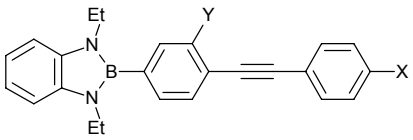
Supplementary Material (ESI) for Dalton Transactions

Supporting Information

Synthetic, structural, photophysical and computational studies on 1,3,2-benzodiazaborolyl – functionalized diphenylacetylenes.

Lothar Weber*[a], Daniel Eickhoff[a], Vanessa Werner[a], Lena Böhling[a], Stefanie Schwedler[a], Anna Chrostowska*[b], Alain Dargelos[b], Małgorzata Maciejczyk[b], Hans-Georg Stammler[a], Beate Neumann[a]

[a]*Fakultät für Chemie der Univerität Bielefeld, D-33615 Bielefeld, GERMANY.*
[b]*Equipe Chimie Physique, IPREM, UMR 5254, Université de Pau et des Pays de l'Adour, 2 Av. du Président Angot, BP 1155, 64013 Pau Cédex, FRANCE;*
e-mail: anna.chrostowska@univ-pau.fr; lothar.weber@uni-bielefeld.de



2: X=H, Y=H

3: X=bdab, Y=H

4: X=H, Y=CN

5: X=OMe, Y=CN

6: X=NMe_2, Y=CN

8: X=CN, Y=CN

9: X=bdab, Y=CN

C-Tables 1 Atomic coordinates for [B3LYP/6-311G(d,p)] optimized geometries, values of total energies of molecule **2** (X=H, Y=H).

C	0.884209477079	-0.500196848608	-7.217535161202
C	0.833546051830	-0.915200711811	-8.541208022747
C	-0.234208965776	-1.706480466031	-9.001005407708
C	-1.239799584528	-2.064735350606	-8.085530153976
C	-1.170929347857	-1.646649882357	-6.763648440534
C	-0.295558415989	-2.133076984178	-10.356111497870
C	-0.347844611891	-2.496510959180	-11.509941709043
C	-0.409364828854	-2.923808291882	-12.865810324426
C	-1.458436063732	-3.749540649667	-13.310043933493
C	0.577549437308	-2.528659838891	-13.787575749835
C	0.513166752409	-2.948274313480	-15.110500775837
C	-0.531082414079	-3.766670267752	-15.539608630858
C	-1.514583137657	-4.164583786135	-14.634767814175
C	-0.111614384930	-0.852083023974	-6.287725607575
C	0.059503061897	0.335279433418	-0.214742786052
C	-0.097780531691	-0.700301058603	-1.139391393937
C	-0.057590711211	-0.391082010047	-2.495833315901
C	0.248684775507	1.651346928572	-0.637646533142
C	0.302210617820	1.967711172970	-1.997484397926
C	0.158378057882	0.939578452751	-2.924533521771
N	-0.189909840073	-1.206271809788	-3.622013107762
N	0.176104268746	0.960704253624	-4.320813859638
B	-0.044161546106	-0.382596992200	-4.796666162307
C	-0.375227612892	-2.649240014315	-3.518896518956
C	-1.798284445382	-3.065906188879	-3.131753286365
C	0.332042360531	2.198100004814	-5.076833470322
C	1.771184277267	2.723322633554	-5.116682363849
H	1.729030942386	0.098959619262	-6.895627214297
H	1.618883670585	-0.634880531957	-9.233143561706
H	-2.071761988320	-2.670011201347	-8.425512753600
H	-1.970708453034	-1.931965695392	-6.088912625326
H	-2.221426148253	-4.057562063010	-12.605460652715
H	1.387895180858	-1.892801274203	-13.452184867737
H	1.280425488887	-2.635779140881	-15.809876589436
H	-0.578114515824	-4.092262272590	-16.572479361423
H	-2.328642085156	-4.801029625565	-14.962986190298
H	0.028790436980	0.110393413104	0.845125914969
H	-0.252345572116	-1.717465257091	-0.800181003517
H	0.360868694336	2.440982092150	0.096343972237
H	0.457794061382	2.991710697862	-2.314965997957
H	-0.112040981201	-3.084697316855	-4.484369576884
H	0.339339481632	-3.045705916973	-2.788740679855
H	-1.866331500973	-4.155307772233	-3.061222030421
H	-2.092779712672	-2.643902271351	-2.168808289416
H	-2.520791408437	-2.727473430843	-3.878281128509
H	-0.021457617682	2.010171047193	-6.092224316050
H	-0.329561571242	2.959664419969	-4.648312657135
H	1.816731959909	3.655315043802	-5.687394688776
H	2.155451350633	2.919664208941	-4.113673892592
H	2.437567013749	1.999834196335	-5.592529912336

Etot =-1063.081938 au

C-Tables 2 Atomic coordinates for [B3LYP/6-311G(d,p)] optimized geometries, values of total energies of molecule **3** (X=bdab, Y=H).

5	0	-2.29225	6.01664	-0.08525
7	0	-2.28754	6.93027	-1.20026
7	0	-2.91067	6.7208	1.01009
6	0	-1.73585	4.55421	-0.0655
6	0	-2.88122	8.12593	-0.78932
6	0	-1.83245	6.71795	-2.56946
6	0	-3.25572	8.00038	0.56916
6	0	-3.11383	6.29199	2.38912
6	0	-0.43144	4.25615	-0.50075
6	0	-2.51555	3.47456	0.38873
6	0	-3.13299	9.30352	-1.487
6	0	-0.50117	7.40412	-2.89396
1	0	-2.6092	7.06921	-3.258
1	0	-1.74078	5.64123	-2.72238
6	0	-3.85335	9.06316	1.2402
6	0	-4.56607	5.93196	2.72058
1	0	-2.76542	7.08535	3.05998
1	0	-2.46977	5.42826	2.56298
6	0	0.07163	2.96248	-0.482
1	0	0.21329	5.0568	-0.84705
6	0	-2.02997	2.17417	0.40732
1	0	-3.53298	3.65177	0.72051
6	0	-3.74408	10.36188	-0.80987
1	0	-2.85975	9.40714	-2.53012
1	0	-0.55848	8.48402	-2.74352
1	0	-0.22572	7.21954	-3.93631
1	0	0.3004	7.02117	-2.25768
6	0	-4.09232	10.24612	0.53627
1	0	-4.13445	8.98104	2.28314
1	0	-5.23829	6.77557	2.55161
1	0	-4.6506	5.63426	3.76971
1	0	-4.91307	5.1005	2.1024
6	0	-0.72212	1.89422	-0.0274
1	0	1.08316	2.76374	-0.81587
1	0	-2.65585	1.36105	0.75556
1	0	-3.94504	11.286	-1.33951
1	0	-4.55895	11.082	1.04465
6	0	-0.21529	0.56594	-0.00752
6	0	0.21529	-0.56594	0.00752
6	0	0.72212	-1.89422	0.0274
6	0	-0.07163	-2.96248	0.482
6	0	2.02997	-2.17417	-0.40732
6	0	0.43144	-4.25615	0.50075
1	0	-1.08316	-2.76374	0.81587
6	0	2.51555	-3.47456	-0.38873
1	0	2.65585	-1.36105	-0.75556
6	0	1.73585	-4.55421	0.0655
1	0	-0.21329	-5.0568	0.84705
1	0	3.53298	-3.65177	-0.72051
5	0	2.29225	-6.01664	0.08525
7	0	2.28754	-6.93027	1.20026
7	0	2.91067	-6.7208	-1.01009
6	0	2.88122	-8.12593	0.78932
6	0	1.83245	-6.71795	2.56946
6	0	3.25572	-8.00038	-0.56916
6	0	3.11383	-6.29199	-2.38912
6	0	3.13299	-9.30352	1.487
6	0	0.50117	-7.40412	2.89396

1	0	2.6092	-7.06921	3.258
1	0	1.74078	-5.64123	2.72238
6	0	3.85335	-9.06316	-1.2402
6	0	4.56607	-5.93196	-2.72058
1	0	2.76542	-7.08535	-3.05998
1	0	2.46977	-5.42826	-2.56298
6	0	3.74408	-10.36188	0.80987
1	0	2.85975	-9.40714	2.53012
1	0	0.55848	-8.48402	2.74352
1	0	0.22572	-7.21954	3.93631
1	0	-0.3004	-7.02117	2.25768
6	0	4.09232	-10.24612	-0.53627
1	0	4.13445	-8.98104	-2.28314
1	0	5.23829	-6.77557	-2.55161
1	0	4.6506	-5.63426	-3.76971
1	0	4.91307	-5.1005	-2.1024
1	0	3.94504	-11.286	1.33951
1	0	4.55895	-11.082	-1.04465

Etot =-1586.5704406 au

C-Tables 3 Atomic coordinates for [B3LYP/6-311G(d,p)] optimized geometries, values of total energies of molecule **4** (X=H, Y=CN).

C,0,-0.4890635746,-7.0487210872,-0.5184425465
C,0,-1.1914983713,-5.8477689279,-0.6416164825
C,0,-0.5101617795,-4.655353789,-0.4156913323
C,0,0.8638283709,-4.6636044513,-0.0815245866
C,0,1.5560819809,-5.8643223392,0.0447657693
C,0,0.8643136058,-7.0571317944,-0.1776226628
N,0,-0.9442912339,-3.3286612828,-0.485495501
B,0,0.1798300591,-2.4749053696,-0.2086711503
N,0,1.3002412827,-3.3415423526,0.0445000065
C,0,0.1897308891,-0.9072804268,-0.2195650233
C,0,-0.6776226907,-0.1599521941,0.5863759589
C,0,-0.6768170372,1.2396725047,0.5749317379
C,0,0.2117096801,1.9495938682,-0.2715661028
C,0,1.078924296,1.2001720136,-1.0837875422
C,0,1.0664806109,-0.1866068667,-1.052817748
C,0,0.2219814296,3.3658936219,-0.2978941412
C,0,0.2093120838,4.5761557973,-0.2999435081
C,0,0.1649230845,5.9967896251,-0.2733537929
C,0,-0.7268289538,6.6559123181,0.5932165005
C,0,-0.7735211399,8.0438568404,0.6229339677
C,0,0.061235469,8.794420287,-0.204805399
C,0,0.9476318679,8.1495365402,-1.0668659597
C,0,1.0028031103,6.7619069078,-1.1044089671
C,0,-2.3092448714,-2.9727345306,-0.859461151
C,0,-3.3295543203,-3.1672616052,0.2665884941
C,0,2.6529081378,-3.0068085079,0.4778211676
C,0,2.8711109294,-3.1744973519,1.9848373545
H,0,-1.0060339517,-7.9860940657,-0.687959884
H,0,-2.2417964889,-5.8528495799,-0.9067436766
H,0,2.6080207942,-5.8808626443,0.3031536417
H,0,1.3888452338,-8.0009604824,-0.0842755921
H,0,-1.3689501367,-0.6617348947,1.2532103847
C,0,-1.5822466059,1.9473254117,1.4255396301
H,0,1.7595575977,1.7274135083,-1.7408317032
H,0,1.7460166085,-0.7258721967,-1.7044400959
H,0,-1.3726311526,6.0665891688,1.2327159546
H,0,-1.4637301638,8.5419958529,1.2941143445
H,0,0.0210983212,9.8773652473,-0.1782460653
H,0,1.5976357372,8.7302194356,-1.7114605421
H,0,1.6898563832,6.2570730098,-1.7727255731
H,0,-2.3023241702,-1.9280812639,-1.1760489816
H,0,-2.6007736354,-3.5646479858,-1.7341576341
H,0,-4.3311692258,-2.9008739827,-0.0822034224
H,0,-3.3536786906,-4.2028178825,0.6117826249
H,0,-3.0904680589,-2.5345546782,1.1247368644
H,0,3.3655290425,-3.624797438,-0.0789755363
H,0,2.8471968247,-1.9711796507,0.1945975517
H,0,3.9049449589,-2.9322434269,2.2470423568
H,0,2.2118999345,-2.5073269361,2.5452547121
H,0,2.6692653375,-4.1982973644,2.3066447176
N,0,-2.321086992,2.5033341946,2.1184682797

Etot =-1155.3458702 au

C-Tables 4 Atomic coordinates for [B3LYP/6-311G(d,p)] optimized geometries, values of total energies of molecule **5** (X=OMe, Y=CN).

8	0	9.37367	-0.15117	0.18885
6	0	8.02283	-0.16716	0.0303
6	0	10.18061	-0.94059	-0.68757
6	0	7.29965	0.6225	0.93649
6	0	7.33979	-0.89783	-0.95044
1	0	9.94371	-2.0065	-0.59891
1	0	11.203	-0.76468	-0.3552
1	0	10.07476	-0.62	-1.72967
6	0	5.91935	0.68013	0.86589
1	0	7.8446	1.18576	1.68541
6	0	5.95076	-0.83714	-1.01444
1	0	7.87425	-1.51238	-1.66322
6	0	5.21699	-0.05494	-0.11128
1	0	5.36585	1.29839	1.56375
1	0	5.42544	-1.39965	-1.77842
6	0	3.79924	-0.00636	-0.17297
6	0	2.58793	0.01465	-0.19027
6	0	1.17182	-0.01343	-0.19362
6	0	0.40853	0.99515	0.44118
6	0	0.47484	-1.0515	-0.8348
6	0	-0.98983	0.94009	0.43591
6	0	1.05592	2.08615	1.10113
6	0	-0.91234	-1.09078	-0.8277
1	0	1.04109	-1.8234	-1.34345
6	0	-1.68906	-0.10304	-0.18813
1	0	-1.5281	1.726	0.95199
7	0	1.54528	2.98572	1.6381
1	0	-1.40768	-1.89636	-1.35966
5	0	-3.25599	-0.16769	-0.2003
7	0	-4.16597	0.87389	-0.60942
7	0	-4.07388	-1.31163	0.12832
6	0	-5.46786	0.3743	-0.52802
6	0	-3.89896	2.24478	-1.03822
6	0	-5.41248	-0.9614	-0.0703
6	0	-3.70894	-2.57525	0.76882
6	0	-6.68899	0.97141	-0.8321
6	0	-4.14091	3.29348	0.06663
1	0	-4.53283	2.46644	-1.90298
1	0	-2.86352	2.288	-1.38243
6	0	-6.57909	-1.70358	0.09647
6	0	-3.94152	-2.57456	2.29275
1	0	-2.65385	-2.76054	0.56564
1	0	-4.27681	-3.38451	0.2974
6	0	-7.85523	0.21989	-0.66603
1	0	-6.74153	1.99293	-1.19172
1	0	-5.17974	3.27499	0.40363
1	0	-3.91718	4.29436	-0.31364
1	0	-3.50167	3.10192	0.93191
6	0	-7.80112	-1.09776	-0.2072
1	0	-6.54765	-2.73027	0.44366
1	0	-3.30687	-1.82538	2.77256
1	0	-3.69556	-3.55595	2.70905
1	0	-4.98291	-2.34838	2.5314
1	0	-8.81574	0.6695	-0.8949
1	0	-8.71989	-1.66166	-0.08549

Etot =-1269.8993663 au

C-Tables 5 Atomic coordinates for [B3LYP/6-311G(d,p)] optimized geometries, values of total energies of molecule **6** (X=NMe_2, Y=CN).

C	0	-0.54789	8.22353	0.34248
C	0	-1.14673	7.01879	0.71851
C	0	-0.51348	5.82766	0.37588
C	0	0.71742	5.84141	-0.3203
C	0	1.30241	7.04534	-0.70169
C	0	0.65551	8.23653	-0.36397
N	0	-0.87902	4.49992	0.61048
B	0	0.14428	3.6476	0.06082
N	0	1.13497	4.52235	-0.51409
C	0	0.17697	2.08267	0.08308
C	0	-0.92428	1.32206	-0.32988
C	0	-0.90678	-0.07729	-0.32083
C	0	0.24457	-0.78055	0.11998
C	0	1.34885	-0.01693	0.53872
C	0	1.31201	1.36861	0.51591
C	0	0.27911	-2.19341	0.13642
C	0	0.28251	-3.40583	0.13725
C	0	0.24327	-4.82077	0.12016
C	0	-0.90131	-5.50111	-0.33772
C	0	-0.95546	-6.88194	-0.36455
C	0	0.13792	-7.66724	0.07391
C	0	1.29006	-6.97988	0.52589
C	0	1.33472	-5.5978	0.54843
C	0	-2.08175	4.14704	1.35751
C	0	-3.37652	4.28256	0.54932
C	0	2.34614	4.19368	-1.25726
C	0	3.63931	4.40728	-0.46324
H	0	-1.02989	9.15943	0.60032
H	0	-2.08555	7.01986	1.25881
H	0	2.23963	7.0668	-1.24442
H	0	1.09907	9.18233	-0.65282
H	0	-1.82172	1.81342	-0.6863
C	0	-2.06287	-0.79265	-0.76239
H	0	2.23505	-0.53508	0.88397
H	0	2.18498	1.91268	0.85952
H	0	-1.75355	-4.92498	-0.67806
H	0	-1.85554	-7.35523	-0.73041
N	0	0.08133	-9.04376	0.06439
H	0	2.15781	-7.53072	0.86043
H	0	2.23095	-5.10069	0.90075
H	0	-1.96573	3.11826	1.70278
H	0	-2.13505	4.77471	2.25395
H	0	-4.2373	4.01686	1.16929
H	0	-3.51906	5.3029	0.18788
H	0	-3.36803	3.62015	-0.31954
H	0	2.26975	3.15037	-1.56839
H	0	2.36972	4.79334	-2.17399
H	0	4.50674	4.15821	-1.08114
H	0	3.74228	5.44328	-0.13452
H	0	3.66234	3.77289	0.42637
N	0	-3.00725	-1.35381	-1.12154
C	0	1.25429	-9.82416	0.42242
C	0	-1.06829	-9.72316	-0.51113
H	0	1.58893	-9.59694	1.44007
H	0	2.09733	-9.65011	-0.25986
H	0	1.00239	-10.88266	0.38642
H	0	-1.19401	-9.50037	-1.57911

H	0	-1.99435	-9.44804	0.00439
H	0	-0.93706	-10.79843	-0.40257

Etot =-1289.3503074 au

C-Tables 6 Atomic coordinates for [B3LYP/6-311G(d,p)] optimized geometries, values of total energies of molecule **8** (X=CN, Y=CN).

C	0	-0.58991	7.66937	0.29391
C	0	-1.20992	6.46267	0.62451
C	0	-0.54704	5.27451	0.33023
C	0	0.73221	5.29383	-0.27113
C	0	1.33901	6.50027	-0.60872
C	0	0.66318	7.68781	-0.32083
N	0	-0.92396	3.94457	0.53675
B	0	0.14251	3.10006	0.06697
N	0	1.17036	3.97629	-0.43148
C	0	0.1814	1.53299	0.09304
C	0	-0.88462	0.76774	-0.39972
C	0	-0.86009	-0.63042	-0.38696
C	0	0.26084	-1.32198	0.13786
C	0	1.32833	-0.55839	0.63536
C	0	1.28553	0.82817	0.60888
C	0	0.29765	-2.73819	0.15661
C	0	0.29556	-3.94827	0.15521
C	0	0.25119	-5.36683	0.13215
C	0	-0.87405	-6.026	-0.39932
C	0	-0.92758	-7.40951	-0.42848
C	0	0.14257	-8.1665	0.07309
C	0	1.267	-7.5167	0.60457
C	0	1.31973	-6.13307	0.63341
C	0	-2.18166	3.58729	1.18597
C	0	-3.40758	3.71811	0.27635
C	0	2.43915	3.65464	-1.0763
C	0	3.66348	3.87633	-0.18202
H	0	-1.09373	8.60321	0.51442
H	0	-2.18657	6.45976	1.09293
H	0	2.31413	6.52612	-1.07966
H	0	1.1225	8.63571	-0.57582
H	0	-1.75531	1.25527	-0.82101
C	0	-1.97391	-1.35934	-0.9089
H	0	2.18947	-1.07209	1.04453
H	0	2.12735	1.37788	1.01448
H	0	-1.69734	-5.43827	-0.78559
H	0	-1.79406	-7.91334	-0.83797
C	0	0.08861	-9.59478	0.04309
H	0	2.09088	-8.10355	0.99087
H	0	2.18705	-5.63097	1.04321
H	0	-2.09034	2.55941	1.54159
H	0	-2.30835	4.21525	2.07451
H	0	-4.31415	3.44728	0.82448
H	0	-3.52549	4.73842	-0.09364
H	0	-3.32611	3.05805	-0.5906
H	0	2.39435	2.61117	-1.39332
H	0	2.53138	4.25453	-1.98825
H	0	4.5785	3.62956	-0.72779
H	0	3.73554	4.91369	0.15033
H	0	3.61846	3.24524	0.70918
N	0	-2.87916	-1.93961	-1.33162
N	0	0.0463	-10.74913	0.0188

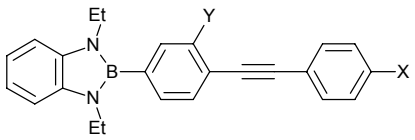
Etot=-1247.6094909 au

C-Tables 7 Atomic coordinates for [B3LYP/6-311G(d,p)] optimized geometries, values of total energies of molecule **9** (X=bdab, Y=CN).

6	0	-10.92132	0.60822	0.25414
6	0	-9.72384	1.22148	0.61056
6	0	-8.52921	0.60942	0.2365
6	0	-8.53768	-0.60107	-0.48878
6	0	-9.74065	-1.20983	-0.84078
6	0	-10.92967	-0.5931	-0.46259
7	0	-7.20541	0.98158	0.44095
5	0	-6.3624	0.00137	-0.14603
7	0	-7.21881	-0.97698	-0.71725
6	0	-4.79762	0.00004	-0.16351
6	0	-4.0571	-0.00186	1.02522
6	0	-2.6576	-0.00391	1.02198
6	0	-1.94439	-0.00078	-0.20334
6	0	-2.68731	0.00255	-1.39482
6	0	-4.07475	0.00123	-1.37029
6	0	-0.52983	-0.00055	-0.22698
6	0	0.68108	-0.00041	-0.22859
6	0	2.10033	-0.0002	-0.20333
6	0	2.84463	-0.00339	-1.39573
6	0	4.23222	-0.0012	-1.35423
6	0	4.93524	-0.00024	-0.13614
6	0	4.17478	0.00083	1.04694
6	0	2.7867	0.00306	1.02369
6	0	-6.82674	2.20972	1.1485
6	0	-6.11425	3.234	0.2582
6	0	-6.85675	-2.2065	-1.43028
6	0	-6.13052	-3.23215	-0.55273
1	0	-11.85907	1.07129	0.53896
1	0	-9.72821	2.15175	1.16714
1	0	-9.75793	-2.14047	-1.39655
1	0	-11.87383	-1.05374	-0.72962
1	0	-4.56682	-0.01043	1.98145
6	0	-1.95275	-0.00996	2.26413
1	0	-2.15583	0.00821	-2.33835
1	0	-4.61167	0.0107	-2.31288
1	0	2.32359	-0.00909	-2.34589
1	0	4.78263	-0.01028	-2.28923
1	0	4.67962	0.00959	2.00718
1	0	2.21857	0.00869	1.9464
1	0	-7.73754	2.66472	1.53889
1	0	-6.20222	1.95502	2.00975
1	0	-5.8816	4.13325	0.8353
1	0	-5.18073	2.83609	-0.13951
1	0	-6.75358	3.51809	-0.58138
1	0	-7.77586	-2.65936	-1.80348
1	0	-6.24728	-1.95392	-2.30314
1	0	-5.91151	-4.13287	-1.13308
1	0	-5.18868	-2.83672	-0.17269
1	0	-6.75452	-3.5137	0.29898
7	0	-1.39339	-0.01458	3.27439
5	0	6.49806	-0.00059	-0.09907
7	0	7.33666	-0.98121	0.49787
6	0	8.66249	-0.60823	0.31177
6	0	8.67989	0.6039	-0.41165
7	0	7.36439	0.97921	-0.65704
6	0	6.94821	-2.20954	1.19855
6	0	6.24522	-3.23127	0.29785
6	0	7.01025	2.20892	-1.37268

6	0	6.27101	3.23185	-0.50274
6	0	9.88715	1.21369	-0.74609
6	0	11.07187	0.59732	-0.35265
6	0	11.05473	-0.60492	0.36192
6	0	9.85246	-1.21962	0.70094
1	0	7.85342	-2.66636	1.60035
1	0	6.31189	-1.9551	2.05122
1	0	6.00371	-4.13127	0.87051
1	0	5.31793	-2.82956	-0.11022
1	0	6.89462	-3.51508	-0.53418
1	0	7.93345	2.66381	-1.73369
1	0	6.41133	1.9567	-2.25282
1	0	6.05714	4.13312	-1.08448
1	0	5.32588	2.83251	-0.13537
1	0	6.88414	3.51342	0.35698
1	0	9.91109	2.14534	-1.30011
1	0	12.01918	1.0593	-0.60619
1	0	11.98882	-1.06793	0.65888
1	0	9.84974	-2.15081	1.25611

Etot =-1678.8346203 au



2: X=H, Y=H

3: X=bdab, Y=H

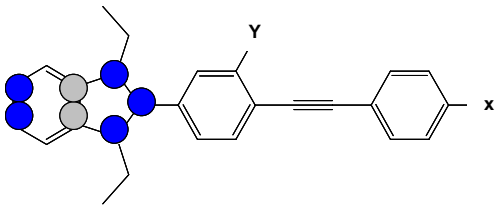
4: X=H, Y=CN

5: X=OMe, Y=CN

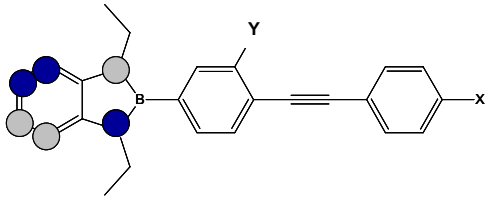
6: X=NMe_2, Y=CN

8: X=CN, Y=CN

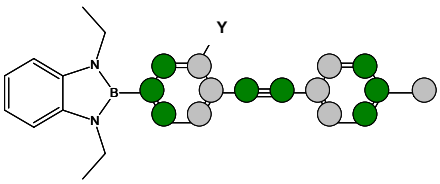
9: X=bdab, Y=CN



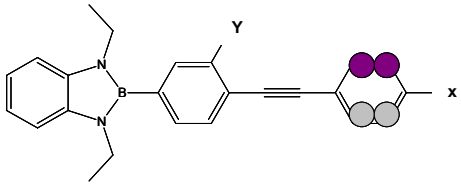
π_3-π_{NBN}



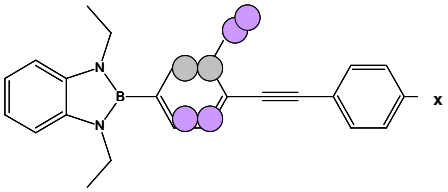
$\pi_{C=C}^{-}$-$n_N^{-\pi}$



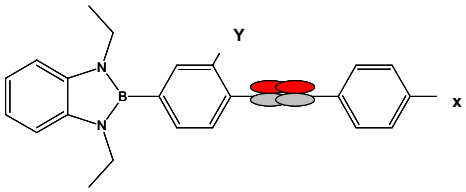
$\pi_2(Ph')$-$\pi_{C\equiv C}^{\pi}$-$\pi_2(Ph'')$



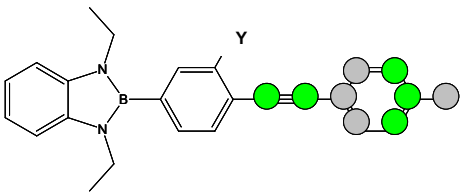
$\pi_3(Ph'')$



$\pi_3(Ph')$- $\pi_{C\equiv N}^{\pi}$



$\pi_{C\equiv C}^{\sigma}$



$\pi_{C\equiv C}^{\pi}$- $\pi_2(Ph'')$-$n_X^{\pi}(X)$

IE-Table 1 Calculated [CAM-B3LYP/6-311G(d,p)] ionization energies (IEs) for molecule **2** (X=H, Y=H). (all values in eV, * value of ΔSCF).

Nature of MO	$-\varepsilon^{K.S.}$	**Corr. IE** (x_{calc}=0.366)	**TD-DFT**
π_3-π_{NBN}	6.86	7.23*	7.23
$\pi_{C=C}^{-}$-$n_N^{-\pi}$	7.42	7.79	7.83
π_2*(Ph')*-$\pi_{C\equiv C}^{\pi}$-π_2*(Ph'')*	7.46	7.83	7.85
π_3*(Ph'')*	8.64	9.01	9.08
π_3*(Ph'')*	8.68	9.04	9.15
$\pi_{C\equiv C}^{\sigma}$	9.03	9.40	9.42

IE-Table 2 Calculated [CAM-B3LYP/6-311G(d,p)] ionization energies (IEs) for molecule **3** (X=H, Y=H). (all values in eV, * value of ΔSCF).

Nature of MO	$-\varepsilon^{K.S.}$	**Corr. IE** (x_{calc}=0.066)	**TD-DFT**
$[\pi_3$-$\pi_{NBN}]^{+}$	6.82	6.89*	6.89*
$[\pi_3$-$\pi_{NBN}]^{-}$	6.96	7.03	7.06
$[\pi_{C=C}^{-}$-$n_N^{-\pi}]^{+}$	7.47	7.54	7.53
$[\pi_{C=C}^{-}$-$n_N^{-\pi}]^{-}$	7.48	7.55	7.54
π_2*(Ph)*-$\pi_{C\equiv C}^{\pi}$-π_2*(Ph)*	7.50	7.56	7.54
$[\pi_3$*(Ph)*$]^{-}$	8.66	8.73	8.09

IE-Table 3 Calculated [CAM-B3LYP/6-311G(d,p)] ionization energies (IEs) for molecule **4** (X=H, Y=CN). (all values in eV, * value of ΔSCF).

Nature of MO	$-\varepsilon^{K.S.}$	**Corr. IE** (x_{calc}=0.361)	**TD-DFT**
π_3-π_{NBN}	7.10	7.46*	7.46*
$\pi_{C=C}^{-}$-$n_N^{-\pi}$	7.63	7.99	8.02
π_2*(Ph')*-$\pi_{C\equiv C}^{\pi}$-π_2*(Ph'')*$^{-}$	7.67	8.03	8.08
π_3*(Ph'')*	8.75	9.10	9.21
π_3*(Ph')*- $\pi_{C\equiv N}^{\pi}$	8.97	9.33	9.38
$\pi_{C\equiv C}^{\sigma}$	9.34	9.70	9.71

IE-Table 4 Calculated [CAM-B3LYP/6-311G(d,p)] ionization energies (IEs) for molecule **5** (X=OMe, Y=CN). (all values in eV, * value of ΔSCF).

Nature of MO	$-\varepsilon^{K.S.}$	**Corr. IE** (x_{calc}=0.357)	**TD-DFT**
π_3-π_{NBN}	6.99	7.35*	7.35*
$\pi_{C\equiv C}^{\pi}$-π_2*(Ph'')*-n_O^{π}*(X)*	7.28	7.64	7.67
$\pi_{C=C}^{-}$-$n_N^{\pi-}$	7.60	7.95	7.97
π_2*(Ph')*-$\pi_{C\equiv C}^{\pi}$- π_2*(Ph'')*-n_O^{π}*(X)*	8.72	9.07	9.09
π_3*(Ph'')*	8.83	9.19	9.28
π_3*(Ph')*-$\pi_{C\equiv N}^{\pi}$	8.95	9.30	9.33

IE-Table 5 Calculated [CAM-B3LYP/6-311G(d,p)] ionization energies (IEs) for molecule **6** (X=NMe_2, Y=CN). (all values in eV, * value of ΔSCF).

Nature of MO IV	$-\varepsilon^{K.S.}$	**Corr. IE** (x_{calc}=0.334)	**TD-DFT**
$\pi_{C\equiv C}^{\pi}$-π_2*(Ph'')*-$n_N^{-\pi}$*(X)*	6.51	6.84*	6.84*
π_3-π_{NBN}	7.05	7.39	7.44
$\pi_{C=C}^{-}$-$n_N^{-\pi}$	7.54	7.87	7.93
π_2*(Ph')*-$\pi_{C\equiv C}^{\pi}$-π_2*(Ph'')*-$n_N^{-\pi}$*(X)*	8.24	8.57	8.50
π_3*(Ph'')*	8.58	8.91	9.03
π_3*(Ph')* -$\pi_{C\equiv N}^{\pi}$	8.79	9.12	9.20

IE-Table 6 Calculated [CAM-B3LYP/6-311G(d,p)] ionization energies (IEs) for molecule **8** (X=CN, Y=CN). (all values in eV, * value of ΔSCF).

Nature of MO	$-\varepsilon^{K.S.}$	**Corr. IE** (x_{calc}=0.353)	**TD-DFT**
π_3-π_{NBN}	7.24	7.59*	7.59*
$\pi_{C=C}^{-}$-$n_N^{-\pi}$	7.76	8.12	8.15
π_2*(Ph')*-$\pi_{C\equiv C}^{\pi}$-π_2*(Ph'')*	8.05	8.41	8.45
π_3*(Ph')*-$\pi_{C\equiv N}^{\pi}$	9.20	9.56	9.62
π_3*(Ph'')*	9.40	9.75	9.82
π_2*(Ph')*-$\pi_{C\equiv C}^{\pi}$- π_2*(Ph'')* -$\pi_{C\equiv N}^{\pi}$	9.58	9.93	9.93

IE-Table 7 Calculated [CAM-B3LYP/6-311G(d,p)] ionization energies (IEs) for molecule **9** (X=bdab, Y=CN). (all values in eV, * value of ΔSCF).

Nature of MO	$-\varepsilon^{K.S.}$	**Corr. IE** (x_{calc}=0.054)	**TD-DFT**
$[\pi_3\text{-}\pi_{NBN}](X)$	6.93	6.89*	6.89*
$\pi_3\text{-}\pi_{NBN}$	7.13	7.18	7.13
$[\pi_{C=C}^{-}\text{-}n_N^{\pi-}](X)$	7.48	7.53	7.57
$\pi_{C=C}^{-}\text{-}n_N^{\pi-}$	7.64	7.70	7.61
$\pi_2(Ph')\text{-}\pi_{C\equiv C}^{\pi}\text{-}\pi_2(Ph'')$	7.69	7.74	7.72
$\pi_3(Ph'')$	8.72	8.77	8.86

H-L-Table 8 Calculated [CAM-B3LYP/6-311G(d,p)] HOMO and LUMO energies ($-\varepsilon^{K.S.}$ in eV), and H-L gap for molecules:**2** – **6**, **8**, **9**.

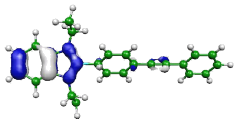
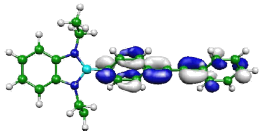
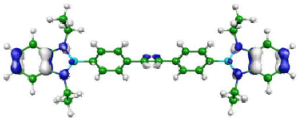
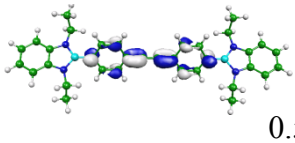
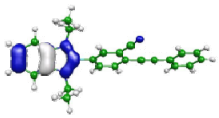
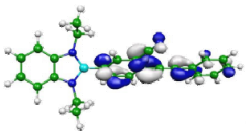
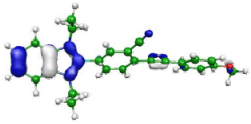
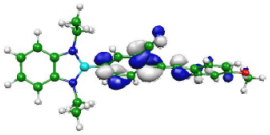
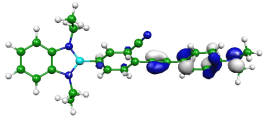
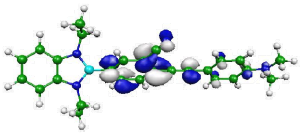
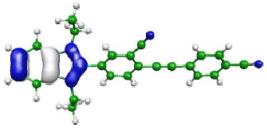
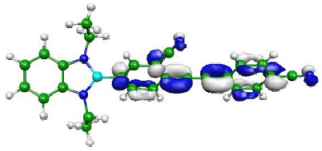
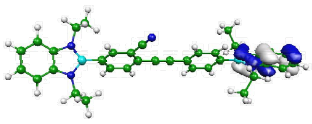
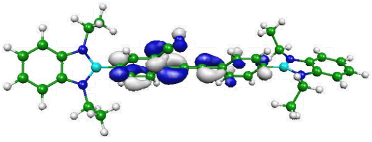
	HOMO	HLG	LUMO
2	 6.86	6.40	 0.47
3	 6.82	6.24	 0.58
4	 6.10	6.13	 0.97
5	 6.99	6.16	 0.83
6	 6.51	5.82	 0.69
8	 7.24	5.72	 1.52
9	 6.93	5.93	 1.00

Table 9 CAM-B3LYB 6-311+G(d,p) calculated (a.u. and esu) α-polarizability and β-hyperpolarizability for molecules **2**, **3**, **4**, **5**, **6**, **8** and **9**.

molecule	α		β	
	a.u.	esu	a.u.	esu
2	341.4	5.1×10^{-23}	583.57	5.0×10^{-30}
3	510.77	7.6×10^{-23}	0.0	0.0
4	355.29	5.3×10^{-23}	648.88	5.6×10^{-30}
5	381.81	5.7×10^{-23}	3913.58	33.8×10^{-30}
6	415.63	6.2×10^{-23}	8893.60	76.8×10^{-30}
8	383.75	5.7×10^{-23}	2441.79	21.1×10^{-30}
9	530.00	7.9×10^{-23}	2615.49	22.6×10^{-30}

Table 1. Crystal data and structure refinement for eick10.

Identification code	eick10
Measurement device	Nonius KappaCCD
Empirical formula	C26 H24 B N3 S
Formula weight	421.35
Temperature	100(2) K
Wavelength	0.71073 A
Crystal system, space group	Triclinic P -1
Unit cell dimensions	a = 10.1351(2) A alpha = 82.5832(13) deg. b = 10.7913(2) A beta = 73.1052(12) deg. c = 10.8348(2) A gamma = 80.0178(12) deg.
Volume	1112.80(4) A^3
Z, Calculated density	2, 1.257 Mg/m^3
Absorption coefficient	0.164 mm^-1
F(000)	444
Crystal size, colour and habit	0.30 x 0.27 x 0.20 mm^3, Colourless block
Theta range for data collection	3.41 to 25.01 deg.
Index ranges	-12<=h<=12, -12<=k<=12, -12<=l<=12
Reflections collected / unique	22441 / 3882 [R(int) = 0.026]
Completeness to theta = 25.01	99.5%
Absorption correction	multi-scan
Max. and min. transmission	0.9680 and 0.9525
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3882 / 0 / 376
Goodness-of-fit on F^2	1.075
Final R indices [I>2sigma(I)]	R1 = 0.0301, wR2 = 0.0772 [3612]
R indices (all data)	R1 = 0.0322, wR2 = 0.0785
Largest diff. peak and hole	0.258 and -0.255 e.A^-3
remarks	Hydrogens were refined isotropically.

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for eick10.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
S(1)	669(1)	-993(1)	2570(1)	25(1)
N(1)	7882(1)	5505(1)	8288(1)	17(1)
N(2)	5848(1)	6898(1)	8594(1)	17(1)
N(3)	7539(1)	2891(1)	3371(1)	27(1)
B(1)	6528(1)	5732(1)	8070(1)	17(1)
C(1)	8008(1)	6512(1)	8924(1)	17(1)
C(2)	6759(1)	7364(1)	9108(1)	18(1)
C(3)	6601(1)	8465(1)	9705(1)	22(1)
C(4)	7703(1)	8700(1)	10118(1)	24(1)
C(5)	8935(1)	7855(1)	9946(1)	23(1)
C(6)	9105(1)	6746(1)	9342(1)	20(1)
C(7)	8984(1)	4429(1)	7997(1)	19(1)
C(8)	10212(1)	4718(1)	6861(1)	26(1)
C(9)	4500(1)	7624(1)	8546(1)	20(1)
C(10)	3384(1)	7535(1)	9826(1)	28(1)
C(11)	5899(1)	4864(1)	7401(1)	18(1)
C(12)	6638(1)	4404(1)	6202(1)	18(1)
C(13)	6058(1)	3669(1)	5588(1)	18(1)
C(14)	4703(1)	3357(1)	6157(1)	19(1)
C(15)	3981(1)	3785(1)	7370(1)	21(1)
C(16)	4565(1)	4522(1)	7967(1)	20(1)
C(17)	6863(1)	3227(1)	4351(1)	20(1)
C(18)	4088(1)	2640(1)	5503(1)	20(1)
C(19)	3560(1)	2063(1)	4939(1)	20(1)
C(20)	2886(1)	1374(1)	4309(1)	18(1)
C(21)	3535(1)	211(1)	3823(1)	21(1)
C(22)	2841(1)	-472(1)	3284(1)	21(1)
C(23)	1479(1)	-19(1)	3217(1)	19(1)
C(24)	842(1)	1152(1)	3668(1)	19(1)
C(25)	1543(1)	1833(1)	4210(1)	19(1)
C(26)	-1027(2)	-108(1)	2673(1)	26(1)

Table 3. Bond lengths [A] and angles [deg] for eick10.

S(1)-C(23)	1.7583(12)
S(1)-C(26)	1.7960(14)
N(1)-C(1)	1.4018(15)
N(1)-B(1)	1.4339(17)
N(1)-C(7)	1.4616(15)
N(2)-C(2)	1.3955(15)
N(2)-B(1)	1.4282(17)
N(2)-C(9)	1.4638(15)
N(3)-C(17)	1.1485(17)
B(1)-C(11)	1.5679(17)
C(1)-C(6)	1.3876(17)
C(1)-C(2)	1.4087(17)
C(2)-C(3)	1.3875(17)
C(3)-C(4)	1.3903(19)
C(3)-H(3)	0.968(15)
C(4)-C(5)	1.3926(19)
C(4)-H(4)	0.993(15)
C(5)-C(6)	1.3979(18)
C(5)-H(5)	0.968(15)
C(6)-H(6)	0.977(15)
C(7)-C(8)	1.5178(18)
C(7)-H(7A)	0.994(14)
C(7)-H(7B)	0.990(14)
C(8)-H(8A)	0.973(17)
C(8)-H(8B)	0.972(16)
C(8)-H(8C)	0.989(17)
C(9)-C(10)	1.5175(18)
C(9)-H(9A)	0.982(15)
C(9)-H(9B)	0.975(15)
C(10)-H(10A)	1.012(18)
C(10)-H(10B)	0.986(17)
C(10)-H(10C)	0.993(17)
C(11)-C(12)	1.4022(17)
C(11)-C(16)	1.4046(17)
C(12)-C(13)	1.3940(17)
C(12)-H(12)	0.975(14)
C(13)-C(14)	1.4123(17)
C(13)-C(17)	1.4438(17)
C(14)-C(15)	1.3984(18)
C(14)-C(18)	1.4340(17)
C(15)-C(16)	1.3865(18)
C(15)-H(15)	0.960(15)
C(16)-H(16)	0.981(14)
C(18)-C(19)	1.2043(18)
C(19)-C(20)	1.4361(17)
C(20)-C(25)	1.3958(18)
C(20)-C(21)	1.4031(18)
C(21)-C(22)	1.3809(18)
C(21)-H(21)	0.975(16)
C(22)-C(23)	1.4020(18)
C(22)-H(22)	0.972(15)
C(23)-C(24)	1.3952(17)
C(24)-C(25)	1.3864(17)
C(24)-H(24)	0.960(14)
C(25)-H(25)	0.966(15)
C(26)-H(26A)	0.977(17)
C(26)-H(26B)	0.986(18)
C(26)-H(26C)	0.971(16)

C(23)-S(1)-C(26)	103.32(6)
C(1)-N(1)-B(1)	107.99(10)
C(1)-N(1)-C(7)	122.05(10)
B(1)-N(1)-C(7)	129.91(10)
C(2)-N(2)-B(1)	108.20(10)
C(2)-N(2)-C(9)	121.68(10)
B(1)-N(2)-C(9)	129.88(10)
N(2)-B(1)-N(1)	106.77(10)
N(2)-B(1)-C(11)	126.28(11)
N(1)-B(1)-C(11)	126.95(11)
C(6)-C(1)-N(1)	130.73(11)
C(6)-C(1)-C(2)	120.96(11)
N(1)-C(1)-C(2)	108.31(10)
C(3)-C(2)-N(2)	130.58(11)
C(3)-C(2)-C(1)	120.68(11)
N(2)-C(2)-C(1)	108.73(10)
C(2)-C(3)-C(4)	118.30(12)
C(2)-C(3)-H(3)	120.3(9)
C(4)-C(3)-H(3)	121.4(9)
C(3)-C(4)-C(5)	121.13(12)
C(3)-C(4)-H(4)	118.2(9)
C(5)-C(4)-H(4)	120.7(9)
C(4)-C(5)-C(6)	120.96(12)
C(4)-C(5)-H(5)	119.9(8)
C(6)-C(5)-H(5)	119.1(8)
C(1)-C(6)-C(5)	117.98(12)
C(1)-C(6)-H(6)	121.0(8)
C(5)-C(6)-H(6)	121.0(8)
N(1)-C(7)-C(8)	113.50(10)
N(1)-C(7)-H(7A)	108.3(8)
C(8)-C(7)-H(7A)	110.5(8)
N(1)-C(7)-H(7B)	107.0(8)
C(8)-C(7)-H(7B)	110.7(8)
H(7A)-C(7)-H(7B)	106.5(11)
C(7)-C(8)-H(8A)	111.9(9)
C(7)-C(8)-H(8B)	110.5(9)
H(8A)-C(8)-H(8B)	107.7(13)
C(7)-C(8)-H(8C)	111.0(9)
H(8A)-C(8)-H(8C)	109.0(13)
H(8B)-C(8)-H(8C)	106.5(13)
N(2)-C(9)-C(10)	113.17(10)
N(2)-C(9)-H(9A)	108.3(8)
C(10)-C(9)-H(9A)	110.4(8)
N(2)-C(9)-H(9B)	108.4(8)
C(10)-C(9)-H(9B)	109.8(8)
H(9A)-C(9)-H(9B)	106.5(11)
C(9)-C(10)-H(10A)	112.0(10)
C(9)-C(10)-H(10B)	110.4(9)
H(10A)-C(10)-H(10B)	108.2(13)
C(9)-C(10)-H(10C)	109.7(9)
H(10A)-C(10)-H(10C)	107.9(13)
H(10B)-C(10)-H(10C)	108.4(13)
C(12)-C(11)-C(16)	116.93(11)
C(12)-C(11)-B(1)	121.48(11)
C(16)-C(11)-B(1)	121.59(11)
C(13)-C(12)-C(11)	121.37(11)
C(13)-C(12)-H(12)	119.5(8)
C(11)-C(12)-H(12)	119.1(8)
C(12)-C(13)-C(14)	120.99(11)
C(12)-C(13)-C(17)	119.01(11)
C(14)-C(13)-C(17)	120.00(11)
C(15)-C(14)-C(13)	117.66(11)
C(15)-C(14)-C(18)	121.41(11)

C(13)-C(14)-C(18)	120.93(11)
C(16)-C(15)-C(14)	120.81(11)
C(16)-C(15)-H(15)	120.0(8)
C(14)-C(15)-H(15)	119.2(8)
C(15)-C(16)-C(11)	122.20(12)
C(15)-C(16)-H(16)	118.0(8)
C(11)-C(16)-H(16)	119.8(8)
N(3)-C(17)-C(13)	177.83(13)
C(19)-C(18)-C(14)	178.50(13)
C(18)-C(19)-C(20)	177.78(13)
C(25)-C(20)-C(21)	118.53(11)
C(25)-C(20)-C(19)	120.26(11)
C(21)-C(20)-C(19)	121.17(11)
C(22)-C(21)-C(20)	120.40(11)
C(22)-C(21)-H(21)	119.0(9)
C(20)-C(21)-H(21)	120.6(9)
C(21)-C(22)-C(23)	120.71(11)
C(21)-C(22)-H(22)	119.0(9)
C(23)-C(22)-H(22)	120.3(9)
C(24)-C(23)-C(22)	119.13(11)
C(24)-C(23)-S(1)	123.96(10)
C(22)-C(23)-S(1)	116.91(9)
C(25)-C(24)-C(23)	119.89(11)
C(25)-C(24)-H(24)	119.9(8)
C(23)-C(24)-H(24)	120.2(8)
C(24)-C(25)-C(20)	121.30(11)
C(24)-C(25)-H(25)	119.5(9)
C(20)-C(25)-H(25)	119.2(9)
S(1)-C(26)-H(26A)	111.4(9)
S(1)-C(26)-H(26B)	106.4(10)
H(26A)-C(26)-H(26B)	108.7(13)
S(1)-C(26)-H(26C)	110.8(9)
H(26A)-C(26)-H(26C)	110.4(13)
H(26B)-C(26)-H(26C)	108.9(13)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for eick10. The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
S(1)	28(1)	22(1)	26(1)	-10(1)	-6(1)	-7(1)
N(1)	18(1)	16(1)	18(1)	-3(1)	-5(1)	-2(1)
N(2)	16(1)	19(1)	17(1)	-2(1)	-5(1)	-2(1)
N(3)	23(1)	32(1)	29(1)	-9(1)	-8(1)	-4(1)
B(1)	19(1)	19(1)	14(1)	1(1)	-4(1)	-5(1)
C(1)	21(1)	17(1)	13(1)	0(1)	-4(1)	-5(1)
C(2)	20(1)	18(1)	15(1)	1(1)	-5(1)	-5(1)
C(3)	26(1)	18(1)	21(1)	-2(1)	-7(1)	1(1)
C(4)	36(1)	18(1)	22(1)	-4(1)	-11(1)	-5(1)
C(5)	28(1)	23(1)	22(1)	-1(1)	-11(1)	-8(1)
C(6)	21(1)	21(1)	19(1)	0(1)	-8(1)	-3(1)
C(7)	20(1)	18(1)	21(1)	-4(1)	-8(1)	0(1)
C(8)	20(1)	30(1)	28(1)	-9(1)	-4(1)	-1(1)
C(9)	18(1)	20(1)	22(1)	-1(1)	-6(1)	0(1)
C(10)	21(1)	28(1)	29(1)	-1(1)	-2(1)	1(1)
C(11)	19(1)	16(1)	19(1)	1(1)	-9(1)	-2(1)
C(12)	16(1)	17(1)	21(1)	1(1)	-7(1)	-3(1)
C(13)	19(1)	16(1)	19(1)	0(1)	-7(1)	-1(1)
C(14)	19(1)	15(1)	23(1)	2(1)	-11(1)	-2(1)
C(15)	17(1)	21(1)	24(1)	2(1)	-7(1)	-5(1)
C(16)	20(1)	20(1)	19(1)	0(1)	-5(1)	-3(1)
C(17)	19(1)	19(1)	26(1)	-2(1)	-11(1)	-4(1)
C(18)	19(1)	18(1)	24(1)	1(1)	-8(1)	-2(1)
C(19)	19(1)	19(1)	21(1)	1(1)	-6(1)	-3(1)
C(20)	21(1)	19(1)	17(1)	2(1)	-6(1)	-7(1)
C(21)	20(1)	21(1)	21(1)	1(1)	-6(1)	-2(1)
C(22)	25(1)	16(1)	20(1)	-2(1)	-5(1)	-1(1)
C(23)	23(1)	19(1)	16(1)	-1(1)	-4(1)	-7(1)
C(24)	18(1)	20(1)	21(1)	-2(1)	-5(1)	-3(1)
C(25)	22(1)	16(1)	20(1)	-3(1)	-5(1)	-3(1)
C(26)	29(1)	30(1)	25(1)	-4(1)	-10(1)	-11(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for eick10.

	x	y	z	U(eq)
H(3)	5738(16)	9043(14)	9834(13)	24(4)
H(4)	7595(15)	9496(15)	10530(14)	29(4)
H(5)	9696(15)	8042(13)	10228(13)	23(4)
H(6)	9986(15)	6174(13)	9183(13)	22(3)
H(7A)	9296(14)	4139(13)	8788(14)	21(3)
H(7B)	8556(14)	3735(13)	7825(13)	18(3)
H(8A)	10665(17)	5382(15)	7021(15)	33(4)
H(8B)	10905(17)	3971(15)	6691(15)	32(4)
H(8C)	9917(17)	4971(15)	6061(16)	35(4)
H(9A)	4631(14)	8508(14)	8272(13)	20(3)
H(9B)	4204(14)	7321(13)	7873(14)	22(3)
H(10A)	3646(18)	7861(16)	10545(17)	42(5)
H(10B)	2492(17)	8026(15)	9746(15)	34(4)
H(10C)	3243(17)	6640(16)	10084(15)	36(4)
H(12)	7570(15)	4619(13)	5783(13)	19(3)
H(15)	3070(15)	3562(13)	7789(13)	22(3)
H(16)	4018(15)	4805(13)	8816(14)	22(3)
H(21)	4475(16)	-133(14)	3870(14)	28(4)
H(22)	3303(15)	-1283(14)	2968(14)	25(4)
H(24)	-81(15)	1486(13)	3610(13)	21(3)
H(25)	1090(15)	2636(14)	4535(13)	24(4)
H(26A)	-971(16)	664(16)	2092(15)	34(4)
H(26B)	-1558(17)	-655(16)	2400(16)	39(4)
H(26C)	-1500(15)	89(14)	3557(16)	29(4)

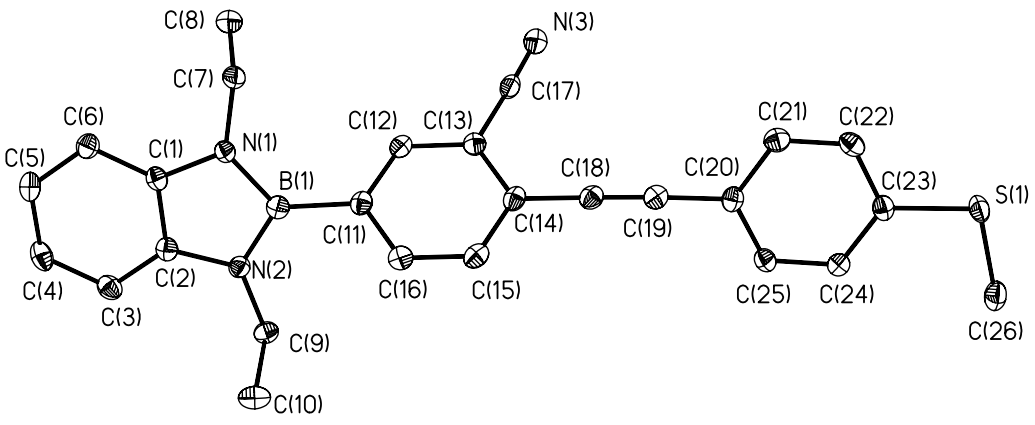


Table 1. Crystal data and structure refinement for eick11.

Identification code	eick11
Measurement device	Nonius KappaCCD
Empirical formula	C27 H27 B N4
Formula weight	418.34
Temperature	100(2) K
Wavelength	0.71073 A
Crystal system, space group	Triclinic P -1
Unit cell dimensions	a = 8.1333(3) A alpha = 92.105(2) deg. b = 8.8483(2) A beta = 94.8037(16) deg. c = 15.7389(5) A gamma = 91.021(2) deg.
Volume	1127.68(6) A^3
Z, Calculated density	2, 1.232 Mg/m^3
Absorption coefficient	0.073 mm^-1
F(000)	444
Crystal size, colour and habit	0.30 x 0.21 x 0.10 mm^3, Colourless fragment
Theta range for data collection	2.93 to 30.00 deg.
Index ranges	0<=h<=11, -12<=k<=12, -22<=l<=22
Reflections collected / unique	22633 / 6329 [R(int) = 0.029]
Completeness to theta = 30.00	96.0%
Absorption correction	multi scan
Max. and min. transmission	0.9927 and 0.9784
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6329 / 0 / 293
Goodness-of-fit on F^2	1.022
Final R indices [I>2sigma(I)]	R1 = 0.0430, wR2 = 0.1082 [5322]
R indices (all data)	R1 = 0.0534, wR2 = 0.1156
Largest diff. peak and hole	0.312 and -0.232 e.A^-3
remarks	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for eick11.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
N(1)	7104(1)	381(1)	4638(1)	17(1)
N(2)	6768(1)	-1579(1)	3635(1)	17(1)
N(3)	10710(1)	5399(1)	2567(1)	26(1)
B(1)	6949(1)	33(1)	3738(1)	17(1)
N(4)	8265(1)	10735(1)	-1287(1)	22(1)
C(1)	7019(1)	-972(1)	5061(1)	17(1)
C(2)	6834(1)	-2180(1)	4447(1)	17(1)
C(3)	6774(1)	-3671(1)	4693(1)	20(1)
C(4)	6879(1)	-3928(1)	5566(1)	24(1)
C(5)	7014(1)	-2736(1)	6173(1)	24(1)
C(6)	7087(1)	-1238(1)	5926(1)	21(1)
C(7)	7275(1)	1835(1)	5110(1)	19(1)
C(8)	9043(1)	2177(1)	5477(1)	25(1)
C(9)	6601(1)	-2551(1)	2863(1)	20(1)
C(10)	4843(1)	-3144(1)	2637(1)	26(1)
C(11)	7011(1)	1204(1)	3016(1)	18(1)
C(12)	8253(1)	2332(1)	3071(1)	18(1)
C(13)	8319(1)	3403(1)	2443(1)	17(1)
C(14)	7129(1)	3397(1)	1735(1)	18(1)
C(15)	5898(1)	2265(1)	1676(1)	20(1)
C(16)	5853(1)	1191(1)	2300(1)	20(1)
C(17)	9642(1)	4525(1)	2513(1)	20(1)
C(18)	7185(1)	4543(1)	1117(1)	20(1)
C(19)	7287(1)	5575(1)	644(1)	21(1)
C(20)	7456(1)	6856(1)	123(1)	20(1)
C(21)	6951(1)	8285(1)	398(1)	21(1)
C(22)	7226(1)	9564(1)	-59(1)	21(1)
C(23)	8011(1)	9467(1)	-824(1)	19(1)
C(24)	8490(1)	8022(1)	-1107(1)	21(1)
C(25)	8219(1)	6751(1)	-642(1)	22(1)
C(26)	8088(2)	12221(1)	-875(1)	26(1)
C(27)	9407(1)	10648(1)	-1951(1)	26(1)

Table 3. Bond lengths [A] and angles [deg] for eick11.

N(1)-C(1)	1.3935(12)
N(1)-B(1)	1.4338(14)
N(1)-C(7)	1.4604(13)
N(2)-C(2)	1.3991(12)
N(2)-B(1)	1.4331(14)
N(2)-C(9)	1.4585(13)
N(3)-C(17)	1.1488(14)
B(1)-C(11)	1.5684(14)
N(4)-C(23)	1.3829(13)
N(4)-C(27)	1.4562(14)
N(4)-C(26)	1.4597(14)
C(1)-C(6)	1.3875(14)
C(1)-C(2)	1.4119(14)
C(2)-C(3)	1.3893(14)
C(3)-C(4)	1.3962(15)
C(4)-C(5)	1.3926(16)
C(5)-C(6)	1.3964(15)
C(7)-C(8)	1.5252(14)
C(9)-C(10)	1.5235(15)
C(11)-C(12)	1.4019(14)
C(11)-C(16)	1.4059(14)
C(12)-C(13)	1.3972(13)
C(13)-C(14)	1.4142(14)
C(13)-C(17)	1.4455(14)
C(14)-C(15)	1.3987(14)
C(14)-C(18)	1.4328(14)
C(15)-C(16)	1.3943(14)
C(18)-C(19)	1.2053(14)
C(19)-C(20)	1.4350(14)
C(20)-C(25)	1.4001(15)
C(20)-C(21)	1.4008(15)
C(21)-C(22)	1.3872(14)
C(22)-C(23)	1.4099(14)
C(23)-C(24)	1.4105(14)
C(24)-C(25)	1.3881(14)

C(1)-N(1)-B(1)	108.23(8)
C(1)-N(1)-C(7)	121.13(8)
B(1)-N(1)-C(7)	130.62(8)
C(2)-N(2)-B(1)	108.18(8)
C(2)-N(2)-C(9)	121.47(8)
B(1)-N(2)-C(9)	130.31(8)
N(2)-B(1)-N(1)	106.57(8)
N(2)-B(1)-C(11)	127.38(9)
N(1)-B(1)-C(11)	126.03(9)
C(23)-N(4)-C(27)	118.67(9)
C(23)-N(4)-C(26)	118.35(9)
C(27)-N(4)-C(26)	116.43(9)
C(6)-C(1)-N(1)	130.50(9)
C(6)-C(1)-C(2)	120.83(9)
N(1)-C(1)-C(2)	108.67(8)
C(3)-C(2)-N(2)	130.73(9)
C(3)-C(2)-C(1)	120.92(9)
N(2)-C(2)-C(1)	108.34(8)
C(2)-C(3)-C(4)	117.73(10)
C(5)-C(4)-C(3)	121.49(10)
C(4)-C(5)-C(6)	120.82(10)
C(1)-C(6)-C(5)	118.16(10)
N(1)-C(7)-C(8)	112.53(8)

N(2)-C(9)-C(10)	113.06(8)
C(12)-C(11)-C(16)	117.17(9)
C(12)-C(11)-B(1)	120.06(9)
C(16)-C(11)-B(1)	122.77(9)
C(13)-C(12)-C(11)	121.15(9)
C(12)-C(13)-C(14)	121.23(9)
C(12)-C(13)-C(17)	119.43(9)
C(14)-C(13)-C(17)	119.34(9)
C(15)-C(14)-C(13)	117.64(9)
C(15)-C(14)-C(18)	122.16(9)
C(13)-C(14)-C(18)	120.18(9)
C(16)-C(15)-C(14)	120.69(9)
C(15)-C(16)-C(11)	122.11(9)
N(3)-C(17)-C(13)	178.97(11)
C(19)-C(18)-C(14)	175.32(11)
C(18)-C(19)-C(20)	176.53(11)
C(25)-C(20)-C(21)	117.80(9)
C(25)-C(20)-C(19)	121.78(9)
C(21)-C(20)-C(19)	120.29(9)
C(22)-C(21)-C(20)	121.45(9)
C(21)-C(22)-C(23)	120.96(9)
N(4)-C(23)-C(22)	121.16(9)
N(4)-C(23)-C(24)	121.43(9)
C(22)-C(23)-C(24)	117.40(9)
C(25)-C(24)-C(23)	121.15(9)
C(24)-C(25)-C(20)	121.22(10)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for eick11. The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
N(1)	16(1)	16(1)	18(1)	2(1)	0(1)	1(1)
N(2)	17(1)	17(1)	16(1)	2(1)	1(1)	0(1)
N(3)	27(1)	23(1)	27(1)	5(1)	1(1)	-3(1)
B(1)	14(1)	18(1)	18(1)	2(1)	1(1)	0(1)
N(4)	27(1)	18(1)	22(1)	4(1)	4(1)	-2(1)
C(1)	13(1)	19(1)	19(1)	3(1)	0(1)	1(1)
C(2)	13(1)	19(1)	18(1)	4(1)	1(1)	1(1)
C(3)	18(1)	18(1)	25(1)	3(1)	1(1)	0(1)
C(4)	22(1)	23(1)	27(1)	10(1)	2(1)	1(1)
C(5)	22(1)	30(1)	21(1)	10(1)	2(1)	3(1)
C(6)	19(1)	26(1)	19(1)	2(1)	1(1)	2(1)
C(7)	18(1)	18(1)	23(1)	-2(1)	1(1)	2(1)
C(8)	19(1)	26(1)	29(1)	-5(1)	-2(1)	0(1)
C(9)	22(1)	19(1)	19(1)	-1(1)	3(1)	0(1)
C(10)	25(1)	27(1)	24(1)	-4(1)	-1(1)	-4(1)
C(11)	18(1)	16(1)	18(1)	1(1)	3(1)	1(1)
C(12)	19(1)	18(1)	18(1)	2(1)	1(1)	1(1)
C(13)	18(1)	15(1)	19(1)	1(1)	3(1)	0(1)
C(14)	20(1)	18(1)	18(1)	2(1)	3(1)	2(1)
C(15)	20(1)	22(1)	19(1)	3(1)	-1(1)	0(1)
C(16)	19(1)	18(1)	21(1)	2(1)	1(1)	-2(1)
C(17)	22(1)	18(1)	19(1)	3(1)	2(1)	2(1)

C(18)	22(1)	21(1)	19(1)	3(1)	1(1)	1(1)
C(19)	21(1)	22(1)	19(1)	2(1)	1(1)	0(1)
C(20)	20(1)	21(1)	19(1)	4(1)	-1(1)	-1(1)
C(21)	24(1)	24(1)	16(1)	2(1)	2(1)	0(1)
C(22)	25(1)	19(1)	19(1)	0(1)	2(1)	1(1)
C(23)	18(1)	19(1)	19(1)	3(1)	-1(1)	-2(1)
C(24)	23(1)	21(1)	21(1)	3(1)	6(1)	1(1)
C(25)	24(1)	19(1)	23(1)	2(1)	4(1)	2(1)
C(26)	33(1)	18(1)	27(1)	2(1)	0(1)	-3(1)
C(27)	29(1)	25(1)	24(1)	6(1)	5(1)	-4(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for eick11.

	x	y	z	U(eq)
H(3)	6666	-4487	4282	24
H(4)	6858	-4938	5750	28
H(5)	7058	-2945	6762	29
H(6)	7180	-425	6339	25
H(7A)	6543	1832	5582	23
H(7B)	6913	2647	4725	23
H(8A)	9425	1355	5840	37
H(8B)	9082	3129	5818	37
H(8C)	9759	2267	5010	37
H(9A)	7341	-3421	2942	24
H(9B)	6961	-1976	2381	24
H(10A)	4485	-3732	3107	39
H(10B)	4806	-3791	2117	39
H(10C)	4107	-2291	2543	39
H(12)	9063	2368	3543	22
H(15)	5084	2227	1206	24
H(16)	5013	425	2241	23
H(21)	6409	8380	908	25
H(22)	6879	10519	147	25
H(24)	9007	7917	-1624	26
H(25)	8558	5792	-846	26
H(26A)	6945	12339	-734	39
H(26B)	8371	13009	-1262	39
H(26C)	8829	12313	-351	39
H(27A)	10502	10383	-1700	38
H(27B)	9475	11630	-2216	38
H(27C)	9013	9873	-2385	38

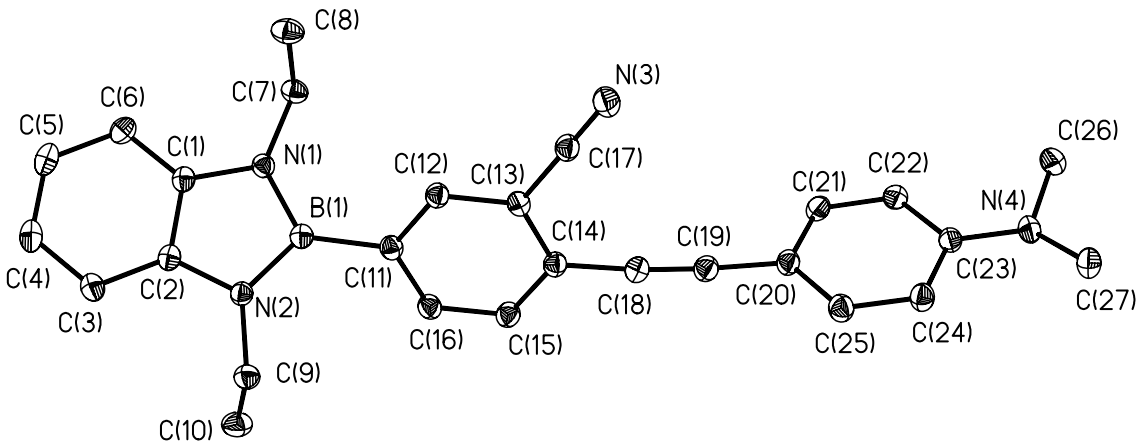


Table 1. Crystal data and structure refinement for vawe11.

Identification code	vawe11
Measurement device	Nonius KappaCCD
Empirical formula	C24 H23 B N2
Formula weight	350.25
Temperature	100(2) K
Wavelength	0.71073 A
Crystal system, space group	Triclinic P -1
Unit cell dimensions	a = 8.22890(10) A alpha = 90.2759(9) deg. b = 9.35640(10) A beta = 94.1820(9) deg. c = 26.2207(3) A gamma = 102.1840(7) deg.
Volume	1967.66(4) A^3
Z, Calculated density	4, 1.182 Mg/m^3
Absorption coefficient	0.068 mm^-1
F(000)	744
Crystal size, colour and habit	0.30 x 0.25 x 0.20 mm^3, Colourless fragment
Theta range for data collection	3.00 to 27.48 deg.
Index ranges	-10<=h<=10, -12<=k<=12, -34<=l<=33
Reflections collected / unique	39445 / 9002 [R(int) = 0.033]
Completeness to theta = 27.48	99.7%
Absorption correction	multi-scan
Max. and min. transmission	0.9865 and 0.9798
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	9002 / 0 / 491
Goodness-of-fit on F^2	1.046
Final R indices [I>2sigma(I)]	R1 = 0.0394, wR2 = 0.0937 [7048]
R indices (all data)	R1 = 0.0554, wR2 = 0.1016
Largest diff. peak and hole	0.243 and -0.215 e.A^-3
remarks	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for vawe11.

U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
N(1)	9287(1)	7213(1)	3912(1)	17(1)
N(2)	11423(1)	7797(1)	3386(1)	18(1)
N(3)	498(1)	102(1)	1478(1)	18(1)
N(4)	-125(1)	2153(1)	1832(1)	19(1)
B(1)	9649(2)	7347(1)	3387(1)	18(1)
B(2)	1037(2)	1203(1)	1876(1)	18(1)
C(1)	10793(1)	7557(1)	4216(1)	17(1)
C(2)	12103(1)	7919(1)	3890(1)	18(1)
C(3)	13746(1)	8339(1)	4089(1)	20(1)
C(4)	14065(2)	8382(1)	4619(1)	23(1)
C(5)	12770(2)	8021(1)	4941(1)	23(1)
C(6)	11115(1)	7604(1)	4744(1)	20(1)
C(7)	7675(1)	6869(1)	4134(1)	22(1)
C(8)	7251(2)	5330(1)	4339(1)	28(1)
C(9)	12482(1)	7915(1)	2957(1)	23(1)
C(10)	13263(2)	6599(2)	2903(1)	34(1)
C(11)	8400(1)	6982(1)	2901(1)	18(1)
C(12)	7368(1)	5586(1)	2830(1)	20(1)
C(13)	6365(1)	5182(1)	2384(1)	20(1)
C(14)	6351(1)	6174(1)	1986(1)	20(1)
C(15)	7327(1)	7591(1)	2057(1)	23(1)
C(16)	8328(1)	7974(1)	2504(1)	22(1)
C(17)	5338(1)	5728(1)	1520(1)	22(1)
C(18)	4472(2)	5299(1)	1138(1)	23(1)
C(19)	3390(1)	4789(1)	690(1)	21(1)
C(20)	2227(2)	3462(1)	696(1)	27(1)
C(21)	1146(2)	2987(1)	270(1)	30(1)
C(22)	1224(2)	3824(1)	-167(1)	26(1)
C(23)	2387(2)	5127(1)	-178(1)	26(1)
C(24)	3461(2)	5615(1)	247(1)	24(1)
C(25)	-919(1)	394(1)	1207(1)	18(1)
C(26)	-1299(1)	1652(1)	1424(1)	19(1)
C(27)	-2673(1)	2180(1)	1231(1)	22(1)
C(28)	-3655(2)	1432(1)	820(1)	26(1)
C(29)	-3288(2)	182(1)	608(1)	26(1)
C(30)	-1921(1)	-359(1)	801(1)	23(1)
C(31)	1122(1)	-1202(1)	1358(1)	22(1)
C(32)	2086(2)	-1050(1)	881(1)	29(1)
C(33)	-165(2)	3507(1)	2111(1)	23(1)
C(34)	402(2)	4880(1)	1808(1)	27(1)
C(35)	2609(1)	1331(1)	2260(1)	19(1)
C(36)	4098(1)	1034(1)	2097(1)	19(1)
C(37)	5520(1)	1151(1)	2425(1)	20(1)
C(38)	5517(1)	1601(1)	2936(1)	21(1)
C(39)	4046(2)	1891(1)	3108(1)	23(1)
C(40)	2628(2)	1747(1)	2777(1)	22(1)
C(41)	7023(1)	1806(1)	3268(1)	22(1)
C(42)	8315(2)	2041(1)	3530(1)	22(1)
C(43)	9866(1)	2344(1)	3841(1)	19(1)
C(44)	10498(1)	1202(1)	4068(1)	21(1)
C(45)	11995(1)	1501(1)	4366(1)	22(1)
C(46)	12882(1)	2929(1)	4440(1)	21(1)
C(47)	12265(2)	4072(1)	4217(1)	24(1)
C(48)	10771(1)	3782(1)	3917(1)	23(1)

Table 3. Bond lengths [A] and angles [deg] for vawe11.

N(1)-C(1)	1.3995(13)
N(1)-B(1)	1.4309(15)
N(1)-C(7)	1.4620(14)
N(2)-C(2)	1.3928(13)
N(2)-B(1)	1.4317(15)
N(2)-C(9)	1.4626(14)
N(3)-C(25)	1.3978(14)
N(3)-B(2)	1.4413(15)
N(3)-C(31)	1.4614(14)
N(4)-C(26)	1.3979(14)
N(4)-B(2)	1.4359(15)
N(4)-C(33)	1.4673(14)
B(1)-C(11)	1.5658(16)
B(2)-C(35)	1.5634(16)
C(1)-C(6)	1.3888(15)
C(1)-C(2)	1.4107(15)
C(2)-C(3)	1.3876(15)
C(3)-C(4)	1.3947(16)
C(4)-C(5)	1.3943(17)
C(5)-C(6)	1.3953(16)
C(7)-C(8)	1.5189(16)
C(9)-C(10)	1.5152(16)
C(11)-C(12)	1.4026(15)
C(11)-C(16)	1.4044(15)
C(12)-C(13)	1.3838(15)
C(13)-C(14)	1.4004(15)
C(14)-C(15)	1.4012(16)
C(14)-C(17)	1.4351(15)
C(15)-C(16)	1.3836(16)
C(17)-C(18)	1.2015(16)
C(18)-C(19)	1.4357(15)
C(19)-C(24)	1.3970(15)
C(19)-C(20)	1.3995(16)
C(20)-C(21)	1.3858(16)
C(21)-C(22)	1.3865(17)
C(22)-C(23)	1.3841(17)
C(23)-C(24)	1.3827(16)
C(25)-C(30)	1.3888(15)
C(25)-C(26)	1.4077(15)
C(26)-C(27)	1.3897(15)
C(27)-C(28)	1.3900(16)
C(28)-C(29)	1.3910(17)
C(29)-C(30)	1.3914(16)
C(31)-C(32)	1.5211(16)
C(33)-C(34)	1.5198(16)
C(35)-C(36)	1.4070(15)
C(35)-C(40)	1.4072(15)
C(36)-C(37)	1.3852(15)
C(37)-C(38)	1.4035(15)
C(38)-C(39)	1.3992(16)
C(38)-C(41)	1.4382(15)
C(39)-C(40)	1.3852(16)
C(41)-C(42)	1.2020(16)
C(42)-C(43)	1.4380(15)
C(43)-C(48)	1.3994(15)
C(43)-C(44)	1.4008(15)
C(44)-C(45)	1.3846(16)
C(45)-C(46)	1.3865(16)

C(46)-C(47)	1.3913(16)
C(47)-C(48)	1.3851(16)
C(1)-N(1)-B(1)	108.39(9)
C(1)-N(1)-C(7)	121.96(9)
B(1)-N(1)-C(7)	129.56(9)
C(2)-N(2)-B(1)	108.49(9)
C(2)-N(2)-C(9)	121.37(9)
B(1)-N(2)-C(9)	129.50(9)
C(25)-N(3)-B(2)	108.37(9)
C(25)-N(3)-C(31)	120.73(9)
B(2)-N(3)-C(31)	130.76(9)
C(26)-N(4)-B(2)	108.52(9)
C(26)-N(4)-C(33)	120.28(9)
B(2)-N(4)-C(33)	131.05(9)
N(1)-B(1)-N(2)	106.35(9)
N(1)-B(1)-C(11)	127.88(10)
N(2)-B(1)-C(11)	125.66(10)
N(4)-B(2)-N(3)	105.98(10)
N(4)-B(2)-C(35)	128.14(10)
N(3)-B(2)-C(35)	125.85(10)
C(6)-C(1)-N(1)	130.93(10)
C(6)-C(1)-C(2)	120.83(10)
N(1)-C(1)-C(2)	108.23(9)
C(3)-C(2)-N(2)	130.59(10)
C(3)-C(2)-C(1)	120.86(10)
N(2)-C(2)-C(1)	108.54(9)
C(2)-C(3)-C(4)	118.12(10)
C(5)-C(4)-C(3)	121.05(11)
C(4)-C(5)-C(6)	121.09(10)
C(1)-C(6)-C(5)	118.05(10)
N(1)-C(7)-C(8)	113.46(9)
N(2)-C(9)-C(10)	112.49(9)
C(12)-C(11)-C(16)	116.81(10)
C(12)-C(11)-B(1)	120.40(9)
C(16)-C(11)-B(1)	122.66(10)
C(13)-C(12)-C(11)	121.93(10)
C(12)-C(13)-C(14)	120.35(10)
C(13)-C(14)-C(15)	118.62(10)
C(13)-C(14)-C(17)	119.76(10)
C(15)-C(14)-C(17)	121.62(10)
C(16)-C(15)-C(14)	120.24(10)
C(15)-C(16)-C(11)	121.99(10)
C(18)-C(17)-C(14)	177.33(12)
C(17)-C(18)-C(19)	178.09(12)
C(24)-C(19)-C(20)	119.00(10)
C(24)-C(19)-C(18)	120.81(10)
C(20)-C(19)-C(18)	120.19(10)
C(21)-C(20)-C(19)	120.40(11)
C(20)-C(21)-C(22)	119.93(11)
C(23)-C(22)-C(21)	120.08(11)
C(24)-C(23)-C(22)	120.37(11)
C(23)-C(24)-C(19)	120.22(11)
C(30)-C(25)-N(3)	130.65(10)
C(30)-C(25)-C(26)	120.77(10)
N(3)-C(25)-C(26)	108.55(9)
C(27)-C(26)-N(4)	130.73(10)
C(27)-C(26)-C(25)	120.68(10)
N(4)-C(26)-C(25)	108.57(9)
C(26)-C(27)-C(28)	118.16(11)
C(27)-C(28)-C(29)	121.19(11)
C(28)-C(29)-C(30)	121.00(11)
C(25)-C(30)-C(29)	118.19(11)

N(3)-C(31)-C(32)	113.11(9)
N(4)-C(33)-C(34)	113.48(9)
C(36)-C(35)-C(40)	116.54(10)
C(36)-C(35)-B(2)	120.55(10)
C(40)-C(35)-B(2)	122.90(10)
C(37)-C(36)-C(35)	122.19(10)
C(36)-C(37)-C(38)	120.11(10)
C(39)-C(38)-C(37)	118.73(10)
C(39)-C(38)-C(41)	121.24(10)
C(37)-C(38)-C(41)	120.00(10)
C(40)-C(39)-C(38)	120.40(10)
C(39)-C(40)-C(35)	122.00(11)
C(42)-C(41)-C(38)	176.55(12)
C(41)-C(42)-C(43)	179.17(12)
C(48)-C(43)-C(44)	119.09(10)
C(48)-C(43)-C(42)	120.42(10)
C(44)-C(43)-C(42)	120.48(10)
C(45)-C(44)-C(43)	120.19(10)
C(44)-C(45)-C(46)	120.33(10)
C(45)-C(46)-C(47)	119.98(11)
C(48)-C(47)-C(46)	120.04(11)
C(47)-C(48)-C(43)	120.37(10)

Symmetry transformations used to generate equivalent atoms:

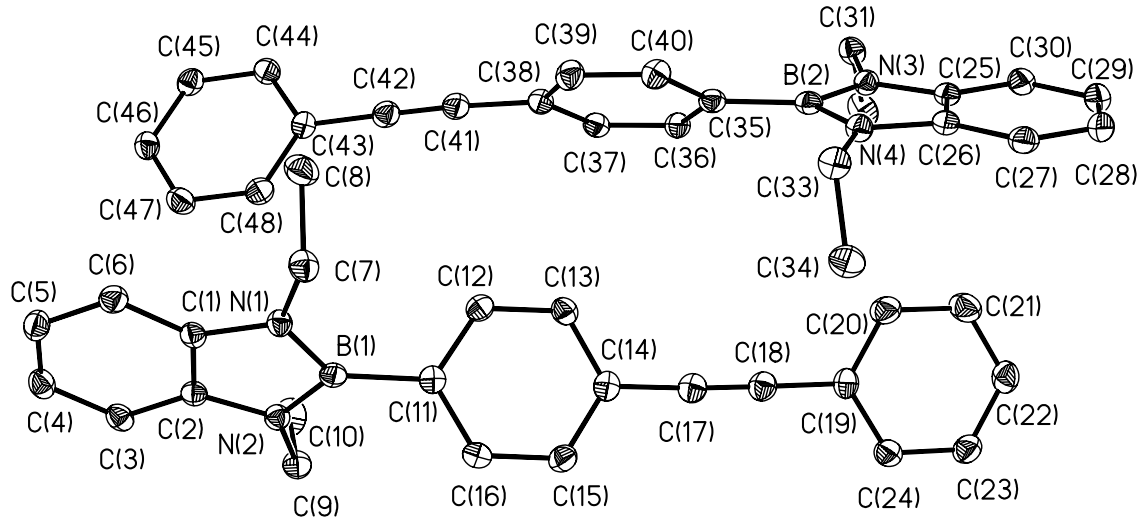
Table 4. Anisotropic displacement parameters (A^2 x 10^3) for vawe11.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

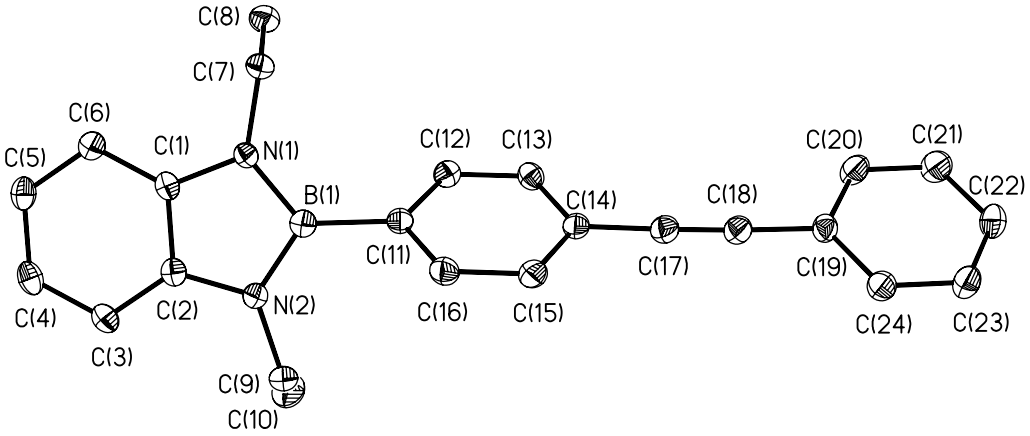
	U11	U22	U33	U23	U13	U12
N(1)	15(1)	18(1)	18(1)	0(1)	0(1)	3(1)
N(2)	18(1)	18(1)	17(1)	0(1)	1(1)	4(1)
N(3)	18(1)	18(1)	18(1)	0(1)	1(1)	4(1)
N(4)	20(1)	18(1)	18(1)	-2(1)	1(1)	4(1)
B(1)	20(1)	14(1)	19(1)	0(1)	1(1)	5(1)
B(2)	19(1)	18(1)	17(1)	2(1)	4(1)	2(1)
C(1)	17(1)	13(1)	20(1)	-1(1)	-2(1)	4(1)
C(2)	20(1)	13(1)	20(1)	0(1)	0(1)	5(1)
C(3)	18(1)	16(1)	26(1)	-1(1)	0(1)	4(1)
C(4)	21(1)	18(1)	28(1)	-2(1)	-6(1)	5(1)
C(5)	26(1)	21(1)	20(1)	-1(1)	-5(1)	7(1)
C(6)	23(1)	18(1)	20(1)	1(1)	1(1)	5(1)
C(7)	17(1)	27(1)	22(1)	-1(1)	3(1)	4(1)
C(8)	26(1)	29(1)	27(1)	-1(1)	6(1)	-4(1)
C(9)	20(1)	27(1)	21(1)	1(1)	5(1)	3(1)
C(10)	32(1)	43(1)	30(1)	-6(1)	5(1)	17(1)
C(11)	17(1)	20(1)	18(1)	-1(1)	2(1)	5(1)
C(12)	21(1)	19(1)	20(1)	2(1)	2(1)	7(1)
C(13)	19(1)	18(1)	23(1)	-2(1)	0(1)	4(1)
C(14)	17(1)	26(1)	18(1)	-1(1)	3(1)	7(1)
C(15)	22(1)	25(1)	20(1)	5(1)	2(1)	4(1)
C(16)	22(1)	19(1)	23(1)	2(1)	2(1)	1(1)
C(17)	22(1)	25(1)	21(1)	0(1)	3(1)	6(1)
C(18)	23(1)	26(1)	20(1)	0(1)	2(1)	6(1)
C(19)	20(1)	25(1)	17(1)	-3(1)	0(1)	7(1)
C(20)	33(1)	26(1)	19(1)	2(1)	2(1)	2(1)
C(21)	33(1)	26(1)	26(1)	-2(1)	1(1)	-2(1)

C(22)	29(1)	28(1)	20(1)	-5(1)	-4(1)	5(1)
C(23)	32(1)	26(1)	20(1)	3(1)	-1(1)	6(1)
C(24)	25(1)	22(1)	23(1)	0(1)	1(1)	2(1)
C(25)	17(1)	19(1)	19(1)	4(1)	3(1)	2(1)
C(26)	17(1)	21(1)	19(1)	3(1)	3(1)	2(1)
C(27)	20(1)	22(1)	26(1)	5(1)	4(1)	4(1)
C(28)	18(1)	29(1)	29(1)	8(1)	-2(1)	4(1)
C(29)	23(1)	29(1)	23(1)	3(1)	-4(1)	-1(1)
C(30)	23(1)	22(1)	21(1)	0(1)	0(1)	1(1)
C(31)	22(1)	18(1)	25(1)	-3(1)	0(1)	4(1)
C(32)	25(1)	30(1)	32(1)	-10(1)	4(1)	4(1)
C(33)	25(1)	21(1)	23(1)	-3(1)	3(1)	8(1)
C(34)	30(1)	22(1)	31(1)	-2(1)	3(1)	5(1)
C(35)	21(1)	15(1)	19(1)	1(1)	2(1)	3(1)
C(36)	21(1)	19(1)	17(1)	-1(1)	1(1)	3(1)
C(37)	19(1)	18(1)	22(1)	1(1)	2(1)	3(1)
C(38)	23(1)	17(1)	21(1)	1(1)	-2(1)	2(1)
C(39)	28(1)	24(1)	17(1)	-2(1)	0(1)	5(1)
C(40)	22(1)	24(1)	20(1)	0(1)	3(1)	7(1)
C(41)	25(1)	19(1)	21(1)	1(1)	-1(1)	4(1)
C(42)	26(1)	19(1)	21(1)	1(1)	0(1)	6(1)
C(43)	20(1)	21(1)	17(1)	-1(1)	0(1)	5(1)
C(44)	25(1)	16(1)	22(1)	-1(1)	0(1)	4(1)
C(45)	25(1)	20(1)	21(1)	1(1)	0(1)	9(1)
C(46)	18(1)	24(1)	21(1)	-1(1)	0(1)	5(1)
C(47)	24(1)	18(1)	29(1)	0(1)	-1(1)	2(1)
C(48)	25(1)	19(1)	26(1)	4(1)	-2(1)	7(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for vawe11.

	x	y	z	U(eq)
H(3)	14629	8590	3870	24
H(4)	15181	8662	4763	27
H(5)	13019	8058	5301	27
H(6)	10234	7360	4964	24
H(7A)	6793	6990	3871	26
H(7B)	7682	7578	4417	26
H(8A)	7132	4619	4056	43
H(8B)	6201	5193	4505	43
H(8C)	8145	5184	4588	43
H(9A)	13377	8806	3006	27
H(9B)	11805	8021	2636	27
H(10A)	13976	6516	3213	51
H(10B)	13935	6717	2607	51
H(10C)	12383	5712	2855	51
H(12)	7357	4899	3095	23
H(13)	5683	4227	2347	24
H(15)	7302	8290	1796	27
H(16)	8986	8938	2544	26
H(20)	2178	2884	993	32
H(21)	351	2090	276	35
H(22)	478	3502	-458	32
H(23)	2447	5689	-479	31
H(24)	4250	6515	237	28
H(27)	-2934	3028	1377	27
H(28)	-4594	1781	681	31
H(29)	-3980	-309	327	32
H(30)	-1681	-1220	659	27
H(31A)	168	-2047	1310	26
H(31B)	1858	-1408	1652	26
H(32A)	1363	-855	587	44
H(32B)	2457	-1959	817	44
H(32C)	3058	-239	931	44
H(33A)	561	3564	2432	27
H(33B)	-1316	3470	2205	27
H(34A)	1583	4986	1748	41
H(34B)	250	5734	2002	41
H(34C)	-262	4804	1480	41
H(36)	4129	744	1751	23
H(37)	6498	925	2304	24
H(39)	4020	2187	3454	28
H(40)	1638	1935	2903	26
H(44)	9899	220	4018	25
H(45)	12416	723	4521	26
H(46)	13911	3128	4644	26
H(47)	12868	5051	4270	29
H(48)	10358	4564	3763	28





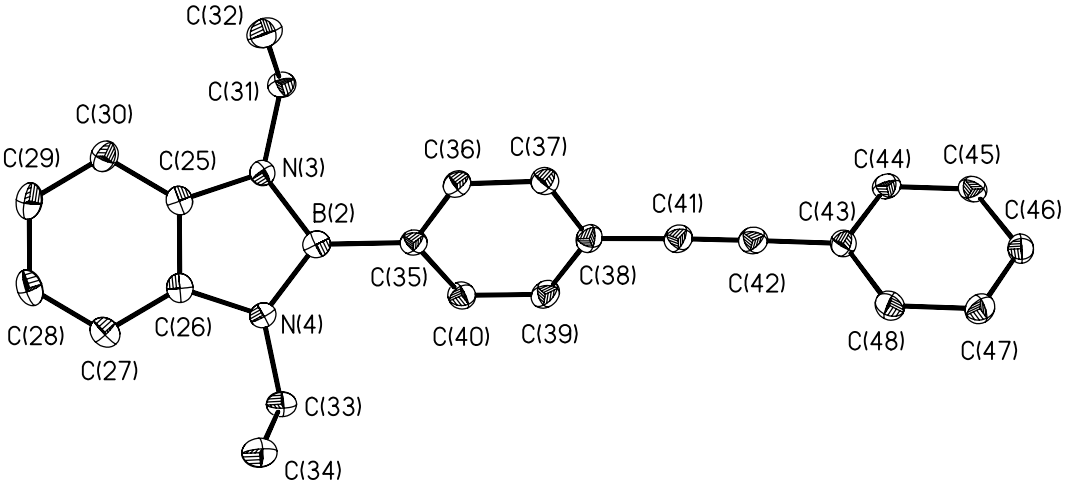


Table 1. Crystal data and structure refinement for vawe12.

Identification code	vawe12
Measurement device	Nonius KappaCCD
Empirical formula	C26 H24 B N3 O
Formula weight	405.29
Temperature	100(2) K
Wavelength	0.71073 A
Crystal system, space group	Triclinic P -1
Unit cell dimensions	a = 7.6596(2) A alpha = 100.4493(11) deg. b = 8.23120(10) A beta = 90.0371(11) deg. c = 18.3644(3) A gamma = 108.9834(10) deg.
Volume	1074.49(4) A^3
Z, Calculated density	2, 1.253 Mg/m^3
Absorption coefficient	0.077 mm^-1
F(000)	428
Crystal size, colour and habit	0.30 x 0.28 x 0.24 mm^3, Colourless fragment
Theta range for data collection	2.97 to 27.48 deg.
Index ranges	-9<=h<=9, -9<=k<=10, -23<=l<=23
Reflections collected / unique	24875 / 4894 [R(int) = 0.028]
Completeness to theta = 27.48	99.6%
Absorption correction	multi-scan
Max. and min. transmission	0.9818 and 0.9774
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4894 / 0 / 283
Goodness-of-fit on F^2	1.058
Final R indices [I>2sigma(I)]	R1 = 0.0379, wR2 = 0.0976 [4247]
R indices (all data)	R1 = 0.0444, wR2 = 0.1018
Largest diff. peak and hole	0.271 and -0.267 e.A^-3
remarks	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for vawe12.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
O(1)	3301(1)	945(1)	565(1)	28(1)
N(1)	9722(1)	4256(1)	7792(1)	16(1)
N(2)	11157(1)	2311(1)	7264(1)	16(1)
N(3)	7571(1)	7057(1)	4999(1)	27(1)
B(1)	9925(2)	3211(1)	7100(1)	16(1)
C(1)	10794(1)	3997(1)	8346(1)	17(1)
C(2)	11671(1)	2804(1)	8022(1)	17(1)
C(3)	12843(1)	2313(1)	8450(1)	20(1)
C(4)	13126(2)	3037(1)	9207(1)	23(1)
C(5)	12255(2)	4212(1)	9525(1)	23(1)
C(6)	11072(1)	4705(1)	9101(1)	20(1)
C(7)	8725(1)	5511(1)	7947(1)	20(1)
C(8)	9996(2)	7397(1)	7997(1)	26(1)
C(9)	12079(1)	1299(1)	6764(1)	19(1)
C(10)	14033(1)	2405(1)	6632(1)	20(1)
C(11)	8952(1)	3024(1)	6327(1)	16(1)
C(12)	8750(1)	4464(1)	6072(1)	17(1)
C(13)	7887(1)	4277(1)	5377(1)	16(1)
C(14)	7208(1)	2627(1)	4901(1)	17(1)
C(15)	7383(1)	1178(1)	5158(1)	17(1)
C(16)	8222(1)	1383(1)	5853(1)	16(1)
C(17)	7700(1)	5811(1)	5153(1)	19(1)
C(18)	6403(1)	2413(1)	4171(1)	18(1)
C(19)	5768(1)	2153(1)	3545(1)	18(1)
C(20)	5062(1)	1815(1)	2789(1)	17(1)
C(21)	5536(1)	3151(1)	2372(1)	18(1)
C(22)	4926(1)	2812(1)	1635(1)	19(1)
C(23)	3831(1)	1130(1)	1294(1)	19(1)
C(24)	3328(1)	-214(1)	1697(1)	19(1)
C(25)	3944(1)	139(1)	2440(1)	19(1)
C(26)	2207(2)	-756(2)	184(1)	39(1)

Table 3. Bond lengths [A] and angles [deg] for vawe12.

O(1)-C(23)	1.3657(12)
O(1)-C(26)	1.4255(13)
N(1)-C(1)	1.3954(12)
N(1)-B(1)	1.4380(13)
N(1)-C(7)	1.4623(12)
N(2)-C(2)	1.3959(12)
N(2)-B(1)	1.4374(13)
N(2)-C(9)	1.4643(12)
N(3)-C(17)	1.1467(14)
B(1)-C(11)	1.5627(14)
C(1)-C(6)	1.3909(13)
C(1)-C(2)	1.4090(14)
C(2)-C(3)	1.3916(14)
C(3)-C(4)	1.3958(14)
C(4)-C(5)	1.3919(16)
C(5)-C(6)	1.3947(15)
C(7)-C(8)	1.5269(15)
C(9)-C(10)	1.5233(14)
C(11)-C(12)	1.4029(13)
C(11)-C(16)	1.4062(13)
C(12)-C(13)	1.3960(13)
C(13)-C(14)	1.4100(13)
C(13)-C(17)	1.4457(13)
C(14)-C(15)	1.4047(13)
C(14)-C(18)	1.4317(13)
C(15)-C(16)	1.3853(13)
C(18)-C(19)	1.2033(14)
C(19)-C(20)	1.4349(13)
C(20)-C(25)	1.3988(14)
C(20)-C(21)	1.4051(14)
C(21)-C(22)	1.3806(13)
C(22)-C(23)	1.3937(14)
C(23)-C(24)	1.3936(14)
C(24)-C(25)	1.3902(13)

C(23)-O(1)-C(26)	117.60(8)
C(1)-N(1)-B(1)	108.32(8)
C(1)-N(1)-C(7)	121.53(8)
B(1)-N(1)-C(7)	130.01(8)
C(2)-N(2)-B(1)	108.13(8)
C(2)-N(2)-C(9)	120.87(8)
B(1)-N(2)-C(9)	130.10(8)
N(2)-B(1)-N(1)	106.29(8)
N(2)-B(1)-C(11)	126.34(9)
N(1)-B(1)-C(11)	127.33(9)
C(6)-C(1)-N(1)	130.69(9)
C(6)-C(1)-C(2)	120.83(9)
N(1)-C(1)-C(2)	108.48(8)
C(3)-C(2)-N(2)	130.41(9)
C(3)-C(2)-C(1)	120.81(9)
N(2)-C(2)-C(1)	108.78(8)
C(2)-C(3)-C(4)	118.12(10)
C(5)-C(4)-C(3)	120.95(10)
C(4)-C(5)-C(6)	121.31(9)
C(1)-C(6)-C(5)	117.99(10)
N(1)-C(7)-C(8)	112.31(8)
N(2)-C(9)-C(10)	111.94(8)
C(12)-C(11)-C(16)	116.76(9)
C(12)-C(11)-B(1)	122.25(8)

C(16)-C(11)-B(1)	120.99(8)
C(13)-C(12)-C(11)	121.54(9)
C(12)-C(13)-C(14)	120.90(9)
C(12)-C(13)-C(17)	118.69(9)
C(14)-C(13)-C(17)	120.41(9)
C(15)-C(14)-C(13)	117.75(9)
C(15)-C(14)-C(18)	120.18(9)
C(13)-C(14)-C(18)	122.06(9)
C(16)-C(15)-C(14)	120.61(9)
C(15)-C(16)-C(11)	122.40(9)
N(3)-C(17)-C(13)	177.80(11)
C(19)-C(18)-C(14)	176.13(10)
C(18)-C(19)-C(20)	177.85(11)
C(25)-C(20)-C(21)	118.31(9)
C(25)-C(20)-C(19)	121.09(9)
C(21)-C(20)-C(19)	120.56(9)
C(22)-C(21)-C(20)	120.75(9)
C(21)-C(22)-C(23)	120.15(9)
O(1)-C(23)-C(24)	124.60(9)
O(1)-C(23)-C(22)	115.21(9)
C(24)-C(23)-C(22)	120.18(9)
C(25)-C(24)-C(23)	119.30(9)
C(24)-C(25)-C(20)	121.30(9)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for vawe12. The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
O(1)	36(1)	24(1)	16(1)	5(1)	-8(1)	0(1)
N(1)	17(1)	17(1)	15(1)	2(1)	0(1)	6(1)
N(2)	18(1)	16(1)	15(1)	1(1)	0(1)	5(1)
N(3)	35(1)	24(1)	25(1)	6(1)	2(1)	13(1)
B(1)	14(1)	14(1)	17(1)	3(1)	1(1)	2(1)
C(1)	16(1)	17(1)	15(1)	4(1)	0(1)	2(1)
C(2)	18(1)	16(1)	15(1)	4(1)	1(1)	2(1)
C(3)	20(1)	20(1)	21(1)	7(1)	1(1)	6(1)
C(4)	21(1)	27(1)	20(1)	10(1)	-2(1)	5(1)
C(5)	23(1)	29(1)	14(1)	5(1)	0(1)	2(1)
C(6)	20(1)	22(1)	16(1)	2(1)	3(1)	4(1)
C(7)	19(1)	22(1)	19(1)	1(1)	2(1)	10(1)
C(8)	26(1)	20(1)	31(1)	-1(1)	0(1)	10(1)
C(9)	20(1)	18(1)	19(1)	-1(1)	0(1)	8(1)
C(10)	20(1)	22(1)	18(1)	2(1)	2(1)	8(1)
C(11)	14(1)	18(1)	16(1)	3(1)	2(1)	5(1)
C(12)	16(1)	16(1)	16(1)	1(1)	1(1)	4(1)
C(13)	16(1)	17(1)	17(1)	4(1)	2(1)	6(1)
C(14)	15(1)	19(1)	15(1)	3(1)	2(1)	6(1)
C(15)	16(1)	16(1)	17(1)	1(1)	1(1)	4(1)
C(16)	16(1)	17(1)	17(1)	4(1)	1(1)	6(1)
C(17)	21(1)	20(1)	16(1)	2(1)	1(1)	7(1)
C(18)	19(1)	17(1)	18(1)	3(1)	1(1)	6(1)

C(19)	18(1)	18(1)	18(1)	3(1)	1(1)	6(1)
C(20)	16(1)	19(1)	15(1)	3(1)	1(1)	7(1)
C(21)	18(1)	16(1)	19(1)	1(1)	0(1)	5(1)
C(22)	20(1)	18(1)	18(1)	7(1)	1(1)	5(1)
C(23)	19(1)	22(1)	15(1)	3(1)	-1(1)	6(1)
C(24)	19(1)	17(1)	20(1)	3(1)	-2(1)	3(1)
C(25)	20(1)	18(1)	19(1)	6(1)	1(1)	5(1)
C(26)	54(1)	27(1)	23(1)	2(1)	-16(1)	-3(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for vawe12.

	x	y	z	U(eq)
H(3)	13434	1508	8233	24
H(4)	13924	2723	9509	28
H(5)	12472	4688	10041	28
H(6)	10474	5501	9322	24
H(7A)	8125	5397	8421	24
H(7B)	7741	5231	7549	24
H(8A)	10951	7693	8400	39
H(8B)	9270	8188	8096	39
H(8C)	10584	7520	7527	39
H(9A)	11345	825	6283	23
H(9B)	12135	296	6979	23
H(10A)	13976	3341	6380	30
H(10B)	14631	1666	6322	30
H(10C)	14747	2920	7109	30
H(12)	9212	5593	6379	20
H(15)	6922	46	4853	20
H(16)	8308	377	6015	20
H(21)	6286	4300	2600	22
H(22)	5254	3728	1359	22
H(24)	2573	-1360	1467	23
H(25)	3598	-776	2716	22
H(26A)	2895	-1572	190	59
H(26B)	1920	-710	-330	59
H(26C)	1054	-1157	432	59

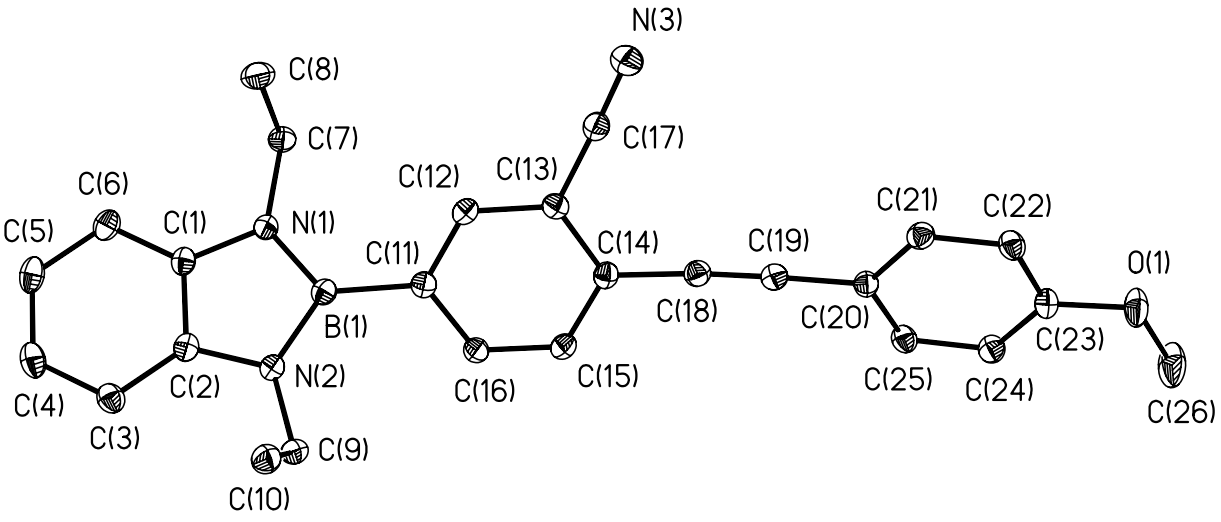


Table 1. Crystal data and structure refinement for vawe14.

Identification code	vawe14
Measurement device	Nonius KappaCCD
Empirical formula	C34 H36 B2 N4
Formula weight	522.29
Temperature	100(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic P 21/n
Unit cell dimensions	a = 9.8599(3) A alpha = 90 deg. b = 11.9000(4) A beta = 103.8752(17) deg. c = 12.5138(3) A gamma = 90 deg.
Volume	1425.44(7) A^3
Z, Calculated density	2, 1.217 Mg/m^3
Absorption coefficient	0.071 mm^-1
F(000)	556
Crystal size, colour and habit	0.22 x 0.14 x 0.06 mm^3, Colourless fragment
Theta range for data collection	2.93 to 27.47 deg.
Index ranges	-12<=h<=12, -15<=k<=15, -16<=l<=16
Reflections collected / unique	19844 / 3195 [R(int) = 0.042]
Completeness to theta = 27.47	97.9%
Absorption correction	multi-scan
Max. and min. transmission	0.9958 and 0.9846
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3195 / 0 / 183
Goodness-of-fit on F^2	1.046
Final R indices [I>2sigma(I)]	R1 = 0.0428, wR2 = 0.1035 [2625]
R indices (all data)	R1 = 0.0541, wR2 = 0.1116
Largest diff. peak and hole	0.249 and -0.249 e.A^-3
remarks	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for vawe14.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
N(1)	2323(1)	5820(1)	-1028(1)	23(1)
N(2)	2240(1)	5599(1)	778(1)	22(1)
B(1)	2555(1)	5024(1)	-144(1)	22(1)
C(1)	1871(1)	6825(1)	-659(1)	24(1)
C(2)	1823(1)	6694(1)	453(1)	23(1)
C(3)	1452(1)	7587(1)	1042(1)	26(1)
C(4)	1119(1)	8607(1)	496(1)	30(1)
C(5)	1142(1)	8728(1)	-606(1)	32(1)
C(6)	1512(1)	7836(1)	-1202(1)	28(1)
C(7)	2466(1)	5707(1)	-2159(1)	26(1)
C(8)	3743(1)	6316(1)	-2357(1)	31(1)
C(9)	2394(1)	5225(1)	1912(1)	24(1)
C(10)	1009(1)	4957(1)	2187(1)	30(1)
C(11)	3086(1)	3787(1)	-154(1)	22(1)
C(12)	4231(1)	3523(1)	-596(1)	24(1)
C(13)	4775(1)	2446(1)	-547(1)	23(1)
C(14)	4180(1)	1577(1)	-62(1)	23(1)
C(15)	3013(1)	1811(1)	358(1)	24(1)
C(16)	2486(1)	2898(1)	313(1)	24(1)
C(17)	4751(1)	462(1)	-11(1)	24(1)

Table 3. Bond lengths [A] and angles [deg] for vawe14.

N(1)-C(1)	1.3939(15)
N(1)-B(1)	1.4315(17)
N(1)-C(7)	1.4613(15)
N(2)-C(2)	1.3973(16)
N(2)-B(1)	1.4383(17)
N(2)-C(9)	1.4593(15)
B(1)-C(11)	1.5635(18)
C(1)-C(6)	1.3856(18)
C(1)-C(2)	1.4116(17)
C(2)-C(3)	1.3913(17)
C(3)-C(4)	1.3929(19)
C(4)-C(5)	1.392(2)
C(5)-C(6)	1.3942(19)
C(7)-C(8)	1.5233(18)
C(9)-C(10)	1.5204(17)
C(11)-C(16)	1.4054(17)
C(11)-C(12)	1.4069(17)
C(12)-C(13)	1.3859(17)

C(13)-C(14)	1.3973(17)
C(14)-C(15)	1.4023(17)
C(14)-C(17)	1.4373(17)
C(15)-C(16)	1.3895(17)
C(17)-C(17)#1	1.202(3)

C(1)-N(1)-B(1)	108.42(10)
C(1)-N(1)-C(7)	120.83(10)
B(1)-N(1)-C(7)	130.74(11)
C(2)-N(2)-B(1)	108.32(10)
C(2)-N(2)-C(9)	121.47(10)
B(1)-N(2)-C(9)	130.04(10)
N(1)-B(1)-N(2)	106.29(11)
N(1)-B(1)-C(11)	127.50(11)
N(2)-B(1)-C(11)	126.19(11)
C(6)-C(1)-N(1)	130.34(11)
C(6)-C(1)-C(2)	120.97(11)
N(1)-C(1)-C(2)	108.70(10)
C(3)-C(2)-N(2)	130.90(11)
C(3)-C(2)-C(1)	120.80(11)
N(2)-C(2)-C(1)	108.26(10)
C(2)-C(3)-C(4)	117.85(12)
C(5)-C(4)-C(3)	121.20(12)
C(4)-C(5)-C(6)	121.26(12)
C(1)-C(6)-C(5)	117.89(12)
N(1)-C(7)-C(8)	112.92(10)
N(2)-C(9)-C(10)	113.21(10)
C(16)-C(11)-C(12)	116.90(11)
C(16)-C(11)-B(1)	122.09(11)
C(12)-C(11)-B(1)	120.96(11)
C(13)-C(12)-C(11)	121.86(11)
C(12)-C(13)-C(14)	120.32(11)
C(13)-C(14)-C(15)	118.94(11)
C(13)-C(14)-C(17)	120.09(11)
C(15)-C(14)-C(17)	120.96(11)
C(16)-C(15)-C(14)	120.11(11)
C(15)-C(16)-C(11)	121.83(11)
C(17)#1-C(17)-C(14)	178.15(18)

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,-y,-z

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for vawe14.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
N(1)	24(1)	23(1)	20(1)	-1(1)	5(1)	2(1)
N(2)	23(1)	23(1)	20(1)	0(1)	5(1)	2(1)
B(1)	20(1)	25(1)	20(1)	-1(1)	3(1)	0(1)
C(1)	22(1)	23(1)	25(1)	-2(1)	4(1)	1(1)
C(2)	20(1)	23(1)	25(1)	-1(1)	5(1)	-1(1)
C(3)	26(1)	27(1)	27(1)	-3(1)	9(1)	-2(1)
C(4)	32(1)	24(1)	38(1)	-6(1)	13(1)	2(1)
C(5)	35(1)	22(1)	39(1)	3(1)	11(1)	4(1)
C(6)	30(1)	27(1)	27(1)	2(1)	7(1)	3(1)

C(7)	30(1)	29(1)	19(1)	0(1)	5(1)	3(1)
C(8)	34(1)	38(1)	23(1)	2(1)	9(1)	2(1)
C(9)	26(1)	29(1)	19(1)	0(1)	5(1)	0(1)
C(10)	30(1)	33(1)	29(1)	-1(1)	12(1)	-3(1)
C(11)	23(1)	24(1)	17(1)	-1(1)	1(1)	2(1)
C(12)	26(1)	24(1)	20(1)	-1(1)	5(1)	0(1)
C(13)	21(1)	27(1)	20(1)	-4(1)	4(1)	2(1)
C(14)	25(1)	23(1)	17(1)	-2(1)	1(1)	4(1)
C(15)	27(1)	24(1)	21(1)	1(1)	7(1)	1(1)
C(16)	24(1)	27(1)	23(1)	0(1)	7(1)	4(1)
C(17)	26(1)	27(1)	19(1)	0(1)	5(1)	3(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for vawe14.

	x	y	z	U(eq)
H(3)	1427	7504	1792	31
H(4)	872	9231	882	36
H(5)	902	9432	-960	38
H(6)	1517	7919	-1956	34
H(7A)	1618	6011	-2667	31
H(7B)	2533	4900	-2330	31
H(8A)	3704	7110	-2158	47
H(8B)	3754	6255	-3135	47
H(8C)	4592	5974	-1903	47
H(9A)	2875	5819	2416	29
H(9B)	2992	4546	2039	29
H(10A)	429	5635	2098	45
H(10B)	1180	4694	2950	45
H(10C)	525	4369	1690	45
H(12)	4642	4100	-939	28
H(13)	5557	2296	-846	28
H(15)	2582	1226	674	29
H(16)	1699	3044	605	29