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Electronic Supplementary Information for

Photonic materials derived from the [*closo*-B₁₀H₁₀]²⁻ anion: Tuning photophysical properties in [*closo*-B₁₀H₈-1-X-10-(4-Y-NC₅H₅)]⁻

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1. Additional synthetic and analytical details.

General. Reagents and solvents were obtained commercially. Anion $[closo-B_{10}H_{10}]^{2^{-}}$ was obtained from $B_{10}H_{14}$ according to a literature procedure.¹ Reactions were conducted in argon atmosphere and subsequent manipulations in air. TLC analyses were conducted on silica gel plates 60-F254. Column chromatography was performed using 70-230 mesh silica gel (Merck). Melting points were recorded uncorrected in capillary tubes or by DSC. NMR spectra were obtained at 500 MHz (¹H), 126 MHz (¹³C) and 160 MHz (¹¹B) in acetone-*d*₆ unless specified otherwise. Chemical shifts were referenced to the solvent (acetone-*d*₆ 2.05 ppm for ¹H and 29.84 ppm for ¹³C)² and to an external sample of neat BF₃•Et₂O in acetone-*d*₆ (¹¹B, $\delta = 0.0$ ppm). ¹¹B NMR chemical shifts were taken from the H-decoupled spectra. IR spectra were recorded for neat samples using an ATR attachment. HR mass spectrometry was conducted with the TOF-MS ES method most often in the negative mode.

Preparation of silica gel SiO₂ passivated with Bu₄NHCO₃:

Aqueous $[Bu_4N]^+[OH]^-$ (2.0 mL, 40% solution) was stirred with a few pieces of solid CO₂ until the solution was homogenous. After concentrating of the aqueous solution under reduced pressure, $[Bu_4N]^+[HCO_3]^-$ was extracted into CH₂Cl₂ (15 mL). The CH₂Cl₂ solution was added to silica gel (~1.5 mL per 10 g of SiO₂), an additional portion of CH₂Cl₂ added, and stirred for 15 min. The freshly prepared passivated SiO₂ was transferred into a column and washed with a few portions of CH₂Cl₂ before using for chromatography.

²⁻ [*closo*-B₁₀H₁₀]²⁻ 2[Et₃HN⁺] (A[Et₃HN]). Prepared according to the literature ²[Et₃HN]⁺ protocol¹ and purified by recrystallization from MeCN/CH₂Cl₂ (3:2); colorless long needles: mp 239 °C; ¹H NMR (500 MHz, acetone- d_6) δ -0.32–0.78 (br m, 8H), 1.41 (t, J = 7.3 Hz, 18H), 3.37 (q, J = 7.3 Hz, 12H), 5.62 (s, 1H); ¹¹B NMR (160 MHz, acetone- d_6) δ -28.0 (d, J = 127 Hz, 8B), -0.1 (d, J = 137 Hz, 2B).

²⁻ [Bu₄N]⁺ [*closo*-B₁₀H₉-1-IPh]⁻ [Bu₄N⁺] (4[Bu₄N]). Prepared in 50% yield according the literature procedure³ using very intense stirring of the reaction mixture: mp 213 °C; ¹H NMR (500 MHz, acetone-*d*₆) δ 0.25 – 1.17 (br m, 8H), 0.98 (t, *J* = 7.4 Hz, 12H), 1.43 (sex, *J* = 7.4 Hz, 8H), 1.81 (quin, *J* = 8.0 Hz, 8H), 3.34 – 3.48 (m, 8H), 4.38 (br q, *J* = 147.6 Hz, 1H), 7.44 (t, *J* = 7.3 Hz, 2H), 7.59 (t, *J* = 7.4 Hz, 1H), 8.24 (d, *J* = 8.3 Hz, 1H); ¹³C NMR (126 MHz, acetone-*d*₆) δ 13.9, 20.4, 24.5, 59.5, 131.0, 131.9, 135.1; ¹¹B NMR (160 MHz, acetone- d_6) δ -27.2 (d, J = 132 Hz, 4B), -23.4 (d, J = 134 Hz, 4H), -2.6 (s, 1B), 10.5 (d, J = 146 Hz, 1B).

 $\begin{bmatrix} closo-B_{10}H_9-1-I]^{2-} & 2[Bu_4N^+] & (5e[Bu_4N]). \text{ Prepared according to the} \\ \text{ literature procedure:}^{3-1}H \text{ NMR (500 MHz, acetone-}d_6) \delta -0.10 - 1.11 (br m, \\ 8H), 0.98 (t, J = 7.3 \text{ Hz}, 24H), 1.45 (sext, J = 7.4 \text{ Hz}, 16H), 1.79 (quint, J = 8.0 \text{ Hz}, \\ 16H), 3.37 - 3.46 (m, 16H), 3.86 (br q, J = 141 \text{ Hz}, 1H); ^{13}C \text{ NMR (126 MHz, acetone-}d_6) \delta \\ 14.0, 20.4, 24.7, 59.5; ^{11}B \text{ NMR (160 MHz, acetone-}d_6) \delta -27.9 (d, J = 122 \text{ Hz}, 4B), -24.5 (d, J = 128 \text{ Hz}, 4H), -7.6 (s, 1B), 0.8 (d, J = 143 \text{ Hz}, 1B). \end{bmatrix}$

Method A. General procedure for the preparation of $[closo-B_{10}H_8-1-X-10-IPh]^{-}[R_4N]^+$ (6) from $[closo-B_{10}H_9-1-IPh]^{-}[Bu_4N]^+$ (4 $[Bu_4N]$).

A solution of phenyliodonium $4[Bu_4N]$ (0.50 mmol) and freshly dried $[Bu_4N]^+X^-$ (0.75 mmol, 1.5 eq) in MeCN (5 mL) was stirred at 55 – 60 °C overnight. All volatiles were removed in vacuum and the brown residue was separated on silica gel (CH₂Cl₂/MeCN 14:1 gradient to 5:1). The resulting product was recrystallized (EtOH/MeCN) giving pure $5[Bu_4N]$. The monosubstituted derivative $5[Bu_4N]$ was dissolved in MeCN (1.0 mL), cooled in an ice bath and PhI(OAc)₂ (1.2 eq) was added in 3 portions over 15 min. The reaction mixture was allowed to gradually reach ambient temperature and stirred overnight (16 – 20 h). Solvent was removed under reduced pressure at room temperature and the residue was chromatographed on silica gel (MeCN/CH₂Cl₂, 1:10). The isolated product $6[Bu_4N]$ was used without further purification.

Method B. Preparation of $[closo-B_{10}H_8-1-X-10-IPh]^{T}[R_4N]^{+}$ (6) from $[closo-B_{10}H_9-1,10-2(IPh)]$ (7). General procedure. A suspension of $[closo-B_{10}H_8-1,10-2(IPh)]^6$ (7, 105 mg, 0.2 mmol) in dry MeCN (5 mL) and appropriate nucleophile salt $[R_4N]^{+}X^{-}$ (X = CN⁻ (1.1 eq), OAc, SCN 1.1–2.5 eq) was stirred at 55 °C (6b) or 60 °C for 1 (CN), 2 or 3 days. Progress of the reaction was monitored with ¹¹B NMR using the supernatant liquid. When ¹¹B NMR demonstrated lack of reaction progress, the reaction mixture was filtered, and the solvent was removed from the brown filtrate under reduced pressure at ambient temperature using a rotary evaporator and an oil pump. The resulting cru de solid was passed through a short SiO₂ plug (MeCN/CH₂Cl₂, 1:9), the main fraction 6[R₄N] was collected, and solvents were removed under vacuum avoiding excess heat. The pure product was isolated by column chromatography and

purified by recrystallization, usually from EtOH/CH₂Cl₂. In a one-pot variation for **6d** and **6e**, volatiles were removed under vacuum after the reaction completed, and the crude mixture was used without purification.

Method C. General procedure for the preparation of [*closo*-B₁₀H₈-1-IPh-10-(4-Xpyridinium)] 6. To a solution of monopyridinium derivative $1a[Bu_4N]$ (0.345 mmol) in MeCN (2 mL) PhI(OAc)₂ (222 mg, 0.690 mmol, 2 eq) was added in 5 portions every 3 h, then the reaction mixture was stirred for 24 h. The reaction was stopped after starting material was consumed based on ¹¹B NMR analysis. Solvents were evaporated under high vacuum, and the residue was washed twice, first with warm EtOH then with cold CH₂Cl₂/hexane (2:1) to obtain sufficiently pure product for the next step. The crude product can be purified on a short silica gel pad using CH₂Cl₂/hexane eluent. After evaporation of solvent at 30 °C, the slightly yellowish residue was recrystallized from EtOH/CH₂Cl₂.

[*closo*-**B**₁₀**H**₉-1-CN]²⁻ 2[**Bu**₄N]⁺ (**5b**[**Bu**₄N]).⁴ Using Method A with [Bu₄N]⁺CN⁻: 157 mg (50% yield) of the product as a gray-blue solid, which was recrystallized from EtOH/MeCN giving pure **5b**[**Bu**₄N] as a light gray microcrystals: R_f = 0.42 (17% MeCN in CH₂Cl₂); mp 216 °C; ¹H NMR (500 MHz, acetone-*d*₆) δ 0.05-0.73 (br m, 8H), 0.98 (t, *J* = 7.4 Hz, 24H), 1.45 (sext, *J* = 7.4 Hz, 16H), 1.77 – 1.83 (m, 16H), 3.40 – 3.44 (m, 16H), 3.73 (br q, *J* = 145.9 Hz, 1H); ¹³C NMR (126 MHz, acetone-*d*₆) δ 13.9, 20.4, 24.6, 59.5; ¹¹B NMR (160 MHz, acetone-*d*₆) δ -27.3 (d, *J* = 148 Hz, 4B), -24.5 (d, *J* = 135 Hz, 4B), -10.1 (s, 1B), 6.6 (d, *J* = 152 Hz, 1B); IR, *v* 2447 (B-H), 2175 (CN), 1480, 1473, 1380, 996, 882, 739 cm⁻¹; HRMS (ESI-) *m/z* calcd. for CH₉B₁₀N: 145.1671, found: 145.1670.

[*closo*-B₁₀H₉-1-N₃]²⁻ 2[Bu₄N]⁺ (5d[Bu₄N]). Using Method A with [Bu₄N]⁺N₃⁻ and chromatography using CH₂Cl₂/MeCN (10:1) to give 307 mg (95% yield) which was recrystallized (EtOH/MeCN) to give pure 5d[Bu₄N] as a white powder: mp 207 °C; R_f = 0.31 (9% MeCN in CH₂Cl₂); ¹H NMR (500 MHz, acetone-*d*₆) δ -0.08-0.78 (br m, 8H), 0.98 (t, *J* = 7.4 Hz, 24H), 1.44 (sext, *J* = 7.4 Hz, 16H), 1.75 – 1.82 (m, 16H), 3.35-3.48 (m, 16H); ¹³C NMR (126 MHz, acetone-*d*₆) δ 14.0, 20.4, 24.6, 59.4; ¹¹B NMR (160 MHz, acetone-*d*₆) δ -29.9 (d, *J* = 131 Hz, 4B), -28.2 (d, *J* = 121 Hz, 4B), -4.2 (d, *J* = 140 Hz 1B), 12.7 (s, 1B); IR, *v* 2447 (BH),

2094 (N₃), 1480, 997, 882, 740 cm⁻¹; HRMS (ESI-) m/z calcd. for B₁₀H₉N₃: 161.1733, found: 161.1732.

[*closo*-B₁₀H₈-1-CN-10-IPh]⁻ [Bu₄N]⁺ (6b[Bu₄N]). Method B using THF/MeCN (1:1) solvent: 62–71 mg (53-60% yield); R_f = 0.82 (9% MeCN in CH₂Cl₂); mp 129 °C; ¹H NMR (500 MHz, acetone- d_6) δ 0.40-1.19 (br m, 8H), 0.97 (t, J = 7.4 Hz, 12H), 1.43 (sext, J = 7.4 Hz, 8H), 1.77 – 1.83 (m, 8H), 3.39 – 3.42 (m, 8H), 7.46 (ddt, J_1 = 7.8 Hz, J_2 = 7.4 Hz J_3 = 1.9 Hz 2H), 7.61 (tt, J_1 = 7.5 Hz, J_2 = 1.1 Hz, 1H), 8.18 (ddm, J_1 = 8.4 Hz, J_2 = 1.1 Hz, 2H); ¹³C NMR (126 MHz, acetone- d_6) δ 13.9, 20.3, 24.4, 59.4, 104.6, 131.4, 132.1, 135.5; ¹¹B NMR (160 MHz, acetone- d_6) δ -24.0 (d, J = 143 Hz, 4B), -23.1 (d, J = 141 Hz, 4B), 0.7 (s, 1B), 2.5 (s, 1B); IR v 2504 (BH), 2192 (CN), 1477, 998, 884, 745, 647 cm⁻¹; HRMS (ESI-) m/z calcd. for C₇H₁₂B₁₀IN: 347.0951, found: 347.0958.

[*closo*-B₁₀H₈-1-OAc-10-IPh]⁻ [Et₄N]⁺ (6c[Et₄N]).⁶ Method B: obtained 46 mg (45% yield); pale grayish crystals from MeCN/EtOH; $R_f = 0.55$ (40% MeCN in CH₂Cl₂); mp 164 °C; ¹H NMR (500 MHz, acetone-*d*₆) δ 0.36-1.11 (br m, 8H), 1.35 (tt, *J*₁ = 7.3 Hz, *J*₂ = 1.9 Hz, 12H), 2.27 (s, 3H), 3.43 (q, *J* = 7.3 Hz, 8H), 7.45 (tm, *J* = 7.8 Hz, 2H), 7.60 (t, *J* = 7.4 Hz, 1H), 8.20 (ddm, *J*₁ = 8.4 Hz, *J*₂ = 1.1 Hz, 2H); ¹³C NMR (126 MHz, acetone-*d*₆) δ 7.8, 23.2, 53.1, 104.0, 131.2, 131.9, 135.3, 172.2; ¹¹B NMR (160 MHz, acetone-*d*₆) δ -28.2 (d, *J* = 133 Hz, 4B), -26.4 (d, *J* = 136 Hz, 4B), - 2.8 (s, 1B), 29.3 (s, 1B); IR, *v* 2495 (BH), 1704 (C=O), 1278 (C-O), 1185, 989, 745, 643 cm⁻¹; HRMS (ESI-) *m/z* calcd. for C₈H₁₆B₁₀IO₂: 381.1131, found: 381.1132.

[*closo*-B₁₀H₈-1-N₃-10-IPh]⁻ [Bu₄N]⁺ (6d[Bu₄N]). Method A: obtained 40-47 mg (66-78% yield); yellowish oil which crystallizes slowly on standing; $R_f = 0.45$ (6% MeCN in CH₂Cl₂); mp 100 °C; ¹H NMR (500 MHz, acetone-*d*₆) δ 0.25 – 1.24 (br m, 8H), 0.98 (t, *J* = 7.4 Hz, 12H), 1.43 (sext, *J* = 7.4 Hz, 8H), 1.78 – 1.84 (m, 8H), 3.41–3.44 (m, 8H), 7.44 (tm, *J* = 7.8 Hz, 2H), 7.61 (tt, *J*₁ = 7.4 Hz, *J*₂ = 1.1 Hz, 1H), 8.19 (dd, *J*₁ = 8.2 Hz, *J*₂ = 1.1 Hz, 2H); ¹³C NMR (126 MHz, acetone-*d*₆) δ 13.9, 20.4, 24.5, 59.5, 104.1, 131.2, 132.0, 135.3; ¹¹B NMR (160 MHz, acetone-*d*₆) δ -27.5 (d, *J* = 131 Hz, 4B), -25.5 (d, *J* = 138 Hz, 4B), -2.0 (s, 1B), 23.3 (s, 1B); IR, *v* 2494 (BH), 2112 (N₃), 1470, 998, 737 cm⁻¹; HRMS (ESI-), calcd. for C₆H₁₃B₁₀IN₃: *m/z* = 364.1090, found: 364.1095.

 $[closo-B_{10}H_8-1-I-10-IPh]^ [Bu_4N]^+$ (6e[Bu_4N]). Method A: obtained 63 mg (91% yield). Alternatively, the following approach gave 33 mg (25% yield or 38% yield relative to recovered starting material). To a solution of 7 (100 mg, 0.191 mmol) in dry THF (8 mL) n-BuLi (2.5 M, 115 μ L, 0.287 mmol, 1.5 eq) was added dropwise at -10 °C under argon atmosphere, and the resulting mixture was stirred for 30 min at -10 °C. Water (10 mL) was added and THF was thoroughly removed under reduced pressure. Then $[Bu_4N]^+HSO_4^-$ (97 mg, 0.287 mmol, 1.5 eq) was added at once at room temperature and the resulting white suspension was stirred overnight. The precipitate was filtered and washed with water, then hexane, and dried under high vacuum. The resulting crude mixture was passed through a short silica gel pad (CH₂Cl₂/MeCN), solvents were removed under reduced pressure, and the crude product was used for the next step without further purification. Pale yellow-green crystals from MeCN/EtOAc; $R_f = 0.15$ (30% MeCN in CH₂Cl₂); mp 70 °C; ¹H NMR (500 MHz, acetone- d_6) δ 1.19 – 0.28 (m, 8H), 0.97 (t, J = 7.3 Hz, 12H), 1.43 (sext, J = 7.4 Hz, 8H), 1.77 - 1.84 (m, 8H), 3.40-3.43 (m, 8H), 7.45 (t, J = 7.9 Hz, 2H), 7.60 (t, J = 7.4 Hz, 1H), 8.19 (dd, $J_1 = 7.7$ Hz, $J_2 = 1.1$ Hz, 2H); ¹³C NMR (126 MHz, acetone- d_6) δ 13.9, 20.4, 24.5, 59.4, 104.0, 131.2, 132.0, 135.4; ¹¹B NMR (160 MHz, acetone- d_6) δ -23.3 (d, J = 135 Hz, 8B), 2.0 (s, 2B); IR, v 2490 (BH), 1474, 1452, 993, 827, 745, 643 cm⁻¹: HRMS (ESI-) m/z calcd. for C₆H₁₃B₁₀I₂: 449.0043, found: 449.0043.

[*closo*-B₁₀H₈-1-SCN-10-IPh]⁻ [Et₄N⁺] (6f[Et₄N]). Method B: obtained 16 mg (16% yield); pale yellow-green crystals from ACN/EtOH; R_f = 0.47 (9% MeCN in CH₂Cl₂); mp 62 °C; ¹H NMR (500 MHz, acetone-*d*₆) δ 0.27-1.16 (br m, 8H), 1.33 (tt, *J*₁ = 7.2 Hz, *J*₂ = 1.8 Hz, 12H), 3.39 (q, *J* = 7.3 Hz, 8H), 7.46 (tm, *J* = 7.8 Hz, 2H), 7.62 (tt, *J*₁ = 7.4 Hz, *J*₂ = 1.1 Hz, 1H), 8.17 (dd, *J*₁ = 8.4 Hz, , *J*₂ = 1.1 Hz, 2H); ¹³C NMR (126 MHz, acetone-*d*₆) δ 7.8, 53.1, 104.5, 118.5, 131.4, 132.1, 135.5; ¹¹B NMR (160 MHz, acetone-*d*₆) δ -23.7 (d, *J* = 133 Hz, 4B), -23.4 (d, *J* = 110 Hz, 4B), 2.3 (s, 1B), 13.9 (s, 1B); IR, *v* 2481 (BH), 2139 (CN), 1470, 1441, 989, 733, 647 cm⁻¹; HRMS (ESI-) *m/z* calcd. for C₇H₁₂B₁₀INS: 379.0671, found: 379.0680.

[*closo*-B₁₀H₈-1-Br-10-IPh]⁻ [Et₄N]⁺ (6g[Et₄N]). Method B: obtained 80 mg (75% yield); pale yellow-green crystals from MeCN/EtOAc; $R_f = 0.15$ (30% MeCN in CH₂Cl₂); mp 165 °C; ¹H NMR (500 MHz, acetone-*d*₆) δ 0.34 – 1.23 (br m, 8H), 1.37 (tt, *J*₁ = 7.3 Hz, *J*₂ = 1.9 Hz, 12H), 3.46 (q, *J* = 7.3 Hz, 8H), 7.45 (tm, *J* = 7.9 Hz, 2H), 7.60 (tt, *J*₁ = 7.4 Hz, *J*₂ = 1.0 Hz, 1H), 8.19 (dd, *J*₁ = 8.3 Hz, *J*₂ = 1.0 Hz, 2H); ¹³C NMR (126 MHz, acetone-*d*₆) δ 7.8, 53.1, 104.1, 131.2,

132.0, 135.4; ¹¹B NMR (160 MHz, acetone- d_6) δ -24.5 (d, J = 147 Hz, 8B), -0.5 (s, 1B), 17.3 (s, 1B); IR, *v* 2486 (BH), 1447, 994, 829, 745, 656 cm⁻¹; HRMS (ESI-) *m/z* calcd. for C₆H₁₂B₁₀BrI: 400.0103, found: 400.0136.

[closo-B₁₀H₈-1-(NHC₄H₈O)-10-IPh] (6k). A mixture of phenyliodonium 4[Bu₄N] (459 mg, 0.905 mmol) and morpholine (3 mL) was stirred overnight at 80 °C. Volatiles were removed in vacuum and the residue was washed with cold hexanes. The residue containing two major species in about equal amounts was dissolved in AcOH (25 mL) and water was added (5 mL). The yellowish mixture was cooled in an ice bath, solid PhI(OAc)₂ (310 mg, 0.96 mmol) was added in one portion and the resulting mixture was stirred for 1.5 hr at 0 °C. Water (25 mL) was added and the resulting precipitate was filtered, washed with water, and dried giving 348 mg of a tan solid. After separation by column chromatography (SiO₂, 5% gradient to 10% EtOAc in CH_2Cl_2) the second band contained 111 mg (30% yield) of the phenyliodonium derivative **6k** as a colorless powder: mp 260 °C dec; ¹H NMR (500 MHz, acetone- d_6) δ 0.32 – 1.47 (br m, 8H), 3.63 - 3.71 (m, 2H), 3.94 (br d, J = 13.3 Hz, 2H), 4.10 (td, $J_1 = 12.2$ Hz, $J_2 = 1.9$ Hz, 2H), 4.19(br dd, $J_1 = 12.5$, $J_2 = 1.6$ Hz, 2H), 7.47 (tm, J = 7.9 Hz, 2H), 7.63 (tt, $J_1 = 7.4$ Hz, $J_2 = 1.1$ Hz, 1H), 8.15 (br s, 1H), 8.18 (dd, $J_1 = 8.4$, $J_2 = 1.1$ Hz, 2H); ¹³C NMR (125 MHz, acetone- d_6) δ 56.0, 65.9, 104.6, 131.5, 132.2, 135.8; ¹¹B NMR (160 MHz, acetone- d_6) δ -25.7 (d, J = 137 Hz, 4B), -23.9 (d, J = 140 Hz, 4B), 2.9 (s, 1B), 22.5 (s, 1B); IR v 3172 (NH), 2491, 2456, (BH), 1259 (C-O), 1125, 987, 738, 679 cm⁻¹; HRMS (ESI-) m/z calcd. for C₁₀H₂₁B₁₀INO: 408.1604, found: 408.1612.

[*closo*-B₁₀H₈-1,10-2(IPh)] (7). Prepared according to the literature procedure:⁴ mp 169 °C dec.; ¹H NMR (500 MHz, acetone- d_6) δ 0.59–1.54 (br m, 8H), 7.49 (t, J = 7.9 Hz, 4H), 7.65 (t, J = 7.4 Hz, 2H), 8.17 (d, J = 8.3 Hz, 4H); ¹³C NMR (126 MHz, acetone- d_6) δ 105.1, 131.7, 132.3, 136.1; ¹¹B NMR (160 MHz, acetone- d_6) δ -22.6 (d, J = 139 Hz, 8B), 7.5 (s, 2B).

Preparation of [*closo*-**B**₁₀**H**₈-1-IPh-10-(NC₅**H**₅)] (8). Method C with reaction time 24 h: 63 mg (69% yield) of product 8 as white fine microcrystals; $R_f = 0.85$ (CH₂Cl₂/hexane 4:1); mp 180 °C; ¹H NMR (500 MHz, acetone-*d*₆) δ 0.74 – 1.53 (br m, 8H), 7.49 (t, *J* = 7.9 Hz, 2H), 7.65 (t, *J* = 7.4 Hz, 1H), 8.09 (t, *J* = 7.1 Hz, 2H), 8.20 (d, J = 7.8 Hz, 2H), 8.55 (t, *J* = 7.8 Hz, 1H), 9.53 (d, *J* = 5.5 Hz, 2H); ¹³C NMR (126 MHz, acetone-*d*₆) δ 104.7, 127.5, 131.6, 132.2, 136.0, 143.7,

148.8; ¹¹B NMR (160 MHz, acetone-d₆) δ -23.4 (d, J = 138 Hz, 8B), 4.1 (s, 1B), 23.1 (s, 1B); IR, *v* 2489 (BH), 1462, 992, 773, 736, 683 cm⁻¹; HRMS (ESI-) *m/z* calcd. for C₁₁H₁₈B₁₀IN: 401.1420, found: 401.1445. Anal. Calcd. for C₁₁H₁₈B₁₀IN: C, 33.09; H, 4.54; N, 3.51. Found: C, 33.35; H, 4.57; N, 3.65.

Preparation of [*closo*-**B**₁₀**H**₈-1-(EtOH)-10-NC₅**H**₅] (9). A suspension of phenyliodonium **8** (150 mg, 0.376 mmol) in EtOH (7 mL) was heated in sealed tube at 110 °C for 2.5 days (¹¹B NMR monitoring), then EtOH was removed in high vacuum and the yellowish residue was washed with warm hexane and purified on short silica gel pad using CH₂Cl₂/MeCN (4:1 gradient to 1:2). Solvents were evaporated, and the yellow product (*ca.* 91% purity) was dried on high vacuum to give 62 mg (69% yield) of **9** as a yellow sticky soft material, which was used for the next step without further purification: $R_f = 0.29$ (CH₂Cl₂/MeCN 1:2); ¹H NMR (500 MHz, acetone-*d*₆) δ 0.56 – 1.31 (m, 8H), 1.68 (t, *J* = 7.0 Hz, 3H), 3.65 (br s, 1H), 4.76 (q, *J* = 7.0 Hz, 2H), 7.96 (tm, *J* = 7.2 Hz, 2H), 8.42 (tt, *J*₁ = 7.5 Hz, *J*₂ = 1.3 Hz, 1H), 9.57 (dd, *J*₁ = 6.4 Hz, *J*₂ = 1.1 Hz, 2H); ¹³C NMR (126 MHz, acetone-*d*₆) δ 16.1, 70.6, 126.6, 142.1, 149.0; ¹¹B NMR (160 MHz, acetone-*d*₆) δ -27.9 (d, *J* = 134 Hz, 4B), -25.9 (d, *J* = 135 Hz, 4B), 12.4 (s, 1B), 27.1 (s, 1B); IR, *v* 2482 (BH), 1462, 1208 (C-O), 1004, 769, 687 cm⁻¹; HRMS (ESI-) *m/z* calcd. for C₇H₂₂B₁₀NO: 244.2481, found: 244.2474.

Preparation of [*closo*-B₁₀H₈-1-IPh-10-(NC₅H₅-4-CN)] (10). Method C starting with 2b[Bu₄N] with increased reaction time (48 h) and amount of PhI(OAc)₂ (1.0 eq added in 3 more portions on the second day): 70.3 mg (48% yield, typically 48-52%) as yellow crystals; $R_f = 0.70$ (CH₂Cl₂ 100%); ¹H NMR (500 MHz, acetone-*d*₆) δ 0.75 – 1.57 (br m, 8H), 7.50 (tm, J = 7.8 Hz, 2H), 7.66 (tt, $J_1 = 7.4$ Hz, $J_2 = 1.1$ Hz, 1H), 8.19 (dd, $J_1 = 8.4$ Hz, $J_2 = 1.1$ Hz, 2H), 8.49 (d, J = 6.8 Hz, 2H), 9.76 (d, J = 6.7 Hz, 2H); ¹³C NMR (126 MHz, acetone-*d*₆) δ 104.8, 116.1, 126.4, 130.1, 131.7, 132.3, 136.1, 149.7; ¹¹B NMR (160 MHz, acetone-*d*₆) δ -22.7 (d, J = 129 Hz, 8B), 5.5 (s, 1B), 22.9 (s, 1B); IR, *v* 2482 (BH), 2240 (CN), 1432, 1235, 998, 840, 750 cm⁻¹; HRMS (ESI, -) *m/z* calcd. for C₁₂H₁₆B₁₀IN₂: 425.1294, found: 425.1291.

NMR tube experiments. To a solution of monoiodonium derivative $4[Bu_4N]$ (5.63 mg, 0.01 mmol) in dry MeCN (0.4 mL) appropriate nucleophile salt $[R_4N]^+X^-$ (1.1 equiv.) was added and the reaction mixtures were stirred at 55 °C. A control sample containing only $4[Bu_4N]$ in

MeCN was also set up under the same conditions to check its stability and to identify chemical shifts coming from decomposition products. The progress of the reactions was monitored using ¹¹B NMR spectroscopy after 3, 6, 22 and 50 h, and the molar percentage of the product in crude mixture was calculated by integration of the signal from the one of two boron atoms located at the apical positions relative to the overall integration of all equatorial boron atom peaks, which was set to 8.00. Then, the resulting value of integrated apical boron signal from product was multiplied by 100% to yield absolute molar percentage of the desired product in the reaction mixture. All boron spectra for crude mixtures were referenced to the corresponding pure products, pure starting material, and decomposition products of the starting material **4[Bu4N]** (formed in MeCN at 55 °C after 40 h). Only reactions with N₃⁻, CN⁻ nucleophiles formed clean product, in which ¹¹B NMR showed two sets of signals – one from product and one from starting material. The reaction with other nucleophiles: X = SCN⁻, OAc⁻, morpholine and pyridine gave complex mixtures of products containing mainly decomposition products of the starting material **4[Bu4N]**. For X = Br⁻, I⁻, only decomposition product.



Figure S1. Spectrum for **4[Bu₄N]** after 16 h at 60 °C in MeCN (referenced to neat BF₃•Et₂O): ¹¹B NMR (160 MHz, MeCN, decoupled) -26.8, -25.4, -25.0, -22.2, -18.8, -1.4, -0.5, 1.9, 8.4, 11.4, 21.7.



Figure S2. ¹H NMR spectrum for A[Et₃HN] recorded in acetone- d_6 at 500 MHz.



Figure S3. ¹¹B{¹H} NMR spectrum for A[Et₃HN] recorded in acetone- d_6 at 160 MHz.



Figure S4. ¹H NMR spectrum for $1a[Bu_4N]$ recorded in acetone- d_6 at 500 MHz.



Figure S5. ¹³C{¹H} NMR spectrum for $1a[Bu_4N]$ recorded in acetone- d_6 at 125 MHz.



Figure S7. ¹H NMR spectrum for $1b[Bu_4N]$, recorded in acetone- d_6 at 500 MHz.





Figure S9. ¹¹B{¹H} NMR spectrum for **1b[Bu₄N]** recorded in acetone- d_6 at 160 MHz.



Figure S10. ¹H NMR spectrum for $1c[Et_4N]$ recorded in acetone- d_6 at 500 MHz.



Figure S11. ¹³C{¹H} NMR spectrum for $1c[Et_4N]$ recorded in acetone- d_6 at 125 MHz.



Figure S12. ¹¹B{¹H} NMR spectrum for $1c[Et_4N]$, recorded in acetone- d_6 at 160 MHz.



Figure S13. ¹H NMR spectrum for $1d[Bu_4N]$ recorded in acetone- d_6 at 500 MHz.



Figure S14. ¹³C{¹H} NMR spectrum for $1d[Bu_4N]$ recorded in acetone- d_6 at 125 MHz.



Figure S15. ¹¹B{¹H} NMR spectrum for $1d[Bu_4N]$ recorded in acetone- d_6 at 160 MHz.



Figure S16. ¹H NMR spectrum for $1e[Bu_4N]$ recorded in acetone- d_6 at 500 MHz.



Figure S17. ¹³C{¹H} NMR spectrum for $1e[Bu_4N]$ recorded in acetone- d_6 at 125 MHz.



Figure S18. ¹¹B{¹H} NMR spectrum for $1e[Bu_4N]$ recorded in acetone- d_6 at 160 MHz.



Figure S19. ¹H NMR spectrum for $1e[Et_4N]$ recorded in acetone- d_6 at 500 MHz.



Figure S21. ¹¹B{¹H} NMR spectrum for $1e[Et_4N]$ recorded in acetone- d_6 at 160 MHz.



Figure S22. ¹H NMR spectrum for $1f[Et_4N]$ recorded in acetone- d_6 at 500 MHz.



Figure S23. ¹³C{¹H} NMR spectrum for $1f[Et_4N]$ recorded in acetone- d_6 at 125 MHz.



Figure S25. ¹H NMR spectrum for $1g[Et_4N]$ recorded in acetone- d_6 at 500 MHz.



Figure S27. ¹¹B{¹H} NMR spectrum for $1g[Et_4N]$ recorded in acetone- d_6 at 160 MHz.



Figure S29. ¹³C $\{^{1}H\}$ NMR spectrum for **1h** recorded in acetone- d_{6} at 125 MHz.

220 210 200 190 180 170 160 150 140 130 120 110 100 90 f1 (ppm)

80 70 60

40 30 20 10 0

50



Figure S31. ¹H NMR spectrum for $1i[Me_4N]$ recorded in acetone- d_6 at 500 MHz.



Figure S33. ¹¹B{¹H} NMR spectrum for $1i[Me_4N]$ recorded in acetone- d_6 at 160 MHz.



Figure S34. ¹H NMR spectrum for 1k recorded in acetone- d_6 at 500 MHz.



Figure S35. ¹³C $\{^{1}H\}$ NMR spectrum for **1k** recorded in acetone- d_{6} at 125 MHz.



Figure S36. ¹¹B $\{^{1}H\}$ NMR spectrum for **1k** recorded in acetone- d_{6} at 160 MHz.



Figure S37. ¹H NMR spectrum for $2b[Bu_4N]$ recorded in acetone- d_6 at 500 MHz.



Figure S38. ¹³C{¹H} NMR spectrum for $2b[Bu_4N]$ recorded in acetone- d_6 at 125 MHz.



Figure S39. ¹¹B{¹H} NMR spectrum for $2b[Bu_4N]$ recorded in acetone- d_6 at 160 MHz.



Figure S40. ¹H NMR spectrum for $2l[Bu_4N]$ recorded in acetone- d_6 at 500 MHz.



Figure S41. ¹³C{¹H} NMR spectrum for $2l[Bu_4N]$ recorded in acetone- d_6 at 125 MHz.



Figure S42. ¹¹B{¹H} NMR spectrum for $2l[Bu_4N]$ recorded in acetone- d_6 at 160 MHz.



Figure S43. ¹H NMR spectrum for 2m[Bu₄N] recorded in acetone-*d*₆ at 500 MHz.



Figure S44. ¹³C{¹H} NMR spectrum for $2m[Bu_4N]$ recorded in acetone- d_6 at 125 MHz.



Figure S45. ¹¹B{¹H} NMR spectrum for $2m[Bu_4N]$ recorded in acetone- d_6 at 160 MHz.



Figure S46. ¹H NMR spectrum for 2n[Bu₄N] recorded in acetone-*d*₆ at 500 MHz.



Figure S47. ¹³C{¹H} NMR spectrum for $2n[Bu_4N]$ recorded in acetone- d_6 at 125 MHz.



Figure S48. ¹¹B{¹H} NMR spectrum for $2n[Bu_4N]$ recorded in acetone- d_6 at 160 MHz.



Figure S49. ¹H NMR spectrum for $3[Bu_4N]$ recorded in acetone- d_6 at 500 MHz.



Figure S51. ¹¹B{¹H} NMR spectrum for $3[Bu_4N]$ recorded in acetone- d_6 at 160 MHz.





Figure S53. ¹¹B{¹H} NMR spectrum of crude **3**[**H**] recorded in acetone- d_6 at 160 MHz.



Figure S54. ¹H NMR spectrum for $4[Bu_4N]$ recorded in acetone- d_6 at 500 MHz.



Figure S55. ¹³C{¹H} NMR spectrum for $4[Bu_4N]$ recorded in acetone- d_6 at 125 MHz.


Figure S56. ¹¹B{¹H} NMR spectrum for $4[Bu_4N]$ recorded in acetone- d_6 at 160 MHz.



Figure S57. ¹H NMR spectrum for 5b[Bu₄N] recorded in acetone-*d*₆ at 500 MHz.



220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 f1 (ppm)

Figure S58. ¹³C{¹H} NMR spectrum for **5b[Bu₄N]** recorded in acetone- d_6 at 125 MHz.



Figure S59. ¹¹B{¹H} NMR spectrum for **5b**[**Bu**₄**N**] recorded in acetone- d_6 at 160 MHz.



Figure S61. ¹³C{¹H} NMR spectrum for **5d[Bu₄N]** recorded in acetone- d_6 at 125 MHz.



Figure S63. ¹H NMR spectrum for $5e[Bu_4N]$ recorded in acetone- d_6 at 500 MHz.



Figure S64. ¹³C{¹H} NMR spectrum for $5e[Bu_4N]$ recorded in acetone- d_6 at 125 MHz.



Figure S65. ¹¹B{¹H} NMR spectrum for $5e[Bu_4N]$ recorded in acetone- d_6 at 160 MHz.



Figure S66. ¹H NMR spectrum for 6b[Bu₄N] recorded in acetone-*d*₆ at 500 MHz.



Figure S67. ¹³C{¹H} NMR spectrum for $6b[Bu_4N]$ recorded in acetone- d_6 at 125 MHz.



Figure S68. ¹¹B{¹H} NMR spectrum for $6b[Bu_4N]$ recorded in acetone- d_6 at 160 MHz.



Figure S69. ¹H NMR spectrum for $6c[Et_4N]$ recorded in acetone- d_6 at 500 MHz.



Figure S70. ¹³C{¹H} NMR spectrum for $6c[Et_4N]$ recorded in acetone- d_6 at 125 MHz.



Figure S71. ¹¹B{¹H} NMR spectrum for $6c[Et_4N]$ recorded in acetone- d_6 at 160 MHz.



Figure S72. ¹H NMR spectrum for $6d[Bu_4N]$ recorded in acetone- d_6 at 500 MHz.



Figure S73. ¹³C{¹H} NMR spectrum for $6d[Bu_4N]$ recorded in acetone- d_6 at 125 MHz.



Figure S75. ¹H NMR spectrum for $6e[Bu_4N]$ recorded in acetone- d_6 at 500 MHz.



Figure S77. ¹¹B{¹H} NMR spectrum for $6e[Bu_4N]$ recorded in acetone- d_6 at 160 MHz.



Figure S78. ¹H NMR spectrum for $6f[Et_4N]$ recorded in acetone- d_6 at 500 MHz.



Figure S79. ¹³C{¹H} NMR spectrum for $6f[Et_4N]$ recorded in acetone- d_6 at 125 MHz.



Figure S80. ¹¹B{¹H} NMR spectrum for **6f[Et₄N]** recorded in acetone- d_6 at 160 MHz.



Figure S81. ¹H NMR spectrum for $6g[Et_4N]$ recorded in acetone- d_6 at 500 MHz.



Figure S83. ¹¹B{¹H} NMR spectrum for $6g[Et_4N]$ recorded in acetone- d_6 at 160 MHz.



Figure S85. ¹³C $\{^{1}H\}$ NMR spectrum for 6k recorded in acetone- d_{6} at 125 MHz.



Figure S87. ¹H NMR spectrum for 7 recorded in acetone- d_6 at 500 MHz.



Figure S88. ¹³C{¹H} NMR spectrum for 7 recorded in acetone- d_6 at 125 MHz.



Figure S89. ¹¹B $\{^{1}H\}$ NMR spectrum for 7 recorded in acetone- d_{6} at 160 MHz.



Figure S90. ¹H NMR spectrum for 8 recorded in acetone- d_6 at 500 MHz.



Figure S91. ¹³C{¹H} NMR spectrum for **8** recorded in acetone- d_6 at 125 MHz.



Figure S93. ¹H NMR spectrum for 9 recorded in acetone- d_6 at 500 MHz.



Figure S94. ¹³C{¹H} NMR spectrum for 9 recorded in acetone- d_6 at 125 MHz.



Figure S95. ¹¹B{¹H} NMR spectrum for **9** recorded in acetone- d_6 at 160 MHz.



Figure S96. ¹H NMR spectrum for 10 recorded in acetone- d_6 at 500 MHz.



Figure S97. ¹³C $\{^{1}H\}$ NMR spectrum for **10** recorded in acetone- d_{6} at 125 MHz.



Figure S98. ¹¹B{¹H} NMR spectrum for **10** recorded in acetone- d_6 at 160 MHz.

3. XRD collection and refinement details, and additional information

Single-crystal X-ray diffraction measurements for $1d[Bu_4N]$, $1g[Et_4N]$, $1e[Et_4N]$, $1c[Et_4N]$, 1k and $1f[Et_4N]$ were performed with a Rigaku XtalLAB SuperNova Pilatus 200K diffractometer whereas data for $1b[Et_4N]$ and 1h were collected using Rigaku XtaLAB Synergy Dualflex Pilatus 300K diffractometer. The measurements were conducted at low temperature (100.0(1) K) using the Cu K_{α} radiation (λ =1.54184 Å). The data were integrated using CrysAlisPro program.⁵ Intensities for absorption were corrected using SCALE3 ABSPACK scaling algorithm implemented in CrysAlisPro program.⁵ All structures were solved with the ShelXT⁶ structure solution program using Intrinsic Phasing and refined by the full-matrix leastsquares minimization on F^2 with the ShelXL⁷ refinement package. All non-hydrogen atoms were refined anisotropically. C–H and B–H hydrogens were generated geometrically using the HFIX command as in ShelXL. Hydrogen atoms were refined isotropically using a riding model.

CCDC	1b[Et4N] 1995610	1c[Et4N] 1995611	1d[Bu ₄ N] 1995612	1e[Et4N] 1995613
Empirical formula	$C_{14}H_{33}B_{10}N_3$	$C_{15}H_{36}B_{10}N_2O_2$	$C_{21}H_{49}B10N_5$	$C_{13}H_{33}B_{10}IN_2$
Formula weight	351.53	384.56	479.75	452.41
Crystal system	Triclinic	Monoclinic	Monoclinic	Monoclinic
Space group	$P\overline{1}$	$P2_{1}/c$	$P2_{1}/c$	$P2_{1}/c$
a/Å	9.6252(3)	13.3761(3)	9.97650(10)	8.64134(14)
<i>b</i> /Å	9.6626(3)	11.0972(2)	17.6586(2)	16.5952(3)
$c/\text{\AA}$	12.8108(4)	15.3153(3)	16.9969(2)	16.9899(3)
a/°	80.569(2)	90	90	90
$\beta/^{\circ}$	74.408(2)	92.873(2)	92.8600(10)	95.5899(16)
$\gamma/^{\circ}$	70.856(2)	90	90	90
Volume/Å ³	1080.39(5)	2270.50(8)	2990.63(6)	2424.85(7)
Z	2	4	4	4
Goodness-of-fit	1.039	1.027	1.043	1.037
Final R indexes	$R_1 = 0.0469,$	$R_1 = 0.0571,$	$R_1 = 0.0469,$	$R_1 = 0.0406,$
[<i>I</i> >=2σ (<i>I</i>)]	$wR_2 = 0.1269$	$wR_2 = 0.1464$	$wR_2 = 0.1269$	$wR_2 = 0.1054$
Final R indexes	$R_1 = 0.0625,$	$R_1 = 0.0818$,	$R_1 = 0.0532,$	$R_1 = 0.0469,$
[all data]	$wR_2 = 0.1559$	$wR_2 = 0.1623$	$wR_2 = 0.1315$	$wR_2 = 0.1090$
CCDC	1f[Et4N] 1995614	1g[Et₄N] 1995615	1h 1995616	1k 1995617
Empirical formula	$C_{14}H_{33}B_{10}N_3S$	$C_{13}H_{33}B_{10}BrN_2$	$C_{10}H_{18}B_{10}N_2$	$C_{9}H_{22}B_{10}N_{2}O$
Formula weight	383.59	405.42	274.36	282.38
Crystal system	Orthorhombic	Triclinic	Monoclinic	Monoclinic
Space group	P2 ₁ 2 ₁ 2 ₁	$P\overline{1}$	C2/c	$P2_1/c$
a/Å	11.6101(2)	9.1777(3)	19.4217(15)	14.9986(2)
b/Å	15.6028(3)	10.0767(3)	6.9015(2)	7.9535(1)
$c/\text{\AA}$	24.7694(2)	12.8183(4)	14.9080(11)	13.6820(2)
$\alpha/^{\circ}$	90	80.275(3)	90	90
$\beta/^{\circ}$	90	76.290(3)	131.094(12)	98.618(1)
γ/°	90	69.530(3)	90	90
Volume/Å ³	4486.9(1)	1074.12(6)	1505.9(3)	1613.72(4)
Ζ	8	2	4	4
Goodness-of-fit	1.042	1.077	1.107	1.074
Final R indexes	$R_1 = 0.0560,$	$R_1 = 0.0278,$	$R_1 = 0.0379,$	$R_1 = 0.0469,$
[<i>I</i> >=2σ (<i>I</i>)]	$wR_2 = 0.1554$	$wR_2 = 0.0718$	$wR_2 = 0.1148$	$wR_2 = 0.1308$
Final <i>R</i> indexes [all data]	$R_1 = 0.0595,$ w $R_2 = 0.1595$	$R_1 = 0.0305,$ w $R_2 = 0.0767$	$R_1 = 0.0399,$ w $R_2 = 0.1170$	$R_1 = 0.0504,$ w $R_2 = 0.1338$

 Table S1. Crystallographic data for derivatives 1.

Two butyl chains of the counterion in $1d[Bu_4N]$ were disordered over two orientations. Occupancies of respective chains were refined independently, which resulted in occupancy ratios of 0.637(11):0.363(11) and 0.760(5):0.240(5), respectively. Similarly, in $1c[Et_4N]$ two ethyl groups of $[Et_4N]^+$ are positionally disordered over two sites. The final refinement resulted in occupancy ratio of 0.853(6):0.147(3). In the crystal system of **1f**[Et_4N], the thiocyanato derivative **1f** exhibits positional disorder of the SCN group in both unique molecules with occupancy ratios of 0.501(7):0.499(7) and 0.79(4):0.21(4), respectively. Moreover, the ethyl groups in 2 unique molecules of $[Et_4N]^+$ are also positionally disordered. Respective occupancy ratios are 0.660(5):0.340(5) and 0.643(6):0.357(6). All disordered structures were refined using the PART command. Atomic displacement parameters were constrained to be equal using SIMU and RIGU instructions. In **1c**[Et_4N] thermal parameters for two atoms were additionally constrained using the EADP instruction. Moreover, in **1c**[Et_4N] geometrical restraint for interatomic distances within one disordered group was applied using the SADI command.

In $1e[Et_4N]$, the solvent molecule positioned about the inversion center was found to be highly disordered. Therefore the best approach to handle this electron density was the SQUEEZE routine of PLATON.⁸ The squeezed void volume was 312 Å³ and the procedure resulted 87 electrons per unit cell confirming the presence of the acetonitrile molecule. The crystal data and structure refinement descriptors for all structures are listed in Table S1.

Files CCDC 1995610-1995617 contain supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via https://www.ccdc.cam.ac.uk/structures/



Figure S99. Infinite molecular double chains of $1b[Et_4N]$ and $1g[Et_4N]$ running along [100] direction. Short intermolecular contacts are depicted as dotted lines B^{...}C (green) and C-H^{...}B (blue).

Analysis of experimental B(1)^{\dots}B(10) distance in series 1 in terms of the Hammett substituent parameter⁹ σ_p exhibits a non-linear correlation shown in Figure S100. For the pyridinium and morpholinium substituents a value of 0.82 for the ⁺NMe₃ was used. For the OAc group a new derived σ_p value of 0.00 was used (see section 5 below). The data point for the CN group is clearly outside the trend.



Figure S100. A correlation of the experimental $B(1)^{\dots}B(10)$ distance in series 1 with the Hammett substituent parameter σ_p .

4. Electronic spectroscopy

a) Solution spectra in MeCN

Electronic absorption spectra were recorded using an Olis 14F UV/Vis/NIR Spectrophotometer. Solutions in spectrophotometric grade MeCN prepared from 1.00-2.00 mg of the analyte in a 25 mL volumetric flask were diluted using volumetric pipets in 10 mL volumetric flasks. Absorbance was measured between 210 to 710 nm for at least three concentrations in a range of 0.15 to 1.5 (M cm)⁻¹. The Beer's Law plot slope was used to determine log ε with typical r^2 of >0.99 for each compound.

Fluorescence spectra were recorded for diluted MeCN solutions using a Hitachi F-4500 Fluorescence Spectrophotometer. The excitation wavelength was set to the absorbance λ_{max} and λ_{em} was scanned from λ_{max} +50 nm to 900 nm. Relative intensity and λ_{em} of fluorescence were somewhat concentration-dependent in weakly fluorescent compounds.

Results are shown in Figures S101–S115.





Figure S101. Clockwise: electronic absorption spectra for $1a[Bu_4N]$ (X=H) in MeCN for 4 concentrations, determination of molar extinction coefficient ε at $\lambda = 365$ nm (best fit function: $\varepsilon = 7093(12) \times \text{conc}$, $r^2 = 0.9999$), molar extinction and normalized fluorescence spectra with indicated excitation wavelength and Stokes shift.



Figure S102. Clockwise: electronic absorption spectra for $1b[Et_4N]$ (X=CN) in MeCN for 3 concentrations, determination of molar extinction coefficient ε at $\lambda = 339.0$ nm (best fit function: $\varepsilon = 7006(114) \times \text{conc}$, $r^2 = 0.9982$), molar extinction and normalized fluorescence spectra with indicated excitation wavelength and Stokes shift.



Figure S103. Clockwise: electronic absorption spectra for $1c[Et_4N]$ (X = OAc) in MeCN for 3 concentrations, determination of molar extinction coefficient ε at $\lambda = 368.5$ nm (best fit function: $\varepsilon = 7574(33) \times \text{conc}$, $r^2 = 0.9999$), molar extinction and normalized fluorescence spectra with indicated excitation wavelength and Stokes shift.





Figure S104. Clockwise: electronic absorption spectra for $1d[Bu_4N]$ (X = N₃) in MeCN for 3 concentrations, determination of molar extinction coefficient ε at λ = 365.0 nm (best fit function: ε = 7924(9)×conc, r^2 = 0.9999), molar extinction spectrum with indicated excitation wavelength and Stokes shift.



Figure S105. Clockwise: electronic absorption spectra for $1e[Et_4N]$ (X = I) in MeCN for 3 concentrations, determination of molar extinction coefficient ε at $\lambda = 357.0$ nm (best fit function: $\varepsilon = 8355 \times \text{conc}$, $r^2 = 0.9999$), molar extinction spectrum. No fluorescence was observed.



Figure S106. Clockwise: electronic absorption spectra for $1f[Et_4N]$ (X = SCN) in MeCN for 3 concentrations, determination of molar extinction coefficient ε at λ = 344.5 nm (best fit function: ε = 6415(48)×conc, r^2 = 0.9997), molar extinction spectrum and normalized fluorescence spectra with indicated excitation wavelength and Stokes shift.





Figure S107. Clockwise: electronic absorption spectra for $1g[Et_4N]$ (X = Br) in MeCN for 3 concentrations, determination of molar extinction coefficient ε at $\lambda = 358.5$ nm (best fit function: $\varepsilon = 8124(7) \times \text{conc}$, $r^2 = 0.9999$), molar extinction spectrum. No fluorescence was observed.



Figure S108. Clockwise: electronic absorption spectra for **1h** (X = ⁺Pyr) in MeCN for 3 concentrations, determination of molar extinction coefficient ε at λ = 335 nm (best fit function: ε = 15917(293)×conc, r^2 = 0.995), molar extinction and normalized fluorescence spectra with indicated excitation wavelength and Stokes shift.



Figure S109. Clockwise: electronic absorption spectra for $1i[Me_4N]$ (X = OEt) in MeCN for 3 concentrations, determination of molar extinction coefficient ε at λ = 393.5 nm (best fit function: ε = 6995(30)×conc, r^2 = 0.999), and molar extinction.





Figure S110. Clockwise: electronic absorption spectra for 1k (X = ⁺MorphH) in MeCN for 3 concentrations, determination of molar extinction coefficient ε at λ = 329.0 nm (best fit function: ε = 6945(36)×conc, r^2 = 0.9998), molar extinction and normalized fluorescence spectra with indicated excitation wavelength and Stokes shift.

A solution of **1k** was degassed with argon bubbled through for 10 minutes. A few crystals of $[Me_4N]^+OH^-\bullet 5H_2O$ were added. The flask was shaken and a golden yellow color appeared. The UV spectrum was measured immediately. The color of the remaining solution gradually turned clear over 30 min.



Figure S111. Electronic absorption spectrum for 1j (X = Morph) in MeCN obtained by *in situ* deprotonation of 1k (see the text).





Figure S112. Clockwise: electronic absorption spectra for $2b[Bu_4N]$ (Y=CN) in MeCN for 3 concentrations, determination of molar extinction coefficient ε at $\lambda = 452$ nm (best fit function: $\varepsilon = 9471(42) \times \text{conc}$, $r^2 = 0.9999$), and molar extinction spectrum. No fluorescence was observed.



Figure S113. Clockwise: electronic absorption spectra for $2l[Bu_4N]$ (Y = COOEt) in MeCN for 3 concentrations, determination of molar extinction coefficient ε at $\lambda = 431.0$ nm (best fit function: $\varepsilon = 8928(13) \times \text{conc}$, $r^2 = 0.9999$), and molar extinction spectrum. No fluorescence was observed.



Figure S114. Clockwise: electronic absorption spectra for $2m[Bu_4N]$ (Y = Me) in MeCN for 3 concentrations, determination of molar extinction coefficient ε at $\lambda = 357.5$ nm (best fit function: $\varepsilon = 8518(9) \times \text{conc}$, $r^2 = 0.9999$), molar extinction and normalized fluorescence spectra with indicate excitation wavelength and Stokes shift.





Figure S115. Clockwise: electronic absorption spectra for $2n[Bu_4N]$ (Y = OMe) in MeCN for 3 concentrations, determination of molar extinction coefficient ε at $\lambda = 339.5$ nm (best fit function: $\varepsilon = 6207(8) \times \text{conc}$, $r^2 = 0.9999$), molar extinction and normalized fluorescence spectra.



Figure S116. Clockwise: electronic absorption spectra for **3**[**Bu**₄**N**] (X = EtO, Y = CN) in MeCN for 3 concentrations, determination of molar extinction coefficient ε at $\lambda = 501.5$ nm (best fit function: $\varepsilon = 8772(8) \times \text{conc}$, $r^2 = 0.9999$) and molar extinction. No fluorescence was observed.

b) Solvent effects on absorption and emission of 1a and 3.

Solvent effects on absorption and emission spectra were investigated in THF, ethyl acetate, acetone, CH₂Cl₂, MeCN, DMF, DMSO and formamide for **1a[Bu₄N]**. Spectra were
obtained as described above, taking into account the UV cutoff for each solvent. Solutions in the range of $1-5 \times 10^{-5}$ M were used for UV and fluorescence measurements and scales normalized for comparison. Compound **1a**[**Bu**₄**N**] was sparingly soluble in toluene and cyclohexanone. Results are shown in Figure S117 and summarized in Table S2.





Figure S117. Normalized absorption and emission spectra for $1a[Bu_4N]$ in a selection of solvents. ΔE stands for the Stokes shift.

Solvent	$E_T 30^{a}$ /kcal mol ⁻¹	Absorption /nm (eV)	Emission /nm (eV)	Stokes shift /eV	DFT excitation ^b /nm (eV)
MeCN	45.6	365.0 (3.397)	568.0 (2.183)	1.214	312.5 (3.968)
DMSO	45.1	371.0 (3.342)	563.0 (2.202)	1.140	311.7 (3.978)
CH_2Cl_2	40.7	374.5 (3.311)	560.0 (2.214)	1.097	328.6 (3.773)
DMF	41.8	381.5 (3.250)	558.5 (2.220)	1.030	312.8 (3.964)
Acetone	42.3	388.5 (3.192)	579.5 (2.140)	1.052	316.4 (3.918)
EtOAc	38.0	393.0 (3.155)	573.5 (2.162)	0.993	338.5 (3.663)
c-hexanone	40.1	_	_	_	319.8 (3.877)
THF	37.5	401.5 (3.088)	582.0 (2.131)	0.957	332.7 (3.726)
toluene	33.9	_	_	_	386.9 (3.205)
formamide	55.9	338.5 (3.663)	542.0 (2.288)	1.375	309.6 (4.004)

Table S2. Summary of the solvatochromic data for 1a[Bu₄N].

^{*a*} From ref.¹⁰. ^{*b*} Calculated at CAM-B3LYP/Def2TZVP// B3LYP/Def2TZVP level of theory in dielectric medium requested with the SCRF(solvent=*name*) keyword.

The absorption spectrum of $3[Bu_4N]$ was recorded in two solvents of most extreme polarity in Table S2 and results are shown in Figure S118.



Figure S118. Normalized absorption spectra for 3[Bu₄N] in three solvents.

c) Solid-state emission

A borosilicate glass capillary was filled with polycrystalline sample of **1** or **2** and placed in the fluorescence spectrometer. The sample was excited at the wavelength of maximum absorption in MeCN solutions. The normalized emission spectra for nine luminescent derivatives in series **1** are shown in Figure S119 and for two in series **2** in Figure S120.

No emission was observed for $1d[Bu_4N]$ (X = N₃), $2b[Bu_4N]$ (Y = CN), $2l[Bu_4N]$ (Y = COOEt), and $3[Bu_4N]$.



Figure S119. Normalized solid-state emission for derivatives in series 1.



Figure S120. Normalized solid-state emission for derivatives for 2m[Bu₄N] and 2n[Bu₄N].

d) Aggregation induced emission (AIE) of 1e[Et₄N]

Emission spectra of iodide $1e[Et_4N]$ dispersed in H₂O (1% and 10% of MeCN solution in H₂O) were measured and compared to solid-state emission in Figure S121.



Figure S121. AIE (MeCN in H₂O) and solid-state spectra for 1e[Et₄N].

5. Correlation analysis of ¹H NMR data for PhX.

To verify σ_p parameters for some substituents and to derive values for some other substituents, a series of 20 monosubstituted derivatives of benzene, Ph–X, were investigated by NMR spectroscopy in acetone- d_6 and results are shown in Tables S3 and S4. The ¹H NMR chemical shifts were assigned on the basis of relative intensities and coupling constant patterns. The effect of substituent X on ¹H NMR resonance at the C(4) position was analyzed in terms of Hammett σ_p parameters⁹ as shown in Figure S122.

Ph-X	ortho-H (d/dd, 2H)	<i>meta</i> -H (t/dd, 2H)	<i>para-</i> H (t/tt, 1H)	Other(s)
Н	7.355	7.355	7.355	-
N_3 ^{<i>a</i>}	7.090	7.416	7.192	_
COMe	7.992	7.513	7.615	2.582
OAc	7.114	7.399	7.237	2.250
Br	7.554	7.332	7.381	_
CF ₃	7.722	7.615	7.684	_
CN	7.780	7.599	7.726	_
COOMe	8.014	7.511	7.633	3.884
F	7.414	7.126	7.195	_
Ι	7.756	7.192	7.408	_
Me	7.171	7.236	7.134	2.313
NMe ₂	6.735	7.172	6.638	2.911
NO ₂	8.256	7.691	7.844	_
OMe	6.921	7.277	6.911	3.781
SCN ^b	7.665	7.554	7.514	_
Ph	7.653	7.462	7.360	_
С≡СН	7.494	7.397	7.381	3.644
CH=CH ₂	7.463	7.337	7.262	6.756, 5.806, 5.228
N-morpholinyl	6.948	7.229	6.807	3.116, 3.768
	7.939	7.577 (overlapped	7.593 (overlapped	2.366 (CH ₃ , tosyl), 3.750 (CH ₂), 4.190 (CH ₂),
[CH ₃ C ₆ H ₄ SO ₃] ⁻ C		with <i>p</i> -H)	with <i>m</i> -H)	5.674 (very broad s) 7.261 (tosyl) and 7.734 (tosyl)

Table S3. ¹H NMR chemical shifts for mono-substituted benzene (500 MHz, acetone- $d_6 \delta = 2.04$).

^{*a*} Prepared in 56% yield according to ref¹¹. ^{*b*} Prepared in 57% yield according to ref¹². ^{*c*} Prepared by mixing equimolar amounts of *N*-phenylmorpholine and TsOH•H₂O.

Н	129.13;
N ₃ ^{<i>a</i>}	119.83, 125.89, 130.79, 140.81;
COMe	26.65, 128.92, 129.32, 133.65, 138.07, 197.84;
OAc	20.95, 122.59, 126.37, 130.11, 151.96, 169.60;
Br	122.83, 127.88, 131.08, 132.14;
CF ₃	125.44, 125.95, 130.00, 131.00, 133.16;
CN	112.96, 119.23, 130.03, 132.75, 133.62;
COOMe	52.27, 129.29, 130.11, 133.73, 167.14;
F	115.95, 125.09, 131.08, 163.74;
Ι	94.70, 128.28, 131.12, 138.05;
Me	21.47, 126.12, 129.03, 129.76, 138.47;
NMe ₂	40.59, 113.31, 117.10, 129.66, 151.64;
NO ₂	124.01, 130.36, 135.63, 149.00;
OMe	55.32, 114.65, 121.25, 130.22, 160.66;
SCN ^b	111.09, 125.63, 130.54, 130.94, 131.33
Ph	127.72, 128.14, 129.69, 141.84;
С≡СН	79.07, 84.14, 123.15, 129.31, 129.62, 132.68
CH=CH ₂	114.06, 126.96, 128.61, 129.33, 137.80, 138.40
N-morpholinyl	49.93, 67.39, 116.27, 120.23, 129.79, 152.52

Table S4. ¹³C NMR chemical shifts for mono-substituted benzene (126 MHz, acetone- $d_6 \delta = 29.84$).

Ph–X

^{*a*} Prepared in 56% yield according to ref¹¹. ^{*b*} Prepared in 57% yield according to ref¹². ^{*c*} Prepared by mixing equimolar amounts of *N*-phenylmorpholine and TsOH•H₂O.



Figure S122. Correlation of ¹H NMR for C(4)–H in a series of PhX with substituent $\sigma_{p(X)}$ parameters (17 datapoints). Best fit line: $\delta_{C4-H} = 7.24(2)+0.745(49) \times \sigma_{p(X)}$; $r^2 = 0.94$.

Analysis of the experimental data in Table S3 for resonance of the C(4)–H nucleus *vs* Hammett $\sigma_{p(X)}$ parameter gave a linear correlation (Figure S122), from which σ_p parameter for the OAc group was calculated to be 0.00(2). This value is significantly different from 0.31 listed in the original publication.¹³

Using correlation in Figure S122 and ¹H NMR data in Table S3 the following values are derived:

<i>N</i> -morpholinyl:	-0.58
AcO:	0.00
N-morpholinium	0.48

6. Computational details

General. Quantum-mechanical calculations were carried out using Gaussian 09 suite of programs. Geometry optimizations were undertaken using the B3LYP^{14, 15} functional with Karlsruhe triple- ζ polarization Def2TZVP basis set^{16, 17} and tight convergence limits with appropriate symmetry constraints. All calculations were performed in PhCl dielectric medium (arbitrarily chosen) with the PCM model¹⁸ requested with SCRF(Solvent= C6H5Cl) keyword, since it was demonstrated¹⁹ that low dielectric medium is important for obtaining accurate geometry of zwitterions, such as 1–3. The ground state nature of stationary points for the obtained equilibrium geometry was confirmed with vibrational frequency calculations.

a) Geometry optimization and method selection

The calculated molecular geometry for series **1** was compared with experimental values. Results shown in Figure S123 demonstrate that both methods B3LYP/TZVP and B3LYP/Def2TZVP reproduce the B(1)^mB(10) and also key B(1)^mX distances accurately. The slope is the latter method is nearly unity and the small uncertainty (1.009±0.042) justifies setting it at unity for the correlation analysis. Removing the data point for dipyridinium derivative **1h** improves all correlations, *e.g.* to $r^2 = 0.993$ for the B3LYP/Def2TZVP method.



Figure S123. Experimental (XRD) versus theoretical B(1)^{...}B(10) distance obtained with four methods for A and series **1.** Best fit lines for B3LYP/Def2TZVP in PhCl medium (red): $d_{\text{Def2TZVP}} = -0.012(1) + d_{\text{XRD}}$, $r^2 = 0.986$; for B3LYP/TZVP in PhCl medium (blue): $d_{\text{TZVP}} = -0.17(13) + 1.045(37) \times d_{\text{XRD}}$, $r^2 = 0.990$; for B3LYP/M062x in PhCl (black): $d_{\text{M062x}} = -0.44(22) + 1.12(6) \times d_{\text{XRD}}$, $r^2 = 0.978$; for B3LYP/M062x in vacuum (green): $d_{\text{M062x}_vac} = -1.32(42) + 1.36(11) \times d_{\text{XRD}}$, $r^2 = 0.946$.

The calculated Pyr–B(1) distances in a series of 9 derivatives **1** fall in a narrow range of the values with the average value closest to the experimental average (1.527(3) Å) found for the B3LYP/Def2TZVP results in PhCl dielectric medium (Figure S124).



Figure S124. Experimental (XRD) versus theoretical B(1)–Pyr distance obtained with four methods with indicated the average value.

Correlation of experimental and DFT calculated other distances such as B–X (C, O, N, Br, I, S), C≡N, C=O, N–N and N≡N is shown in Figure S125. The S–CN and SC≡N distances

were not used in the correlation, because of the disorder of the SCN group and hence a relatively large error.



Figure S125. Experimental (XRD) versus theoretical miscellaneous distances obtained with four methods. Best fit lines for B3LYP/Def2TZVP in PhCl medium (red): $d_{\text{Def2TZVP}} = -0.023(16) + 1.02(1) \times d_{\text{XRD}}$, $r^2 = 0.999$; for B3LYP/TZVP in PhCl medium (blue): $d_{\text{TZVP}} = -0.034(17) + 1.028(11) \times d_{\text{XRD}}$, $r^2 = 0.999$; for B3LYP/M062x in PhCl (black): $d_{\text{M062x}} = -0.014(20) + 1.01(1) \times d_{\text{XRD}}$, $r^2 = 0.998$; for B3LYP/M062x in vacuum (green): $d_{\text{M062x},\text{vac}} = -0.01(2) + 1.004(12) \times d_{\text{XRD}}$, $r^2 = 0.999$.

b) Electronic excitation energies

Excitation energies for compounds in series **1** and **2** and derivative **3** were obtained using the TD-DFT²⁰ method at CAM-B3LYP/Def2TZVP// B3LYP/Def2TZVP level of theory using TD(NStates=20) SCF=tight in MeCN dielectric medium using the PCM model¹⁸ requested with the SCRF(Solvent= CH3CN) keyword.

The lowest excitation energy, classified as $\pi \rightarrow \pi^*$ intramolecular CT excitation, and also the energies of the involved frontier MOs are listed in Table S5.

compound	π→π*	HOMO π	LUMO, π*
	$HOMO \rightarrow LUMO$	/eV	
19 H	$\frac{7 \text{nm}(f)}{312.5(0.291)}$	-7.038	-0.871
1a, 11	512.5 (0.251)	-7.050	-0.071
1b, CN	295.7 (0.334)	-7.346	-0.948
1c, OAc	316.1 (0.278)	-6.967	-0.884
1d , N ₃	322.6 (0.328)	-6.757	-0.900
1e, I	305.3 (0.337)	-7.056	-0.919
1f, SCN	306.6 (0.324)	-7.040	-0.930
1g , Br	306.8 (0.314)	-7.088	-0.912
1h , Pyr	298.8 (0.550)	-7.474	-1.072
1i, OEt	345.2 (0.293)	-6.469	-0.852
1j, Morph	370.0 (0.279)	-6.000	-0.853
1k, MorphH	287.4 (0.323)	-7.567	-0.983
2b , Y=CN	390.3 (0.417)	-7.092	-1.912
2l, Y=COOEt	368.5 (0.403)	-7.066	-1.690
2m , Y=Me	302.9 (0.336)	-7.005	-0.719
2n, Y=OMe	288.4 (0.370)	-6.969	-0.445
2 , Y=OAc	312.8 (0.357)	-7.037	-0.915
2 , Y=CH ₂ CN	319.2 (0.342)	-7.051	-0.993
3	448.8 (0.436)	-6.499	-1.902

Table S5. Calculated electronic transition energies and oscillator strength for the lowest energy transition and energies of the FMOs involved in these transitions.^a

^a CAM-B3LYP/Def2TZVP // B3LYP/Def2TZVP method in MeCN dielectric medium.

Solvent effects on excitation energies of **1a** and energy level of the involved FMOs were calculated using the same protocol and changing solvent in the SCRF(solvent=*name*) keyword. Results are shown in Table S6.

TD-DFT calculated solvent effects on the $\pi \rightarrow \pi^*$ excitation energy in **1a** were correlated with the E_r30 solvent parameters and results are graphically shown in Figure S126. Solvents effects on the FMO energy levels are shown in Figure S127. Data show much stronger solvent impact of the solvent polarity on the HOMO level than on the LUMO.

ε	$E_{T}30^{b}$	π→ π*	HOMO, π	LUMO, π*
	/kcal mol ⁻¹	HOMO→ LUMO	/eV	/eV
		/nm		
2.2706	34.300	390.46	-5.3588	-0.065852
2.3741	33.900	386.88	-5.4333	-0.10776
8.9300	40.700	328.62	-6.6815	-0.72546
7.4257	37.500	332.73	-6.5866	-0.68437
15.619	40.100	319.84	-6.8840	-0.80982
20.493	42.300	316.44	-6.9488	-0.83594
5.9867	38.000	338.52	-6.4521	-0.62423
35.688	45.600	312.50	-7.0377	-0.87077
37.219	41.800	312.81	-7.0429	-0.87295
46.826	45.100	311.71	-7.0666	-0.88193
108.94	55.900	309.62	-7.1191	-0.90206
	 ε 2.2706 2.3741 8.9300 7.4257 15.619 20.493 5.9867 35.688 37.219 46.826 108.94 	ε E.30 ^b /kcal mol ⁻¹ 2.2706 34.300 2.3741 33.900 8.9300 40.700 7.4257 37.500 15.619 40.100 20.493 42.300 5.9867 38.000 35.688 45.600 37.219 41.800 46.826 45.100 108.94 55.900	ε E.30 b $\pi \rightarrow \pi^{*}$ /kcal mol ⁻¹ HOMO \rightarrow LUMO /nm2.270634.300390.462.374133.900386.888.930040.700328.627.425737.500332.7315.61940.100319.8420.49342.300316.445.986738.000338.5235.68845.600312.5037.21941.800312.8146.82645.100311.71108.9455.900309.62	ε E.30 b $\pi \rightarrow \pi^{*}$ HOMO, π /kcal mol ⁻¹ HOMO \rightarrow LUMO/eV 2.2706 34.300390.46-5.35882.374133.900386.88-5.43338.930040.700328.62-6.68157.425737.500332.73-6.586615.61940.100319.84-6.884020.49342.300316.44-6.94885.986738.000338.52-6.452135.68845.600312.50-7.037737.21941.800312.81-7.042946.82645.100311.71-7.0666108.9455.900309.62-7.1191

Table S6. Calculated lowest energy electronic transitions for **1a** and energies of the FMOs involved.^a

^{*a*} CAM-B3LYP/Def2TZVP // B3LYP/Def2TZVP method. ^{*b*} Ref¹⁰.



Figure S126. Calculated lowest energy excitations (CAM-B3LYP/Def2TZVP // B3LYP/Def2TZVP method in MeCN dielectric medium) versus the $E_T 30$ parameter. Best fit lines: $E_{CT} = 3.03 + \exp(-0.0018 \times (E_T 30/60)^{-12}), r^2 = 0.966$.



Figure S127. Calculated FMO energies (CAM-B3LYP/Def2TZVP // B3LYP/Def2TZVP method in solvent dielectric medium versus the E_T30 parameter.

c) partial output data for TD-DFT calculations

CAM-B3LYP/Def2TZVP TD(NStates=20) SCF=tight Geom(NoAngle, noDistance) SCRF(solvent=CH3CN)

1a (X = H)

Excitation energies and oscillator strengths: Excited State Singlet-A1 3.9675 eV 312.50 nm f=0.2908 <S**2>=0.000 1: 47 -> 52 0.11400 51 -> 52 0.69074 This state for optimization and/or second-order correction. Total Energy, E(TD-HF/TD-KS) = -502.183485410Copying the excited state density for this state as the 1-particle RhoCI density. Singlet-A2 4.0504 eV 306.10 nm f=0.0000 <S**2>=0.000 Excited State 2: 46 -> 52 0.13800 50 -> 52 0.68510 Excited State Singlet-B2 3: 4.8432 eV 255.99 nm f=0.0007 <S**2>=0.000 40 -> 53 0.10804 44 -> 52 0.25767 47 -> 53 0.13597 51 -> 53 0.62696 Excited State Singlet-B1 5.0543 eV 245.31 nm f=0.0014 <S**2>=0.000 4: 49 -> 52 0.69967 Excited State 5: Singlet-B2 5.2034 eV 238.27 nm f=0.0005 <S**2>=0.000 44 -> 52 0.11012 48 -> 52 0.67582 51 -> 53 -0.14710 Excited State 5.2169 eV 237.66 nm f=0.0009 <S**2>=0.000 6: Singlet-B1 46 -> 53 0.13109 50 -> 53 0.69032 Excited State 7: Singlet-B2 5.6080 eV 221.09 nm f=0.1079 <S**2>=0.000 40 -> 53 0.17179 44 -> 52 0.60805 48 -> 52 -0.1598551 -> 53 -0.26142

1b (X = CN)

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A1 4.1934 eV 295.67 nm f=0.3340 <S**2>=0.000 53 -> 58 -0.12345 57 -> 58 0.68681 This state for optimization and/or second-order correction. Total Energy, E(TD-HF/TD-KS) = -594.455829884 Copying the excited state density for this state as the 1-particle RhoCI density. 4.2814 eV 289.59 nm f=0.0000 <S**2>=0.000 Excited State 2: Singlet-A2 52 -> 58 0.14473 56 -> 58 0.67955 Excited State 3: Singlet-B2 5.0372 eV 246.14 nm f=0.0056 <S**2>=0.000 47 -> 59 -0.13023 51 -> 58 -0.36082 53 -> 59 -0.14106 54 -> 58 -0.14331 57 -> 59 0.55391

Excited 55	State -> 58	4:	Singlet-B1 0.69805	5.2758 eV	235.01 nm	f=0.0024	<s**2>=0.000</s**2>
Excited 51 54 57	State -> 58 -> 58 -> 59	5 :	Singlet-B2 0.10897 0.64675 0.23882	5.3885 eV	230.09 nm	f=0.0015	<s**2>=0.000</s**2>
Excited 57	State -> 60	6 :	Singlet-A2 0.68033	5.4788 eV	226.30 nm	f=0.0000	<s**2>=0.000</s**2>
Excited 52 56	State -> 59 -> 59	7 :	Singlet-B1 0.14226 0.68746	5.4843 eV	226.07 nm	f=0.0008	<s**2>=0.000</s**2>
Excited 47 51 54 57	State -> 59 -> 58 -> 58 -> 59	8:	Singlet-B2 0.11709 0.55504 -0.21764 0.33921	5.6813 eV	218.23 nm	f=0.1104	<s**2>=0.000</s**2>

1c (X = OAc)

Excitation energies and oscillator strengths:

Excited 62	State -> 67	1:	Singlet-A 0.11942 0.68766	3.9228 eV	316.06 nm	f=0.2776	<s**2>=0.000</s**2>
This sta	ate fo	r optin	mization and/or	second-order	correction.		
Copying	the e	xcited	state density	for this state	as the 1-pa	rticle Rho	CI density.
Excited	State	2:	Singlet-A	4.0235 eV	308.15 nm	f=0.0306	<s**2>=0.000</s**2>
61	-> 0/		-0.13135				
05	-> 07		0.00402				
Excited	State	3:	Singlet-A	4.8226 eV	257.09 nm	f=0.0005	<s**2>=0.000</s**2>
59	-> 67		-0.24571				
62	-> 68		0.14364				
65	-> 68		0.12131				
66	-> 68		0.62086				
Excited	State	4•	Singlet_A	5 1709 eV	239 77 nm	f=0 0004	<\$**2>=0 000
63	-> 67		0.54901	5.1705 60	209177 111	1 0.0001	
65	-> 68		0.41420				
		_					
Excited	State	5:	Singlet-A	5.1913 eV	238.83 nm	f=0.0023	<s**2>=0.000</s**2>
63	-> 67		-0.42622				
64	-> 67		0.10474				
65	-> 68		0.52377				
66	-> 68		-0.12812				
Excited	State	6:	Singlet-A	5.2678 eV	235.36 nm	f=0.0019	<s**2>=0.000</s**2>
59	-> 67		-0.15405				
64	-> 67		0.65509				
65	-> 68		-0.10334				
66	-> 68		-0.12707				
Excited	State	7:	Singlet-A	5.5683 eV	222.66 nm	f=0.0063	<s**2>=0.000</s**2>
65	-> 69		0.16208				
66	-> 69		0.51731				
66	-> 71		0.29497				
66	- > 72		0.21402				
66	-> 74		-0.10953				
66	-> 80		-0.13976				

Excited	State	8:	Singlet-A	5.6064 eV	221.15 nm	f=0.1053	<s**2>=0.000</s**2>
54	-> 68		0.15526				
59	-> 67		0.59963				
64	-> 67		0.20412				
66	-> 68		0.23164				

$1d (X = N_3)$

Excitation energies and oscillator strengths:

3.8429 eV 322.63 nm f=0.3275 <S**2>=0.000 Excited State 1: Singlet-A' 57 -> 62 0.17151 61 -> 62 0.67870 This state for optimization and/or second-order correction. Total Energy, E(TD-HF/TD-KS) = -665.817335887Copying the excited state density for this state as the 1-particle RhoCI density. Excited State 4.0874 eV 303.33 nm f=0.0000 <S**2>=0.000 2: Singlet-A" 56 -> 62 0.16221 60 -> 62 0.67873 Excited State 3: Singlet-A" 4.5026 eV 275.36 nm f=0.0005 <S**2>=0.000 55 -> 64 -0.22916 57 -> 64 -0.29030 61 -> 64 0.55194 Excited State 4.7652 eV 260.19 nm f=0.0002 <S**2>=0.000 4: Singlet-A' 53 -> 62 -0.2179757 -> 63 0.19874 61 -> 63 0.63236 Excited State Singlet-A" 5.2211 eV 237.47 nm f=0.0013 <S**2>=0.000 5: 59 -> 62 0.67945 60 -> 63 -0.16538 Excited State Singlet-A" 5.2672 eV 235.39 nm f=0.0013 <S**2>=0.000 6: 56 -> 63 0.14912 59 -> 62 0.17210 60 -> 63 0.66656 Excited State 5.2987 eV 233.99 nm f=0.0052 <S**2>=0.000 7: Singlet-A' 53 -> 62 0.22016 58 -> 62 0.64544 61 -> 63 0.14494 Excited State 5.3498 eV 231.76 nm f=0.0080 <S**2>=0.000 8: Singlet-A' 54 -> 64 0.20364 56 -> 64 0.14986 57 -> 62 0.18529 57 -> 65 -0.13049 60 -> 64 -0.33427 60 -> 66 -0.13127 61 -> 65 0.43511 61 -> 71 0.11467 Excited State 5.4723 eV 226.57 nm f=0.0001 <S**2>=0.000 9: Singlet-A" 61 -> 66 0.52723 61 -> 67 -0.38620 61 -> 70 -0.12078 61 -> 76 -0.14025 Excited State 10: 5.5874 eV 221.90 nm f=0.0974 <S**2>=0.000 Singlet-A' 50 -> 63 -0.17035 53 -> 62 0.58594 58 -> 62 -0.26231 61 -> 63 0.21753

1e X = I) Excitation energies and oscillator strengths: 4.0606 eV 305.34 nm f=0.3324 <s**2>=0.000 Excited State 1: Singlet-A1 59 -> 64 -0.20020 63 -> 640.66988 This state for optimization and/or second-order correction. Total Energy, E(TD-HF/TD-KS) = -799.336318218Copying the excited state density for this state as the 1-particle RhoCI density. 4.1423 eV 299.31 nm f=0.0000 <S**2>=0.000 Excited State 2: Singlet-A2 58 -> 64 -0.22787 62 -> 64 0.65807 Excited State 4.9402 eV 250.97 nm f=0.0020 <S**2>=0.000 Singlet-B2 3: 51 -> 65 -0.11604 54 -> 64 -0.29746 59 -> 65 -0.21000 60 -> 64 -0.10133 63 -> 65 0.58201 Excited State 4: Singlet-B1 5.2417 eV 236.54 nm f=0.0017 <S**2>=0.000 0.69124 61 -> 64 62 -> 65 -0.10090 Excited State 5: Singlet-B1 5.3161 eV 233.23 nm f=0.0009 <S**2>=0.000 58 -> 65 -0.21205 0.10968 61 -> 64 62 -> 65 0.66132 5.3396 eV 232.20 nm f=0.0034 <S**2>=0.000 Excited State 6: Singlet-B2 54 -> 64 0.16593 60 -> 64 0.64919 63 -> 65 0.19562 Excited State 7: Singlet-B2 5.6338 eV 220.07 nm f=0.1030 <S**2>=0.000 51 -> 65 0.15816 54 -> 64 0.57195 60 -> 64 -0.23627 63 -> 65 0.28091 1f (X = SCN)Excitation energies and oscillator strengths: Excited State 1: Singlet-A 4.0440 eV 306.59 nm f=0.3242 <S**2>=0.000 61 -> 66 -0.18186 65 -> 66 0.67510 This state for optimization and/or second-order correction. Total Energy, E(TD-HF/TD-KS) = -992.671008363Copying the excited state density for this state as the 1-particle RhoCI density. Excited State 2: Singlet-A 4.3698 eV 283.73 nm f=0.0000 <S**2>=0.000 60 -> 66 0.13835 64 -> 66 0.68380 Excited State 4.9311 eV 251.43 nm f=0.0018 <S**2>=0.000 3: Singlet-A 54 -> 67 -0.11230 57 -> 66 0.28928 61 -> 67 -0.20017 65 -> 67 0.59272 Excited State 5.2383 eV 236.69 nm f=0.0010 <S**2>=0.000 4: Singlet-A 59 -> 68 0.12531 61 -> 68 0.25739 61 -> 71 -0.13692 65 -> 68 0.57812

65	-> 71		-0.14633				
Excited 63	State -> 66	5 :	Singlet-A 0.69476	5.2966 eV	234.08 nm	f=0.0018	<s**2>=0.000</s**2>
Excited	State	6 :	Singlet-A	5.3775 eV	230.56 nm	f=0.0075	<s**2>=0.000</s**2>
57	-> 66		0.21606				
62	-> 66		0.62694				
65	-> 67		-0.20705				
Excited	State	7 :	Singlet-A	5.3988 eV	229.65 nm	f=0.0000	<s**2>=0.000</s**2>
61	-> 68		0.11339				
65	-> 69		0.62861				
65	-> 71		-0.16453				
65	_> 74		-0.12156				
xcited	State	8:	Singlet-A	5.5539 eV	223.24 nm	f=0.0008	<s**2>=0.000</s**2>
60	-> 67		0.13295				
64	-> 67		0.69001				
cited	State	9 :	Singlet-A	5.6390 eV	219.87 nm	f=0.1011	<s**2>=0.000</s**2>
54	-> 67		-0.15489				
57	-> 66		0.55878				
62	-> 66		-0.28943				
65	-> 67		-0.26225				
(X =) citatio	Br) on ener	gies a	and oscillator st	rengths:			
	State	1.	Singlet_A1	4 0418 eV	306 75 nm	f=0.3139	<5**2>=0 000
64	-> 69	1.	-0.15003	1.0110 CV	500 . 75 IIII	1 0.5155	
68	-> 69		0.68324				
otal E opying	nergy, the ex	E(TD-H cited	HF/TD-KS) = -307 state density for	5.91340495 r this state	as the 1-pa	rticle Rhc	CI density.
Excited	State	2:	Singlet-A2	4.1234 eV	300.68 nm	f=0.0000	<s**2>=0.000</s**2>
63	-> 69		0.17257				
67	-> 69		0.67581				
xcited	State	3:	Singlet-B2	4.9205 eV	251.98 nm	f=0.0017	<s**2>=0.000</s**2>
56	-> 70		-0.11170				
60	-> 69		-0.28904				
64	-> 70		-0.17163				
68	<u> </u>		0.60191				
xcited	State	4:	Singlet-B1	5.2387 eV	236.67 nm	f=0.0016	<s**2>=0.000</s**2>
66	-> 69		0.68764				
67	-> 70		0.12727				
xcited	State	5 :	Singlet-B1	5.2997 eV	233.94 nm	f=0.0010	<s**2>=0.000</s**2>
xcited 63	State -> 70	5:	Singlet-B1 0.15932	5.2997 eV	233.94 nm	f=0.0010	<s**2>=0.000</s**2>
xcited 63 66	State -> 70 -> 69	5:	Singlet-B1 0.15932 -0.13380	5.2997 eV	233.94 nm	f=0.0010	<s**2>=0.000</s**2>
xcited 63 66 67	State -> 70 -> 69 -> 70	5:	Singlet-B1 0.15932 -0.13380 0.67255	5.2997 eV	233.94 nm	f=0.0010	<s**2>=0.000</s**2>
xcited 63 66 67 xcited	State -> 70 -> 69 -> 70 State	5: 6:	Singlet-B1 0.15932 -0.13380 0.67255 Singlet-B2	5.2997 eV 5.3319 eV	233.94 nm 232.53 nm	f=0.0010 f=0.0031	<s**2>=0.000</s**2>
xcited 63 66 67 xcited 60	State -> 70 -> 69 -> 70 State -> 69	5: 6:	Singlet-B1 0.15932 -0.13380 0.67255 Singlet-B2 0.16743	5.2997 eV 5.3319 eV	233.94 nm 232.53 nm	f=0.0010 f=0.0031	<s**2>=0.000 <s**2>=0.000</s**2></s**2>
xcited 63 66 67 xcited 60 65	State -> 70 -> 69 -> 70 State -> 69 -> 69	5: 6:	Singlet-B1 0.15932 -0.13380 0.67255 Singlet-B2 0.16743 0.65169	5.2997 eV 5.3319 eV	233.94 nm 232.53 nm	f=0.0010 f=0.0031	<s**2>=0.000</s**2>
xcited 63 66 67 xcited 60 65 68	State -> 70 -> 69 -> 70 State -> 69 -> 69 -> 70	5:	Singlet-B1 0.15932 -0.13380 0.67255 Singlet-B2 0.16743 0.65169 0.18882	5.2997 eV 5.3319 eV	233.94 nm 232.53 nm	f=0.0010 f=0.0031	<5**2>=0.000
xcited 63 66 67 xcited 60 65 68 xcited	State -> 70 -> 69 -> 70 State -> 69 -> 69 -> 70 State	5: 6: 7:	Singlet-B1 0.15932 -0.13380 0.67255 Singlet-B2 0.16743 0.65169 0.18882 Singlet-B2	5.2997 eV 5.3319 eV 5.6331 eV	233.94 nm 232.53 nm 220.10 nm	f=0.0010 f=0.0031 f=0.1064	<s**2>=0.000 <s**2>=0.000 <s**2>=0.000</s**2></s**2></s**2>
xcited 63 66 67 xcited 60 65 68 xcited 56	State -> 70 -> 69 -> 70 State -> 69 -> 70 State -> 70	5: 6: 7:	Singlet-B1 0.15932 -0.13380 0.67255 Singlet-B2 0.16743 0.65169 0.18882 Singlet-B2 0.16041	5.2997 eV 5.3319 eV 5.6331 eV	233.94 nm 232.53 nm 220.10 nm	f=0.0010 f=0.0031 f=0.1064	<s**2>=0.000 <s**2>=0.000 <s**2>=0.000</s**2></s**2></s**2>
Excited 63 66 67 Excited 60 65 68 Excited 56 60	State -> 70 -> 69 -> 70 State -> 69 -> 70 State -> 70 State -> 70	5: 6: 7:	Singlet-B1 0.15932 -0.13380 0.67255 Singlet-B2 0.16743 0.65169 0.18882 Singlet-B2 0.16041 0.57975	5.2997 eV 5.3319 eV 5.6331 eV	233.94 nm 232.53 nm 220.10 nm	f=0.0010 f=0.0031 f=0.1064	<s**2>=0.000 <s**2>=0.000 <s**2>=0.000</s**2></s**2></s**2>
Excited 63 66 67 Excited 60 65 68 Excited 56 60 65	State -> 70 -> 69 -> 70 State -> 69 -> 70 State -> 70 State -> 70 -> 69 -> 69	5: 6: 7:	Singlet-B1 0.15932 -0.13380 0.67255 Singlet-B2 0.16743 0.65169 0.18882 Singlet-B2 0.16041 0.57975 -0.23471	5.2997 eV 5.3319 eV 5.6331 eV	233.94 nm 232.53 nm 220.10 nm	f=0.0010 f=0.0031 f=0.1064	<s**2>=0.000 <s**2>=0.000 <s**2>=0.000</s**2></s**2></s**2>
Excited 63 66 67 Excited 60 65 68 Excited 56 60 65 68	State -> 70 -> 69 -> 70 State -> 69 -> 70 State -> 70 State -> 70 -> 69 -> 69 -> 70	5: 6: 7:	Singlet-B1 0.15932 -0.13380 0.67255 Singlet-B2 0.16743 0.65169 0.18882 Singlet-B2 0.16041 0.57975 -0.23471 0.27477	5.2997 eV 5.3319 eV 5.6331 eV	233.94 nm 232.53 nm 220.10 nm	f=0.0010 f=0.0031 f=0.1064	<s**2>=0.00 <s**2>=0.00 <s**2>=0.00</s**2></s**2></s**2>

1h (X = Pyr)

Excitation energies and oscillator strengths: Excited State 1: Singlet-A 4.1500 eV 298.76 nm f=0.5503 <S**2>=0.000 67 -> 73 -0.11792 71 -> 72 0.68858 This state for optimization and/or second-order correction. Total Energy, E(TD-HF/TD-KS) = -749.719533135Copying the excited state density for this state as the 1-particle RhoCI density. Excited State 2: Singlet-A 4.3165 eV 287.23 nm f=0.0000 <S**2>=0.000 66 -> 73 -0.11374 70 -> 72 0.68253 4.3845 eV 282.78 nm f=0.0000 <S**2>=0.000 Excited State 3: Singlet-A 67 -> 72 -0.12807 71 -> 73 0.68263 Excited State 4: Singlet-A 4.5305 eV 273.67 nm f=0.0940 <S**2>=0.000 -0.15260 66 -> 72 70 -> 73 0.68369 Excited State 5: Singlet-B 5.0799 eV 244.07 nm f=0.0137 <S**2>=0.000 61 -> 75 -0.11509 64 -> 72 -0.28025 65 -> 73 -0.26834 67 -> 75 -0.12593 69 -> 72 0.14277 70 -> 75 0.13749 71 -> 74 0.51342 6**:** Excited State Singlet-B 5.0839 eV 243.87 nm f=0.0021 <S**2>=0.000 61 -> 74 -0.11578 64 -> 73 -0.27067 65 -> 72 -0.28525 67 -> 74 -0.12664 68 -> 72 0.12560 70 -> 74 0.14038 71 -> 75 0.51181 5.3551 eV 231.52 nm f=0.0027 <S**2>=0.000 Excited State 7: Singlet-B 0.66973 68 -> 72 69 -> 73 -0.13851 71 -> 75 -0.12035 5.3596 eV 231.33 nm f=0.0000 <S**2>=0.000 Excited State 8: Singlet-B 68 -> 73 -0.17023 69 -> 72 0.65471 71 -> 74 -0.16738 Excited State 5.5256 eV 224.38 nm f=0.0048 <S**2>=0.000 9: Singlet-B 64 -> 73 -0.13533 65 -> 72 -0.17398 69 -> 73 0.53540 70 -> 74 0.18922 71 -> 75 -0.33057 Excited State 10: 5.5450 eV 223.59 nm f=0.0353 <S**2>=0.000 Singlet-B 64 -> 72 -0.19511 65 -> 73 -0.15757 68 -> 73 0.51906 70 -> 75 0.19779 71 -> 74 -0.33853 5.5948 eV 221.60 nm f=0.0016 <S**2>=0.000 Excited State 11: Singlet-B 66 -> 75 -0.10764 69 -> 73 -0.31819 70 -> 74 0.60031

71	-> 75		-0.13562				
Excited	State	12:	Singlet-B	5.5996 eV	221.42 nm	f=0.0000	<s**2>=0.000</s**2>
66	-> 74		-0.11226				
68	- > 73		-0.29809				
69	-> 72		-0.11815				
70	- > 75		0.60820				
Excited	State	13:	Singlet-B	5.7409 eV	215.97 nm	f=0.0222	<s**2>=0.000</s**2>
64	-> 73		0.34367				
65	-> 72		0.36175				
68	-> 72		0.12598				
69	-> 73		0.27660				
70	-> 74		0.24327				
71	-> 75		0.27457				
Excited	State	14:	Singlet-B	5.7485 eV	215.68 nm	f=0.1620	<s**2>=0.000</s**2>
64	-> 72		0.35468				
65	-> 73		0.33622				
68	-> 73		0.31603				
69	-> 72		0.14885				
70	-> 75		0.22649				
71	-> 74		0.25463				

lj (X=OEt)

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 3.5915 eV 345.22 nm f=0.2933 <S**2>=0.000 59 -> 64 -0.13242 63 -> 64 0.68812 This state for optimization and/or second-order correction. Total Energy, E(TD-HF/TD-KS) = -656.067041486Copying the excited state density for this state as the 1-particle RhoCI density. 3.8722 eV 320.19 nm f=0.0000 <S**2>=0.000 Excited State 2: Singlet-A 58 -> 64 -0.14023 62 -> 64 0.68522 Excited State 4.5160 eV 274.55 nm f=0.0001 <S**2>=0.000 3: Singlet-A 56 -> 64 0.15657 59 -> 65 -0.16000 63 -> 65 0.66455 Singlet-A Excited State 5.0350 eV 246.25 nm f=0.0005 <S**2>=0.000 4: 58 -> 65 -0.13348 62 -> 65 0.68721 Excited State 5: Singlet-A 5.1105 eV 242.61 nm f=0.0015 <S**2>=0.000 61 -> 64 0.69734 Excited State 6: Singlet-A 5.1954 eV 238.64 nm f=0.0030 <S**2>=0.000 56 -> 64 0.18136 60 -> 64 0.66895 Excited State 7: 5.2817 eV 234.74 nm f=0.0001 <S**2>=0.000 Singlet-A 63 -> 67 0.64410 63 -> 70 0.12685 63 -> 76 0.19585 Excited State 8: Singlet-A 5.4734 eV 226.52 nm f=0.0638 <S**2>=0.000 56 -> 64 0.10126 59 -> 64 0.65630 63 -> 64 0.12060

1j (X=Morpholine)

Excitation energies and oscillator strengths: Excited State 1: Singlet-A 3.3509 eV 370.01 nm f=0.2787 <S**2>=0.000 72 -> 75 -0.17949 74 -> 75 0.67661 This state for optimization and/or second-order correction. Total Energy, E(TD-HF/TD-KS) = -788.800345460Copying the excited state density for this state as the 1-particle RhoCI density. Excited State 2: Singlet-A 3.9301 eV 315.47 nm f=0.0186 <S**2>=0.000 68 -> 75 0.13527 73 -> 75 0.68526 4.3120 eV 287.53 nm f=0.0003 <S**2>=0.000 Excited State 3: Singlet-A 66 -> 75 -0.11356 72 -> 76 -0.19804 74 -> 76 0.66017 5.0123 eV 247.36 nm f=0.0455 <S**2>=0.000 Excited State 4: Singlet-A 69 -> 75 0.18954 71 -> 75 0.35447 72 -> 75 0.51354 74 -> 75 0.14634 74 -> 78 -0.14678 Excited State 5: Singlet-A 5.0288 eV 246.55 nm f=0.0007 <S**2>=0.000 71 -> 75 0.12167 72 -> 75 0.10349 72 -> 78 -0.11109 74 -> 78 0.61656 74 -> 81 -0.13352 74 -> 88 -0.15622 Excited State 6: 5.0674 eV 244.67 nm f=0.0110 <S**2>=0.000 Singlet-A 69 -> 75 -0.14120 70 -> 75 -0.14385 71 -> 75 0.43964 72 -> 75 -0.25405 73 -> 76 -0.403715.0893 eV 243.62 nm f=0.0063 <S**2>=0.000 Excited State 7: Singlet-A 69 -> 75 -0.10518 71 -> 75 0.38259 72 -> 75 -0.16264 73 -> 76 0.53523 Excited State 8: 5.1755 eV 239.56 nm f=0.0025 <S**2>=0.000 Singlet-A 66 -> 75 -0.17831 70 -> 75 0.65042 73 -> 76 -0.11906 Excited State 9: Singlet-A 5.4085 eV 229.24 nm f=0.0307 <S**2>=0.000 -0.10067 73 -> 78 74 -> 77 0.47890 -0.45145 74 -> 79 74 -> 82 0.11306 5.4934 eV 225.70 nm f=0.0731 <S**2>=0.000 Excited State 10: Singlet-A 61 -> 76 -0.16545 66 -> 75 0.58828 70 -> 75 0.21449 0.15488 72 -> 76 74 -> 76 0.15600

1k (X=Morpholinium)

Excitation energies and oscillator strengths:

Excited State 1: 4.3139 eV 287.40 nm f=0.3231 <S**2>=0.000 Singlet-A 70 -> 75 -0.10837 74 -> 75 0.69025 This state for optimization and/or second-order correction. Total Energy, E(TD-HF/TD-KS) = -789.244520139Copying the excited state density for this state as the 1-particle RhoCI density. Excited State 2: Singlet-A 4.4089 eV 281.21 nm f=0.0002 <S**2>=0.000 69 -> 75 0.13076 73 -> 75 0.68448 Excited State 5.1002 eV 243.09 nm f=0.0096 <S**2>=0.000 3: Singlet-A 63 -> 76 0.15116 67 -> 75 0.40654 70 -> 76 -0.11905 71 -> 75 0.15570 74 -> 76 0.51981 Excited State 5.3829 eV 230.33 nm f=0.0023 <S**2>=0.000 4: Singlet-A 72 -> 75 0.69748 Excited State 5: Singlet-A 5.4853 eV 226.03 nm f=0.0029 <S**2>=0.000 67 -> 75 0.11038 71 -> 75 0.63164 74 -> 76 -0.27723 Excited State 6: Singlet-A 5.6006 eV 221.38 nm f=0.0009 <S**2>=0.000 69 -> 76 0.12589 73 -> 76 0.69072 Excited State 5.7390 eV 216.04 nm f=0.1083 <S**2>=0.000 7: Singlet-A 63 -> 76 0.12863 67 -> 75 0.52472 71 -> 75 -0.25180 74 -> 76 -0.36846

2b (Y=CN)

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A1 3.1767 eV 390.30 nm f=0.4169 <S**2>=0.000 0.10075 53 -> 58 57 -> 58 0.69262 This state for optimization and/or second-order correction. Total Energy, E(TD-HF/TD-KS) = -594.443371725 Copying the excited state density for this state as the 1-particle RhoCI density. Excited State 2: Singlet-A2 3.2733 eV 378.78 nm f=0.0000 <S**2>=0.000 52 -> 58 0.13086 56 -> 58 0.68619 Excited State Singlet-B1 4.2200 eV 293.80 nm f=0.0005 3: <S**2>=0.000 55 -> 58 0.70098 4.3708 eV 283.67 nm f=0.0001 Excited State 4: Singlet-B2 <S**2>=0.000 49 -> 58 0.12604 54 -> 58 0.67101 57 -> 59 0.15276

Excited State <pre><s**2>=0.000</s**2></pre>	5:	Singlet-B2	4.5125 eV	274.76 nm	f=0.0025
49 -> 58		0.23638			
53 -> 59		0 12770			
54 -> 58		-0 19466			
54 = 250 57 = 250		0 61661			
57 -2 59		0.01001			
Excited State	6:	Singlet-A1	4.8765 eV	254.25 nm	f=0.0583
<s**2>=0.000</s**2>					
50 -> 58		-0.10834			
53 - > 58		0.68389			
57 -> 58		-0.10311			
Excited State <pre><s**2>=0.000</s**2></pre>	7 :	Singlet-A2	4.9203 eV	251.99 nm	f=0.0000
48 -> 58		-0.11796			
52 -> 58		0.67571			
56 -> 58		-0.13124			
Excited State	8:	Singlet-B1	4.9331 eV	251.33 nm	f=0.0006
52 -> 59		0.13542			
56 -> 59		0.69134			
Excited State <s**2>=0.000</s**2>	9 :	Singlet-B2	5.1670 eV	239.95 nm	f=0.1058
47 - > 59		-0.14094			
49 - > 58		0.62489			
57 -> 59		-0.28197			
21 (Y=COOEt) Excitation ener	gies a	nd oscillator str	engths:		
Excited State <pre><s**2>=0.000</s**2></pre>	1:	Singlet-A'	3.3642 eV	368.54 nm	f=0.4033
66 - > 71		0.10398			
70 -> 71		0.69020			
This state for	optim	ization and/or se	econd-order o	correction.	
Total Energy.	E(TD-H	F/TD-KS) = -769	399731694		
Copving the ex	cited	state density for	this state	as the 1-pa	rticle RhoCT
density.					
Excited State	2:	Singlet-A"	3.4753 eV	356.76 nm	f=0.0000
<s**2>=0.000</s**2>		2			
65 -> 71		-0.12873			
69 -> 71		0.68411			
69 -> 73		0.10161			
05 7 70		0.10101			
Excited State	3:	Singlet-A"	4.4345 eV	279.59 nm	f=0.0007
<pre><s**2>=0 000</s**2></pre>	0.	bingice n	1.1010 01		1 000007
68 5 71		0 69858			
00 -> /1		0.09030			
Excited State	4:	Singlet-A'	4.5540 eV	272.25 nm	f=0.0016
<s**2>=0.000</s**2>	-	J			
63 -> 71		0.22933			
67 <u>-></u> 71		0.61340			
70 -> 72		-0.23328			
, 5 - <i>7</i> 7 Z		3.23320			
Excited State <pre><s**2>=0.000</s**2></pre>	5:	Singlet-A'	4.6919 eV	264.25 nm	f=0.0063

63	-> 71	L	-0.28487			
66	-> 72	2	0.11429			
67	-> 71	L	0.32644			
70	-> 72	2	0.53430			
Excited <\$**2>=0.	State	e 6:	Singlet-A"	4.8361 eV	256.37 nm	f=0.0001
60	-> 71	L	0.65566			
60	-> 73	3	-0.23702			
Excited <s**2>=0.</s**2>	State	e 7:	Singlet-A'	5.0943 eV	243.38 nm	f=0.0593
62	-> 71	L	-0.10626			
66	-> 71	L	0.68089			
70	-> 71	L	-0.10768			
Excited <\$**2>=0.	State	e 8:	Singlet-A"	5.1245 eV	241.95 nm	f=0.0007
65	-> 72	2	-0.13388			
69	-> 72	2	0.69128			
Excited <\$**2>=0.	State	e 9:	Singlet-A"	5.1300 eV	241.69 nm	f=0.0000
61	-> 71	L	-0.11731			
65	-> 71	L	0.67259			
69	-> 71	L	0.12898			
Excited <\$**2>=0.	State	e 10:	Singlet-A'	5.1888 eV	238.95 nm	f=0.0833
57	-> 72	2	-0.10966			
63	-> 71	L	0.57731			
70	-> 72	2	0.37664			
2m (Y=Me) Excitatio	on ene	ergies a	and oscillator str	rengths:		
Excited	State	e 1:	Singlet-A'	4.0932 eV	302.90 nm	f=0.3357
51 55	-> 56 -> 56	5 5	0.11469 0.68966			
This sta	ate fo	or optin	nization and/or se	cond-order c	orrection.	
TOTAL EI	iergy,	, E(TD-I	1F/TD-KS) = -541.	488915896		
density.	tne e	excited	state density for	this state	as tne 1-pa	rticle Rhoci
Excited <s**2>=0.</s**2>	State	e 2:	Singlet-A"	4.2025 eV	295.02 nm	f=0.0000
50	-> 56	5	0.13482			
54	-> 56	5	0.68431			
Excited <\$**2>=0.	State	e 3:	Singlet-A"	4.8573 eV	255.25 nm	f=0.0002
45	-> 57	7	0.11158			
48	-> 56	5	0.24590			
51	-> 57	7	0.14065			
55	-> 57	7	0.63195			
Excited <\$**2>=0.	State	e 4:	Singlet-A'	5.2101 eV	237.97 nm	f=0.0010
53	-> 56	5	0.66044			

54 -> 57 -0.22761 Excited State 5: Singlet-A' 5.2481 eV 236.25 nm f=0.0015 <S**2>=0.000 0.12003 50 -> 57 53 -> 56 0.23342 54 -> 57 0.65341 Excited State 6: Singlet-A" 5.3469 eV 231.88 nm f=0.0016 <S**2>=0.000 48 -> 56 0.16289 52 -> 56 0.66347 55 **-**> 57 -0.14461 Excited State 7: Singlet-A" 5.6775 eV 218.38 nm f=0.0935 <S**2>=0.000 45 -> 57 0.18968 48 -> 56 0.58900 52 **-**> 56 -0.20944 55 **-**> 57 -0.25087 2n (Y=OMe) Excitation energies and oscillator strengths: Singlet-A' 4.2990 eV 288.40 nm f=0.3698 Excited State 1: <S**2>=0.000 55 -> 60 0.12145 59 -> 60 0.68763 This state for optimization and/or second-order correction. Total Energy, E(TD-HF/TD-KS) = -616.704871954Copying the excited state density for this state as the 1-particle RhoCI density. Excited State 2: Singlet-A" 4.4578 eV 278.13 nm f=0.0000 <S**2>=0.000 -0.13281 54 -> 60 58 **-**> 60 0.68305 Singlet-A' 4.7872 eV 258.99 nm f=0.0075 Excited State 3: <S**2>=0.000 51 -> 60 -0.17250 53 -> 61 -0.10443 0.16004 55 -> 61 59 -> 61 0.65321 Excited State 4: Singlet-A" 5.1891 eV 238.93 nm f=0.0006 <S**2>=0.000 54 -> 61 -0.13159 58 -> 61 0.69070 5: Singlet-A" 5.4763 eV 226.40 nm f=0.0024 Excited State <S**2>=0.000 57 -> 60 0.69873 Singlet-A' 5.5949 eV 221.60 nm f=0.0005 Excited State 6: <S**2>=0.000 51 -> 60 0.18569 56 -> 60 0.65245 59 -> 61 0.11119

Excited	State	7:	Singlet-A"	5.7295	eV	216.40	nm	f=0.0000
<s**2>=0.</s**2>	000							
59	-> 63	0	.58841					
59	-> 64	0	.17416					
59	-> 66	0	.22161					
59	-> 73	0	.18843					
Excited	State	8:	Singlet-A'	5.8614	eV	211.53	nm	f=0.0349
<s**2>=0.</s**2>	000							
51	-> 60	0	.47641					
53	-> 61	0	.32713					
55	-> 60	0	.15883					
55	-> 61	-0	.14858					
56	-> 60	-0	.22374					
59	-> 61	0	.20825					
Excited	State	9:	Singlet-A'	5.8797	eV	210.87	nm	f=0.1705
<s**2>=0.</s**2>	000							
51	-> 60	-0	.11442					
51	-> 61	0	.15328					
53	-> 60	-0	.38287					
55	-> 60	0	.40844					
58	-> 63	0	.23107					
59	-> 65	0	.19553					
3 (Y=CN, X	= OEt)							
Excited	State	1:	Singlet-A	2.7624	eV	448.83	nm	f=0.4361
<s**2>=0.</s**2>	000							
65	-> 70	-0	.11070					
69	-> 70	0	. 69197					
This sta	te for d	ontimiza.	tion and/or seco	ond-orde	er co	vrectio	n.	
Total En	erav El	ישט_אד/שו שט_אד/שו	-KS) = -748 32	28385973	21 00	,1100010		
Conving	the exci	ted sta	te density for t	-hig gt2	, ato a	as the '	l_nar	ticle RhoCT
density.	che exel	lica sta	te density for t				-pui	
Duraitad	C+	2.	Cinalat D	2 0642	o17	101 61	~ ~	£-0 0000
Excited	State	2:	Singlet-A	3.0643	ev	404.61	nm	I=0.0000
<\$**2>=0.	000	0	10065					
64	-> 70	-0	.12965					
68	_> 70	0	.68692					
Excited	a							
<\$**2>=0.	State	3:	Singlet-A	4.1522	eV	298.60	nm	f=0.0001
6 1	State 000	3:	Singlet-A	4.1522	eV	298.60	nm	f=0.0001
01	State 000 -> 70	3:	Singlet-A .16266	4.1522	eV	298.60	nm	f=0.0001
61 65	5tate 000 -> 70 -> 71	3: _0 _0	Singlet-A .16266 .15698	4.1522	eV	298.60	nm	f=0.0001
61 65 69	State 000 -> 70 -> 71 -> 71	3: _0 _0 0	Singlet-A .16266 .15698 .66073	4.1522	eV	298.60	nm	f=0.0001
61 65 69 Excited	State 000 -> 70 -> 71 -> 71 State	3: 0 -0 0 4:	Singlet-A .16266 .15698 .66073 Singlet-A	4.1522	eV eV	298.60	nm	f=0.0001
61 65 69 Excited <s**2>=0.</s**2>	State 000 -> 70 -> 71 -> 71 State	3: 0 -0 0 4:	Singlet-A .16266 .15698 .66073 Singlet-A	4.1522	eV eV	298.60 290.67	nm nm	f=0.0001 f=0.0004
61 65 69 Excited <s**2>=0. 67</s**2>	State 000 -> 70 -> 71 -> 71 State 000 -> 70	3: 0 -0 0 4:	Singlet-A .16266 .15698 .66073 Singlet-A .70093	4.1522 4.2655	eV eV	298.60 290.67	nm nm	f=0.0001 f=0.0004
61 65 69 Excited <s**2>=0. 67</s**2>	State 000 -> 70 -> 71 -> 71 State 000 -> 70	3: 0 -0 0 4: 0	Singlet-A .16266 .15698 .66073 Singlet-A .70093	4.1522 4.2655	eV eV	298.60 290.67	nm nm	f=0.0001 f=0.0004
61 65 69 Excited <s**2>=0. 67 Excited</s**2>	State 000 -> 70 -> 71 -> 71 State 000 -> 70 State	3: 0 -0 0 4: 0 5:	Singlet-A .16266 .15698 .66073 Singlet-A .70093 Singlet-A	4.1522 4.2655 4.3719	eV eV eV	298.60 290.67 283.59	nm nm nm	f=0.0001 f=0.0004 f=0.0021
<pre>61 65 69 Excited <s**2>=0. 67 Excited <s**2>=0.</s**2></s**2></pre>	State 000 -> 70 -> 71 -> 71 State 000 -> 70 State 000	3: 0 -0 0 4: 0 5:	Singlet-A .16266 .15698 .66073 Singlet-A .70093 Singlet-A	4.1522 4.2655 4.3719	eV eV eV	298.60 290.67 283.59	nm nm nm	f=0.0001 f=0.0004 f=0.0021
<pre>61 65 69 Excited <s**2>=0. 67 Excited <s**2>=0. 66</s**2></s**2></pre>	State 000 -> 70 -> 71 -> 71 State 000 -> 70 State 000 -> 70	3: 0 -0 0 4: 0 5: 0	Singlet-A .16266 .15698 .66073 Singlet-A .70093 Singlet-A	4.1522 4.2655 4.3719	eV eV eV	298.60 290.67 283.59	nm nm	f=0.0001 f=0.0004 f=0.0021
61 65 69 Excited <s**2>=0. 67 Excited <s**2>=0. 66</s**2></s**2>	State 000 -> 70 -> 71 -> 71 State 000 -> 70 State 000 -> 70	3: 0 -0 0 4: 0 5: 0	Singlet-A .16266 .15698 .66073 Singlet-A .70093 Singlet-A .69255	4.1522 4.2655 4.3719	eV eV eV	298.60 290.67 283.59	nm nm nm	f=0.0001 f=0.0004 f=0.0021
<pre>61 65 69 Excited <s**2>=0. 67 Excited <s**2>=0. 66 Excited</s**2></s**2></pre>	State 000 -> 70 -> 71 -> 71 State 000 -> 70 State 000 -> 70 State	3: 0 -0 0 4: 0 5: 0 6:	Singlet-A .16266 .15698 .66073 Singlet-A .70093 Singlet-A .69255 Singlet-A	 4.1522 4.2655 4.3719 4.5950 	eV eV eV	298.60 290.67 283.59 269.82	nm nm nm	f=0.0001 f=0.0004 f=0.0021 f=0.1020
<pre>61 65 69 Excited <s**2>=0. 67 Excited <s**2>=0. 66 Excited <s**2>=0.</s**2></s**2></s**2></pre>	State 000 -> 70 -> 71 -> 71 State 000 -> 70 State 000 -> 70 State 000	3: 0 -0 0 4: 0 5: 0 6:	Singlet-A .16266 .15698 .66073 Singlet-A .70093 Singlet-A .69255 Singlet-A	4.1522 4.2655 4.3719 4.5950	eV eV eV	298.60 290.67 283.59 269.82	nm nm nm	f=0.0001 f=0.0004 f=0.0021 f=0.1020
<pre>61 65 69 Excited <s**2>=0. 67 Excited <s**2>=0. 66 Excited <s**2>=0. 65</s**2></s**2></s**2></pre>	State 000 -> 70 -> 71 -> 71 State 000 -> 70 State 000 -> 70 State 000 -> 70 State 000 -> 70	3: 0 -0 0 4: 0 5: 0 6: 0	Singlet-A .16266 .15698 .66073 Singlet-A .70093 Singlet-A .69255 Singlet-A .67970	4.1522 4.2655 4.3719 4.5950	eV eV eV	298.60 290.67 283.59 269.82	nm nm nm	f=0.0001 f=0.0004 f=0.0021 f=0.1020

7. Archive for DFT results

A

1\1\GINC-LOCALHOST\FOpt\RB3LYP\def2TZVP\B10H10(2-)\PIOTR\10-Jun-2020\0 \\#P B3LYP/Def2TZVP FOpt(tight) geom(noangle, nodistance) fcheck #P SC RF(Solvent=C6H5Cl)\\B10H10 anion, D4d sym\\-2,1\B,-0.000000006,1.2957 240704,-0.7581610836\B,0.000000006,-1.2957240703,-0.7581610836\B,-1.2 957240703,-0.000000006,-0.7581610836\B,1.2957240703,0.000000006,-0.7 581610836\B,0.915966411,0.9159664119,0.758390132\B,-0.9159664119,0.915 9664111,0.758390132\B,-0.915966411,-0.9159664118,0.758390132\B,0.91596 64119,-0.915966411,0.758390132\B,0.,0.,1.8524476948\B,0.,0.,-1.8531518 459\H,-0.0000000011,2.4276697171,-1.1607416045\H,0.0000000011,-2.42766 97171,-1.1607416045\H,-2.4276697171,-0.0000000011,-1.1607416045\H,2.42 76697171,0.0000000011,-1.1607416045\H,1.7165238536,1.7165238552,1.1608 451813\H,-1.7165238552,1.7165238536,1.1608451813\H,-1.7165238536,-1.71 65238551,1.1608451813\H,1.7165238552,-1.7165238536,1.1608451813\H,0.,0 .,-3.049567886\H,0.,0.,3.0489415151\\Version=ES64L-G09RevD.01\State=1-A1\HF=-254.9669623\RMSD=7.342e-09\RMSF=2.286e-06\Dipole=0.,0.,0.004994 4\Ouadrupole=2.1626917,2.1626917,-4.3253833,0.,0.,0.\PG=C04V [C4(H1B1B 1H1),2SGV(B2H2),2SGD(B2H2)]\\

1a

1\1\GINC-LOCALHOST\F0pt\RB3LYP\def2TZVP\C5H14B10N1(1-)\PIOTR\08-Jun-20 20\0\\#P B3LYP/Def2TZVP FOpt(tight) geom(noangle, nodistance) fcheck # P SCRF(Solvent=C6H5C1)\\B10-1-Pyridine, C2v\\-1,1\B,0.,0.,0.1004669108 \B,1.3009082385,0.,2.6639787152\B,0.,1.2995441316,2.65961425\B,-1.3009 082385,0.,2.6639787152\B,0.,-1.2995441316,2.65961425\B,0.9276001595,-0 .9194110773,1.1561683107\B,0.9276001595,0.9194110773,1.1561683107\B,-0 .9276001595,0.9194110773,1.1561683107\B,-0.9276001595,-0.9194110773,1. 1561683107\B,0.,0.,3.7508598325\N,0.,0.,-1.4257287664\C,1.1950061319,0 .,-3.4894423797\C,-1.1950061319,0.,-3.4894423797\C,1.1634271736,0.,-2. 109774387\C,-1.1634271736,0.,-2.109774387\C,0.,0.,-4.1981969318\H,2.42 57431357,0.,3.0733868298\H,0.,2.4265774397,3.0625202638\H,-2.425743135 7,0.,3.0733868298\H,0.,-2.4265774397,3.0625202638\H,2.1502769405,0.,-3 .9944269036\H,-2.1502769405,0.,-3.9944269036\H,1.7112917794,-1.7099039 616,0.7153541943\H,1.7112917794,1.7099039616,0.7153541943\H,-1.7112917 794,1.7099039616,0.7153541943\H,-1.7112917794,-1.7099039616,0.71535419 43\H,2.0578133254,0.,-1.5062694654\H,-2.0578133254,0.,-1.5062694654\H, 0.,0.,-5.2797590301\H,0.,0.,4.942748398\\Version=ES64L-G09RevD.01\Stat e=1-A1\HF=-502.6726892\RMSD=4.723e-09\RMSF=2.108e-06\Dipole=0.,0.,-9.1 622476\Quadrupole=8.2566338,-0.2269991,-8.0296346,0.,0.,0.\PG=C02V [C2 (H1B1B1N1C1H1), SGV(C4H6B2), SGV'(H2B2), X(H4B4)]

1b

1\1\GINC-LOCALHOST\FOpt\RB3LYP\def2TZVP\C6H13B10N2(1-)\PIOTR\08-Jun-20 20\0\\#P B3LYP/Def2TZVP FOpt(tight) geom(noangle, nodistance) fcheck # P SCRF(Solvent=C6H5C1)\\CB-10-B10-1-Pyridine, C2v\\-1,1\B,0.,1.3079071 673,-2.0619270955\B,0.,-1.3079071673,-2.0619270955\B,1.3067100182,0.,-2.0587438247\B,-1.3067100182,0.,-2.0587438247\B,-0.9217129395,0.927946 7331,-0.5610664469\B,0.9217129395,0.9279467331,-0.5610664469\B,0.92171 29395,-0.9279467331,-0.5610664469\B,-0.9217129395,-0.9279467331,-0.561 0664469\B,0.,0.,0.4923771873\B,0.,0.,-3.133518571\N,0.,0.,2.0193586377 \C,0.,1.195460812,4.0812752987\C,0.,-1.195460812,4.0812752987\C,0.,1.1 639605706,2.7017024211\C,0.,-1.1639605706,2.7017024211\C,0.,0.,4.78895 51812\H,0.,2.4235527178,-2.4855232307\H,0.,-2.4235527178,-2.4855232307 \H,2.424373285,0.,-2.4766032996\H,-2.424373285,0.,-2.4766032996\H,-1.7 102734865,1.7103646951,-0.1200835318\H,1.7102734865,1.7103646951,-0.12 00835318\H,1.7102734865,-1.7103646951,-0.1200835318\H,-1.7102734865,-1 .7103646951,-0.1200835318\H,0.,2.1503901644,4.5866550378\H,0.,-2.15039 01644,4.5866550378\H,0.,2.0587446093,2.0987874981\H,0.,-2.0587446093,2

.0987874981\H,0.,0.,5.870510495\C,0.,0.,-4.6656155395\N,0.,0.,-5.82323 31819\\Version=ES64L-G09RevD.01\State=1-A1\HF=-594.9937748\RMSD=3.259e -09\RMSF=1.740e-06\Dipole=0.,0.,10.6869728\Quadrupole=6.0651034,14.722 2843,-20.7873878,0.,0.,0.\PG=C02V [C2(H1C1N1B1B1C1N1),SGV(C4H6B2),SGV' (H2B2),X(H4B4)]\\

1c

1\1\GINC-LOCALHOST\FOpt\RB3LYP\def2TZVP\C7H16B10N102(1-)\PIOTR\09-Jun-2020\0\\#P B3LYP/Def2TZVP FOpt(tight) geom(noangle, nodistance) fcheck #P SCRF(Solvent=C6H5C1)\\MeCOO-B10-Pyr, C1\\-1,1\B,1.0804164208,-1.21 87652971,1.1070890628\B,-0.740329922,-1.2657466522,-0.7632646321\B,-0. 7565916018,-1.3850586438,1.0848084241\B,1.0961438223,-1.0917584315,-0. 726782887\B,1.3389591764,0.3696047156,0.3021107949\B,0.0315994571,0.16 39511408,1.5796985288\B,-1.2661450711,0.1300574412,0.2491056192\B,0.04 58415452,0.3378942592,-1.0291608421\B,-0.0609028957,1.2971591435,0.344 6350589\B,0.261707387,-2.3119606582,0.1041462952\N,-0.2089958074,2.812 5188737,0.444353181\C,0.4135331235,4.8866445946,1.4435881861\C,-1.2396 286677,4.8372365606,-0.2814757138\C,0.5281862672,3.5162034494,1.329434 963\C,-1.0814268311,3.4681541774,-0.350138461\C,-0.4831292343,5.565722 3748,0.6280614574\H,1.8971617665,-1.6414599834,1.8714859431\H,-1.47947 01545,-1.6922518563,-1.5982649966\H,-1.5101482744,-1.9188372715,1.8417 203003\H,1.9297517966,-1.4003891035,-1.5266672144\H,2.4074888671,0.906 0489685,0.3441486042\H,-0.0242244742,0.524104493,2.7193336311\H,-2.412 9340607,0.4704436936,0.2644632335\H,0.0198853493,0.8501441661,-2.11023 30884\H,1.0242996849,5.4077605696,2.1667285076\H,-1.9504173949,5.31875 67622,-0.9375429108\H,1.2064400237,2.9363042908,1.9358881891\H,-1.6413 981275,2.851531025,-1.0358103378\H,-0.5900668227,6.6395730691,0.699748 2395\0,0.5501961192,-3.7383308895,0.0211917292\C,-0.3235551203,-4.7244 591311,-0.0753511769\0,-1.5323785168,-4.5999023874,-0.1196523833\C,0.3 63106189,-6.0724471949,-0.1199013087\H,1.0887408535,-6.0976465719,-0.9 341801032\H,0.9123445813,-6.2356740052,0.8092973587\H,-0.3700253834,-6 .8640015015,-0.2532642115\\Version=ES64L-G09RevD.01\State=1-A\HF=-730. 6969465\RMSD=5.152e-09\RMSF=5.758e-06\Dipole=0.1659392.6.8391101.0.503 4113\Quadrupole=-12.4693011,19.2773616,-6.8080605,-11.1799543,3.266868 8,1.6815989\PG=C01 [X(C7H16B10N102)]\\

1d

1\1\GINC-LOCALHOST\F0pt\RB3LYP\def2TZVP\C5H13B10N4(1-)\PIOTR\08-Jun-20 20\0\\#P B3LYP/Def2TZVP FOpt(tight) geom(noangle, nodistance) fcheck # P SCRF(Solvent=C6H5C1)\\N3-B10-Pyr, Cs\\-1,1\B,-1.8077376607,0.9314216 313,0.\B,-1.5319093567,-1.6623754743,0.\B,-1.6593304863,-0.3665392084, -1.3058271082\B,-1.6593304863,-0.3665392084,1.3058271082\B,-0.27260743 ,0.7166096827,0.9218996492\B,-0.27260743,0.7166096827,-0.9218996492\B, -0.0744219853,-1.1291418232,-0.9213300603\B,-0.0744219853,-1.129141823 2,0.9213300603\B,0.8743412524,-0.0936370987,0.\B,-2.7342701789,-0.4802 922983,0.\N,2.3912357416,0.0681415344,0.\C,4.3171718598,1.4748151413,0 .\C,4.5701826663,-0.9016031704,0.\C,2.9486818463,1.2976036308,0.\C,3.1 951616169, -1.0163280221, 0.\C, 5.1485617353, 0.3616539431, 0.\H, -2.3543444 443,1.9947530888,0.\H,-1.8409178072,-2.8169078169,0.\H,-2.0858717557,-0.4108308743,-2.4211377684\H,-2.0858717557,-0.4108308743,2.4211377684\ H,0.0816593892,1.543236975,1.7102464118\H,0.0816593892,1.543236975,-1. 7102464118\H,0.4457095439,-1.8622134,-1.7102759992\H,0.4457095439,-1.8 622134,1.7102759992\H,4.7181444001,2.4781465892,0.\H,5.1731998705,-1.7 982017057,0.\H,2.2550895857,2.1240872098,0.\H,2.6912869421,-1.97031513 25,0.\H,6.2240101616,0.4761589706,0.\N,-5.8802830891,0.9761920365,0.\N ,-4.2264014444,-0.680889943,0.\N,-5.0381627199,0.2068566338,0.\\Versio n=ES64L-G09RevD.01\State=1-A'\HF=-666.3696011\RMSD=4.854e-09\RMSF=3.43 1e-06\Dipole=8.828228,0.6345435,0.\Quadrupole=-3.249954,4.5469331,-1.2 969791,4.8970199,0.,0.\PG=CS [SG(C5H7B4N4),X(H6B6)]\\

1e

1\1\GINC-LOCALHOST\FOpt\RB3LYP\def2TZVP\C5H13B10I1N1(1-)\PIOTR\08-Jun-2020\0\\#P B3LYP/Def2TZVP FOpt(tight) geom(noangle, nodistance) fcheck #P SCRF(Solvent=C6H5C1)\\I-10-B10-1-Pyridine, C2v\\-1,1\B,0.,1.308488 7025,0.1946860813\B,0.,-1.3084887025,0.1946860813\B,-1.3073036199,0.,0 .1910360634\B,1.3073036199,0.,0.1910360634\B,0.9213339253,0.9281655164 ,-1.3092657925\B,-0.9213339253,0.9281655164,-1.3092657925\B,-0.9213339 253,-0.9281655164,-1.3092657925\B,0.9213339253,-0.9281655164,-1.309265 7925\B,0.,0.,-2.3619994742\B,0.,0.,1.2522136357\N,0.,0.,-3.8884389127\ C,0.,1.1952338999,-5.9512014671\C,0.,-1.1952338999,-5.9512014671\C,0., 1.1637444054,-4.571621822\C,0.,-1.1637444054,-4.571621822\C,0.,0.,-6.6 593669486\H,0.,2.4251330905,0.617043076\H,0.,-2.4251330905,0.617043076 \H,-2.4261113355,0.,0.6072255676\H,2.4261113355,0.,0.6072255676\H,1.71 02825143,1.7108319317,-1.7503082961\H,-1.7102825143,1.7108319317,-1.75 03082961\H,-1.7102825143,-1.7108319317,-1.7503082961\H,1.7102825143,-1 .7108319317,-1.7503082961\H,0.,2.1503378405,-6.4563425053\H,0.,-2.1503 378405,-6.4563425053\H,0.,2.0585106433,-3.9687157131\H,0.,-2.058510643 3,-3.9687157131\H,0.,0.,-7.7409162847\I,0.,0.,3.4625967941\\Version=ES 64L-G09RevD.01\State=1-A1\HF=-799.916861\RMSD=4.791e-09\RMSF=1.244e-06 \Dipole=0.,0.,-7.133442\Ouadrupole=-14.1375417,-5.547559,19.6851007,0. ,0.,0.\PG=C02V [C2(H1C1N1B1B1I1),SGV(C4H6B2),SGV'(H2B2),X(H4B4)]\\

1f

1\1\GINC-LOCALHOST\FOpt\RB3LYP\def2TZVP\C6H13B10N2S1(1-)\PIOTR\08-Jun-2020\0\\#P B3LYP/Def2TZVP FOpt(tight) geom(noangle, nodistance) fcheck #P SCRF(Solvent=C6H5C1)\\Pr-B10-SCN, C1\\-1,1\B,-1.4891923647,0.98977 44612,0.0337291382\B,-1.2516372038,-1.608813999,-0.0411468462\B,-1.355 9087,-0.2721780335,-1.3138328358\B,-1.3508023465,-0.3472077526,1.30633 83519\B,0.0503390708,0.7164602495,0.9496802946\B,0.0467289864,0.769494 0932,-0.9023508485\B,0.2149778549,-1.0717868316,-0.9537882267\B,0.2185 803007,-1.1247284146,0.8950132654\B,1.1804279499,-0.0811025878,-0.0021 389336\B,-2.4181870121,-0.4017371711,-0.0043081457\N,2.7000139973,0.06 2448218,-0.0009903805\C,4.6395774503,1.4473014133,0.0348927869\C,4.865 9778163,-0.9318319392,-0.0336914102\C,3.2692901371,1.2854256081,0.0329 280692\C,3.4897142962,-1.0311217656,-0.0338522352\C,5.4575811573,0.324 8101067,0.0011478631\H,-2.0038309339,2.0652357324,0.0655296482\H,-1.57 09246742,-2.7597582827,-0.0734827297\H,-1.7857538229,-0.2832325284,-2. 4270882702\H,-1.7763114631,-0.4219972571,2.4188019569\H,0.419043276,1. 5150708999,1.7586955166\H,0.412370071,1.6131324817,-1.6657696166\H,0.7 227760413,-1.7911000642,-1.7620334902\H,0.7294422034,-1.8890573396,1.6 587882807\H,5.0522359652,2.4454045764,0.0626757419\H,5.4596489414,-1.8 341411511,-0.0606928124\H,2.5837613531,2.118229422,0.0581176439\H,2.97 39698337,-1.9784858342,-0.0599814969\H,6.5342506578,0.4272783581,0.001 9837388\S,-4.2743199077,-0.7464703289,-0.0105553497\C,-4.9762631134,0. 7826791822,0.0345650515\N,-5.525155818,1.804495478,0.0648712803\\Versi on=ES64L-G09RevD.01\State=1-A\HF=-993.2098756\RMSD=4.406e-09\RMSF=2.61 4e-06\Dipole=9.3312846,-0.454897,-0.0311838\Quadrupole=-2.3300942,2.78 48345,-0.4547403,14.5009577,0.4185479,0.0647394\PG=C01 [X(C6H13B10N2S1)] \ \

1g

1\1\GINC-LOCALHOST\FOpt\RB3LYP\def2TZVP\C5H13B10Br1N1(1-)\PIOTR\08-Jun -2020\0\\#P B3LYP/Def2TZVP FOpt(tight) geom(noangle, nodistance) fchec k #P SCRF(Solvent=C6H5C1)\\Br-10-B10-1-Pyridine, C2v\\-1,1\B,0.,1.3075 844996,0.8105272142\B,0.,-1.3075844996,0.8105272142\B,-1.306388181,0., 0.8067369507\B,1.306388181,0.,0.8067369507\B,0.9212222673,0.9283358453 ,-0.692900286\B,-0.9212222673,0.9283358453,-0.692900286\B,-0.921222267 3,-0.9283358453,-0.692900286\B,0.9212222673,-0.9283358453,-0.692900286 \B,0.,0.,-1.7458288516\B,0.,0.,1.870244177\N,0.,0.,-3.271858312\C,0.,1 $.1951571546, -5.334933707\C, 0., -1.1951571546, -5.334933707\C, 0., 1.1636753565, -3.9553555323\C, 0., -1.1636753565, -3.9553555323\C, 0., 0., -6.0432650542\H, 0., 2.4226850355, 1.2378344777\H, 0., -2.4226850355, 1.2378344777\H, -2.4237497831, 0., 1.2277211955\H, 2.4237497831, 0., 1.2277211955\H, 1.7102321139, 1.711038855, -1.134223425\H, -1.7102321139, -1.711038855, -1.134223425\H, 1.7102321139, -1.711038855, -1.134223425\H, 1.7102321139, -1.711038855, -1.134223425\H, 0., 2.1503180272, -5.8399972346\H, 0., -2.1503180272, -5.8399972346\H, 0., -2.0584426554, -3.3524644192\H, 0., -2.0584426554, -3.3524644192\H, 0., -2.0584426554, -3.3524644192\H, 0., 0., -7.1248121038\Br, 0., 0., 3.8746579192\Version=ES64L-G09RevD.01\State=1-A1\HF=-3076.3032858\RMSD=3.896e-09\RMSF=3.226e-06\Dipole=0., 0., -7.9152922\Quadrupole=-9.5859934, -1.0166478, 10.6026412, 0., 0., 0.\PG=C02V [C2(H1C1N1B1B1Br1), SGV(C4H6B2), SGV'(H2B2), X(H4B4)]\$

1h

1\1\GINC-LOCALHOST\FOpt\RB3LYP\def2TZVP\C10H18B10N2\PIOTR\10-Jun-2020\ 0\\#P B3LYP/Def2TZVP FOpt(tight) geom(noangle, nodistance) fcheck #P S CRF(Solvent=C6H5C1)\\1-Pyridine-B10-1-Pyridine, C2 staggered\\0,1\B,0. ,0.,1.800181\B,1.211733,0.497672,-0.749867\B,0.50421,-1.208205,-0.7475 6\B,-1.211733,-0.497672,-0.749867\B,-0.50421,1.208205,-0.74756\B,0.504 374,1.208136,0.74756\B,1.211666,-0.497836,0.749866\B,-0.504374,-1.2081 36,0.74756\B,-1.211666,0.497836,0.749866\B,0.,0.,-1.80018\N,0.,0.,3.32 8038\C,1.122476,0.412099,5.389164\C,-1.122476,-0.412099,5.389164\C,1.0 92883,0.401217,4.009746\C,-1.092883,-0.401217,4.009746\C,0.,0.,6.09629 5\H,2.235313,0.925638,-1.190774\H,0.925812,-2.235906,-1.184386\H,-2.23 5313,-0.925638,-1.190774\H,-0.925812,2.235906,-1.184386\H,2.018661,0.7 41063,5.894909\H,-2.018661,-0.741063,5.894909\H,0.926117,2.23578,1.184 384\H,2.235187,-0.925942,1.190773\H,-0.926117,-2.23578,1.184384\H,-2.2 35187,0.925942,1.190773\H,1.933782,0.708773,3.407764\H,-1.933782,-0.70 8773,3.407764\H,0.,0.,7.177814\N,0.,0.,-3.328037\C,-1.092883,0.401217, -4.009746\C,1.092883,-0.401217,-4.009746\C,-1.122476,0.412098,-5.38916 4\C,1.122476,-0.412098,-5.389164\C,0.,0.,-6.096295\H,-1.933783,0.70877 ,-3.407763\H,1.933783,-0.70877,-3.407763\H,-2.018662,0.741061,-5.89490 9\H,2.018662,-0.741061,-5.894909\H,0.,0.,-7.177814\\Version=ES64L-G09R evD.01\State=1-A\HF=-750.360128\RMSD=8.858e-09\RMSF=2.099e-07\Dipole=0 .,0.,0.0000051\Quadrupole=-25.7824445,-39.1612049,64.9436494,0.0000234 ,0.,0.\PG=C02 [C2(H1C1N1B1B1N1C1H1),X(C8H16B8)]\\

1i

1\1\GINC-LOCALHOST\F0pt\RB3LYP\def2TZVP\C7H18B10N101(1-)\PIOTR\11-Jun-2020\0\\#P B3LYP/Def2TZVP FOpt(tight) geom(noangle, nodistance) fcheck #P SCRF(Solvent=C6H5Cl)\\EtO-B10-Pyr, C1\\-1,1\B,0.1358761853,-1.8237 600199,0.3373681657\B,-2.0469735733,-0.4350330077,0.1035907565\B,-1.00 60301653,-0.9894656793,1.5162169933\B,-0.888274839,-1.2409555839,-1.07 72468286\B,0.6755335911,-0.4448492598,-0.70091985\B,0.5921210689,-0.26 67052014,1.1361718426\B,-0.9650579165,0.7222298436,0.9673950832\B,-0.8 818407987,0.5445031607,-0.8653940079\B,0.4267085835,1.0248963997,0.074 3369402\B,-1.5465472504,-2.0457958139,0.2825092466\N,1.2498474853,2.30 22897929,-0.0121580277\C,3.3703179425,3.3962206145,-0.0219579713\C,1.3 635997101,4.6751854141,-0.2370933517\C,2.5982872979,2.2553726836,0.053 6166694\C,0.6437707702,3.5009005797,-0.1559061465\C,2.7509308796,4.631 5158146,-0.1698677178\H,0.8571905418,-2.7696415683,0.4618420804\H,-3.2 177905387,-0.1990770366,0.0275492652\H,-1.2908460289,-1.244889326,2.65 00911631\H,-1.0723543564,-1.7115224404,-2.1620111073\H,1.6092288367,-0 .5716547116, -1.4394803877\H, 1.4545982595, -0.2414096426, 1.9661304871\H, -1.4237043153,1.5871791897,1.6561528374\H,-1.2692509831,1.2573123291,-.610051177,-0.3517988728\H,3.022956974,1.270191882,0.1684317196\H,-0.4 338387305,3.4739275834,-0.2022188246\H,3.3359397966,5.5390558664,-0.23 13100677\0,-2.3708777196,-3.2055179327,0.3575397079\C,-1.7658950576,-4 .4702694535,0.507645245\H,-1.0798002778,-4.6674471057,-0.3283235615\H,

-1.1593692118,-4.4975274928,1.4240689894\C,-2.8365787027,-5.5461880917 ,0.5633555073\H,-2.3826075374,-6.5335892587,0.6797119338\H,-3.51076594 53,-5.3765670157,1.4058459921\H,-3.4308987149,-5.5471218631,-0.3530902 472\\Version=ES64L-G09RevD.01\State=1-A\HF=-656.6122796\RMSD=3.131e-09 \RMSF=1.193e-06\Dipole=4.1976635,5.2785577,-0.3212765\Quadrupole=-2.86 04173,13.8530598,-10.9926425,5.4689469,-0.1517784,-2.1807895\PG=C01 [X (C7H18B10N101)]\\

1j

1\1\GINC-LOCALHOST\FOpt\RB3LYP\def2TZVP\C9H21B10N2O1(1-)\PIOTR\24-Jul-2020\0\\#P B3LYP/Def2TZVP FOpt(tight) geom(noangle, nodistance) fcheck #P SCRF(Solvent=C6H5C1)\\10-Morpholine=B10-1-Pyr, C1\\-1,1\B,0.579518 8228,1.2589203811,-0.2041976106\B,0.564172622,-1.2662950425,0.37064637 91\B,0.5274510673,0.2835290919,1.3522418076\B,0.5770784472,-0.28887525 55,-1.189263775\B,-0.9193302519,0.694333869,-1.0522606376\B,-0.9471312 767,1.1052073062,0.747571107\B,-0.9643688737,-0.6977711737,1.156954791 4\B,-0.9220891125,-1.1096807832,-0.6430749002\B,-1.9955254092,-0.00128 14681,0.0305492246\B,1.6704180548,-0.0075469912,0.1065087321\N,-3.5166 527446,0.0024045754,-0.0028763259\C,-5.5759472087,1.1924562265,-0.2025 435661\C, -5.5888906749, -1.1776950941, 0.0964509202\C, -4.1973466828, 1.15 84418211,-0.1653786335\C,-4.2099425047,-1.1503215359,0.1265664791\C,-6 .2927237002,0.0090377024,-0.0704911317\H,0.994155204,2.3544914309,-0.4 477668062\H,0.9689197897,-2.3636186602,0.6270755999\H,0.9368095158,0.5 272514699,2.4497874061\H,1.020621225,-0.5374208551,-2.2728520685\H,-1. 337087433,1.2889179957,-2.0036081298\H,-1.3957018684,2.0478596386,1.33 39806527\H,-1.4197714588,-1.2900523137,2.0922627769\H,-1.3481002238,-2 .0522512811,-1.2460634772\H,-6.0748324563,2.1418243148,-0.3352088512\H ,-6.0982136591,-2.1246588127,0.2042939635\H,-3.5904641248,2.0450996881 ,-0.2633222239\H,-3.6126883096,-2.0399550371,0.2528425593\H,-7.3738557 119,0.0115781549,-0.0970634696\N,3.1565207481,-0.0214162532,0.15702167 9\C,3.8529847344,-1.1431134913,-0.4487665476\C,3.8668773566,1.21746509 24,-0.1038123384\C,5.2977395941,-1.2044772911,0.024715216\C,5.31342754 91,1.123484023,0.3594571097\0,5.9883080054,0.0169957249,-0.2389919571\ H,3.854690997,-1.0765461156,-1.553701633\H,3.3473082171,-2.0726034697, -0.1822718491\H,3.8615762799,1.4758485509,-1.180752074\H,3.3768773283, 2.0382190402,0.4222655849\H,5.8492604334,-1.987443065,-0.4997466512\H, 5.3255609859,-1.4133471454,1.1036593326\H,5.8748799474,2.0154052934,0. 0740137525\H,5.3447707603,1.0211437441,1.4537515833\\Version=ES64L-G09 RevD.01\State=1-A\HF=-789.4010982\RMSD=1.449e-09\RMSF=3.651e-06\Dipole =-5.6405819,0.0000928,-0.108825\Quadrupole=16.229585,-2.0542117,-14.17 53733,-0.2221418,2.660466,-0.5119114\PG=C01 [X(C9H21B10N2O1)]\\

1k

1\1\GINC-LOCALHOST\FOpt\RB3LYP\def2TZVP\C9H22B10N2O1\PIOTR\11-Jun-2020 \0\\#P B3LYP/Def2TZVP FOpt(tight) geom(noangle, nodistance) fcheck #P SCRF(Solvent=C6H5Cl)\\10-Morpholinium-B10-1-Pyr, C1\\0,1\B,0.583146734 7,1.2642189693,-0.1048693265\B,0.5437074798,-1.295202363,0.4489804355\ B,0.4994999834,0.2604059323,1.4468703438\B,0.6261805303,-0.2924328502, -1.1084473019\B,-0.8754750262,0.7000476586,-0.9990169922\B,-0.96409785 78,1.0915433465,0.8043971965\B,-0.9922460325,-0.7210689409,1.197214093 4\B,-0.9039448981,-1.1148688767,-0.6046654705\B,-1.9832445655,-0.00656 10924,0.0464278339\B,1.6107958176,-0.0219387057,0.2204909711\N,-3.5093 826512,0.0032368582,-0.0337476389\C,-5.5472883597,1.1869410981,-0.3856 881973\C,-5.5877767088,-1.1545059256,0.0987244194\C,-4.1703171558,1.14 72591968,-0.3059636437\C,-4.2097390012,-1.1322771612,0.1657733691\C,-6 .2737010833,0.0206753701,-0.1810212692\H,1.0211773617,2.3532370966,-0. 3173452119\H,0.9596003915,-2.3849236378,0.7070667762\H,0.8875373635,0. 4890911608,2.5538996399\H,1.0944460163,-0.5323565343,-2.1797417847\H,-1.2670516155,1.3003555764,-1.9539476544\H,-1.4273980897,2.0261656646,1 .3851951356\H,-1.4761456235,-1.3177257312,2.110968943\H,-1.3151771293,

-2.0453716568,-1.2295051532\H,-6.0360480316,2.124929969,-0.6057914767\ H,-6.1090764888,-2.0860077791,0.2651544867\H,-3.5540274599,2.020083267 6,-0.4555715414\H,-3.6235304029,-2.0126939847,0.3788484087\H,-7.353677 694,0.0275345612,-0.2381709747\N,3.1688117937,-0.05940355,0.3637641282 \C,3.8214190503,-1.1650099975,-0.4192235358\C,3.8472600695,1.242994207 9,0.0452582653\C,5.3226224149,-1.1706922908,-0.1923390468\C,5.34819185 69,1.1317142967,0.2486201783\0,5.9071795255,0.0805778659,-0.5267293255 \H,3.5830369791,-0.9906441094,-1.4664222042\H,3.3691590064,-2.10454015 54,-0.1094954732\H,3.6068918133,1.4789606082,-0.989745532\H,3.41826934 32,2.0107425909,0.6850696255\H,5.7852018932,-1.9213776168,-0.831783304 1\H,5.5515153319,-1.4227828182,0.8527777604\H,5.8286485059,2.055680571 2,-0.0704800073\H,5.5790308776,0.9754262034,1.3116137973\H,3.346928155 1,-0.2512267623,1.3510896584\\Version=ES64L-G09RevD.01\State=1-A\HF=-7 89.8908783\RMSD=7.000e-09\RMSF=3.835e-06\Dipole=-0.9757274,-0.0775423, 0.2895324\Quadrupole=47.9296547,-18.0394455,-29.8902092,-1.1151413,8.2 415148,-0.9988511\PG=C01 [X(C9H22B10N2O1)]\\

2b

1\1\GINC-LOCALHOST\FOpt\RB3LYP\def2TZVP\C6H13B10N2(1-)\PIOTR\07-Jun-20 20\0\\#P B3LYP/Def2TZVP FOpt(tight) geom(noangle, nodistance) fcheck # P SCRF(Solvent=C6H5C1)\\H-B10-Pyr-4-CN, Cs\\-1,1\B,0.,-1.3020545449,-3 .3603429997\B,0.,1.3020545449,-3.3603429997\B,-1.300448398,0.,-3.34960 4992\B,1.300448398,0.,-3.349604992\B,0.916624887,-0.9335051982,-1.8525 757718\B,-0.916624887,-0.9335051982,-1.8525757718\B,-0.916624887,0.933 5051982,-1.8525757718\B,0.916624887,0.9335051982,-1.8525757718\B,0.,0. ,-0.7962206136\B,0.,0.,-4.4445095992\N,0.,0.,0.7180516422\C,0.,-1.2021 61486,2.7800688883\C,0.,1.202161486,2.7800688883\C,0.,-1.1651635378,1. 4043856452\C,0.,1.1651635378,1.4043856452\C,0.,0.,3.4930894419\H,0.,-2 .4250630613,-3.7718066066\H,0.,2.4250630613,-3.7718066066\H,-2.4264974 477,0.,-3.7521505524\H,2.4264974477,0.,-3.7521505524\H,1.7071506682,-1 .7127291153,-1.4066829207\H,-1.7071506682,-1.7127291153,-1.4066829207\ H,-1.7071506682,1.7127291153,-1.4066829207\H,1.7071506682,1.7127291153 ,-1.4066829207\H,0.,-2.1548842404,3.2881346556\H,0.,2.1548842404,3.288 1346556\H,0.,-2.0612972716,0.8041457057\H,0.,2.0612972716,0.8041457057 \C,0.,0.,4.9207010544\N,0.,0.,6.0730584041\H,0.,0.,-5.63536481\\Versio n=ES64L-G09RevD.01\State=1-A1\HF=-594.9466776\RMSD=8.657e-09\RMSF=2.18 8e-06\Dipole=0.,0.,7.6608233\Quadrupole=18.8808667,28.2150628,-47.0959 296,0.,0.,0.\PG=C02V [C2(H1B1B1N1C1C1N1),SGV(C4H6B2),SGV'(H2B2),X(H4B4)] \ \

21

1\1\GINC-LOCALHOST\FOpt\RB3LYP\def2TZVP\C8H18B10N102(1-)\PIOTR\08-Jun-2020\0\\#P B3LYP/Def2TZVP FOpt(tight) geom(noangle, nodistance) fcheck #P SCRF(Solvent=C6H5C1)\\H-B10-Pyr-4-COOEt, Cs\\-1,1\B,-4.434842104,-1.5612365607,0.\B,-4.7414365266,1.0236797498,0.\B,-4.5790094736,-0.268 7221124,1.3001563267\B,-4.5790094736,-0.2687221124,-1.3001563267\B,-2. 9803266574,-1.0165586877,-0.9170887216\B,-2.9803266574,-1.0165586877,0 .9170887216\B,-3.2000348341,0.8330897055,0.9176141208\B,-3.2000348341, 0.8330897055,-0.9176141208\B,-2.0408010196,0.0331189839,0.\B,-5.664737 3144,-0.3971096807,0.\N,-0.5312888131,0.2026021192,0.\C,1.6503715891,-0.7639928693,0.\C,1.3909664438,1.6134656394,0.\C,0.2773772343,-0.87952 91049,0.\C,0.0254264733,1.434284685,0.\C,2.2317779138,0.5025987655,0.\ H,-4.7106610545,-2.7256335523,0.\H,-5.2827433728,2.0908852577,0.\H,-4. 9791082529,-0.3158075442,2.426731787\H,-4.9791082529,-0.3158075442,-2. 426731787\H,-2.4489428537,-1.7406151537,-1.7078377682\H,-2.4489428537, -1.7406151537,1.7078377682\H,-2.8526135499,1.6618840958,1.7076859812\H *,*−2.8526135499,1.6618840958,−1.7076859812\H,2.256110832,−1.6568754075, 0.\H,1.8036203544,2.6114488087,0.\H,-0.2226796182,-1.8352459368,0.\H,-0.6684064709,2.2603417274,0.\C,3.7114711665,0.7150990145,0.\0,4.226078 6174,1.8102690174,0.\0,4.3876350267,-0.4352805235,0.\C,5.8377570929,-0

.3478375925,0.\C,6.3838393668,-1.75548982,0.\H,6.1456396601,0.21222724 28,0.8833166255\H,6.1456396601,0.2122272428,-0.8833166255\H,7.47434779 99,-1.7183775372,0.\H,6.0605524211,-2.3025729246,0.8864172948\H,6.0605 524211,-2.3025729246,-0.8864172948\H,-6.8479611358,-0.5390333945,0.\\V ersion=ES64L-G09RevD.01\State=1-A'\HF=-769.9781351\RMSD=5.839e-09\RMSF =3.063e-06\Dipole=12.2715934,-0.1028072,0.\Quadrupole=-52.8752088,27.8 776212,24.9975876,-14.8203375,0.,0.\PG=CS [SG(C8H8B4N102),X(H10B6)]\\

2m

1\1\GINC-LOCALHOST\FOpt\RB3LYP\def2TZVP\C6H16B10N1(1-)\PIOTR\07-Jun-20 20\0\\#P B3LYP/Def2TZVP FOpt(tight) geom(noangle, nodistance) fcheck # P SCRF(Solvent=C6H5C1)\\H-B10-Pyr-4-Me, Cs\\-1,1\B,-0.003447364,-3.129 0783316,1.300737025\B,-0.003447364,-3.1290783316,-1.300737025\B,-1.302 8134031,-3.1230074811,0.\B,1.2959583375,-3.1288215819,0.\B,0.919636602 6,-1.6233721103,0.9265702591\B,-0.9199177126,-1.6193027493,0.926553567 7\B,-0.9199177126,-1.6193027493,-0.9265535677\B,0.9196366026,-1.623372 1103,-0.9265702591\B,0.0022244297,-0.565027593,0.\B,-0.0058052276,-4.2 165865981,0.\N,0.0043340865,0.9619936808,0.\C,0.009572441,3.0290791368 ,1.1884684543\C,0.009572441,3.0290791368,-1.1884684543\C,0.0067454415, $1.6515165391, 1.1593999794 \ C, 0.0067454415, 1.6515165391, -1.1593999794 \ C,$ 0.0085254115,3.7611245323,0.\H,-0.004382721,-3.5381541443,2.4258991544 \H,-0.004382721,-3.5381541443,-2.4258991544\H,-2.4309061738,-3.5235286 397,0.\H,2.4223025909,-3.5342229271,0.\H,1.7111987065,-1.1854285806,1. 7110942248\H,-1.7094606291,-1.177629486,1.7110257545\H,-1.7094606291,-1.177629486,-1.7110257545\H,1.7111987065,-1.1854285806,-1.7110942248\H ,0.0150339978,3.5294395141,2.1473370671\H,0.0150339978,3.5294395141,-2 .1473370671\H,0.0085376675,1.0532205087,2.0574912414\H,0.0085376675,1. 0532205087,-2.0574912414\C,-0.0179191199,5.2599290689,0.\H,0.468930373 ,5.6650700684,-0.8868129662\H,-1.0518090246,5.6170431833,0.\H,0.468930 373,5.6650700684,0.8868129662\H,-0.008677236,-5.4086621252,0.\\Version =ES64L-G09RevD.01\State=1-A'\HF=-542.0071681\RMSD=3.981e-09\RMSF=5.623 e-07\Dipole=-0.0118572,10.4272318,0.\Ouadrupole=3.9177474,-15.801702,1 1.8839546,-0.2532979,0.,0.\PG=CS [SG(C2H4B4N1),X(C4H12B6)]\\

2n

1\1\GINC-LOCALHOST\F0pt\RB3LYP\def2TZVP\C6H16B10N101(1-)\PIOTR\07-Jun-2020\0\\#P B3LYP/Def2TZVP FOpt(tight) geom(noangle, nodistance) fcheck #P SCRF(Solvent=C6H5C1)\\H-B10-Pyr-4-OMe, Cs\\-1,1\B,-1.2034363557,3. 5842673187,0.\B,1.3945565789,3.4587067439,0.\B,0.0945778481,3.51947717 88,1.299298061\B,0.0945778481,3.5194771788,-1.299298061\B,-0.902478461 7,2.0597228851,-0.9202895163\B,-0.9024784617,2.0597228851,0.9202895163 \B,0.9459693605,1.9710571116,0.9205283525\B,0.9459693605,1.9710571116, -0.9205283525\B,-0.0291085865,0.9599838687,0.\B,0.1473080683,4.6075953 27,0.\N,-0.1079581575,-0.567812991,0.\C,-1.4162889887,-2.5637290164,0. \C,0.9801500058,-2.697984536,0.\C,-1.3059185725,-1.1978275607,0.\C,1.0 081979325,-1.3199766554,0.\C,-0.2566608966,-3.3496868735,0.\H,-2.30778 67054,4.0473685595,0.\H,2.5383293526,3.8138644399,0.\H,0.1145427701,3. 9222404916,2.4267530529\H,0.1145427701,3.9222404916,-2.4267530529\H,-1 .7090283817,1.6621602202,-1.7114007869\H,-1.7090283817,1.6621602202,1. 7114007869\H,1.7105283842,1.4947499913,1.7100853256\H,1.7105283842,1.4 947499913,-1.7100853256\H,-2.3896097824,-3.0325342758,0.\H,1.915184731 ,-3.2354271735,0.\H,-2.1714745996,-0.553658823,0.\H,1.9392301282,-0.77 39092391,0.\0,-0.4277695212,-4.6761053101,0.\C,0.7232812836,-5.5294473 998,0.\H,1.3265884788,-5.3665594862,0.894451734\H,0.3343193177,-6.5432 060678,0.\H,1.3265884788,-5.3665594862,-0.894451734\H,0.2031708399,5.7 989498002,0.\\Version=ES64L-G09RevD.01\State=1-A'\HF=-617.2492628\RMSD =7.815e-09\RMSF=4.124e-06\Dipole=0.2357671,-11.565461,0.\Quadrupole=15 .764201,-23.2571054,7.4929045,-7.1869357,0.,0.\PG=CS [SG(C6H8B4N101),X (H8B6)]\\

3

1\1\GINC-LOCALHOST\FOpt\RB3LYP\def2TZVP\C8H17B10N2O1(1-)\PIOTR\17-Sep-
2020\0\\#P B3LYP/Def2TZVP FOpt(tight) geom(noangle, nodistance) fcheck
<pre>#P SCRF(Solvent=C6H5Cl)\\EtO-B10-PyrCN, C1\\-1,1\B,-1.5442997689,-1.0</pre>
711618168,0.000003701\B,-1.3707975781,1.5245495222,-0.0000003693\B,-1.
434084936,0.2258069744,1.305500507\B,-1.434086329,0.2258029773,-1.3054
972082\B,-0.0161019041,-0.8019107374,-0.9192191665\B,-0.0161008544,-0.
8019079394,0.9192240696\B,0.1068614873,1.0616552393,0.9174193008\B,0.1
068605328,1.0616524734,-0.9174201346\B,1.1022088323,0.0583718263,0.000
0005318\B,-2.5462885412,0.3006784364,0.0000021131\N,2.604827666,-0.040
4010379,-0.0000002476\C,4.5877351884,-1.373704468,-0.0000000758\C,4.74
37924619,1.0250930459,-0.0000029369\C,3.2188168787,-1.2488615337,0.000
0007405\C,3.3701204868,1.0783289924,-0.0000020469\C,5.3806552493,-0.22
0674407,-0.0000019594\H,-2.0334565619,-2.1613917671,0.0000058036\H,-1.
7290600473,2.6651109355,-0.000001985\H,-1.8655357597,0.2550866298,2.41
98544917\H,-1.8655383382,0.2550791747,-2.4198508272\H,0.3754182123,-1.
6108229782,-1.7081751194\H,0.3754201091,-1.6108177195,1.7081821182\H,0
.6030947595,1.8110252229,1.706067737\H,0.6030929054,1.8110200234,-1.70
6071442\H,5.0321796095,-2.3578459886,0.0000007515\H,5.3117641473,1.943
4980211,-0.000004413\H,2.5626848897,-2.1048683013,0.0000022012\H,2.830
7689519,2.0122827873,-0.000002766\0,-3.9550526018,0.4615677007,0.00000
24946\C,-4.7849411587,-0.6813189777,-0.000000385\H,-4.5749647118,-1.30
26724597,-0.8813178804\H,-4.5749718636,-1.3026716277,0.8813194597\C,-6
.2420335114,-0.2545515273,-0.000006641\H,-6.8965894211,-1.129667275,-0
.0000083511\H,-6.4692446213,0.344330246,0.8846118572\H,-6.4692374457,0
.3443283905,-0.8846282439\C,6.8033356829,-0.3126822493,-0.000002889\N,
7.953976923,-0.387340018,-0.0000036344\\Version=ES64L-G09RevD.01\State
=1-A\HF=-748.887503\RMSD=1.904e-09\RMSF=1.123e-06\Dipole=4.6863855,-0.
9816561,-0.0000052\Quadrupole=-28.9761375,18.5497268,10.4264107,8.7065
542,0.0000408,-0.0000161\PG=C01 [X(C8H17B10N2O1)]\\

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 $(X = CN, [OCRNMe_2]^+, OCOR, and [OH_2]^+)$ derivatives, *Eur. J. Inorg. Chem.*, 2020, 3083-3093.

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