

Electronic Supplementary Information for:

A General Method for the Synthesis of Covalent and Ionic Amine Borane Complexes Containing Trinitromethyl Fragments

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Table S1. The chemical shift of hydrides in BH₂ group in 3a-3g in ¹H NMR^a.

Entry	Comps.	A	¹ H NMR (ppm)
1	3a	NH ₃	2.61
2	3b	CH ₃ NH ₂	2.53
3	3c	(CH ₃) ₂ NH	2.47
4	3d	(CH ₃) ₃ N	-
5	3e	(NH ₂ CH ₂) ₂	2.02 ^b
6	3f	(CH ₃) ₃ N	-
7	3g	(NH ₃) ₂	2.56

^a "A" is a Lewis base; ^b molecular formula [NH₂CH₂BH₂C(NO₂)₃]₂.

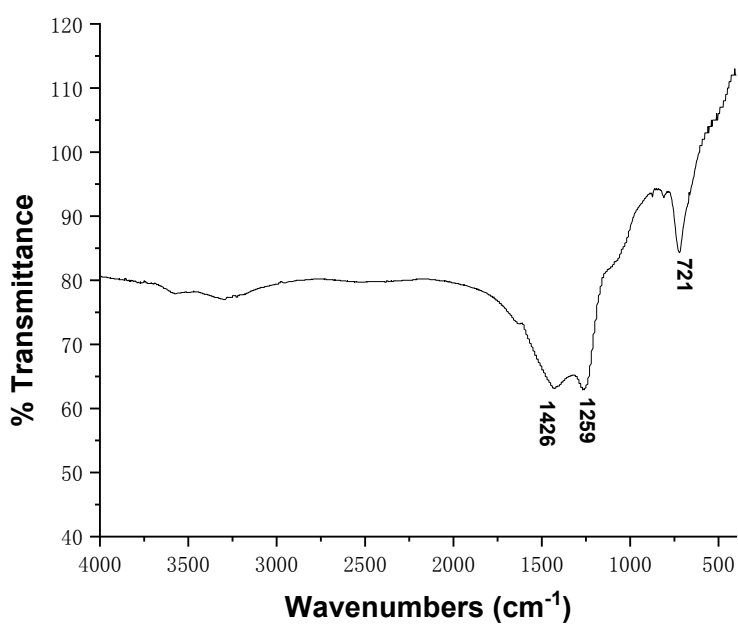


Fig. S1. IR spectrum of the residue from the TGA-MS experiment of NH₃BH₂C(NO₂)₃ (3a) (The spectrum is similar to that of B₂O₃).

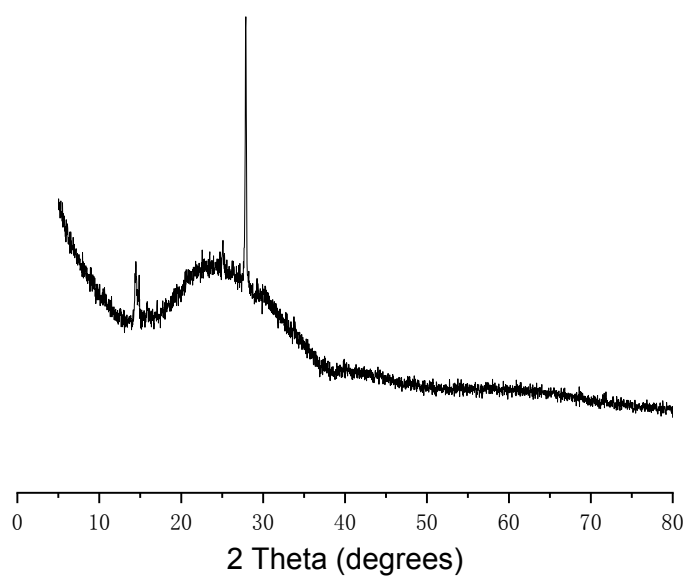


Fig. S2. X-ray powder diffraction pattern of the residue from the TGA-MS experiment of $\text{NH}_3\text{BH}_2\text{C}(\text{NO}_2)_3$ (3a) (The peaks are related to B_2O_3).

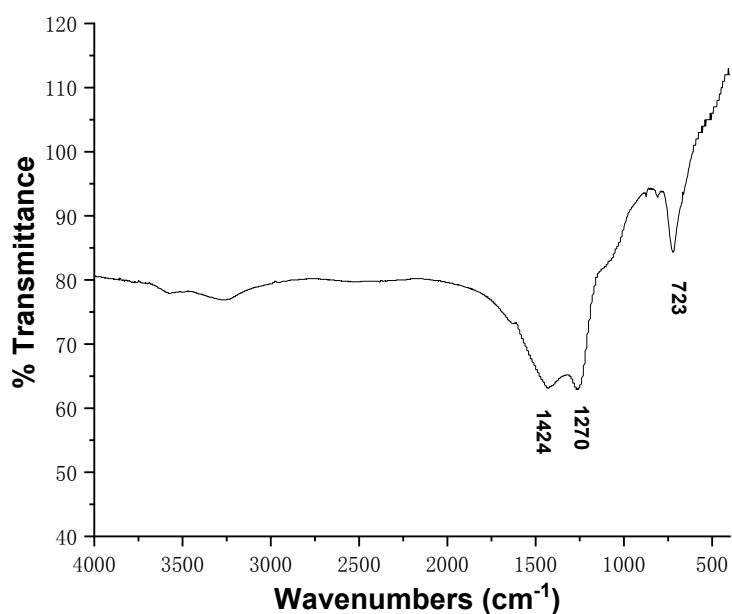


Fig. S3. IR spectrum of the residue from the TGA-MS experiment of $[\text{H}_2\text{B}(\text{NH}_3)_2][\text{C}(\text{NO}_2)_3]$ (3g) (The spectrum is similar to that of B_2O_3).

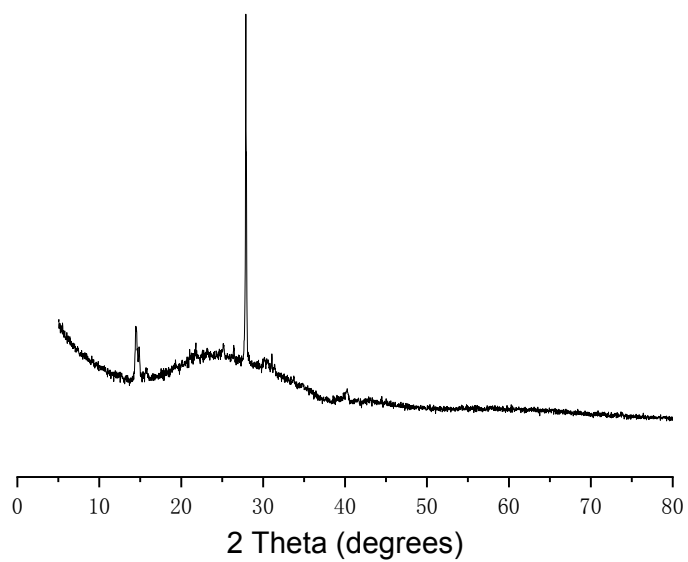


Fig. S4. X-ray powder diffraction pattern of the residue from the TGA-MS experiment of $[\text{H}_2\text{B}(\text{NH}_3)_2][\text{C}(\text{NO}_2)_3]$ (3g) (The peaks are related to B_2O_3).

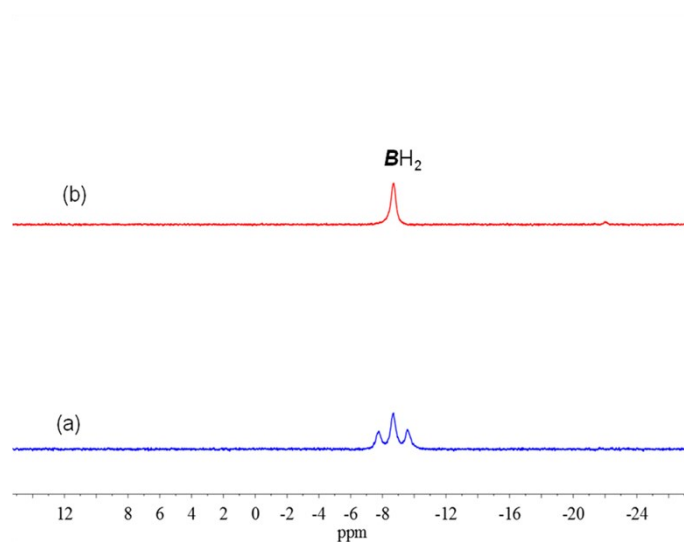


Fig. S5. ^{11}B (a) and $^{11}\text{B}\{^1\text{H}\}$ NMR (b) spectra of $\text{NH}_3\text{BH}_2\text{Cl}$ (1a) in THF.

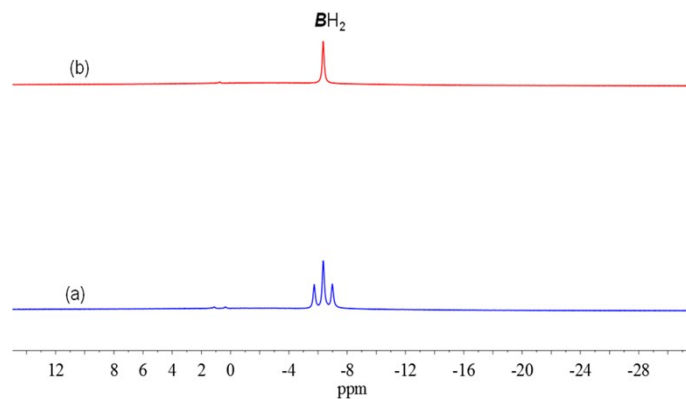


Fig. S6. ^{11}B (a) and $^{11}\text{B}\{^1\text{H}\}$ NMR (b) spectra of $\text{CH}_3\text{NH}_2\text{BH}_2\text{Cl}$ (1b) in THF.

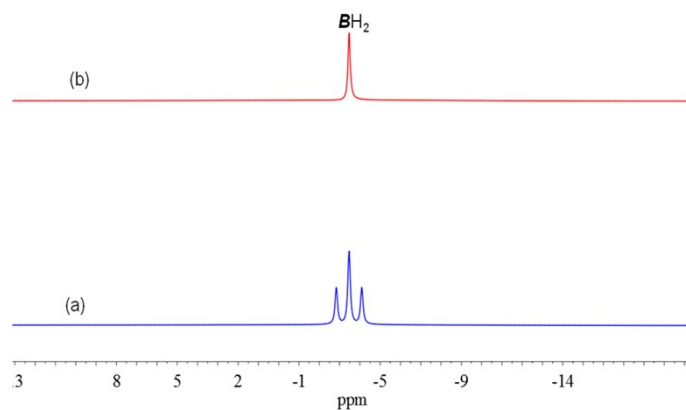


Fig. S7. ^{11}B (a) and $^{11}\text{B}\{^1\text{H}\}$ NMR (b) spectra of $(\text{CH}_3)_2\text{NHBH}_2\text{Cl}$ (1c) in THF.

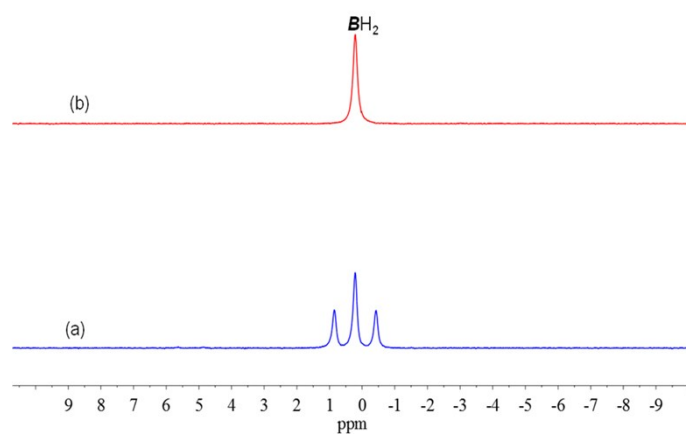


Fig. S8. ^{11}B (a) and $^{11}\text{B}\{^1\text{H}\}$ NMR (b) spectra of $(\text{CH}_3)_3\text{NBH}_2\text{Cl}$ (1d) in THF.

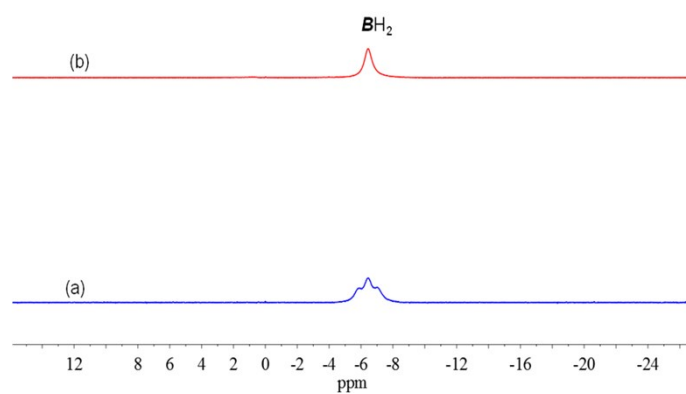


Fig. S9. ^{11}B (a) and $^{11}\text{B}\{^1\text{H}\}$ NMR (b) spectra of $\text{ClBH}_2\text{NH}_2\text{CH}_2\text{CH}_2\text{NH}_2\text{BH}_2\text{Cl}$ (1e) in THF.

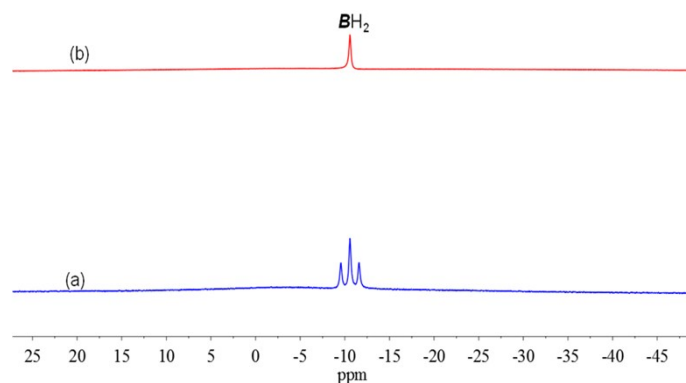


Fig. S10. ^{11}B (a) and $^{11}\text{B}\{^1\text{H}\}$ NMR (b) spectra of $(\text{CH}_3)_3\text{NBH}_2\text{I}$ (1f) in toluene.

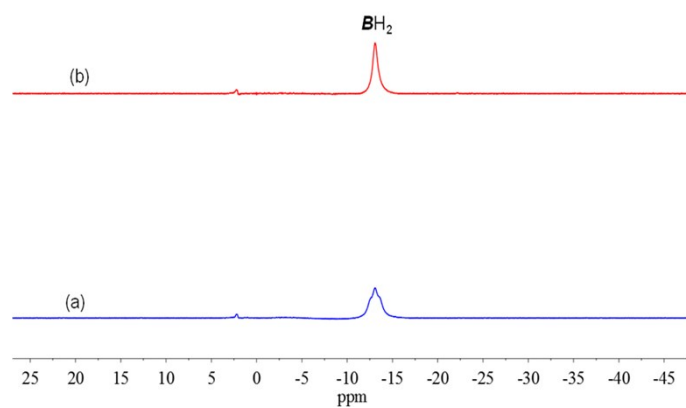


Fig. S11. ^{11}B (a) and $^{11}\text{B}\{^1\text{H}\}$ NMR (b) spectra of $(\text{NH}_3)_2\text{BH}_2\text{Cl}$ (1g) in DMF.

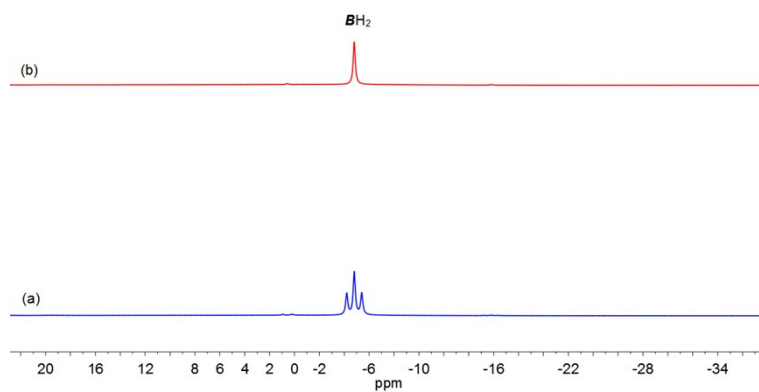


Fig. S12. ^{11}B (a) and $^{11}\text{B}\{^1\text{H}\}$ NMR (b) spectra of $\text{NH}_3\text{BH}_2\text{C}(\text{NO}_2)_3$ (3a) in CD_3CN .

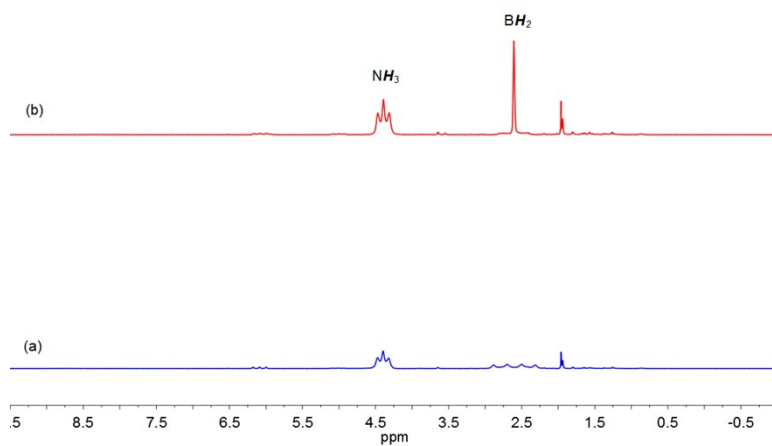


Fig. S13. ^1H (a) and $^1\text{H}\{^{11}\text{B}\}$ NMR (b) spectra of $\text{NH}_3\text{BH}_2\text{C}(\text{NO}_2)_3$ (3a) in CD_3CN .

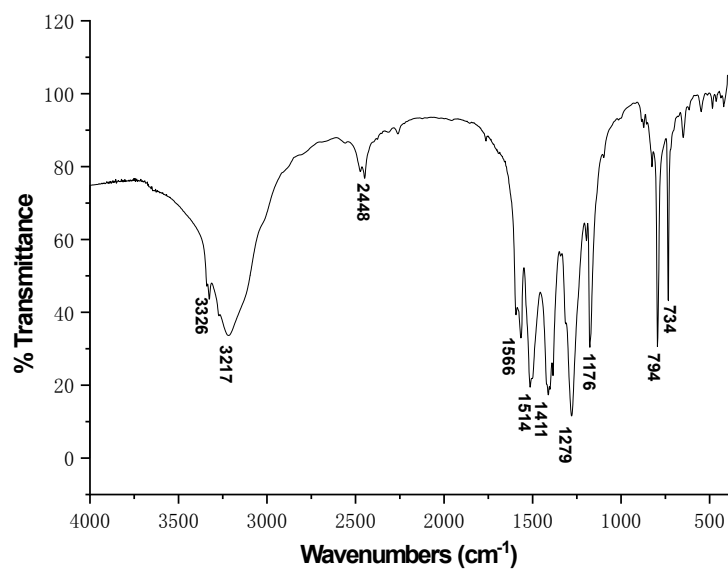


Fig. S14. IR spectrum of $\text{NH}_3\text{BH}_2\text{C}(\text{NO}_2)_3$ (3a).

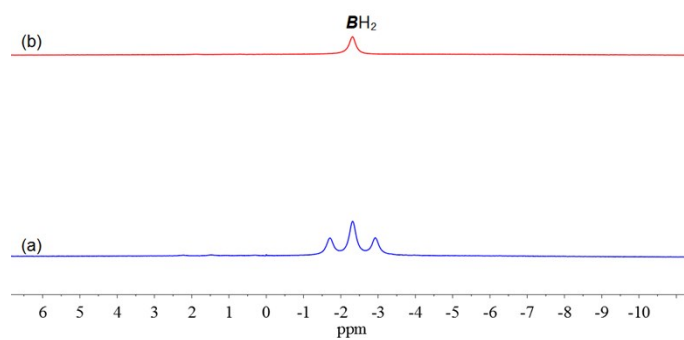


Fig. S15. ^{11}B (a) and $^{11}\text{B}\{^1\text{H}\}$ NMR (b) spectra of $\text{CH}_3\text{NH}_2\text{BH}_2\text{C}(\text{NO}_2)_3$ (3b) in CD_3CN .

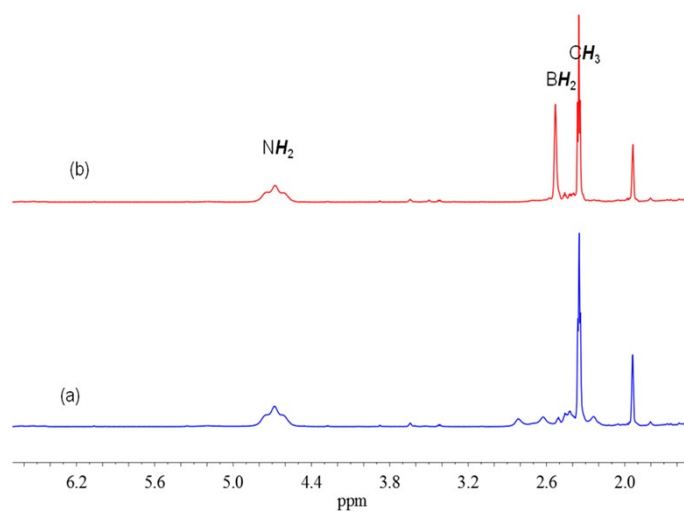


Fig. S16. ^1H (a) and $^1\text{H}\{^{11}\text{B}\}$ NMR (b) spectra of $\text{CH}_3\text{NH}_2\text{BH}_2\text{C}(\text{NO}_2)_3$ (3b) in CD_3CN .

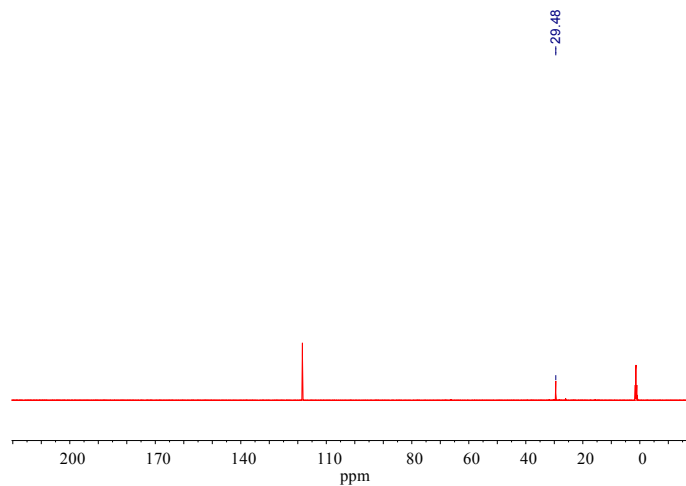


Fig. S17. ^{13}C NMR spectrum of $\text{CH}_3\text{NH}_2\text{BH}_2\text{C}(\text{NO}_2)_3$ (**3b**) in CD_3CN .

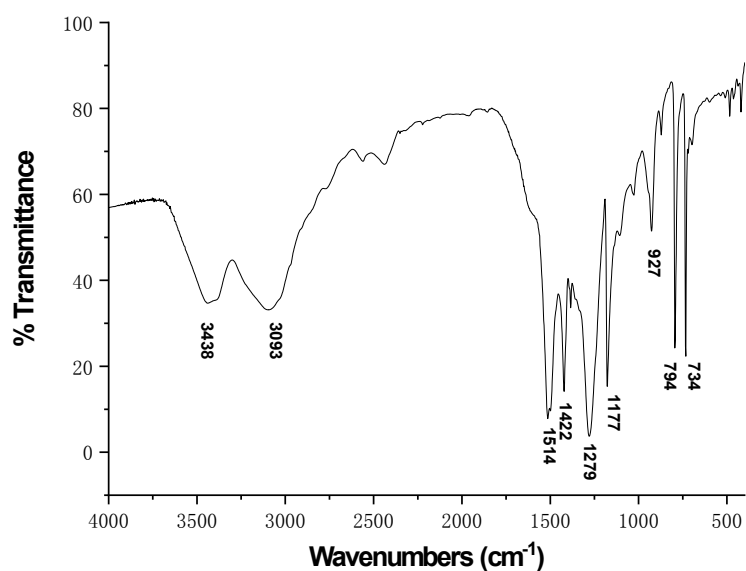


Fig. S18. IR spectrum of $\text{CH}_3\text{NH}_2\text{BH}_2\text{C}(\text{NO}_2)_3$ (**3b**).

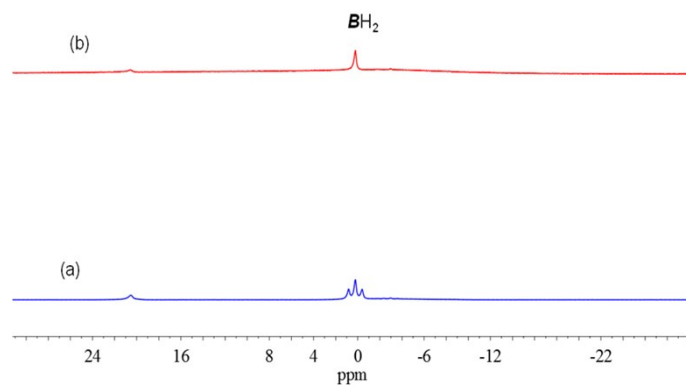


Fig. S19. ^{11}B (a) and $^{11}\text{B}\{^1\text{H}\}$ NMR (b) spectra of $(\text{CH}_3)_2\text{NHBH}_2\text{C}(\text{NO}_2)_3$ (**3c**) in CD_3CN .

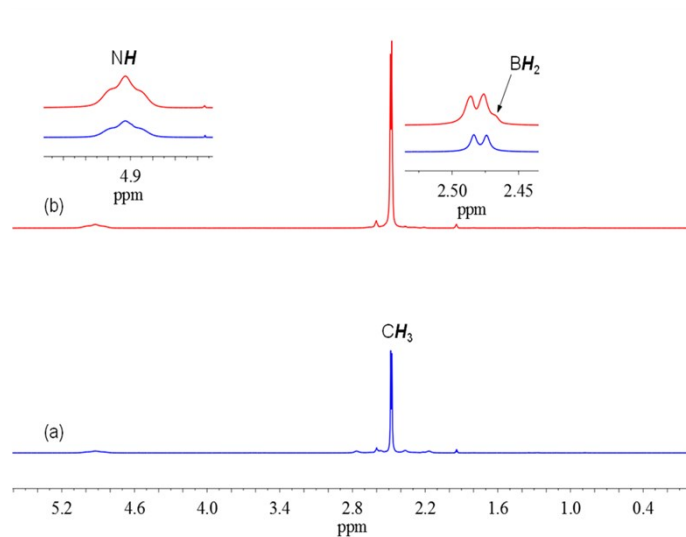


Fig. S20. ^1H (a) and $^1\text{H}\{^{11}\text{B}\}$ NMR (b) spectra of $(\text{CH}_3)_2\text{NHBH}_2\text{C}(\text{NO}_2)_3$ (**3c**) in CD_3CN .

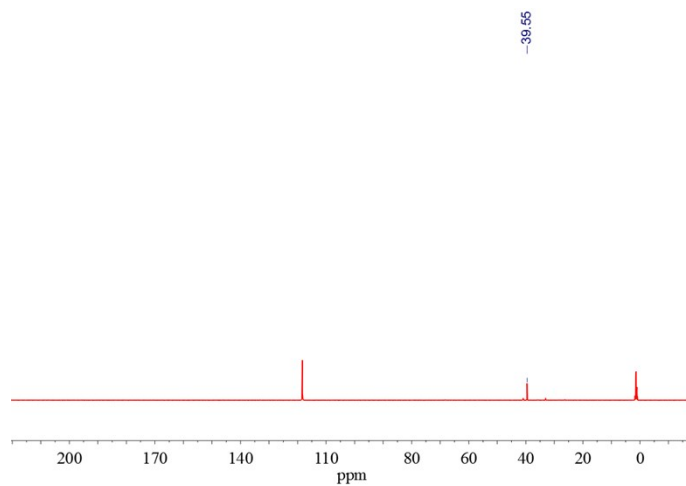


Fig. S21. ^{13}C NMR spectrum of $(\text{CH}_3)_2\text{NHBH}_2\text{C}(\text{NO}_2)_3$ (**3c**) in CD_3CN .

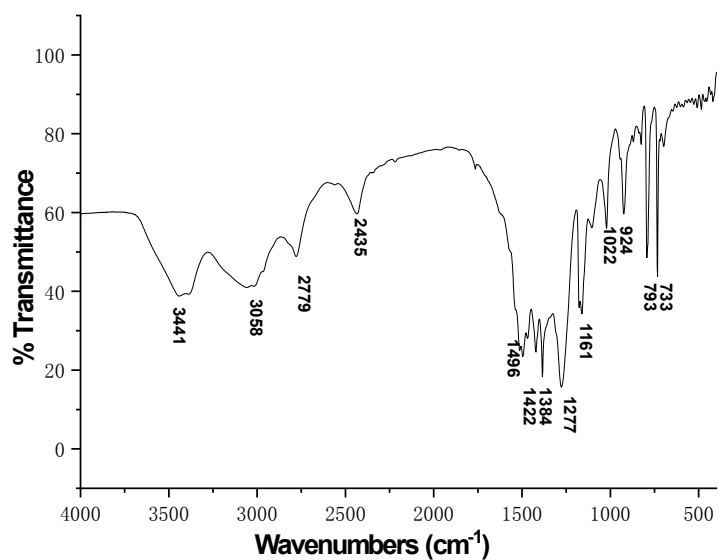


Fig. S22. IR spectrum of $(\text{CH}_3)_2\text{NHBH}_2\text{C}(\text{NO}_2)_3$ (**3c**).

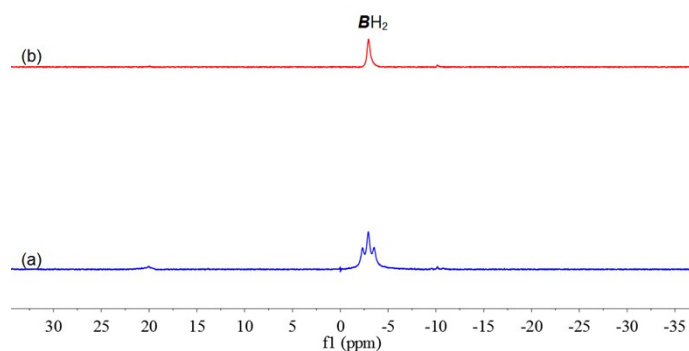


Fig. S23. ^{11}B (a) and $^{11}\text{B}\{^1\text{H}\}$ NMR (b) spectra of $[\text{CH}_2\text{NH}_2\text{BH}_2\text{C}(\text{NO}_2)_3]_2$ (**3e**) in CD_3CN .

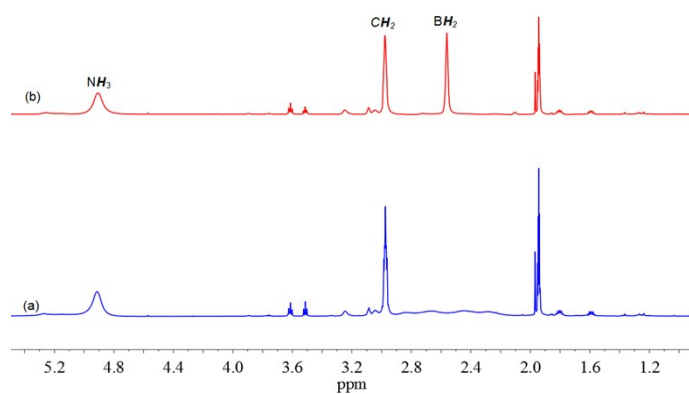


Fig. S24. ^1H (a) and $^1\text{H}\{^{11}\text{B}\}$ NMR (b) spectra of $[\text{CH}_2\text{NH}_2\text{BH}_2\text{C}(\text{NO}_2)_3]_2$ (**3e**) in CD_3CN .

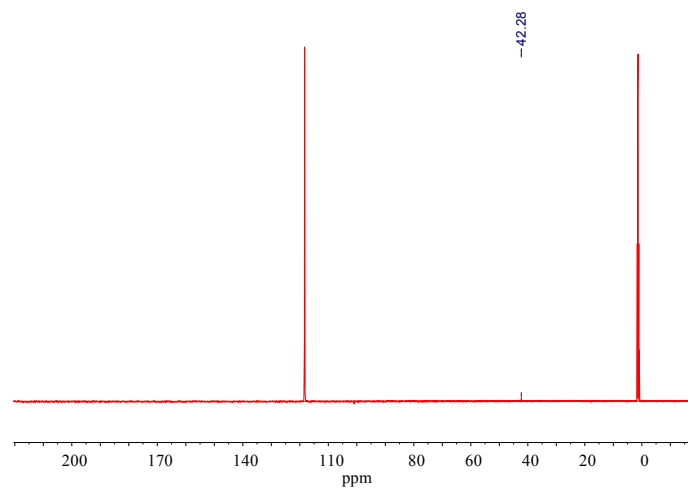


Fig. S25. ^{13}C NMR spectrum of $[\text{CH}_2\text{NH}_2\text{BH}_2\text{C}(\text{NO}_2)_3]_2$ (**3e**) in CD_3CN .

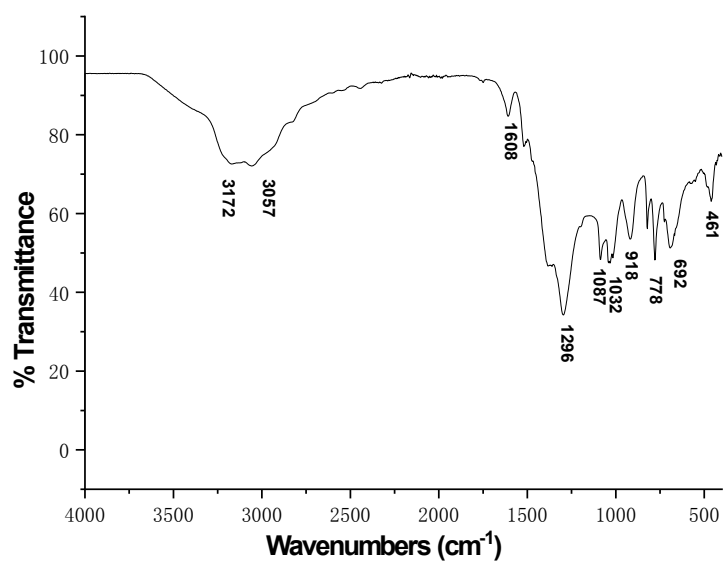


Fig. S26. IR spectrum of $[\text{CH}_2\text{NH}_2\text{BH}_2\text{C}(\text{NO}_2)_3]_2$ (**3e**).

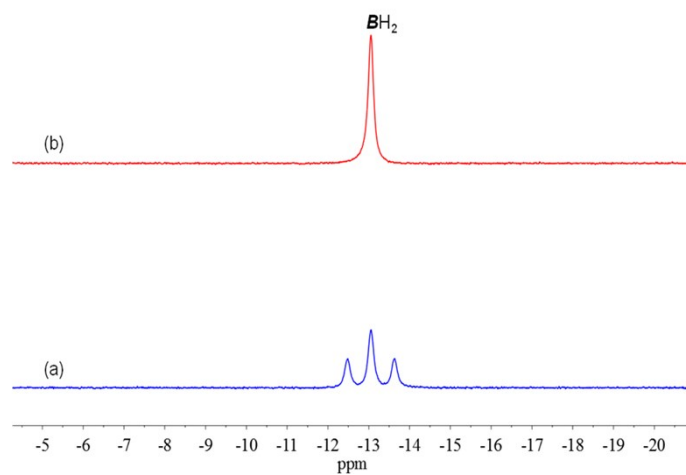


Fig. S27. ^{11}B (a) and $^{11}\text{B}\{^1\text{H}\}$ NMR (b) spectra of $[\text{H}_2\text{B}(\text{NH}_3)_2][\text{C}(\text{NO}_2)_3]$ (3g) in CD_3CN .

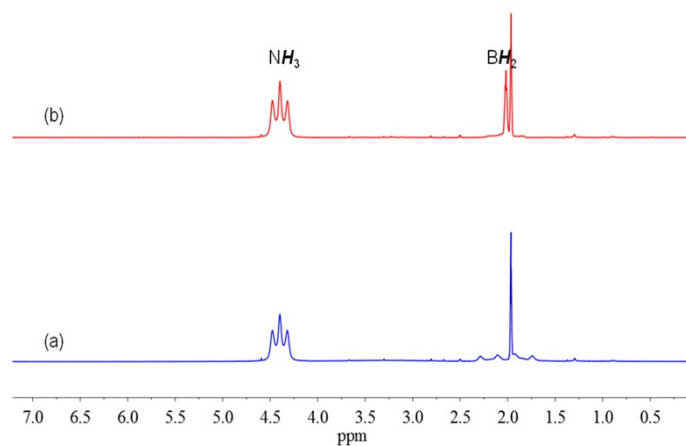


Fig. S28. ^1H (a) and $^1\text{H}\{^{11}\text{B}\}$ NMR (b) spectra of $[\text{H}_2\text{B}(\text{NH}_3)_2][\text{C}(\text{NO}_2)_3]$ (3g) in CD_3CN .

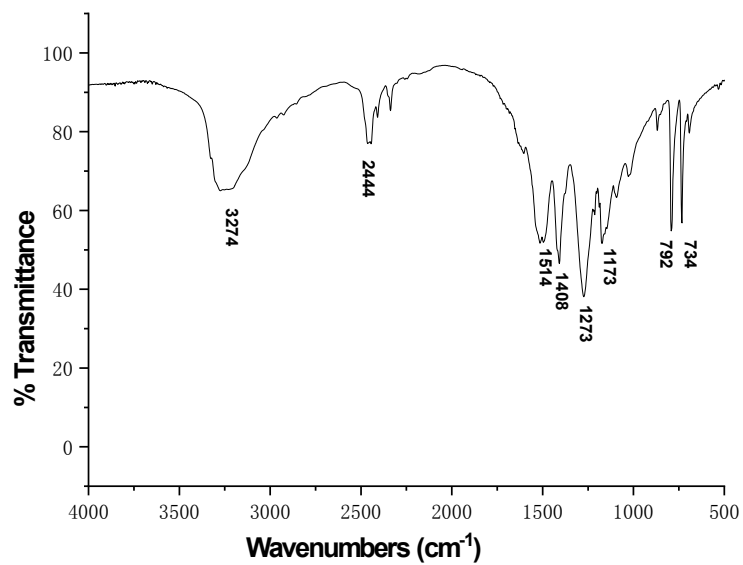


Fig. S29. IR spectrum of $[\text{H}_2\text{B}(\text{NH}_3)_2][\text{C}(\text{NO}_2)_3]$ (3g).

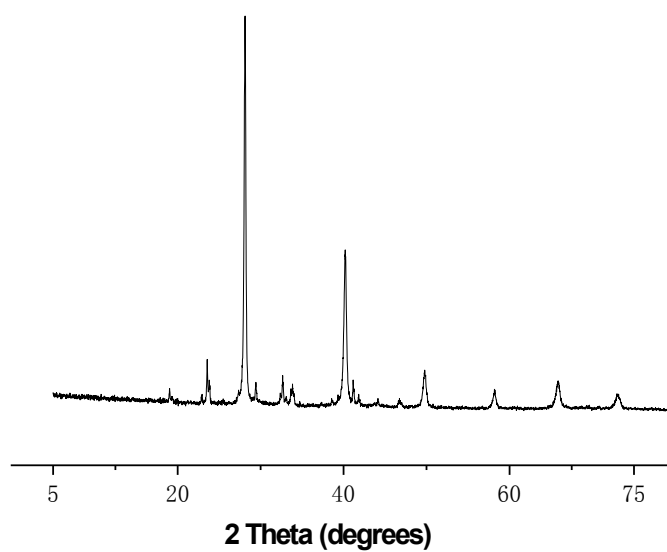


Fig. S30. X-ray powder diffraction pattern of KCl.

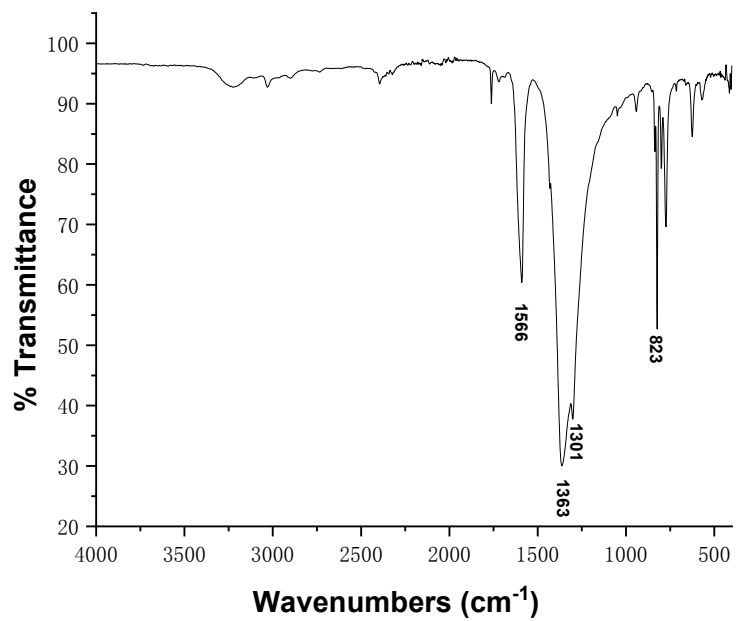


Fig. S31. IR spectrum of K[C(NO₂)₃].