ADVANCED FUNCTIONAL MATERIALS

Supporting Information

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Supporting Information

From Blue to Red: Syntheses, Structures, Electronic and Electroluminescent Properties of Tunable Luminescent N^N chelate Boron Complexes

Qin-De Liu,[a] Maria S. Mudadu,[b] Randolph Thummel,[b] Ye Tao,[c] Suning Wang*,[a]

Synthesis of ligands

*2,4-Difluorophenylhydrazine (**6a**)*:[1] A mixture of 2,4-difluoroaniline (1.29 g, 10.0 mmol) in concentrated HCl (7 mL) was warmed until complete dissolution of the solid. The solution was slowly cooled to 5-10 •C and a solution of $NaNO_2$ (0.70 g, 10.1 mmol) in water (3.5 mL) was added dropwise. The solution turned slightly yellow and a white precipitate formed. The mixture was stirred for 1 h at 5-10 •C and then was added dropwise to a cooled (5-10 •C) solution of stannous chloride dihydrate (14.33 g, 63.5 mmol) in concentrated HCl (7 mL). A white foamy solid formed and the mixture was stirred for 50 min. Then, 50% NaOH was added until pH 14 was reached. The mixture turned gray and it was extracted with Et_2O (4 x 40 mL) and the resulting emulsion was filtered through Celite. The combined organic phase was washed with water (30 mL), brine (30 mL), dried ($MgSO_4$) and concentrated to provide **6a** as a white solid (1.06 g, 73%): mp 62-63 •C; ^{1}H-NMR ($CDCl_3$) δ 7.08 (m, 1H), 6.73-6.85 (overlapping m, 2H), 5.30 (s, 1H), 3.57 (s, 2H).

*2,5-Difluorophenylhydrazine (**7a**)*: In the same manner described above for **6a**, the reaction of 2,5-difluoroaniline (1.99 g, 15.4 mmol), $NaNO_2$ (1.08 g, 15.6 mmol) and stannous choride dihydrate (21.71 g, 97.7 mmol) provided **7a** as a white solid (1.85 g, 83%): mp 71-73 ˚C; ^{1}H-NMR ($CDCl_3$) δ 6.81-6.93 (overlapping m, 2H), 6.36 (m, 1H), 5.50 (s, 1H), 3.57 (s, 2H).

*2,3,4-Trifluorophenylhydrazine (**8a**)*: In the same manner described above for **6a**, the reaction of 2,3,4-trifluoroaniline (1.91 g, 13.0 mmol), $NaNO_2$ (0.91 g, 13.2 mmol) and stannous chloride dihydrate (18.3 g, 82.5 mmol) provided **8a** as a white solid (1.68 g, 80%): mp 84-85 ˚C; ^{1}H-NMR ($CDCl_3$) δ 6.94-6.79 (overlapping m, 2H), 5.35 (s, 1H), 3.58 (s, 2H).

*2,3,4,5-Tetrafluorophenylhydrazine (**9a**)*: In the same manner described above for **2a**, the reaction of 2,3,4,5-tetrafluoroaniline (**1e**, 0.90 g, 5.5 mmol), $NaNO_2$ (0.49 g, 7.0 mmol) and stannous chloride dihydrate (7.99 g, 35.4 mmol) provided **2e** as a light brown solid (0.33 g, 34%): mp 59-60 ˚C; ^{1}H-NMR ($CDCl_3$) δ 6.86 (m, 1H), 5.43 (s, 1H), 3.60 (s, 2H).

*2',4'-Difluorophenylhydrazone of 2-acetylpyridine (**6b**)*:[2] A mixture of 2-acetylpyridine (0.58 g, 4.8 mmol), 2,4-difluorophenylhydrazine (**6a**, 0.80 g, 6.0 mmol), and glacial HOAc (2 drops) in absolute EtOH (16 mL) was refluxed for 4

h. After cooling to room temperature, the mixture was concentrated and the product was recrystallized from hexanes to provide **6b** as a light orange solid (0.92 g, 78%): mp 59-60 ˚C; ^{1}H-NMR ($CDCl_3$) δ 8.57 (d, 1H, *J* = 4.2 Hz), 8.15 (d, 1H, *J* = 8.1 Hz), 7.57-7.72 (overlapping m, 2H), 7.53 (bs, 1H), 7.22 (t, 1H, *J* = 5.1 Hz), 6.92-6.82 (overlapping m, 2H), 2.41 (s, 3H).

*2',5'-Difluorophenylhydrazone of 2-acetylpyridine (**7b**)*: In the same manner described above for **6b**, a mixture of 2-acetylpyridine (1.19 g, 9.8 mmol) and 2,5-difluorophenylhydrazine (**7a**, 1.70 g, 11.8 mmol) provided **7b** as a white solid (1.81 g, 75%): mp 119-120 ˚C; ^{1}H-NMR ($CDCl_3$) δ 8.58 (dd, 1H, *J* = 5.1, 1.2 Hz), 8.16 (d, 1H, *J* = 8.1 Hz), 7.72 (td, 1H, *J* = 7.8, 1.5 Hz), 7.66 (bs, 1H), 7.36 (ddd, 1H, *J* = 9.9, 6.6, 3.0 Hz), 7.23 (ddd, 1H, *J* = 7.5, 4.8, 0.6 Hz), 7.01 (ddd, 1H, *J* = 13.8, 9.0, 4.8 Hz), 6.51 (m, 1H), 2.43 (s, 3H).

*2',3',4'-Trifluorophenylhydrazone of 2-acetylpyridine (**8b**)*: In the same manner described above for **6b**, a mixture of 2-acetylpyridine (0.90 g, 7.4 mmol) and 2,3,4-trifluorophenylhydrazine (**8a**, 1.44 g, 8.9 mmol) provided **8b** as a white solid (1.90 g, 97%): mp 91-93 ˚C; ^{1}H-NMR ($CDCl_3$) δ 8.59 (dd, 1H, *J* = 4.8, 0.6 Hz), 8.13 (dd, 1H, *J* = 8.1, 0.6 Hz), 7.70 (t, 1H, *J* = 9.0 Hz), 7.51 (bs, 1H), 7.21-7.39 (overlapping m, 2H), 6.97 (m, 1H), 2.43 (s, 3H).

*2',3',4',5'-Tetrafluorophenylhydrazone of 2-acetylpyridine (**9b**)*: In the same manner described above for **6a**, a mixture of 2-acetylpyridine (0.11 g, 0.9 mmol) and 2,3,4,5-tetrafluorophenylhydrazine (**9a**, 0.14 g, 0.8 mmol) provided a brown oil. Chromatography on silica gel, eluting with CH_2Cl_2, provided **9b** as a yellow solid (0.13 g, 60%): mp 74-77 ˚C; ^{1}H-NMR ($CDCl_3$) δ 9.88 (bs, 1H), 8.71 (dd, 1H, *J* = 5.1, 0.9 Hz), 7.86 (td, 1H, *J* = 7.8, 1.8 Hz), 7.51 (d, 1H, *J* = 8.1 Hz), 7.25-7.35 (overlapping m, 2H), 2.43 (s, 3H).

*5,7-Difluoro-2-(2'-pyridyl)indole (**6L**)*:[3] A mixture of **6b** (3.33 g, 13.5 mmol) and PPA (10.0 g) was mechanically stirred at 100-120 ˚C for 3 h. While cooling to room temperature, 10% NaOH was added until pH 14 was obtained. The mixture was extracted with CH_2Cl_2 (3 x 30 mL) and the combined organic phase was washed with brine (20 mL), dried ($MgSO_4$) and concentrated. Chromatography on silica gel, eluting with CH_2Cl_2 provided **5a** (1.23 g, 40%) as an orange solid: mp 131-132 ˚C; ^{1}H-NMR ($CDCl_3$) δ 9.78 (s, 1H), 8.60 (d, 1H, *J* = 5.1 Hz), 7.78 (d, 1H, *J* = 8.1 Hz), 7.75 (td, 1H, *J* = 7.8, 1.5 Hz), 7.23 (m, 1H), 7.09 (dd, 1H, *J* = 9.0, 1.8 Hz), 6.98 (t, 1H, *J* = 2.7 Hz), 6.75 (dt, 1H, *J* = 10.8, 2.1 Hz); ^{13}C-NMR ($CDCl_3$) δ 157.2 (dd, $J_{C\text{-}F}$ = 236.8, 9.5 Hz), 149.7, 149.3, 149.0 (dd, $J_{C\text{-}F}$ = 247.6, 14.2 Hz), 139.1, 137.0, 131.4 (dd, $J_{C\text{-}F}$ = 11.1, 6.6 Hz), 122.7, 122.0 (d, $J_{C\text{-}F}$ = 13.1 Hz), 120.3, 101.4 (dd, $J_{C\text{-}F}$ = 24.0, 2.8 Hz), 101.3, 98.3 (dd, $J_{C\text{-}F}$ = 34.3, 20.4 Hz); Anal. Calcd for $C_{13}H_8N_2F_2$(1/3 H_2O): C, 66.21; H, 3.25; N, 11.88. Found: C, 66.73; H, 3.02; N, 11.61.

*4,7-Difluoro-2-(2'-pyridyl)indole (**7L**)*: In the same manner described above for **6L**, a mixture of **7b** (1.53 g, 6.2 mmol) and PPA (7.00 g) provided **7L** as a white solid (0.30 g, 21%): mp 110-112 ˚C; ^{1}H-NMR ($CDCl_3$) δ 9.86 (bs, 1H), 8.61 (dd, 1H, *J* = 3.9, 1.2 Hz), 7.82 (dd, 1H, *J* = 9.0, 1.2 Hz), 7.76 (td, 1H, *J* = 8.1, 1.8 Hz), 7.23 (td, 1H, *J* = 5.4, 1.2 Hz), 7.08 (t, 1H, *J* = 2.4 Hz), 6.81 (ddd, 1H, *J* = 12.0, 8.4, 3.3 Hz), 6.66 (dd, 1H, *J* = 9.3, 3.3 Hz); ^{13}C-NMR ($CDCl_3$) δ 152.6 (dd, J_{C-F} = 242.9, 2.4 Hz), 149.5, 149.3, 146.4 (dd, J_{C-F} = 239.5, 3.4 Hz), 137.9, 137.0, 126.9 (dd, J_{C-F} = 16.0, 11.0 Hz), 122.7, 121.2 (dd, J_{C-F} = 24.4, 5.1 Hz), 120.3, 107.4 (dd, J_{C-F} = 21.9, 7.2 Hz), 97.4; Anal. Calcd for $C_{13}H_8N_2F_2$: C, 67.83; H, 3.48; N, 12.17. Found: C, 67.71; H, 3.23; N, 12.10.

*5,6,7-Trifluoro-2-(2'-pyridyl)indole (**8L**)*: In the same manner described above for **6L**, a mixture of **8b** (1.59 g, 6.0 mmol) and PPA (6.00 g) provided **8L** as a white solid (0.58 g, 39%): mp 135-136 ˚C; ^{1}H-NMR ($CDCl_3$) δ 9.83 (bs, 1H), 8.60 (d, 1H, *J* = 4.8 Hz), 7.76 (dd, 1H, *J* = 4.5, 1.2 Hz), 7.14-7.24 (overlapping m, 2H), 6.96 (t, 1H, *J* = 2.4 Hz); ^{13}C-NMR ($CDCl_3$) δ 149.4, 149.3, 147.2 (dd, J_{C-F} = 241.7, 10.7 Hz), 138.2 (ddd, J_{C-F} = 248.7, 13.8, 4.49 Hz), 139.1 (d, J_{C-F} = 3.5 Hz), 137.1, 137.8 (ddd, J_{C-F} = 243.0, 18.4, 12.5 Hz), 127.8, 123.3 (ddd, J_{C-F} = 214.3, 4.6, 2.3 Hz), 122.8, 120.1, 101.7 (ddd, J_{C-F} = 99.1, 5.7, 2.7 Hz), 101.0; Anal. Calcd for $C_{13}H_7N_2F_3$(1/4 H_2O): C, 61.78; H, 2.97; N, 11.09. Found: C, 61.40; H, 2.74; N, 10.94.

*4,5,6,7-Tetrafluoro-2-(2'-pyridyl)indole (**9L**)*: In the same manner described above for **5a**, a mixture of **4e** (0.18 g, 0.7 mmol) and PPA (2.00 g) provided **5e** as a white solid, which was recrystallized from CH_2Cl_2/hexane (0.06 g, 24%): mp 136-138 ˚C; ^{1}H-NMR ($CDCl_3$) δ 9.88 (bs, 1H), 8.54 (d, 1H, *J* = 5.4 Hz), 7.73 (overlapping m, 2H), 7.20 (m, 1H), 7.02 (t, 1H, *J* = 3.0 Hz); ^{13}C-NMR ($CDCl_3$) δ 149.4, 148.3, 138.9, 137.3, 123.2, 120.3, 97.3 (fluorinated carbons difficult to assign due to complicated couplings); Anal. Calcd for $C_{13}H_6N_2F_4$(1/4 H_2O): C, 57.67; H, 2.40; N, 10.35. Found: C, 57.38; H, 1.76; N, 10.13.

*Phenylhydrazone of 2-acetylthiazole (**11a, 11a'**)*: In the same manner described for **6b**, a mixture of 2-acetylthiazole (1.27 g, 10.0 mmol), phenylhydrazine (1.30 g, 12.0 mmol), and glacial HOAc (4 drops) in absolute EtOH (10 mL) provided a brown oil. Chromatography on alumina, eluting with CH_2Cl_2/petroleum ether (1:1), provided the E and Z isomers (**11a** and **11a'**) as a yellow oil (2.16 g, 99%) in an approximately 1:1 ratio by TLC: (**11a**) R_f = 0.89; ^{1}H-NMR ($CDCl_3$) δ 12.99 (bs, 1H), 7.98 (d, 1H, *J* = 3.3 Hz), 7.34 (d, 1H, *J* = 3.3 Hz), 7.23-7.32 (overlapping m, 4H), 6.89 (tt, 1H, *J* = 6.9, 1.5 Hz),

2.45 (s, 3H); (**11a'**) R_f = 0.46; ^{1}H-NMR ($CDCl_3$) δ 7.76 (d, 1H, *J* = 3.3 Hz), 7.64 (bs, 1H), 7.33 (d, 1H, *J* = 7.5 Hz), 7.30 (d, 1H, *J* = 7.2 Hz), 7.25 (d, 1H, *J* = 3.3 Hz), 7.19 (dd, 2H, *J* = 8.1, 1.5 Hz), 6.95 (t, 1H, *J* = 8.4 Hz), 2.43 (s, 3H).

*2-(2'-Thiazolyl)indole (**11L**)*:[2, 3] A mixture of the phenylhydrazone of 2-acetylthiazole (**11a** and **11a'**, 1.67 g, 7.7 mmol), $ZnCl_2$ (5.44 g) and glacial HOAc (110 mL) was refluxed under Argon protection. After 24 h, more $ZnCl_2$ (2.72 g) was added, and the mixture was refluxed for a further 48 h. After cooling to room temperature, the reaction mixture was concentrated. The residue was dissolved with CH_2Cl_2 (50 mL) and 10% NaOH was added until pH 14 was obtained. The mixture was sonicated for 15 min and the white residue filtered. The two layers were separated and the aqueous phase was extracted with CH_2Cl_2 (3 x 50 mL). The combined organic phase was washed with brine (50 mL), dried ($MgSO_4$) and concentrated. Chromatography on silica gel, eluting with CH_2Cl_2 provided **11L** (0.92 g, 56%) as a white solid: mp 125-126 °C; ^{1}H-NMR ($CDCl_3$) δ 9.65 (bs, 1H), 7.81 (d, 1H, *J* = 3.3 Hz), 7.65 (d, 1H, *J* = 7.8 Hz), 7.40 (dd, 1H, *J* = 8.1, 1.2 Hz), 7.32 (d, 1H, *J* = 3.3 Hz), 7.26 (td, 1H, *J* = 8.1, 1.2 Hz), 7.13 (td, 1H, *J* = 7.8, 1.5 Hz), 7.04 (dd, 1H, *J* = 1.8, 0.9 Hz); ^{13}C-NMR ($CDCl_3$) δ 161.6, 142.7, 137.2, 131.5, 128.5, 124.0, 121.4, 120.5, 118.5, 111.7, 103.6.

*1-Phenylsulfonyl-2-(8'-quinolyl)indole (**12a**)*: Under nitrogen protection, to a solution of 1-phenylsulfonyl-indole (1.00 g, 3.89 mmol) in 5 mL THF at 0 °C was slowly added a solution of LDA (1.5 M in cyclohexane, 2.8 mL, 4.20 mmol). The resulting mixture was stirred for 30 min at this temperature, and then a solution of anhydrous $ZnCl_2$ (0.5 M in THF, 8.4 mL, 4.2 mmol) was added slowly. The mixture was stirred at room temperature for another 30 min. In a separate flask, a solution of 8-bromoqunoline (0.673 g, 3.23 mmol) in 5 mL THF was added to a solution containing a catalyst prepared by the reaction of $Pd(PPh_3)_2Cl_2$ (0.10g, 0.14 mmol) and diisobutylaluminum hydride (1.0 M in hexane, 0.28 mL, 0.28 mmol), and the mixture was stirred for 20 min at room temperature. The resulting mixture was added slowly to the former mixture solution. The final mixed solution was refluxed for 6 h under nitrogen protection, then cooled to room temperature, and poured into saturated aqueous Na_2CO_3. The aqueous phase was extracted with Et_2O, and the organic extracts were combined and concentrated to give a brown residue, which was purified by column chromatography (hexane/ethyl acetate, 3/1) to obtain the product as white powder (1.07 g, 86% yield). ^{1}H NMR ($CDCl_3$, δ, ppm): 8.83 (dd, 1H, J = 4.2, 1.7 Hz), 8.20 – 8.27 (m, 2H) , 7.96 (dd, 1H, J = 8.2, 1.4 Hz), 7.80 (dd, 1H, J = 7.1, 1.4 Hz), 7.64 (dd, 1H, J = 8.1, 7.2 Hz), 7.53 – 7.62 (m, 3H), 7.23 – 7.45 (m, 6H), 6.80 (s, 1H).

*1-Phenylsulfonyl-2-(8'-quinolyl)-7-azaindole (**13a**)*: In the same manner as described for **12a**, the reaction of 1-phenylsulfonyl-7-azaindole (3.79 g, 14.4 mmol) and 8-bromoquinoline (2.50 g, 12.0 mmol) afforded 1-phenylsulfonyl-2-(8'-Quinolyl)-7-azaindole as white powder (4.56 g, 96% yield). ^{1}H NMR ($CDCl_3$, δ, ppm): 8.80 (1H, m), 8.48 (1H, d, J =

4.8 Hz), 8.26 (1H, d, J = 8.4 Hz), 8.00 (3H, m), 7.87 (2H, m), 7.68 (1H, m), 7.36-7.52 (4H, m), 7.22 (1H, dd, J = 7.8, 4.8 Hz), 6.68 (1H, s).

*2-(8'-Quinolyl)indole (**12L**)*: A mixture of 1-phenylsulfonyl-2-(8'-quinolyl)indole (**12a**, 0.90 g, 2.34 mmol) in EtOH (150 mL) and 10% aqueous NaOH (10 mL) was heated at reflux for 10 h. The resulting mixture was concentrated, and the residue was dissolved in CH_2Cl_2. The solution was washed with water and aqueous Na_2CO_3, dried over $MgSO_4$, and concentrated . Column chromatography (hexane/ethyl acetate, 3/1) of the residue afforded the product as yellow powder (0.53 g, 93% yield), mp 153 – 154 ^oC. ^1H NMR (CD_2Cl_2, δ, ppm): 9.08 (dd, 1H, J = 4.2, 1.8 Hz, quin), 8.44 (dd, 1H, J = 7.5, 1.3 Hz, quin), 8.31 (dd, 1H, J = 8.3, 1.7 Hz, quin), 7.82 (dd, 1H, J = 8.0, 1.1 Hz, quin), 7.71 (dd, 1H, J = 7.9, 0.8 Hz, indl), 7.67 (t, 1H, J = 7.8 Hz, quin), 7.60 (dd, 1H, J = 8.1, 0.8 Hz, indl), 7.55 (dd, 1H, J = 8.3, 4.2 Hz, quin), 7.23 – 7.26 (m, 2H, indl), 7.15 (ddd, 1H, J = 7.9, 7.1, 0.9 Hz, indl). ^{13}C NMR (CD_2Cl_2, δ, ppm): 149.6, 145.6, 138.1, 137.7, 137.2, 129.7, 128.9, 128.5, 127.8, 127.6, 127.1, 122.4, 121.6, 120.7, 120.1, 111.9, 100.5. Anal Calcd for $C_{17}H_{12}N_2$: C, 83.60; H, 4.92; N, 11.47. Found: C, 83.29; H, 4.85; N, 11.44.

*2-(8'-Quinolyl)-7-azaindole (**13L**)*: In the same manner as described for **12L**, the treatment of 1-phenylsulfonyl-2-(8'-quinolyl)-7-azaindole (**13a**, 4.5 g, 11.5 mmol) with 10% aqueous NaOH solution (64 mL) afforded the product as yellow microcrystalline solid (2.3 g, 82% yield), mp 132 – 133 ^oC. ^1H NMR (CD_2Cl_2, δ, ppm): 9.06 (dd, 1H, J = 4.2, 1.8 Hz, quin), 8.43 (dd, 1H, J = 7.6, 1.2 Hz, quin), 8.34 (dd, 1H, J = 4.6, 1.5 Hz, azaindl), 8.30 (dd, 1H, J = 8.3, 1.8 Hz, quin), 8.00 (d, 1H, J = 7.8, 1.2 Hz, azaindl), 7.85 (dd, 1H, J = 8.0 1.1 Hz, quin), 7.67 (d, 1H, J = 7.7 Hz, quin), 7.55 (dd, 1H, J = 8.3, 4.2 Hz, quin), 7.16 (s, 1H, azaindl), 7.11 (dd, 1H, J = 7.8, 4.7 Hz, azaindl). ^{13}C NMR (CD_2Cl_2, δ, ppm): 149.9, 149.5, 145.5, 143.9, 138.2, 137.6, 129.6, 128.4, 128.3, 128.2, 127.9, 127.0, 121.7, 120.7, 116.5, 98.6. Anal Calcd. for $C_{16}H_{11}N_3$: C, 78.37; H, 4.49; N, 17.14. Found: C, 78.39; H, 4.55; N, 17.07.

References

[1] Y. T. Tao, C. W. Ko, E. Balasubramaniam, *Thin Solid Films*, **2002**, *417*, 61.

[2] K. H. Pilgram, *Synth. Commun.* 1985, *15*, 697-706.

[3] B. Robinson, *The Fischer Indole Synthesis*; John Wiley & Sons: Chichester New York Brisbane Toronto Singapore, 1982.

Figure^^S1. Molecular structure of 6

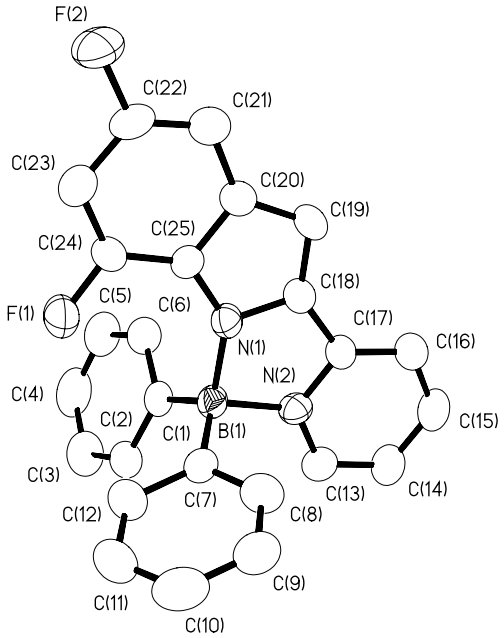


Figure.^^S2. Molecular structure of **8.**

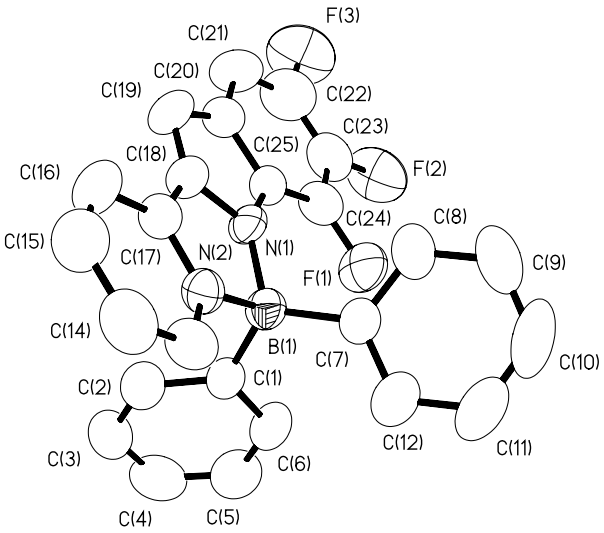


Figure.^^S3. Molecular structure of **13**.

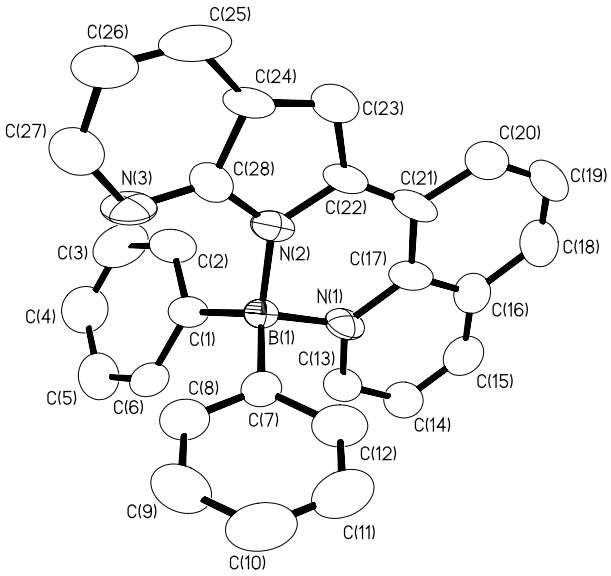
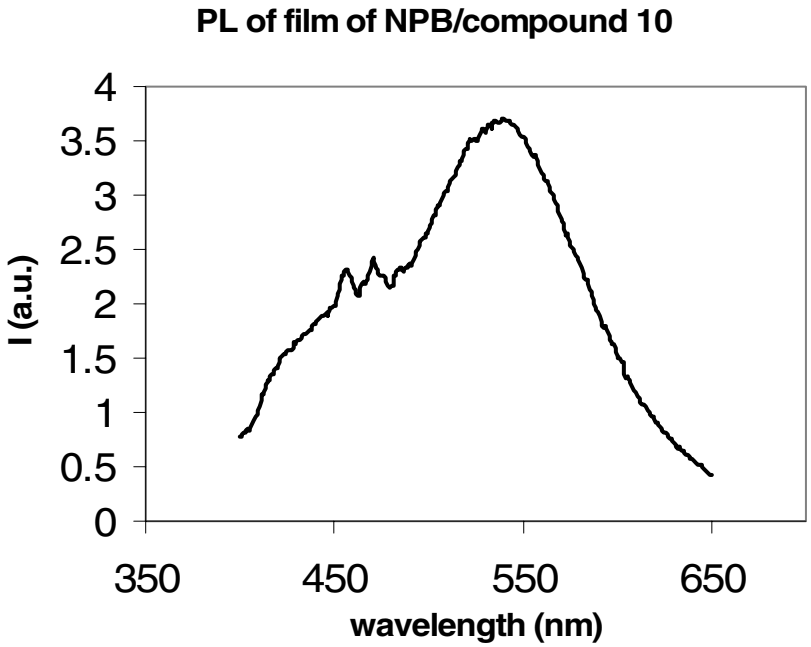
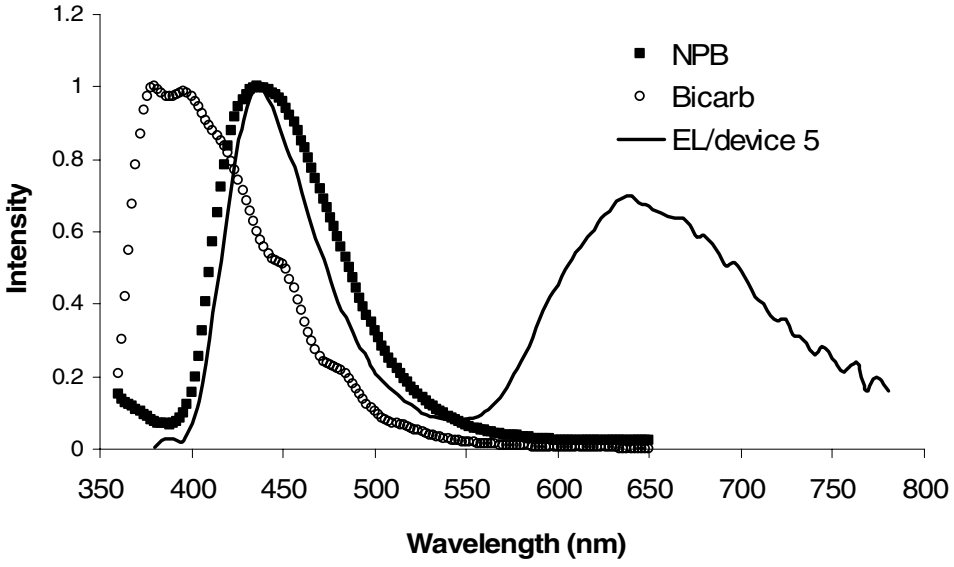


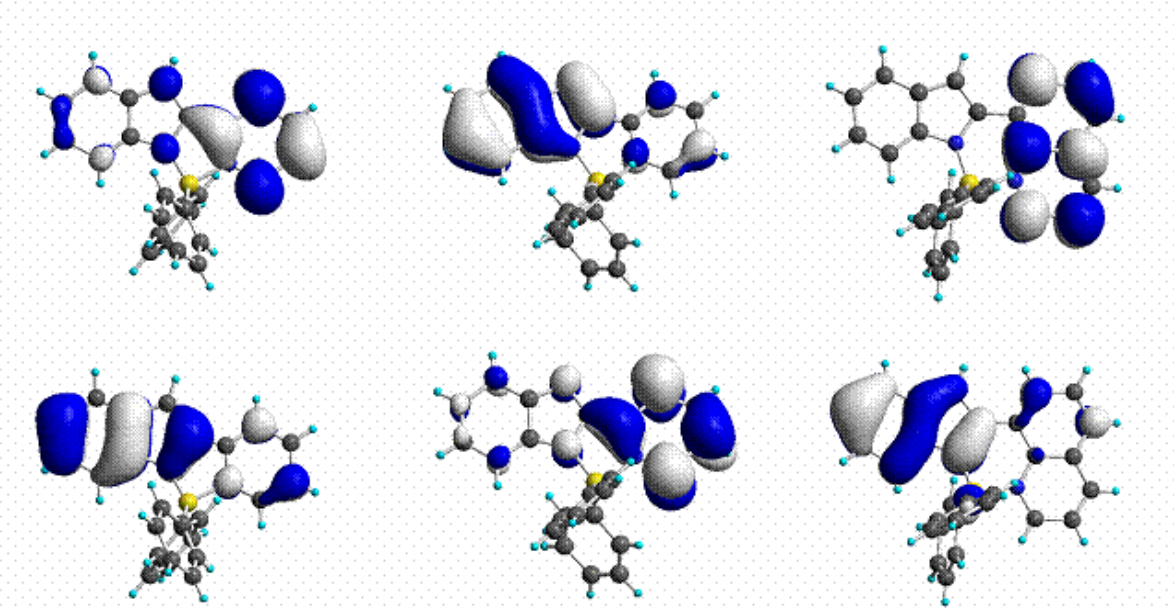
Figure S4.


PL of film of NPB/compound 10
I (a.u.)
4
3.5
3
2.5
2
1.5
1
0.5
0
350
450
550
650
wavelength (nm)

Figure^^S5. PL spectra of NPB and Bicarb and EL of device 5.



Figure^^S6. HOMO-1 and LUMO+1 for **1**, **10**, and **12**



1 **10** **12**

Table 1. Crystal data and structure refinement for **6**.

Identification code	**6**	
Empirical formula	C25 H17 B F2 N2	
Formula weight	394.22	
Temperature	293(2) K	
Wavelength	0.71073 [Å]	
Crystal system	Monoclinic	
Space group	$P2_1$	
Unit cell dimensions	a = 9.188(3) [Å]	α= 90°.
	b = 11.721(4) [Å]	β= 91.697(7)°.
	c = 18.737(6) [Å]	γ = 90°.
Volume	2017.0(11) [$Å^3$]	
Z	4	
Density (calculated)	1.298 [Mgm^{-1}]	
Absorption coefficient	0.089 [mm^{-1}]	
F(000)	816	
Crystal size	0.30 x 0.10 x 0.10 [mm^3]	
Theta range for data collection	2.05 to 28.33°.	
Index ranges	-12<=h<=11, -15<=k<=15, -24<=l<=22	
Reflections collected	14468	
Independent reflections	8108 [R(int) = 0.0371]	
Completeness to theta = 28.33°	94.8 %	
Absorption correction	Empirical	
Max. and min. transmission	1.000 and 0.712	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	8108 / 1 / 541	
Goodness-of-fit on F^2	0.817	
Final R indices [I>2sigma(I)]	R1 = 0.0474, wR2 = 0.0856	
R indices (all data)	R1 = 0.1430, wR2 = 0.1032	
Absolute structure parameter	-0.9(8)	
Largest diff. peak and hole	0.218 and -0.130 e.[$Å^{-3}$]	

Table 2. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for **6**. U[eq] is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U[eq]
B(1)	8982(4)	6119(3)	505(2)	49(1)
B(2)	9040(5)	-42(4)	5623(2)	54(1)
N(1)	9089(3)	5018(2)	988(1)	48(1)
N(2)	10690(3)	6463(2)	647(2)	48(1)
N(3)	8103(3)	1081(2)	5587(2)	51(1)
N(4)	8910(3)	-282(3)	4764(2)	56(1)
C(1)	8003(3)	7093(3)	847(2)	47(1)
C(2)	7456(4)	8035(3)	453(2)	59(1)
C(3)	6632(4)	8876(3)	770(3)	77(1)
C(4)	6302(5)	8809(4)	1472(3)	78(1)
C(5)	6810(5)	7910(4)	1874(2)	75(1)
C(6)	7650(4)	7077(3)	1568(2)	58(1)
C(7)	8746(4)	5788(3)	-314(2)	48(1)
C(8)	9830(4)	5321(3)	-702(2)	64(1)
C(9)	9686(5)	4985(3)	-1402(2)	74(1)
C(10)	8367(6)	5130(3)	-1761(2)	79(1)
C(11)	7232(5)	5613(3)	-1407(2)	71(1)
C(12)	7413(4)	5932(3)	-689(2)	61(1)
C(13)	11355(4)	7385(3)	380(2)	58(1)
C(14)	12819(4)	7557(3)	503(2)	65(1)
C(15)	13601(4)	6771(4)	901(2)	67(1)
C(16)	12918(4)	5823(3)	1180(2)	63(1)
C(17)	11458(4)	5695(3)	1041(2)	48(1)
C(18)	10464(4)	4800(3)	1263(2)	50(1)
C(19)	10499(4)	3824(3)	1682(2)	61(1)
C(20)	9052(4)	3420(3)	1675(2)	52(1)
C(21)	8372(5)	2479(3)	2002(2)	66(1)
C(22)	6952(5)	2359(3)	1891(2)	65(1)
C(23)	6061(4)	3087(3)	1467(2)	64(1)
C(24)	6730(4)	3973(3)	1154(2)	53(1)
C(25)	8211(4)	4169(3)	1241(2)	44(1)
C(26)	8272(4)	-1063(3)	6037(2)	54(1)
C(27)	6831(4)	-1010(3)	6233(2)	68(1)
C(28)	6167(5)	-1870(4)	6596(2)	91(2)
C(29)	6918(5)	-2876(4)	6746(2)	79(1)
C(30)	8308(5)	-2972(4)	6549(2)	80(1)
C(31)	9008(5)	-2080(3)	6214(2)	66(1)
C(32)	10704(4)	239(3)	5843(2)	49(1)
C(33)	11302(4)	39(3)	6520(2)	68(1)
C(34)	12700(5)	368(4)	6721(3)	90(2)
C(35)	13551(5)	919(4)	6242(3)	96(2)
C(36)	13025(5)	1134(4)	5573(3)	85(1)
C(37)	11613(5)	792(3)	5365(2)	72(1)
C(38)	9436(4)	-1192(3)	4419(2)	70(1)
C(39)	9225(5)	-1295(4)	3695(3)	81(1)
C(40)	8432(5)	-476(5)	3330(2)	87(1)
C(41)	7898(4)	468(4)	3685(2)	75(1)
C(42)	8127(4)	529(3)	4404(2)	56(1)
C(43)	7658(4)	1385(3)	4902(2)	57(1)
C(44)	6861(4)	2382(3)	4889(2)	67(1)

C(45)	6757(4)	2721(3)	5609(2)	56(1)
C(46)	6065(4)	3630(3)	5959(2)	70(1)
C(47)	6113(4)	3641(3)	6669(3)	66(1)
C(48)	6881(5)	2864(3)	7107(2)	67(1)
C(49)	7566(4)	2005(3)	6768(2)	58(1)
C(50)	7546(4)	1903(3)	6034(2)	50(1)
F(1)	5936(2)	4700(2)	726(1)	75(1)
F(2)	6234(3)	1474(2)	2220(1)	91(1)
F(3)	8338(3)	1224(2)	7164(1)	86(1)
F(4)	5418(3)	4505(2)	7027(1)	93(1)

Table 3. Bond lengths [Å] and angles [°] for **6**.

B(1)-N(1)	1.578(5)	C(24)-C(25)	1.386(4)
B(1)-C(7)	1.593(5)	C(26)-C(27)	1.386(5)
B(1)-C(1)	1.598(5)	C(26)-C(31)	1.405(5)
B(1)-N(2)	1.634(5)	C(27)-C(28)	1.369(5)
B(2)-N(3)	1.573(5)	C(28)-C(29)	1.390(6)
B(2)-C(26)	1.600(5)	C(29)-C(30)	1.344(5)
B(2)-C(32)	1.606(5)	C(30)-C(31)	1.388(5)
B(2)-N(4)	1.635(5)	C(32)-C(33)	1.387(5)
N(1)-C(18)	1.373(4)	C(32)-C(37)	1.401(5)
N(1)-C(25)	1.374(4)	C(33)-C(34)	1.383(5)
N(2)-C(13)	1.345(4)	C(34)-C(35)	1.371(6)
N(2)-C(17)	1.350(4)	C(35)-C(36)	1.353(5)
N(3)-C(43)	1.382(4)	C(36)-C(37)	1.402(5)
N(3)-C(50)	1.385(4)	C(38)-C(39)	1.371(5)
N(4)-C(38)	1.345(4)	C(39)-C(40)	1.374(6)
N(4)-C(42)	1.359(4)	C(40)-C(41)	1.387(6)
C(1)-C(6)	1.399(4)	C(41)-C(42)	1.359(5)
C(1)-C(2)	1.412(4)	C(42)-C(43)	1.445(5)
C(2)-C(3)	1.388(5)	C(43)-C(44)	1.379(5)
C(3)-C(4)	1.361(5)	C(44)-C(45)	1.413(5)
C(4)-C(5)	1.370(5)	C(45)-C(46)	1.411(5)
C(5)-C(6)	1.380(5)	C(45)-C(50)	1.430(4)
C(7)-C(8)	1.364(4)	C(46)-C(47)	1.331(5)
C(7)-C(12)	1.404(4)	C(47)-F(4)	1.381(4)
C(8)-C(9)	1.372(5)	C(47)-C(48)	1.402(5)
C(9)-C(10)	1.378(5)	C(48)-C(49)	1.355(5)
C(10)-C(11)	1.374(5)	C(49)-F(3)	1.364(4)
C(11)-C(12)	1.403(5)	C(49)-C(50)	1.380(4)
C(13)-C(14)	1.373(4)		
C(14)-C(15)	1.375(5)	N(1)-B(1)-C(7)	111.0(3)
C(15)-C(16)	1.386(5)	N(1)-B(1)-C(1)	112.4(3)
C(16)-C(17)	1.368(4)	C(7)-B(1)-C(1)	119.8(3)
C(17)-C(18)	1.459(5)	N(1)-B(1)-N(2)	93.8(3)
C(18)-C(19)	1.387(4)	C(7)-B(1)-N(2)	108.6(3)
C(19)-C(20)	1.412(4)	C(1)-B(1)-N(2)	108.0(3)
C(20)-C(25)	1.411(4)	N(3)-B(2)-C(26)	113.5(3)
C(20)-C(21)	1.415(5)	N(3)-B(2)-C(32)	110.8(3)
C(21)-C(22)	1.323(5)	C(26)-B(2)-C(32)	117.3(3)
C(22)-F(2)	1.383(4)	N(3)-B(2)-N(4)	94.4(3)
C(22)-C(23)	1.411(5)	C(26)-B(2)-N(4)	109.2(3)
C(23)-C(24)	1.351(4)	C(32)-B(2)-N(4)	109.2(3)
C(24)-F(1)	1.366(3)	C(18)-N(1)-C(25)	106.2(3)

C(18)-N(1)-B(1)	114.1(3)	C(23)-C(24)-C(25)	122.2(3)
C(25)-N(1)-B(1)	139.7(3)	F(1)-C(24)-C(25)	118.2(3)
C(13)-N(2)-C(17)	120.2(3)	N(1)-C(25)-C(24)	131.6(3)
C(13)-N(2)-B(1)	125.6(3)	N(1)-C(25)-C(20)	109.4(3)
C(17)-N(2)-B(1)	114.1(3)	C(24)-C(25)-C(20)	119.0(3)
C(43)-N(3)-C(50)	106.1(3)	C(27)-C(26)-C(31)	115.6(4)
C(43)-N(3)-B(2)	113.8(3)	C(27)-C(26)-B(2)	122.2(3)
C(50)-N(3)-B(2)	140.1(3)	C(31)-C(26)-B(2)	122.2(4)
C(38)-N(4)-C(42)	120.6(3)	C(28)-C(27)-C(26)	122.8(4)
C(38)-N(4)-B(2)	126.3(3)	C(27)-C(28)-C(29)	119.9(4)
C(42)-N(4)-B(2)	113.0(3)	C(30)-C(29)-C(28)	119.0(4)
C(6)-C(1)-C(2)	115.2(3)	C(29)-C(30)-C(31)	121.2(4)
C(6)-C(1)-B(1)	121.7(3)	C(30)-C(31)-C(26)	121.3(4)
C(2)-C(1)-B(1)	123.0(3)	C(33)-C(32)-C(37)	115.8(3)
C(3)-C(2)-C(1)	121.5(4)	C(33)-C(32)-B(2)	123.2(3)
C(4)-C(3)-C(2)	120.8(4)	C(37)-C(32)-B(2)	120.8(3)
C(3)-C(4)-C(5)	119.7(4)	C(34)-C(33)-C(32)	122.8(4)
C(4)-C(5)-C(6)	120.0(4)	C(35)-C(34)-C(33)	119.7(5)
C(5)-C(6)-C(1)	122.7(4)	C(36)-C(35)-C(34)	120.0(5)
C(8)-C(7)-C(12)	115.0(3)	C(35)-C(36)-C(37)	120.4(4)
C(8)-C(7)-B(1)	122.0(3)	C(32)-C(37)-C(36)	121.3(4)
C(12)-C(7)-B(1)	123.0(3)	N(4)-C(38)-C(39)	120.2(4)
C(7)-C(8)-C(9)	124.9(4)	C(38)-C(39)-C(40)	119.2(4)
C(8)-C(9)-C(10)	119.3(4)	C(39)-C(40)-C(41)	120.6(4)
C(11)-C(10)-C(9)	119.0(4)	C(42)-C(41)-C(40)	118.1(4)
C(10)-C(11)-C(12)	120.1(4)	C(41)-C(42)-N(4)	121.3(4)
C(11)-C(12)-C(7)	121.7(4)	C(41)-C(42)-C(43)	129.6(4)
N(2)-C(13)-C(14)	120.7(4)	N(4)-C(42)-C(43)	109.2(3)
C(13)-C(14)-C(15)	119.1(4)	C(44)-C(43)-N(3)	112.2(3)
C(14)-C(15)-C(16)	120.4(4)	C(44)-C(43)-C(42)	138.2(4)
C(17)-C(16)-C(15)	118.0(4)	N(3)-C(43)-C(42)	109.5(3)
N(2)-C(17)-C(16)	121.6(3)	C(43)-C(44)-C(45)	105.7(3)
N(2)-C(17)-C(18)	108.3(3)	C(46)-C(45)-C(44)	134.3(4)
C(16)-C(17)-C(18)	130.1(3)	C(46)-C(45)-C(50)	118.4(4)
N(1)-C(18)-C(19)	111.8(3)	C(44)-C(45)-C(50)	107.2(3)
N(1)-C(18)-C(17)	109.7(3)	C(47)-C(46)-C(45)	118.0(4)
C(19)-C(18)-C(17)	138.5(3)	C(46)-C(47)-F(4)	119.4(4)
C(18)-C(19)-C(20)	105.4(3)	C(46)-C(47)-C(48)	125.5(4)
C(25)-C(20)-C(19)	107.2(3)	F(4)-C(47)-C(48)	115.0(4)
C(25)-C(20)-C(21)	119.5(3)	C(49)-C(48)-C(47)	116.1(4)
C(19)-C(20)-C(21)	133.3(3)	C(48)-C(49)-F(3)	119.0(4)
C(22)-C(21)-C(20)	117.5(4)	C(48)-C(49)-C(50)	122.6(4)
C(21)-C(22)-F(2)	119.4(4)	F(3)-C(49)-C(50)	118.3(4)
C(21)-C(22)-C(23)	125.2(4)	C(49)-C(50)-N(3)	132.0(3)
F(2)-C(22)-C(23)	115.4(4)	C(49)-C(50)-C(45)	119.2(4)
C(24)-C(23)-C(22)	116.5(4)	N(3)-C(50)-C(45)	108.7(3)
C(23)-C(24)-F(1)	119.6(3)		

Table 4. Anisotropic displacement parameters [$Å^2 \times 10^3$] for **6**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
B(1)	40(3)	44(2)	61(3)	10(2)	8(2)	6(2)
B(2)	60(3)	55(3)	47(3)	5(2)	6(2)	4(2)
N(1)	42(2)	46(2)	57(2)	3(1)	4(2)	5(2)
N(2)	51(2)	42(2)	51(2)	4(2)	4(2)	-4(2)
N(3)	55(2)	52(2)	47(2)	4(2)	4(2)	5(2)
N(4)	55(2)	58(2)	53(2)	-1(2)	5(2)	5(2)
C(1)	37(2)	46(2)	58(2)	-4(2)	-2(2)	-5(2)
C(2)	51(3)	52(2)	74(3)	6(2)	0(2)	4(2)
C(3)	69(3)	37(2)	123(4)	0(3)	5(3)	10(2)
C(4)	63(3)	66(3)	106(4)	-39(3)	10(3)	0(2)
C(5)	64(3)	88(3)	73(3)	-28(3)	4(2)	-6(3)
C(6)	57(3)	58(2)	61(3)	-7(2)	6(2)	7(2)
C(7)	46(2)	43(2)	54(2)	3(2)	7(2)	-3(2)
C(8)	74(3)	62(3)	55(3)	-4(2)	-1(2)	3(2)
C(9)	81(3)	83(3)	59(3)	-6(2)	16(3)	6(3)
C(10)	111(4)	69(3)	58(3)	-10(2)	5(3)	-24(3)
C(11)	73(3)	74(3)	64(3)	-2(2)	-19(2)	-7(3)
C(12)	62(3)	50(2)	72(3)	4(2)	-6(2)	0(2)
C(13)	60(3)	53(2)	60(3)	4(2)	8(2)	0(2)
C(14)	50(3)	59(2)	85(3)	-1(2)	3(2)	-10(2)
C(15)	43(3)	85(3)	73(3)	-10(2)	0(2)	-8(2)
C(16)	48(3)	72(3)	69(3)	10(2)	-4(2)	-1(2)
C(17)	41(2)	49(2)	52(2)	1(2)	0(2)	2(2)
C(18)	46(2)	53(2)	52(2)	2(2)	2(2)	8(2)
C(19)	49(3)	61(2)	74(3)	21(2)	-7(2)	8(2)
C(20)	55(3)	47(2)	55(2)	4(2)	2(2)	3(2)
C(21)	67(3)	59(3)	74(3)	13(2)	2(2)	-3(2)
C(22)	74(3)	61(3)	60(3)	11(2)	4(2)	-25(3)
C(23)	55(3)	65(3)	70(3)	2(2)	1(2)	-16(2)
C(24)	50(3)	45(2)	62(3)	11(2)	-2(2)	6(2)
C(25)	43(2)	49(2)	40(2)	-2(2)	3(2)	-5(2)
C(26)	55(3)	51(2)	56(2)	0(2)	7(2)	3(2)
C(27)	56(3)	60(3)	87(3)	15(2)	5(2)	1(2)
C(28)	77(3)	94(3)	105(4)	13(3)	33(3)	-17(3)
C(29)	85(4)	62(3)	88(3)	11(3)	0(3)	-21(3)
C(30)	98(4)	53(3)	89(3)	4(2)	15(3)	0(3)
C(31)	72(3)	62(3)	65(3)	0(2)	8(2)	5(2)
C(32)	46(2)	48(2)	54(2)	-4(2)	-3(2)	1(2)
C(33)	66(3)	76(3)	62(3)	-8(2)	6(2)	2(2)
C(34)	65(3)	118(4)	85(4)	-21(3)	-20(3)	13(3)
C(35)	49(3)	105(4)	133(5)	-30(4)	2(3)	0(3)
C(36)	59(3)	92(3)	103(4)	5(3)	9(3)	-14(3)
C(37)	62(3)	72(3)	84(3)	11(2)	9(3)	6(2)
C(38)	75(3)	68(3)	65(3)	-7(2)	4(2)	6(2)
C(39)	91(4)	87(3)	66(3)	-17(3)	11(3)	6(3)
C(40)	89(4)	119(4)	51(3)	-14(3)	3(3)	-20(3)
C(41)	87(3)	83(3)	56(3)	2(2)	11(2)	2(3)
C(42)	57(3)	66(3)	44(3)	6(2)	2(2)	-2(2)
C(43)	62(3)	64(3)	43(3)	9(2)	0(2)	8(2)
C(44)	85(3)	58(3)	59(3)	14(2)	-1(2)	11(2)

C(45)	54(3)	56(2)	58(3)	12(2)	1(2)	7(2)
C(46)	73(3)	49(2)	88(3)	7(2)	18(3)	10(2)
C(47)	63(3)	56(3)	80(3)	-10(3)	23(3)	5(2)
C(48)	72(3)	61(3)	68(3)	-6(2)	19(2)	-6(2)
C(49)	60(3)	58(2)	54(3)	7(2)	-3(2)	3(2)
C(50)	46(2)	51(2)	53(3)	1(2)	10(2)	-3(2)
F(1)	51(1)	75(1)	100(2)	21(1)	-8(1)	-6(1)
F(2)	97(2)	74(2)	101(2)	26(1)	-2(2)	-27(1)
F(3)	105(2)	94(2)	60(1)	3(1)	3(1)	26(2)
F(4)	105(2)	61(1)	113(2)	-12(1)	30(2)	9(1)

Table 5. Hydrogen coordinates [x 10^4] and isotropic displacement parameters [Å^2 x 10^3] for **6**.

	x	y	z	U[eq]
H(2A)	7653	8092	-30	71
H(3A)	6300	9494	499	92
H(4A)	5736	9371	1677	94
H(5A)	6587	7860	2354	90
H(6A)	7997	6481	1853	70
H(8A)	10735	5224	-474	76
H(9A)	10470	4663	-1632	89
H(10A)	8248	4904	-2234	95
H(11A)	6341	5728	-1645	85
H(12A)	6631	6248	-455	73
H(13A)	10817	7911	110	69
H(14A)	13275	8197	319	78
H(15A)	14595	6877	984	80
H(16A)	13437	5290	1453	76
H(19A)	11306	3504	1917	73
H(21A)	8904	1966	2284	80
H(23A)	5065	2963	1407	76
H(27A)	6291	-363	6113	81
H(28A)	5215	-1782	6742	109
H(29A)	6466	-3473	6979	94
H(30A)	8809	-3649	6640	96
H(31A)	9984	-2157	6104	79
H(33A)	10739	-333	6852	81
H(34A)	13061	215	7180	107
H(35A)	14489	1147	6376	115
H(36A)	13604	1509	5249	102
H(37A)	11273	936	4901	87
H(38A)	9945	-1754	4673	84
H(39A)	9614	-1911	3452	97
H(40A)	8250	-556	2842	104
H(41A)	7398	1041	3438	90
H(44A)	6472	2755	4488	81
H(46A)	5591	4204	5700	84
H(48A)	6918	2934	7601	80

Table 1. Crystal data and structure refinement for **8**.

Identification code	**8**	
Empirical formula	C25 H16 B F3 N2	
Formula weight	412.21	
Temperature	293(2) [K]	
Wavelength	0.71073 [Å]	
Crystal system	Monoclinic	
Space group	P2(1)	
Unit cell dimensions	a = 9.015(4) [Å]	α= 90°.
	b = 11.936(5) [Å]	β= 91.464(6)°.
	c = 9.341(4) [Å]	γ = 90°.
Volume	1004.8(7) [$Å^3$]	
Z	2	
Density (calculated)	1.362 [Mgm^{-3}]	
Absorption coefficient	0.099 [mm^{-1}]	
F(000)	424	
Crystal size	0.30 x 0.30 x 0.10 [mm^3]	
Theta range for data collection	2.18 to 28.36°.	
Index ranges	-10<=h<=11, -15<=k<=15, -12<=l<=12	
Reflections collected	6658	
Independent reflections	4104 [R(int) = 0.0396]	
Completeness to theta = 28.36°	94.6 %	
Absorption correction	Empirical	
Max. and min. transmission	1.000 and 0.605	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4104 / 0 / 280	
Goodness-of-fit on F^2	0.707	
Final R indices [I>2sigma(I)]	R1 = 0.0402, wR2 = 0.0604	
R indices (all data)	R1 = 0.1433, wR2 = 0.0711	
Absolute structure parameter	-0.4(7)	
Largest diff. peak and hole	0.109 and -0.128 [$e.Å^{-3}$]	

Table 2. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **8**. U[eq] is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U[eq]
B(1)	988(4)	8374(3)	4000(4)	48(1)
N(1)	1954(3)	9457(2)	4138(3)	49(1)
N(2)	1231(3)	8044(2)	5697(3)	50(1)
C(1)	-713(4)	8708(2)	3729(3)	47(1)
C(2)	-1525(4)	9257(3)	4760(3)	66(1)
C(3)	-2925(4)	9670(3)	4514(4)	76(1)
C(4)	-3586(4)	9531(3)	3204(5)	83(1)
C(5)	-2850(5)	8991(3)	2149(4)	78(1)
C(6)	-1432(4)	8587(2)	2401(3)	62(1)
C(7)	1677(4)	7429(3)	3029(3)	48(1)
C(8)	3163(4)	7481(3)	2654(3)	64(1)
C(9)	3790(4)	6665(4)	1811(4)	84(1)
C(10)	2967(7)	5772(4)	1358(4)	89(2)
C(11)	1523(6)	5697(3)	1688(4)	82(1)
C(12)	882(4)	6518(3)	2524(4)	68(1)
C(13)	771(4)	7106(3)	6321(4)	63(1)
C(14)	1034(4)	6928(3)	7769(4)	78(1)
C(15)	1771(4)	7740(4)	8539(4)	78(1)
C(16)	2255(4)	8705(3)	7899(4)	70(1)

C(17)	1982(4)	8836(3)	6440(4)	53(1)
C(18)	2403(4)	9733(3)	5507(4)	55(1)
C(19)	3102(4)	10708(3)	5577(4)	67(1)
C(20)	3146(4)	11117(3)	4154(4)	58(1)
C(21)	3758(4)	12080(3)	3508(5)	78(1)
C(22)	3590(5)	12169(3)	2085(6)	87(1)
C(23)	2880(4)	11398(4)	1235(5)	73(1)
C(24)	2279(4)	10486(3)	1836(4)	60(1)
C(25)	2413(4)	10317(3)	3303(4)	47(1)
F(1)	1570(2)	9719(2)	996(2)	78(1)
F(2)	2742(2)	11554(2)	-196(2)	104(1)
F(3)	4175(3)	13082(2)	1394(3)	126(1)

Table 3. Bond lengths [Å] and angles [°] for **8**.

B(1)-N(1)	1.562(4)	N(1)-B(1)-N(2)	93.3(2)
B(1)-C(7)	1.584(4)	C(7)-B(1)-N(2)	109.7(3)
B(1)-C(1)	1.598(5)	C(1)-B(1)-N(2)	108.4(2)
B(1)-N(2)	1.643(4)	C(25)-N(1)-C(18)	105.4(3)
N(1)-C(25)	1.360(4)	C(25)-N(1)-B(1)	139.0(3)
N(1)-C(18)	1.371(3)	C(18)-N(1)-B(1)	115.3(3)
N(2)-C(13)	1.333(3)	C(13)-N(2)-C(17)	121.5(3)
N(2)-C(17)	1.346(4)	C(13)-N(2)-B(1)	126.0(3)
C(1)-C(2)	1.389(4)	C(17)-N(2)-B(1)	112.5(3)
C(1)-C(6)	1.393(4)	C(2)-C(1)-C(6)	115.2(3)
C(2)-C(3)	1.369(4)	C(2)-C(1)-B(1)	121.9(3)
C(3)-C(4)	1.358(4)	C(6)-C(1)-B(1)	122.5(3)
C(4)-C(5)	1.365(5)	C(3)-C(2)-C(1)	123.6(3)
C(5)-C(6)	1.380(4)	C(4)-C(3)-C(2)	119.3(4)
C(7)-C(12)	1.379(4)	C(3)-C(4)-C(5)	119.9(4)
C(7)-C(8)	1.395(4)	C(4)-C(5)-C(6)	120.5(4)
C(8)-C(9)	1.382(4)	C(5)-C(6)-C(1)	121.6(3)
C(9)-C(10)	1.361(5)	C(12)-C(7)-C(8)	116.3(3)
C(10)-C(11)	1.349(5)	C(12)-C(7)-B(1)	123.3(3)
C(11)-C(12)	1.388(5)	C(8)-C(7)-B(1)	120.3(3)
C(13)-C(14)	1.384(4)	C(9)-C(8)-C(7)	121.4(4)
C(14)-C(15)	1.368(5)	C(10)-C(9)-C(8)	120.1(4)
C(15)-C(16)	1.374(5)	C(11)-C(10)-C(9)	120.2(4)
C(16)-C(17)	1.388(4)	C(10)-C(11)-C(12)	120.0(4)
C(17)-C(18)	1.438(4)	C(7)-C(12)-C(11)	121.9(4)
C(18)-C(19)	1.324(4)	N(2)-C(13)-C(14)	120.6(3)
C(19)-C(20)	1.417(4)	C(15)-C(14)-C(13)	118.3(4)
C(20)-C(25)	1.398(4)	C(14)-C(15)-C(16)	121.4(3)
C(20)-C(21)	1.417(4)	C(15)-C(16)-C(17)	118.1(4)
C(21)-C(22)	1.338(5)	N(2)-C(17)-C(16)	120.1(3)
C(22)-C(23)	1.364(5)	N(2)-C(17)-C(18)	110.4(3)
C(22)-F(3)	1.377(4)	C(16)-C(17)-C(18)	129.5(4)
C(23)-C(24)	1.346(4)	C(19)-C(18)-N(1)	112.7(3)
C(23)-F(2)	1.352(4)	C(19)-C(18)-C(17)	139.2(4)
C(24)-F(1)	1.355(4)	N(1)-C(18)-C(17)	108.1(3)
C(24)-C(25)	1.388(4)	C(18)-C(19)-C(20)	106.3(3)
		C(25)-C(20)-C(21)	119.7(3)
N(1)-B(1)-C(7)	114.3(3)	C(25)-C(20)-C(19)	105.9(3)
N(1)-B(1)-C(1)	109.7(3)	C(21)-C(20)-C(19)	134.4(3)
C(7)-B(1)-C(1)	118.4(3)	C(22)-C(21)-C(20)	116.9(4)

C(21)-C(22)-C(23)	124.4(4)	C(23)-C(24)-F(1)	119.6(4)
C(21)-C(22)-F(3)	119.5(5)	C(23)-C(24)-C(25)	120.2(4)
C(23)-C(22)-F(3)	116.1(4)	F(1)-C(24)-C(25)	120.1(3)
C(24)-C(23)-F(2)	119.7(4)	N(1)-C(25)-C(24)	131.0(3)
C(24)-C(23)-C(22)	119.4(4)	N(1)-C(25)-C(20)	109.6(3)
F(2)-C(23)-C(22)	120.9(4)	C(24)-C(25)-C(20)	119.4(3)

Table 4. Anisotropic displacement parameters [$Å^2 x\ 10^3$] for **8**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
B(1)	52(3)	53(3)	38(2)	0(2)	1(2)	-5(2)
N(1)	55(2)	59(2)	32(2)	-7(2)	1(1)	-12(2)
N(2)	52(2)	61(2)	38(2)	3(2)	2(1)	-3(2)
C(1)	55(2)	41(2)	46(2)	-3(2)	4(2)	-2(2)
C(2)	64(3)	75(3)	58(2)	-6(2)	-1(2)	3(2)
C(3)	60(3)	85(3)	82(3)	-15(3)	11(2)	8(2)
C(4)	54(3)	83(3)	111(3)	7(3)	-6(3)	4(2)
C(5)	73(3)	83(3)	76(3)	-2(2)	-16(3)	6(2)
C(6)	72(3)	68(2)	46(2)	-9(2)	-9(2)	5(2)
C(7)	56(3)	55(2)	32(2)	4(2)	-2(2)	3(2)
C(8)	69(3)	83(3)	42(2)	1(2)	3(2)	14(2)
C(9)	76(3)	125(4)	51(3)	8(3)	11(2)	38(3)
C(10)	148(5)	74(3)	47(3)	-8(2)	1(3)	42(3)
C(11)	126(4)	61(3)	60(3)	-10(2)	-8(3)	1(3)
C(12)	89(3)	62(3)	53(2)	-4(2)	-1(2)	-1(2)
C(13)	60(3)	72(3)	56(3)	11(2)	3(2)	-3(2)
C(14)	83(3)	96(3)	54(3)	22(3)	8(2)	3(3)
C(15)	82(3)	108(4)	45(3)	14(3)	-7(2)	3(3)
C(16)	83(3)	84(3)	41(2)	-8(2)	-12(2)	-1(2)
C(17)	48(2)	68(3)	45(2)	-2(2)	-1(2)	2(2)
C(18)	59(3)	63(3)	44(2)	-6(2)	-1(2)	-9(2)
C(19)	75(3)	69(3)	55(3)	-18(2)	-8(2)	-13(2)
C(20)	55(2)	52(2)	67(3)	-5(2)	8(2)	-8(2)
C(21)	75(3)	54(3)	104(4)	-4(3)	-3(3)	-16(2)
C(22)	95(3)	71(3)	95(4)	28(3)	6(3)	-5(3)
C(23)	72(3)	81(3)	65(3)	16(3)	12(3)	3(2)
C(24)	58(3)	65(3)	56(3)	14(2)	6(2)	-1(2)
C(25)	49(2)	46(2)	46(2)	-2(2)	6(2)	-2(2)
F(1)	97(2)	93(2)	44(1)	3(1)	0(1)	-16(1)
F(2)	104(2)	126(2)	83(2)	48(2)	7(1)	-9(2)
F(3)	141(2)	86(2)	153(2)	49(2)	15(2)	-24(2)

Table 5. Hydrogen coordinates [$x\ 10^4$] and isotropic displacement parameters [$Å^2 x\ 10^3$] for **8**.

	x	y	z	U(eq)
H(2A)	-1094	9349	5668	79
H(3A)	-3418	10041	5237	91
H(4A)	-4539	9804	3026	99
H(5A)	-3306	8894	1253	93
H(6A)	-946	8225	1666	74
H(8A)	3744	8078	2978	77
H(9A)	4776	6727	1554	100
H(10A)	3401	5211	819	107
H(11A)	956	5095	1356	99
H(12A)	-113	6451	2750	82
H(13A)	268	6567	5778	75
H(14A)	718	6274	8208	93
H(15A)	1947	7636	9515	94
H(16A)	2753	9255	8429	84
H(19A)	3487	11055	6396	80
H(21A)	4253	12625	4047	93

Table 1. Crystal data and structure refinement for **9**.

Identification code	**9**	
Empirical formula	C25 H15 B F4 N2	
Formula weight	430.20	
Temperature	293(2) K	
Wavelength	0.71073 [Å]	
Crystal system	Orthorhombic	
Space group	Pna2(1)	
Unit cell dimensions	a = 19.128(4) [Å]	α= 90°.
	b = 9.0418(17) [Å]	β= 90°.
	c = 11.663(3) [Å]	γ = 90°.
Volume	2017.2(7) [$Å^3$]	
Z	4	
Density (calculated)	1.417 [Mgm^{-3}]	
Absorption coefficient	0.109 [mm^{-1}]	
F(000)	880	
Crystal size	0.20 x 0.15 x 0.05 [mm^3]	
Theta range for data collection	2.13 to 28.33°.	
Index ranges	-25<=h<=24, -11<=k<=12, -15<=l<=13	
Reflections collected	14058	
Independent reflections	4460 [R(int) = 0.1102]	
Completeness to theta = 28.33°	98.2 %	
Absorption correction	Empirical	
Max. and min. transmission	1.000 and 0.853	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4460 / 1 / 289	
Goodness-of-fit on F^2	0.609	
Final R indices [I>2sigma(I)]	R1 = 0.0377, wR2 = 0.0337	
R indices (all data)	R1 = 0.2227, wR2 = 0.0485	
Absolute structure parameter	-0.7(6)	
Largest diff. peak and hole	0.136 and -0.139 [e.$Å^{-3}$]	

Table 2. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$x 10^3] for **9**.

U[eq] is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U[eq]
B(1)	516(2)	1012(5)	-593(5)	50(2)
F(1)	2034(1)	1592(2)	702(2)	80(1)
F(2)	2672(1)	2866(3)	2469(2)	90(1)
F(3)	1966(1)	4492(3)	4042(2)	96(1)
F(4)	562(1)	4747(2)	3852(2)	95(1)
N(1)	495(2)	1978(3)	534(3)	47(1)
N(2)	-308(2)	1259(4)	-866(3)	52(1)
C(1)	664(2)	-677(5)	-253(4)	51(1)
C(2)	1324(2)	-1284(5)	-368(4)	66(1)
C(3)	1482(3)	-2688(5)	32(4)	83(2)
C(4)	966(3)	-3512(5)	544(5)	93(2)
C(5)	305(3)	-2971(6)	651(4)	89(2)
C(6)	152(2)	-1549(5)	242(3)	70(2)
C(7)	980(2)	1781(5)	-1563(3)	49(1)
C(8)	1157(2)	3263(5)	-1551(4)	63(2)
C(9)	1570(2)	3922(6)	-2384(5)	78(2)
C(10)	1797(3)	3110(7)	-3280(5)	92(2)
C(11)	1636(3)	1652(7)	-3341(4)	84(2)
C(12)	1236(2)	1005(5)	-2496(4)	65(1)
C(13)	-649(3)	2028(5)	-27(5)	60(1)
C(14)	-1364(3)	2295(5)	-126(4)	73(2)
C(15)	-1706(3)	1806(5)	-1078(5)	88(2)
C(16)	-1349(3)	1059(5)	-1922(5)	80(2)
C(17)	-657(3)	769(5)	-1803(4)	67(2)
C(18)	-165(3)	2447(4)	858(4)	55(1)
C(19)	-160(3)	3208(5)	1846(4)	63(2)
C(20)	547(2)	3270(5)	2207(5)	52(1)
C(21)	938(3)	2452(5)	1382(5)	49(1)
C(22)	1654(3)	2356(5)	1474(5)	54(1)
C(23)	1976(2)	2994(6)	2370(5)	62(1)
C(24)	1612(3)	3798(6)	3168(5)	70(2)
C(25)	920(3)	3918(5)	3095(4)	65(2)

Table 3. Bond lengths [Å] and angles [°] for **9**.

B(1)-N(1)	1.579(5)	C(4)-C(5)	1.361(5)
B(1)-C(7)	1.597(5)	C(5)-C(6)	1.402(5)
B(1)-C(1)	1.603(5)	C(7)-C(8)	1.382(4)
B(1)-N(2)	1.623(5)	C(7)-C(12)	1.384(5)
F(1)-C(22)	1.348(5)	C(8)-C(9)	1.386(5)
F(2)-C(23)	1.341(4)	C(9)-C(10)	1.349(6)
F(3)-C(24)	1.375(5)	C(10)-C(11)	1.355(5)
F(4)-C(25)	1.345(4)	C(11)-C(12)	1.378(5)
N(1)-C(21)	1.371(5)	C(13)-C(14)	1.394(5)
N(1)-C(18)	1.384(5)	C(13)-C(18)	1.437(6)
N(2)-C(17)	1.356(4)	C(14)-C(15)	1.363(6)
N(2)-C(13)	1.366(5)	C(15)-C(16)	1.376(6)
C(1)-C(6)	1.383(4)	C(16)-C(17)	1.356(5)
C(1)-C(2)	1.384(5)	C(18)-C(19)	1.342(5)
C(2)-C(3)	1.386(5)	C(19)-C(20)	1.419(5)
C(3)-C(4)	1.374(6)	C(20)-C(25)	1.386(6)

C(20)-C(21)	1.425(5)	C(10)-C(11)-C(12)	120.1(5)
C(21)-C(22)	1.378(5)	C(11)-C(12)-C(7)	122.9(5)
C(22)-C(23)	1.343(6)	N(2)-C(13)-C(14)	119.8(5)
C(23)-C(24)	1.370(6)	N(2)-C(13)-C(18)	110.0(5)
C(24)-C(25)	1.333(5)	C(14)-C(13)-C(18)	130.2(5)
		C(15)-C(14)-C(13)	118.9(5)
N(1)-B(1)-C(7)	111.3(4)	C(14)-C(15)-C(16)	120.2(5)
N(1)-B(1)-C(1)	109.0(4)	C(17)-C(16)-C(15)	120.4(5)
C(7)-B(1)-C(1)	119.5(4)	N(2)-C(17)-C(16)	120.0(5)
N(1)-B(1)-N(2)	93.5(3)	C(19)-C(18)-N(1)	112.7(5)
C(7)-B(1)-N(2)	109.9(4)	C(19)-C(18)-C(13)	139.1(6)
C(1)-B(1)-N(2)	110.5(3)	N(1)-C(18)-C(13)	108.1(4)
C(21)-N(1)-C(18)	105.7(4)	C(18)-C(19)-C(20)	106.4(5)
C(21)-N(1)-B(1)	139.2(4)	C(25)-C(20)-C(19)	136.8(6)
C(18)-N(1)-B(1)	114.9(4)	C(25)-C(20)-C(21)	117.0(5)
C(17)-N(2)-C(13)	120.6(4)	C(19)-C(20)-C(21)	106.2(5)
C(17)-N(2)-B(1)	126.2(4)	N(1)-C(21)-C(22)	130.6(5)
C(13)-N(2)-B(1)	113.2(4)	N(1)-C(21)-C(20)	109.0(5)
C(6)-C(1)-C(2)	117.4(4)	C(22)-C(21)-C(20)	120.1(5)
C(6)-C(1)-B(1)	121.4(4)	C(23)-C(22)-F(1)	119.6(5)
C(2)-C(1)-B(1)	121.0(4)	C(23)-C(22)-C(21)	119.2(5)
C(1)-C(2)-C(3)	122.0(5)	F(1)-C(22)-C(21)	121.1(5)
C(4)-C(3)-C(2)	119.1(5)	F(2)-C(23)-C(22)	119.0(5)
C(5)-C(4)-C(3)	120.8(5)	F(2)-C(23)-C(24)	119.4(6)
C(4)-C(5)-C(6)	119.5(5)	C(22)-C(23)-C(24)	121.7(5)
C(1)-C(6)-C(5)	121.1(5)	C(25)-C(24)-C(23)	120.3(6)
C(8)-C(7)-C(12)	114.4(4)	C(25)-C(24)-F(3)	120.0(6)
C(8)-C(7)-B(1)	123.4(4)	C(23)-C(24)-F(3)	119.8(6)
C(12)-C(7)-B(1)	122.2(4)	C(24)-C(25)-F(4)	120.6(6)
C(7)-C(8)-C(9)	123.3(5)	C(24)-C(25)-C(20)	121.6(5)
C(10)-C(9)-C(8)	119.5(6)	F(4)-C(25)-C(20)	117.7(5)
C(9)-C(10)-C(11)	119.8(6)		

Table 4. Anisotropic displacement parameters [$Å^2 x\ 10^3$] for **9**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
B(1)	39(4)	57(4)	55(4)	-1(3)	-1(3)	0(3)
F(1)	48(2)	100(2)	93(2)	-26(2)	-2(2)	11(2)
F(2)	59(2)	112(2)	98(2)	-21(2)	-25(2)	1(2)
F(3)	84(2)	134(2)	69(2)	-33(2)	-20(2)	-9(2)
F(4)	88(2)	116(2)	81(2)	-38(2)	11(2)	-7(2)
N(1)	37(3)	52(2)	51(3)	-4(2)	2(2)	0(2)
N(2)	43(3)	59(3)	54(3)	0(2)	0(3)	-4(2)
C(1)	51(3)	56(3)	45(3)	-3(3)	5(3)	-10(3)
C(2)	63(4)	66(4)	69(4)	5(3)	11(3)	9(3)
C(3)	92(5)	63(4)	93(5)	9(3)	-8(4)	1(4)
C(4)	122(6)	57(4)	98(5)	14(4)	-8(5)	7(4)
C(5)	123(6)	64(4)	81(4)	10(4)	10(4)	-32(4)
C(6)	64(4)	70(3)	77(4)	4(3)	7(3)	-9(3)
C(7)	41(3)	59(3)	46(4)	1(3)	3(3)	6(3)
C(8)	60(4)	53(3)	77(4)	7(3)	13(3)	11(3)
C(9)	55(4)	83(4)	96(5)	33(4)	-8(4)	-11(3)
C(10)	71(4)	128(6)	78(5)	35(4)	3(4)	-28(4)
C(11)	69(4)	122(6)	61(4)	-3(4)	25(3)	-15(4)

C(12)	53(3)	76(4)	67(4)	-8(3)	8(3)	-5(3)
C(13)	53(4)	54(3)	71(4)	2(3)	15(4)	-3(3)
C(14)	42(4)	92(4)	86(5)	-12(3)	-13(3)	0(3)
C(15)	50(4)	89(5)	124(6)	-21(4)	-2(4)	0(3)
C(16)	51(4)	99(4)	91(5)	-7(3)	-37(4)	-1(4)
C(17)	64(4)	72(4)	64(4)	-16(3)	-12(3)	-2(3)
C(18)	52(4)	59(3)	55(4)	-2(3)	-3(3)	3(3)
C(19)	66(4)	69(4)	55(4)	-9(3)	22(3)	-3(3)
C(20)	50(4)	48(3)	58(4)	6(3)	8(4)	-7(3)
C(21)	43(3)	45(3)	60(4)	-8(3)	7(4)	-3(3)
C(22)	46(4)	51(4)	63(4)	-7(3)	7(4)	2(3)
C(23)	39(3)	68(4)	80(4)	-6(3)	-14(4)	3(3)
C(24)	73(5)	79(4)	57(4)	-13(3)	-12(4)	-15(4)
C(25)	78(4)	65(4)	51(4)	-24(3)	19(4)	2(4)

Table 5. Hydrogen coordinates [x 10^4] and isotropic displacement parameters [$Å^2$x 10^3] for **9**.

	x	y	z	U[eq]
H(2A)	1673	-733	-724	79
H(3A)	1932	-3067	-46	99
H(4A)	1069	-4452	821	111
H(5A)	-42	-3539	993	107
H(6A)	-301	-1185	306	84
H(8A)	992	3847	-953	76
H(9A)	1688	4917	-2326	93
H(10A)	2063	3549	-3853	111
H(11A)	1797	1088	-3953	101
H(12A)	1134	3	-2555	78
H(14A)	-1603	2798	448	88
H(15A)	-2183	1978	-1158	105
H(16A)	-1583	751	-2579	96
H(17A)	-422	234	-2364	80
H(19A)	-545	3614	2220	76

Table 1. Crystal data and structure refinement for **10**.

Identification code	**10**	
Empirical formula	C24 H18 B N3	
Formula weight	359.22	
Temperature	293(2) [K]	
Wavelength	0.71073 [Å]	
Crystal system	Monoclinic	
Space group	Cc	
Unit cell dimensions	a = 15.360(4) [Å]	α= 90°.
	b = 17.116(5) [Å]	β= 106.685(5)°.
	c = 7.302(2) [Å]	γ = 90°.
Volume	1838.8(8) [$Å^3$]	
Z	4	
Density (calculated)	1.298 [Mgm^{-3}]	
Absorption coefficient	0.077 [mm^{-1}]	
F(000)	752	
Crystal size	0.10 x 0.10 x 0.05 [mm^3]	
Theta range for data collection	1.83 to 28.30°.	
Index ranges	-18<=h<=20, -22<=k<=21, -9<=l<=9	
Reflections collected	6450	
Independent reflections	3407 [R(int) = 0.0790]	
Completeness to theta = 28.30°	95.4 %	
Absorption correction	Empirical	
Max. and min. transmission	1.000 and 0.839	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3407 / 2 / 253	
Goodness-of-fit on F^2	0.712	
Final R indices [I>2sigma(I)]	R1 = 0.0542, wR2 = 0.0383	
R indices (all data)	R1 = 0.2251, wR2 = 0.0522	
Absolute structure parameter	4(3)	
Largest diff. peak and hole	0.159 and -0.179 [$e.Å^{-3}$]	

Table 2. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$x 10^3] for **10**. U[eq] is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U[eq]
B(1)	6628(5)	1974(4)	14881(10)	46(2)
N(1)	6892(3)	2755(2)	13997(6)	42(1)
N(2)	6124(3)	2470(3)	16235(6)	45(1)
N(3)	6814(3)	4087(2)	13923(7)	55(1)
C(1)	7482(4)	1527(3)	16165(8)	49(2)
C(2)	8363(4)	1699(3)	16176(8)	57(2)
C(3)	9100(4)	1275(4)	17205(9)	67(2)
C(4)	8984(5)	671(4)	18371(9)	83(2)
C(5)	8126(5)	493(3)	18420(8)	77(2)
C(6)	7370(4)	905(3)	17281(8)	65(2)
C(7)	5898(4)	1485(3)	13331(7)	43(1)
C(8)	6194(4)	958(4)	12148(9)	58(2)
C(9)	5598(5)	560(3)	10708(9)	66(2)
C(10)	4677(5)	647(3)	10364(9)	69(2)
C(11)	4362(5)	1168(4)	11426(9)	70(2)
C(12)	4966(4)	1578(3)	12886(8)	54(2)
C(13)	7301(4)	2988(4)	12615(8)	43(2)
C(14)	7697(4)	2573(3)	11407(8)	54(2)
C(15)	8038(4)	2998(4)	10239(9)	65(2)

C(16)	7990(4)	3810(5)	10195(9)	72(2)
C(17)	7600(4)	4237(4)	11367(9)	72(2)
C(18)	7237(4)	3819(4)	12587(9)	56(2)
C(19)	6635(4)	3428(4)	14682(9)	42(2)
C(20)	6183(4)	3240(4)	16109(8)	44(2)
C(21)	5837(4)	3750(4)	17181(8)	62(2)
C(22)	5406(5)	3456(5)	18442(8)	76(2)
C(23)	5320(4)	2632(5)	18542(8)	73(2)
C(24)	5702(4)	2155(3)	17450(9)	65(2)

Table 3. Bond lengths [Å] and angles [°] for **10**.

B(1)-C(1)	1.575(9)	C(13)-N(1)-B(1)	139.2(5)
B(1)-C(7)	1.584(9)	C(20)-N(2)-C(24)	119.8(5)
B(1)-N(1)	1.586(7)	C(20)-N(2)-B(1)	114.6(5)
B(1)-N(2)	1.655(7)	C(24)-N(2)-B(1)	125.6(5)
N(1)-C(19)	1.358(5)	C(19)-N(3)-C(18)	102.0(5)
N(1)-C(13)	1.392(7)	C(6)-C(1)-C(2)	116.6(6)
N(2)-C(20)	1.325(6)	C(6)-C(1)-B(1)	120.2(6)
N(2)-C(24)	1.353(6)	C(2)-C(1)-B(1)	123.1(5)
N(3)-C(19)	1.321(6)	C(3)-C(2)-C(1)	122.8(5)
N(3)-C(18)	1.395(7)	C(2)-C(3)-C(4)	120.1(6)
C(1)-C(6)	1.380(6)	C(5)-C(4)-C(3)	118.7(7)
C(1)-C(2)	1.383(7)	C(4)-C(5)-C(6)	120.7(6)
C(2)-C(3)	1.372(7)	C(1)-C(6)-C(5)	120.9(6)
C(3)-C(4)	1.383(7)	C(12)-C(7)-C(8)	115.0(5)
C(4)-C(5)	1.364(7)	C(12)-C(7)-B(1)	125.4(5)
C(5)-C(6)	1.408(8)	C(8)-C(7)-B(1)	119.3(5)
C(7)-C(12)	1.383(6)	C(9)-C(8)-C(7)	121.9(6)
C(7)-C(8)	1.411(6)	C(8)-C(9)-C(10)	121.1(6)
C(8)-C(9)	1.362(7)	C(11)-C(10)-C(9)	119.0(7)
C(9)-C(10)	1.371(7)	C(10)-C(11)-C(12)	120.0(7)
C(10)-C(11)	1.359(7)	C(7)-C(12)-C(11)	122.8(6)
C(11)-C(12)	1.387(7)	N(1)-C(13)-C(14)	132.8(6)
C(13)-C(14)	1.400(7)	N(1)-C(13)-C(18)	104.7(6)
C(13)-C(18)	1.425(6)	C(14)-C(13)-C(18)	122.5(7)
C(14)-C(15)	1.337(7)	C(15)-C(14)-C(13)	116.5(6)
C(15)-C(16)	1.391(7)	C(14)-C(15)-C(16)	122.0(7)
C(16)-C(17)	1.385(7)	C(17)-C(16)-C(15)	122.8(7)
C(17)-C(18)	1.379(7)	C(18)-C(17)-C(16)	116.9(7)
C(19)-C(20)	1.444(7)	C(17)-C(18)-N(3)	129.5(7)
C(20)-C(21)	1.377(7)	C(17)-C(18)-C(13)	119.2(7)
C(21)-C(22)	1.374(8)	N(3)-C(18)-C(13)	111.2(6)
C(22)-C(23)	1.421(8)	N(3)-C(19)-N(1)	116.8(5)
C(23)-C(24)	1.384(7)	N(3)-C(19)-C(20)	134.0(6)
C(1)-B(1)-C(7)	117.8(5)	N(1)-C(19)-C(20)	109.1(5)
C(1)-B(1)-N(1)	112.7(5)	N(2)-C(20)-C(21)	123.2(6)
C(7)-B(1)-N(1)	111.5(5)	N(2)-C(20)-C(19)	109.1(5)
C(1)-B(1)-N(2)	110.3(5)	C(21)-C(20)-C(19)	127.7(6)
C(7)-B(1)-N(2)	110.0(5)	C(22)-C(21)-C(20)	119.1(7)
N(1)-B(1)-N(2)	91.6(4)	C(21)-C(22)-C(23)	117.9(6)
C(19)-N(1)-C(13)	105.3(4)	C(24)-C(23)-C(22)	119.6(7)
C(19)-N(1)-B(1)	115.4(4)	N(2)-C(24)-C(23)	120.4(6)

Table 4. Anisotropic displacement parameters [$Å^2 x\ 10^3$] for **10**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
B(1)	41(4)	53(5)	48(5)	1(4)	21(4)	-2(4)
N(1)	46(3)	24(3)	59(4)	-2(3)	20(3)	-4(3)
N(2)	47(3)	47(4)	36(3)	6(3)	5(2)	-1(3)
N(3)	63(3)	43(4)	53(4)	2(3)	9(3)	-3(3)
C(1)	48(4)	53(4)	44(4)	1(3)	11(3)	-9(4)
C(2)	59(4)	62(5)	44(4)	5(3)	6(3)	4(4)
C(3)	55(5)	68(6)	64(6)	10(4)	-2(4)	3(4)
C(4)	57(5)	76(6)	91(7)	6(5)	-16(5)	9(4)
C(5)	87(5)	65(5)	61(5)	18(4)	-10(5)	-4(5)
C(6)	54(4)	61(5)	64(5)	12(4)	-7(4)	-14(4)
C(7)	46(4)	42(4)	47(4)	5(3)	20(3)	1(3)
C(8)	66(5)	57(5)	46(5)	1(4)	9(4)	-6(4)
C(9)	72(5)	53(5)	67(6)	-8(4)	11(4)	8(4)
C(10)	100(7)	51(5)	43(5)	-7(3)	0(5)	-14(5)
C(11)	53(4)	107(6)	46(5)	-7(4)	8(4)	-17(5)
C(12)	52(4)	60(4)	54(4)	-11(4)	18(4)	-11(4)
C(13)	39(4)	48(5)	40(4)	0(4)	9(4)	2(4)
C(14)	63(5)	57(4)	47(5)	-2(4)	24(4)	-3(4)
C(15)	65(5)	68(6)	66(6)	3(5)	26(4)	-4(5)
C(16)	68(5)	109(7)	38(5)	13(5)	12(4)	-20(5)
C(17)	81(5)	68(5)	56(5)	13(5)	2(4)	-21(5)
C(18)	66(5)	45(5)	50(5)	8(4)	6(4)	-14(4)
C(19)	40(3)	41(4)	38(4)	-5(4)	1(3)	-9(4)
C(20)	43(4)	56(5)	32(4)	-1(4)	9(3)	4(4)
C(21)	62(5)	85(6)	42(5)	-11(4)	17(4)	-3(4)
C(22)	83(6)	112(7)	32(5)	-15(4)	16(4)	26(5)
C(23)	67(5)	101(6)	60(6)	-3(4)	31(4)	7(5)
C(24)	70(5)	75(5)	49(4)	11(4)	16(4)	2(5)

Table 5. Hydrogen coordinates [$x\ 10^4$] and isotropic displacement parameters [$Å^2 x\ 10^3$] for **10**.

	x	y	z	U[eq]
H(2A)	8461	2120	15455	68
H(3A)	9678	1394	17119	80
H(4A)	9482	392	19106	99
H(5A)	8038	94	19215	93
H(6A)	6788	757	17281	78
H(8A)	6814	880	12358	69
H(9A)	5818	224	9945	79
H(10A)	4275	354	9418	83
H(11A)	3740	1250	11173	84
H(12A)	4735	1931	13597	65
H(14A)	7722	2030	11416	65
H(15A)	8316	2744	9431	78
H(16A)	8229	4078	9342	87
H(17A)	7584	4780	11334	87
H(21A)	5895	4287	17054	75

H(22A)	5178	3786	19205	91
H(23A)	5008	2414	19337	88
H(24A)	5668	1615	17553	78

Table 1. Crystal data and structure refinement for **11**.

Identification code	**11**	
Empirical formula	C23 H17 B N2 S	
Formula weight	364.26	
Temperature	293(2) [K]	
Wavelength	0.71073 [Å]	
Crystal system	Monoclinic	
Space group	P2(1)/n	
Unit cell dimensions	a = 9.033(2) [Å]	α= 90°.
	b = 15.711(4) [Å]	β= 105.643(5)°.
	c = 13.500(3) [Å]	γ = 90°.
Volume	1844.9(8) [$Å^3$]	
Z	4	
Density (calculated)	1.311 [Mgm^{-3}]	
Absorption coefficient	0.185 [mm^{-1}]	
F(000)	760	
Crystal size	0.20 x 0.10 x 0.05 [mm^3]	
Theta range for data collection	2.03 to 28.25°.	
Index ranges	-11<=h<=11, -20<=k<=20, -17<=l<=16	
Reflections collected	12982	
Independent reflections	4366 [R(int) = 0.0880]	
Completeness to theta = 28.25°	95.9 %	
Absorption correction	Empirical(SADABS)	
Max. and min. transmission	1.000 and 0.833	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4366 / 0 / 244	
Goodness-of-fit on F^2	0.787	
Final R indices [I>2sigma(I)]	R1 = 0.0603, wR2 = 0.0874	
R indices (all data)	R1 = 0.2021, wR2 = 0.1067	
Largest diff. peak and hole	0.368 and -0.244 [e.$Å^{-3}$]	

Table 2. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **11**. U[eq] is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U[eq]
B(1)	7966(4)	1076(2)	-2401(3)	41(1)
S(1)	9825(1)	1684(1)	550(1)	62(1)
N(1)	8843(2)	1919(2)	-2459(2)	39(1)
N(2)	8406(3)	1066(2)	-1162(2)	41(1)
C(1)	8732(4)	268(2)	-2791(2)	41(1)
C(2)	10015(4)	317(2)	-3148(2)	56(1)
C(3)	10685(4)	-387(3)	-3476(3)	72(1)
C(4)	10060(5)	-1173(3)	-3424(3)	69(1)
C(5)	8796(4)	-1256(2)	-3074(2)	59(1)
C(6)	8123(4)	-552(2)	-2769(2)	50(1)
C(7)	6149(3)	1163(2)	-2892(2)	40(1)
C(8)	5484(4)	919(2)	-3905(2)	53(1)
C(9)	3958(4)	1057(2)	-4382(3)	59(1)
C(10)	3028(4)	1441(2)	-3871(3)	60(1)
C(11)	3622(4)	1673(2)	-2858(2)	60(1)
C(12)	5163(4)	1535(2)	-2391(2)	49(1)
C(13)	9589(3)	2256(2)	-1523(2)	42(1)
C(14)	10308(3)	3009(2)	-1625(2)	52(1)
C(15)	9982(3)	3153(2)	-2696(2)	46(1)
C(16)	10354(4)	3802(2)	-3302(3)	64(1)
C(17)	9813(4)	3742(2)	-4348(3)	63(1)
C(18)	8935(4)	3061(2)	-4815(3)	60(1)
C(19)	8554(3)	2414(2)	-4251(2)	51(1)
C(20)	9077(3)	2465(2)	-3186(2)	40(1)
C(21)	9305(3)	1719(2)	-744(2)	43(1)
C(22)	8784(3)	778(2)	530(2)	55(1)
C(23)	8110(3)	532(2)	-442(2)	48(1)

Table 3. Bond lengths [Å] and angles [°] for **11**.

B(1)-N(1)	1.555(4)	C(13)-C(14)	1.374(4)
B(1)-C(1)	1.602(4)	C(13)-C(21)	1.424(4)
B(1)-C(7)	1.602(4)	C(14)-C(15)	1.414(4)
B(1)-N(2)	1.612(4)	C(15)-C(16)	1.403(4)
S(1)-C(21)	1.683(3)	C(15)-C(20)	1.409(4)
S(1)-C(22)	1.703(3)	C(16)-C(17)	1.368(4)
N(1)-C(20)	1.362(3)	C(17)-C(18)	1.378(4)
N(1)-C(13)	1.368(3)	C(18)-C(19)	1.369(4)
N(2)-C(21)	1.336(3)	C(19)-C(20)	1.389(4)
N(2)-C(23)	1.363(3)	C(22)-C(23)	1.345(4)
C(1)-C(2)	1.372(4)	N(1)-B(1)-C(1)	112.8(3)
C(1)-C(6)	1.403(4)	N(1)-B(1)-C(7)	112.7(3)
C(2)-C(3)	1.389(4)	C(1)-B(1)-C(7)	114.6(3)
C(3)-C(4)	1.368(4)	N(1)-B(1)-N(2)	94.3(2)
C(4)-C(5)	1.355(4)	C(1)-B(1)-N(2)	109.0(2)
C(5)-C(6)	1.378(4)	C(7)-B(1)-N(2)	111.6(3)
C(7)-C(12)	1.384(4)	C(21)-S(1)-C(22)	90.73(16)
C(7)-C(8)	1.391(3)	C(20)-N(1)-C(13)	106.8(2)
C(8)-C(9)	1.372(4)	C(20)-N(1)-B(1)	138.8(3)
C(9)-C(10)	1.363(4)	C(13)-N(1)-B(1)	114.4(2)
C(10)-C(11)	1.377(4)	C(21)-N(2)-C(23)	112.7(3)
C(11)-C(12)	1.381(4)	C(21)-N(2)-B(1)	112.5(3)

C(23)-N(2)-B(1)	134.8(3)	N(1)-C(13)-C(21)	108.1(3)
C(2)-C(1)-C(6)	115.6(3)	C(14)-C(13)-C(21)	140.1(3)
C(2)-C(1)-B(1)	123.4(3)	C(13)-C(14)-C(15)	105.4(3)
C(6)-C(1)-B(1)	120.9(3)	C(16)-C(15)-C(20)	118.9(3)
C(1)-C(2)-C(3)	123.3(3)	C(16)-C(15)-C(14)	134.1(3)
C(4)-C(3)-C(2)	118.8(4)	C(20)-C(15)-C(14)	107.0(3)
C(5)-C(4)-C(3)	120.2(4)	C(17)-C(16)-C(15)	118.4(3)
C(4)-C(5)-C(6)	120.6(4)	C(16)-C(17)-C(18)	121.9(3)
C(5)-C(6)-C(1)	121.6(3)	C(19)-C(18)-C(17)	121.4(3)
C(12)-C(7)-C(8)	115.6(3)	C(18)-C(19)-C(20)	117.8(3)
C(12)-C(7)-B(1)	123.8(3)	N(1)-C(20)-C(19)	129.3(3)
C(8)-C(7)-B(1)	120.4(3)	N(1)-C(20)-C(15)	109.2(3)
C(9)-C(8)-C(7)	122.0(3)	C(19)-C(20)-C(15)	121.5(3)
C(10)-C(9)-C(8)	120.7(3)	N(2)-C(21)-C(13)	110.7(3)
C(9)-C(10)-C(11)	119.4(3)	N(2)-C(21)-S(1)	112.4(2)
C(10)-C(11)-C(12)	119.1(3)	C(13)-C(21)-S(1)	136.9(3)
C(11)-C(12)-C(7)	123.0(3)	C(23)-C(22)-S(1)	111.0(2)
N(1)-C(13)-C(14)	111.7(3)	C(22)-C(23)-N(2)	113.3(3)

Table 4. Anisotropic displacement parameters [$Å^2 \times 10^3$] for **11**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
B(1)	49(3)	41(3)	31(2)	3(2)	9(2)	-3(2)
S(1)	75(1)	69(1)	35(1)	0(1)	4(1)	-4(1)
N(1)	47(2)	35(2)	31(2)	-2(1)	6(1)	-6(1)
N(2)	46(2)	41(2)	35(2)	6(1)	11(1)	3(2)
C(1)	46(2)	45(3)	29(2)	4(2)	8(2)	1(2)
C(2)	69(3)	41(3)	64(2)	6(2)	29(2)	1(2)
C(3)	80(3)	70(3)	78(3)	16(3)	46(2)	19(3)
C(4)	89(3)	54(3)	64(3)	1(2)	22(2)	21(3)
C(5)	67(3)	47(3)	56(2)	-4(2)	2(2)	2(2)
C(6)	48(2)	51(3)	47(2)	1(2)	7(2)	-1(2)
C(7)	48(2)	33(2)	39(2)	-1(2)	13(2)	-1(2)
C(8)	60(2)	57(3)	38(2)	-8(2)	5(2)	6(2)
C(9)	59(3)	63(3)	46(2)	-6(2)	0(2)	2(2)
C(10)	43(2)	70(3)	58(2)	8(2)	-2(2)	-2(2)
C(11)	45(2)	81(3)	55(2)	-2(2)	15(2)	-1(2)
C(12)	49(2)	57(3)	38(2)	-1(2)	6(2)	-3(2)
C(13)	48(2)	43(2)	35(2)	-3(2)	10(2)	-3(2)
C(14)	53(2)	44(3)	51(2)	-2(2)	-1(2)	-9(2)
C(15)	44(2)	42(2)	51(2)	3(2)	9(2)	3(2)
C(16)	63(3)	54(3)	73(3)	8(2)	15(2)	-11(2)
C(17)	64(3)	58(3)	69(3)	21(2)	23(2)	1(2)
C(18)	70(3)	70(3)	42(2)	8(2)	19(2)	1(2)
C(19)	59(2)	56(3)	40(2)	2(2)	17(2)	-2(2)
C(20)	42(2)	39(2)	39(2)	2(2)	12(2)	1(2)
C(21)	45(2)	48(2)	34(2)	-4(2)	5(2)	1(2)
C(22)	55(2)	69(3)	42(2)	12(2)	15(2)	1(2)
C(23)	50(2)	49(2)	47(2)	6(2)	15(2)	3(2)

Table 5. Hydrogen coordinates [$\times 10^4$] and isotropic displacement parameters [$Å^2 \times 10^3$] for **11**.

	x	y	z	U[eq]
H(2A)	10459	848	-3171	67
H(3A)	11542	-325	-3727	86
H(4A)	10505	-1652	-3630	83
H(5A)	8379	-1793	-3039	71
H(6A)	7245	-621	-2543	60
H(8A)	6093	656	-4271	64
H(9A)	3553	886	-5061	71
H(10A)	2001	1546	-4204	72
H(11A)	2995	1919	-2492	72
H(12A)	5557	1701	-1709	59
H(14A)	10887	3351	-1100	63
H(16A)	10954	4263	-2999	77
H(17A)	10044	4172	-4756	75
H(18A)	8594	3041	-5529	72
H(19A)	7964	1955	-4570	61
H(22A)	8693	491	1113	66
H(23A)	7503	47	-606	58

Table 1. Crystal data and structure refinement for **12**.

Identification code	**12**	
Empirical formula	C29 H21 B N2	
Formula weight	408.29	
Temperature	293(2) [K]	
Wavelength	0.71073 [Å]	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 20.290(12) [Å]	α= 90°.
	b = 11.619(6) [Å]	β= 90.570(10)°.
	c = 17.856(11) [Å]	γ = 90°.
Volume	4210(4) [$Å^3$]	
Z	8	
Density (calculated)	1.288 [Mgm^{-3}]	
Absorption coefficient	0.075 [mm^{-1}]	
F(000)	1712	
Crystal size	0.15 x 0.10 x 0.10 [mm^3]	
Theta range for data collection	2.01 to 28.43°.	
Index ranges	-26<=h<=26, -15<=k<=14, -22<=l<=23	
Reflections collected	15017	
Independent reflections	5048 [R(int) = 0.2284]	
Completeness to theta = 28.43°	95.2 %	
Absorption correction	Empirical(SADABS)	
Max. and min. transmission	1.000 and 0.792	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5048 / 0 / 290	
Goodness-of-fit on F^2	0.657	
Final R indices [I>2sigma(I)]	R1 = 0.0581, wR2 = 0.0481	
R indices (all data)	R1 = 0.3483, wR2 = 0.0723	
Extinction coefficient	0.00025(3)	
Largest diff. peak and hole	0.194 and -0.179 [$e.Å^{-3}$]	

Table 2. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **12**. U[eq] is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
B(1)	-2071(3)	-1016(4)	-1784(3)	42(2)
N(1)	-2054(2)	135(3)	-1360(2)	40(1)
N(2)	-2858(2)	-1350(3)	-1835(2)	36(1)
C(1)	-1733(2)	-2022(4)	-1292(2)	35(1)
C(2)	-1726(2)	-1966(3)	-527(2)	54(2)
C(3)	-1463(2)	-2829(4)	-76(2)	71(2)
C(4)	-1199(2)	-3796(4)	-404(3)	70(2)
C(5)	-1210(2)	-3890(4)	-1153(3)	62(2)
C(6)	-1455(2)	-3007(3)	-1593(2)	45(1)
C(7)	-1816(2)	-863(3)	-2621(2)	39(1)
C(8)	-1169(2)	-1045(3)	-2822(3)	52(1)
C(9)	-950(2)	-814(3)	-3535(3)	60(2)
C(10)	-1370(3)	-386(4)	-4064(3)	64(2)
C(11)	-2015(3)	-173(4)	-3889(3)	64(2)
C(12)	-2230(2)	-416(3)	-3176(3)	50(1)
C(13)	-1500(3)	724(4)	-1137(2)	44(1)
C(14)	-847(3)	404(3)	-1129(2)	57(2)
C(15)	-380(2)	1166(4)	-867(2)	67(2)
C(16)	-561(3)	2271(4)	-634(3)	83(2)
C(17)	-1200(3)	2604(4)	-629(3)	72(2)
C(18)	-1676(3)	1839(4)	-888(3)	51(2)
C(19)	-2363(3)	1894(3)	-951(2)	54(2)
C(20)	-2575(2)	881(4)	-1239(2)	41(1)
C(21)	-3233(3)	489(4)	-1385(2)	45(1)
C(22)	-3763(3)	1186(4)	-1254(3)	59(2)
C(23)	-4407(3)	824(4)	-1356(3)	73(2)
C(24)	-4547(2)	-257(4)	-1596(2)	66(2)
C(25)	-4018(3)	-1015(4)	-1763(3)	48(1)
C(26)	-4142(2)	-2124(4)	-2016(2)	58(2)
C(27)	-3628(2)	-2804(3)	-2185(2)	53(2)
C(28)	-2986(2)	-2404(3)	-2097(2)	47(1)
C(29)	-3372(3)	-623(4)	-1663(2)	43(1)

Table 3. Bond lengths [Å] and angles [°] for **12**.

B(1)-N(1)	1.537(5)	B(1)-C(1)	1.611(5)
B(1)-C(7)	1.596(6)	B(1)-N(2)	1.645(5)

N(1)-C(13)	1.372(5)	C(29)-N(2)-B(1)	125.4(4)
N(1)-C(20)	1.386(4)	C(2)-C(1)-C(6)	115.2(4)
N(2)-C(28)	1.335(4)	C(2)-C(1)-B(1)	120.7(4)
N(2)-C(29)	1.379(4)	C(6)-C(1)-B(1)	124.1(4)
C(1)-C(2)	1.367(4)	C(1)-C(2)-C(3)	123.0(4)
C(1)-C(6)	1.387(4)	C(4)-C(3)-C(2)	119.5(5)
C(2)-C(3)	1.389(4)	C(5)-C(4)-C(3)	119.1(5)
C(3)-C(4)	1.378(5)	C(4)-C(5)-C(6)	120.6(5)
C(4)-C(5)	1.343(5)	C(5)-C(6)-C(1)	122.6(4)
C(5)-C(6)	1.380(4)	C(8)-C(7)-C(12)	116.1(4)
C(7)-C(8)	1.379(5)	C(8)-C(7)-B(1)	123.0(5)
C(7)-C(12)	1.393(5)	C(12)-C(7)-B(1)	120.5(5)
C(8)-C(9)	1.378(5)	C(9)-C(8)-C(7)	121.8(5)
C(9)-C(10)	1.361(5)	C(10)-C(9)-C(8)	120.4(5)
C(10)-C(11)	1.371(5)	C(9)-C(10)-C(11)	120.0(5)
C(11)-C(12)	1.379(5)	C(10)-C(11)-C(12)	119.0(5)
C(13)-C(14)	1.376(5)	C(11)-C(12)-C(7)	122.6(5)
C(13)-C(18)	1.418(5)	N(1)-C(13)-C(14)	130.9(5)
C(14)-C(15)	1.375(5)	N(1)-C(13)-C(18)	109.7(5)
C(15)-C(16)	1.400(5)	C(14)-C(13)-C(18)	119.4(5)
C(16)-C(17)	1.352(6)	C(15)-C(14)-C(13)	119.2(5)
C(17)-C(18)	1.389(5)	C(14)-C(15)-C(16)	120.7(5)
C(18)-C(19)	1.397(5)	C(17)-C(16)-C(15)	121.2(6)
C(19)-C(20)	1.353(5)	C(16)-C(17)-C(18)	118.6(5)
C(20)-C(21)	1.432(5)	C(17)-C(18)-C(19)	133.4(5)
C(21)-C(22)	1.369(5)	C(17)-C(18)-C(13)	120.8(5)
C(21)-C(29)	1.412(5)	C(19)-C(18)-C(13)	105.8(5)
C(22)-C(23)	1.382(5)	C(20)-C(19)-C(18)	107.7(4)
C(23)-C(24)	1.357(5)	C(19)-C(20)-N(1)	111.3(4)
C(24)-C(25)	1.421(5)	C(19)-C(20)-C(21)	129.7(5)
C(25)-C(26)	1.387(5)	N(1)-C(20)-C(21)	118.9(4)
C(25)-C(29)	1.398(5)	C(22)-C(21)-C(29)	116.5(5)
C(26)-C(27)	1.344(5)	C(22)-C(21)-C(20)	120.9(5)
C(27)-C(28)	1.392(5)	C(29)-C(21)-C(20)	122.6(5)
		C(21)-C(22)-C(23)	122.7(5)
N(1)-B(1)-C(7)	111.0(4)	C(24)-C(23)-C(22)	121.2(5)
N(1)-B(1)-C(1)	110.8(4)	C(23)-C(24)-C(25)	118.9(5)
C(7)-B(1)-C(1)	116.8(4)	C(26)-C(25)-C(29)	120.7(5)
N(1)-B(1)-N(2)	104.4(4)	C(26)-C(25)-C(24)	120.6(6)
C(7)-B(1)-N(2)	107.4(4)	C(29)-C(25)-C(24)	118.7(5)
C(1)-B(1)-N(2)	105.4(3)	C(27)-C(26)-C(25)	118.8(5)
C(13)-N(1)-C(20)	105.5(4)	C(26)-C(27)-C(28)	120.3(4)
C(13)-N(1)-B(1)	126.2(4)	N(2)-C(28)-C(27)	121.7(4)
C(20)-N(1)-B(1)	127.4(4)	N(2)-C(29)-C(25)	118.9(5)
C(28)-N(2)-C(29)	119.6(4)	N(2)-C(29)-C(21)	119.3(5)
C(28)-N(2)-B(1)	114.9(4)	C(25)-C(29)-C(21)	121.8(5)

Table 4. Anisotropic displacement parameters [$Å^2 x\ 10^3$] for **12**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}

B(1)	43(4)	41(4)	41(4)	-6(3)	4(4)	-2(3)
N(1)	47(3)	39(2)	35(3)	-3(2)	-3(2)	1(2)
N(2)	45(3)	32(2)	33(2)	1(2)	3(2)	6(2)
C(1)	34(3)	43(3)	27(3)	2(3)	1(3)	6(2)
C(2)	69(4)	48(3)	44(4)	11(3)	4(3)	14(3)
C(3)	95(5)	73(4)	45(4)	13(3)	-10(4)	2(4)
C(4)	64(4)	68(4)	77(5)	28(4)	-7(4)	12(3)
C(5)	62(4)	50(3)	73(4)	7(3)	-6(4)	14(3)
C(6)	42(3)	47(3)	45(3)	6(3)	3(3)	9(3)
C(7)	47(4)	35(3)	34(3)	1(2)	-3(3)	-10(3)
C(8)	57(4)	54(3)	45(4)	3(3)	15(3)	5(3)
C(9)	68(4)	60(4)	51(4)	2(3)	26(4)	-4(3)
C(10)	98(5)	57(4)	38(4)	3(3)	13(4)	-20(4)
C(11)	82(5)	66(4)	43(4)	10(3)	-5(4)	-13(4)
C(12)	66(4)	42(3)	42(3)	-4(3)	15(3)	-10(3)
C(13)	58(4)	42(3)	33(3)	-6(3)	1(3)	2(3)
C(14)	65(4)	52(4)	52(4)	-16(3)	4(3)	-10(3)
C(15)	59(4)	75(4)	68(4)	-16(3)	-2(3)	-7(4)
C(16)	94(6)	59(4)	96(5)	-10(4)	31(5)	-29(4)
C(17)	102(5)	53(4)	61(4)	-17(3)	21(5)	-23(4)
C(18)	61(4)	39(3)	54(4)	-12(3)	12(4)	-7(4)
C(19)	82(5)	35(3)	46(4)	-10(3)	3(4)	4(3)
C(20)	46(4)	43(3)	34(3)	4(3)	-4(3)	7(3)
C(21)	58(4)	37(3)	38(3)	4(3)	7(3)	17(3)
C(22)	64(4)	53(4)	59(4)	-3(3)	-7(4)	15(4)
C(23)	71(5)	62(4)	87(5)	-12(4)	-3(4)	34(4)
C(24)	49(4)	90(4)	59(4)	-1(4)	1(3)	20(4)
C(25)	46(4)	56(4)	42(3)	5(3)	5(3)	12(4)
C(26)	51(4)	75(4)	49(4)	6(3)	-10(3)	7(4)
C(27)	54(4)	52(3)	53(4)	-2(3)	-9(4)	0(3)
C(28)	52(4)	48(3)	40(3)	-5(3)	2(3)	7(3)
C(29)	50(4)	44(3)	34(3)	2(3)	10(3)	7(3)

Table 5. Hydrogen coordinates [x 10^4] and isotropic displacement parameters [$Å^2$x 10^3] for **12**.

	x	y	z	U[eq]
H(2A)	-1905	-1320	-298	64
H(3A)	-1465	-2754	442	85
H(4A)	-1015	-4376	-110	84
H(5A)	-1051	-4554	-1379	74
H(6A)	-1433	-3077	-2111	54
H(8A)	-874	-1331	-2467	62
H(9A)	-512	-952	-3654	72
H(10A)	-1220	-239	-4545	77
H(11A)	-2303	131	-4245	76
H(12A)	-2669	-277	-3061	60
H(14A)	-722	-320	-1300	68
H(15A)	60	946	-845	81
H(16A)	-236	2786	-479	99
H(17A)	-1317	3330	-456	86
H(19A)	-2626	2516	-819	65
H(22A)	-3688	1935	-1089	71

H(23A)	-4750	1331	-1258	88
H(24A)	-4982	-499	-1651	79
H(26A)	-4572	-2391	-2068	70
H(27A)	-3703	-3546	-2362	64
H(28A)	-2637	-2882	-2223	56

Table 1. Crystal data and structure refinement for **13**.

Identification code	**13**	
Empirical formula	C28 H20 B N3	
Formula weight	409.28	
Temperature	297(2) [K]	
Wavelength	0.71073 [Å]	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 20.246(9) [Å]	α= 90°.
	b = 11.547(5) [Å]	β= 91.728(9)°.
	c = 17.962(8) [Å]	γ = 90°.
Volume	4197(3) [$Å^3$]	
Z	8	
Density (calculated)	1.295 [Mgm^{-3}]	
Absorption coefficient	0.076 [mm^{-1}]	
F(000)	1712	
Crystal size	0.40 x 0.30 x 0.05 [mm^3]	
Theta range for data collection	2.01 to 28.29°.	
Index ranges	-25<=h<=26, -15<=k<=15, -23<=l<=21	
Reflections collected	14223	
Independent reflections	4958 [R(int) = 0.2297]	
Completeness to theta = 28.29°	95.1 %	
Absorption correction	Empirical	
Max. and min. transmission	1.000 and 0.582	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4958 / 0 / 290	
Goodness-of-fit on F^2	0.720	
Final R indices [I>2sigma(I)]	R1 = 0.0857, wR2 = 0.1511	
R indices (all data)	R1 = 0.3565, wR2 = 0.1964	
Extinction coefficient	0.00090(17)	
Largest diff. peak and hole	0.211 and -0.212 [$e.Å^{-3}$]	

Table 2. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$x 10^3] for **13**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U[eq]

B(1)	2018(4)	-979(6)	1761(4)	37(2)
N(1)	2009(3)	217(4)	1353(2)	38(1)
N(2)	2816(3)	-1300(4)	1843(2)	41(1)
N(3)	838(3)	423(4)	1139(3)	59(2)
C(1)	1680(3)	-1976(5)	1248(3)	38(2)
C(2)	1721(3)	-1936(5)	497(3)	49(2)
C(3)	1480(4)	-2817(6)	38(4)	73(2)
C(4)	1212(3)	-3793(6)	340(4)	65(2)
C(5)	1185(3)	-3880(5)	1098(4)	63(2)
C(6)	1414(3)	-2982(5)	1547(3)	40(2)
C(7)	1756(3)	-816(4)	2597(3)	37(2)
C(8)	1103(3)	-944(4)	2751(3)	47(2)
C(9)	867(3)	-743(5)	3454(4)	55(2)
C(10)	1281(4)	-387(5)	4011(4)	62(2)
C(11)	1936(4)	-229(5)	3888(4)	61(2)
C(12)	2177(3)	-461(4)	3183(4)	50(2)
C(13)	2946(3)	-2371(5)	2097(3)	41(2)
C(14)	3593(4)	-2764(5)	2211(3)	52(2)
C(15)	4099(3)	-2104(6)	2043(3)	52(2)
C(16)	3987(4)	-969(6)	1790(3)	48(2)
C(17)	3330(4)	-577(5)	1683(3)	40(2)
C(18)	4513(4)	-192(7)	1624(3)	70(2)
C(19)	4381(4)	901(6)	1407(4)	70(3)
C(20)	3730(4)	1249(5)	1295(3)	53(2)
C(21)	3193(4)	542(5)	1407(3)	47(2)
C(22)	2542(4)	922(5)	1231(3)	36(2)
C(23)	2330(4)	1945(5)	918(3)	49(2)
C(24)	1647(4)	1897(5)	838(3)	49(2)
C(25)	1155(4)	2635(5)	586(4)	69(2)
C(26)	520(4)	2260(6)	594(4)	71(2)
C(27)	390(4)	1165(6)	875(4)	71(2)
C(28)	1455(4)	803(5)	1112(3)	42(2)

Table 3. Bond lengths [Å] and angles [°] for **13**.

B(1)-N(1)	1.563(7)	C(9)-C(10)	1.350(7)
B(1)-C(1)	1.614(8)	C(10)-C(11)	1.362(8)
B(1)-C(7)	1.618(8)	C(11)-C(12)	1.396(7)
B(1)-N(2)	1.661(8)	C(13)-C(14)	1.395(7)
N(1)-C(28)	1.370(6)	C(14)-C(15)	1.319(7)
N(1)-C(22)	1.374(6)	C(15)-C(16)	1.403(7)
N(2)-C(13)	1.342(6)	C(16)-C(17)	1.412(7)
N(2)-C(17)	1.372(6)	C(16)-C(18)	1.431(8)
N(3)-C(27)	1.324(7)	C(17)-C(21)	1.408(7)
N(3)-C(28)	1.327(7)	C(18)-C(19)	1.346(8)
C(1)-C(2)	1.355(7)	C(19)-C(20)	1.386(8)
C(1)-C(6)	1.395(7)	C(20)-C(21)	1.380(7)
C(2)-C(3)	1.388(7)	C(21)-C(22)	1.415(7)
C(3)-C(4)	1.371(8)	C(22)-C(23)	1.372(7)
C(4)-C(5)	1.369(8)	C(23)-C(24)	1.388(7)
C(5)-C(6)	1.384(7)	C(24)-C(25)	1.375(8)
C(7)-C(8)	1.367(7)	C(24)-C(28)	1.414(7)
C(7)-C(12)	1.398(7)	C(25)-C(26)	1.359(8)
C(8)-C(9)	1.384(7)	C(26)-C(27)	1.389(8)

N(1)-B(1)-C(1)	111.4(5)
N(1)-B(1)-C(7)	109.5(5)
C(1)-B(1)-C(7)	117.9(5)
N(1)-B(1)-N(2)	103.6(5)
C(1)-B(1)-N(2)	106.6(5)
C(7)-B(1)-N(2)	106.8(5)
C(28)-N(1)-C(22)	107.2(5)
C(28)-N(1)-B(1)	125.6(5)
C(22)-N(1)-B(1)	126.9(5)
C(13)-N(2)-C(17)	119.3(6)
C(13)-N(2)-B(1)	114.6(5)
C(17)-N(2)-B(1)	126.0(5)
C(27)-N(3)-C(28)	114.0(6)
C(2)-C(1)-C(6)	116.6(6)
C(2)-C(1)-B(1)	120.4(6)
C(6)-C(1)-B(1)	122.4(5)
C(1)-C(2)-C(3)	122.3(6)
C(4)-C(3)-C(2)	120.2(7)
C(5)-C(4)-C(3)	118.9(7)
C(4)-C(5)-C(6)	120.1(6)
C(5)-C(6)-C(1)	121.7(6)
C(8)-C(7)-C(12)	116.8(6)
C(8)-C(7)-B(1)	121.4(6)
C(12)-C(7)-B(1)	121.6(6)
C(7)-C(8)-C(9)	122.0(6)
C(10)-C(9)-C(8)	120.2(7)
C(9)-C(10)-C(11)	120.4(7)
C(10)-C(11)-C(12)	119.4(7)
C(11)-C(12)-C(7)	121.1(7)
N(2)-C(13)-C(14)	121.6(6)
C(15)-C(14)-C(13)	120.7(6)
C(14)-C(15)-C(16)	119.6(7)
C(15)-C(16)-C(17)	119.1(6)
C(15)-C(16)-C(18)	122.6(7)
C(17)-C(16)-C(18)	118.3(6)
N(2)-C(17)-C(21)	119.3(6)
N(2)-C(17)-C(16)	119.5(6)
C(21)-C(17)-C(16)	121.2(6)
C(19)-C(18)-C(16)	120.4(7)
C(18)-C(19)-C(20)	119.5(7)
C(21)-C(20)-C(19)	123.9(7)
C(20)-C(21)-C(17)	116.4(7)
C(20)-C(21)-C(22)	121.1(7)
C(17)-C(21)-C(22)	122.4(6)
C(23)-C(22)-N(1)	109.8(6)
C(23)-C(22)-C(21)	129.5(6)
N(1)-C(22)-C(21)	120.7(6)
C(22)-C(23)-C(24)	107.8(6)
C(25)-C(24)-C(23)	135.9(6)
C(25)-C(24)-C(28)	117.7(7)
C(23)-C(24)-C(28)	106.4(6)
C(26)-C(25)-C(24)	118.4(7)
C(25)-C(26)-C(27)	118.9(7)
N(3)-C(27)-C(26)	125.8(7)
N(3)-C(28)-N(1)	126.1(6)
N(3)-C(28)-C(24)	125.2(6)
N(1)-C(28)-C(24)	108.7(6)

Table 4. Anisotropic displacement parameters [$Å^2 x\ 10^3$] for **13**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
B(1)	33(5)	44(5)	35(5)	16(4)	0(4)	-4(4)
N(1)	56(4)	30(3)	29(3)	3(2)	7(3)	-7(3)
N(2)	61(4)	23(3)	38(3)	3(3)	1(3)	-15(3)
N(3)	65(5)	38(3)	75(4)	35(3)	7(4)	17(3)
C(1)	53(5)	31(4)	30(4)	2(3)	2(3)	-5(3)
C(2)	83(5)	29(4)	35(4)	-4(3)	2(4)	-14(3)
C(3)	116(7)	67(5)	34(5)	-18(4)	-14(5)	4(5)
C(4)	80(6)	55(5)	59(5)	-17(4)	-2(5)	-4(4)
C(5)	64(6)	43(5)	83(6)	1(4)	-11(5)	-11(4)
C(6)	51(5)	38(4)	30(4)	-2(3)	-3(3)	2(3)
C(7)	51(5)	24(4)	35(4)	1(3)	-6(4)	-4(3)
C(8)	68(5)	33(4)	40(5)	-3(3)	-1(4)	-3(4)
C(9)	76(6)	43(4)	49(5)	-16(4)	28(4)	-1(4)
C(10)	105(7)	36(4)	46(5)	-8(4)	14(5)	23(5)
C(11)	93(7)	41(4)	47(5)	-5(3)	-5(5)	17(5)
C(12)	71(5)	27(4)	50(4)	1(3)	9(4)	14(4)
C(13)	61(5)	27(4)	36(4)	-2(3)	-1(4)	-11(4)
C(14)	53(5)	41(4)	61(5)	15(4)	-6(4)	-1(4)
C(15)	55(5)	64(5)	37(4)	-6(4)	0(4)	3(4)
C(16)	51(5)	41(4)	50(5)	-3(4)	-7(4)	-2(4)
C(17)	58(5)	42(4)	20(4)	0(3)	15(4)	-3(4)
C(18)	68(6)	92(6)	51(5)	-4(5)	-2(4)	-30(5)
C(19)	85(7)	70(6)	56(5)	9(4)	-3(5)	-48(5)
C(20)	76(6)	42(5)	42(4)	1(3)	-5(4)	-15(5)
C(21)	76(6)	35(4)	30(4)	0(3)	15(4)	-25(4)
C(22)	62(5)	21(4)	27(4)	0(3)	10(4)	-9(4)
C(23)	78(6)	19(4)	49(5)	-2(3)	-5(4)	-14(4)
C(24)	65(6)	33(4)	50(5)	19(4)	8(4)	-3(4)
C(25)	108(7)	38(4)	61(5)	21(4)	13(5)	24(5)
C(26)	85(7)	58(6)	72(6)	26(4)	18(5)	17(5)
C(27)	62(6)	66(5)	86(6)	25(5)	10(5)	1(5)
C(28)	43(5)	37(4)	46(4)	2(3)	11(4)	-1(4)

Table 5. Hydrogen coordinates [x 10^4] and isotropic displacement parameters [$Å^2 x\ 10^{\ 3}$] for **13**.

	x	y	z	U[eq]
H(2A)	1918	-1296	281	59
H(3A)	1500	-2743	-477	87
H(4A)	1052	-4387	35	78
H(5A)	1012	-4543	1313	76
H(6A)	1389	-3052	2061	48
H(8A)	809	-1173	2371	56
H(9A)	421	-853	3543	66
H(10A)	1119	-249	4482	74
H(11A)	2219	31	4269	73
H(12A)	2627	-377	3103	59
H(13A)	2597	-2863	2201	49
H(14A)	3668	-3500	2407	62

H(15A)	4528	-2389	2091	63
H(18A)	4948	-445	1665	84
H(19A)	4724	1420	1334	84
H(20A)	3651	2004	1135	64
H(23A)	2597	2562	783	59
H(25A)	1256	3372	414	83
H(26A)	177	2729	414	85
H(27A)	-50	933	879	85