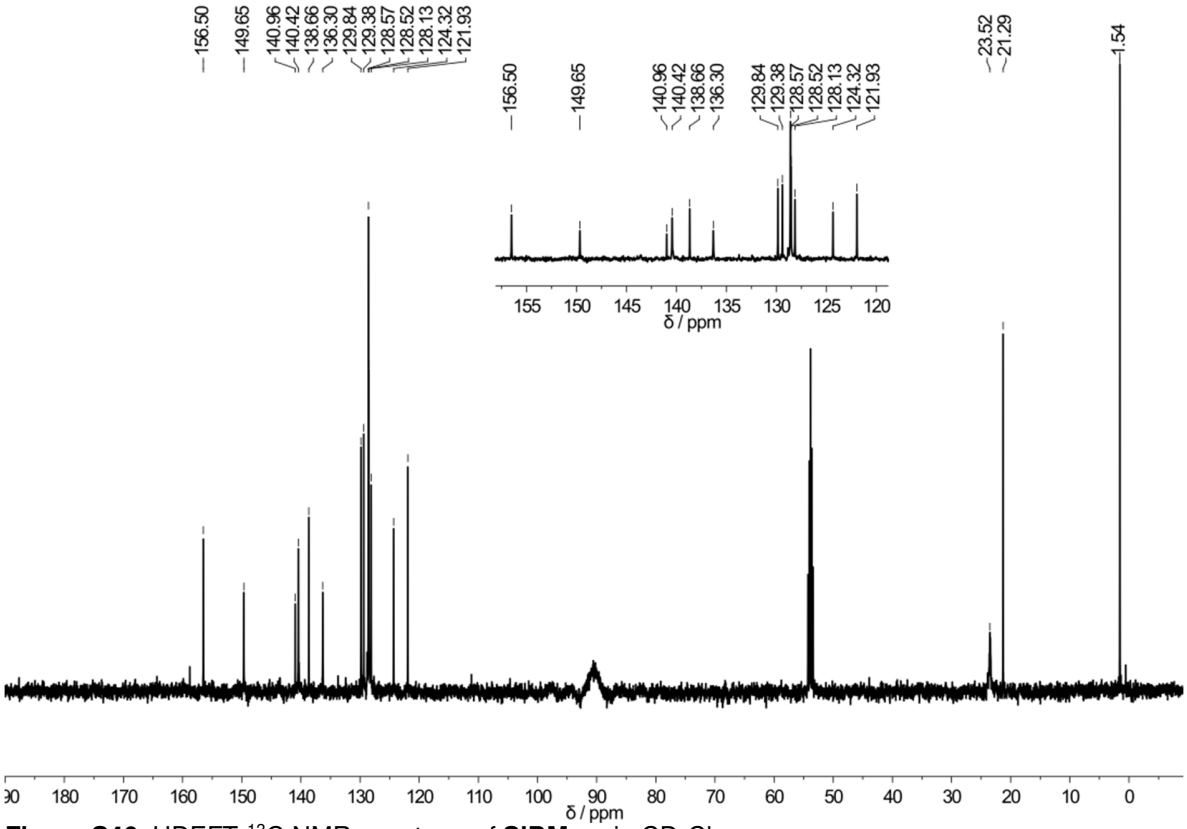


Figure S46. UDEFT-^{13}C NMR-spectrum of **SiBMes$_2$** in CD_2Cl_2.