Supporting Information

Catalytic Activation of Nitrous Oxide: Boryl vs Hydride Nickel Species

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1. Experimental procedures

General considerations. All manipulations were carried out using standard Schlenk and glovebox techniques, under an atmosphere of argon or high purity nitrogen, respectively. All solvents were dried and degassed prior to use. n-Pentane, THF and toluene were distilled over Na/K alloy and stored under molecular sieves. CH_2Cl_2 was distilled over CaH_2. C_6D_6 was distilled over Na/K alloy and stored under molecular sieves. NMR spectra were recorded on Bruker DRX-500, DRX-400 and DPX-300 spectrometers, and they were referenced to external $SiMe_4$ (δ 0 ppm) using the residual protio solvent peaks as internal standard (^{1}H NMR experiments) or the characteristic resonances of the solvent nuclei (^{13}C NMR experiments). ^{11}B NMR spectra were referenced to an external standard of $BF_3{\cdot}Et_2O$ (δ 0 ppm). ^{31}P NMR chemical shifts were referenced to an external 85% solution of H_3PO_4 (δ 0 ppm) in the appropriate solvent. The following reagents were purchased and used as received: B_2Cat_2, B_2pin_2, HBcat and HBpin from Aldrich and N_2O from Air-Liquide. Compounds **1a**, **1b**, **2a, 3** and **4a** were prepared according to the literature procedures.[1-3] $B_2Cat'_2$ was prepared following a method previously reported.[4]

2. Stoichiometric reactions

2.1 Preparation of ^{tBu}PBPNiBcat' (**5a**)

85 mg (0.167 mmol) of ^{tBu}PBPNiMe (**2a**) were suspended in 2.5 mL of pentane and then 46 mg (0.175 mmol) of $B_2cat'_2$ were added as a solid. Then, the mixture was stirred at room temperature 19h. The yellow solid that precipitate was washed with pentane (2 x 3 mL). Afterwards the solid was dried under vacuum to lead **5a** as a bright yellow solid (73 mg, 70%). Elemental Analysis $C_{31}H_{50}B_2N_2NiO_2P_2$ (625.01) Calcd: C 59.57, H 8.06, N 4.48; found: C 59.56; H 7.82, N 4.70.

^{1}H NMR (400 MHz, C_6D_6): *δ* (ppm) = 1.17 (vt, 36 H, $^3J_{HP}$ = 7 Hz, ^{t}Bu), 2.19 (s, 3 H, CH_3-Cat), 3.84 (s, 4 H, CH_2), 6.69 (d, 1 H, $^3J_{HH}$ = 8 Hz, CH), 7.04 (dd, 2 H, $^3J_{HH}$ = 6, $^4J_{HH}$ = 3 Hz, CH), 7.15 (s, CH; overlapped with the signal of benzene), 7.17 (dd, 2 H, $^3J_{HH}$ = 6, $^4J_{HH}$ = 3 Hz, CH), 7.24 (d, 1 H, $^3J_{HH}$ = 8 Hz, CH).

^{13}C{^{1}H} NMR (100 MHz, C_6D_6): *δ* (ppm) = 21.4 (s, CH_3-Cat), 29.9 (s, CH_3-^{t}Bu), 35.7 (t, $^1J_{PC}$ = 8 Hz, Cq-^{t}Bu), 43.2 (t, $^1J_{PC}$ = 17 Hz, CH_2), 109.7 (s, CH), 110.4 (s, CH), 111.7 (s, CH), 118.7 (s, CH), 121.1 (s, CH), 130.0 (s, Cq), 139.9 (t, $^3J_{PC}$ = 8 Hz, Cq), 149.3 (s, Cq -Bcat'), 151.4 (s, Cq-Bcat').

^{31}P{^{1}H} NMR (162 MHz, C_6D_6): *δ* (ppm) = 117.3 (s).

^{11}B{^{1}H} NMR (128 MHz, C_6D_6): *δ* (ppm) = 60 and 50 (bs).

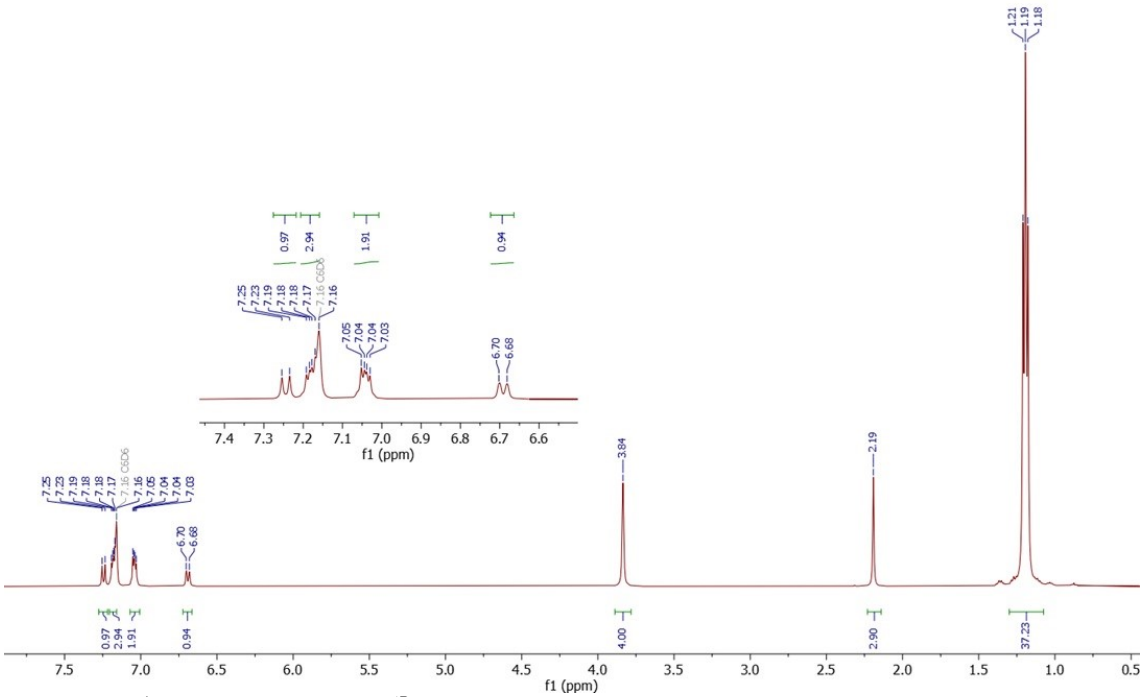


Figure S1. ^{1}H NMR spectrum of ^{tBu}PBPNiBcat' (**5a**) (400 MHz, C_6D_6).

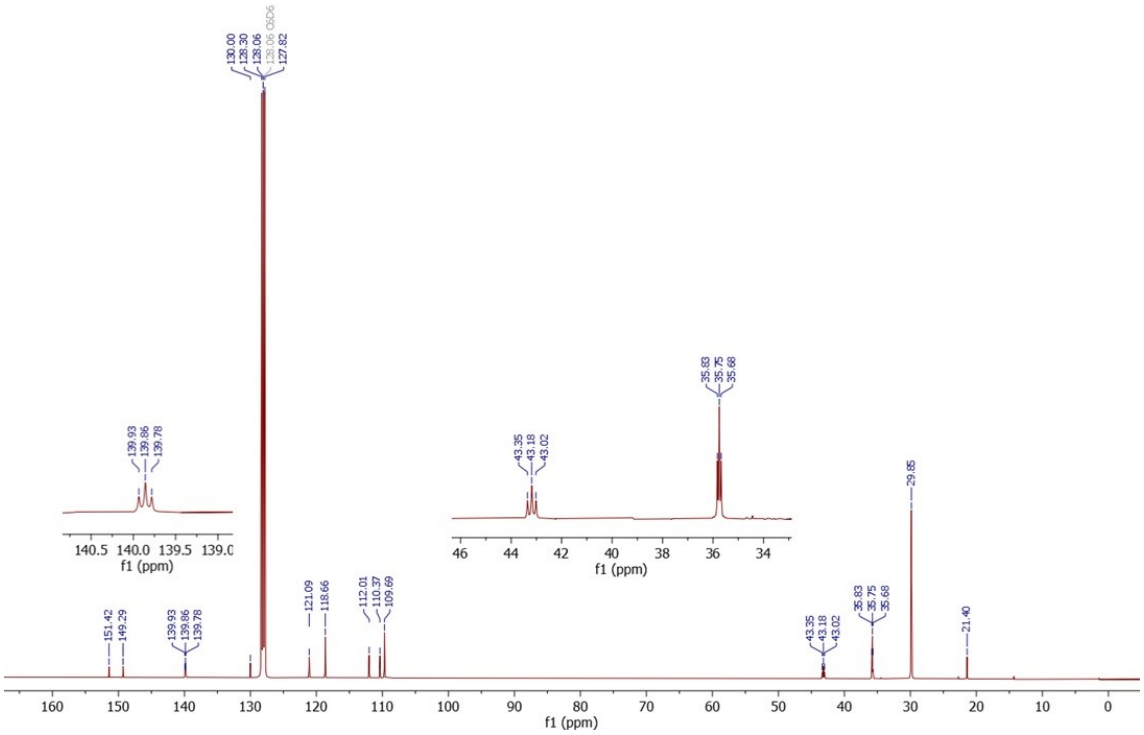


Figure S2. $^{13}C\{^{1}H\}$ NMR spectrum of ^{tBu}PBPNiBcat' (**5a**) (100 MHz, C_6D_6).

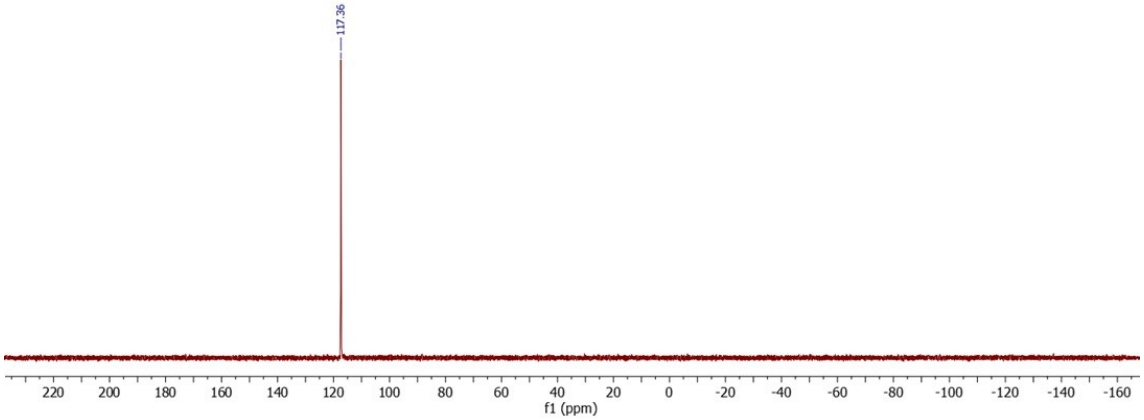


Figure S3. $^{31}P\{^{1}H\}$ NMR spectrum of ^{tBu}PBPNiBcat' (**5a**) (162 MHz, C_6D_6).

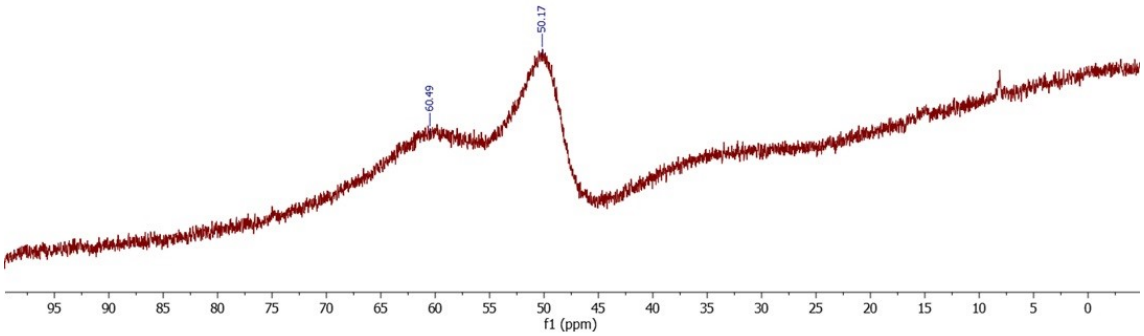


Figure S4. $^{11}B\{^{1}H\}$ NMR spectrum of ^{tBu}PBPNiBcat' (**5a**) (128 MHz, C_6D_6).

2.2 Preparation of ^{tBu}PBPNiOBcat (**6a**)

A Fischer-Porter vessel (6 mL) containing ^{tBu}PBPNiBcat (**4a**) (20 mg, 0.033 mmol) in C_6D_6 (500 µL) was degassed via freeze-pump-thaw cycles. Then, the Fischer-Porter tube was backfilled with N_2O (1 bar) and was stirred at room temperature for 30 minutes turning from bright yellow to dark yellow. Afterwards, the solution was dried under vacuum to afford **6a** as a pale-yellow solid (16 mg, 81%). Elemental Analysis $C_{30}H_{48}B_2N_2NiO_3P_2$ (626.99) Calcd: C 57.47, H 7.72, N 4.47; found: C 57.56; H 7.55, N 4.29.

^{1}H NMR (400 MHz, C_6D_6): δ (ppm) = 1.26 (vt, 36 H, $^{3}J_{HP}$ = 7 Hz, ^{t}Bu), 3.45 (s, 4 H, CH_2), 6.82 (dd, 2 H, $^{3}J_{HH}$ = 6, $^{4}J_{HH}$ = 3 Hz, CH), 6.87 (dd, 2 H, $^{3}J_{HH}$ = 6, $^{4}J_{HH}$ = 3 Hz, CH), 7.11 (dd, 2 H, $^{3}J_{HH}$ = 6, $^{4}J_{HH}$ = 3 Hz, CH), 7.18–7.13 (m, 2 H, CH).

^{13}C{^{1}H} NMR (100 MHz, C_6D_6): δ (ppm) = 29.5 (s, CH_3-^{t}Bu), 34.9 (t, $^{1}J_{PC}$ = 6 Hz, Cq-^{t}Bu), 39.6 (t, $^{1}J_{PC}$ = 18 Hz, CH_2), 108.5 (s, CH), 110.7 (s, CH), 118.8 (s, CH), 120.4 (s, CH), 139.4 (t, $^{3}J_{PC}$ = 8 Hz, Cq), 151.3 (s, Cq-Bcat).

^{31}P{^{1}H} NMR (162 MHz, C_6D_6): *δ* (ppm) = 84.0 (s).

^{11}B{^{1}H} NMR (128 MHz, C_6D_6): *δ* (ppm) = 38 and 24 (bs).

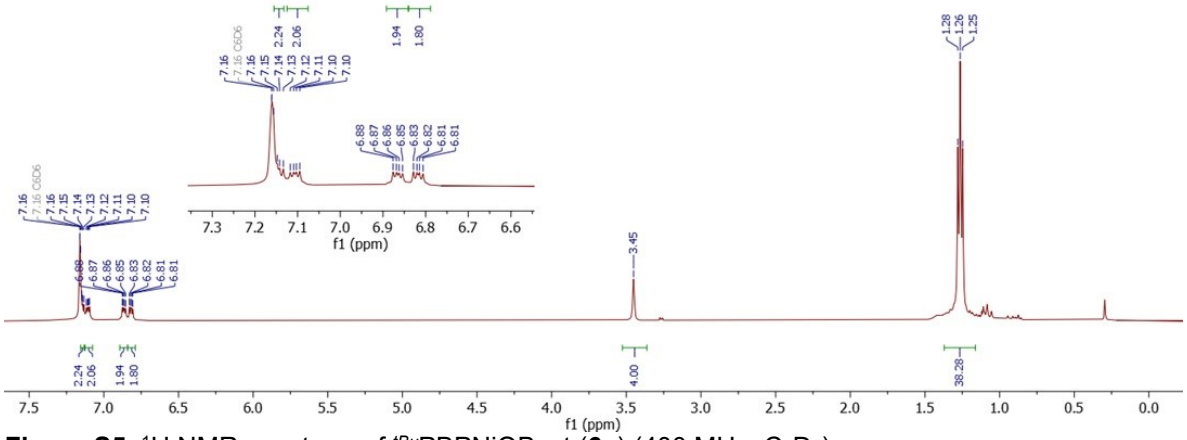


Figure S5. ^{1}H NMR spectrum of ^{tBu}PBPNiOBcat (**6a**) (400 MHz, C_6D_6).

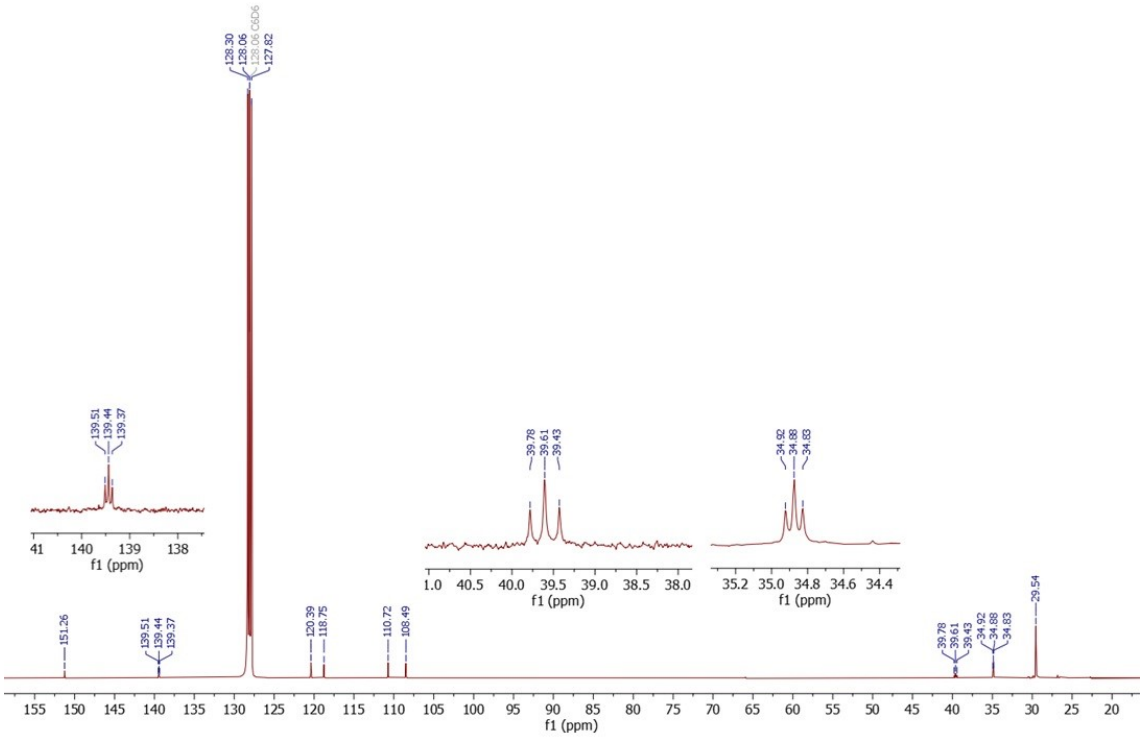


Figure S6. $^{13}C\{^{1}H\}$ NMR spectrum of ^{tBu}PBPNiOBcat (**6a**) (400 MHz, C_6D_6).

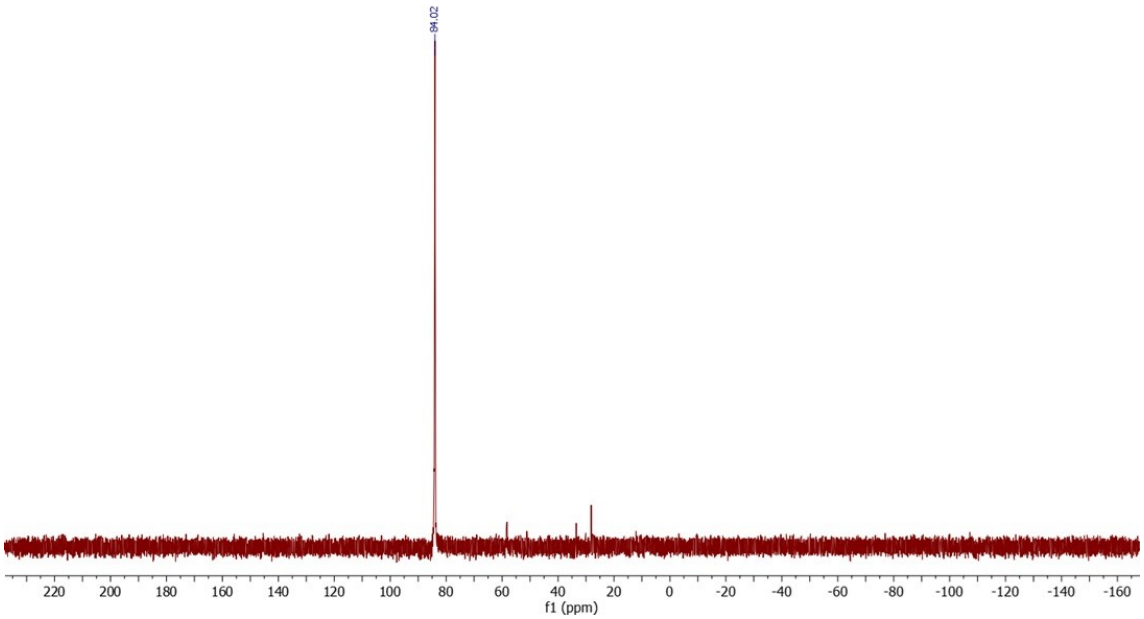


Figure S7. $^{31}P\{^{1}H\}$ NMR spectrum of ^{tBu}PBPNiOBcat (**6a**) (162 MHz, C_6D_6).

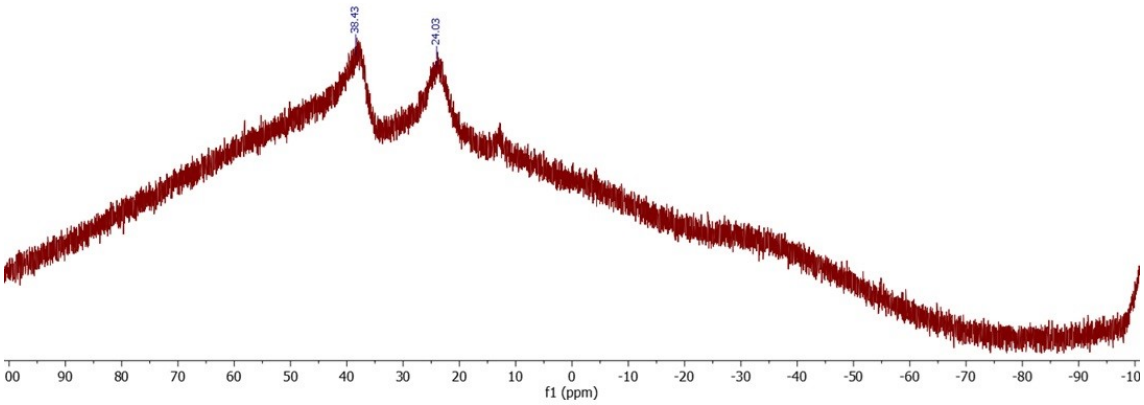


Figure S8. $^{11}B\{^{1}H\}$ NMR spectrum of ^{tBu}PBPNiOBcat (**6a**) (128 MHz, C_6D_6).

2.3 Preparation of ^{tBu}PBPNiOBcat' (**7a**)

To a Fischer-Porter vessel (6 mL) containing ^{tBu}PBPNiBcat' (**5a**) (20 mg, 0.032 mmol) in C_6D_6 (500 µL) was degassed via freeze-pump-thaw cycles. Then, the Fischer-Porter tube was backfilled with N_2O (1 bar) and was stirred at room temperature for 30 minutes turning from bright yellow to dark yellow. Afterwards, the solution was dried under vacuum to afford **7a** as a pale-yellow solid (18 mg, 87%). Elemental Analysis $C_{31}H_{50}B_2N_2NiO_3P_2$ (641.01) Calcd: C 58.09, H 7.86, N 4.37; found: C 58.45; H 7.59, N 4.01.

^{1}H NMR (400 MHz, C_6D_6): δ (ppm) = 1.27 (vt, 36 H, $^{3}J_{HP}$ = 7 Hz, ^{t}Bu), 2.17 (s, 3 H, CH_3-Cat), 3.46 (s, 4 H, CH_2), 6.63 (dd, 1 H, $^{3}J_{HH}$ = 8, $^{4}J_{HH}$ = 2 Hz, CH), 6.87 (dd, 2 H, $^{3}J_{HH}$ = 6, $^{4}J_{HH}$ = 3 Hz, CH), 7.00 (d, 1 H, $^{4}J_{HH}$ = 2 Hz, CH), 7.06 (d, 1 H, $^{3}J_{HH}$ = 8 Hz; CH) 7.11 (dd, 2 H, $^{3}J_{HH}$ = 6, $^{4}J_{HH}$ = 3 Hz, CH).

$^{13}C\{^1H\}$ NMR (126 MHz, C_6D_6): δ (ppm) = 21.5 (s, CH_3-Cat), 29.6 (s, CH_3-^{t}Bu), 34.9 (t, $^1J_{PC}$ = 5 Hz, Cq-^{t}Bu), 39.6 (t, $^1J_{PC}$ = 18 Hz, CH_2), 108.5 (s, CH), 110.1 (s, CH-), 111.7 (s, CH), 118.7 (s, CH), 120.4 (s, CH), 129.4 (s, Cq-Bcat'), 139.5 (t, $^3J_{PC}$ = 7 Hz, Cq), 149.1 (s, Cq- Bcat'), 151.3 (s, Cq-Bcat').

$^{31}P\{^1H\}$ NMR (162 MHz, C_6D_6): δ (ppm) = 84.0 (s).

$^{11}B\{^1H\}$ NMR (128 MHz, C_6D_6): δ (ppm) = 37 and 23 (bs).

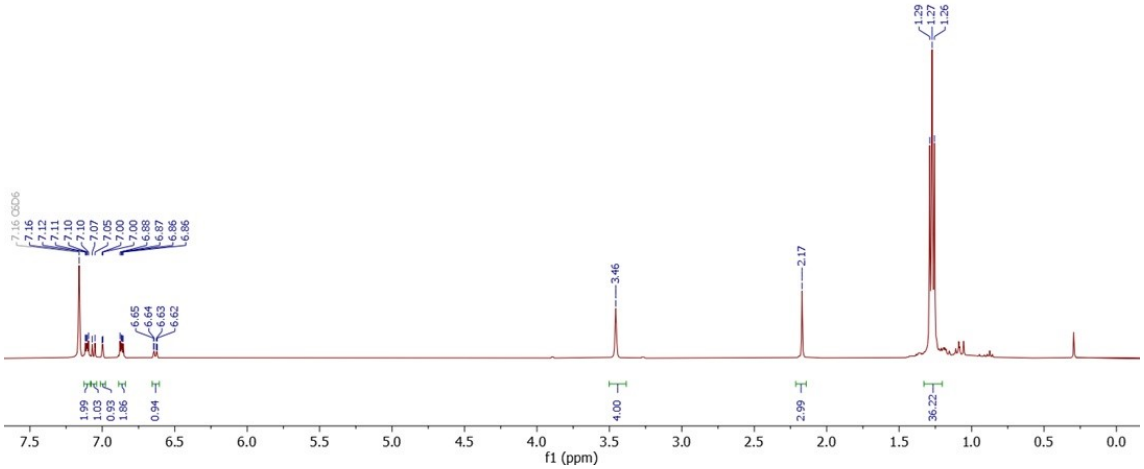


Figure S9. ^{1}H NMR spectrum of ^{tBu}PBPNiOBcat' (**7a**) (400 MHz, C_6D_6).

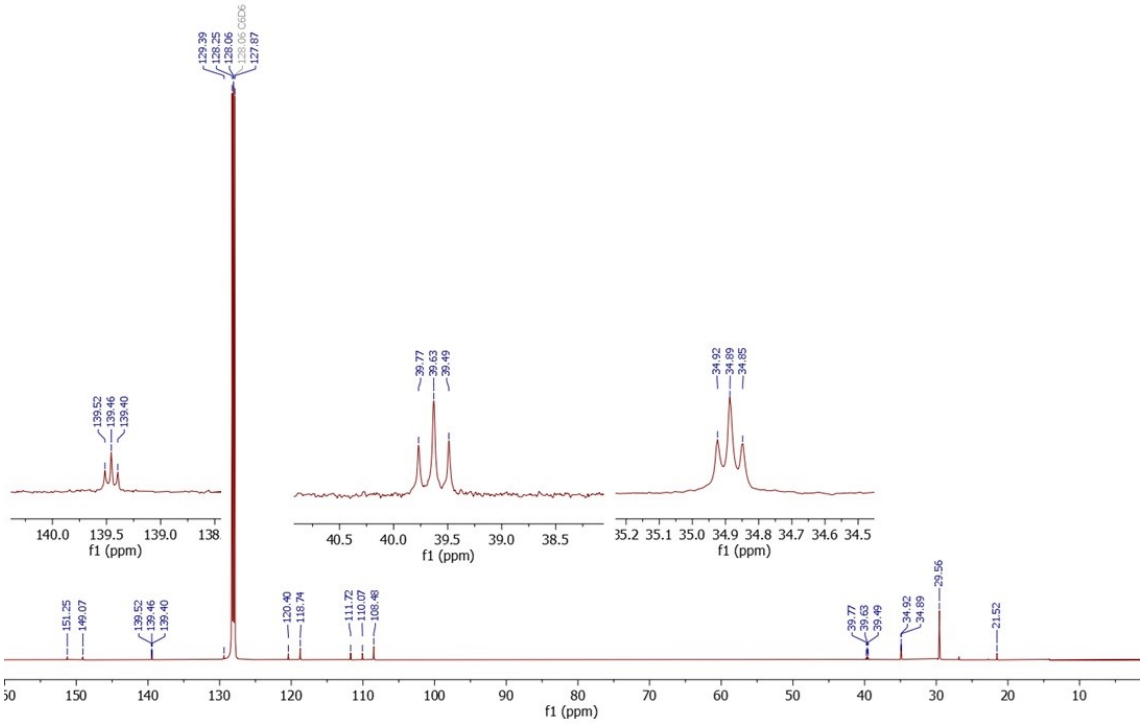


Figure S10. $^{13}C\{^1H\}$ NMR spectrum of ^{tBu}PBPNiOBcat' (**7a**) (126 MHz, C_6D_6).

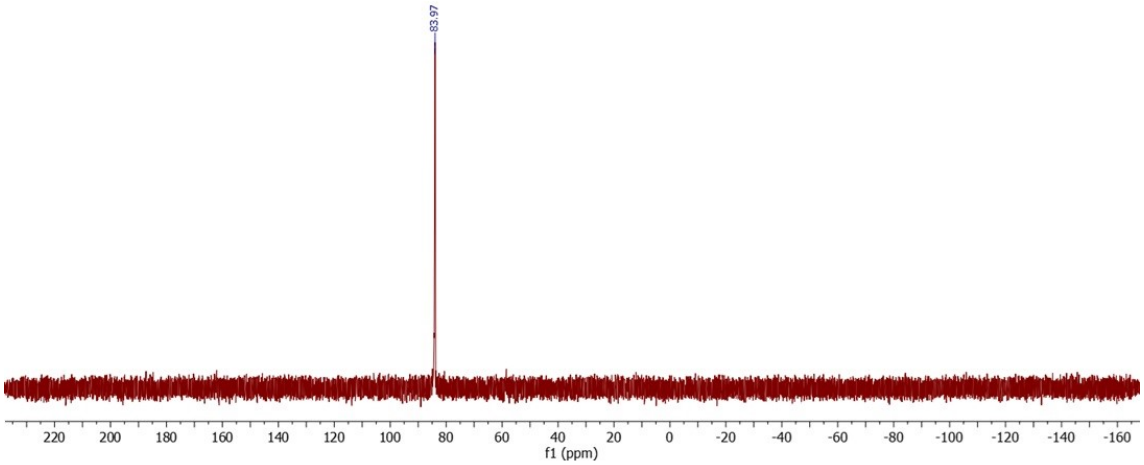


Figure S11. $^{31}P\{^{1}H\}$ NMR spectrum of ^{tBu}PBPNiOBcat' (**7a**) (162 MHz, C_6D_6).

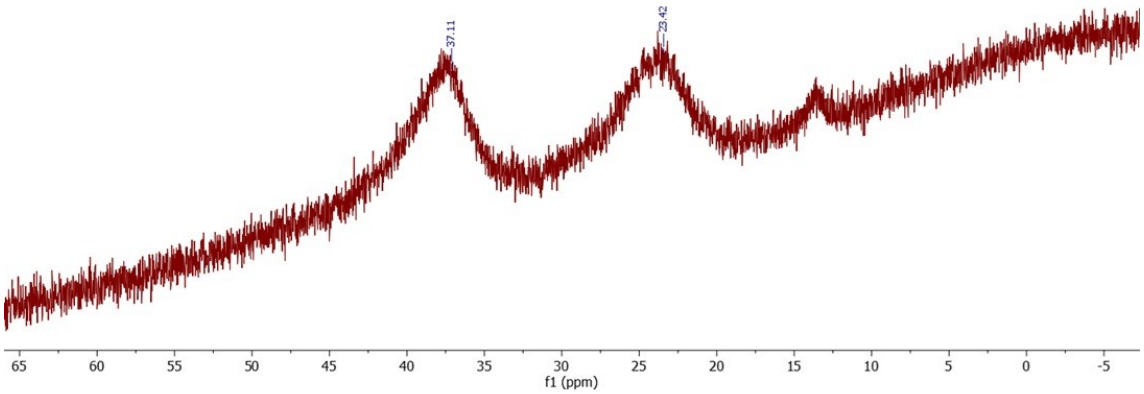


Figure S12. $^{11}B\{^{1}H\}$ NMR spectrum of ^{tBu}PBPNiOBcat' (**7a**) (128 MHz, C_6D_6).

2.4 Preparation of ^{Cy}PBPNiCH$_3$ (**2b**)

2b was prepared following a modified procedure to that previously reported.[3]

A mixture of 200mg (0.287 mmol) of ^{Cy}PBPNiBr (**1b**) and 50 mg (0.287 mmol) of $MgMe_2$(tmeda) were suspended in 4 mL of pentane. Then, the mixture was stirred at room temperature during 12 hours. The solution was filtered and all volatiles removed under vacuum to yield **2b** as a bright yellow solid (62 mg, 35%). The NMR data obtained was identical to those reported in the literature.[3]

3. *In Situ* NMR Studies

3.1- NMR reaction of ^{tBu}PBPNiBcat (**4a**) with N_2O

A solution of ^{tBu}PBPNiBcat (**4a**) (8 mg, 0.013 mmol) in C_6D_6 (500 µL) was prepared in a J. Young valve NMR tube, freeze-pump-thaw degassed, placed under N_2O (2 bar) and thereafter monitored at room temperature by NMR spectroscopy. After 3h at room temperature, complete formation of ^{tBu}PBPNiOBcat (**6a**) is observed (δ_{31P} = 84 ppm).

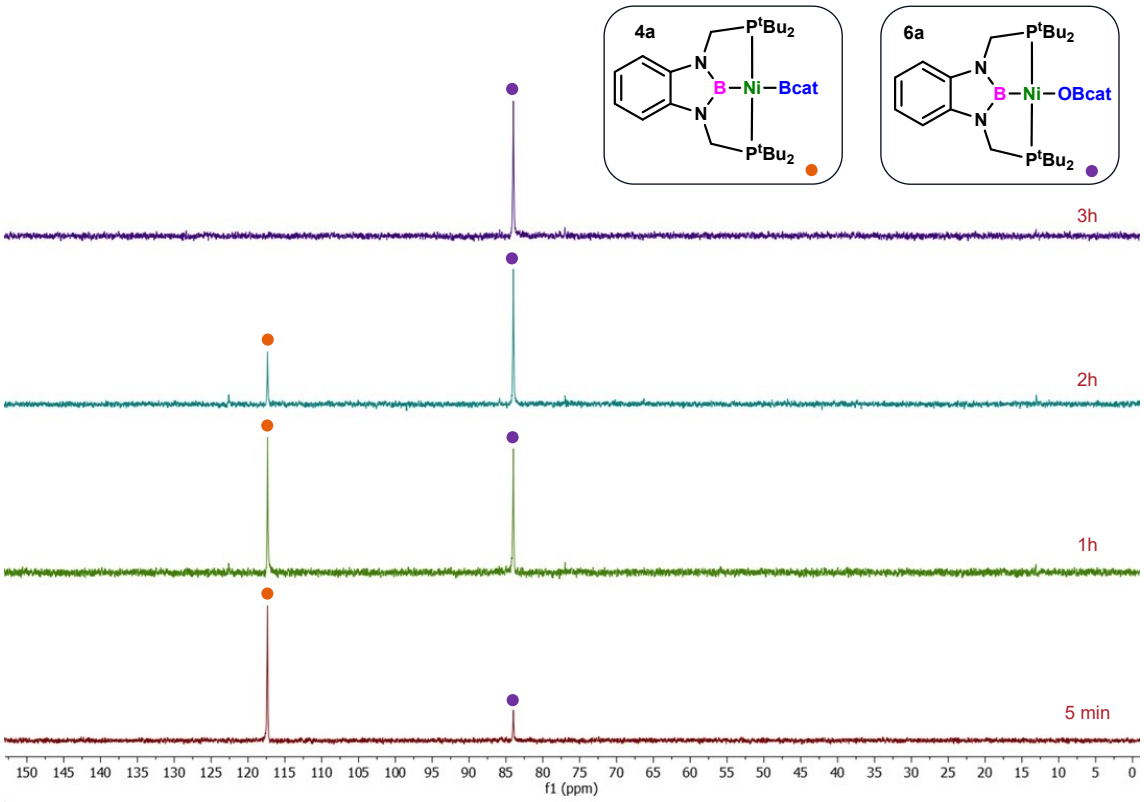


Figure S13. $^{31}P\{^1H]$ NMR spectrum of ^{tBu}PBPNiBcat (**4a**) + N_2O (2 bar) in a J. Young NMR tube (162 MHz, C_6D_6, 298K).

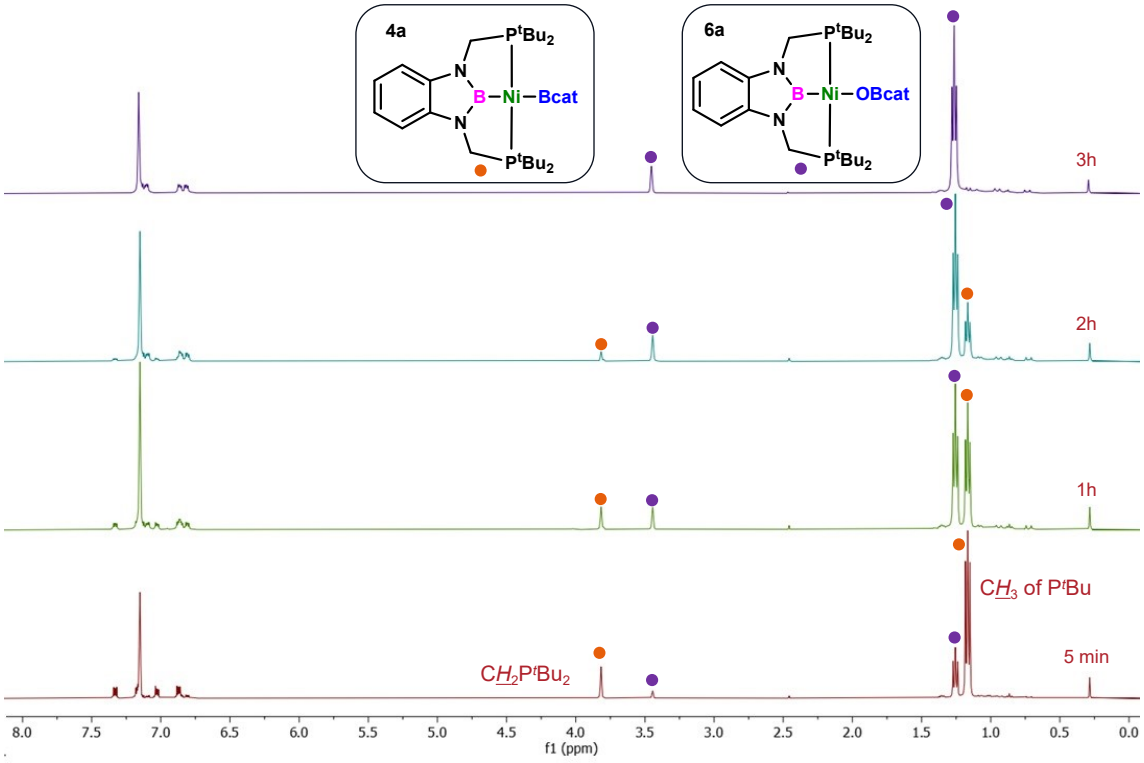


Figure S14. ^1H NMR spectrum of ^{tBu}PBPNiBcat (**4a**) + N_2O (2 bar) in a J. Young NMR tube (400 MHz, C_6D_6, 298K).

3.2-NMR reaction of [(^{tBu}PBP)-NiH$_2$Bcat] (**8**) with N_2O

A solution of ^{tBu}PBPNiH$_2$Bcat (**8**) (15 mg, 0.024 mmol) in C_6D_6 (500 µL) was prepared in a J. Young valve NMR tube, freeze-pump-thaw degassed, placed under N_2O (2 bar) and thereafter the reaction was monitored at room temperature by NMR spectroscopy. After 5 min complete formation of ^{tBu}PBPNiOBcat (**6a**) is observed (δ_{31P} = 84 ppm).

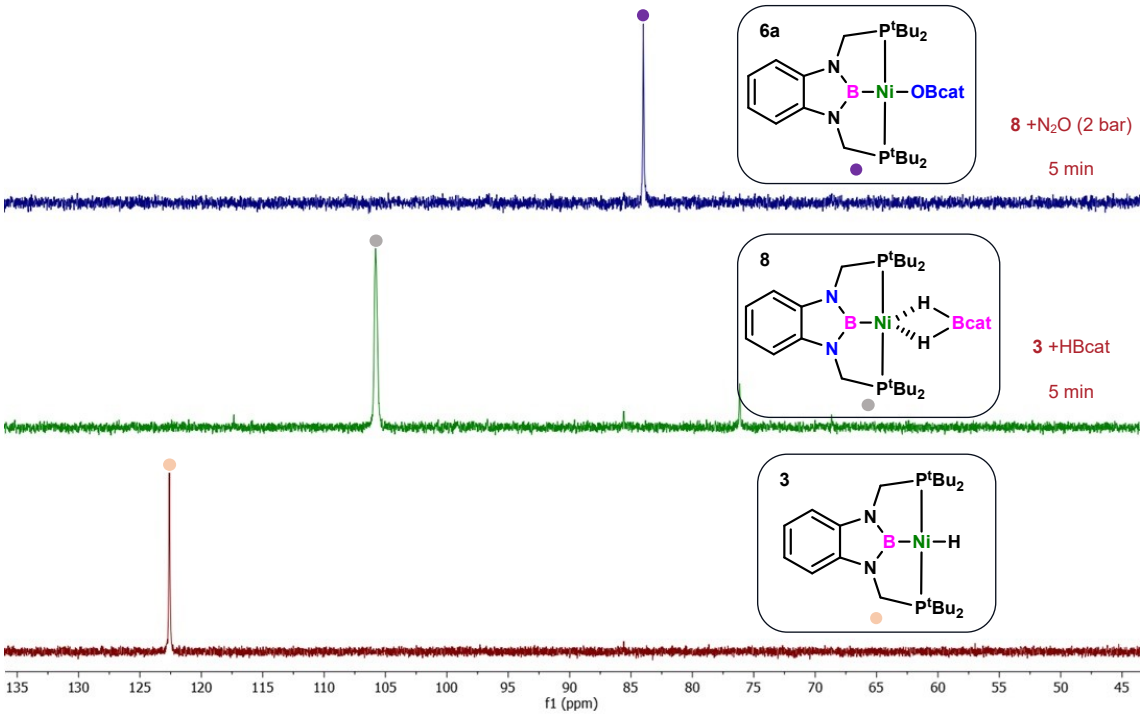


Figure S15. $^{31}P\{^1H\}$ NMR spectrum of ^{tBu}PBPNiH$_2$Bcat (**8**) + N_2O (2 bar) in a J. Young NMR tube (162 MHz, C_6D_6, 298K).

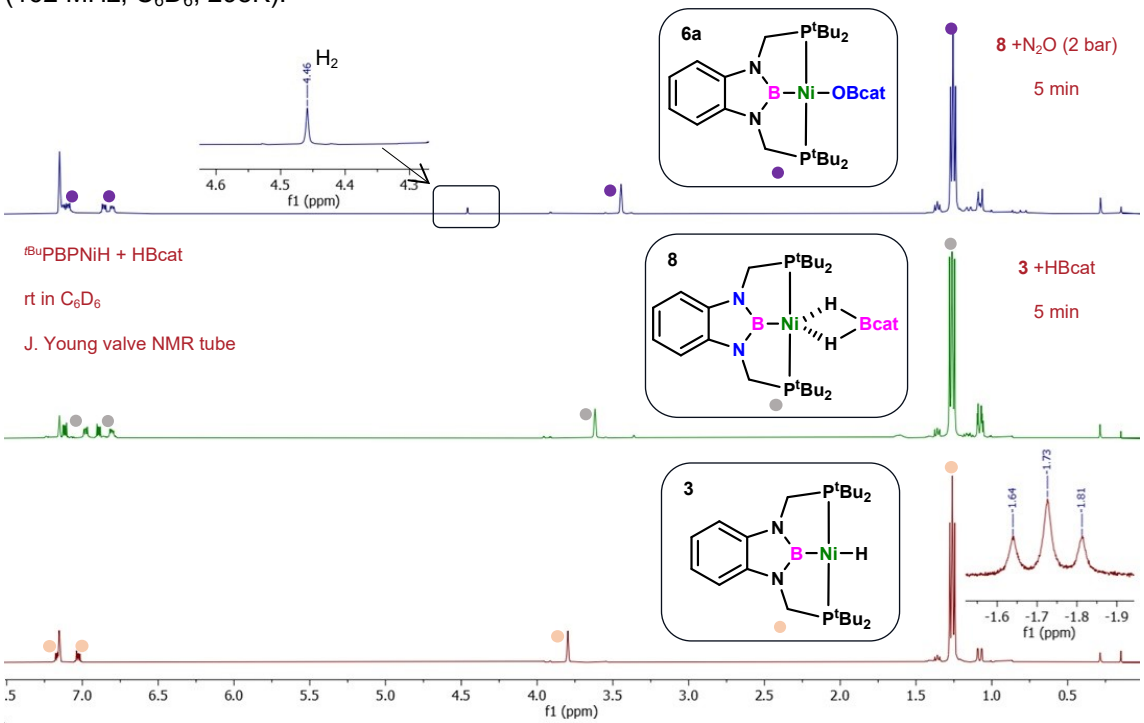


Figure S16. ^1H NMR spectrum of ^{tBu}PBPNiH$_2$Bcat (**8**) + N_2O (2 bar) in a J. Young NMR tube (400 MHz, C_6D_6, 298K).

3.3-NMR scale reaction of ^{tBu}PBPNiOBcat (6a) with B_2cat_2

A solution of ^{tBu}PBPNiOBcat (**6a**) (8 mg, 0.013 mmol) and B_2cat_2 (3 mg, 0.013 mmol) in C_6D_6 (500 µL) was prepared in a J. Young valve NMR tube and thereafter monitored at room temperature by NMR spectroscopy. Analysis within 5 min indicated quantitative spectroscopic formation of ^{tBu}PBPNiBcat (**4a**) (δ_{31P} = 117 ppm) and O(Bcat)$_2$ (δ_{11B} = 22 ppm).

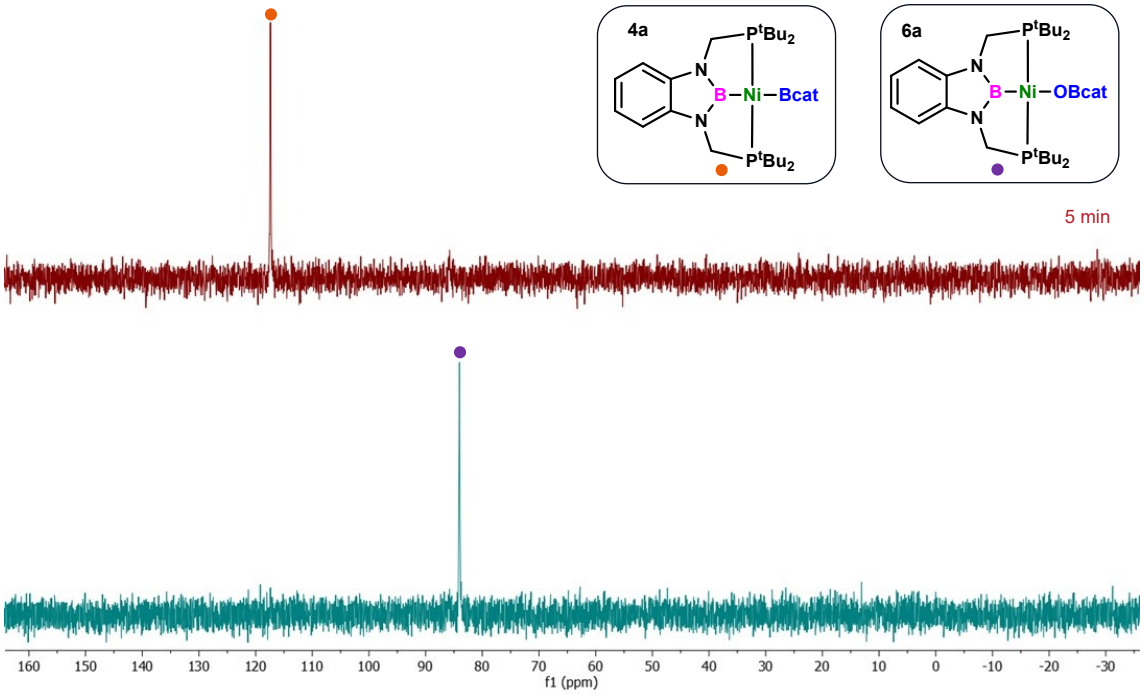


Figure S17. $^{31}P\{^1H\}$ NMR spectrum of ^{tBu}PBPNiOBcat (**6a**) + B_2cat_2 recorded after 5 min (162 MHz, C_6D_6).

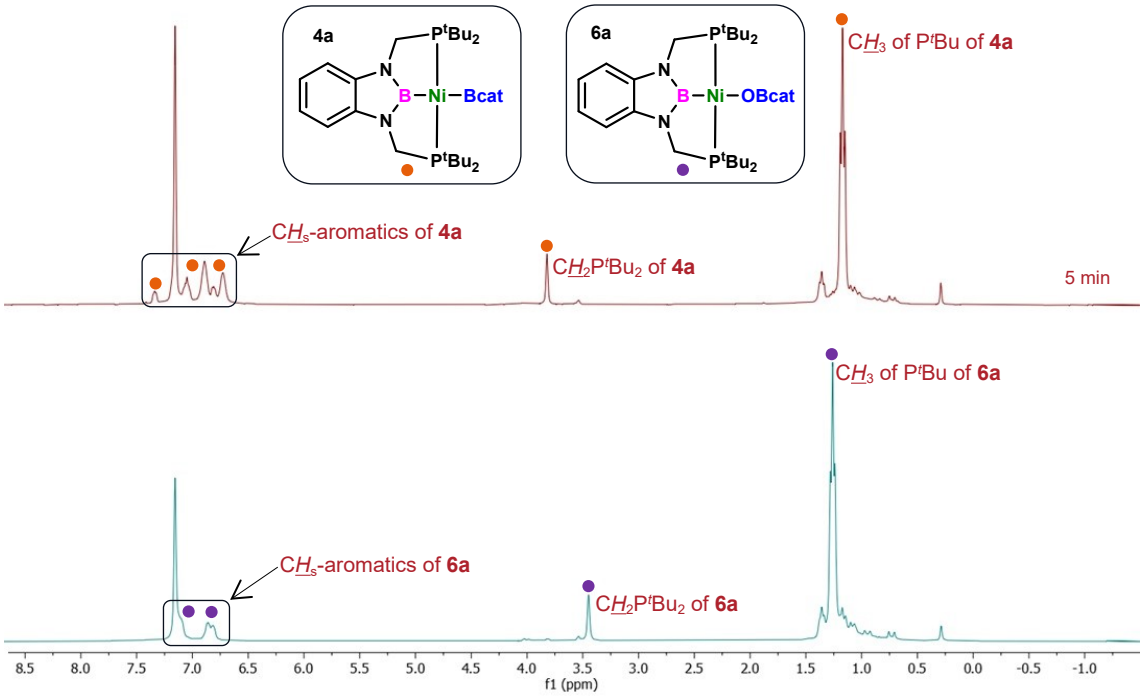


Figure S18. ^{1}H NMR spectrum of ^{tBu}PBPNiOBcat (**6a**) + B_2cat_2 recorded after 5 min (300 MHz, C_6D_6).

3.4-NMR scale reaction of ^{tBu}PBPNiOBcat (**6a**) with HBcat

A solution of ^{tBu}PBPNiOBcat (**6a**) (8 mg, 0.013 mmol) and HBcat (2 mg, 0.013 mmol) in C_6D_6 (500 µL) was prepared in a J. Young valve NMR tube and monitored at room temperature by NMR spectroscopy. Analysis within 5 min indicated the formation of ^{tBu}PBPNiH (**3**) which ^{31}P chemical shift is slightly upfield (δ_{31P} = 108 ppm) probably due to the interaction with HBcat and still the presence of ^{tBu}PBPNiOBcat (**6a**) (δ_{11B} = 84 ppm). Adding a second equivalent of HBcat resulted in the complete transformation of **6a** to **3•HBcat**.[2]

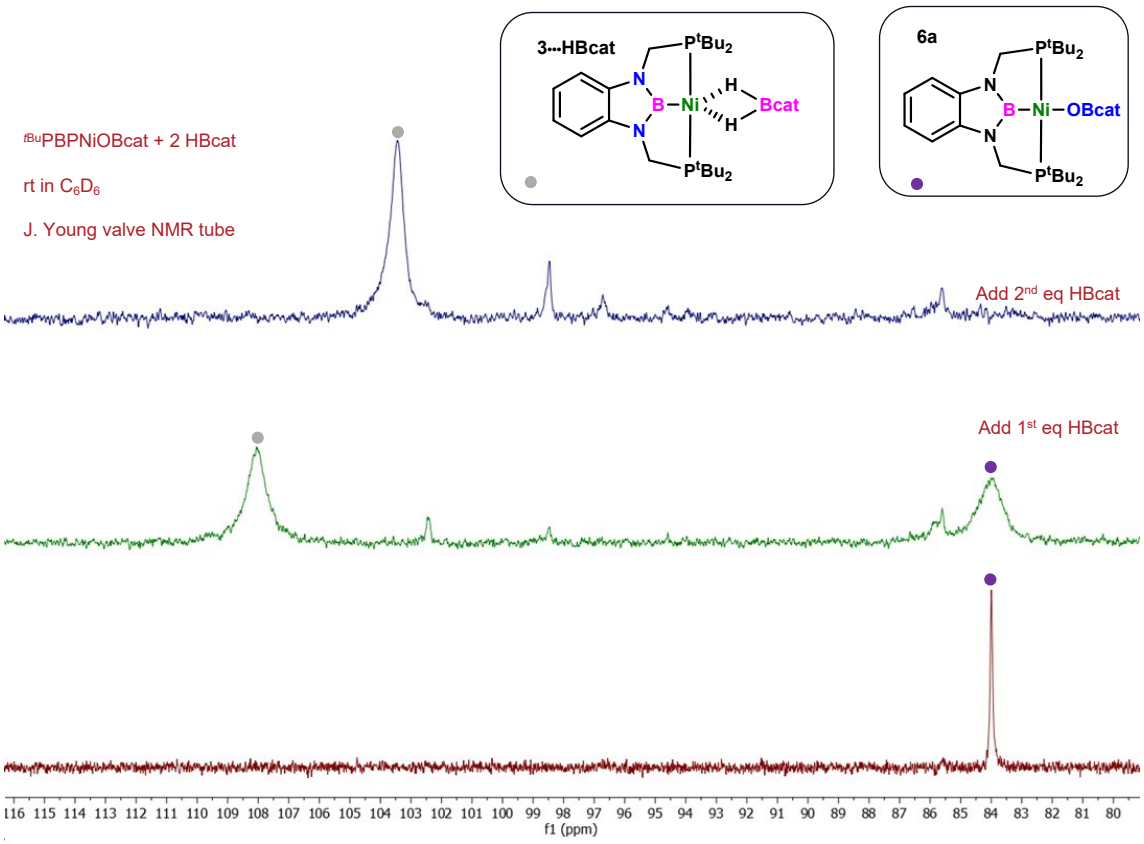


Figure S19. $^{31}P\{^{1}H\}$ NMR spectrum of ^{tBu}PBPNiOBcat (**6a**) + HBcat recorded after 5 min (162 MHz, C_6D_6).

3.5- NMR scale synthesis of ^{Cy}PBPNiBR (R = Cat (**4b**); 4-MeCat (**5b**))

A solution of ^{Cy}PBPNiMe (**2b**) (30 mg, 0.049 mmol) and B_2cat_2/$B_2cat'_2$ (0.049 mmol) in C_6D_6 (500 µL) was prepared in a J. Young valve NMR tube and monitored at room temperature by NMR spectroscopy. After 15 min the $^{31}P\{^{1}H\}$ NMR indicated quantitative spectroscopic formation of ^{Cy}PBPNiBR, R = Cat **4b**; 4-MeCat **5b** (δ_{31P} = 87.8 ppm). The $^{11}B\{^{1}H\}$ NMR spectrum confirms the formation of MeBcat (δ_{11B} = 35 ppm) along with **4b** and **5b**. All attempts to remove MeBcat from the reaction mixture led to the decomposition of bis(boryl)nickel complexes **4b** and **5b**, and the addition of N_2O (2 bar) to the solution of **4b** and **5b** resulted in the formation of several products.

NMR data for 4b:

^{1}H NMR (500 MHz, C_6D_6): δ (ppm) = 1.03 (m, 4H, CH_2), 1.11 (m, 4H, CH_2), 1.22 (m, 8 H, CH_2, $P(C_6H_{11})_2$, overlapped with signal of pentane), 1.38 (m, 4 H, CH_2, $P(C_6H_{11})_2$), 1.55 (m, 8 H, CH_2, $P(C_6H_{11})_2$), 1.63 (m, 8 H, CH_2, $P(C_6H_{11})_2$), 1.97 (m, 8 H, CH_2, $P(C_6H_{11})_2$), 3.66 (s, 4 H, CH_2), 6.88 (dd, 2 H, $^{3}J_{HH}$ = 5.7, $^{4}J_{HH}$ = 3.2 Hz, C*H*), 7.12 (dd, 2 H, $^{3}J_{HH}$ = 5.6, $^{4}J_{HH}$ = 3.2 Hz, C*H*), 7.21 (dd, 2 H, $^{3}J_{HH}$ = 5.6, $^{4}J_{HH}$ = 3.2 Hz, C*H*), 7.35 (dd, 2 H, $^{3}J_{HH}$ = 5.7, $^{4}J_{HH}$ = 3.2 Hz, C*H*).

$^{13}C\{^{1}H\}$ NMR (126 MHz, C_6D_6): δ (ppm) = 26.1 (s, CH_2), 26.8 (t, $^{2}J_{PC}$ = 5.4 Hz,CH_2), 26.9 (t, $^{2}J_{PC}$ = 6.4 Hz,CH_2), 28.6 (s, CH_2), 28.9 (s, CH_2), 35.8 (t, $^{1}J_{PC}$ = 11.8 Hz, CH), 43.7 (t, $^{1}J_{PC}$ = 17.7 Hz, CH_2), 109.6 (s, CH-$_{PBP}$), 110.1 (s, CH-$_{BCat}$), 118.7 (s, CH-$_{PBP}$), 120.4 (s, CH-aromatic), 139.5 (t, $^{3}J_{PC}$ = 7 Hz, *C*q-$_{PBP}$), 150.8 (s, Cq-Bcat).

$^{31}P\{^{1}H\}$ NMR (202 MHz, C_6D_6): δ (ppm) = 87.8 (s).

$^{11}B\{^{1}H\}$ NMR (160 MHz, C_6D_6): δ (ppm) = 57 and 49 (bs).

NMR data for 5b:

^{1}H NMR (500 MHz, C_6D_6): δ (ppm) = 1.04 (m, 4H, CH_2), 1.13 (m, 4 H, CH_2, $P(C_6H_{11})_2$,), 1.24 (m, 8 H, CH_2, $P(C_6H_{11})_2$ overlapped with signal of pentane), 1.41 (m, 8 H, CH_2, $P(C_6H_{11})_2$), 1.55 (m, 8 H, CH_2, $P(C_6H_{11})_2$), 1.65 (m, 8 H, CH_2, $P(C_6H_{11})_2$), 1.98 (m, 8 H, CH_2, $P(C_6H_{11})_2$), 2.18 (s, 3 H, CH_3), 3.66 (s, 4 H, CH_2), 6.68 (d, 1 H, CH), 6.88 (s, 1 H, CH), 7.12 (dd, 2 H, $^{3}J_{HH}$ = 5.6, $^{4}J_{HH}$ = 3.2 Hz, CH), 7.22 (dd, 2 H, $^{3}J_{HH}$ = 5.7, $^{4}J_{HH}$ = 3.2 Hz, CH), 7.26 (d, $^{3}J_{HH}$ = 8.1 Hz, CH).

^{13}C{^{1}H} NMR (126 MHz, C_6D_6): δ (ppm) = 21.03 (s, CH_3), 26.1 (s, CH_2), 26.8 (t, $^{2}J_{PC}$ = 5.4 Hz,CH_2), 26.9 (t, $^{2}J_{PC}$ = 6.4 Hz,CH_2), 28.6 (s, CH_2), 28.9 (s, CH_2), 35.8 (t, $^{1}J_{PC}$ = 11.8 Hz, CH), 43.7 (t, $^{1}J_{PC}$ = 17.7 Hz, CH_2), 109.6 (s, CH-$_{PBP}$), 110.1 (s, CH-$_{Bcat'}$), 112.1 (s, CH-$_{Bcat'}$), 118.3 (s, CH-$_{PBP}$), 120.4 (s, CH-$_{Bcat'}$), 139.9 (t, $^{3}J_{PC}$ = 7 Hz, Cq-$_{PBP}$), 150.8 (s, Cq-Bcat).

^{31}P{^{1}H} NMR (202 MHz, C_6D_6): δ (ppm) = 87.8 (s).

^{11}B{^{1}H} NMR (160 MHz, C_6D_6): δ (ppm) = 56 and 49 (bs).

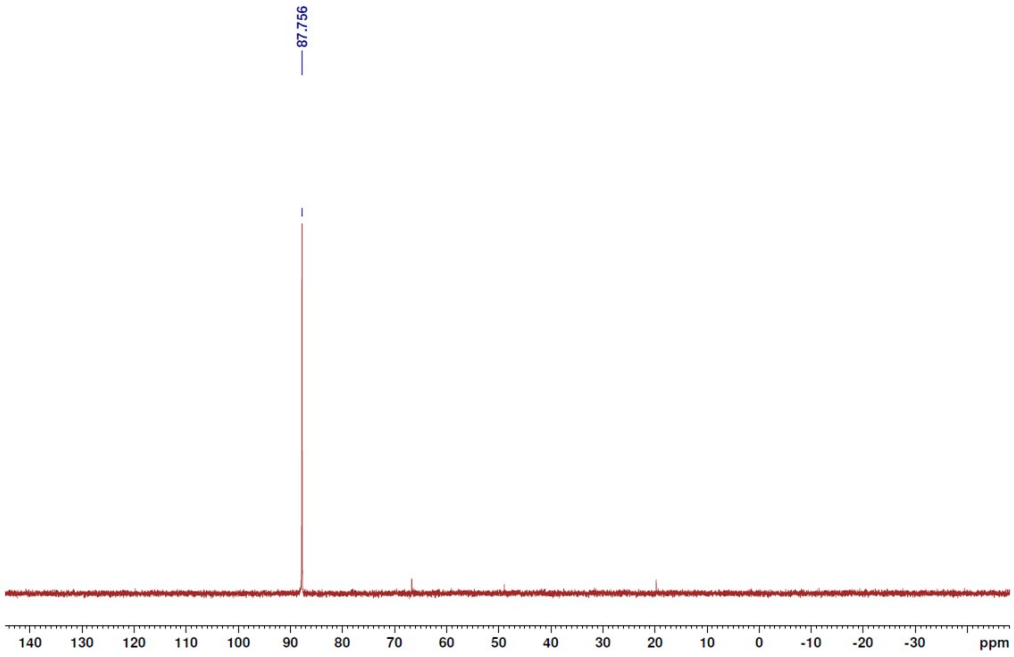


Figure S20. ^{31}P{^{1}H} NMR spectrum of ^{Cy}PBPNiBcat (**4b**) (202 MHz, C_6D_6).

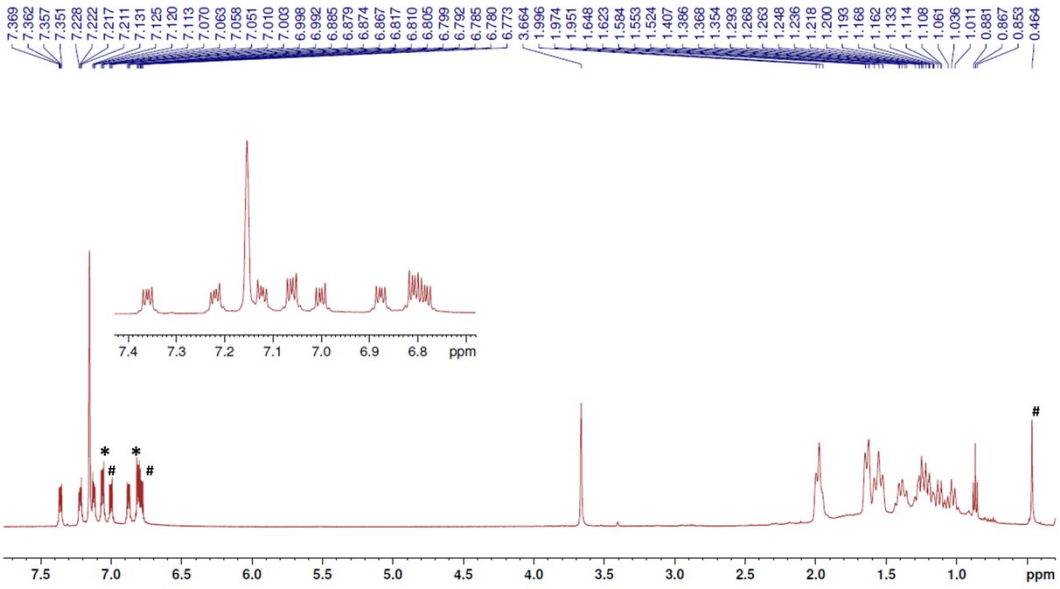


Figure S21. ^{1}H NMR spectrum of ^{Cy}PBPNiBcat (**4b**) (500 MHz, C_6D_6). * denotes B_2Cat_2 and # denotes MeBcat.

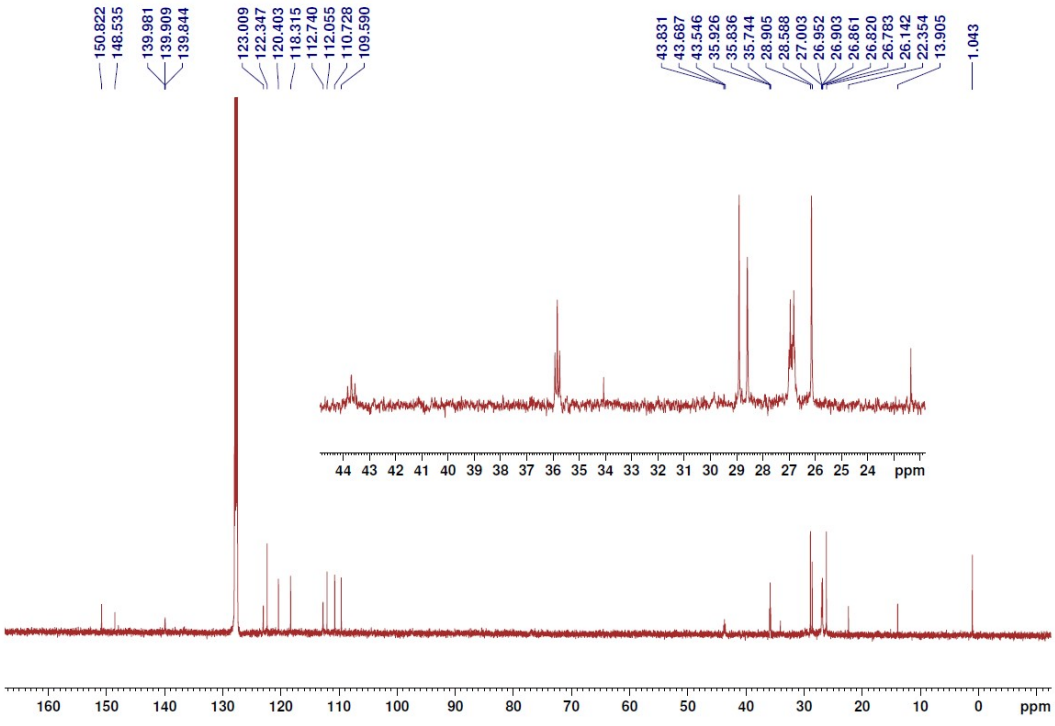


Figure S22. $^{13}C\{^{1}H\}$ NMR spectrum of ^{Cy}PBPNiBcat (**4b**) (126 MHz, C_6D_6).

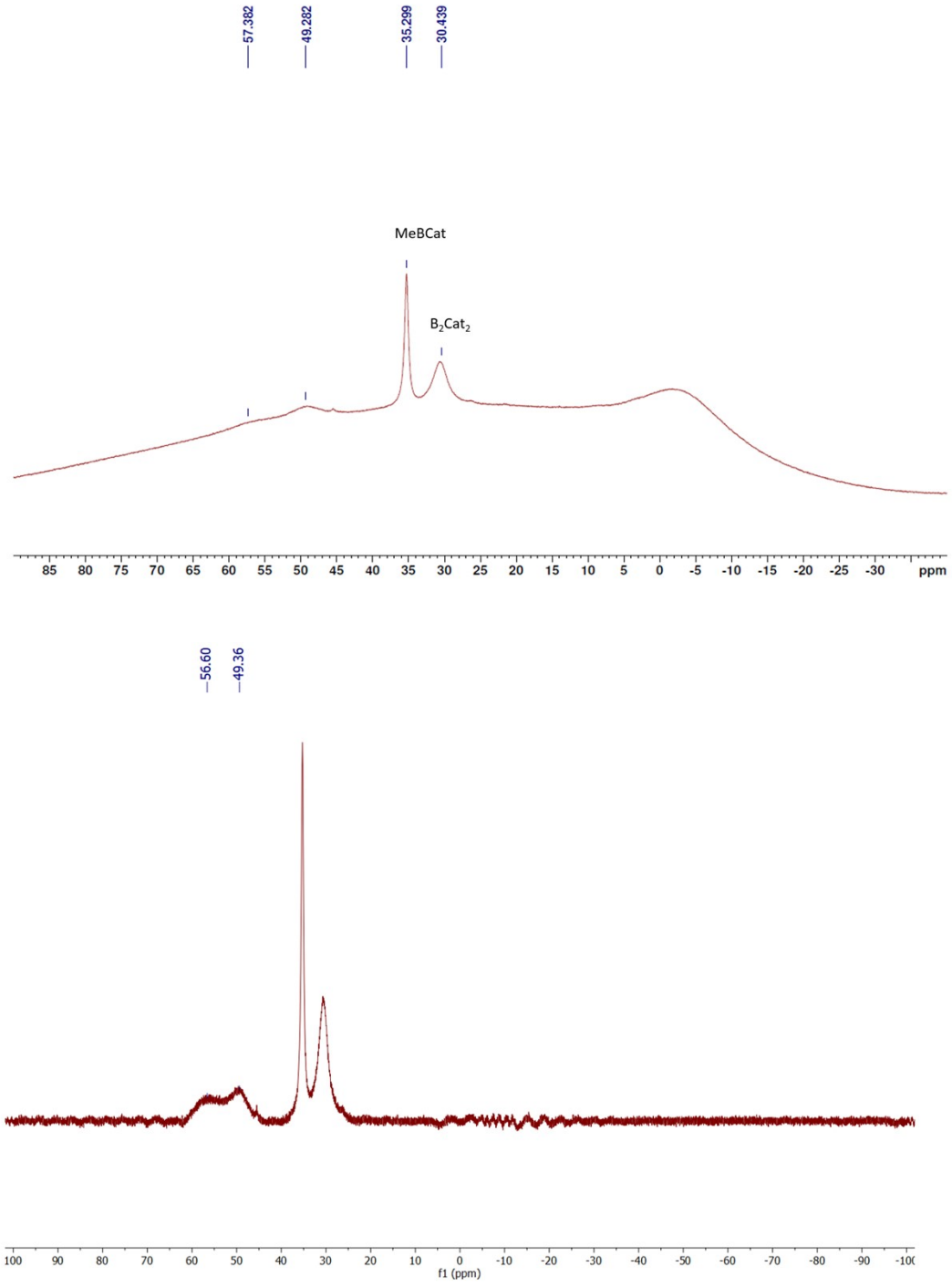


Figure S23. Top: $^{11}B\{^{1}H\}$ NMR spectrum of ^{Cy}PBPNiBcat (**4b**) (160 MHz, C_6D_6). Bottom: processed $^{11}B\{^{1}H\}$ spectra where the signal from borosilicate glass has been minimized by using the smooth segments algorithm included in the multipoint baseline correction option in MestReNova. Signals at 35 and 30 ppm correspond to MeBCat and B_2Cat_2, respectively.

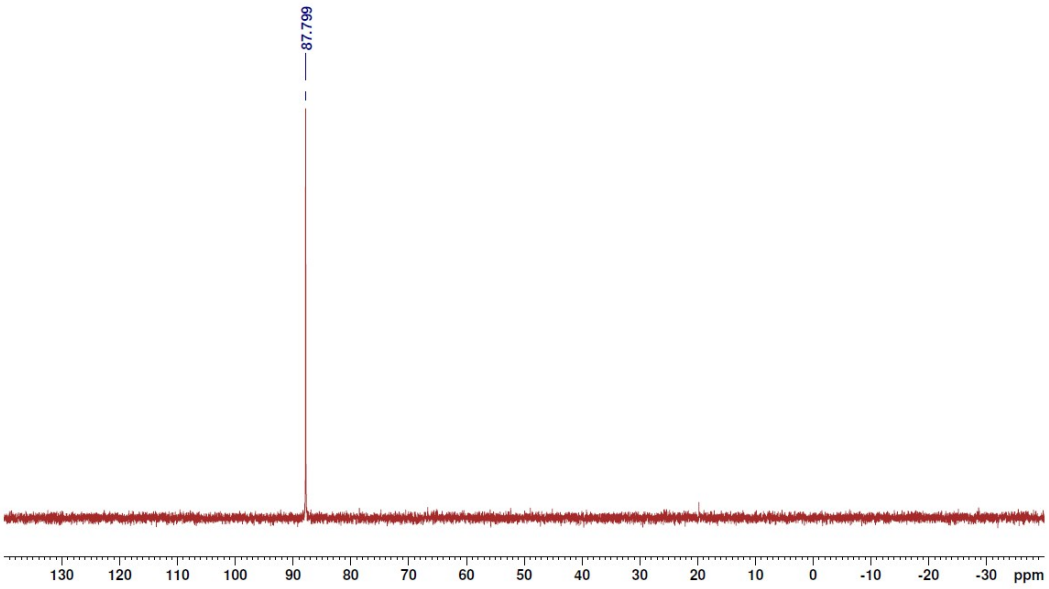


Figure S24. $^{31}P\{^{1}H\}$ NMR spectrum of ^{Cy}PBPNiBcat' (**5b**) (202 MHz, C_6D_6).

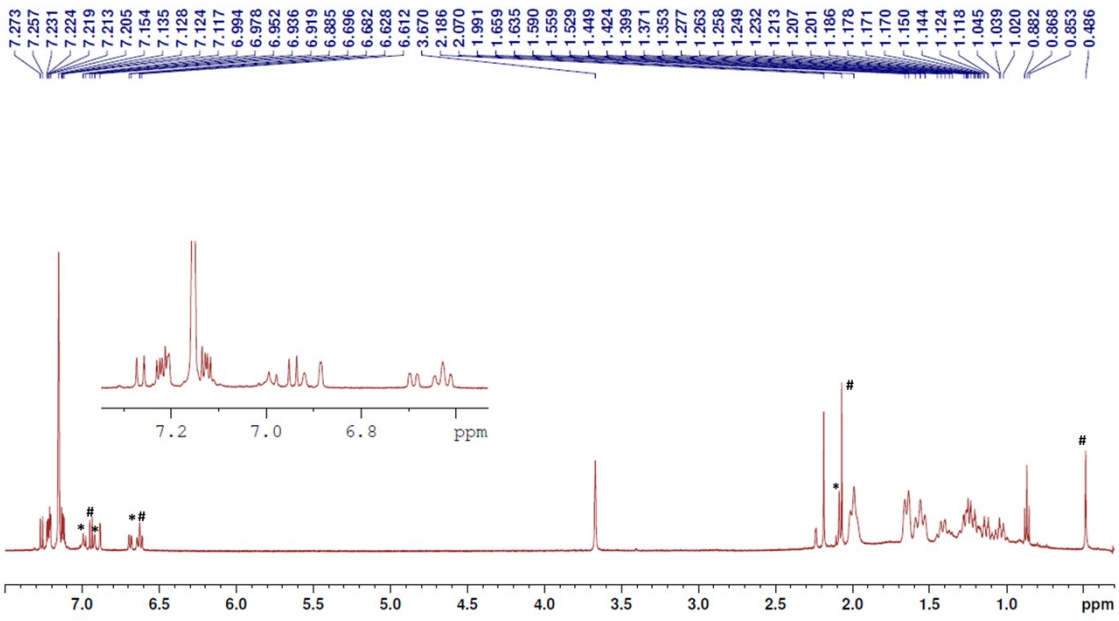


Figure S25. ^{1}H NMR spectrum of ^{Cy}PBPNiBcat' (**5b**) (500 MHz, C_6D_6). * denotes $B_2Cat'_2$ and # denotes MeBcat'.

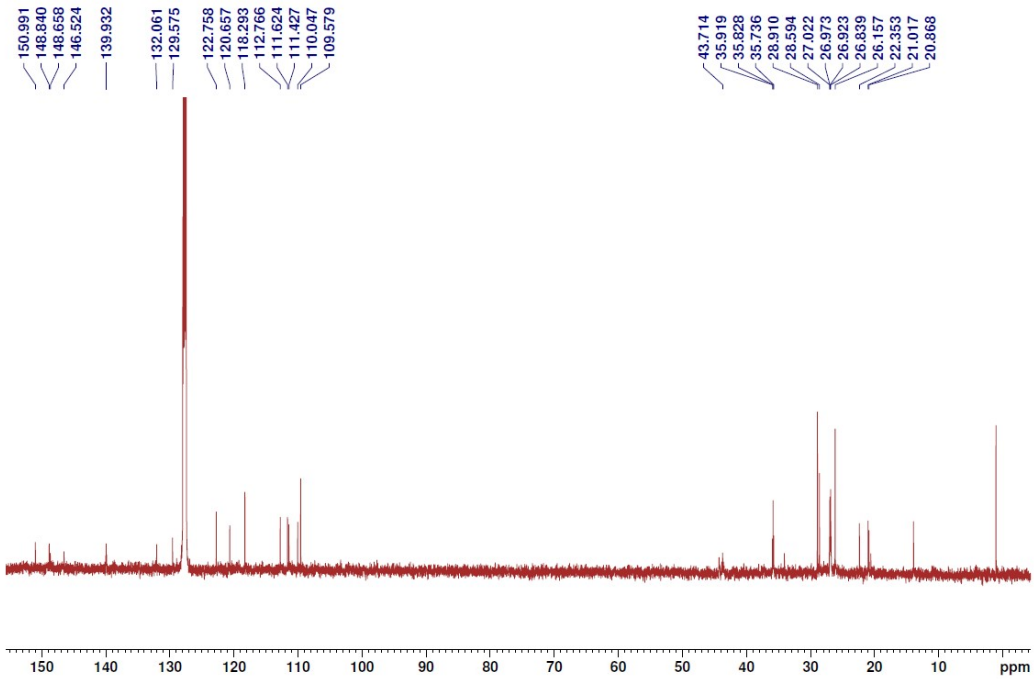
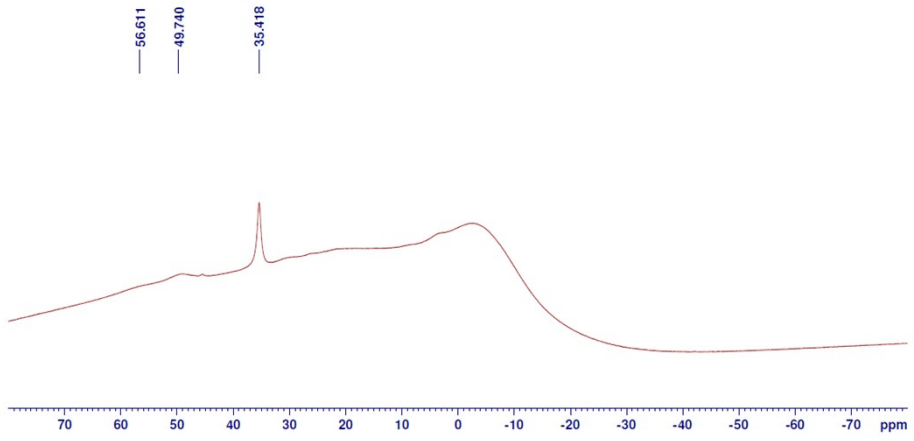


Figure S26. $^{13}C\{^{1}H\}$ NMR spectrum of ^{Cy}PBPNiBcat' (**5b**) (126 MHz, C_6D_6).



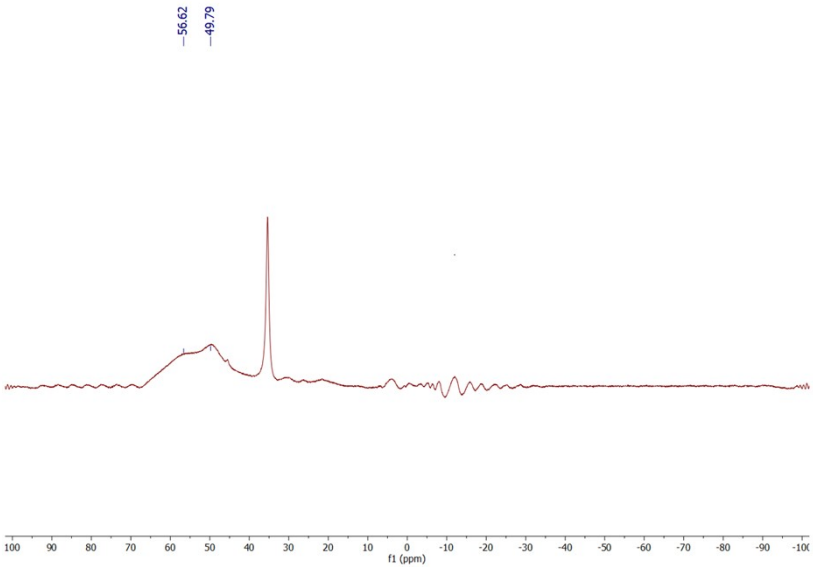


Figure S27. Top: $^{11}B\{^1H\}$ NMR spectrum of ^{Cy}PBPNiBcat' (**5b**) (160 MHz, C_6D_6). Bottom: processed $^{11}B\{^1H\}$ spectra where the signal from borosilicate glass has been minimized by using the smooth segments algorithm included in the multipoint baseline correction option in MestReNova. Signal at 35 ppm corresponds to MeBCat'.

3.6- NMR scale reaction of ^{tBu}PBPNiH (3) with N_2O

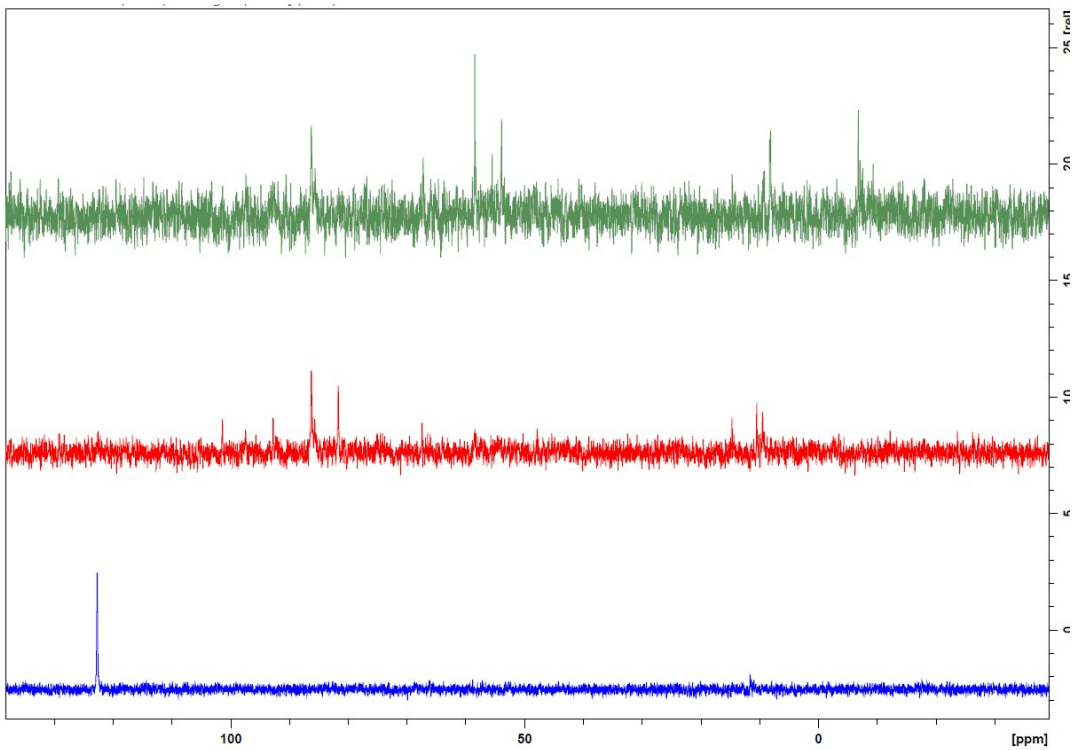


Figure S28. $^{31}P\{^1H\}$ NMR spectrum of: ^{tBu}PBPNiH (**3**) (bottom) and after addition of 2 bar NO_2; t = 15 min (middle) and 2 h (top) (162 MHz, C_6D_6).

3.7- NMR scale reaction of ^{tBu}PBPNiH (3) with HBpin and N_2O

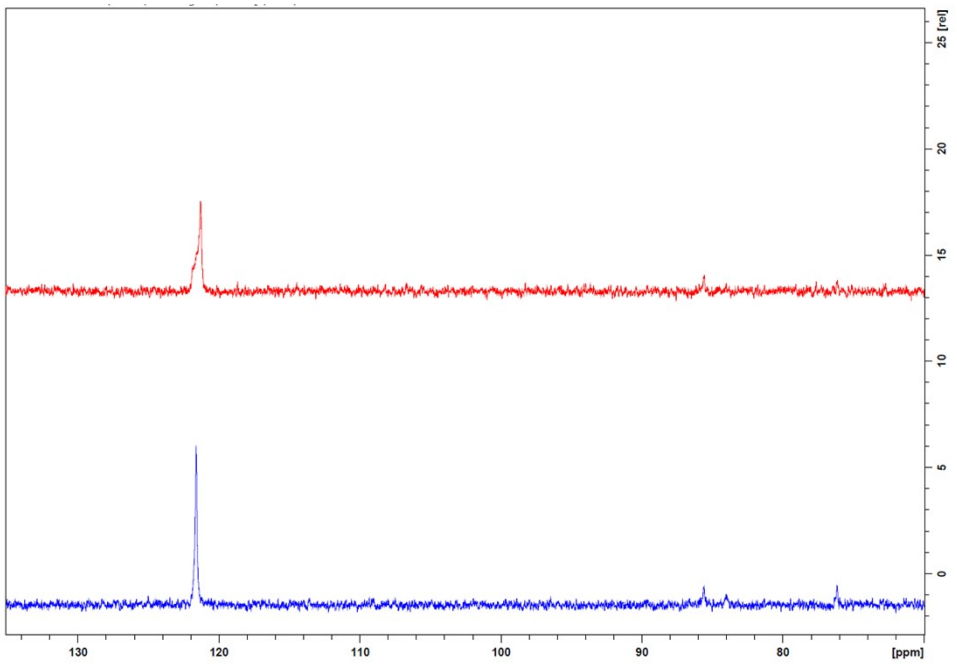
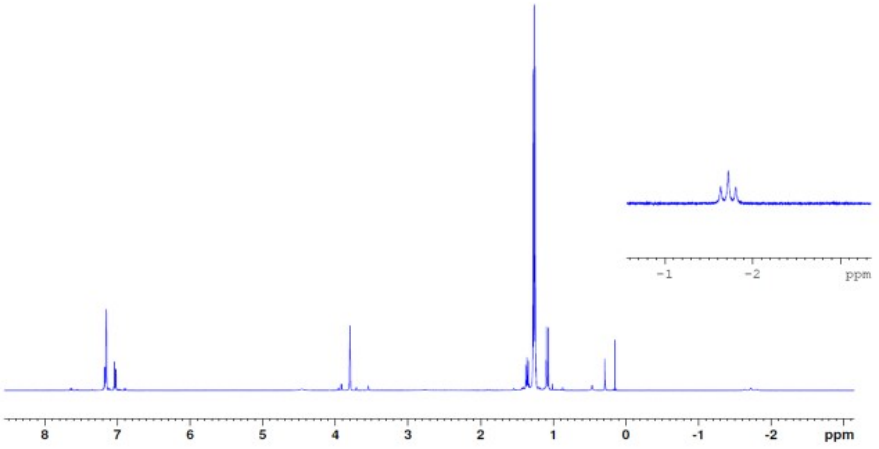


Figure S29. $^{31}P\{^1H\}$ NMR spectrum of: ^{tBu}PBPNiH (**3**) (bottom) and after addition of 10 equiv. of HBpin (top) (162 MHz, C_6D_6).



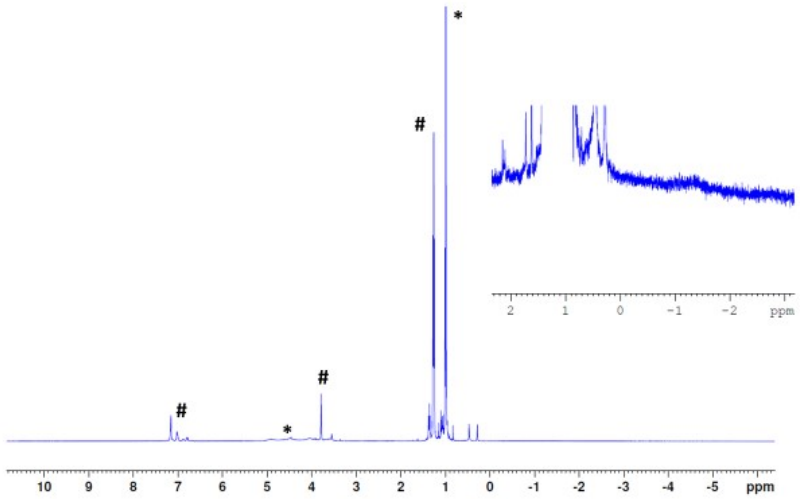


Figure S30. ^{1}H NMR spectrum of: ^{tBu}PBPNiH (**3**) (bottom) and after addition of 10 equiv. of HBpin (top) (400 MHz, C_6D_6) showing an expansion of the hydride region in both cases. * denotes resonances corresponding to HBpin and # resonances corresponding to **3**.

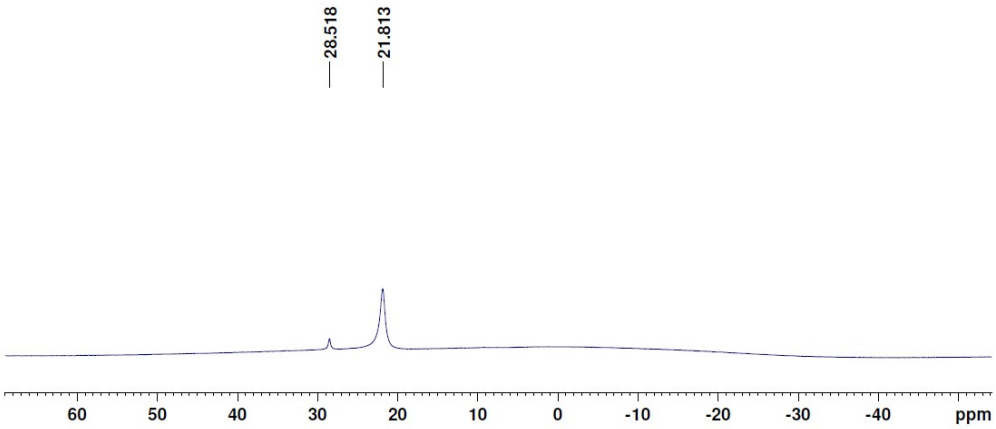


Figure S31. ^{11}B{^{1}H} NMR spectrum of **3** after addition of HBpin and N_2O (128 MHz, C_6D_6).

4. Catalytic reactions

4.1 General Method

All reactions were performed in duplicate in deuterated solvent. To a high-pressure J. Young valve NMR tube containing the catalyst or precatalyst (5 or 2 mol %), C_6D_6 (500 µL) and borane or diborane (0.08 mmol) were added and the J. Young valve NMR tube was degassed via three freeze-pump-thaw cycles. Then, the J. Young valve NMR tube was backfilled with N_2O gas. The reaction mixture was monitored by ^{11}B{^{1}H} NMR spectroscopy (see Table S1).

Entry	[Ni]	Solvent	T	Reductant	Cat. loading mol %	Time (h)	Conv. (%)[a]
1	**2a**	C_6D_6	25	B_2Cat_2	5	19	36
2	**2a**	toluene	25	B_2Cat_2	5	19	36
3	**2a**	C_6H_5F	25	B_2Cat_2	5	19	8
4	**2a**	THF	25	B_2Cat_2	5	19	0
5	**2a**	CH_2Cl_2	25	B_2Cat_2	5	19	0
6	**2a**	C_6D_6	50	B_2Cat_2	5	10	99
7	**2a**	C_6D_6	50	$B_2Cat'_2$	5	6	99
8	**2a**	C_6D_6	50	B_2pin_2	5	19	0
9	**2b**	C_6D_6	50	B_2Cat_2	5	4	99
10	**2b**	C_6D_6	50	$B_2Cat'_2$	5	3.5	99
11	**2a**	C_6D_6	25	HBcat	5	0.5	99
12[b]	**2a**	C_6D_6	25	HBcat	2	1	99
13	**2a**	C_6D_6	25	HBpin	5	1	99
14	**2a**	C_6D_6	25	9-BBN	5	19	0
15	**2b**	C_6D_6	25	HBcat	5	19	99
16	**3**	C_6D_6	25	HBcat	5	0.5	99
17	**3**	C_6D_6	25	HBpin	5	1.5	99

Table S1. Catalyst screening for the diborane and borane reduction of N_2O

a NMR spectroscopic yield by $^{11}B^{1}\{H\}$ NMR analysis using $BH_3(NMe_3)$ as an internal standard. *b* Reaction carried out in a Fischer Porter reactor; P_{N2O} = 1 bar.

4.2 Catalytic reactions using ^{tBu}PBPNiMe (**2a**) as precatalyst

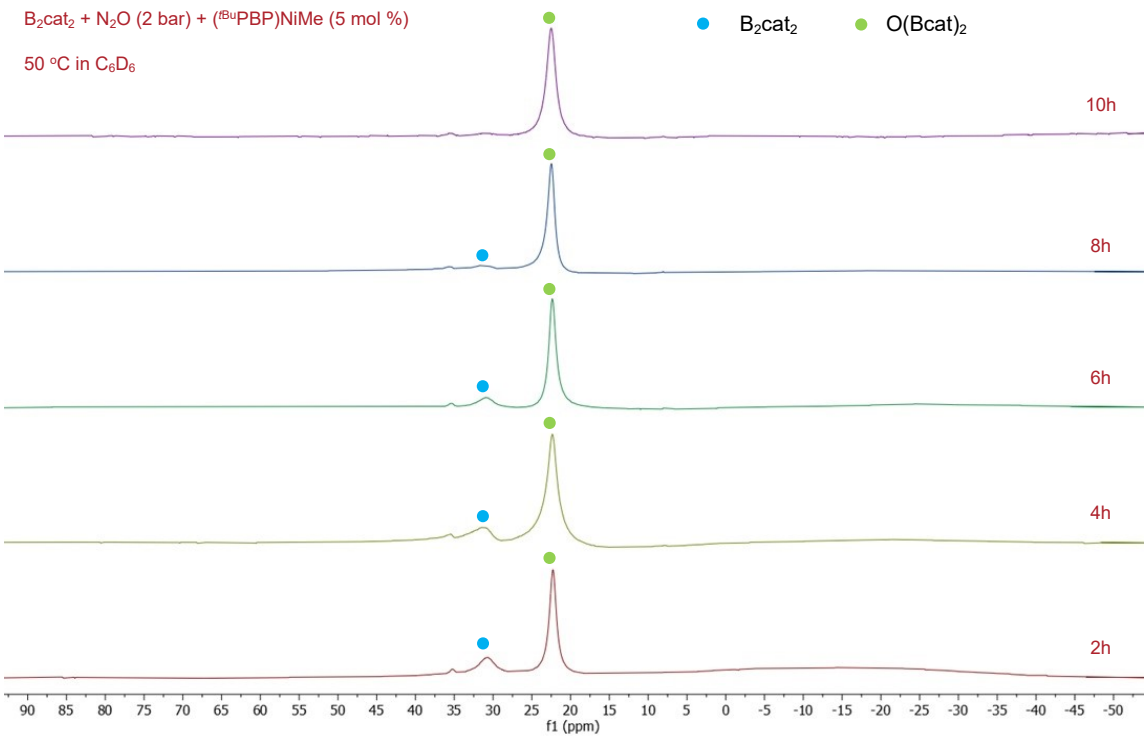


Figure S32. $^{11}B\{^{1}H\}$NMR spectrum of B_2cat_2 reduction of N_2O at 50 °C after 10h in a J. Young NMR tube (entry 6; 128 MHz, C_6D_6).

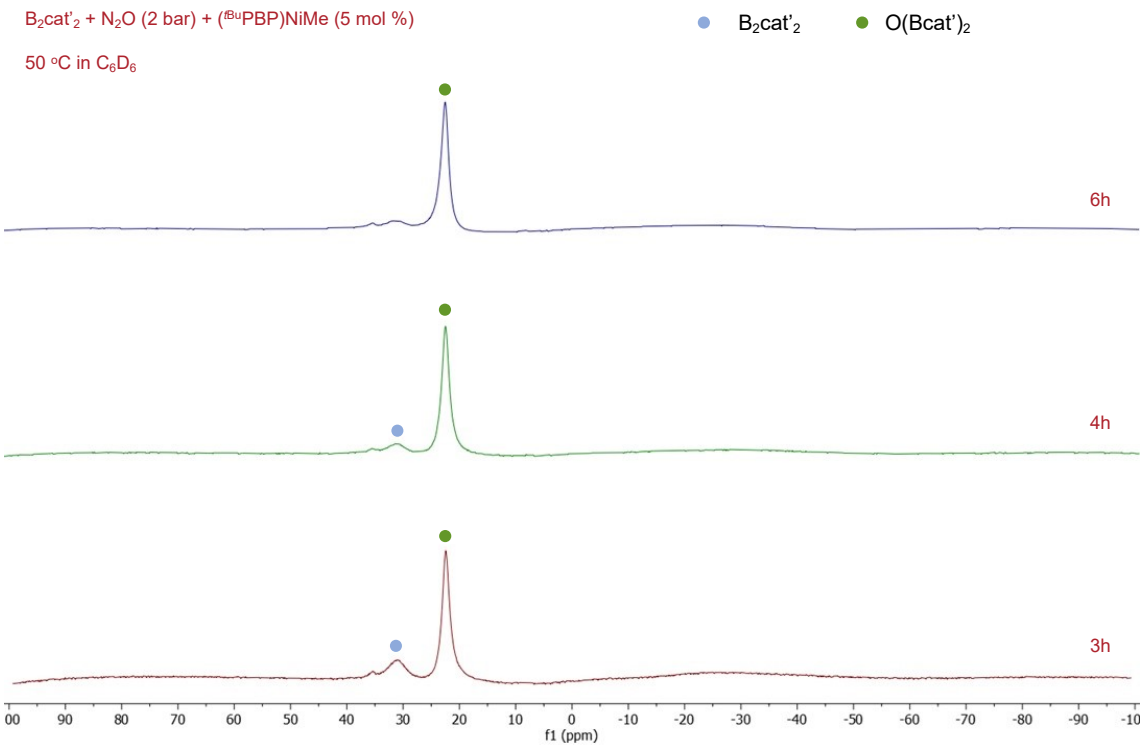


Figure S33. $^{11}B\{^1H\}$NMR spectrum of $B_2cat'_2$ reduction of N_2O at 50 °C after 6h in a J. Young NMR tube (entry 7; 128 MHz, C_6D_6).

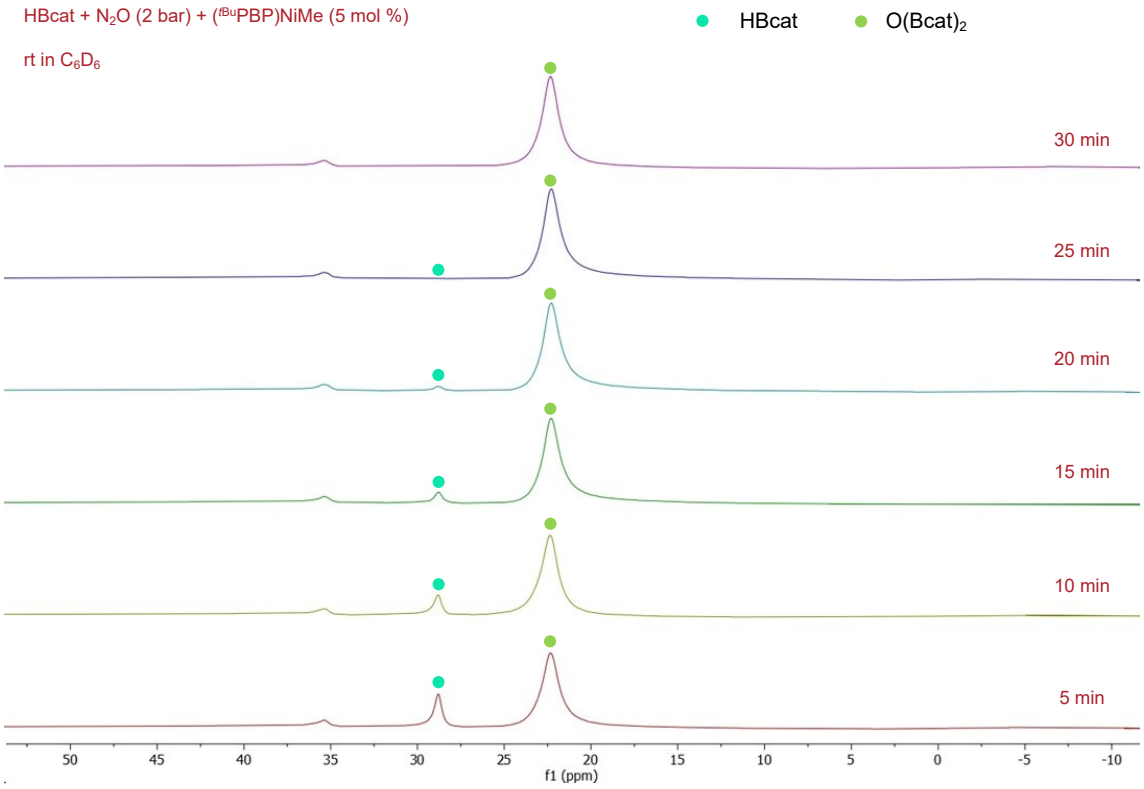


Figure S34. $^{11}B\{^1H\}$NMR spectrum of HBcat reduction of N_2O at room temperature after 30 min in a J. Young NMR tube (entry 11; 128 MHz, C_6D_6).

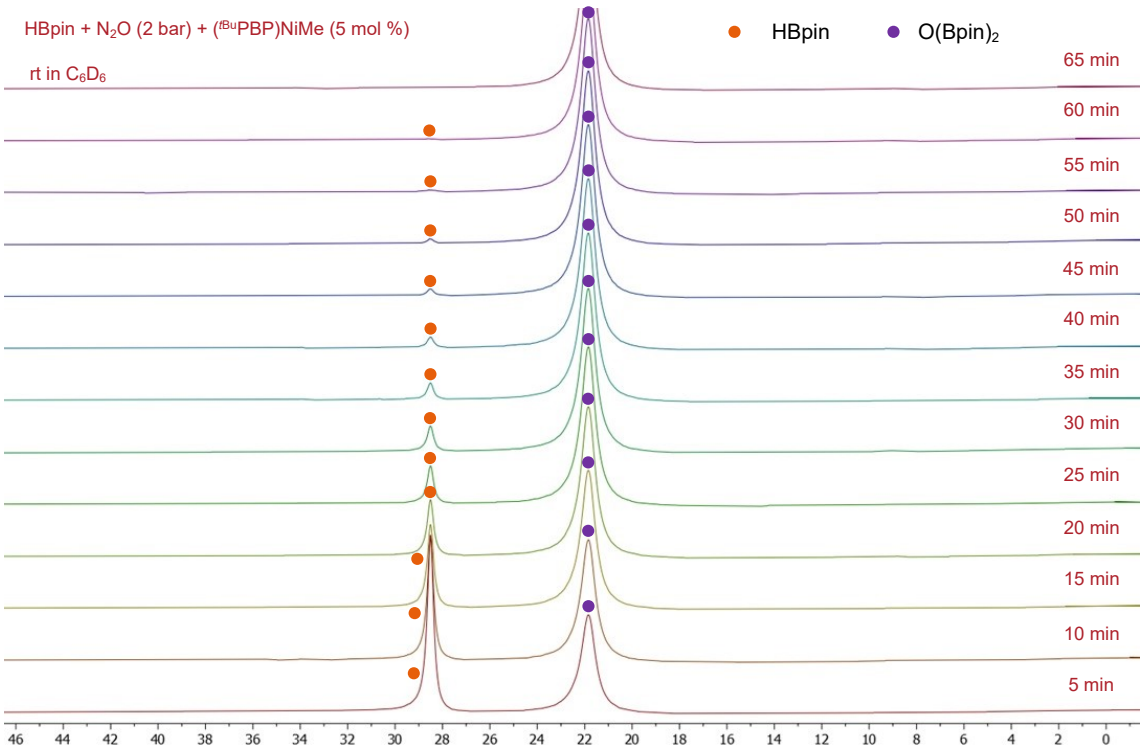


Figure S35. $^{11}B\{^{1}H\}$NMR spectrum of HBpin reduction of N_2O at room temperature after 1h in a J. Young NMR tube (entry 13; 128 MHz, C_6D_6).

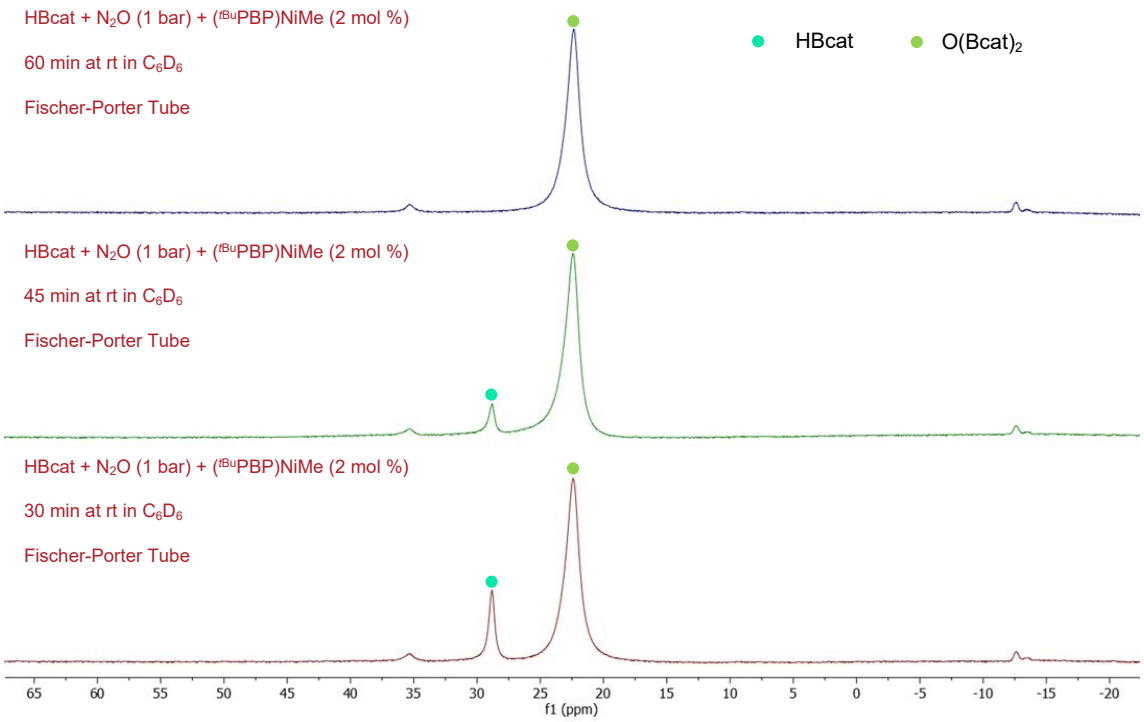


Figure S36. $^{11}B\{^{1}H\}$NMR spectrum of HBcat reduction of N_2O at room temperature after 30; 45 and 60 min in a Fischer-Porter tube (entry 12; 128 MHz, C_6D_6).

N_2 detection by GC-TCD.

GC-TCD analysis were carried out using an Agilent 7820A apparatus equipped with a Carboxen 1010 Plot (30 m × 0.53 mm) column. Helium carrier gas was supplied at a head pressure of 2.4 psi to provide an initial flow rate of 2.5 mL/min. The injector temperature was setup to 230 °C, and the oven temperature was initially held at 30 °C for 7 min, then gradually increased to 220 °C at 25 °C/min.

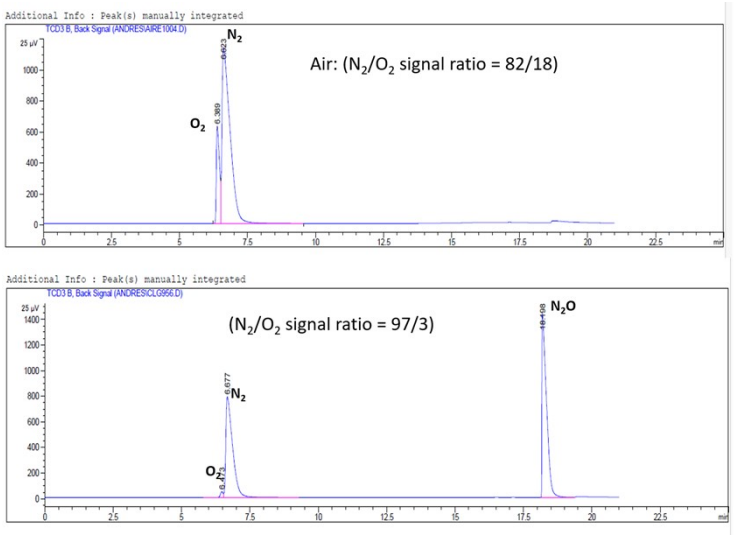


Figure S37. N_2 detection by GC-TCD of HBcat reduction of N_2O at room temperature using ^{tBu}PBPNiMe as the precatalyst after 1h (entry 12). top: control experiment: air (N_2 + O_2); bottom: catalytic reaction (Table 1, entry 12).

4.3 Catalytic reactions using as precatalyst ^{Cy}PBPNiMe (**2b**)

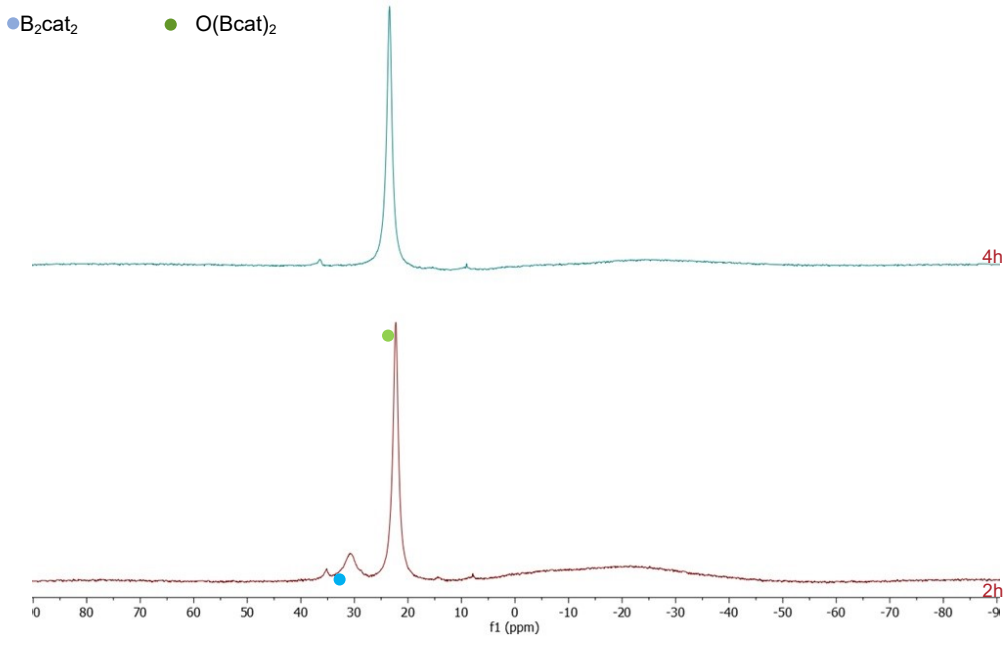


Figure S38. $^{11}B\{^1H\}$NMR spectrum of B_2cat_2 reduction of N_2O at 50 °C after 4h (entry 9; 128 MHz, C_6D_6).

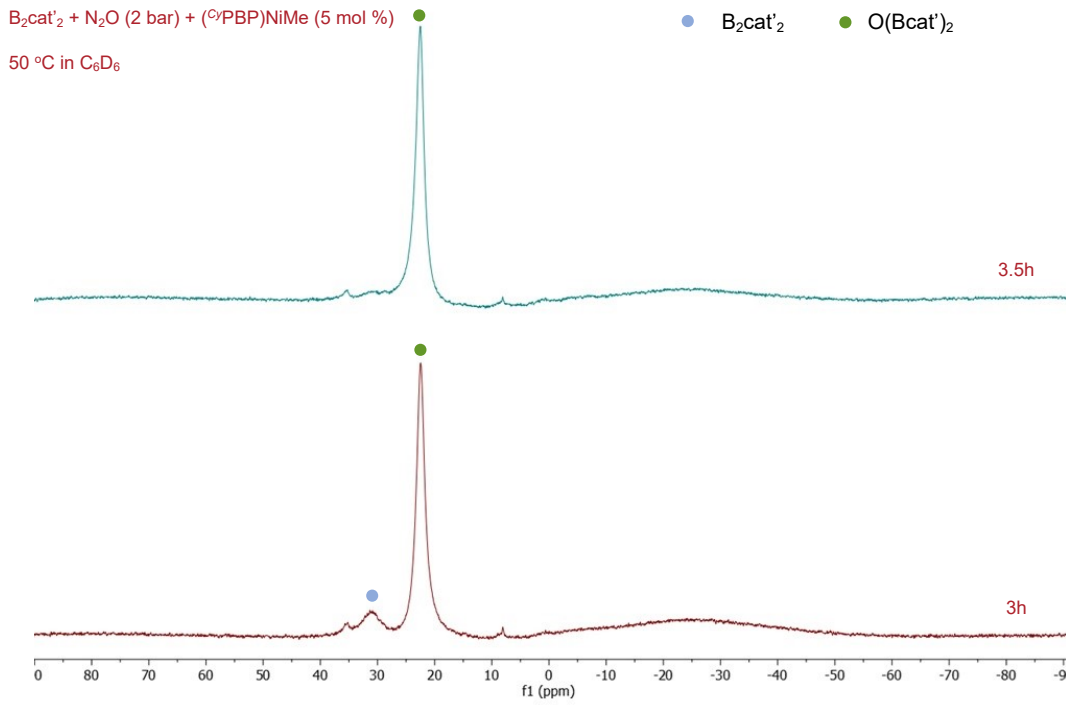


Figure S39. $^{11}B\{^1H\}$NMR spectrum of $B_2cat'_2$ reduction of N_2O at 50 °C after 3.5 h (entry 10; 128 MHz, C_6D_6).

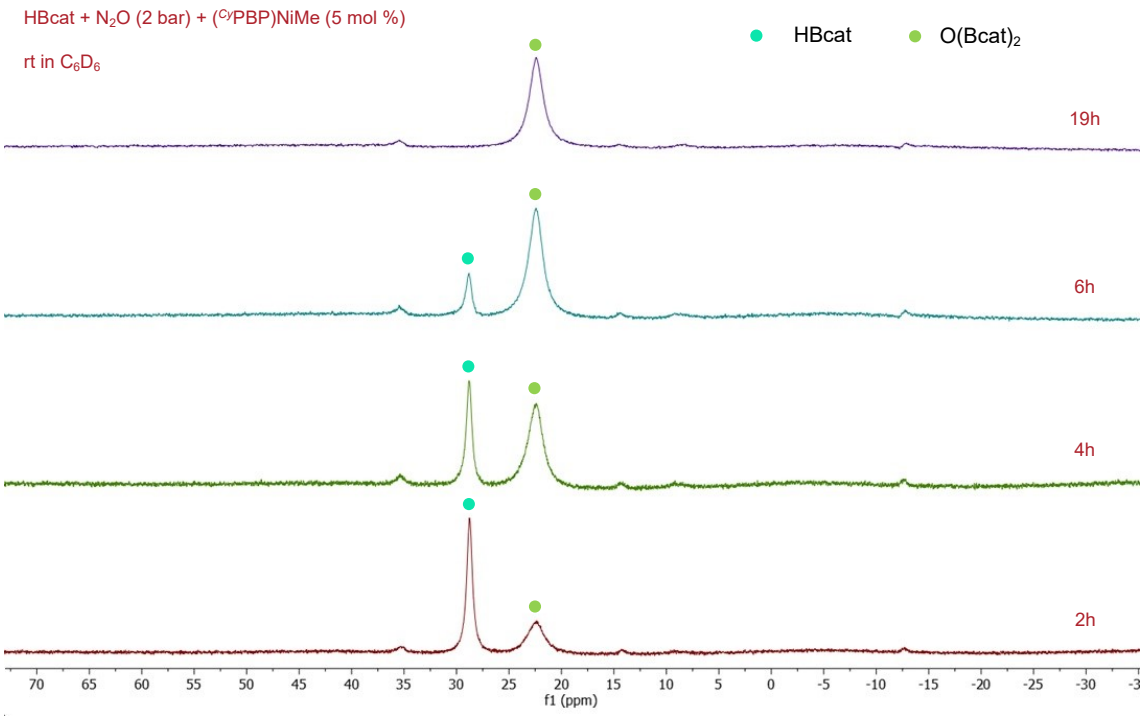


Figure S40. $^{11}B\{^1H\}$NMR spectrum of HBcat reduction of N_2O at room temperature after 19h (entry 15; 128 MHz, C_6D_6).

4.4 Catalytic reactions using as catalyst ^{tBu}PBPNiH (**3**)

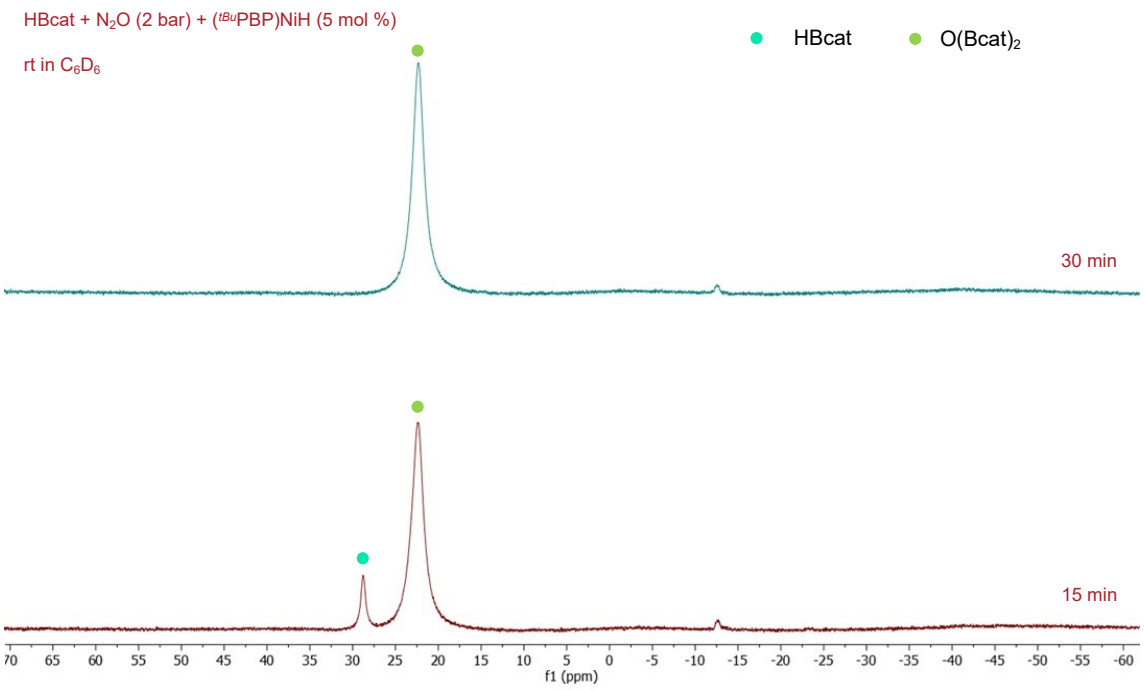


Figure S41. $^{11}B\{^1H\}$NMR spectrum of HBcat reduction of N_2O at room temperature after 30 min (entry 16; 96 MHz, C_6D_6).

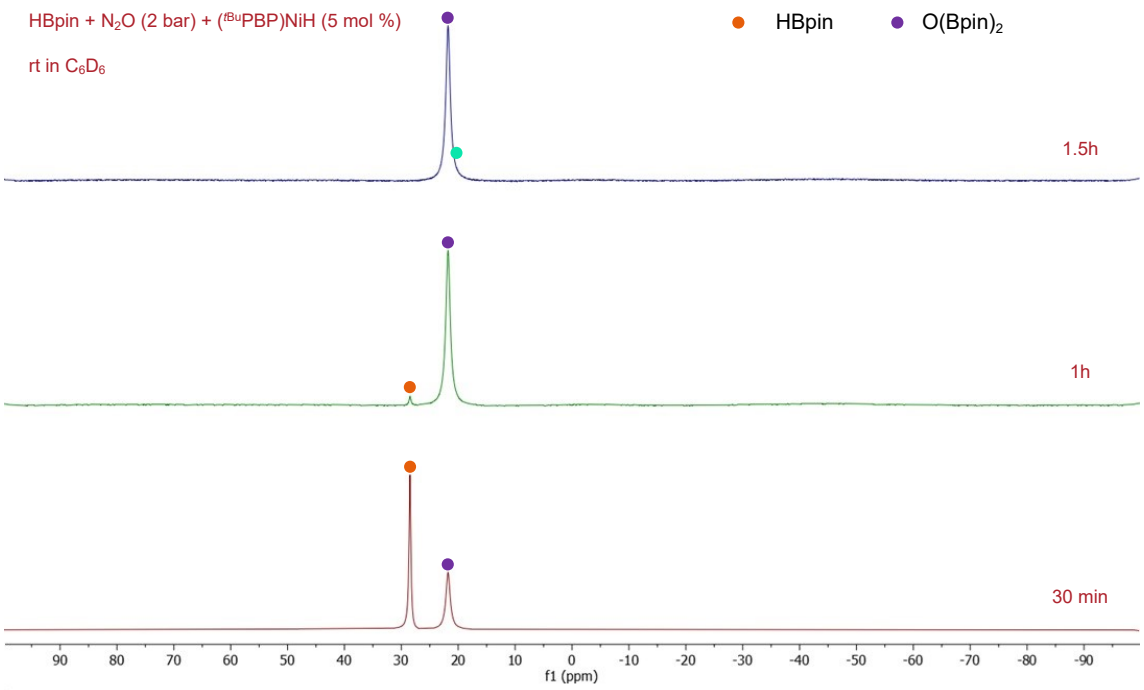


Figure S42. $^{11}B\{^1H\}$NMR spectrum of HBpin reduction of N_2O at room temperature after 1.5h (entry 17; 96 MHz, C_6D_6).

5. Kinetic studies

5.1- Order in catalyst

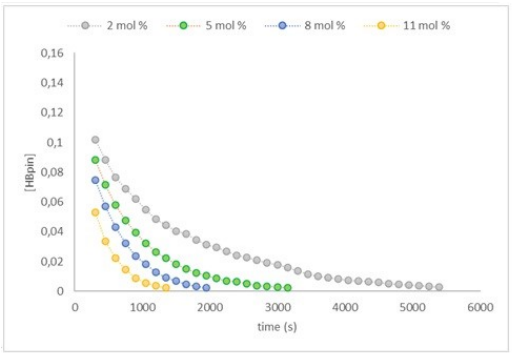
A J. Young tube valve NMR was charged with precatalyst **2a** and HBcat (2, 5, 8 or 11 mol %), HBpin (0.08 mmol) in C_6D_6 (500 µL) and was degassed via three freeze-pump-thaw cycles. Then, the solution was backfilled with N_2O gas (4 bar) and inserted in an NMR apparatus. The progression of the reaction was monitored by $^{11}B\{^1H\}$ NMR using the following parameters for each spectrum; d1 = 0.4, ns = 40.

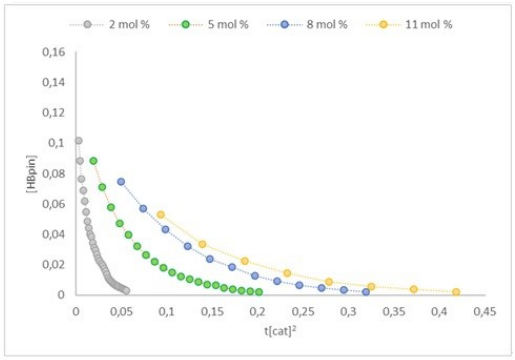
Table S2. Concentration values for each component used to determine the order of catalyst in the reaction rate.

Entry	[HBpin]	N_2O	[^{tBu}PBP-NiMe]/HBcat
1*	0.16 mM	4 bar	3.20E-03 mM
2*	0.16 mM	4 bar	8.00E-03 mM
3*	0.16 mM	4 bar	12.8 E-03 mM
4*	0.16 mM	4 bar	17.6 E-03 mM

*Repeated two times

The order in catalyst was confirmed visually by Variable Time Normalization Analysis (VTNA) as well. The concentration plots obtained by NMR (Figure S39) show the concentration of HBpin against a normalized time scale to a zeroth- , first- and second- order dependence on the initial catalyst concentration, according to the method developed by Burés.[5] This analysis indicates that the reaction is first-order with respect to the catalyst.





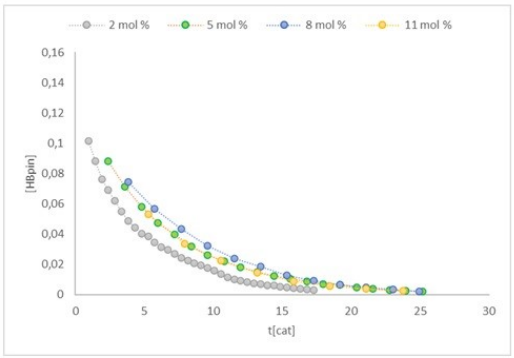
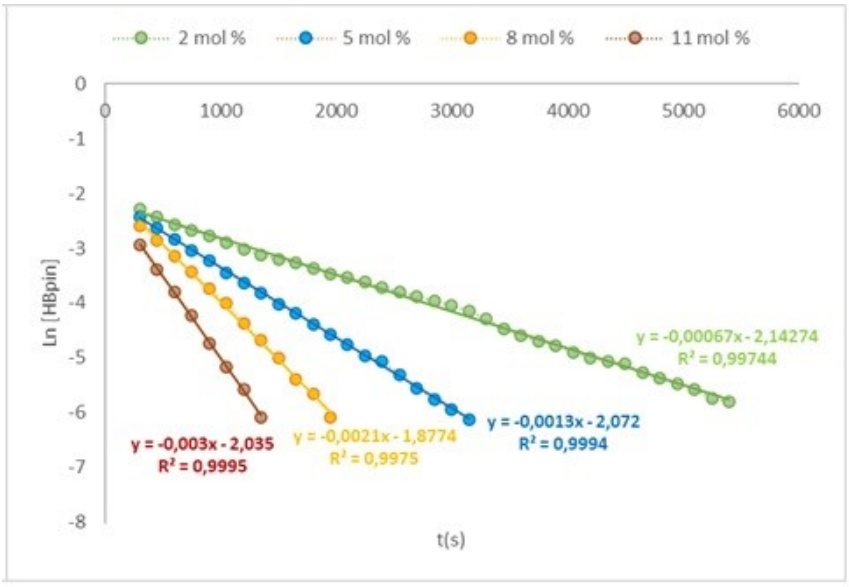


Figure S43. Plots obtained of the NMR data where the concentration of ^{tBu}PBPNiMe (**2a**) is elevated to different exponents.



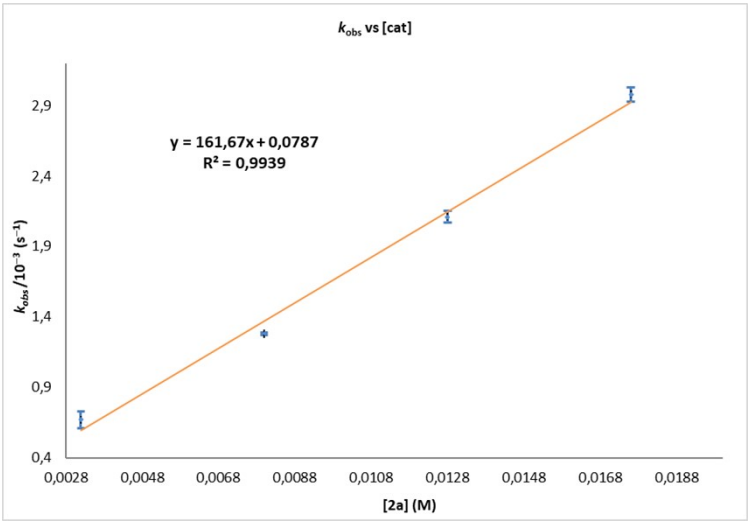


Figure S44. Kinetic plots of ln[HBpin] vs initial time (s) in C_6D_6 using catalyst loading of **2a** from 2 to 11 mol %; P_{N2O} = 4 bar; [HBpin] = 0.16m M (top). Variation of k_{obs} *vs* [**2a**] (bottom).

Table S3. Concentration values for each component used to determine the order of gas in the reaction rate.

Entry	[**2a**] (M)	% **2a** (mol/mol)	k_{obs} (s^{-1})/10^{-3}
1	0.032	2	0.67 ± 0.06
2	0.008	5	1.28 ± 0.01
3	0.0128	8	2.11 ± 0.04
3	0.0176	11	2.98 ± 0.05

5.2- Order in N_2O

A J. Young tube valve NMR was charged with precatalyst **2a** and HBcat (5 mol %), HBpin (0.08 mmol) in C_6D_6 (500 µL) and was degassed via three freeze-pump-thaw cycles. Then, the solution was backfilled with N_2O gas (2 or 4 bar) and inserted in an NMR apparatus. The progression of the reaction was monitored by $^{11}B\{^1H\}$ NMR using the following parameters for each spectrum; d1 = 0.4, ns = 40. Analysis of the kinetics (Figure S41) indicates that the reaction is zero order in N_2O.

Table S4. Concentration values for each component used to determine the order of gas in the reaction rate.

Entry	[HBpin]	N_2O	[$^{(tBu)}$PBP-NiMe]/HBcat
1*	0.16 mM	2 bar	8.00E-03 mM
2*	0.16 mM	4 bar	8.00E-03 mM

*Repeated two times

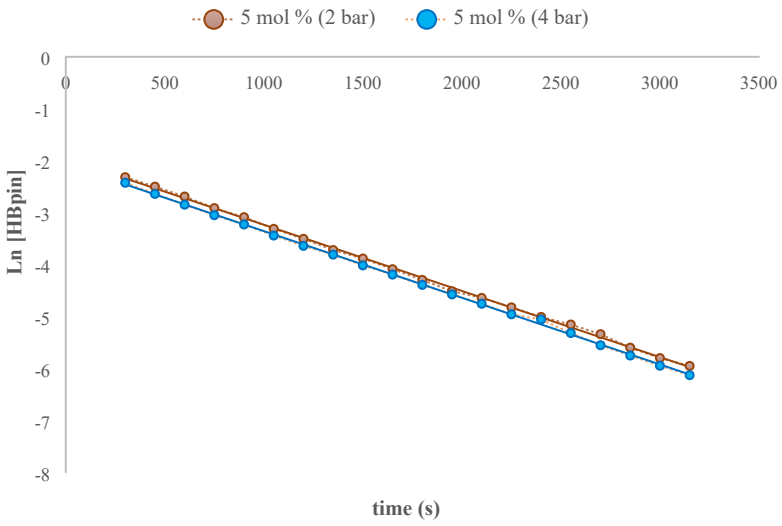


Figure S45. Kinetic plot of ln[HBpin] vs initial time (s) in C_6D_6 using catalyst **2a** for P_{N_2O} = 2 bar and 4 bar; [HBpin] = 0.16 mM; 5 mol % of **2a.**

5.3- Order in HBpin

A J. Young tube valve NMR was charged with precatalyst **2a** and HBcat (5 mol %), HBpin (0.08 or 0.16 mmol) in C_6D_6 (500 µL) and was degassed via three freeze-pump-thaw cycles. Then, the solution was backfilled with N_2O gas (2 or 4 bar) and inserted in an NMR apparatus. The progression of the reaction was monitored by $^{11}B\{^1H\}$ NMR using the following parameters for each spectrum; d1 = 0.4, ns = 40. Analysis of the kinetics (Figure S42) indicates that the reaction is first order in HBpin.

Table S5. Concentration values for each component used to determine the order of gas in the reaction rate.

Entry	[HBpin]	N_2O	[^{tBu}PBP-NiMe]/HBcat
1*	0.16 mM	4 bar	8.00E-03 mM
2*	0.32 mM	4 bar	8.00E-03 mM

*Repeated two times

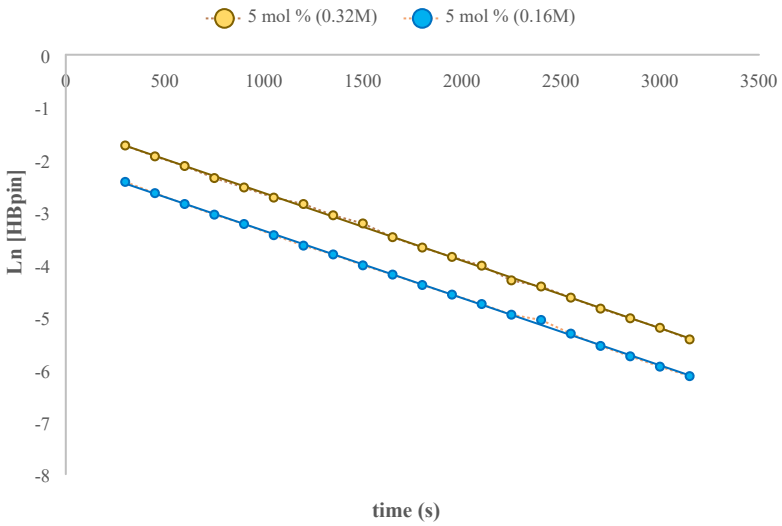


Figure S46. Kinetic plot of ln[HBpin] vs initial time (s) in C_6D_6 using catalyst **2a** for P_{N_2O} = 4 bar; [HBpin] = 0.16 mM and 0.32 mM; 5 mol % of **2a.**

5.4- Variable temperature $^{11}B\{^1H\}$ NMR study of reaction of ^{tBu}PBPNiMe (2a) with N_2O in presence of HBpin and line-shape data analysis

A J. Young tube valve NMR was charged with catalyst **2a** (5 mol %) and HBpin (0.08 mmol) in C_6D_6 (500 µL) and was degassed via three freeze-pump-thaw cycles. Then, the solution was backfilled with N_2O gas (4 bar) and inserted in an NMR apparatus at different temperatures (in the range 288–308 K; Figure S43). The progression of the reaction was monitored by $^{11}B\{^1H\}$ NMR using the following parameters for each spectrum; d1 = 0.4, ns = 40. The line-shape analysis plot of a variable temperature $^{11}B\{^1H\}$ NMR study provided the data listed in Table S5. The corresponding Eyring plot is (Figure S44) permitted to estimate the following activation energy: $\Delta G^{\#}$ (298.15 K) = (18.5 ± 0.9) kcal·mol^{-1}.

Table S6. k_{obs} values calculated at different temperatures ([**2a**]).

T (K)	$k_{obs}/10^{-3}$ (s^{-1})	$k/10^{-1}$ ($s^{-1}M^{-1}$)	*ln(k/T)*
288	0.541 ± 0.003	0.675 ± 0.004	-8.36
293	0.91 ± 0.02	1.14 ± 0.03	-7.85
298	1.28 ± 0.01	1.60 ± 0.01	-7.53
303	2.11 ± 0.05	2.64 ± 0.06	-7.05
308	3.58 ± 0.08	4.5 ± 0.1	-6.53

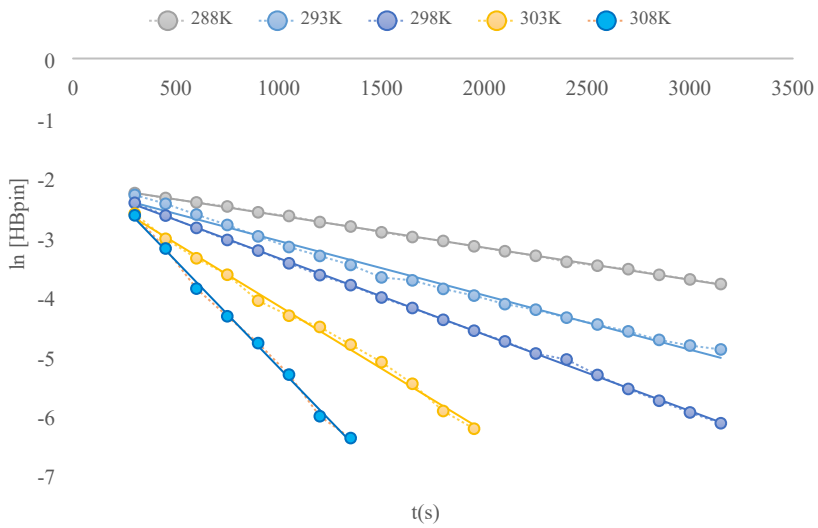


Figure S47. Kinetic plots of ln [HBpin] vs initial time (s) in C_6D_6 using catalyst **2a** for P_{N_2O} = 4 bar; [HBpin] = 0.16 mM; 5 mol% of **2a** at Temperature = 288, 293, 298, 303 and 308 K

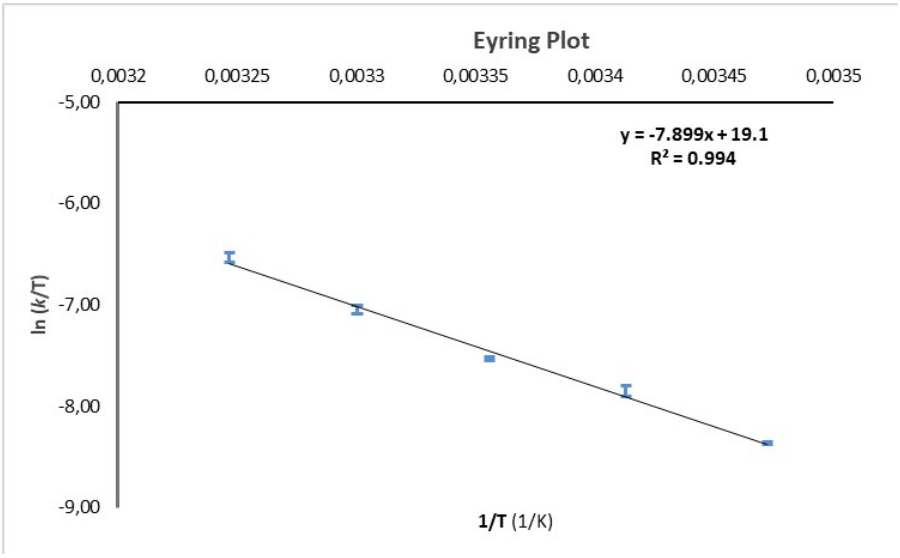


Figure S48. Eyring plot and activation parameters for the reaction of catalyst **2a** with N_2O (4 bar) and HBpin. $\Delta H^{\ddagger}$ = 15.7 (± 0.7) kcal·mol^{-1} $\Delta S^{\ddagger}$ = –9.4 (± 0.6) cal·mol^{-1} K^{-1} $\Delta G^{\ddagger}$ (298.15) = 18.5 (± 0.9) kcal·mol^{-1}

6. Computational details

Gibbs energy profiles

Unless otherwise stated, calculations were performed using the PBE0 functional,[6] as implemented in Gaussian 09[7] along with Grimme's D3 dispersion correction.[8] Geometry optimizations were performed in solution (solvent = benzene, ε = 2.27) using the continuum SMD model[9] and basis set 1 (BS1). BS1 uses the double-ζ 6-31G(d,p)[10] basis set for the H, C, N, O,

B, and P atoms and the scalar relativistic Stuttgart−Dresden SDD pseudopotential[11] and its associated double-ζ basis set, complemented with a set of polarization functions, for the Ni atom.[12] The nature of the stationary points was confirmed by frequency analysis. Connections between the transition states and the minima were checked by perturbing the transition state geometry along the TS coordinate and optimizing until the corresponding minima. All energies in solution were corrected by single-point calculations with the larger basis set 2 (BS2) including triple-ζ def2TZVP basis set for the H, C, N, O, B, and P atoms, and def2QZVP for the Ni atom.[13] The scalar relativistic Stuttgart−Dresden SDD pseudopotential and its associated basis set for Ni was used in the energy profile calculations. Gibbs energies in benzene were calculated at 298.15 K. Gibbs energy corrections were obtained based on vibrational frequencies of the BS1 optimized structures using the quasi-harmonic approximation. Thermal contributions to the Gibbs energies were corrected by employing the approximation described by Grimme, where entropic terms for frequencies below a cut-off of 100 cm^{-1} were calculated using the free-rotor approximation.[14] The GoodVibes program developed by Paton and Funes-Ardoiz was employed to introduce these corrections.[15] All reported energies in the main text correspond to PBE0-D3/BS2 Gibbs energies in benzene solvent (1 M) at 298.15 K in kcal mol^{-1}. Structure visualization was performed with Chemcraft software.[16]

7. High-energy transition states

*Calculations to obtain Ni hydroxo species (hydride complex **3** and N_2O as energy reference (BS1))*

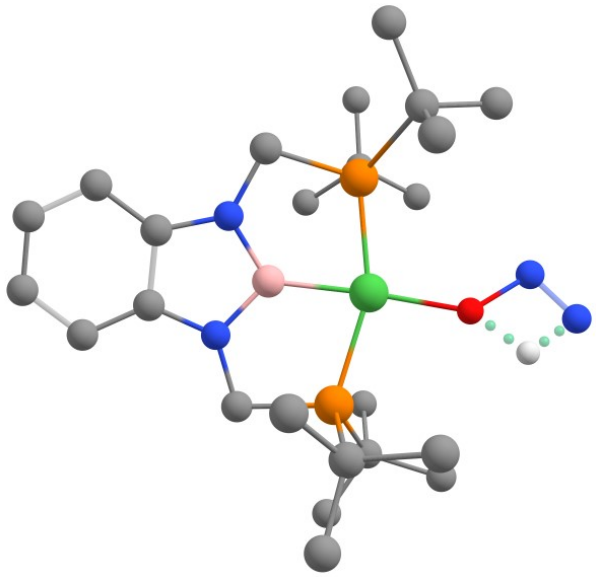


Figure S49. Transition state involving a 4-membered ring for the extrusion of N_2 (**TS-NiOH-1**). The energy required to overcome this barrier is 32.0 kcal mol^{-1}. Most of the H atoms have been omitted for clarity.

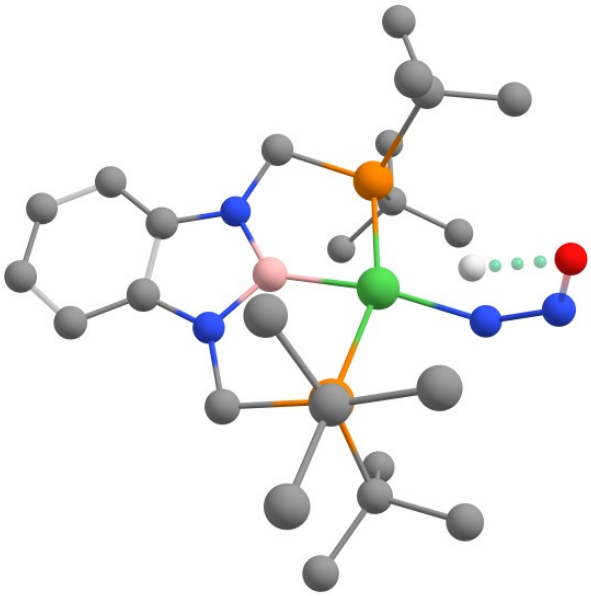


Figure S50. Transition state involving a 5-membered ring for the extrusion of N_2 (**TS-NiOH-2**). The energy required to overcome this barrier is 36.5 kcal mol^{-1}. Most of the H atoms have been omitted for clarity.

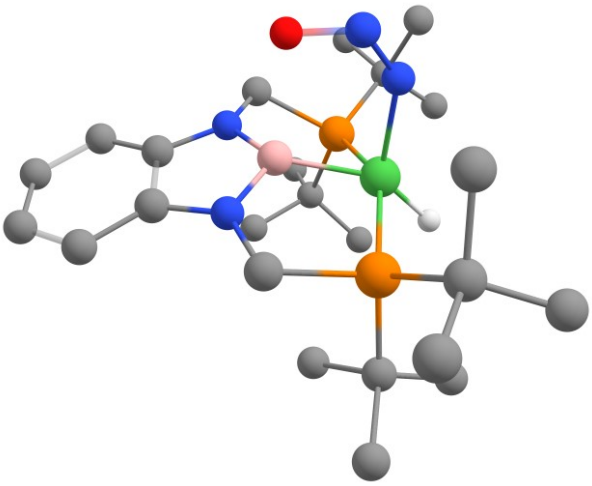


Figure S51. Transition state for the activation of N_2O mediated by the PBP ligand (**TS-NiOH-3**). The energy required to overcome this barrier is 31.2 kcal mol^{-1}. Most of the H atoms have been omitted for clarity.

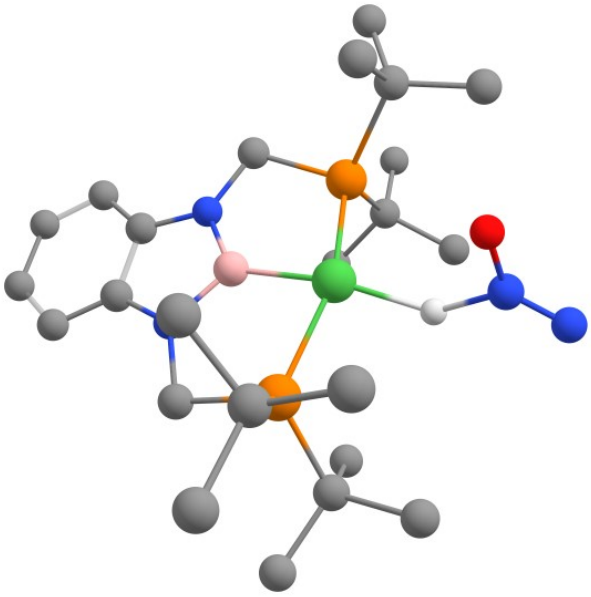


Figure S52. Transition state involving hydride attack to the central atom of N_2O (**TS-NiOH-4**). The energy required to overcome this barrier is 30 kcal mol^{-1}. Most of the H atoms have been omitted for clarity.

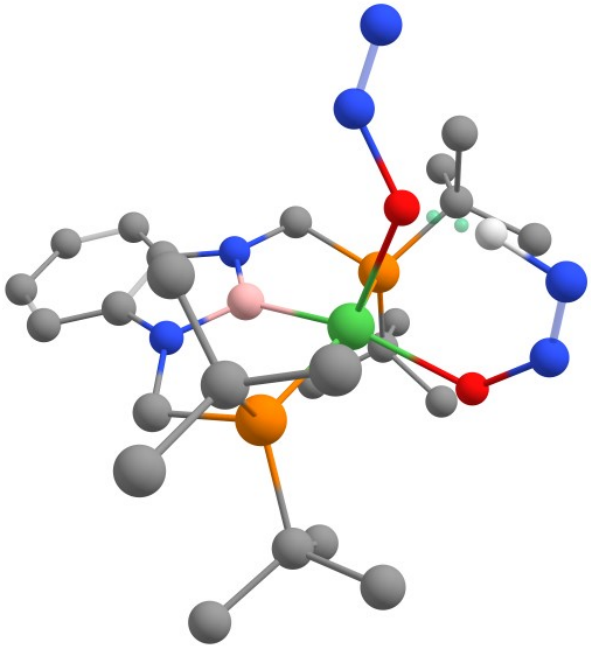


Figure S53. Transition state involving the participation of two N_2O molecules (**TS-NiOH-5**). The energy required to overcome this barrier is 40.1 kcal mol^{-1}. Most of the H atoms have been omitted for clarity.

*Calculations from boryl complex **4a** (boryl complex **4a** and N_2O as energy reference (BS1))*

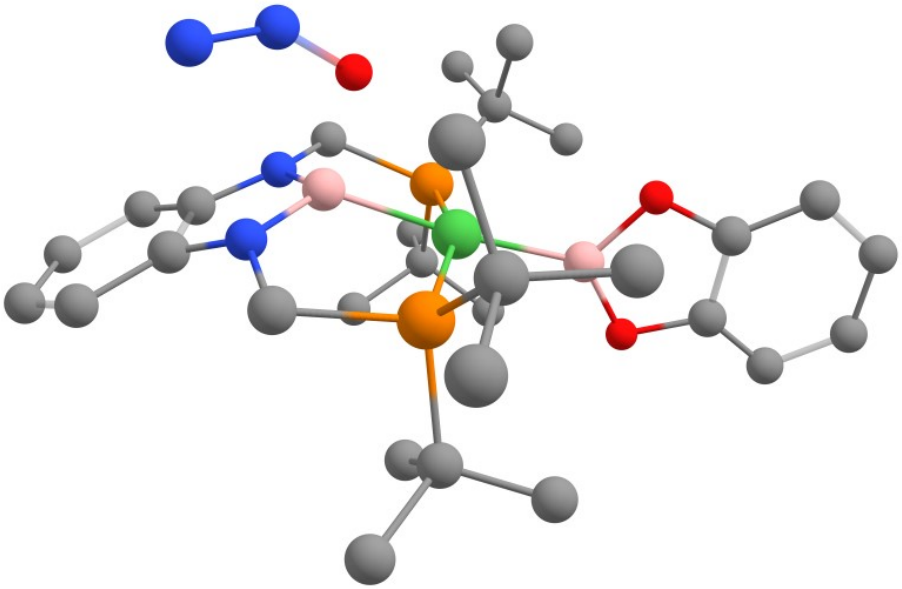


Figure S54. Transition state involving the interaction between the boron atom from the PBP ligand and the oxygen atom of N_2O (**TS-NiBcat-1**). The energy required to overcome this barrier is 35.3 kcal mol^{-1}. H atoms have been omitted for clarity.

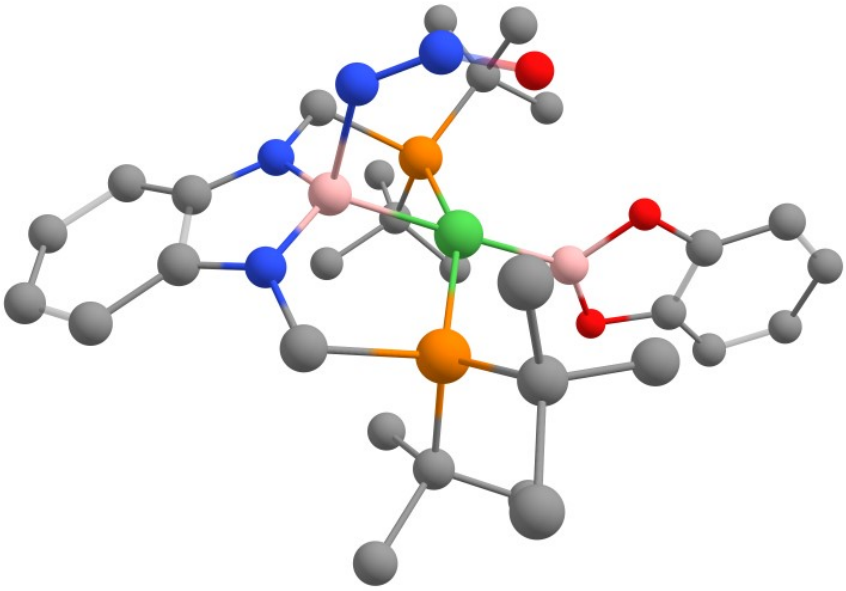


Figure S55. Transition state involving the interaction between the boron atom from the PBP ligand and the terminal nitrogen atom of N_2O (**TS-NiBcat-2**). The energy required to overcome this barrier is 34.7 kcal mol^{-1}. H atoms have been omitted for clarity.

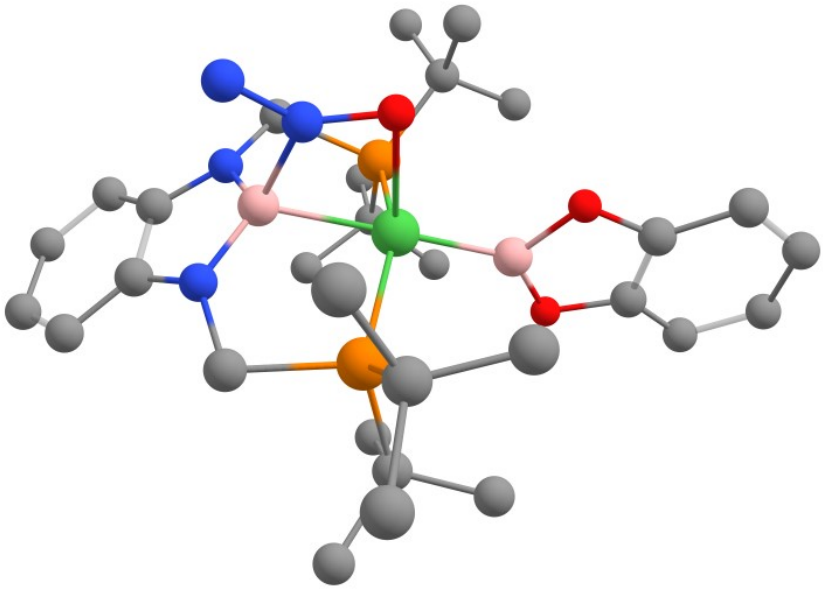


Figure S56. Transition state involving the interaction between the boron atom from the PBP ligand and the central nitrogen atom of N_2O (**TS-NiBcat-3**). The energy required to overcome this barrier is 46.0 kcal mol^{-1}. H atoms have been omitted for clarity.

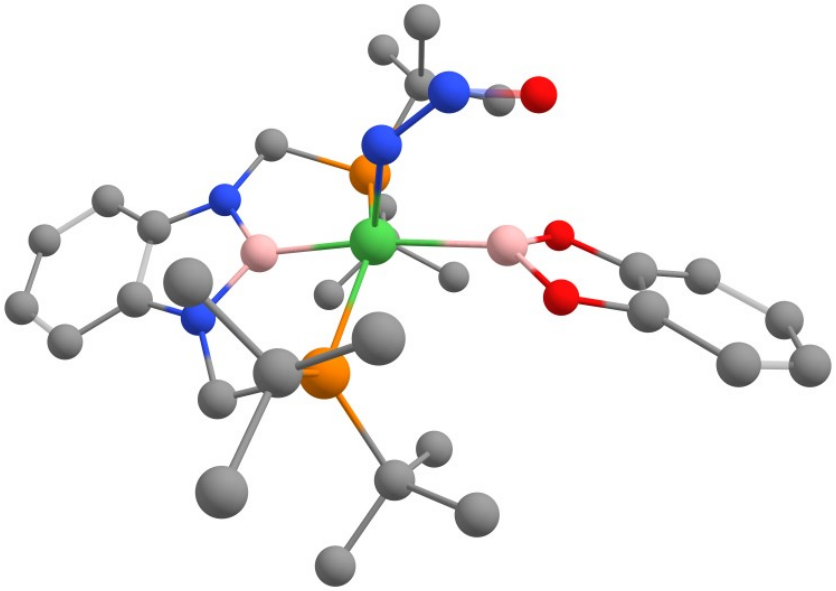


Figure S57. Transition state involving the interaction between the boron atom from the Bcat ligand and the oxygen atom of N_2O (**TS-NiBcat-4**). The energy required to overcome this barrier is 32.2 kcal mol^{-1}. H atoms have been omitted for clarity.

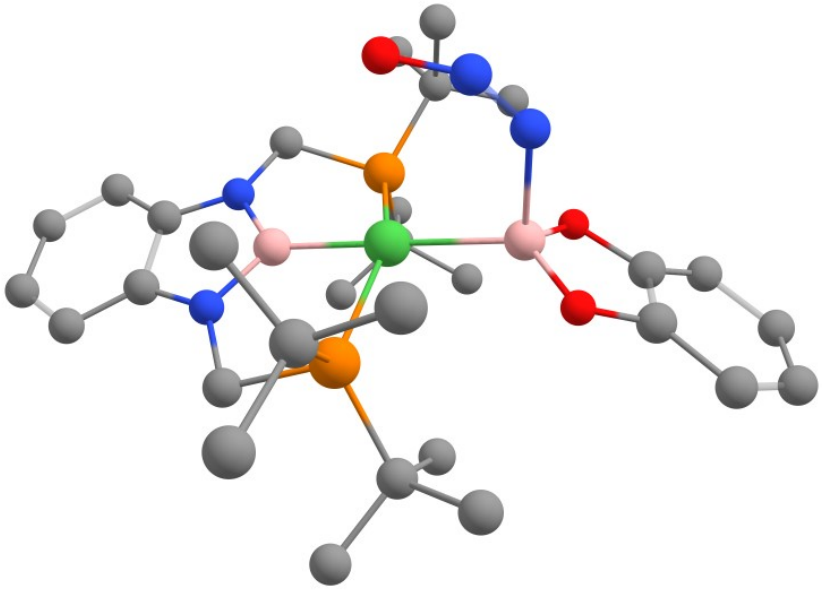


Figure S58. Transition state involving the interaction between the boron atom from the Bcat ligand and the terminal nitrogen atom of N_2O (**TS-NiBcat-5**). The energy required to overcome this barrier is 35.2 kcal mol^{-1}. H atoms have been omitted for clarity.

*Calculations from hydridoborate complexes **8** and **9** (BS2))*

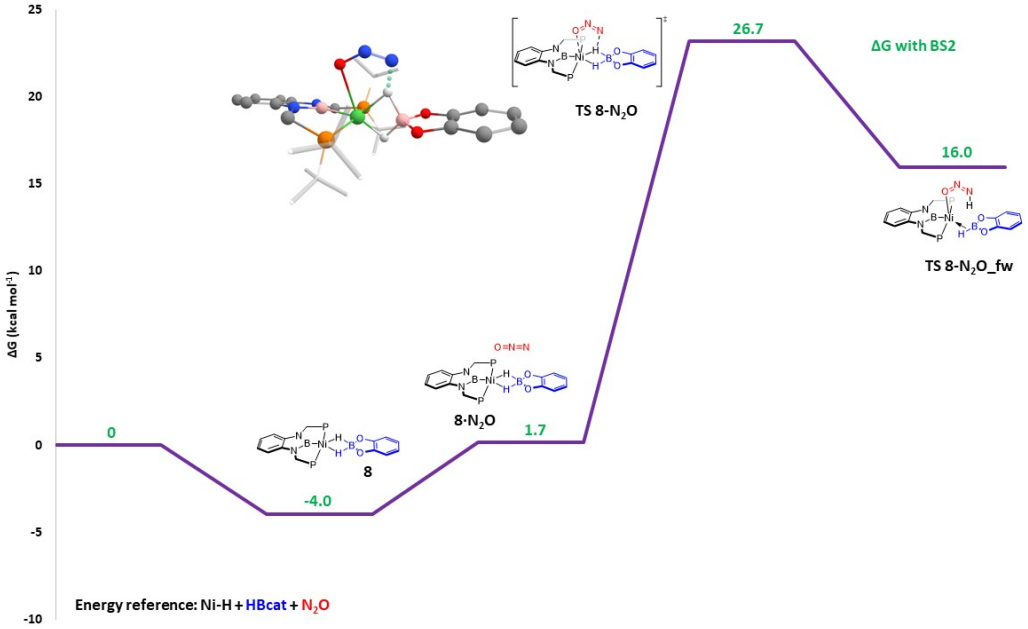


Figure S59. Computed Gibbs energy profile in benzene (SMD) for the activation of N_2O mediated by hydridoborate complex **8**. Relative Gibbs energies computed at 298 K and 1 M are given in kcal mol^{-1}. The Gibbs energy of **3** + N_2O + HBcat has been taken as zero energy. All data have been computed at the SMD-PBE0-D3/def2-TZVP/def2-QZVP&SDD//SMD-PBE0-D3/6-31G(d,p)&SDD(+f) level.

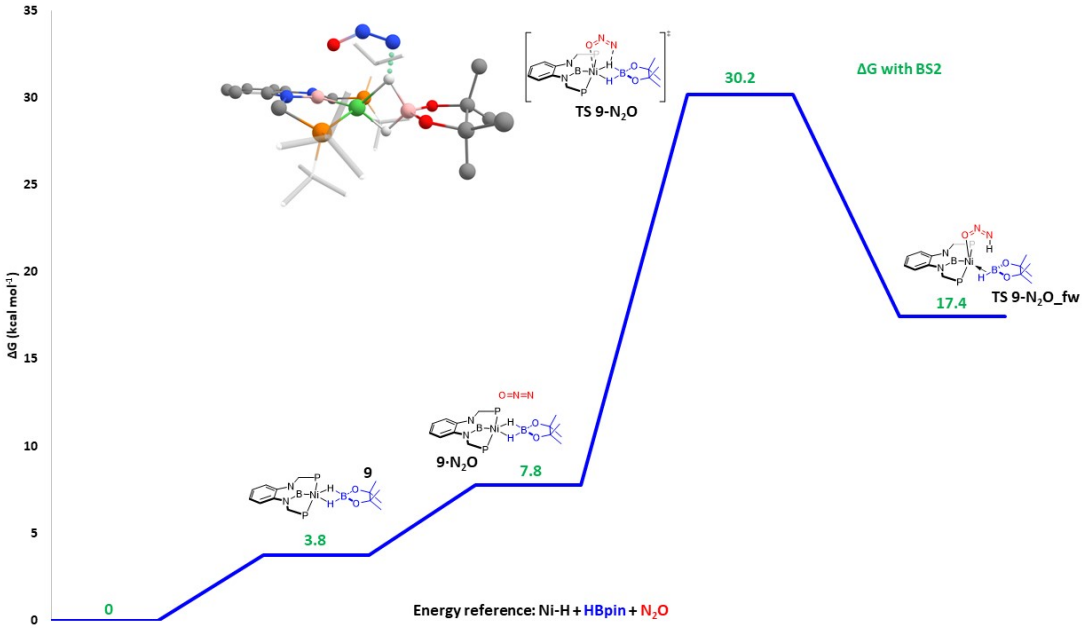
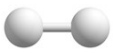


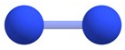
Figure S60. Computed Gibbs energy profile in benzene (SMD) for the activation of N_2O mediated by hydridoborate complex **9**. Relative Gibbs energies computed at 298 K and 1 M are given in kcal mol^{-1}. The Gibbs energy of **3** + N_2O + HBpin has been taken as zero energy. All data have been computed at the SMD-PBE0-D3/def2-TZVP/def2-QZVP&SDD//SMD-PBE0-D3/6-31G(d,p)&SDD(+f) level.

8. Cartesian coordinates of the optimized structures



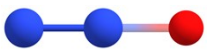
H_2

H	0.000000000	0.000000000	0.372138000
H	0.000000000	0.000000000	-0.372138000



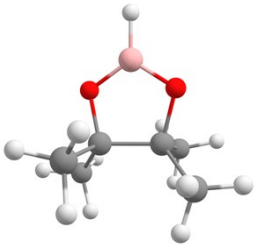
N_2

N	0.000000000	0.000000000	0.551046000
N	0.000000000	0.000000000	-0.551046000



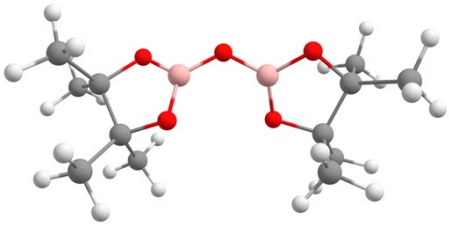
N_2O

O	0.000000000	0.000000000	1.112369000
N	0.000000000	0.000000000	-0.071094000
N	0.000000000	0.000000000	-1.200184000



HBpin

B	2.374923000	-0.005081000	-0.003124000
O	3.119026000	-1.024887000	-0.519386000
O	3.113368000	1.018241000	0.514318000
C	4.493264000	-0.771579000	-0.133596000
C	4.489422000	0.771386000	0.130865000
H	1.182924000	-0.007838000	-0.004277000
C	4.747969000	-1.594004000	1.124433000
H	4.528295000	-2.644118000	0.912099000
H	5.788934000	-1.519226000	1.452193000
H	4.099411000	-1.273487000	1.945544000
C	5.406845000	-1.226946000	-1.255787000
H	6.449680000	-0.982235000	-1.029478000
H	5.332334000	-2.311959000	-1.373905000
H	5.137840000	-0.765901000	-2.208054000
C	5.398919000	1.231163000	1.254581000
H	6.443354000	0.991828000	1.029972000
H	5.318638000	2.315760000	1.372714000
H	5.130661000	0.768613000	2.206337000
C	4.742283000	1.594905000	-1.126821000
H	4.517282000	2.643981000	-0.914974000
H	5.784131000	1.525027000	-1.452880000
H	4.096563000	1.271137000	-1.948892000

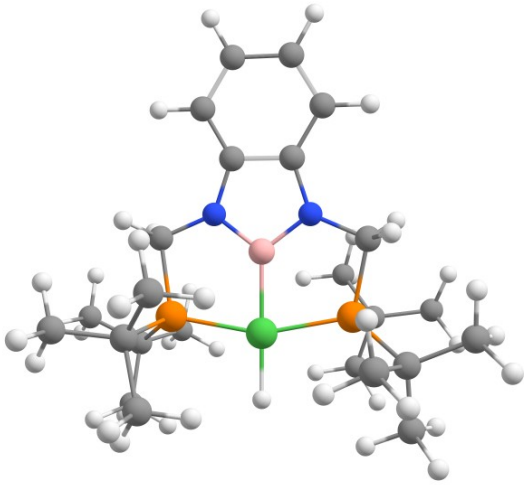


pinBOBpin

B	2.456648000	-0.144223000	-0.422068000
O	2.992823000	-0.973127000	0.525933000

O	3.388421000	0.506469000	-1.189326000
C	4.412391000	-0.702504000	0.536586000
C	4.651953000	-0.130937000	-0.902323000
O	1.111164000	0.034705000	-0.542841000
B	0.451533000	0.351499000	-1.692638000
O	-0.715290000	1.066538000	-1.681488000
O	0.855747000	-0.042160000	-2.942202000
C	-1.253482000	0.975562000	-3.019251000
C	0.027191000	0.685830000	-3.874329000
C	-2.240776000	-0.185890000	-3.021701000
H	-2.994604000	-0.012593000	-2.248446000
H	-2.750331000	-0.281809000	-3.984918000
H	-1.738227000	-1.131911000	-2.797137000
C	-0.204968000	-0.175453000	-5.100480000
H	-0.899477000	0.313234000	-5.791364000
H	0.741603000	-0.331582000	-5.626527000
H	-0.607489000	-1.154336000	-4.832599000
C	0.791258000	1.951674000	-4.245972000
H	1.773638000	1.669328000	-4.634931000
H	0.268081000	2.531776000	-5.011846000
H	0.947617000	2.588691000	-3.369945000
C	-1.961256000	2.275472000	-3.350662000
H	-2.311112000	2.272737000	-4.388025000
H	-2.832523000	2.396954000	-2.700298000
H	-1.307841000	3.137708000	-3.203003000
C	5.154350000	-1.989012000	0.842860000
H	6.236296000	-1.837723000	0.771875000
H	4.924441000	-2.314681000	1.861700000
H	4.866509000	-2.790832000	0.160087000
C	4.657180000	0.329867000	1.631092000
H	4.263604000	-0.055335000	2.575997000
H	5.723197000	0.538357000	1.760887000
H	4.142324000	1.269782000	1.408681000
C	5.757387000	0.902127000	-1.004247000
H	6.719392000	0.470171000	-0.709928000
H	5.844343000	1.248189000	-2.038515000

H	5.555139000	1.770488000	-0.374013000
C	4.841455000	-1.223320000	-1.948873000
H	4.772045000	-0.775043000	-2.943949000
H	5.816101000	-1.710891000	-1.854173000
H	4.059693000	-1.985111000	-1.869260000



Complex 3 (NiH)

Ni	-0.000072000	-1.029031000	-0.000019000
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P	2.123210000	-0.639679000	0.055173000
N	-1.125983000	1.765480000	-0.173161000
N	1.126224000	1.765321000	0.173324000
C	-2.888908000	-0.874775000	1.657295000
C	-3.094624000	-1.496067000	-1.427199000
C	2.425053000	1.196113000	0.406595000
H	2.753080000	1.339062000	1.443500000
H	3.199669000	1.615584000	-0.247763000
C	-0.688198000	5.474939000	-0.112943000
H	-1.217494000	6.419634000	-0.200923000
C	-2.424946000	1.196504000	-0.406157000
H	-2.753321000	1.339734000	-1.442912000
H	-3.199286000	1.615947000	0.248547000
C	-0.705282000	3.080993000	-0.113310000
C	2.888886000	-0.874588000	-1.657367000
C	-1.400878000	4.277756000	-0.229548000
H	-2.472792000	4.278827000	-0.407985000

C	1.401449000	4.277551000	0.229944000
H	2.473362000	4.278465000	0.408389000
C	0.705692000	3.080888000	0.113633000
C	3.094349000	-1.496788000	1.426954000
C	0.688931000	5.474837000	0.113428000
H	1.218354000	6.419454000	0.201479000
C	2.515112000	-2.264627000	-2.184580000
H	1.432826000	-2.422203000	-2.150669000
H	2.852300000	-2.355191000	-3.225215000
H	2.982089000	-3.070015000	-1.613481000
C	4.406090000	-0.695421000	-1.691473000
H	4.920682000	-1.493125000	-1.148183000
H	4.751580000	-0.735083000	-2.732345000
H	4.726321000	0.267182000	-1.278596000
C	2.223065000	0.167780000	-2.568219000
H	1.133068000	0.061015000	-2.563660000
H	2.460108000	1.197762000	-2.285049000
H	2.577005000	0.018474000	-3.596005000
C	2.184707000	-1.364331000	2.657473000
H	1.218287000	-1.848701000	2.479225000
H	2.660859000	-1.846938000	3.520507000
H	1.996963000	-0.318103000	2.925153000
C	4.459735000	-0.877101000	1.735584000
H	4.911957000	-1.416166000	2.577898000
H	5.154475000	-0.945711000	0.895812000
H	4.387073000	0.173672000	2.031562000
C	3.259678000	-2.980781000	1.096067000
H	3.611888000	-3.512840000	1.988762000
H	2.309400000	-3.426477000	0.785049000
H	4.000673000	-3.142487000	0.306875000
C	-3.260217000	-2.980100000	-1.096618000
H	-3.612215000	-3.511965000	-1.989515000
H	-2.310096000	-3.426031000	-0.785432000
H	-4.001483000	-3.141856000	-0.307689000
C	-2.185004000	-1.363510000	-2.657716000
H	-1.996866000	-0.317254000	-2.925020000

H	-1.218737000	-1.848267000	-2.479704000
H	-2.661376000	-1.845615000	-3.520910000
C	-4.459890000	-0.876043000	-1.735735000
H	-4.912649000	-1.415522000	-2.577493000
H	-5.154386000	-0.943649000	-0.895686000
H	-4.386778000	0.174467000	-2.032542000
C	-2.515965000	-2.265259000	2.183923000
H	-1.433842000	-2.423779000	2.149269000
H	-2.852548000	-2.355758000	3.224759000
H	-2.984055000	-3.070108000	1.612982000
C	-2.222313000	0.166777000	2.568512000
H	-2.576730000	0.017700000	3.596170000
H	-1.132429000	0.058825000	2.564272000
H	-2.458118000	1.197058000	2.285412000
C	-4.406011000	-0.694770000	1.691709000
H	-4.921059000	-1.491849000	1.147936000
H	-4.751413000	-0.734956000	2.732591000
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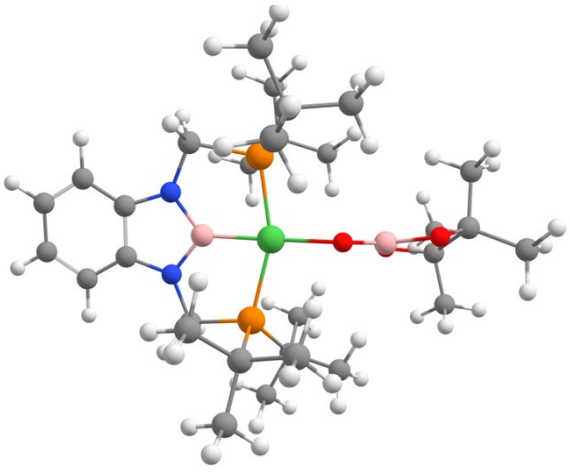

Complex 6a-Bpin (NiOBpin)

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P	0.494948000	-2.158828000	0.232191000
P	0.739385000	2.174211000	0.141322000
N	2.900050000	-1.247649000	-0.111574000
N	2.952305000	0.988207000	-0.522226000

C	-0.039664000	-2.925204000	-1.407488000
C	-0.173755000	-3.068253000	1.739963000
C	2.451001000	2.329849000	-0.620210000
H	2.377401000	2.666478000	-1.661212000
H	3.072884000	3.052862000	-0.077799000
C	6.564576000	-1.011173000	-0.791210000
H	7.484049000	-1.587542000	-0.841898000
C	2.341722000	-2.510131000	0.282729000
H	2.649069000	-2.793618000	1.296818000
H	2.620896000	-3.328711000	-0.392474000
C	4.206288000	-0.900544000	-0.402093000
C	0.959503000	2.861894000	1.886259000
C	5.369377000	-1.657220000	-0.460841000
H	5.347786000	-2.723345000	-0.251892000
C	5.430307000	1.131145000	-0.997212000
H	5.454062000	2.197469000	-1.204914000
C	4.237375000	0.500342000	-0.668488000
C	-0.324704000	3.272916000	-0.954168000
C	6.594503000	0.358986000	-1.054585000
H	7.536710000	0.835962000	-1.309438000
C	-0.323727000	2.606155000	2.687085000
H	-0.685276000	1.580967000	2.558611000
H	-0.119252000	2.781761000	3.750782000
H	-1.135118000	3.276994000	2.395677000
C	1.323272000	4.345691000	1.935975000
H	0.503825000	4.980196000	1.586403000
H	1.531763000	4.629660000	2.975379000
H	2.217936000	4.580852000	1.349541000
C	2.088403000	2.035231000	2.520740000
H	1.845999000	0.967120000	2.524083000
H	3.049486000	2.160897000	2.012195000
H	2.219925000	2.356937000	3.561239000
C	-0.620941000	2.403077000	-2.185246000
H	-1.232289000	1.535987000	-1.915521000
H	-1.177243000	2.996619000	-2.922564000
H	0.296130000	2.048899000	-2.671717000

C	0.355419000	4.572515000	-1.395368000
H	-0.345633000	5.141074000	-2.019681000
H	0.635319000	5.211914000	-0.554846000
H	1.248941000	4.394909000	-2.001538000
C	-1.640349000	3.597011000	-0.244940000
H	-2.343403000	4.024960000	-0.969562000
H	-2.097567000	2.700471000	0.179750000
H	-1.501557000	4.333630000	0.551748000
C	-1.696318000	-3.196562000	1.654393000
H	-2.075211000	-3.561996000	2.617301000
H	-2.165912000	-2.229228000	1.457590000
H	-2.006198000	-3.915962000	0.890611000
C	0.168294000	-2.136188000	2.912678000
H	1.245404000	-1.946923000	2.993642000
H	-0.348111000	-1.177435000	2.800531000
H	-0.157005000	-2.600258000	3.852467000
C	0.452466000	-4.445286000	1.976918000
H	0.031820000	-4.868824000	2.897842000
H	0.241550000	-5.149793000	1.169233000
H	1.537120000	-4.398213000	2.114172000
C	-1.486541000	-2.518376000	-1.699143000
H	-1.626411000	-1.435197000	-1.655085000
H	-1.755439000	-2.856467000	-2.708326000
H	-2.194143000	-2.974673000	-1.003580000
C	0.852458000	-2.291171000	-2.484712000
H	0.526961000	-2.651620000	-3.468407000
H	0.766154000	-1.199360000	-2.477549000
H	1.910416000	-2.547436000	-2.372292000
C	0.093321000	-4.447285000	-1.454872000
H	-0.618986000	-4.938350000	-0.786014000
H	-0.124591000	-4.795160000	-2.472708000
H	1.100747000	-4.794579000	-1.202125000
O	-1.585467000	0.116713000	0.939516000
B	-2.780803000	0.140170000	0.401763000
O	-3.977576000	-0.012139000	1.123572000
O	-3.072383000	0.304899000	-0.968823000

C	-5.025294000	-0.250538000	0.185242000
C	-4.487025000	0.442542000	-1.113033000
C	-6.321446000	0.329255000	0.725903000
H	-7.132102000	0.236381000	-0.004853000
H	-6.617497000	-0.212789000	1.629568000
H	-6.207428000	1.382558000	0.991043000
C	-4.805948000	1.934809000	-1.153307000
H	-4.227492000	2.398218000	-1.958221000
H	-5.867734000	2.123412000	-1.340691000
H	-4.525776000	2.417925000	-0.212785000
C	-5.161093000	-1.763755000	0.025689000
H	-5.323061000	-2.208095000	1.012375000
H	-6.000105000	-2.039679000	-0.620915000
H	-4.244656000	-2.192742000	-0.390122000
C	-4.916367000	-0.214012000	-2.414395000
H	-6.006139000	-0.202285000	-2.523169000
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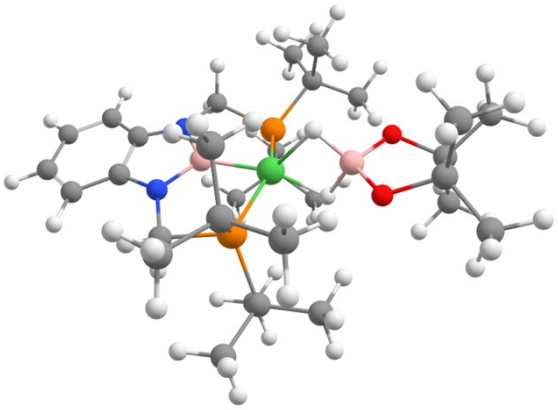

Complex 9 (NiH2Bpin)

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P	0.316275000	-2.180374000	0.195425000
P	0.540836000	2.159922000	0.008791000
N	2.694847000	-1.228318000	-0.249017000
N	2.715109000	0.978455000	-0.776744000
C	-0.162888000	-3.310676000	-1.265856000
C	-0.268838000	-2.860538000	1.864010000

C	2.214599000	2.319006000	-0.820144000
H	2.094893000	2.684336000	-1.846360000
H	2.862546000	3.023420000	-0.283981000
C	6.403578000	-0.869047000	-0.481651000
H	7.342957000	-1.405472000	-0.381753000
C	2.175405000	-2.449562000	0.288116000
H	2.490652000	-2.600824000	1.327827000
H	2.492814000	-3.327850000	-0.279067000
C	4.013426000	-0.843045000	-0.406226000
C	0.905592000	2.600204000	1.817478000
C	5.200328000	-1.550907000	-0.273163000
H	5.191611000	-2.604733000	-0.008472000
C	5.225177000	1.207712000	-0.949510000
H	5.235664000	2.262537000	-1.209947000
C	4.025261000	0.539401000	-0.743634000
C	-0.416366000	3.556706000	-0.852230000
C	6.415558000	0.486205000	-0.813257000
H	7.364225000	0.991923000	-0.969735000
C	-0.346373000	2.304530000	2.650954000
H	-0.680861000	1.272485000	2.510309000
H	-0.114166000	2.450932000	3.713268000
H	-1.182624000	2.960378000	2.399327000
C	1.345021000	4.047444000	2.046525000
H	0.547358000	4.765112000	1.840794000
H	1.623628000	4.168961000	3.100922000
H	2.221864000	4.320816000	1.450553000
C	2.030938000	1.670016000	2.291754000
H	1.771182000	0.617107000	2.147833000
H	2.979185000	1.858302000	1.778571000
H	2.196702000	1.836645000	3.363479000
C	-0.884355000	2.969995000	-2.191764000
H	-1.639581000	2.197163000	-2.040578000
H	-1.329047000	3.772618000	-2.794067000
H	-0.057153000	2.542444000	-2.770690000
C	0.458964000	4.786534000	-1.137181000
H	-0.169160000	5.544191000	-1.622365000

H	0.873261000	5.241730000	-0.235746000
H	1.283065000	4.574666000	-1.824283000
C	-1.636522000	3.996400000	-0.040791000
H	-2.240697000	4.672955000	-0.659299000
H	-2.265088000	3.143124000	0.220872000
H	-1.355713000	4.548746000	0.860519000
C	-1.788952000	-2.756262000	2.005181000
H	-2.061229000	-3.002214000	3.039504000
H	-2.146689000	-1.750071000	1.779535000
H	-2.322325000	-3.444320000	1.348847000
C	0.350690000	-1.939580000	2.925081000
H	1.444666000	-1.963725000	2.940714000
H	0.034445000	-0.903289000	2.770489000
H	0.004892000	-2.256838000	3.916495000
C	0.176088000	-4.305304000	2.098831000
H	-0.078394000	-4.597998000	3.125516000
H	-0.336518000	-5.001435000	1.428974000
H	1.256103000	-4.442883000	1.980398000
C	-1.641754000	-3.698245000	-1.198620000
H	-2.287961000	-2.841448000	-0.990267000
H	-1.934023000	-4.124758000	-2.167044000
H	-1.819018000	-4.469505000	-0.441730000
C	0.089003000	-2.474475000	-2.527927000
H	-0.100298000	-3.096930000	-3.411944000
H	-0.566925000	-1.601074000	-2.570194000
H	1.124314000	-2.119013000	-2.582568000
C	0.672694000	-4.593771000	-1.371183000
H	0.707731000	-5.168645000	-0.442552000
H	0.214605000	-5.235488000	-2.133800000
H	1.698139000	-4.402802000	-1.700384000
C	-4.422294000	-0.583772000	-0.552997000
C	-4.340817000	0.893940000	-0.062753000
B	-2.206423000	0.075447000	-0.384210000
O	-3.024883000	1.257790000	-0.461585000
O	-3.103767000	-1.049898000	-0.295442000
C	-4.682072000	-0.674862000	-2.056319000

H	-4.508495000	-1.704513000	-2.384453000
H	-5.709677000	-0.401114000	-2.317155000
H	-3.994610000	-0.023482000	-2.604281000
C	-5.407669000	-1.458385000	0.204218000
H	-6.428437000	-1.069568000	0.119893000
H	-5.398401000	-2.472383000	-0.209091000
H	-5.143571000	-1.526793000	1.262074000
C	-5.330956000	1.842548000	-0.717165000
H	-6.363042000	1.522760000	-0.536638000
H	-5.213371000	2.849691000	-0.303814000
H	-5.164903000	1.902713000	-1.795155000
C	-4.436340000	1.000806000	1.459539000
H	-4.164122000	2.016720000	1.763044000
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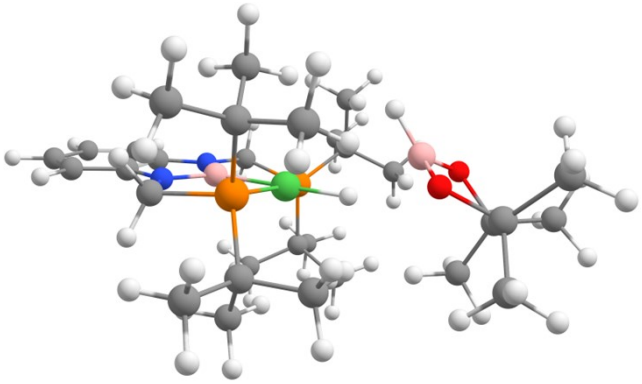

TS-HBpin

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P	0.456482000	-2.146871000	0.059935000
P	0.680943000	2.136886000	-0.084852000
N	2.903479000	-1.221768000	0.020776000
N	2.993911000	1.008182000	-0.405286000
C	0.008820000	-3.143074000	-1.486935000
C	-0.274391000	-2.857093000	1.646959000
C	2.483765000	2.334371000	-0.603115000
H	2.547385000	2.647949000	-1.652209000

H	3.003661000	3.087107000	0.003301000
C	6.625661000	-0.946868000	-0.082165000
H	7.548006000	-1.512695000	0.014660000
C	2.306620000	-2.504751000	0.253948000
H	2.529564000	-2.892662000	1.255833000
H	2.650323000	-3.251697000	-0.467688000
C	4.234631000	-0.861017000	-0.068444000
C	0.707157000	2.739146000	1.709629000
C	5.400503000	-1.605106000	0.059374000
H	5.357031000	-2.671024000	0.266217000
C	5.515075000	1.182002000	-0.476915000
H	5.560035000	2.247214000	-0.686734000
C	4.291427000	0.539037000	-0.338074000
C	-0.202643000	3.338608000	-1.238409000
C	6.681673000	0.422995000	-0.344519000
H	7.647183000	0.909766000	-0.450224000
C	-0.631574000	2.372348000	2.357030000
H	-0.833294000	1.301383000	2.256015000
H	-0.601533000	2.625675000	3.424571000
H	-1.470812000	2.907376000	1.909013000
C	0.969314000	4.237273000	1.863426000
H	0.151422000	4.843342000	1.465274000
H	1.061243000	4.476993000	2.930479000
H	1.900400000	4.551337000	1.379755000
C	1.813550000	1.962023000	2.437389000
H	1.672847000	0.880445000	2.347572000
H	2.815427000	2.201518000	2.069187000
H	1.783051000	2.222669000	3.502757000
C	-0.334827000	2.556873000	-2.553627000
H	-0.914885000	1.640733000	-2.409125000
H	-0.851508000	3.176704000	-3.297299000
H	0.640368000	2.281408000	-2.972535000
C	0.558047000	4.642470000	-1.501015000
H	-0.017816000	5.244490000	-2.215429000
H	0.688570000	5.246251000	-0.600475000
H	1.543066000	4.476395000	-1.947175000

C	-1.600790000	3.655423000	-0.708389000
H	-2.157150000	4.206747000	-1.477241000
H	-2.166983000	2.746825000	-0.489321000
H	-1.565805000	4.288836000	0.183392000
C	-1.791483000	-2.645269000	1.663611000
H	-2.160157000	-2.800979000	2.685625000
H	-2.052315000	-1.633552000	1.340405000
H	-2.320363000	-3.342994000	1.012714000
C	0.321726000	-1.990631000	2.767242000
H	1.413551000	-2.043398000	2.825060000
H	0.039762000	-0.940191000	2.632305000
H	-0.075234000	-2.326956000	3.733143000
C	0.055632000	-4.330996000	1.877640000
H	-0.311559000	-4.636293000	2.865967000
H	-0.431892000	-4.974454000	1.139376000
H	1.131478000	-4.533853000	1.854131000
C	-1.497033000	-3.402828000	-1.534218000
H	-2.090511000	-2.523412000	-1.281290000
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C	0.403081000	-2.220209000	-2.649381000
H	0.204520000	-2.726470000	-3.602963000
H	-0.173349000	-1.289069000	-2.625666000
H	1.467437000	-1.959022000	-2.621654000
C	0.742420000	-4.480004000	-1.638181000
H	0.640890000	-5.123992000	-0.760592000
H	0.309378000	-5.018132000	-2.490560000
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C	-4.909758000	-0.640960000	-0.078541000
C	-4.647407000	0.888237000	0.108503000
B	-3.025278000	-0.018691000	-1.201204000
O	-3.703874000	1.162251000	-0.942757000
O	-3.661700000	-1.106998000	-0.616051000
C	-5.977172000	-0.932565000	-1.130259000
H	-5.959736000	-2.001329000	-1.363401000
H	-6.980968000	-0.672116000	-0.780288000

H	-5.773558000	-0.383074000	-2.054280000
C	-5.219239000	-1.398705000	1.200377000
H	-6.141616000	-1.025747000	1.658308000
H	-5.360608000	-2.460101000	0.973867000
H	-4.409156000	-1.314989000	1.926848000
C	-5.863402000	1.774477000	-0.094934000
H	-6.645276000	1.537891000	0.634421000
H	-5.580633000	2.823071000	0.040727000
H	-6.276467000	1.666735000	-1.099973000
C	-3.977297000	1.212580000	1.438580000
H	-3.688414000	2.267265000	1.441671000
H	-4.649957000	1.042436000	2.284638000
H	-3.071078000	0.615488000	1.570259000
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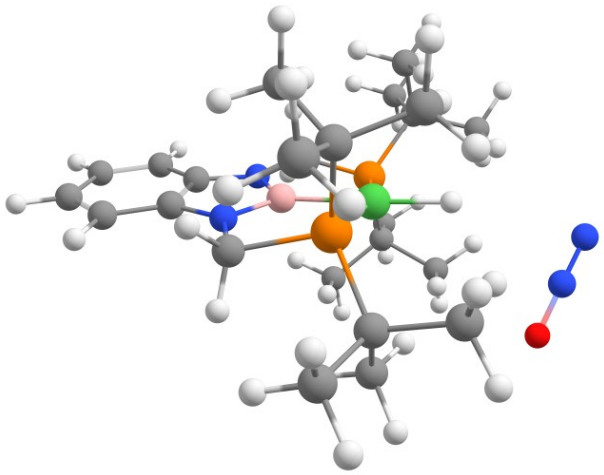

Complex 3·N_2O

Ni	-0.543990000	0.358125000	0.213500000
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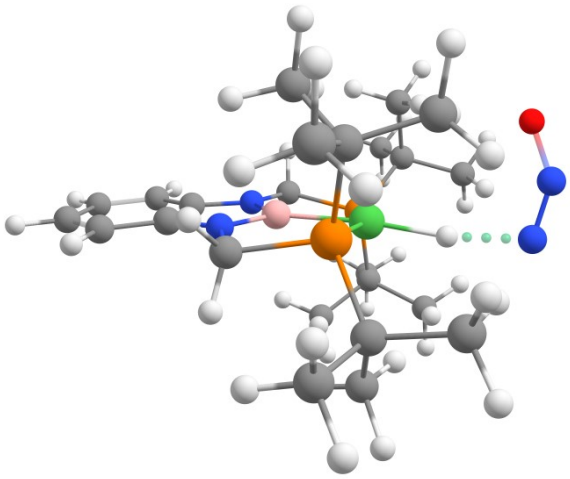
P	0.892140000	1.972286000	0.101981000
N	1.258857000	-2.054959000	0.005040000
N	2.383373000	-0.110735000	-0.372159000
C	-2.074991000	-2.085162000	-1.464976000
C	-2.397771000	-2.152509000	1.667828000
C	2.551355000	1.308023000	-0.526155000
H	2.707513000	1.588508000	-1.575194000

H	3.395782000	1.702213000	0.053164000
C	4.629553000	-3.585867000	-0.490724000
H	5.168605000	-4.529048000	-0.503090000
C	0.134049000	-2.884902000	0.336404000
H	0.208715000	-3.282868000	1.355952000
H	0.014644000	-3.737053000	-0.345109000
C	2.586512000	-2.368815000	-0.216045000
C	1.322430000	2.601423000	1.831528000
C	3.256605000	-3.585492000	-0.226605000
H	2.723256000	-4.512095000	-0.032068000
C	4.654190000	-1.164648000	-0.726909000
H	5.189857000	-0.239073000	-0.919929000
C	3.290362000	-1.150076000	-0.462770000
C	0.497244000	3.355090000	-1.114894000
C	5.316196000	-2.396129000	-0.737361000
H	6.382961000	-2.424538000	-0.941181000
C	0.026383000	2.955706000	2.569185000
H	-0.675677000	2.116532000	2.552743000
H	0.262700000	3.199074000	3.613005000
H	-0.482264000	3.819134000	2.134317000
C	2.272491000	3.798271000	1.839798000
H	1.794204000	4.700125000	1.447049000
H	2.573776000	4.014643000	2.872716000
H	3.186282000	3.613579000	1.265214000
C	1.972757000	1.419635000	2.566864000
H	1.315531000	0.543564000	2.571498000
H	2.930453000	1.118491000	2.131545000
H	2.161004000	1.710317000	3.607945000
C	-0.011965000	2.612427000	-2.359438000
H	-0.891023000	2.006082000	-2.118471000
H	-0.296968000	3.340236000	-3.129703000
H	0.751426000	1.955088000	-2.791643000
C	1.682128000	4.242218000	-1.506083000
H	1.345772000	4.968390000	-2.257189000
H	2.084055000	4.809771000	-0.664029000
H	2.501541000	3.675073000	-1.957839000

C	-0.635800000	4.219249000	-0.558434000
H	-1.031567000	4.858058000	-1.357697000
H	-1.455535000	3.601647000	-0.179736000
H	-0.288178000	4.876134000	0.244945000
C	-3.774297000	-1.501377000	1.526723000
H	-4.328817000	-1.620977000	2.465982000
H	-3.687865000	-0.430765000	1.317234000
H	-4.368353000	-1.968408000	0.735064000
C	-1.687068000	-1.534440000	2.881249000
H	-0.679197000	-1.940383000	3.025983000
H	-1.604847000	-0.447648000	2.768297000
H	-2.263112000	-1.746172000	3.790979000
C	-2.552760000	-3.660661000	1.882560000
H	-3.147691000	-3.830032000	2.789046000
H	-3.071355000	-4.152848000	1.057286000
H	-1.593538000	-4.165570000	2.030852000
C	-3.081219000	-0.987941000	-1.829184000
H	-2.596736000	-0.007095000	-1.827433000
H	-3.474616000	-1.178896000	-2.835947000
H	-3.929385000	-0.946476000	-1.141549000
C	-0.937632000	-2.032234000	-2.495679000
H	-1.360531000	-2.183270000	-3.496722000
H	-0.433556000	-1.060231000	-2.482213000
H	-0.179878000	-2.805826000	-2.338643000
C	-2.750232000	-3.454963000	-1.518348000
H	-3.649775000	-3.493378000	-0.897085000
H	-3.060393000	-3.664613000	-2.550112000
H	-2.081126000	-4.265202000	-1.209459000
H	-1.855541000	1.152148000	0.495892000
O	-3.465079000	2.524803000	-1.750907000
N	-4.097176000	2.116816000	-0.837211000
N	-4.711810000	1.731149000	0.025826000



TS1

Ni	-0.021283000	-0.701213000	0.061057000
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P	-2.145505000	-0.216718000	0.042119000
N	1.224643000	2.034137000	-0.041648000
N	-1.029310000	2.104285000	-0.359238000
C	2.947419000	-0.867279000	-1.511607000
C	3.009403000	-1.127863000	1.630588000
C	-2.363828000	1.586760000	-0.475169000
H	-2.736125000	1.643920000	-1.504828000
H	-3.079916000	2.112857000	0.168742000
C	0.927451000	5.750019000	-0.269935000
H	1.492874000	6.676807000	-0.231120000
C	2.494039000	1.444548000	0.278304000
H	2.806196000	1.688607000	1.300921000
H	3.296641000	1.761883000	-0.399060000
C	0.853023000	3.361054000	-0.161882000
C	-2.797667000	-0.246435000	1.813828000
C	1.596000000	4.533332000	-0.107676000
H	2.669342000	4.501198000	0.058299000
C	-1.210807000	4.619838000	-0.533968000
H	-2.284186000	4.653779000	-0.699319000
C	-0.558116000	3.404466000	-0.371194000
C	-3.254463000	-1.133650000	-1.174352000
C	-0.451875000	5.792368000	-0.480065000

H	-0.946224000	6.751655000	-0.604854000
C	-2.472289000	-1.606713000	2.443095000
H	-1.404007000	-1.832711000	2.369712000
H	-2.752361000	-1.584945000	3.503899000
H	-3.015346000	-2.430032000	1.973871000
C	-4.294703000	0.037101000	1.934784000
H	-4.899409000	-0.772932000	1.517361000
H	-4.559756000	0.124630000	2.996015000
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C	-2.006534000	0.826503000	2.577026000
H	-0.928615000	0.641320000	2.517773000
H	-2.194572000	1.839881000	2.209548000
H	-2.299180000	0.798691000	3.633914000
C	-2.427848000	-1.182874000	-2.467894000
H	-1.494278000	-1.733547000	-2.315072000
H	-3.002729000	-1.699269000	-3.246824000
H	-2.187632000	-0.181786000	-2.844910000
C	-4.595038000	-0.448024000	-1.455160000
H	-5.143769000	-1.043898000	-2.195456000
H	-5.226749000	-0.370761000	-0.567825000
H	-4.476893000	0.553774000	-1.878504000
C	-3.504059000	-2.560778000	-0.682811000
H	-3.928002000	-3.155556000	-1.500835000
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C	3.130663000	-2.646067000	1.490710000
H	3.440534000	-3.070659000	2.453786000
H	2.178713000	-3.107918000	1.212747000
H	3.887789000	-2.927768000	0.752928000
C	2.060746000	-0.812899000	2.796684000
H	1.902684000	0.264135000	2.926289000
H	1.084196000	-1.285062000	2.642028000
H	2.487008000	-1.199676000	3.730790000
C	4.387906000	-0.526882000	1.919229000
H	4.785786000	-0.982484000	2.834896000
H	5.108139000	-0.720211000	1.121276000

H	4.351539000	0.552793000	2.091336000
C	2.547300000	-2.298963000	-1.882627000
H	1.460554000	-2.416151000	-1.911202000
H	2.942076000	-2.532024000	-2.879600000
H	2.946250000	-3.042905000	-1.189061000
C	2.341868000	0.077610000	-2.560573000
H	2.720840000	-0.202941000	-3.550913000
H	1.249424000	0.000125000	-2.580715000
H	2.601923000	1.127292000	-2.392304000
C	4.470052000	-0.733697000	-1.510014000
H	4.943318000	-1.484610000	-0.871078000
H	4.844993000	-0.893076000	-2.528881000
H	4.809042000	0.256968000	-1.189218000
H	-0.073651000	-2.271826000	0.409567000
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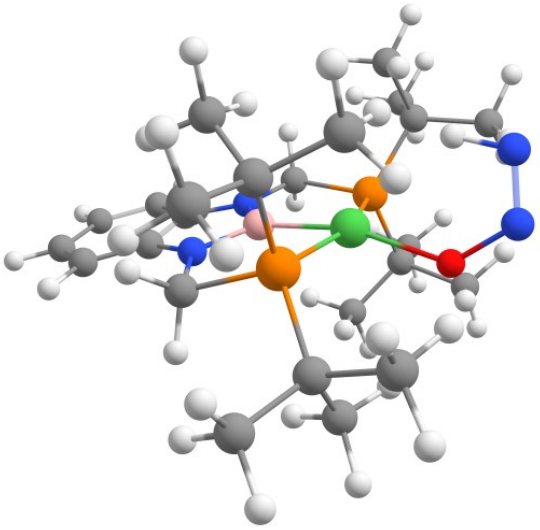

Int1

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P	-2.189800000	-0.400797000	-0.047797000
N	1.068037000	2.015727000	0.237993000
N	-1.184371000	1.987002000	-0.059053000
C	2.866248000	-0.532424000	-1.722343000

C	3.291794000	-1.109520000	1.350076000
C	-2.475685000	1.429721000	-0.342977000
H	-2.772135000	1.603372000	-1.384549000
H	-3.268577000	1.829225000	0.301621000
C	0.591636000	5.717400000	0.134754000
H	1.112080000	6.668913000	0.196208000
C	2.395628000	1.496299000	0.382630000
H	2.782335000	1.647180000	1.396953000
H	3.106591000	1.954543000	-0.316001000
C	0.632075000	3.326740000	0.173049000
C	-2.931102000	-0.688615000	1.663133000
C	1.319975000	4.530709000	0.255170000
H	2.395409000	4.545992000	0.409392000
C	-1.492500000	4.493888000	-0.145001000
H	-2.567480000	4.480525000	-0.302533000
C	-0.778828000	3.308572000	-0.023337000
C	-3.167947000	-1.225050000	-1.433178000
C	-0.790310000	5.699381000	-0.062602000
H	-1.330976000	6.637025000	-0.154857000
C	-2.535683000	-2.085369000	2.152163000
H	-1.449779000	-2.184226000	2.226238000
H	-2.954742000	-2.245633000	3.153268000
H	-2.897174000	-2.888331000	1.507304000
C	-4.451376000	-0.531723000	1.703842000
H	-4.958520000	-1.323337000	1.145892000
H	-4.789382000	-0.599343000	2.745397000
H	-4.785865000	0.435979000	1.315336000
C	-2.281650000	0.338006000	2.602443000
H	-1.188917000	0.265831000	2.580383000
H	-2.556366000	1.370429000	2.365883000
H	-2.614453000	0.135274000	3.627831000
C	-2.258388000	-1.093282000	-2.664846000
H	-1.335055000	-1.661783000	-2.521020000
H	-2.779551000	-1.495279000	-3.542802000
H	-2.001993000	-0.050005000	-2.885111000
C	-4.516700000	-0.557582000	-1.719760000

H	-4.988937000	-1.076041000	-2.563603000
H	-5.207094000	-0.616273000	-0.875780000
H	-4.416802000	0.493115000	-2.007549000
C	-3.382351000	-2.711358000	-1.137763000
H	-3.797157000	-3.191363000	-2.032982000
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H	-4.097093000	-2.871062000	-0.324853000
C	3.575506000	-2.582328000	1.049655000
H	4.051130000	-3.036513000	1.927745000
H	2.669887000	-3.156614000	0.837444000
H	4.269679000	-2.696115000	0.211873000
C	2.482852000	-0.992309000	2.650538000
H	2.242420000	0.048070000	2.897530000
H	1.541959000	-1.547826000	2.598812000
H	3.068010000	-1.403566000	3.481901000
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H	5.181758000	-0.879392000	2.345450000
H	5.256730000	-0.411470000	0.648203000
H	4.508428000	0.664707000	1.837717000
C	2.622952000	-1.966799000	-2.205549000
H	1.574775000	-2.259617000	-2.098031000
H	2.897781000	-2.031524000	-3.266038000
H	3.229125000	-2.697936000	-1.665610000
C	2.027121000	0.412858000	-2.596640000
H	2.351228000	0.309856000	-3.639536000
H	0.961912000	0.159775000	-2.548694000
H	2.135901000	1.465845000	-2.318072000
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H	4.988683000	-0.920799000	-1.370238000
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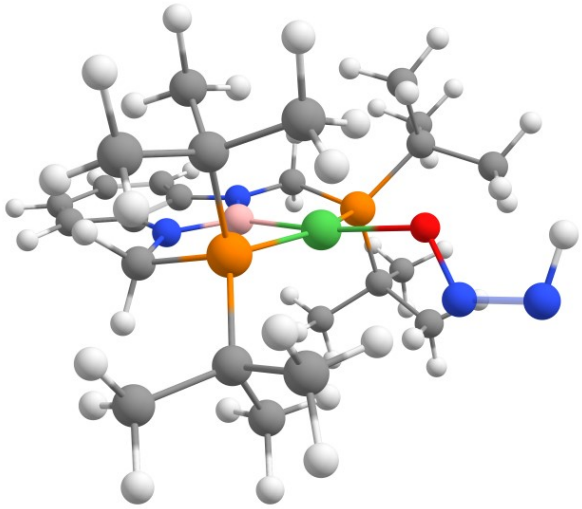

Int1'

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P	2.164110000	-0.411571000	0.082045000
N	-1.017198000	2.078746000	-0.215777000
N	1.224744000	1.998999000	0.160362000
C	-2.914748000	-0.382061000	1.703987000
C	-3.226661000	-1.086696000	-1.346594000
C	2.506876000	1.403899000	0.414980000
H	2.828012000	1.548396000	1.453755000
H	3.297529000	1.795623000	-0.237504000
C	-0.435204000	5.767841000	-0.231061000
H	-0.925223000	6.730425000	-0.346857000
C	-2.341291000	1.577133000	-0.449522000
H	-2.640846000	1.694737000	-1.497566000
H	-3.099822000	2.069670000	0.171998000
C	-0.546063000	3.378693000	-0.179667000
C	2.856060000	-0.696398000	-1.648106000
C	-1.193803000	4.598023000	-0.331005000
H	-2.262292000	4.637723000	-0.524209000
C	1.601152000	4.497705000	0.165507000
H	2.669858000	4.460029000	0.358142000
C	0.857788000	3.328832000	0.065748000
C	3.119951000	-1.309877000	1.432429000

C	0.938229000	5.718712000	0.013173000
H	1.503350000	6.643512000	0.087007000
C	2.376979000	-2.064540000	-2.147104000
H	1.286212000	-2.146156000	-2.114486000
H	2.697410000	-2.195117000	-3.188258000
H	2.785293000	-2.896351000	-1.569746000
C	4.379636000	-0.604930000	-1.726663000
H	4.867226000	-1.419944000	-1.184712000
H	4.690513000	-0.680109000	-2.776274000
H	4.762683000	0.346012000	-1.340733000
C	2.228758000	0.375852000	-2.551131000
H	1.134920000	0.337104000	-2.516210000
H	2.540764000	1.392388000	-2.292787000
H	2.541297000	0.188569000	-3.585796000
C	2.227255000	-1.170899000	2.675023000
H	1.266714000	-1.673226000	2.521384000
H	2.725016000	-1.635819000	3.535308000
H	2.030887000	-0.123727000	2.933622000
C	4.500417000	-0.715521000	1.723400000
H	4.963062000	-1.282283000	2.541248000
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H	4.449066000	0.328513000	2.047020000
C	3.250549000	-2.795135000	1.087996000
H	3.628402000	-3.331780000	1.967421000
H	2.280948000	-3.223645000	0.817559000
H	3.960143000	-2.966775000	0.273205000
C	-3.581785000	-2.520558000	-0.946560000
H	-4.026410000	-3.025465000	-1.813250000
H	-2.703972000	-3.099163000	-0.650682000
H	-4.321431000	-2.550661000	-0.141065000
C	-2.306126000	-1.127591000	-2.575547000
H	-1.975465000	-0.127095000	-2.879163000
H	-1.422510000	-1.743274000	-2.376354000
H	-2.847094000	-1.567840000	-3.422508000
C	-4.513857000	-0.329374000	-1.690075000
H	-5.038766000	-0.876383000	-2.483354000

H	-5.197453000	-0.252451000	-0.841145000
H	-4.326196000	0.678899000	-2.070090000
C	-2.635251000	-1.790362000	2.243404000
H	-1.578873000	-2.058321000	2.141757000
H	-2.906343000	-1.825668000	3.306099000
H	-3.216998000	-2.558507000	1.729206000
C	-2.146266000	0.622760000	2.574935000
H	-2.503515000	0.541006000	3.608944000
H	-1.070782000	0.413997000	2.570009000
H	-2.287968000	1.660371000	2.256864000
C	-4.410954000	-0.080134000	1.768382000
H	-5.001913000	-0.830466000	1.236418000
H	-4.736437000	-0.092380000	2.816182000
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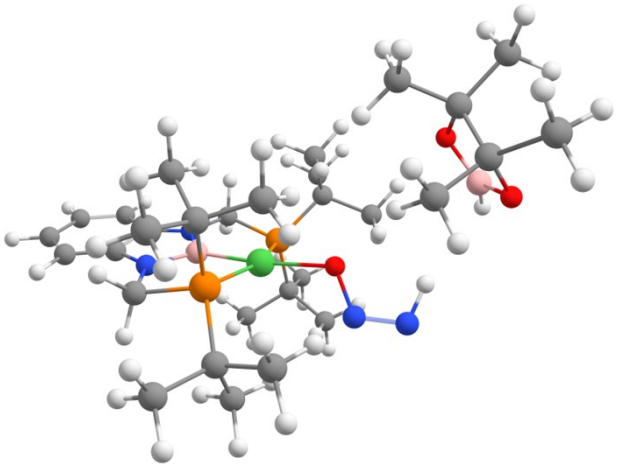

Int1'·HBpin

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P	0.758278000	2.140933000	0.358532000
N	3.293175000	-0.906600000	-0.437967000
N	2.934172000	1.314827000	-0.766839000
C	0.394963000	-2.897140000	-1.264392000

C	0.951247000	-3.310360000	1.801987000
C	2.215760000	2.558716000	-0.747577000
H	1.863925000	2.845878000	-1.746063000
H	2.809200000	3.390584000	-0.347182000
C	6.597014000	-0.155006000	-2.007451000
H	7.542255000	-0.596265000	-2.310599000
C	3.000531000	-2.250308000	-0.027826000
H	3.542321000	-2.526889000	0.884454000
H	3.241496000	-2.992502000	-0.799441000
C	4.425043000	-0.376794000	-1.029929000
C	1.253052000	2.831904000	2.043027000
C	5.625807000	-0.962908000	-1.409193000
H	5.803386000	-2.021626000	-1.241251000
C	5.168660000	1.807226000	-1.840585000
H	4.993491000	2.866259000	-2.009115000
C	4.196692000	1.014437000	-1.244053000
C	-0.688978000	3.049530000	-0.426969000
C	6.372520000	1.206258000	-2.219200000
H	7.144490000	1.810831000	-2.686777000
C	0.280659000	2.285842000	3.094401000
H	0.267689000	1.191874000	3.096039000
H	0.601947000	2.623961000	4.087470000
H	-0.745765000	2.625736000	2.944226000
C	1.289306000	4.358907000	2.090014000
H	0.293298000	4.795172000	1.978169000
H	1.679092000	4.680180000	3.064048000
H	1.942438000	4.784776000	1.320739000
C	2.647928000	2.274529000	2.359795000
H	2.656212000	1.179586000	2.339930000
H	3.419261000	2.632501000	1.671331000
H	2.932312000	2.595548000	3.369492000
C	-1.105240000	2.143487000	-1.595914000
H	-1.414736000	1.161039000	-1.226998000
H	-1.959120000	2.590689000	-2.117535000
H	-0.297342000	2.005321000	-2.324809000
C	-0.344349000	4.444747000	-0.954221000

H	-1.238943000	4.871334000	-1.425020000
H	-0.034544000	5.130223000	-0.162307000
H	0.440866000	4.426774000	-1.716501000
C	-1.856859000	3.136437000	0.557311000
H	-2.744675000	3.489096000	0.020617000
H	-2.086281000	2.153941000	0.978831000
H	-1.660998000	3.841706000	1.370449000
C	-0.512484000	-3.720589000	1.981861000
H	-0.620621000	-4.220891000	2.952205000
H	-1.181421000	-2.857085000	1.985072000
H	-0.840074000	-4.427749000	1.213996000
C	1.370312000	-2.433370000	2.992091000
H	2.395031000	-2.056236000	2.889952000
H	0.690375000	-1.582609000	3.102764000
H	1.328360000	-3.028049000	3.913328000
C	1.828807000	-4.566217000	1.756900000
H	1.648605000	-5.148217000	2.669406000
H	1.599726000	-5.212979000	0.907268000
H	2.898198000	-4.336081000	1.733250000
C	-1.115256000	-2.643661000	-1.213667000
H	-1.326366000	-1.587130000	-1.023681000
H	-1.561885000	-2.924615000	-2.175911000
H	-1.614356000	-3.221053000	-0.432724000
C	0.966878000	-2.091241000	-2.439909000
H	0.484015000	-2.428808000	-3.365476000
H	0.769116000	-1.019798000	-2.326441000
H	2.045957000	-2.222735000	-2.564678000
C	0.679756000	-4.382149000	-1.479972000
H	0.203828000	-5.006837000	-0.719535000
H	0.275872000	-4.689199000	-2.453038000
H	1.752259000	-4.604180000	-1.489233000
H	-3.223367000	0.091080000	2.100233000
O	-1.306348000	-0.074980000	1.076268000
N	-1.471049000	-0.496091000	2.317031000
N	-2.608193000	-0.355869000	2.808339000
B	-4.976512000	1.428312000	0.314659000

O	-5.588147000	0.262343000	0.663755000
O	-4.566036000	1.478315000	-0.985075000
C	-5.418917000	-0.654548000	-0.446772000
C	-5.120253000	0.313695000	-1.645222000
H	-4.828640000	2.330148000	1.078908000
C	-4.104515000	-0.208054000	-2.644185000
H	-3.146491000	-0.423843000	-2.168350000
H	-4.470026000	-1.121549000	-3.124360000
H	-3.936471000	0.540385000	-3.424466000
C	-6.377255000	0.787298000	-2.365878000
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H	-6.624656000	-2.134959000	-1.461213000
H	-6.820997000	-2.098429000	0.298189000
H	-7.572327000	-0.842315000	-0.693650000
C	-4.243209000	-1.555689000	-0.094733000
H	-4.449313000	-2.053287000	0.857581000
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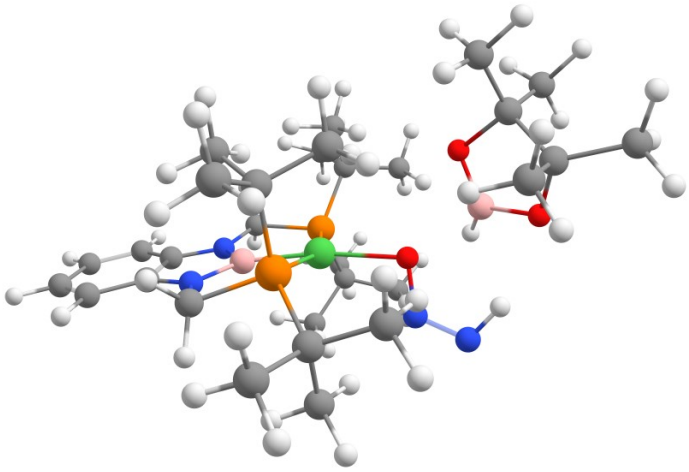

TS2

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P	0.750027000	2.201232000	0.145622000
N	3.089700000	-1.197011000	0.012644000
N	3.068407000	1.051964000	-0.267554000
C	0.272176000	-2.641310000	-1.651667000
C	0.072254000	-3.455632000	1.393128000
C	2.519914000	2.357906000	-0.466275000
H	2.532250000	2.630588000	-1.526673000
H	3.064528000	3.135484000	0.082398000
C	6.710367000	-0.828362000	-0.814685000
H	7.639492000	-1.375975000	-0.944707000
C	2.565078000	-2.517881000	0.192412000
H	2.856101000	-2.954045000	1.154811000
H	2.882768000	-3.208682000	-0.599534000
C	4.375012000	-0.800272000	-0.304331000
C	0.823425000	3.100665000	1.804358000
C	5.549945000	-1.523828000	-0.463357000
H	5.563391000	-2.600504000	-0.317727000
C	5.517587000	1.292248000	-0.840174000
H	5.505309000	2.368487000	-0.988724000
C	4.359514000	0.610322000	-0.489383000
C	-0.185374000	3.187220000	-1.179654000
C	6.694325000	0.555237000	-1.000363000
H	7.610736000	1.069991000	-1.274755000
C	-0.531286000	3.010715000	2.511165000
H	-0.855890000	1.974273000	2.622074000
H	-0.430823000	3.435919000	3.517791000
H	-1.315149000	3.568435000	1.996163000
C	1.248580000	4.565776000	1.697797000
H	0.499441000	5.172180000	1.181216000
H	1.357628000	4.977108000	2.709136000
H	2.209879000	4.698504000	1.191175000
C	1.844458000	2.314578000	2.640877000
H	1.537324000	1.268854000	2.753454000
H	2.852741000	2.330016000	2.214880000
H	1.899613000	2.759078000	3.642207000
C	-0.453532000	2.166473000	-2.293643000

H	-1.137255000	1.384796000	-1.950086000
H	-0.920735000	2.673385000	-3.147916000
H	0.472052000	1.699768000	-2.653103000
C	0.612847000	4.367544000	-1.750217000
H	-0.045597000	4.935614000	-2.419057000
H	0.963924000	5.056671000	-0.978112000
H	1.472534000	4.055189000	-2.348636000
C	-1.514921000	3.725680000	-0.652134000
H	-2.107495000	4.090651000	-1.500331000
H	-2.105790000	2.960786000	-0.152254000
H	-1.369912000	4.568847000	0.029861000
C	-1.453080000	-3.536309000	1.308903000
H	-1.833809000	-4.101517000	2.168197000
H	-1.910536000	-2.545552000	1.326746000
H	-1.783233000	-4.056930000	0.404143000
C	0.481465000	-2.878754000	2.758489000
H	1.569225000	-2.860047000	2.888240000
H	0.099851000	-1.866107000	2.909582000
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C	0.674557000	-4.858311000	1.260427000
H	0.331506000	-5.462016000	2.110129000
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C	-1.167917000	-2.186828000	-1.899312000
H	-1.326529000	-1.150951000	-1.580573000
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H	-1.889704000	-2.815352000	-1.373933000
C	1.192841000	-1.810836000	-2.557722000
H	0.912385000	-1.994621000	-3.602148000
H	1.085038000	-0.739166000	-2.362335000
H	2.250246000	-2.069731000	-2.450018000
C	0.416728000	-4.120613000	-2.006048000
H	-0.324715000	-4.737218000	-1.491583000
H	0.251954000	-4.247784000	-3.083354000
H	1.413287000	-4.514099000	-1.780350000
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N	-1.367435000	-0.216319000	2.337016000
N	-2.342506000	-0.417065000	3.080290000
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O	-4.520277000	0.259248000	0.991753000
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C	-4.537191000	0.431714000	-1.331370000
H	-2.948315000	1.802433000	1.271237000
C	-4.279376000	-0.321479000	-2.622728000
H	-3.553387000	-1.123261000	-2.485435000
H	-5.207952000	-0.754128000	-3.009867000
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C	-5.436988000	1.635623000	-1.600668000
H	-4.914728000	2.319859000	-2.276086000
H	-6.383722000	1.345523000	-2.066647000
H	-5.652793000	2.176316000	-0.674229000
C	-6.557954000	-0.524788000	-0.010739000
H	-7.004940000	-0.974317000	-0.903802000
H	-6.819767000	-1.149407000	0.848806000
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C	-4.437841000	-1.842424000	-0.136370000
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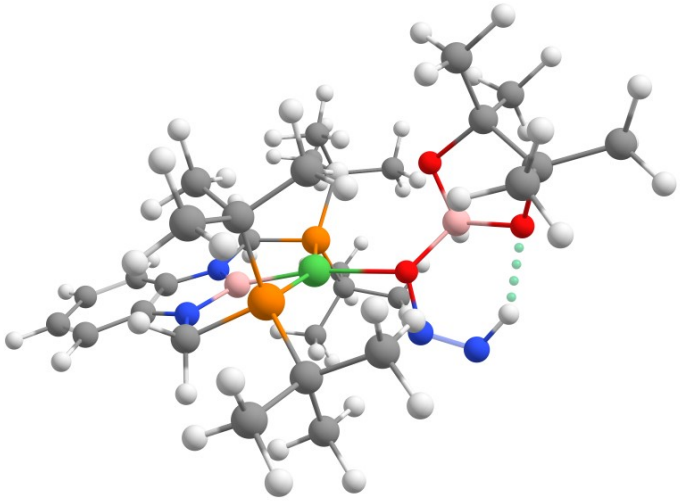

Int2

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P	0.726845000	2.210856000	0.123405000
N	3.005632000	-1.236134000	0.060863000
N	3.020485000	1.007012000	-0.263156000
C	0.211616000	-2.651361000	-1.664889000
C	-0.065765000	-3.459248000	1.381276000
C	2.494112000	2.315091000	-0.499427000
H	2.502873000	2.553591000	-1.568353000
H	3.053572000	3.100792000	0.022222000
C	6.642890000	-0.933741000	-0.718292000
H	7.565940000	-1.496489000	-0.824325000
C	2.459782000	-2.548999000	0.233372000
H	2.726038000	-2.987210000	1.201683000
H	2.786840000	-3.243579000	-0.550999000
C	4.301503000	-0.862918000	-0.244363000
C	0.844506000	3.089428000	1.791998000
C	5.467806000	-1.606314000	-0.372098000
H	5.463507000	-2.680187000	-0.206909000
C	5.481381000	1.202848000	-0.801327000
H	5.486492000	2.276003000	-0.970809000
C	4.308772000	0.543212000	-0.456185000
C	-0.171266000	3.241250000	-1.194087000
C	6.649427000	0.446466000	-0.929297000
H	7.577138000	0.943003000	-1.199059000
C	-0.496296000	2.994713000	2.521431000
H	-0.798774000	1.956368000	2.663353000
H	-0.391067000	3.448591000	3.514933000
H	-1.301612000	3.515789000	2.001165000
C	1.268081000	4.555197000	1.692664000
H	0.497565000	5.170046000	1.219662000
H	1.419958000	4.948207000	2.705700000
H	2.207356000	4.695527000	1.148186000
C	1.881959000	2.298278000	2.602469000
H	1.600332000	1.242349000	2.684166000

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H	1.928885000	2.713377000	3.616671000
C	-0.403546000	2.257523000	-2.349422000
H	-1.090952000	1.460911000	-2.049016000
H	-0.854004000	2.794504000	-3.194379000
H	0.533484000	1.813718000	-2.708026000
C	0.647943000	4.436773000	-1.699787000
H	0.033708000	4.985545000	-2.424510000
H	0.914719000	5.138333000	-0.906432000
H	1.562685000	4.145538000	-2.222553000
C	-1.518446000	3.763030000	-0.695316000
H	-2.055625000	4.205193000	-1.543763000
H	-2.143470000	2.970103000	-0.284796000
H	-1.399145000	4.549841000	0.056005000
C	-1.591327000	-3.517568000	1.279608000
H	-1.989600000	-4.070855000	2.138708000
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C	0.338368000	-2.897308000	2.754081000
H	1.424215000	-2.901231000	2.898734000
H	-0.024927000	-1.878002000	2.904659000
H	-0.095308000	-3.531397000	3.536981000
C	0.514613000	-4.871240000	1.247814000
H	0.155011000	-5.471942000	2.092687000
H	0.199879000	-5.378606000	0.334625000
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C	-1.234625000	-2.235486000	-1.941235000
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H	0.886200000	-1.982074000	-3.595139000
H	0.978004000	-0.722232000	-2.352462000
H	2.192720000	-2.011586000	-2.404651000
C	0.403667000	-4.123484000	-2.028446000
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H	0.267932000	-4.241791000	-3.110722000
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H	-3.362630000	-0.152934000	2.604743000
O	-1.697304000	-0.118268000	1.041697000
N	-1.491446000	-0.226630000	2.412252000
N	-2.478004000	-0.223660000	3.142286000
B	-2.956980000	0.715201000	0.561840000
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C	-4.248732000	0.459831000	-1.327528000
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C	-4.895335000	1.838991000	-1.469520000
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H	-4.944764000	2.347204000	-0.501871000
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H	-6.756637000	-0.793944000	0.821609000
H	-6.624890000	0.865999000	0.231125000
C	-4.581776000	-1.867636000	-0.280897000
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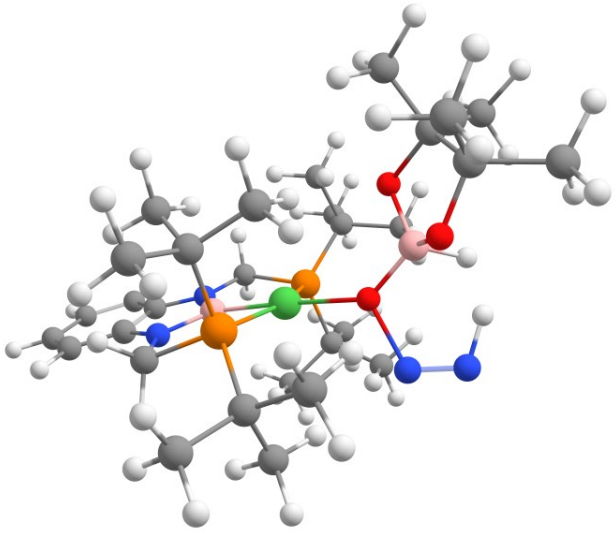

TS3

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P	0.880218000	2.185374000	0.166715000
N	2.900984000	-1.344315000	-0.172455000
N	2.980307000	0.877184000	-0.625542000
C	-0.155592000	-2.848578000	-1.321873000
C	-0.069608000	-3.188517000	1.806086000
C	2.516943000	2.227093000	-0.747093000
H	2.363826000	2.512434000	-1.794189000
H	3.206689000	2.953769000	-0.300124000
C	6.459382000	-1.254521000	-1.295451000
H	7.344203000	-1.865089000	-1.451277000
C	2.337643000	-2.602478000	0.221179000
H	2.714382000	-2.937610000	1.194659000
H	2.533834000	-3.400348000	-0.505936000
C	4.174667000	-1.050055000	-0.622048000
C	1.345046000	2.893423000	1.859179000
C	5.292357000	-1.852468000	-0.812077000
H	5.257673000	-2.915136000	-0.588327000
C	5.387444000	0.927715000	-1.391330000
H	5.423267000	1.989962000	-1.616877000
C	4.222492000	0.342776000	-0.911752000
C	-0.159368000	3.373632000	-0.867019000

C	6.506381000	0.111743000	-1.579099000
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H	-0.012483000	1.605882000	2.957900000
H	0.423275000	3.100353000	3.797810000
H	-0.755586000	3.135915000	2.478845000
C	1.726722000	4.373197000	1.839037000
H	0.866282000	5.013492000	1.627107000
H	2.103920000	4.654681000	2.830237000
H	2.516443000	4.599291000	1.115019000
C	2.531804000	2.068962000	2.379664000
H	2.302647000	0.997972000	2.395307000
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C	-0.507623000	2.573771000	-2.131426000
H	-1.115453000	1.697989000	-1.891257000
H	-1.096461000	3.212502000	-2.802671000
H	0.385193000	2.260206000	-2.684584000
C	0.576814000	4.653956000	-1.277958000
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H	1.500354000	4.455829000	-1.830324000
C	-1.445788000	3.737821000	-0.124489000
H	-2.099618000	4.303022000	-0.800192000
H	-1.998896000	2.851014000	0.192679000
H	-1.248974000	4.374532000	0.744050000
C	-1.600085000	-3.245048000	1.835568000
H	-1.926447000	-3.582722000	2.827048000
H	-2.060421000	-2.274912000	1.634142000
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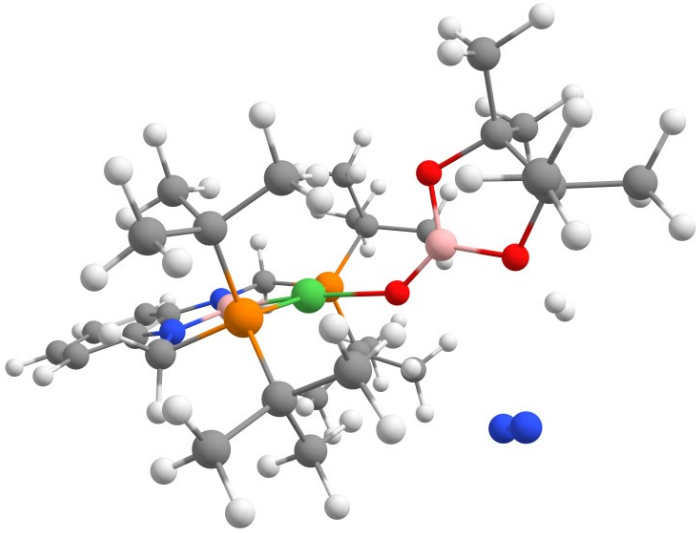
C	0.445013000	-2.394324000	3.016186000
H	1.537461000	-2.304041000	3.019424000
H	0.015963000	-1.390501000	3.049996000
H	0.157477000	-2.916369000	3.937346000
C	0.500177000	-4.609613000	1.876300000
H	0.140513000	-5.079564000	2.800387000

H	0.177698000	-5.240577000	1.046270000
H	1.593926000	-4.626116000	1.915878000
C	-1.591759000	-2.348004000	-1.485321000
H	-1.651527000	-1.256359000	-1.449711000
H	-1.966526000	-2.680846000	-2.462398000
H	-2.267668000	-2.728044000	-0.718750000
C	0.693030000	-2.214550000	-2.433193000
H	0.265299000	-2.499778000	-3.402208000
H	0.681331000	-1.121159000	-2.370595000
H	1.735908000	-2.546018000	-2.423793000
C	-0.112996000	-4.370630000	-1.448344000
H	-0.816929000	-4.853463000	-0.765535000
H	-0.406021000	-4.651109000	-2.467811000
H	0.884996000	-4.785559000	-1.271338000
H	-3.336794000	0.967414000	2.260285000
O	-1.638370000	0.035732000	1.009931000
N	-1.711075000	0.123135000	2.668309000
N	-2.712624000	0.577945000	3.087572000
B	-2.903809000	0.349419000	0.394569000
O	-3.863273000	-0.734470000	0.427723000
O	-2.816445000	0.776891000	-0.978330000
C	-4.835663000	-0.437176000	-0.558854000
C	-4.124082000	0.637561000	-1.517477000
H	-3.426200000	1.350415000	1.079355000
C	-3.976052000	0.187460000	-2.966663000
H	-3.434837000	-0.757090000	-3.043287000
H	-4.948396000	0.075567000	-3.457291000
H	-3.404589000	0.942468000	-3.516821000
C	-4.791511000	2.014885000	-1.505992000
H	-4.212583000	2.690587000	-2.143997000
H	-5.816742000	1.984053000	-1.888445000
H	-4.807634000	2.442547000	-0.500657000
C	-6.089181000	0.098420000	0.138342000
H	-6.886973000	0.346088000	-0.569881000
H	-6.467160000	-0.672477000	0.817530000
H	-5.869098000	0.985414000	0.737508000

C	-5.201971000	-1.744054000	-1.256820000
H	-5.577866000	-2.448417000	-0.507668000
H	-5.984019000	-1.601835000	-2.010283000
H	-4.335963000	-2.203523000	-1.736090000



6a-Bpin (NiOBpin)·H_2·N_2

Ni	0.338881000	0.028838000	0.101719000
B	2.214115000	-0.062802000	-0.208465000
P	0.650560000	-2.159729000	0.094323000
P	0.856129000	2.174877000	0.057558000
N	3.061445000	-1.220935000	-0.118427000
N	3.113258000	1.020064000	-0.500913000
C	0.200808000	-2.949141000	-1.557985000
C	-0.077578000	-3.054704000	1.582552000
C	2.605407000	2.358981000	-0.605256000
H	2.585894000	2.711336000	-1.643569000
H	3.190444000	3.078633000	-0.018781000
C	6.756418000	-0.939581000	-0.580721000
H	7.683426000	-1.506010000	-0.583965000
C	2.496689000	-2.492799000	0.234148000
H	2.756242000	-2.785100000	1.259257000
H	2.818441000	-3.301105000	-0.434300000
C	4.378535000	-0.857080000	-0.328712000
C	0.971673000	2.819219000	1.828292000
C	5.551053000	-1.601359000	-0.327694000
H	5.528705000	-2.669975000	-0.132009000

C	5.613140000	1.193511000	-0.828878000
H	5.637570000	2.262367000	-1.022990000
C	4.409921000	0.546963000	-0.577251000
C	-0.158031000	3.290568000	-1.067424000
C	6.786893000	0.433822000	-0.826739000
H	7.737192000	0.923201000	-1.020799000
C	-0.354217000	2.530412000	2.544631000
H	-0.707699000	1.513926000	2.349369000
H	-0.210945000	2.654960000	3.625324000
H	-1.149227000	3.214476000	2.240190000
C	1.318003000	4.303612000	1.938317000
H	0.516309000	4.940842000	1.554462000
H	1.457914000	4.561712000	2.995785000
H	2.245719000	4.561584000	1.416339000
C	2.068567000	1.984736000	2.507172000
H	1.832460000	0.915649000	2.474537000
H	3.056405000	2.126340000	2.057566000
H	2.138317000	2.284767000	3.560044000
C	-0.385884000	2.445651000	-2.330024000
H	-1.003387000	1.568576000	-2.111122000
H	-0.908333000	3.051659000	-3.081846000
H	0.556708000	2.107394000	-2.777617000
C	0.536977000	4.601925000	-1.445374000
H	-0.137337000	5.185357000	-2.085195000
H	0.778424000	5.219806000	-0.577400000
H	1.456556000	4.440238000	-2.015924000
C	-1.509905000	3.592210000	-0.418451000
H	-2.180828000	4.026046000	-1.169516000
H	-1.978394000	2.686044000	-0.028204000
H	-1.416803000	4.315904000	0.396405000
C	-1.597001000	-3.162766000	1.434058000
H	-2.027520000	-3.495215000	2.386921000
H	-2.039888000	-2.194884000	1.184386000
H	-1.881548000	-3.898633000	0.676100000
C	0.233894000	-2.119611000	2.761418000
H	1.311199000	-1.972670000	2.902748000

H	-0.231798000	-1.140877000	2.610566000
H	-0.163273000	-2.555431000	3.686902000
C	0.522955000	-4.436492000	1.851763000
H	0.074014000	-4.843292000	2.766947000
H	0.322345000	-5.147935000	1.047590000
H	1.604565000	-4.401863000	2.014753000
C	-1.238654000	-2.572522000	-1.920577000
H	-1.402189000	-1.492119000	-1.894120000
H	-1.452714000	-2.924776000	-2.937887000
H	-1.968786000	-3.037605000	-1.254557000
C	1.131147000	-2.304897000	-2.596484000
H	0.856222000	-2.672351000	-3.592844000
H	1.029475000	-1.214331000	-2.596409000
H	2.186425000	-2.545664000	-2.435263000
C	0.362484000	-4.469012000	-1.586760000
H	-0.380305000	-4.967178000	-0.957230000
H	0.209782000	-4.826748000	-2.612930000
H	1.358418000	-4.797938000	-1.271882000
H	-3.959313000	2.791136000	2.216954000
O	-1.507934000	0.104368000	0.624776000
N	-3.261601000	-0.867534000	3.478009000
N	-2.626987000	0.016236000	3.650945000
B	-2.666571000	0.133547000	0.015569000
O	-3.907900000	0.025588000	0.674071000
O	-2.880660000	0.261317000	-1.371567000
C	-4.901148000	-0.239395000	-0.316191000
C	-4.283791000	0.414994000	-1.597474000
H	-3.943314000	2.111978000	1.904560000
C	-4.651175000	-0.267700000	-2.904027000
H	-4.313964000	-1.306595000	-2.919866000
H	-5.733614000	-0.247207000	-3.069568000
H	-4.171675000	0.252932000	-3.739224000
C	-4.578597000	1.909732000	-1.687446000
H	-3.948417000	2.348746000	-2.466775000
H	-5.625267000	2.106273000	-1.940469000
H	-4.348051000	2.409519000	-0.742282000

C	-6.224884000	0.355315000	0.133061000
H	-6.993690000	0.234110000	-0.637691000
H	-6.568584000	-0.156463000	1.037452000
H	-6.128220000	1.417688000	0.367033000
C	-5.026213000	-1.756880000	-0.437128000
H	-5.243627000	-2.170835000	0.552018000
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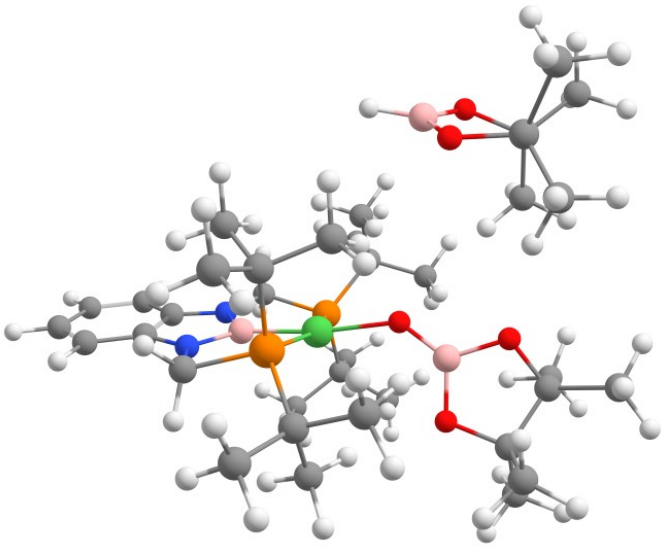
H	-4.086694000	-2.196008000	-0.785883000



Complex 6a-Bpin(NiOBpin)·HBpin

Ni	-0.951939000	-0.142659000	0.216431000
B	-2.804638000	0.068300000	-0.164853000
P	-1.266767000	-1.768353000	-1.246261000
P	-1.437663000	1.620349000	1.458503000
N	-3.552221000	-0.545195000	-1.228738000
N	-3.743738000	0.948367000	0.475193000
C	-1.557731000	-3.438813000	-0.417663000
C	-0.002465000	-1.841157000	-2.640117000
C	-3.307608000	1.791310000	1.552591000
H	-3.676888000	1.443158000	2.525050000
H	-3.626945000	2.833587000	1.426583000
C	-7.127174000	0.351753000	-1.830255000
H	-7.981360000	0.158780000	-2.473168000
C	-2.893157000	-1.447082000	-2.130897000
H	-2.707492000	-0.984294000	-3.108029000
H	-3.457886000	-2.372706000	-2.299494000

C	-4.844042000	-0.053299000	-1.239692000
C	-0.887915000	3.187029000	0.563245000
C	-5.923195000	-0.316281000	-2.073381000
H	-5.829162000	-1.019750000	-2.896179000
C	-6.167543000	1.534900000	0.066392000
H	-6.262071000	2.242265000	0.885829000
C	-4.966305000	0.877625000	-0.166008000
C	-0.913983000	1.576435000	3.263503000
C	-7.247149000	1.261813000	-0.779151000
H	-8.194027000	1.767740000	-0.612743000
C	0.606081000	3.076288000	0.239043000
H	0.863844000	2.105650000	-0.192266000
H	0.877539000	3.855359000	-0.481648000
H	1.237979000	3.216480000	1.118977000
C	-1.165618000	4.480217000	1.328382000
H	-0.552459000	4.558853000	2.230643000
H	-0.911621000	5.335388000	0.689318000
H	-2.217792000	4.588242000	1.613177000
C	-1.656358000	3.197792000	-0.767045000
H	-1.452610000	2.292210000	-1.348917000
H	-2.740236000	3.281058000	-0.638787000
H	-1.324577000	4.060373000	-1.357858000
C	-1.209070000	0.136563000	3.710071000
H	-0.588921000	-0.581215000	3.163693000
H	-0.983147000	0.036529000	4.779862000
H	-2.263264000	-0.132581000	3.572467000
C	-1.668478000	2.556637000	4.165976000
H	-1.290897000	2.452288000	5.191261000
H	-1.526882000	3.598643000	3.870921000
H	-2.743226000	2.354143000	4.199751000
C	0.590853000	1.829943000	3.368416000
H	0.934478000	1.551772000	4.371993000
H	1.145759000	1.233532000	2.640283000
H	0.837807000	2.884959000	3.218370000
C	1.286418000	-2.505412000	-2.151015000
H	2.062051000	-2.376012000	-2.915205000

H	1.645662000	-2.044049000	-1.227828000
H	1.162136000	-3.581354000	-1.995448000
C	0.295597000	-0.365719000	-2.950263000
H	-0.599153000	0.178482000	-3.276327000
H	0.702499000	0.135109000	-2.066163000
H	1.035987000	-0.299449000	-3.756405000
C	-0.494687000	-2.544842000	-3.908067000
H	0.300018000	-2.499046000	-4.663490000
H	-0.728356000	-3.599755000	-3.745140000
H	-1.375052000	-2.063036000	-4.344240000
C	-0.396648000	-3.733313000	0.536599000
H	-0.224067000	-2.913936000	1.239074000
H	-0.631805000	-4.635949000	1.115426000
H	0.540031000	-3.920524000	0.007116000
C	-2.830434000	-3.285515000	0.427715000
H	-2.996963000	-4.216295000	0.984110000
H	-2.731167000	-2.470179000	1.152471000
H	-3.724374000	-3.095991000	-0.173886000
C	-1.730038000	-4.592096000	-1.405506000
H	-0.803329000	-4.808546000	-1.944234000
H	-2.005832000	-5.500554000	-0.855107000
H	-2.520812000	-4.404717000	-2.139673000
O	0.963895000	-0.237891000	0.401316000
B	1.779102000	-0.873980000	1.204374000
O	3.177856000	-0.910794000	1.039886000
O	1.422189000	-1.628976000	2.339738000
C	3.691047000	-1.940624000	1.882960000
C	2.618095000	-2.008961000	3.023036000
B	2.606978000	2.374068000	-2.841540000
O	3.431413000	1.536311000	-3.532641000
O	3.113391000	2.800214000	-1.651092000
C	4.513931000	1.182355000	-2.631925000
C	4.489526000	2.352819000	-1.589475000
H	1.540650000	2.717540000	-3.250784000
C	2.420665000	-3.386246000	3.633317000
H	3.343781000	-3.748384000	4.098433000

H	1.648279000	-3.338222000	4.407654000
H	2.097277000	-4.112422000	2.883871000
C	2.873395000	-0.981817000	4.122396000
H	1.990833000	-0.925443000	4.766513000
H	3.734685000	-1.250279000	4.742227000
H	3.045985000	0.010188000	3.695291000
C	3.745479000	-3.223347000	1.055938000
H	4.341613000	-3.039540000	0.157001000
H	4.197458000	-4.053680000	1.607422000
H	2.741606000	-3.521272000	0.738677000
C	5.087726000	-1.558702000	2.342651000
H	5.479415000	-2.284692000	3.063194000
H	5.766226000	-1.536891000	1.483723000
H	5.098776000	-0.567560000	2.801714000
C	4.804353000	1.941506000	-0.163090000
H	4.713516000	2.812895000	0.493228000
H	4.130734000	1.163059000	0.201795000
H	5.833160000	1.572124000	-0.089955000
C	4.151447000	-0.163696000	-2.021403000
H	3.989567000	-0.882696000	-2.829736000
H	4.954451000	-0.539929000	-1.381912000
H	3.244090000	-0.107073000	-1.415436000
C	5.794459000	1.073338000	-3.438489000
H	6.648071000	0.877930000	-2.781443000
H	5.714421000	0.240892000	-4.144083000
H	5.993870000	1.981909000	-4.010690000
C	5.343694000	3.545420000	-2.004358000
H	5.125970000	4.386102000	-1.339167000
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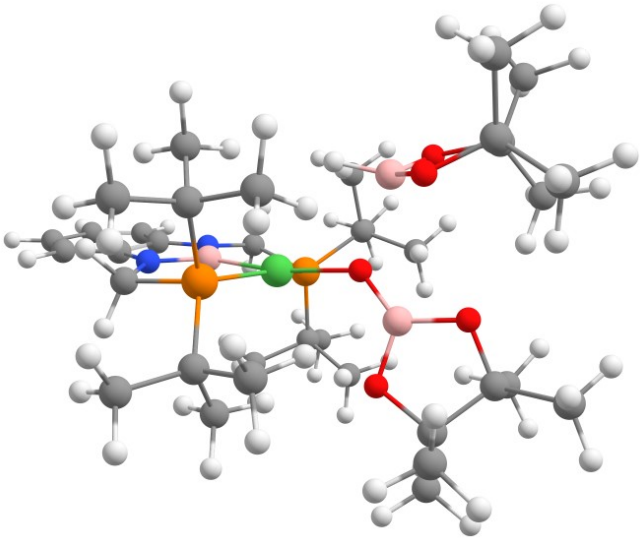

TS4

Ni	-0.759187000	0.035239000	-0.047269000
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P	-1.396627000	2.221601000	-0.043521000
N	-3.415304000	-1.329367000	-0.528918000
N	-3.638901000	0.915369000	-0.324708000
C	-1.269440000	-2.600558000	2.045206000
C	0.014868000	-3.389608000	-0.736838000
C	-3.273797000	2.267002000	-0.032196000
H	-3.644722000	2.577610000	0.951525000
H	-3.661879000	2.977113000	-0.771852000
C	-7.124841000	-1.223868000	-0.927108000
H	-8.006525000	-1.838046000	-1.086960000
C	-2.785167000	-2.613167000	-0.453012000
H	-2.714144000	-3.103479000	-1.430127000
H	-3.317007000	-3.293562000	0.223758000
C	-4.757477000	-1.026800000	-0.654873000
C	-0.979801000	3.140652000	-1.637858000
C	-5.868936000	-1.834196000	-0.860180000
H	-5.761608000	-2.910191000	-0.966763000
C	-6.150606000	0.979688000	-0.587387000
H	-6.259736000	2.055303000	-0.478964000
C	-4.898544000	0.382348000	-0.520147000
C	-0.975814000	3.222779000	1.499975000

C	-7.263228000	0.158810000	-0.793398000
H	-8.251395000	0.606625000	-0.849216000
C	0.542544000	3.218947000	-1.796848000
H	1.048754000	2.323772000	-1.439547000
H	0.794800000	3.335183000	-2.857319000
H	0.961377000	4.078182000	-1.267582000
C	-1.570335000	4.545998000	-1.757702000
H	-1.119542000	5.241336000	-1.044742000
H	-1.352584000	4.930704000	-2.762128000
H	-2.657130000	4.575113000	-1.630717000
C	-1.560165000	2.246529000	-2.745292000
H	-1.136231000	1.237883000	-2.706246000
H	-2.650566000	2.159228000	-2.689138000
H	-1.311170000	2.680142000	-3.721557000
C	-1.183782000	2.244676000	2.664271000
H	-0.487205000	1.404257000	2.597198000
H	-0.997421000	2.765104000	3.612872000
H	-2.209166000	1.857651000	2.699235000
C	-1.853984000	4.459924000	1.714485000
H	-1.518903000	4.967493000	2.628037000
H	-1.779779000	5.181067000	0.897561000
H	-2.910082000	4.214569000	1.857982000
C	0.488828000	3.655461000	1.454828000
H	0.782156000	4.026666000	2.443904000
H	1.149106000	2.824828000	1.200361000
H	0.647850000	4.468995000	0.742408000
C	1.451055000	-3.295266000	-0.218749000
H	2.102266000	-3.893071000	-0.867321000
H	1.818310000	-2.267701000	-0.239114000
H	1.541039000	-3.699339000	0.794292000
C	-0.044963000	-2.895115000	-2.190542000
H	-1.016643000	-3.099586000	-2.652757000
H	0.162193000	-1.827119000	-2.270633000
H	0.718246000	-3.415662000	-2.778921000
C	-0.457953000	-4.845808000	-0.701190000
H	0.140437000	-5.419815000	-1.420103000

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H	-2.233721000	-0.671807000	2.402958000
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H	-2.406475000	-4.469028000	1.758650000
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O	3.446284000	0.014260000	0.900671000
O	1.687983000	0.562301000	2.257852000
C	3.922676000	-0.128229000	2.240657000
C	2.871485000	0.695547000	3.057028000
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O	2.897972000	1.085007000	-1.996290000
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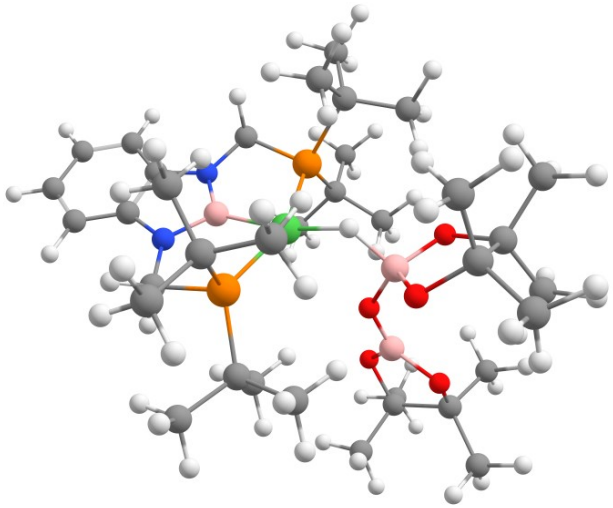

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C	-1.296725000	-3.621346000	-0.538051000
C	-2.762273000	2.601629000	-0.301998000
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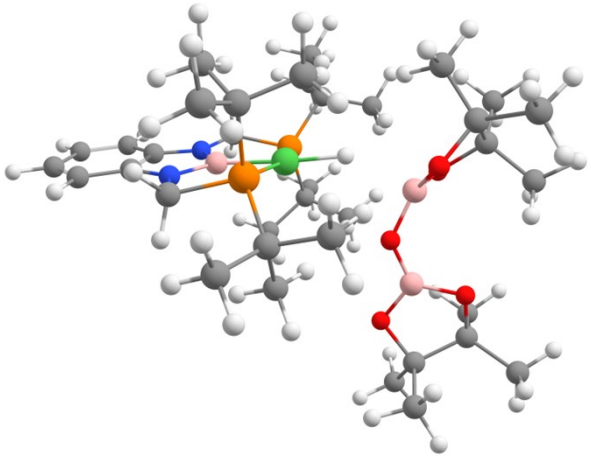

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C	-3.113293000	-2.471973000	-0.196815000
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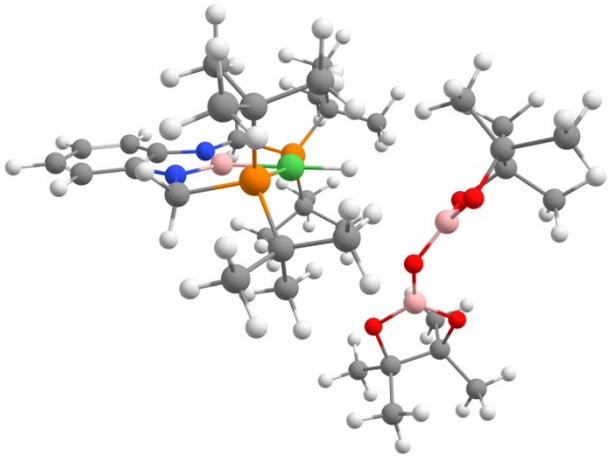

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H	-8.086898000	1.819809000	-1.812980000
C	-1.219650000	-3.893141000	-0.450481000
H	-0.943148000	-3.318104000	0.437922000
H	-1.585993000	-4.879185000	-0.136206000
H	-0.311728000	-4.043581000	-1.037938000
C	-2.670435000	-3.980794000	-2.493690000
H	-1.790341000	-4.184793000	-3.109530000
H	-3.089306000	-4.950031000	-2.193638000
H	-3.420270000	-3.482210000	-3.117092000
C	-3.553284000	-3.064094000	-0.338684000
H	-3.329024000	-2.500553000	0.573115000
H	-4.401572000	-2.580302000	-0.832461000
H	-3.872282000	-4.072813000	-0.046922000
C	-0.045160000	0.162791000	-2.967485000
H	0.448911000	0.364608000	-2.013122000
H	0.684838000	0.339138000	-3.767559000
H	-0.859884000	0.885384000	-3.097838000
C	-1.147458000	-1.559889000	-4.413034000
H	-0.369383000	-1.416112000	-5.173733000
H	-1.519399000	-2.581518000	-4.518625000
H	-1.963397000	-0.872750000	-4.657735000
C	0.639908000	-2.228054000	-2.789118000
H	1.454215000	-1.973395000	-3.478627000
H	1.027657000	-2.133346000	-1.772497000
H	0.372338000	-3.274009000	-2.972449000
C	0.603707000	-0.101689000	3.751011000
H	0.828844000	-0.797329000	4.569480000
H	1.044503000	-0.493977000	2.829175000
H	1.090886000	0.848627000	3.989750000
C	-1.542912000	-1.344876000	3.519725000
H	-2.628389000	-1.298421000	3.372968000
H	-1.110459000	-1.901446000	2.680744000
H	-1.355941000	-1.905306000	4.444879000
C	-1.470647000	0.768538000	4.855990000
H	-1.186942000	0.205026000	5.754247000
H	-1.077960000	1.781289000	4.969964000

H	-2.563372000	0.826276000	4.848126000
C	1.039160000	2.165714000	1.273351000
H	1.057733000	1.469408000	0.431428000
H	1.522464000	3.099536000	0.960951000
H	1.635039000	1.730540000	2.078146000
C	-1.091331000	3.171570000	0.515009000
H	-0.542614000	4.090134000	0.271334000
H	-1.088094000	2.530529000	-0.372578000
H	-2.127817000	3.451764000	0.726554000
C	-0.394687000	3.413941000	2.909392000
H	0.198699000	3.010140000	3.734649000
H	0.058219000	4.372314000	2.624399000
H	-1.402345000	3.629054000	3.280914000
O	2.741052000	-0.226854000	-0.979454000
B	3.356133000	0.959919000	-1.205022000
O	4.692302000	1.187018000	-0.984622000
O	2.690395000	2.034234000	-1.734213000
C	4.893639000	2.605760000	-1.154761000
C	3.697913000	3.002308000	-2.089840000
B	3.060382000	-1.149415000	-0.027986000
O	3.402515000	-0.838248000	1.264990000
O	3.126018000	-2.487362000	-0.314833000
C	4.013768000	-2.029572000	1.804899000
C	3.359429000	-3.161348000	0.940647000
H	0.253451000	-1.000231000	0.467781000
C	3.139646000	4.393203000	-1.856130000
H	3.900846000	5.155878000	-2.049683000
H	2.300377000	4.570962000	-2.535121000
H	2.775294000	4.512438000	-0.833631000
C	4.004743000	2.792345000	-3.568371000
H	3.074312000	2.882168000	-4.136486000
H	4.714316000	3.533549000	-3.947572000
H	4.413470000	1.792954000	-3.747436000
C	4.802873000	3.231876000	0.232210000
H	5.538426000	2.751283000	0.883561000
H	5.010361000	4.305776000	0.208200000

H	3.814232000	3.074204000	0.672899000
C	6.270053000	2.838307000	-1.748723000
H	6.423623000	3.900230000	-1.966436000
H	7.037448000	2.525469000	-1.034365000
H	6.413851000	2.267196000	-2.668143000
C	4.254004000	-4.360436000	0.686502000
H	3.723872000	-5.089258000	0.066066000
H	5.170616000	-4.077115000	0.164667000
H	4.522326000	-4.849872000	1.628426000
C	5.514258000	-1.892198000	1.567284000
H	5.859812000	-0.961907000	2.027249000
H	6.073887000	-2.724651000	2.004037000
H	5.741044000	-1.839386000	0.497952000
C	3.720796000	-2.114180000	3.289674000
H	4.144782000	-3.030811000	3.712716000
H	4.174913000	-1.261782000	3.804237000
H	2.649031000	-2.099946000	3.490033000
C	2.003765000	-3.607845000	1.472336000
H	1.535302000	-4.264541000	0.734100000
H	2.100659000	-4.161119000	2.411413000
H	1.340211000	-2.749903000	1.617674000

Cartesian coordinates of the high energy transition states

TS-NiOH-1

Ni	-0.025529000	-0.754531000	-0.053842000
B	0.089587000	1.148819000	0.007092000
P	-2.174508000	-0.199919000	-0.067067000
P	2.158031000	-0.474764000	0.051815000
N	-0.964749000	2.097303000	-0.211799000
N	1.261003000	1.953615000	0.218493000
C	-2.896131000	-0.272842000	1.675810000
C	-3.299567000	-0.999032000	-1.359476000
C	2.524195000	1.321762000	0.466937000
H	2.831793000	1.418654000	1.514809000
H	3.332380000	1.724500000	-0.156370000
C	-0.288757000	5.769710000	-0.160753000

H	-0.750551000	6.746312000	-0.275377000
C	-2.286675000	1.627054000	-0.506706000
H	-2.530185000	1.742313000	-1.569599000
H	-3.064140000	2.140186000	0.073524000
C	-0.463189000	3.383810000	-0.145231000
C	2.944626000	-0.703999000	-1.648979000
C	-1.074813000	4.621564000	-0.296519000
H	-2.136476000	4.691944000	-0.516720000
C	1.702879000	4.441038000	0.269976000
H	2.765003000	4.372669000	0.488919000
C	0.931857000	3.293822000	0.135633000
C	3.045737000	-1.416189000	1.425844000
C	1.076099000	5.681252000	0.117564000
H	1.662975000	6.589788000	0.218645000
C	2.539049000	-2.069975000	-2.213616000
H	1.453512000	-2.204094000	-2.199460000
H	2.884777000	-2.139903000	-3.252619000
H	2.983693000	-2.902218000	-1.663121000
C	4.466537000	-0.568051000	-1.648476000
H	4.947188000	-1.386267000	-1.104820000
H	4.831626000	-0.605296000	-2.682462000
H	4.804906000	0.380453000	-1.218007000
C	2.323459000	0.378090000	-2.544930000
H	1.231348000	0.294692000	-2.569693000
H	2.576981000	1.394512000	-2.228797000
H	2.697588000	0.247570000	-3.567786000
C	2.096351000	-1.301087000	2.627563000
H	1.135632000	-1.780571000	2.412438000
H	2.543246000	-1.799146000	3.497034000
H	1.901954000	-0.258722000	2.905866000
C	4.415645000	-0.839370000	1.797896000
H	4.836609000	-1.438765000	2.614883000
H	5.127526000	-0.873672000	0.970039000
H	4.359449000	0.192213000	2.157124000
C	3.202300000	-2.892869000	1.061431000
H	3.551942000	-3.442723000	1.943915000

H	2.252648000	-3.332744000	0.748790000
H	3.941361000	-3.044446000	0.269154000
C	-3.772747000	-2.386147000	-0.921579000
H	-4.248747000	-2.880454000	-1.777897000
H	-2.948911000	-3.018888000	-0.584312000
H	-4.520712000	-2.332794000	-0.124659000
C	-2.391049000	-1.149842000	-2.588782000
H	-1.976975000	-0.188882000	-2.918165000
H	-1.555226000	-1.823394000	-2.372589000
H	-2.968865000	-1.565383000	-3.423878000
C	-4.523501000	-0.150449000	-1.723672000
H	-5.109274000	-0.690515000	-2.478097000
H	-5.181133000	0.028498000	-0.869430000
H	-4.258427000	0.816300000	-2.160734000
C	-2.633999000	-1.669202000	2.250708000
H	-1.569452000	-1.920297000	2.213085000
H	-2.955588000	-1.689704000	3.299702000
H	-3.173136000	-2.455823000	1.719700000
C	-2.118284000	0.743602000	2.523772000
H	-2.467645000	0.675948000	3.561527000
H	-1.043325000	0.535156000	2.513276000
H	-2.264208000	1.776204000	2.192281000
C	-4.387831000	0.053845000	1.740015000
H	-4.996795000	-0.692579000	1.224020000
H	-4.707715000	0.065774000	2.789492000
H	-4.618594000	1.038766000	1.320720000
H	0.583054000	-3.792611000	-0.370419000
O	-0.003391000	-2.649700000	-0.265412000
N	-0.962274000	-3.785934000	0.168874000
N	-0.254422000	-4.735115000	0.003533000

TS-NiOH-2

Ni	0.020154000	-0.780192000	-0.110930000
B	-0.037299000	1.136657000	-0.073384000
P	2.180697000	-0.299111000	0.006397000
P	-2.173229000	-0.425571000	-0.080983000
N	1.054546000	2.043024000	0.128101000

N	-1.192558000	1.976996000	-0.198697000
C	2.978695000	-0.488116000	-1.697970000
C	3.176769000	-1.096854000	1.397297000
C	-2.487983000	1.397736000	-0.403609000
H	-2.844712000	1.547970000	-1.429101000
H	-3.245349000	1.803534000	0.277988000
C	0.483939000	5.730785000	0.251133000
H	0.978143000	6.689292000	0.381455000
C	2.372743000	1.535692000	0.370348000
H	2.680092000	1.687534000	1.411627000
H	3.132566000	1.996248000	-0.273203000
C	0.587171000	3.345009000	0.133198000
C	-2.870384000	-0.693208000	1.650678000
C	1.242014000	4.558104000	0.303327000
H	2.314502000	4.590622000	0.474152000
C	-1.564096000	4.475702000	-0.135070000
H	-2.636757000	4.444954000	-0.305143000
C	-0.820276000	3.303843000	-0.082284000
C	-3.174465000	-1.273595000	-1.436627000
C	-0.894945000	5.690372000	0.035194000
H	-1.459133000	6.617873000	-0.002071000
C	-2.551346000	-2.114211000	2.125804000
H	-1.487075000	-2.350741000	2.044067000
H	-2.839440000	-2.204180000	3.180665000
H	-3.101084000	-2.877291000	1.571137000
C	-4.376585000	-0.447520000	1.750927000
H	-4.947720000	-1.209697000	1.213622000
H	-4.676169000	-0.501284000	2.804882000
H	-4.676004000	0.537532000	1.378169000
C	-2.118801000	0.292685000	2.557606000
H	-1.037079000	0.125871000	2.513214000
H	-2.310183000	1.340505000	2.305870000
H	-2.443502000	0.136598000	3.593539000
C	-2.304783000	-1.142124000	-2.696305000
H	-1.370900000	-1.699887000	-2.581598000
H	-2.851324000	-1.550056000	-3.555721000

H	-2.060568000	-0.098034000	-2.927015000
C	-4.538736000	-0.622582000	-1.690535000
H	-5.037462000	-1.169028000	-2.500669000
H	-5.196751000	-0.661439000	-0.819964000
H	-4.459165000	0.419587000	-2.012749000
C	-3.374558000	-2.757781000	-1.122583000
H	-3.784025000	-3.252595000	-2.011992000
H	-2.433815000	-3.253444000	-0.871327000
H	-4.089877000	-2.910109000	-0.309029000
C	3.448305000	-2.572040000	1.098809000
H	3.900210000	-3.029757000	1.987699000
H	2.529905000	-3.125180000	0.883299000
H	4.156378000	-2.698753000	0.274797000
C	2.270972000	-0.996015000	2.633894000
H	1.996570000	0.039076000	2.869041000
H	1.354552000	-1.577775000	2.498314000
H	2.803827000	-1.401184000	3.502967000
C	4.503582000	-0.385053000	1.686552000
H	4.983244000	-0.882512000	2.538502000
H	5.201839000	-0.433136000	0.848981000
H	4.374387000	0.665192000	1.963799000
C	2.751618000	-1.907437000	-2.227579000
H	1.691145000	-2.172342000	-2.231845000
H	3.128991000	-1.960964000	-3.256519000
H	3.278996000	-2.665014000	-1.643691000
C	2.229213000	0.486038000	-2.619970000
H	2.626716000	0.383291000	-3.637113000
H	1.158129000	0.259124000	-2.652007000
H	2.343686000	1.533713000	-2.324692000
C	4.473566000	-0.168503000	-1.710851000
H	5.053628000	-0.926301000	-1.177425000
H	4.826456000	-0.162445000	-2.749561000
H	4.706965000	0.812052000	-1.283443000
H	0.173754000	-2.288477000	0.727404000
N	0.135069000	-3.759817000	-0.153894000
O	0.320158000	-3.719006000	1.134077000

N	-0.012409000	-2.644503000	-0.661006000

TS-NiOH-3

Ni	0.099240000	-1.092309000	-0.236608000
B	-0.046662000	0.794732000	-0.774111000
P	2.228014000	-0.479295000	0.183695000
P	-2.098865000	-0.812269000	0.067193000
N	0.948489000	1.755815000	-0.423079000
N	-1.291934000	1.502952000	-0.829121000
C	3.651315000	-1.227150000	-0.820345000
C	2.639915000	-0.498175000	2.039113000
C	-2.529556000	0.766793000	-0.855707000
H	-2.843776000	0.534632000	-1.880980000
H	-3.344945000	1.308527000	-0.365361000
C	0.000760000	5.337007000	0.060500000
H	0.397024000	6.321068000	0.294313000
C	2.316917000	1.358458000	-0.247115000
H	2.815193000	1.925205000	0.547373000
H	2.893670000	1.494010000	-1.170039000
C	0.349875000	3.000361000	-0.324850000
C	-2.568548000	-0.362925000	1.852573000
C	0.875284000	4.248482000	-0.019345000
H	1.941103000	4.373910000	0.150278000
C	-1.907378000	3.927129000	-0.475355000
H	-2.971490000	3.808952000	-0.660668000
C	-1.049102000	2.839107000	-0.563931000
C	-3.268971000	-2.125106000	-0.630829000
C	-1.367163000	5.178222000	-0.160135000
H	-2.025633000	6.039802000	-0.095214000
C	-1.968647000	-1.385571000	2.822082000
H	-0.883996000	-1.449830000	2.719282000
H	-2.204559000	-1.081497000	3.849352000
H	-2.370582000	-2.390409000	2.672274000
C	-4.078041000	-0.273031000	2.094060000
H	-4.570614000	-1.248051000	2.060513000
H	-4.243565000	0.136242000	3.098525000
H	-4.578228000	0.397814000	1.388069000

C	-1.971166000	1.021156000	2.149062000
H	-0.926176000	1.106937000	1.848246000
H	-2.521304000	1.825564000	1.653132000
H	-2.029994000	1.205524000	3.228537000
C	-2.699346000	-2.562350000	-1.985742000
H	-1.717930000	-3.029206000	-1.883742000
H	-3.386722000	-3.291125000	-2.433020000
H	-2.597126000	-1.727838000	-2.686115000
C	-4.691967000	-1.602398000	-0.863368000
H	-5.278790000	-2.396797000	-1.341444000
H	-5.209168000	-1.328516000	0.056091000
H	-4.711630000	-0.741679000	-1.539298000
C	-3.292353000	-3.343995000	0.294856000
H	-3.830250000	-4.159990000	-0.203362000
H	-2.280064000	-3.698349000	0.516826000
H	-3.807070000	-3.144230000	1.238419000
C	2.459042000	-1.901688000	2.626041000
H	2.539948000	-1.838516000	3.718292000
H	1.476963000	-2.312137000	2.375429000
H	3.219044000	-2.605613000	2.281855000
C	1.605415000	0.417361000	2.701229000
H	1.656068000	1.454285000	2.355791000
H	0.596462000	0.045671000	2.519637000
H	1.771413000	0.422268000	3.785384000
C	4.045334000	0.006894000	2.373378000
H	4.124950000	0.128387000	3.460849000
H	4.820137000	-0.703723000	2.074669000
H	4.271685000	0.978843000	1.923566000
C	3.958673000	-2.637646000	-0.310083000
H	3.050106000	-3.239176000	-0.198663000
H	4.607391000	-3.144464000	-1.034989000
H	4.488736000	-2.625226000	0.646267000
C	3.166429000	-1.331329000	-2.270540000
H	4.004445000	-1.660083000	-2.897549000
H	2.360330000	-2.059891000	-2.370693000
H	2.810059000	-0.375285000	-2.667675000

C	4.932346000	-0.383496000	-0.810866000
H	5.364729000	-0.254239000	0.181130000
H	5.681794000	-0.895719000	-1.427177000
H	4.784089000	0.605881000	-1.253366000
H	0.109358000	-2.115975000	0.873533000
O	0.365264000	0.630902000	-3.196904000
N	0.210526000	-0.603969000	-3.077093000
N	0.060031000	-1.291284000	-2.120551000

TS-NiOH-4

Ni	-0.002044000	-0.709573000	-0.077949000
B	0.063251000	1.180655000	-0.179068000
P	2.168493000	-0.415617000	0.026006000
P	-2.164436000	-0.262561000	-0.039417000
N	1.218078000	2.014963000	-0.032742000
N	-1.044669000	2.082170000	-0.280369000
C	3.006882000	-0.848612000	-1.603032000
C	3.002740000	-1.157246000	1.546173000
C	-2.378912000	1.570361000	-0.410776000
H	-2.769416000	1.708589000	-1.425351000
H	-3.083422000	2.038669000	0.287474000
C	0.877926000	5.732408000	0.044480000
H	1.434753000	6.660043000	0.141089000
C	2.503178000	1.429235000	0.220764000
H	2.852736000	1.649283000	1.236180000
H	3.274588000	1.773809000	-0.478940000
C	0.828990000	3.343283000	-0.037164000
C	-2.785687000	-0.437937000	1.732596000
C	1.563038000	4.515282000	0.089796000
H	2.641058000	4.482684000	0.221450000
C	-1.256283000	4.601312000	-0.249812000
H	-2.334097000	4.635834000	-0.382226000
C	-0.586197000	3.385520000	-0.202902000
C	-3.290206000	-1.074265000	-1.316099000
C	-0.507318000	5.774342000	-0.123530000
H	-1.014383000	6.734369000	-0.157865000
C	-2.415533000	-1.835037000	2.244075000

H	-1.333364000	-1.997364000	2.210358000
H	-2.737763000	-1.929945000	3.288524000
H	-2.886669000	-2.640798000	1.676937000
C	-4.287049000	-0.199237000	1.891572000
H	-4.880444000	-0.985288000	1.416362000
H	-4.539814000	-0.202346000	2.959244000
H	-4.603537000	0.767359000	1.484888000
C	-2.008481000	0.591324000	2.566259000
H	-0.926650000	0.467948000	2.445592000
H	-2.261094000	1.625468000	2.312413000
H	-2.250147000	0.443085000	3.625806000
C	-2.473209000	-1.024355000	-2.616303000
H	-1.549739000	-1.602009000	-2.511999000
H	-3.063941000	-1.460411000	-3.431478000
H	-2.217431000	0.001328000	-2.907489000
C	-4.623045000	-0.344653000	-1.518458000
H	-5.180027000	-0.859587000	-2.311048000
H	-5.250362000	-0.351686000	-0.624531000
H	-4.498859000	0.692859000	-1.841768000
C	-3.566823000	-2.535169000	-0.957128000
H	-4.116490000	-2.999746000	-1.785326000
H	-2.641190000	-3.098868000	-0.824794000
H	-4.188940000	-2.629891000	-0.062417000
C	3.104539000	-2.677833000	1.414938000
H	3.421239000	-3.095699000	2.378364000
H	2.148269000	-3.142661000	1.158447000
H	3.849041000	-2.975256000	0.671327000
C	2.049703000	-0.824244000	2.703672000
H	1.894197000	0.254019000	2.824507000
H	1.071307000	-1.293825000	2.553830000
H	2.470419000	-1.205545000	3.642156000
C	4.389261000	-0.578643000	1.843317000
H	4.769087000	-1.034997000	2.765873000
H	5.112131000	-0.793475000	1.053485000
H	4.373407000	0.502775000	2.006395000
C	2.672492000	-2.296342000	-1.977469000

H	1.594175000	-2.486548000	-1.961468000
H	3.041818000	-2.491682000	-2.992053000
H	3.148912000	-3.021152000	-1.313017000
C	2.357705000	0.073735000	-2.646649000
H	2.762095000	-0.172968000	-3.635709000
H	1.271857000	-0.067766000	-2.680087000
H	2.554417000	1.135027000	-2.464482000
C	4.522176000	-0.646733000	-1.595181000
H	5.025747000	-1.383392000	-0.962887000
H	4.904503000	-0.781262000	-2.614611000
H	4.819521000	0.354011000	-1.264595000
H	0.042818000	-2.313164000	0.449801000
O	-0.387946000	-3.267627000	-1.262409000
N	-0.199495000	-3.450145000	-0.015481000
N	-0.197620000	-4.339896000	0.749042000

TS-NiOH-5

Ni	0.055842000	-0.737468000	0.009799000
B	0.008923000	1.147080000	-0.278549000
P	-2.155981000	-0.283358000	0.265406000
P	2.229028000	-0.216899000	0.296595000
N	-1.143082000	1.953586000	-0.579353000
N	1.090863000	2.083434000	-0.153622000
C	-2.485279000	0.047225000	2.106634000
C	-3.532462000	-1.350924000	-0.479775000
C	2.363002000	1.654727000	0.353413000
H	2.513107000	1.994980000	1.385573000
H	3.209029000	2.018700000	-0.241326000
C	-0.878280000	5.673357000	-0.753353000
H	-1.447904000	6.583830000	-0.916362000
C	-2.458966000	1.379979000	-0.541374000
H	-2.887528000	1.242481000	-1.541272000
H	-3.157818000	1.991069000	0.044218000
C	-0.779790000	3.288763000	-0.604342000
C	3.347247000	-0.668404000	-1.158203000
C	-1.529558000	4.438140000	-0.817256000
H	-2.593482000	4.375108000	-1.028500000

C	1.252764000	4.602873000	-0.271480000
H	2.316171000	4.667637000	-0.058171000
C	0.614946000	3.370934000	-0.331819000
C	2.969040000	-0.742871000	1.955434000
C	0.489124000	5.754158000	-0.485927000
H	0.970509000	6.726946000	-0.441722000
C	3.207593000	-2.161888000	-1.470423000
H	2.168409000	-2.423184000	-1.672773000
H	3.795423000	-2.390382000	-2.368534000
H	3.580649000	-2.797286000	-0.664807000
C	4.823119000	-0.328458000	-0.946752000
H	5.293643000	-0.985950000	-0.210585000
H	5.356189000	-0.472382000	-1.895038000
H	4.985029000	0.710424000	-0.640153000
C	2.806178000	0.134108000	-2.350479000
H	1.733658000	-0.024128000	-2.486318000
H	2.984361000	1.209328000	-2.251354000
H	3.315869000	-0.199898000	-3.262466000
C	1.872471000	-0.453837000	2.987722000
H	0.971327000	-1.034010000	2.776103000
H	2.232005000	-0.731119000	3.986599000
H	1.601820000	0.607335000	3.019850000
C	4.235451000	0.021395000	2.354990000
H	4.543497000	-0.316541000	3.352563000
H	5.072979000	-0.159577000	1.679913000
H	4.076333000	1.101766000	2.420910000
C	3.260385000	-2.245716000	1.954500000
H	3.502195000	-2.560292000	2.977425000
H	2.394731000	-2.824409000	1.621647000
H	4.120925000	-2.494624000	1.327306000
C	-3.675243000	-2.655189000	0.308016000
H	-4.315822000	-3.345725000	-0.254055000
H	-2.710695000	-3.149678000	0.459775000
H	-4.142825000	-2.498898000	1.283927000
C	-3.096130000	-1.689325000	-1.909621000
H	-2.884361000	-0.795123000	-2.505655000

H	-2.207760000	-2.319337000	-1.918032000
H	-3.907338000	-2.232328000	-2.409631000
C	-4.887081000	-0.635749000	-0.559805000
H	-5.605781000	-1.312797000	-1.038842000
H	-5.296175000	-0.366984000	0.413901000
H	-4.845289000	0.268289000	-1.175399000
C	-2.047119000	-1.184139000	2.909333000
H	-1.060312000	-1.540769000	2.606646000
H	-2.013066000	-0.924518000	3.974710000
H	-2.741640000	-2.020304000	2.799459000
C	-1.600877000	1.234347000	2.513278000
H	-1.704318000	1.394492000	3.593456000
H	-0.546043000	1.044276000	2.299227000
H	-1.887720000	2.164876000	2.013953000
C	-3.934586000	0.388594000	2.452479000
H	-4.603276000	-0.465575000	2.321366000
H	-3.985235000	0.676733000	3.510051000
H	-4.321455000	1.230733000	1.869160000
H	-0.105283000	-3.026102000	-1.570608000
O	0.127089000	-2.607266000	0.894969000
N	-0.029063000	-3.726898000	0.308537000
N	-0.143157000	-3.975854000	-0.865333000
O	0.058373000	-1.862022000	-2.019429000
N	-0.199742000	-1.259969000	-3.365595000
N	-0.714392000	-1.596844000	-4.315096000

TS-NiBcat-1

Ni	-0.162783000	0.006647000	0.198135000
B	1.801385000	-0.067443000	0.709393000
P	0.315414000	2.132207000	-0.083468000
P	0.135551000	-2.164257000	0.140355000
N	2.717469000	1.012217000	0.336893000
N	2.584932000	-1.283456000	0.506600000
C	-0.356092000	3.365084000	1.187790000
C	-0.009909000	2.742271000	-1.858812000
C	1.918694000	-2.544981000	0.653772000
H	1.938055000	-2.884277000	1.696103000

H	2.366450000	-3.332913000	0.039304000
C	5.984901000	0.227469000	-1.297021000
H	6.848144000	0.679257000	-1.776928000
C	2.199432000	2.324747000	0.025791000
H	2.586434000	2.655605000	-0.941942000
H	2.490184000	3.077325000	0.767476000
C	3.865243000	0.449632000	-0.204850000
C	0.131460000	-2.820363000	-1.636034000
C	4.960079000	1.046948000	-0.813858000
H	5.019231000	2.128172000	-0.903287000
C	4.820035000	-1.774293000	-0.548049000
H	4.772602000	-2.854418000	-0.441776000
C	3.787662000	-0.969584000	-0.073501000
C	-0.901721000	-3.230656000	1.301491000
C	5.914548000	-1.159878000	-1.162029000
H	6.725908000	-1.776670000	-1.538536000
C	-1.158081000	-2.409905000	-2.350340000
H	-1.282449000	-1.326271000	-2.366621000
H	-1.118578000	-2.768990000	-3.386784000
H	-2.052095000	-2.834230000	-1.887973000
C	0.300635000	-4.337985000	-1.730521000
H	-0.581889000	-4.875488000	-1.372174000
H	0.440124000	-4.612800000	-2.783804000
H	1.175342000	-4.705346000	-1.184121000
C	1.308512000	-2.136681000	-2.348172000
H	1.284270000	-1.051611000	-2.215447000
H	2.282941000	-2.494057000	-2.003971000
H	1.244740000	-2.348320000	-3.422628000
C	-0.988434000	-2.402225000	2.591347000
H	-1.492978000	-1.448166000	2.410067000
H	-1.561935000	-2.958509000	3.343815000
H	-0.000267000	-2.188485000	3.012160000
C	-0.286722000	-4.597496000	1.620174000
H	-0.944009000	-5.120743000	2.326258000
H	-0.185716000	-5.234102000	0.739006000
H	0.693307000	-4.518181000	2.099337000

C	-2.312675000	-3.430793000	0.743708000
H	-2.941348000	-3.885394000	1.519492000
H	-2.781294000	-2.485061000	0.460119000
H	-2.325244000	-4.100523000	-0.120837000
C	-1.491914000	3.066178000	-2.059001000
H	-1.680856000	3.201195000	-3.131550000
H	-2.141109000	2.260060000	-1.712134000
H	-1.778642000	3.997601000	-1.562060000
C	0.362285000	1.548602000	-2.746273000
H	1.413754000	1.262532000	-2.629128000
H	-0.260607000	0.679477000	-2.512845000
H	0.206001000	1.810380000	-3.800526000
C	0.815729000	3.955476000	-2.304192000
H	0.511120000	4.218582000	-3.324981000
H	0.657524000	4.837411000	-1.681592000
H	1.889518000	3.753189000	-2.344840000
C	-1.875222000	3.204144000	1.311200000
H	-2.140927000	2.192031000	1.624994000
H	-2.241774000	3.903098000	2.073758000
H	-2.409764000	3.421893000	0.384661000
C	0.249276000	2.989310000	2.545480000
H	-0.182189000	3.641210000	3.315028000
H	0.016701000	1.955184000	2.812684000
H	1.334221000	3.125481000	2.580045000
C	-0.006876000	4.818480000	0.866480000
H	-0.540325000	5.183903000	-0.014784000
H	-0.303790000	5.453403000	1.710817000
H	1.067050000	4.967464000	0.710417000
C	-4.288153000	0.027941000	0.510272000
C	-4.220935000	0.074483000	-0.880906000
C	-5.496444000	0.007149000	1.181157000
C	-5.357489000	0.104569000	-1.666319000
C	-6.655429000	0.036654000	0.395600000
H	-5.537693000	-0.030537000	2.265170000
C	-6.587718000	0.084449000	-0.997376000
H	-5.292434000	0.140861000	-2.749211000

H	-7.626029000	0.021590000	0.883006000
H	-7.506315000	0.106038000	-1.576639000
B	-2.119630000	0.036773000	-0.086649000
O	-2.912559000	0.083672000	-1.264119000
O	-3.023611000	0.002546000	1.016405000
O	1.463153000	0.018240000	2.454902000
N	2.412874000	0.605255000	3.072316000
N	3.337209000	1.269126000	2.926913000

TS-NiBcat-2

Ni	-0.077511000	0.033448000	0.336830000
B	1.888117000	0.017023000	0.935494000
P	0.324467000	2.219074000	0.064979000
P	0.301368000	-2.148780000	0.116405000
N	2.710989000	1.122818000	0.491038000
N	2.678112000	-1.161030000	0.631889000
C	-0.554830000	3.499531000	1.151387000
C	0.212843000	2.738062000	-1.771309000
C	2.057742000	-2.453208000	0.738961000
H	2.034939000	-2.792463000	1.782532000
H	2.575638000	-3.216291000	0.150518000
C	6.068997000	0.527797000	-1.018674000
H	6.931857000	1.024805000	-1.452637000
C	2.174786000	2.454567000	0.392744000
H	2.644602000	3.003304000	-0.425955000
H	2.342557000	3.030527000	1.309850000
C	3.904674000	0.640375000	0.001203000
C	0.476873000	-2.694141000	-1.695885000
C	4.996749000	1.295285000	-0.560034000
H	5.015161000	2.379273000	-0.630722000
C	4.963306000	-1.538309000	-0.363987000
H	4.955291000	-2.621871000	-0.285688000
C	3.885710000	-0.786914000	0.096891000
C	-0.756723000	-3.371819000	1.095365000
C	6.052856000	-0.866204000	-0.920284000
H	6.903761000	-1.438551000	-1.278608000
C	-0.755945000	-2.274944000	-2.499157000

H	-0.898061000	-1.194284000	-2.494737000
H	-0.624659000	-2.598485000	-3.539631000
H	-1.679277000	-2.725544000	-2.128043000
C	0.692151000	-4.199992000	-1.859142000
H	-0.203160000	-4.775925000	-1.612850000
H	0.932158000	-4.406366000	-2.909813000
H	1.525368000	-4.579072000	-1.258670000
C	1.700919000	-1.965470000	-2.267901000
H	1.685019000	-0.897172000	-2.046997000
H	2.645292000	-2.367858000	-1.892093000
H	1.706949000	-2.086445000	-3.358079000
C	-0.981859000	-2.688311000	2.448051000
H	-1.488888000	-1.727845000	2.330888000
H	-1.601570000	-3.334351000	3.082748000
H	-0.039518000	-2.514146000	2.978787000
C	-0.089590000	-4.730854000	1.334202000
H	-0.736588000	-5.322036000	1.994528000
H	0.050969000	-5.308691000	0.419507000
H	0.878600000	-4.641260000	1.835840000
C	-2.115149000	-3.576360000	0.421421000
H	-2.764052000	-4.146590000	1.097765000
H	-2.616457000	-2.626697000	0.216863000
H	-2.040478000	-4.141555000	-0.511286000
C	-1.240707000	2.985277000	-2.180542000
H	-1.282270000	3.095135000	-3.271669000
H	-1.889243000	2.149891000	-1.913302000
H	-1.645716000	3.903915000	-1.748135000
C	0.743154000	1.528046000	-2.544660000
H	1.781818000	1.299778000	-2.280868000
H	0.132233000	0.643940000	-2.343840000
H	0.710887000	1.732473000	-3.622446000
C	1.053564000	3.957028000	-2.172630000
H	0.845599000	4.178017000	-3.226941000
H	0.825249000	4.858184000	-1.602873000
H	2.128904000	3.769548000	-2.105760000
C	-2.050702000	3.161696000	1.162461000

H	-2.225465000	2.162502000	1.571116000
H	-2.574750000	3.885249000	1.799567000
H	-2.507748000	3.206394000	0.170972000
C	-0.042676000	3.366929000	2.590082000
H	-0.614070000	4.056908000	3.223398000
H	-0.202599000	2.362671000	2.981181000
H	1.012172000	3.634592000	2.698153000
C	-0.335936000	4.944574000	0.699717000
H	-0.793747000	5.159798000	-0.268371000
H	-0.800570000	5.615937000	1.432787000
H	0.726885000	5.205005000	0.650181000
C	-4.167976000	-0.140523000	0.212207000
C	-3.994087000	-0.014757000	-1.164543000
C	-5.423294000	-0.243669000	0.781311000
C	-5.064332000	0.017326000	-2.037666000
C	-6.516378000	-0.213205000	-0.093356000
H	-5.547747000	-0.342157000	1.854977000
C	-6.341310000	-0.085396000	-1.472067000
H	-4.915385000	0.116473000	-3.108259000
H	-7.521080000	-0.290653000	0.312089000
H	-7.211606000	-0.064984000	-2.121666000
B	-1.968901000	-0.010374000	-0.204148000
O	-2.659649000	0.065013000	-1.438499000
O	-2.947259000	-0.145650000	0.817506000
O	-0.520807000	0.230528000	3.328008000
N	0.690327000	0.120307000	3.395305000
N	1.681177000	0.036355000	2.775460000

TS-NiBcat-3

Ni	0.099792000	0.058413000	-0.470332000
B	-1.935333000	0.076446000	-0.941696000
P	-0.252710000	2.227340000	0.021830000
P	-0.276416000	-2.128434000	-0.134374000
N	-2.697641000	1.153630000	-0.373903000
N	-2.675759000	-1.134125000	-0.714606000
C	0.379704000	3.484951000	-1.250946000
C	0.180017000	2.805491000	1.785249000

C	-2.019101000	-2.411345000	-0.803927000
H	-1.957039000	-2.751484000	-1.844573000
H	-2.546961000	-3.181401000	-0.233429000
C	-5.987929000	0.409738000	1.232862000
H	-6.826646000	0.868959000	1.748063000
C	-2.131329000	2.416430000	0.026063000
H	-2.457113000	2.650102000	1.044232000
H	-2.445124000	3.249926000	-0.614219000
C	-3.875386000	0.610228000	0.122686000
C	-0.481857000	-2.635172000	1.682714000
C	-4.932439000	1.213727000	0.790267000
H	-4.941013000	2.287516000	0.955151000
C	-4.918707000	-1.587330000	0.348424000
H	-4.917141000	-2.660262000	0.177838000
C	-3.864349000	-0.798363000	-0.094857000
C	0.773886000	-3.383502000	-1.083193000
C	-5.981064000	-0.967214000	1.013414000
H	-6.815337000	-1.570940000	1.359097000
C	0.767031000	-2.279635000	2.491633000
H	0.976157000	-1.211454000	2.469553000
H	0.599254000	-2.570575000	3.536340000
H	1.664187000	-2.797357000	2.146544000
C	-0.788751000	-4.121375000	1.875651000
H	0.076432000	-4.752637000	1.656442000
H	-1.054193000	-4.289582000	2.926936000
H	-1.634256000	-4.467513000	1.273001000
C	-1.655682000	-1.809886000	2.226233000
H	-1.555207000	-0.750492000	1.974940000
H	-2.623137000	-2.154949000	1.852911000
H	-1.676936000	-1.898895000	3.319173000
C	1.033466000	-2.747080000	-2.454319000
H	1.571351000	-1.801080000	-2.365415000
H	1.635087000	-3.438986000	-3.057303000
H	0.108012000	-2.548378000	-3.003901000
C	0.084036000	-4.736579000	-1.293320000
H	0.735054000	-5.363639000	-1.915334000

H	-0.093707000	-5.278857000	-0.363468000
H	-0.867965000	-4.644420000	-1.824348000
C	2.117249000	-3.599996000	-0.382990000
H	2.770209000	-4.186661000	-1.040813000
H	2.633377000	-2.658086000	-0.174835000
H	2.013887000	-4.154747000	0.553194000
C	1.679569000	3.085002000	1.919184000
H	1.915168000	3.231498000	2.980752000
H	2.290990000	2.253575000	1.565484000
H	1.980621000	3.995244000	1.394107000
C	-0.189297000	1.621538000	2.684006000
H	-1.258977000	1.389162000	2.637042000
H	0.369877000	0.727813000	2.401086000
H	0.049012000	1.864664000	3.726964000
C	-0.591406000	4.037987000	2.275265000
H	-0.281669000	4.242923000	3.307638000
H	-0.387323000	4.936106000	1.692380000
H	-1.673901000	3.885507000	2.300759000
C	1.855179000	3.166566000	-1.521850000
H	1.973558000	2.137763000	-1.874084000
H	2.227902000	3.838723000	-2.304870000
H	2.490240000	3.303605000	-0.642771000
C	-0.383902000	3.294689000	-2.569054000
H	-0.053349000	4.071172000	-3.269788000
H	-0.158018000	2.329298000	-3.020916000
H	-1.468019000	3.397679000	-2.465680000
C	0.217514000	4.940816000	-0.809567000
H	0.836969000	5.193273000	0.053682000
H	0.532729000	5.593645000	-1.632911000
H	-0.823663000	5.191436000	-0.578700000
C	4.124387000	-0.164476000	-0.351928000
C	3.936664000	-0.121561000	1.027716000
C	5.383586000	-0.255840000	-0.913540000
C	4.994671000	-0.163703000	1.914413000
C	6.465018000	-0.300850000	-0.025577000
H	5.519325000	-0.290512000	-1.989608000

C	6.275569000	-0.255776000	1.356634000
H	4.833728000	-0.128734000	2.987090000
H	7.473011000	-0.372751000	-0.423447000
H	7.138248000	-0.292778000	2.015367000
B	1.936332000	-0.027737000	0.049109000
O	2.597888000	-0.034124000	1.292144000
O	2.909518000	-0.109548000	-0.970953000
O	0.106758000	0.162403000	-2.724484000
N	-1.151782000	0.197539000	-2.558637000
N	-2.113586000	0.294404000	-3.234670000

TS-NiBcat-4

Ni	0.022452000	0.039608000	0.480458000
B	-1.920295000	-0.147064000	0.192084000
P	-0.186231000	-2.172541000	-0.067824000
P	-0.690999000	2.157067000	0.079266000
N	-2.649585000	-1.305337000	-0.216648000
N	-2.913381000	0.865312000	0.395947000
C	-0.111409000	-3.343072000	1.422229000
C	0.839574000	-2.851736000	-1.526783000
C	-2.500262000	2.225806000	0.578693000
H	-2.591989000	2.556574000	1.619793000
H	-3.069613000	2.919924000	-0.051922000
C	-6.355018000	-1.174442000	-0.653230000
H	-7.223600000	-1.758019000	-0.944701000
C	-1.948628000	-2.466033000	-0.673704000
H	-1.975012000	-2.534712000	-1.766346000
H	-2.362895000	-3.397931000	-0.273037000
C	-3.998394000	-1.004667000	-0.291399000
C	-0.763062000	2.453646000	-1.804795000
C	-5.092755000	-1.773228000	-0.667132000
H	-4.966321000	-2.809185000	-0.969050000
C	-5.423488000	0.940616000	0.108346000
H	-5.551048000	1.977174000	0.407780000
C	-4.163749000	0.354754000	0.097822000
C	-0.015833000	3.703490000	0.957837000
C	-6.517149000	0.159661000	-0.273486000

H	-7.510380000	0.599472000	-0.272413000
C	0.626013000	2.197061000	-2.396017000
H	0.966509000	1.183948000	-2.175542000
H	0.573711000	2.313780000	-3.485983000
H	1.384550000	2.884075000	-2.018289000
C	-1.236718000	3.855044000	-2.196079000
H	-0.534808000	4.636742000	-1.898685000
H	-1.324031000	3.899644000	-3.288864000
H	-2.223082000	4.092838000	-1.785445000
C	-1.733593000	1.442632000	-2.428772000
H	-1.451150000	0.412186000	-2.195418000
H	-2.768806000	1.592743000	-2.109141000
H	-1.703343000	1.562342000	-3.518849000
C	0.258252000	3.298018000	2.410539000
H	1.158917000	2.688619000	2.483982000
H	0.425342000	4.205588000	3.003824000
H	-0.574530000	2.753877000	2.869237000
C	-1.033556000	4.854455000	0.972740000
H	-0.562572000	5.715451000	1.463221000
H	-1.346574000	5.180613000	-0.019306000
H	-1.928173000	4.612708000	1.553861000
C	1.299102000	4.186532000	0.342248000
H	1.724946000	4.959720000	0.993912000
H	2.027120000	3.376299000	0.261423000
H	1.159898000	4.636892000	-0.644506000
C	2.190303000	-3.415563000	-1.077180000
H	2.809319000	-3.582323000	-1.967459000
H	2.724543000	-2.731358000	-0.419908000
H	2.081122000	-4.379448000	-0.573003000
C	1.079364000	-1.655901000	-2.454094000
H	0.143110000	-1.175771000	-2.761294000
H	1.706994000	-0.901540000	-1.971993000
H	1.593172000	-1.992942000	-3.362927000
C	0.108792000	-3.948040000	-2.317035000
H	0.814885000	-4.379877000	-3.036771000
H	-0.252698000	-4.764696000	-1.687106000

H	-0.733847000	-3.562885000	-2.897306000
C	1.238516000	-3.213804000	2.135288000
H	1.493339000	-2.175054000	2.342883000
H	1.180426000	-3.747080000	3.092397000
H	2.056500000	-3.654183000	1.563308000
C	-1.220698000	-2.880681000	2.379337000
H	-1.198602000	-3.518240000	3.271860000
H	-1.070445000	-1.846462000	2.698033000
H	-2.220063000	-2.965219000	1.941523000
C	-0.348191000	-4.810688000	1.056537000
H	0.442124000	-5.216418000	0.420571000
H	-0.356124000	-5.402341000	1.980445000
H	-1.310129000	-4.978998000	0.562491000
C	4.161154000	-0.425424000	-0.019572000
C	3.999135000	0.865494000	-0.517382000
C	5.354047000	-1.111822000	-0.148380000
C	5.019542000	1.532440000	-1.167809000
C	6.396922000	-0.445202000	-0.802818000
H	5.472364000	-2.116212000	0.245558000
C	6.233563000	0.848008000	-1.301894000
H	4.881076000	2.538488000	-1.550922000
H	7.353082000	-0.946505000	-0.922180000
H	7.064406000	1.336020000	-1.803175000
B	2.075033000	0.235929000	0.426410000
O	2.727268000	1.283452000	-0.262239000
O	2.991471000	-0.837213000	0.542635000
O	2.481246000	0.852851000	2.682710000
N	1.363081000	0.398335000	2.987679000
N	0.439594000	0.013638000	2.362925000

TS-NiBcat-5

Ni	0.024832000	0.013729000	0.335055000
B	-1.897471000	-0.084356000	0.058563000
P	-0.252510000	-2.177942000	-0.080230000
P	-0.563290000	2.167027000	0.062666000
N	-2.669791000	-1.219117000	-0.346799000
N	-2.858002000	0.968784000	0.221384000

C	-0.294855000	-3.246724000	1.480521000
C	0.782028000	-3.001560000	-1.452208000
C	-2.401124000	2.309458000	0.429705000
H	-2.554945000	2.648303000	1.460855000
H	-2.890510000	3.026843000	-0.241171000
C	-6.357354000	-0.951078000	-0.862342000
H	-7.242624000	-1.505537000	-1.160667000
C	-2.003043000	-2.421311000	-0.741916000
H	-1.989731000	-2.523287000	-1.832270000
H	-2.468819000	-3.323637000	-0.329712000
C	-4.002210000	-0.868089000	-0.457535000
C	-0.472774000	2.494492000	-1.814519000
C	-5.119295000	-1.599259000	-0.840843000
H	-5.028700000	-2.644938000	-1.121650000
C	-5.356447000	1.139087000	-0.120729000
H	-5.448167000	2.185375000	0.157546000
C	-4.120995000	0.504467000	-0.095892000
C	0.085674000	3.683856000	1.017553000
C	-6.473584000	0.394974000	-0.509980000
H	-7.448281000	0.873869000	-0.536345000
C	0.945575000	2.157659000	-2.285736000
H	1.204220000	1.124736000	-2.038237000
H	0.999306000	2.275334000	-3.375532000
H	1.705840000	2.799291000	-1.837237000
C	-0.829044000	3.924229000	-2.226714000
H	-0.125904000	4.666005000	-1.842415000
H	-0.798165000	3.988604000	-3.321670000
H	-1.840694000	4.207962000	-1.918644000
C	-1.445301000	1.548522000	-2.532585000
H	-1.228026000	0.498953000	-2.314067000
H	-2.491470000	1.738603000	-2.275299000
H	-1.337804000	1.698563000	-3.614364000
C	0.238989000	3.231011000	2.474124000
H	1.121464000	2.602216000	2.590771000
H	0.375866000	4.112105000	3.113114000
H	-0.631212000	2.681404000	2.847638000

C	-0.896814000	4.864804000	0.985469000
H	-0.438168000	5.702843000	1.525330000
H	-1.123889000	5.216471000	-0.021742000
H	-1.839614000	4.642984000	1.493024000
C	1.452045000	4.153937000	0.513891000
H	1.839402000	4.909516000	1.209315000
H	2.169936000	3.332936000	0.470191000
H	1.395232000	4.623194000	-0.472197000
C	2.075608000	-3.624278000	-0.920158000
H	2.716723000	-3.874081000	-1.775173000
H	2.625689000	-2.941469000	-0.275247000
H	1.886765000	-4.555205000	-0.378107000
C	1.130499000	-1.869092000	-2.425187000
H	0.235920000	-1.355238000	-2.795903000
H	1.777831000	-1.126534000	-1.950312000
H	1.662069000	-2.278210000	-3.293581000
C	0.017143000	-4.095014000	-2.212479000
H	0.720048000	-4.600710000	-2.885787000
H	-0.405597000	-4.856861000	-1.551688000
H	-0.786622000	-3.698148000	-2.837989000
C	1.041358000	-3.138106000	2.221480000
H	1.369129000	-2.103053000	2.318575000
H	0.924746000	-3.555103000	3.229328000
H	1.839687000	-3.691857000	1.724358000
C	-1.396244000	-2.636356000	2.359043000
H	-1.417081000	-3.165284000	3.320015000
H	-1.202780000	-1.578416000	2.562461000
H	-2.390433000	-2.725108000	1.910755000
C	-0.611769000	-4.721284000	1.221852000
H	0.164996000	-5.221406000	0.637548000
H	-0.676087000	-5.240270000	2.186486000
H	-1.571623000	-4.867714000	0.717088000
C	4.154904000	-0.532013000	-0.131240000
C	4.034043000	0.840706000	-0.352072000
C	5.289455000	-1.232182000	-0.499310000
C	5.041177000	1.574141000	-0.952036000

C	6.317183000	-0.497432000	-1.102727000
H	5.374527000	-2.299913000	-0.324092000
C	6.195754000	0.875312000	-1.324539000
H	4.936273000	2.641186000	-1.121360000
H	7.227175000	-1.008461000	-1.403662000
H	7.012786000	1.414442000	-1.795249000
B	2.133136000	0.119880000	0.616433000
O	2.818955000	1.257097000	0.083567000
O	3.014627000	-0.994981000	0.439259000
N	1.271069000	0.253300000	3.261931000
N	2.086617000	0.344457000	2.435283000
O	0.106665000	0.078028000	3.553924000

*Cartesian coordinates of the calculations using hydridoborates **8** and **9***

Complex 8 (NiH_2Bcat)

Ni	0.024014000	-0.000043000	-0.000212000
B	-1.891364000	-0.000212000	-0.000014000
N	-2.775913000	1.124753000	-0.122846000
N	-2.775699000	-1.125273000	0.123529000
C	-4.092330000	0.705603000	-0.084542000
C	-5.285932000	1.409224000	-0.176344000
H	-5.286817000	2.486963000	-0.314368000
C	-6.482629000	0.691819000	-0.086322000
H	-7.427402000	1.223536000	-0.154953000
C	-6.482486000	-0.692708000	0.090188000
H	-7.427149000	-1.224515000	0.159640000
C	-5.285640000	-1.409993000	0.179170000
H	-5.286294000	-2.487731000	0.317205000
C	-4.092189000	-0.706253000	0.086323000
P	-0.414172000	-2.205575000	0.050291000
C	-2.250372000	-2.432844000	0.354990000
H	-2.676615000	-3.191265000	-0.313190000
H	-2.427910000	-2.758671000	1.385826000
C	0.308787000	-3.266481000	1.450364000
C	0.231453000	-2.376805000	2.698854000
H	-0.790654000	-2.036257000	2.903468000
H	0.866756000	-1.492375000	2.599178000

H	0.571093000	-2.948812000	3.571160000
C	-0.485854000	-4.554481000	1.714263000
H	0.014555000	-5.099132000	2.524396000
H	-0.518173000	-5.220486000	0.850130000
H	-1.511355000	-4.371855000	2.045708000
C	1.765184000	-3.648869000	1.187542000
H	2.383396000	-2.788064000	0.928575000
H	1.849202000	-4.388363000	0.385022000
H	2.174581000	-4.109102000	2.095716000
C	-0.177557000	-2.985359000	-1.658072000
C	-0.500481000	-4.479767000	-1.695813000
H	-1.499731000	-4.711905000	-1.313631000
H	0.231568000	-5.069258000	-1.137340000
H	-0.465719000	-4.822599000	-2.737282000
C	-1.124660000	-2.226152000	-2.598820000
H	-0.981388000	-2.600393000	-3.619942000
H	-0.907343000	-1.152673000	-2.596420000
H	-2.180872000	-2.357813000	-2.344136000
C	1.255719000	-2.763281000	-2.147888000
H	2.001848000	-3.247974000	-1.516630000
H	1.504649000	-1.700946000	-2.191890000
H	1.346588000	-3.177799000	-3.159847000
P	-0.414545000	2.205538000	-0.050092000
C	-2.250925000	2.432512000	-0.353979000
H	-2.677070000	3.190560000	0.314686000
H	-2.428912000	2.758749000	-1.384606000
C	-0.177295000	2.984857000	1.658349000
C	-1.123787000	2.225187000	2.599334000
H	-0.979971000	2.599021000	3.620527000
H	-0.906379000	1.151727000	2.596369000
H	-2.180154000	2.356871000	2.345305000
C	-0.500491000	4.479196000	1.696715000
H	-0.465260000	4.821718000	2.738270000
H	-1.499984000	4.711240000	1.315113000
H	0.231141000	5.069020000	1.138040000
C	1.256285000	2.762887000	2.147353000

H	2.002007000	3.247755000	1.515745000
H	1.505366000	1.700568000	2.191059000
H	1.347665000	3.177266000	3.159323000
C	0.307406000	3.267138000	-1.450184000
C	0.229797000	2.377795000	-2.698898000
H	-0.792281000	2.036913000	-2.903108000
H	0.865458000	1.493564000	-2.599776000
H	0.568803000	2.950170000	-3.571209000
C	-0.487876000	4.554903000	-1.713304000
H	0.011944000	5.099997000	-2.523502000
H	-0.520043000	5.220630000	-0.848948000
H	-1.513462000	4.371992000	-2.044326000
C	1.763762000	3.650104000	-1.187985000
H	2.172398000	4.111024000	-2.096153000
H	2.382560000	2.789483000	-0.929831000
H	1.847873000	4.389220000	-0.385125000
H	1.444546000	0.093048000	-1.030584000
B	2.209027000	0.000192000	-0.001299000
O	3.100806000	-1.162311000	-0.141655000
O	3.100679000	1.162796000	0.138967000
C	4.365952000	-0.695961000	-0.081941000
C	4.365877000	0.696511000	0.079877000
C	5.545516000	-1.411244000	-0.162754000
C	5.545362000	1.411863000	0.161228000
H	5.533883000	-2.489847000	-0.288024000
C	6.748493000	-0.690520000	-0.079643000
C	6.748418000	0.691208000	0.078670000
H	5.533611000	2.490466000	0.286482000
H	7.692203000	-1.225452000	-0.140870000
H	7.692070000	1.226192000	0.140337000
H	1.445064000	-0.092805000	1.028499000

Complex 8·N_2O

Ni	0.086100000	0.008123000	-0.149012000
B	-1.801238000	0.099846000	0.189893000
N	-2.671831000	1.218282000	-0.039556000
N	-2.684335000	-0.977918000	0.539191000

C	-3.989802000	0.831257000	0.123735000
C	-5.179196000	1.531607000	-0.025481000
H	-5.174478000	2.579085000	-0.314150000
C	-6.379519000	0.849638000	0.197138000
H	-7.320874000	1.380026000	0.084965000
C	-6.386498000	-0.498221000	0.558109000
H	-7.333321000	-1.003899000	0.725008000
C	-5.193736000	-1.211702000	0.711695000
H	-5.200029000	-2.260201000	0.996319000
C	-3.996362000	-0.543070000	0.492908000
P	-0.539448000	-2.138363000	-0.322664000
C	-2.177993000	-2.317683000	0.566071000
H	-2.840139000	-3.023556000	0.049276000
H	-2.019192000	-2.683371000	1.586952000
C	0.446789000	-3.588834000	0.407683000
C	0.967448000	-3.108370000	1.768894000
H	0.150370000	-2.803384000	2.430796000
H	1.673111000	-2.283357000	1.661728000
H	1.491885000	-3.938120000	2.259086000
C	-0.426590000	-4.830323000	0.643943000
H	0.208677000	-5.615570000	1.072498000
H	-0.864378000	-5.234088000	-0.270115000
H	-1.232742000	-4.651150000	1.360996000
C	1.631407000	-3.974384000	-0.481068000
H	2.264107000	-3.115523000	-0.711210000
H	1.309441000	-4.453312000	-1.409665000
H	2.250953000	-4.701041000	0.059814000
C	-0.973975000	-2.469532000	-2.141950000
C	-1.408157000	-3.906423000	-2.435600000
H	-2.259869000	-4.220593000	-1.823728000
H	-0.597507000	-4.626302000	-2.301014000
H	-1.725235000	-3.970921000	-3.483948000
C	-2.122635000	-1.528847000	-2.531203000
H	-2.324481000	-1.650608000	-3.602668000
H	-1.861778000	-0.480719000	-2.353804000
H	-3.051098000	-1.745555000	-1.994263000

C	0.242683000	-2.108563000	-3.001665000
H	1.113413000	-2.733167000	-2.791408000
H	0.533395000	-1.065379000	-2.849346000
H	-0.015957000	-2.240214000	-4.059697000
P	-0.298661000	2.203174000	-0.359982000
C	-2.141806000	2.417116000	-0.614736000
H	-2.515021000	3.331482000	-0.138487000
H	-2.370287000	2.480005000	-1.686088000
C	-0.016373000	3.201841000	1.228834000
C	-0.995021000	2.644369000	2.272132000
H	-0.768535000	3.100353000	3.243685000
H	-0.902877000	1.559662000	2.372523000
H	-2.040788000	2.865429000	2.039244000
C	-0.269482000	4.701115000	1.059900000
H	-0.208116000	5.178621000	2.045726000
H	-1.262018000	4.924210000	0.655668000
H	0.481666000	5.177238000	0.424498000
C	1.406182000	2.985891000	1.750609000
H	2.172786000	3.330077000	1.055617000
H	1.605766000	1.933009000	1.956928000
H	1.521695000	3.544348000	2.688048000
C	0.412259000	3.075415000	-1.885875000
C	0.334522000	2.039188000	-3.014002000
H	-0.684313000	1.664879000	-3.167802000
H	0.982114000	1.183347000	-2.805996000
H	0.663322000	2.500607000	-3.953403000
C	-0.385033000	4.317684000	-2.303576000
H	0.096457000	4.753328000	-3.188065000
H	-0.406358000	5.091533000	-1.534568000
H	-1.415822000	4.086722000	-2.586794000
C	1.875393000	3.464579000	-1.668395000
H	2.299526000	3.794011000	-2.625215000
H	2.473277000	2.629280000	-1.296458000
H	1.974457000	4.297404000	-0.966171000
H	1.513323000	-0.087856000	-0.991978000
B	2.231416000	-0.071082000	0.114641000

O	3.088302000	-1.262346000	0.145424000
O	3.147460000	1.075369000	0.084534000
C	4.365094000	-0.827622000	0.066158000
C	4.399737000	0.572760000	0.028006000
C	5.523756000	-1.579073000	0.025381000
C	5.595184000	1.261217000	-0.052788000
H	5.484443000	-2.663759000	0.057456000
C	6.742516000	-0.885929000	-0.056282000
C	6.777338000	0.504178000	-0.095125000
H	5.611003000	2.346642000	-0.080258000
H	7.671174000	-1.448843000	-0.090018000
H	7.733099000	1.016920000	-0.158728000
H	1.416043000	-0.033833000	1.089270000
O	-0.826284000	-0.733440000	3.560827000
N	0.307517000	-0.419811000	3.705401000
N	1.386513000	-0.121932000	3.840868000

TS 8-N_2O

Ni	0.084965000	0.004576000	0.011588000
B	-1.811772000	-0.089256000	-0.352736000
N	-2.685817000	-1.206612000	-0.149705000
N	-2.674671000	0.988803000	-0.737633000
C	-3.998039000	-0.815400000	-0.361069000
C	-5.192727000	-1.511378000	-0.244142000
H	-5.199767000	-2.556858000	0.051700000
C	-6.384011000	-0.828077000	-0.509482000
H	-7.329918000	-1.355191000	-0.423615000
C	-6.374755000	0.516623000	-0.880704000
H	-7.314021000	1.023663000	-1.082667000
C	-5.175620000	1.226266000	-1.000751000
H	-5.170070000	2.272402000	-1.293680000
C	-3.987783000	0.556379000	-0.738515000
P	-0.585634000	2.157833000	0.230375000
C	-2.159095000	2.324620000	-0.764348000
H	-2.849486000	3.047208000	-0.312421000
H	-1.920564000	2.658596000	-1.780282000
C	0.426634000	3.646108000	-0.383506000

C	1.077974000	3.224324000	-1.704948000
H	0.343314000	2.891265000	-2.442983000
H	1.809680000	2.429903000	-1.554240000
H	1.606194000	4.088625000	-2.126650000
C	-0.461685000	4.868036000	-0.660336000
H	0.183803000	5.687358000	-1.000828000
H	-1.000611000	5.225475000	0.218072000
H	-1.186156000	4.685922000	-1.459073000
C	1.530242000	4.036881000	0.602863000
H	2.165534000	3.187434000	0.861542000
H	1.134107000	4.487462000	1.516575000
H	2.170778000	4.788696000	0.124654000
C	-1.144410000	2.443807000	2.024371000
C	-1.637980000	3.861756000	2.318672000
H	-2.459004000	4.162955000	1.660287000
H	-0.844052000	4.608607000	2.249839000
H	-2.022107000	3.893776000	3.345879000
C	-2.290195000	1.469566000	2.329123000
H	-2.547412000	1.555505000	3.392170000
H	-1.999352000	0.432702000	2.134804000
H	-3.194496000	1.683223000	1.751962000
C	0.024949000	2.099294000	2.954024000
H	0.886145000	2.756965000	2.819816000
H	0.357947000	1.069704000	2.799142000
H	-0.306138000	2.192905000	3.995722000
P	-0.336647000	-2.198548000	0.330354000
C	-2.192744000	-2.384003000	0.496521000
H	-2.548723000	-3.314357000	0.039224000
H	-2.476955000	-2.402045000	1.556144000
C	0.036518000	-3.325403000	-1.146573000
C	-0.866407000	-2.848044000	-2.292567000
H	-0.582480000	-3.385393000	-3.205658000
H	-0.759660000	-1.777120000	-2.481805000
H	-1.925524000	-3.053119000	-2.108660000
C	-0.246136000	-4.804694000	-0.875938000
H	-0.125508000	-5.357131000	-1.815970000

H	-1.266967000	-4.987725000	-0.525759000
H	0.453218000	-5.237316000	-0.155920000
C	1.496897000	-3.166110000	-1.576298000
H	2.203435000	-3.469291000	-0.802188000
H	1.732318000	-2.138538000	-1.855379000
H	1.671180000	-3.797243000	-2.456670000
C	0.273516000	-2.962788000	1.960604000
C	0.157686000	-1.853530000	3.012301000
H	-0.852870000	-1.433359000	3.072160000
H	0.852870000	-1.037134000	2.801317000
H	0.404702000	-2.263260000	3.999484000
C	-0.572270000	-4.158855000	2.418200000
H	-0.133736000	-4.554073000	3.342985000
H	-0.587924000	-4.973966000	1.693507000
H	-1.605152000	-3.885855000	2.650688000
C	1.737183000	-3.398251000	1.862307000
H	2.094224000	-3.657963000	2.866829000
H	2.379953000	-2.608753000	1.467588000
H	1.858773000	-4.287462000	1.237229000
H	1.369672000	0.098843000	0.971470000
B	2.269961000	0.081290000	0.049764000
O	3.083064000	1.265066000	0.062418000
O	3.151378000	-1.049654000	0.124463000
C	4.368207000	0.840484000	-0.046073000
C	4.409402000	-0.555913000	-0.006321000
C	5.516938000	1.598444000	-0.164154000
C	5.601672000	-1.249540000	-0.081987000
H	5.471533000	2.682356000	-0.196037000
C	6.731327000	0.903421000	-0.243903000
C	6.772769000	-0.489220000	-0.203070000
H	5.621515000	-2.334272000	-0.051502000
H	7.656509000	1.464006000	-0.341466000
H	7.729868000	-0.998385000	-0.269585000
H	1.632556000	0.022318000	-1.226149000
O	-0.323925000	0.453577000	-2.600951000
N	0.814535000	0.312337000	-3.070124000

N	1.893176000	0.098280000	-2.631880000

TS 8-N_2O_fw

Ni	0.458150000	-0.372153000	-1.045605000
B	-1.485342000	-0.390946000	-0.982685000
N	-2.399742000	0.661110000	-1.301137000
N	-2.308967000	-1.499996000	-0.612665000
C	-3.700128000	0.204729000	-1.164869000
C	-4.919870000	0.825649000	-1.393937000
H	-4.963144000	1.856270000	-1.735199000
C	-6.086998000	0.086074000	-1.179120000
H	-7.052158000	0.553621000	-1.351816000
C	-6.030141000	-1.239788000	-0.747852000
H	-6.952141000	-1.791217000	-0.586924000
C	-4.805767000	-1.873194000	-0.514155000
H	-4.763479000	-2.903502000	-0.172347000
C	-3.641225000	-1.146622000	-0.724616000
P	-0.076821000	-2.584844000	-1.317725000
C	-1.721320000	-2.796618000	-0.457788000
H	-2.324715000	-3.586105000	-0.922083000
H	-1.557388000	-3.053975000	0.594440000
C	0.940183000	-3.995191000	-0.540864000
C	1.463432000	-3.466366000	0.798238000
H	0.662487000	-3.098921000	1.444728000
H	2.177935000	-2.654069000	0.663570000
H	1.975720000	-4.282210000	1.323479000
C	0.077723000	-5.235409000	-0.260944000
H	0.724491000	-6.006598000	0.176021000
H	-0.375661000	-5.663823000	-1.156263000
H	-0.713478000	-5.040701000	0.467950000
C	2.131769000	-4.409149000	-1.408428000
H	2.761835000	-3.559329000	-1.674256000
H	1.827433000	-4.928881000	-2.320666000
H	2.751194000	-5.107892000	-0.831856000
C	-0.452820000	-2.983141000	-3.137007000
C	-0.847118000	-4.437867000	-3.401305000
H	-1.714277000	-4.747447000	-2.809460000

H	-0.031132000	-5.139339000	-3.215098000
H	-1.126371000	-4.541529000	-4.457271000
C	-1.608770000	-2.087240000	-3.600211000
H	-1.757509000	-2.238028000	-4.676778000
H	-1.386815000	-1.028525000	-3.434818000
H	-2.553358000	-2.319704000	-3.099890000
C	0.781448000	-2.619019000	-3.970838000
H	1.665115000	-3.204279000	-3.707650000
H	1.027557000	-1.558993000	-3.860806000
H	0.565207000	-2.802076000	-5.030668000
P	-0.082465000	1.785133000	-1.536477000
C	-1.917039000	1.863672000	-1.904859000
H	-2.372301000	2.771215000	-1.492095000
H	-2.092554000	1.861565000	-2.987394000
C	0.076853000	2.955481000	-0.057417000
C	-0.922663000	2.455645000	0.996101000
H	-0.767977000	3.031130000	1.917160000
H	-0.768302000	1.397812000	1.226764000
H	-1.963983000	2.601942000	0.692076000
C	-0.229554000	4.418016000	-0.383303000
H	-0.223621000	4.988240000	0.553853000
H	-1.217504000	4.554940000	-0.835023000
H	0.520176000	4.868366000	-1.039195000
C	1.488876000	2.847379000	0.523882000
H	2.263280000	3.162171000	-0.178726000
H	1.714923000	1.830213000	0.846753000
H	1.555261000	3.494154000	1.407436000
C	0.641588000	2.557675000	-3.119829000
C	0.681047000	1.435665000	-4.164065000
H	-0.295615000	0.959471000	-4.306767000
H	1.397877000	0.657824000	-3.889053000
H	0.990402000	1.852136000	-5.130708000
C	-0.220379000	3.701547000	-3.673995000
H	0.284021000	4.113513000	-4.557007000
H	-0.351804000	4.520248000	-2.965449000
H	-1.208763000	3.370042000	-4.002847000

C	2.061941000	3.082557000	-2.900021000
H	2.484618000	3.369896000	-3.871027000
H	2.720586000	2.335463000	-2.455370000
H	2.076353000	3.972748000	-2.265361000
H	1.706823000	-0.374135000	-2.025941000
B	2.689276000	-0.357007000	-1.238689000
O	3.484001000	-1.496210000	-1.114072000
O	3.469957000	0.789409000	-1.081370000
C	4.723415000	-1.046885000	-0.747075000
C	4.714785000	0.344762000	-0.728148000
C	5.851320000	-1.779763000	-0.433894000
C	5.834710000	1.081211000	-0.394730000
H	5.842576000	-2.864444000	-0.445943000
C	6.992176000	-1.045806000	-0.096068000
C	6.983915000	0.351261000	-0.076995000
H	5.814031000	2.165587000	-0.376262000
H	7.903717000	-1.576092000	0.162447000
H	7.889289000	0.884751000	0.196172000
H	2.360007000	-0.309516000	0.762172000
O	0.207085000	-0.553643000	1.076088000
N	1.059966000	-0.492745000	2.048306000
N	2.273415000	-0.352380000	1.813333000

Complex 9·N_2O

Ni	0.061022000	-0.001170000	-0.152809000
B	-1.815995000	0.123215000	0.223033000
N	-2.676439000	1.250378000	-0.013088000
N	-2.711457000	-0.938372000	0.596819000
C	-3.997162000	0.882180000	0.166663000
C	-5.179404000	1.594560000	0.017653000
H	-5.163831000	2.638123000	-0.285270000
C	-6.386585000	0.930969000	0.259231000
H	-7.322038000	1.471942000	0.147457000
C	-6.407349000	-0.411757000	0.638232000
H	-7.358746000	-0.903381000	0.819486000
C	-5.221727000	-1.137858000	0.791544000
H	-5.238810000	-2.182859000	1.089457000

C	-4.017888000	-0.487605000	0.554854000
P	-0.594708000	-2.129812000	-0.296055000
C	-2.221361000	-2.284807000	0.621178000
H	-2.902027000	-2.984478000	0.120597000
H	-2.048826000	-2.647728000	1.641158000
C	0.390478000	-3.580587000	0.437724000
C	0.935357000	-3.086376000	1.784721000
H	0.131523000	-2.758733000	2.452288000
H	1.651977000	-2.274466000	1.649709000
H	1.453886000	-3.917009000	2.280918000
C	-0.484662000	-4.814950000	0.699673000
H	0.151283000	-5.595394000	1.137247000
H	-0.929344000	-5.232754000	-0.204653000
H	-1.286000000	-4.622250000	1.418696000
C	1.562637000	-3.975518000	-0.462253000
H	2.196102000	-3.114451000	-0.685688000
H	1.229991000	-4.448167000	-1.390507000
H	2.181423000	-4.708654000	0.071510000
C	-1.064901000	-2.486572000	-2.103117000
C	-1.508613000	-3.925642000	-2.369392000
H	-2.348289000	-4.229568000	-1.736207000
H	-0.696377000	-4.644606000	-2.240214000
H	-1.846693000	-4.004380000	-3.410371000
C	-2.217101000	-1.545851000	-2.482083000
H	-2.439331000	-1.677340000	-3.548319000
H	-1.948516000	-0.497229000	-2.319134000
H	-3.136521000	-1.752873000	-1.925956000
C	0.135410000	-2.140929000	-2.991298000
H	1.011561000	-2.758264000	-2.782526000
H	0.425615000	-1.094814000	-2.861940000
H	-0.141255000	-2.294135000	-4.042042000
P	-0.292829000	2.187314000	-0.401108000
C	-2.138163000	2.427876000	-0.624594000
H	-2.488450000	3.359078000	-0.163543000
H	-2.385319000	2.470544000	-1.693008000
C	0.032774000	3.213331000	1.164507000

C	-0.931521000	2.689653000	2.237784000
H	-0.679255000	3.160814000	3.196120000
H	-0.851321000	1.605832000	2.356275000
H	-1.978871000	2.921157000	2.022367000
C	-0.203141000	4.712583000	0.974009000
H	-0.112780000	5.207730000	1.948786000
H	-1.201547000	4.941928000	0.588477000
H	0.539034000	5.165908000	0.312198000
C	1.462406000	2.985922000	1.662031000
H	2.217351000	3.313627000	0.946825000
H	1.652490000	1.931329000	1.867648000
H	1.601897000	3.551040000	2.592725000
C	0.401583000	3.033678000	-1.951123000
C	0.305805000	1.979771000	-3.061127000
H	-0.715423000	1.603773000	-3.193302000
H	0.953710000	1.126548000	-2.844009000
H	0.622077000	2.424831000	-4.012894000
C	-0.395049000	4.272821000	-2.378908000
H	0.080963000	4.696319000	-3.272351000
H	-0.408223000	5.055739000	-1.618681000
H	-1.428672000	4.041386000	-2.651067000
C	1.870463000	3.415836000	-1.758750000
H	2.288124000	3.713095000	-2.729502000
H	2.461158000	2.584355000	-1.364018000
H	1.983026000	4.270277000	-1.084538000
H	1.430574000	-0.144604000	-1.040756000
B	2.201799000	-0.099292000	0.057810000
O	3.022540000	-1.277419000	0.164194000
O	3.091485000	1.025618000	-0.074639000
C	4.344814000	-0.914614000	-0.217368000
C	4.405634000	0.576687000	0.230319000
H	1.366538000	-0.031042000	1.044671000
O	-0.757149000	-0.666462000	3.583655000
N	0.384194000	-0.372422000	3.702462000
N	1.470594000	-0.092535000	3.815542000
C	5.327149000	-1.836925000	0.483785000

H	5.221894000	-2.856722000	0.099683000
H	6.360519000	-1.516293000	0.312201000
H	5.140651000	-1.864164000	1.559745000
C	4.466583000	-1.063924000	-1.734336000
H	5.484820000	-0.873800000	-2.089906000
H	4.194269000	-2.086346000	-2.015119000
H	3.783763000	-0.378305000	-2.245475000
C	4.626429000	0.716005000	1.736906000
H	5.649558000	0.458971000	2.031123000
H	4.437158000	1.753938000	2.028184000
H	3.930933000	0.078121000	2.290500000
C	5.406387000	1.434051000	-0.526665000
H	5.370352000	2.462492000	-0.152101000
H	6.428164000	1.062035000	-0.392420000
H	5.180569000	1.459197000	-1.595246000

TS 9-N_2O

Ni	0.064314000	0.011610000	-0.023314000
B	-1.836978000	-0.118030000	-0.349069000
N	-2.683141000	-1.250503000	-0.099553000
N	-2.740657000	0.945807000	-0.685414000
C	-4.010671000	-0.880619000	-0.241655000
C	-5.185935000	-1.595591000	-0.061379000
H	-5.160123000	-2.641011000	0.233870000
C	-6.401571000	-0.932729000	-0.263047000
H	-7.332496000	-1.475889000	-0.127264000
C	-6.434511000	0.411188000	-0.634505000
H	-7.391447000	0.902430000	-0.786871000
C	-5.254937000	1.140740000	-0.817359000
H	-5.282264000	2.186835000	-1.109472000
C	-4.043459000	0.491560000	-0.618515000
P	-0.627746000	2.146276000	0.184991000
C	-2.248571000	2.289841000	-0.735890000
H	-2.928771000	3.001812000	-0.252431000
H	-2.062756000	2.625925000	-1.762240000
C	0.343113000	3.637037000	-0.486206000
C	0.937341000	3.209683000	-1.832910000

H	0.171697000	2.861994000	-2.531662000
H	1.686397000	2.426742000	-1.706428000
H	1.433258000	4.077384000	-2.286531000
C	-0.562912000	4.852913000	-0.729443000
H	0.060388000	5.669922000	-1.114254000
H	-1.055239000	5.220398000	0.171929000
H	-1.329104000	4.658667000	-1.485460000
C	1.490549000	4.033251000	0.445911000
H	2.139286000	3.180897000	0.660297000
H	1.137807000	4.476437000	1.380898000
H	2.102430000	4.790990000	-0.060205000
C	-1.109402000	2.448908000	1.999440000
C	-1.594179000	3.868015000	2.302388000
H	-2.440096000	4.163556000	1.673543000
H	-0.804591000	4.615785000	2.198494000
H	-1.939539000	3.907125000	3.343184000
C	-2.239047000	1.474080000	2.358595000
H	-2.451145000	1.564441000	3.431308000
H	-1.954619000	0.437025000	2.155827000
H	-3.167403000	1.683284000	1.819084000
C	0.097343000	2.115088000	2.883864000
H	0.953849000	2.767122000	2.701568000
H	0.421005000	1.082979000	2.728034000
H	-0.188922000	2.225647000	3.937295000
P	-0.297423000	-2.187307000	0.331556000
C	-2.144931000	-2.405791000	0.551443000
H	-2.494546000	-3.352089000	0.122496000
H	-2.399108000	-2.410115000	1.619161000
C	0.047835000	-3.324041000	-1.146700000
C	-0.894540000	-2.869655000	-2.270219000
H	-0.622542000	-3.401655000	-3.190115000
H	-0.821847000	-1.796822000	-2.463538000
H	-1.943429000	-3.098638000	-2.057659000
C	-0.210291000	-4.804583000	-0.857305000
H	-0.109148000	-5.363677000	-1.795877000
H	-1.219478000	-4.996193000	-0.478804000

H	0.512090000	-5.224636000	-0.152763000
C	1.493109000	-3.151966000	-1.620132000
H	2.222700000	-3.448165000	-0.865229000
H	1.708972000	-2.121045000	-1.900286000
H	1.646206000	-3.781229000	-2.506154000
C	0.375424000	-2.936221000	1.945475000
C	0.302412000	-1.815269000	2.988405000
H	-0.703732000	-1.390304000	3.080699000
H	0.992213000	-1.005003000	2.738979000
H	0.584944000	-2.214617000	3.970635000
C	-0.451209000	-4.127093000	2.448079000
H	0.028002000	-4.519259000	3.353842000
H	-0.501406000	-4.944970000	1.727867000
H	-1.472004000	-3.850217000	2.725352000
C	1.835827000	-3.368944000	1.795886000
H	2.234778000	-3.604774000	2.790932000
H	2.452321000	-2.582417000	1.354392000
H	1.934980000	-4.272912000	1.188001000
H	1.355177000	0.180075000	0.873421000
B	2.246841000	0.119500000	-0.089662000
O	3.025288000	1.289141000	-0.203549000
O	3.093122000	-0.993371000	0.067530000
C	4.374411000	0.947998000	0.139556000
C	4.434231000	-0.571510000	-0.214583000
H	1.456243000	0.010750000	-1.319630000
O	-0.587559000	0.480568000	-2.750581000
N	0.551583000	0.309355000	-3.193181000
N	1.630167000	0.078964000	-2.770670000
C	5.318248000	1.829598000	-0.657390000
H	5.204897000	2.871966000	-0.343085000
H	6.360741000	1.537253000	-0.492637000
H	5.101606000	1.775966000	-1.726235000
C	4.539520000	1.207778000	1.635825000
H	5.566971000	1.038825000	1.973024000
H	4.278708000	2.249566000	1.845787000
H	3.870508000	0.567137000	2.219557000

C	4.715922000	-0.824001000	-1.692744000
H	5.756713000	-0.598982000	-1.946544000
H	4.530897000	-1.879959000	-1.911939000
H	4.057315000	-0.229843000	-2.329952000
C	5.383127000	-1.390349000	0.643911000
H	5.345046000	-2.439726000	0.334935000
H	6.414833000	-1.042089000	0.527402000
H	5.114255000	-1.341626000	1.701431000

TS 9-N_2O_fw

Ni	-0.000465000	0.030787000	-0.104487000
B	1.907239000	0.058320000	-0.298475000
N	2.813113000	1.139361000	-0.058864000
N	2.733192000	-1.040662000	-0.696250000
C	4.113079000	0.709050000	-0.263961000
C	5.329556000	1.361590000	-0.122211000
H	5.368698000	2.400421000	0.193874000
C	6.499551000	0.643838000	-0.390775000
H	7.461799000	1.136948000	-0.285991000
C	6.448782000	-0.692107000	-0.789657000
H	7.372374000	-1.226420000	-0.993719000
C	5.227672000	-1.357785000	-0.936246000
H	5.189643000	-2.396236000	-1.253097000
C	4.060305000	-0.653841000	-0.671723000
P	0.583096000	-2.160673000	0.192296000
C	2.166038000	-2.354253000	-0.782905000
H	2.822084000	-3.120406000	-0.351899000
H	1.929731000	-2.634294000	-1.815327000
C	-0.468114000	-3.600575000	-0.473668000
C	-1.115736000	-3.086597000	-1.762261000
H	-0.379282000	-2.744247000	-2.492989000
H	-1.791457000	-2.253904000	-1.563900000
H	-1.698216000	-3.898283000	-2.216715000
C	0.383270000	-4.831939000	-0.814000000
H	-0.284662000	-5.613928000	-1.197031000
H	0.908680000	-5.248922000	0.047183000
H	1.115386000	-4.631622000	-1.600938000

C	-1.577526000	-4.014855000	0.496700000
H	-2.200411000	-3.168315000	0.790828000
H	-1.191972000	-4.508342000	1.392651000
H	-2.227287000	-4.738210000	-0.012946000
C	1.105599000	-2.519104000	1.982580000
C	1.539965000	-3.962729000	2.243207000
H	2.365631000	-4.270405000	1.593516000
H	0.723863000	-4.679435000	2.128688000
H	1.897999000	-4.044298000	3.277290000
C	2.280411000	-1.598793000	2.337944000
H	2.513581000	-1.724628000	3.402777000
H	2.031654000	-0.546641000	2.168452000
H	3.187203000	-1.829846000	1.771478000
C	-0.067735000	-2.149504000	2.897596000
H	-0.955165000	-2.762007000	2.725090000
H	-0.345788000	-1.100263000	2.762956000
H	0.233338000	-2.285605000	3.943891000
P	0.480895000	2.204286000	0.315886000
C	2.335901000	2.343549000	0.548431000
H	2.734500000	3.252044000	0.082391000
H	2.587053000	2.375686000	1.615765000
C	0.178977000	3.353107000	-1.157781000
C	1.099534000	2.849599000	-2.279477000
H	0.861966000	3.403048000	-3.196474000
H	0.946583000	1.784107000	-2.476626000
H	2.159319000	3.017870000	-2.062632000
C	0.482127000	4.825434000	-0.877383000
H	0.402546000	5.381374000	-1.819884000
H	1.495135000	4.987221000	-0.494704000
H	-0.230329000	5.272509000	-0.178779000
C	-1.271984000	3.213569000	-1.625389000
H	-1.996660000	3.519851000	-0.868504000
H	-1.503878000	2.189939000	-1.921490000
H	-1.418580000	3.850086000	-2.507076000
C	-0.159581000	2.971802000	1.935410000
C	-0.084624000	1.860118000	2.988432000

H	0.919213000	1.429029000	3.073301000
H	-0.779828000	1.048519000	2.759476000
H	-0.353493000	2.270615000	3.969842000
C	0.685621000	4.156958000	2.421659000
H	0.227497000	4.554640000	3.336086000
H	0.730504000	4.973830000	1.700230000
H	1.708879000	3.871569000	2.680353000
C	-1.614339000	3.426758000	1.799319000
H	-1.998972000	3.684255000	2.794522000
H	-2.256929000	2.650314000	1.379183000
H	-1.705738000	4.321099000	1.176585000
H	-1.310084000	0.031168000	0.891970000
B	-2.432324000	-0.029666000	0.375902000
O	-3.147581000	-1.181655000	0.431881000
O	-3.169606000	1.077585000	0.101389000
C	-4.503431000	-0.899621000	-0.011863000
C	-4.562275000	0.683636000	-0.010011000
H	-2.014200000	0.139844000	-1.752407000
O	0.069068000	-0.234940000	-2.277356000
N	-0.868974000	-0.176260000	-3.164994000
N	-2.044959000	0.036310000	-2.794986000
C	-4.662450000	-1.533308000	-1.387358000
H	-4.473613000	-2.607522000	-1.302264000
H	-5.680722000	-1.397738000	-1.763528000
H	-3.960804000	-1.124164000	-2.118544000
C	-5.448558000	-1.569078000	0.971962000
H	-6.490713000	-1.362290000	0.710559000
H	-5.300758000	-2.652255000	0.934145000
H	-5.272608000	-1.240534000	1.998252000
C	-5.106511000	1.296268000	-1.288496000
H	-6.148192000	1.002197000	-1.449494000
H	-5.070735000	2.386790000	-1.208580000
H	-4.512662000	1.003124000	-2.156895000
C	-5.260979000	1.277210000	1.205956000
H	-5.150254000	2.365189000	1.182494000
H	-6.329348000	1.043222000	1.209436000

H -4.819882000 0.915190000 2.139092000

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