Supporting Information

Nano-sized nickel catalyst for deep hydrogenation of lignin monomers and first-principles insight into the catalyst preparation

Shi-Chao Qi[a], Lu Zhang[a], Hisahiro Einaga[b], Shinji Kudo[a], Koyo Norinaga[a] and Jun-ichiro Hayashi*[a]

[a]*Institute for Materials Chemistry and Engineering, Kyushu University, 6-1, Kasuga Koen, Kasuga, Fukuoka 816-8580, Japan*

[b]*Faculty of Engineering Sciences, Kyushu University, 6-1, Kasuga Koen, Kasuga, Fukuoka 816-8580, Japan*

* Corresponding author. *E-mail address:* junichiro_hayashi@cm.kyushu-u.ac.jp (J. -i. Hayashi)

Reagents and Materials

Nickel(II) nitrate hexahydrate (> 98.0%), sodium borohydride (> 90.0%), pyridine (> 99.0%), ethanol (> 99.5%), isopropanol (> 99.7%), phenol (> 99.0%), *o*-methoxyphenol (> 98.0%), *o*-ethoxyphenol (> 98.0%), syringol (> 99.0%), *p*-hydroxybenzaldehyde (> 98.0%), vanillin (> 98.0%), catechol (> 99.0%), and pyrogallol (> 99.0%) were purchased from Wako Pure Chemical Industries, Ltd., Japan. *p*-Propylphenol (> 99.0%), orcinol (> 97.0%), and syringaldehyde (> 98.0%) were purchased from SIGAMA-ALDRICH Co., Ltd.. *p*-Cresol (> 99.0%) and 2,4-dimethylphenol (> 99.0%) were purchased from Tokyo Chemical Industry Co., Ltd., Japan. 2,3,5-Trimethylphenol (> 98.0%) was purchased from Kanto Chemical Co., Inc., Japan. ZSM-5 zeolite (CBV 3024E, SiO_2/Al_2O_3 = 30) was purchased from ZEOLYST Int. Inc..

Characterizations

High-resolution transmission electron microscopy (TEM) was performed at 200 kV. XRD was carried out with Cu−Kα radiation and a scanning angle range from 5 °to 80 °(scanning step; 0.02 °, scanning time per step; 0.1 s). The N_2 adsorption/desorption isotherms were recorded at −195.8 ℃. Each sample was outgassed at 300 ℃ for 3 h prior to the measurements. Specific surface areas were calculated by applying BET method to isotherms at the relative pressure of 0.05−0.4. XPS measurements were performed adopting Al Kα radiation and a beam spot size of 900 μm (energy step size; 1.000 eV, pass energy; 50.0 eV). Accurate binding energies (E_B) were determined by referencing to the C 1s peak at 284.5 eV. XAFS spectra were taken at ambient temperature and with operation energy at 1.4 GeV.

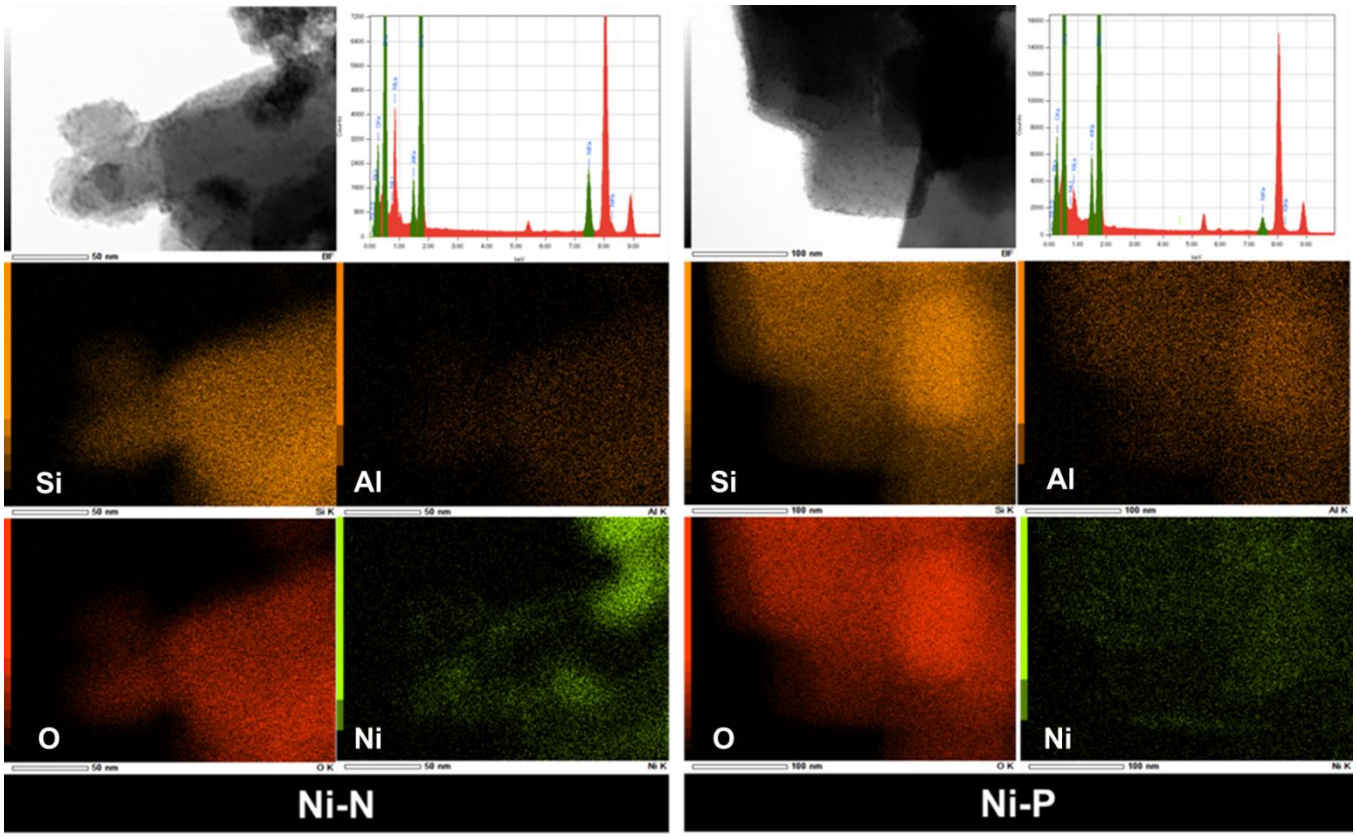


Fig. S1 Elemental Si, Al, O, and Ni maps for Ni-N and Ni-P.

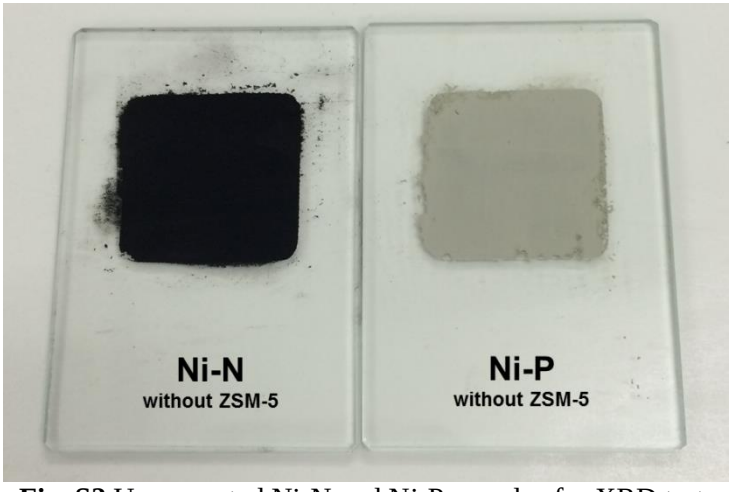


Fig. S2 Unsupported Ni-N and Ni-P samples for XRD test.

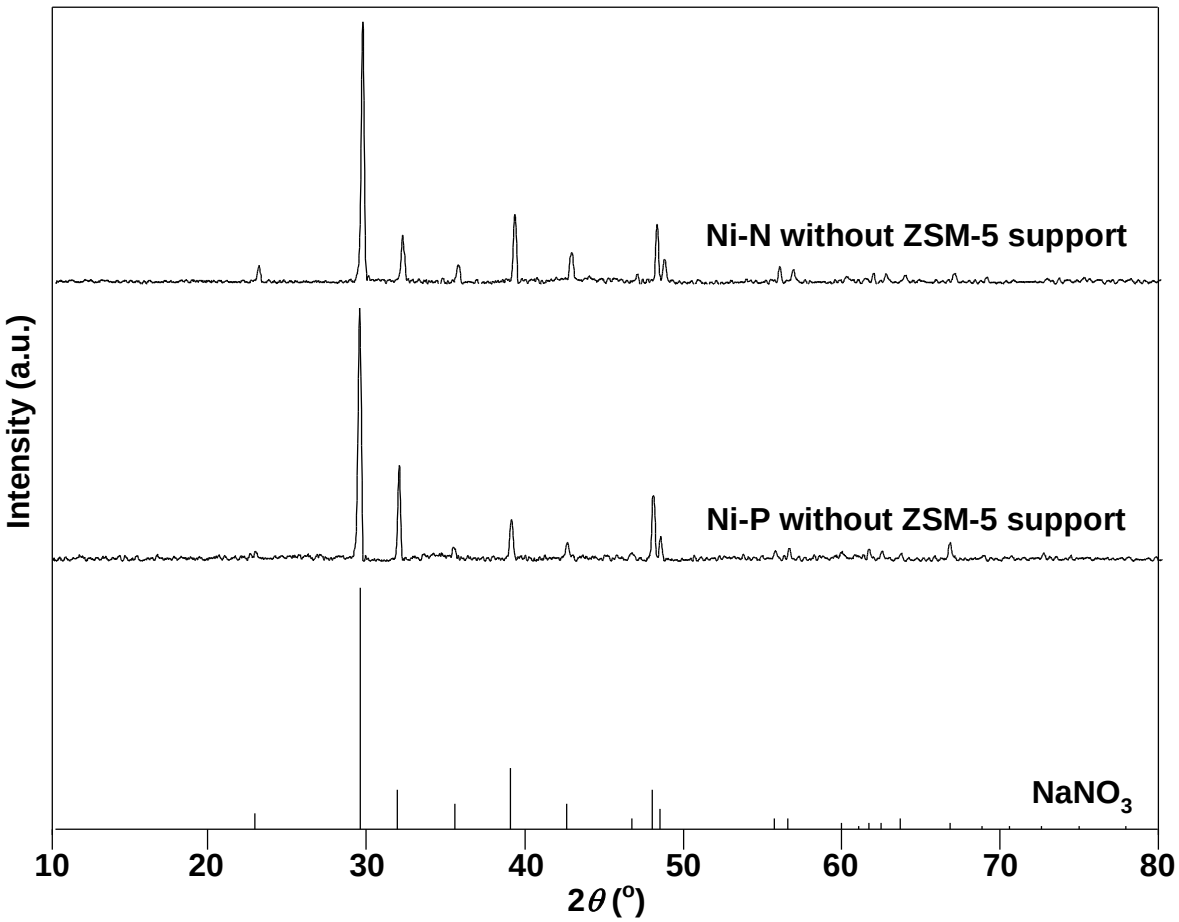


Fig. S3 XRD patterns of Ni-N and Ni-P without ZSM-5 support (these peaks only indicate the presence of sodium nitrate crystal as the by-product).

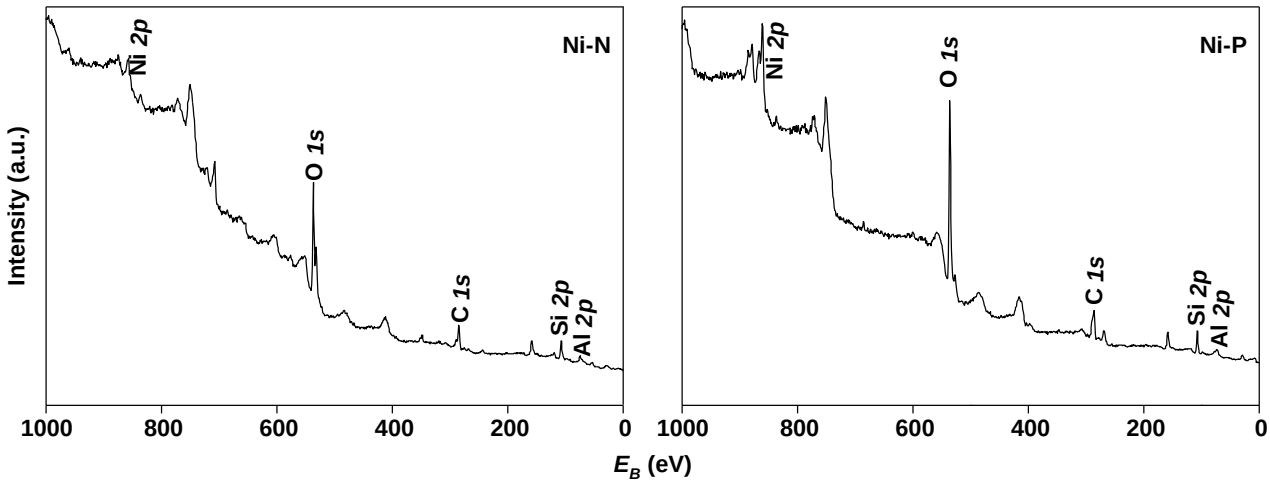


Fig. S4 XPS spectra of Ni-N and Ni-P (B species are undetected at the E_B range of 186−196 eV).

Table S1. Ni K-edge EXAFS curve-fitting results for Ni-N and Ni-P samples.

Catalyst	Shell	CN	R / Å	σ / Å	ΔE / eV	R_f / % [a]
Ni-N	Ni-O	3.7 ±0.10	2.036 ±0.01	0.0860	-3.2880	
	Ni-Ni	1.3 ±0.10	2.474 ±0.01	0.0940	-8.4590	1.7
	Ni-O-Ni	1.9 ±0.20	3.074 ±0.01	0.0980	-3.4030	
$Ni\text{-}N_{spent}$	Ni-O	1.5 ±0.10	2.039 ±0.01	0.065	-9.929	0.1
	Ni-Ni	8.4 ±0.10	2.474 ±0.01	0.075	-6.916	
Ni-P	Ni-O	5.90 ±0.10	2.034 ±0.01	0.075	-7.429	2.5
	Ni-O-Ni	4.80 ±0.20	3.072 ±0.01	0.082	-4.279	
$Ni\text{-}P_{spent}$	Ni-O	5.90 ±0.10	2.036 ±0.01	0.076	-7.011	2.6
	Ni-O-Ni	6.10 ±0.20	3.076 ±0.01	0.092	-3.1080	

[a]The residual factor: $R_f(\%) = \frac{\sum \{k^3\chi(k)_{obs} - k^3\chi(k)_{calc}\}^2}{\sum \{k^3\chi(k)_{obs}\}^2} \times 100$

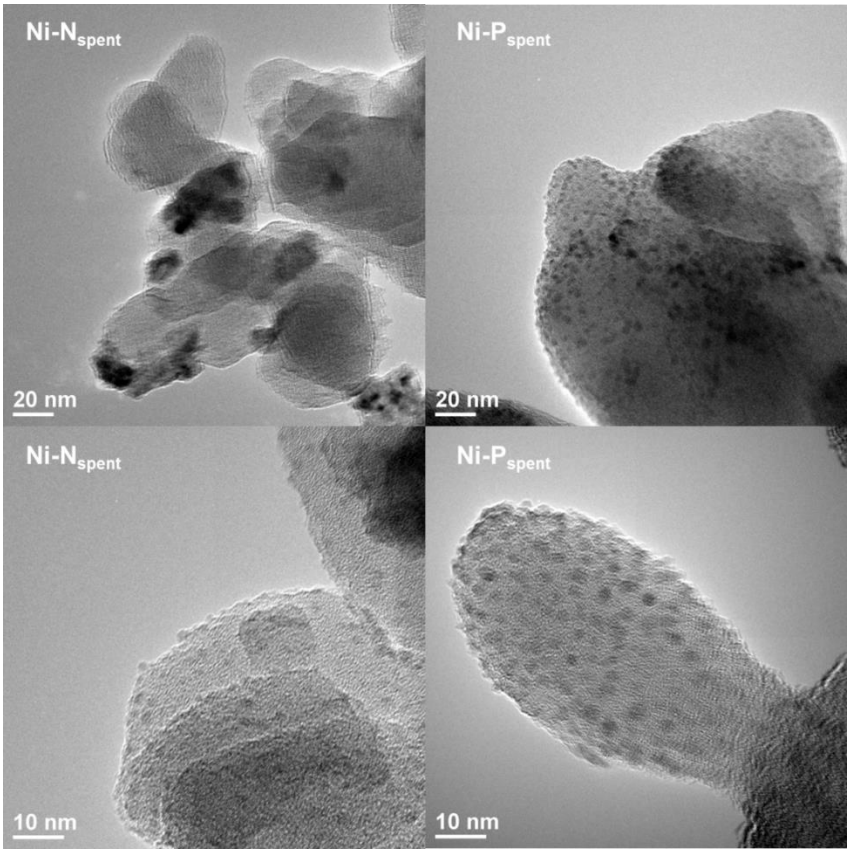
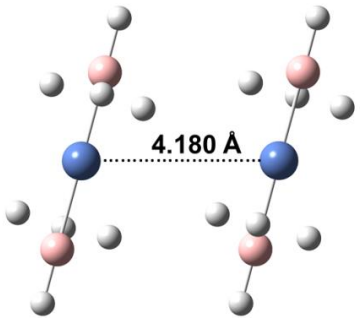
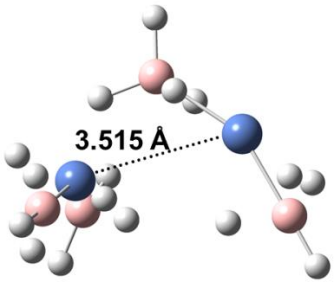
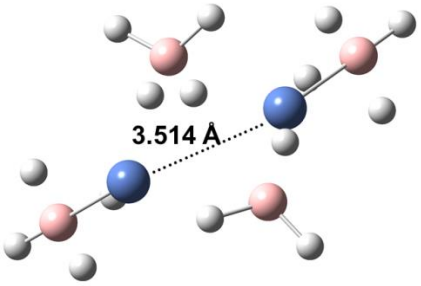


Fig. S5 TEM images for $Ni\text{-}N_{spent}$ and $Ni\text{-}P_{spent}$.

Table S2. Examples of geometry-optimized bimolecular $Ni(BH_4)_2$ systems based on collision theory model.

Geom.			
E_G **(a.u.)**	−447.383666	−447.381584	−447.380782

In Fig. S6, according to Boltzmann distribution, the molar fractions of $[Ni_2(BH_4)_3]^+$-Case1 to -Case5 are 1.6%, 9.7%, 70.5%, 9.3%, and 9.0%, respectively. In Table S3, in consideration of the influences from two ethanol molecules coordinated with Ni atoms, the molar fractions of the five $[Ni_2(BH_4)_3]^+$ geometries are 16.5%, 30.3%, 34.5%, 5.4%, and 13.3%, respectively.

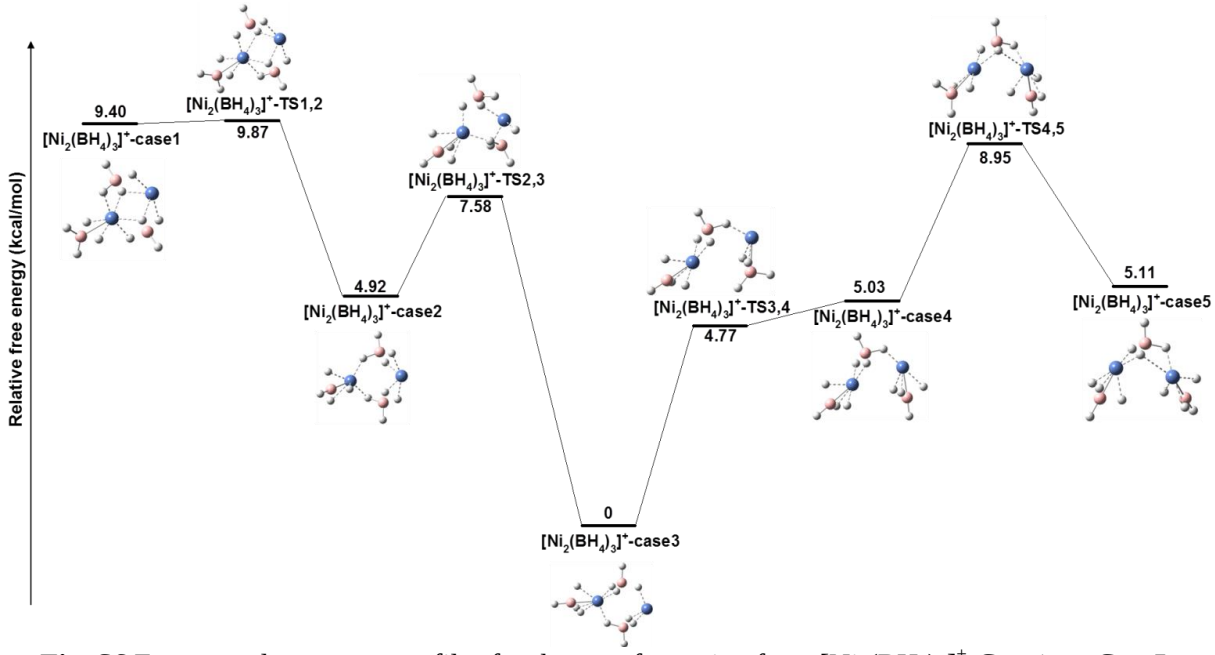


Fig. S6 Energy and geometry profiles for the transformation from $[Ni_2(BH_4)_3]^+$-Case1 to -Case5.

Table S3. E_0 and E_G of $[Ni_2(BH_4)_3]^+$ with two ethanol molecules.

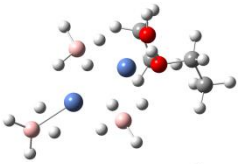
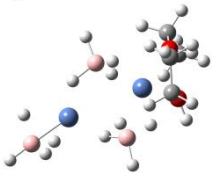
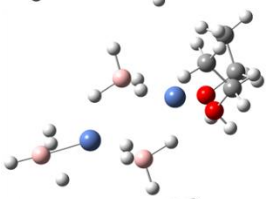
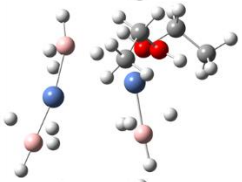
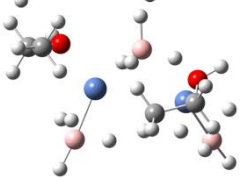
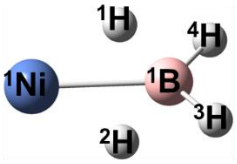
2Ethanol-Ion	Geom.	Energy (a.u.)
2Et.-$[Ni_2(BH_4)_3]^+$-Case1		E_0 = –729.783436 E_G = –729.833150
2Et.-$[Ni_2(BH_4)_3]^+$-Case2		E_0 = –729.786295 E_G = –729.835554
2Et.-$[Ni_2(BH_4)_3]^+$-Case3		E_0 = –729.788593 E_G = –729.836067
2Et.-$[Ni_2(BH_4)_3]^+$-Case4		E_0 = –729.780722 E_G = –729.828757
2Et.-$[Ni_2(BH_4)_3]^+$-Case5		E_0 = –729.784367 E_G = –729.832292

Table S4. Population analysis by matching up the α and β orbitals for $NiBH_4$.

Geom.	[a] Occ.	Overlap	Contributions of relevant atoms
	$\alpha\beta$	1.000	^1Ni_d = 1.00
	$\alpha\beta$	1.000	^1Ni_d = 0.98
	$\alpha\beta$	1.000	^1B_p = 0.32, ^1H_s = 0.27, and ^2H_s = 0.27
	$\alpha\beta$	1.000	^1Ni_d = 0.97
	$\alpha\beta$	0.998	^1Ni_d = 0.94
	α	1.000	^1Ni_d = 0.90

[a] Occ., occupied patterns of the highest several orbitals.

Table S5 show some other potential INTs or TS following INT-4T. $^3BH_2$ of INT-4T might rotate slightly to the left with the formation of TS-4T(2) through TS-4T-4T(2). $^3BH_2$ might also directly bond with ^2B to generate INT-5T(2); however, we did not find the TS between INT-4T(2) and INT-5T(2). INT-5T(3) is unproductive either since no effective reactions initiate from it.

Table S5. Some other potential INTs and TS for the decomposition of INT-4T.

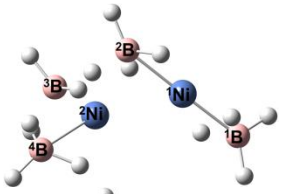
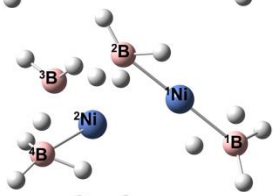
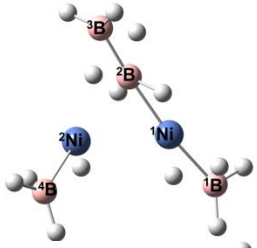
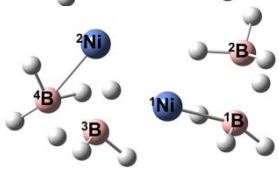
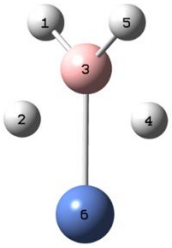
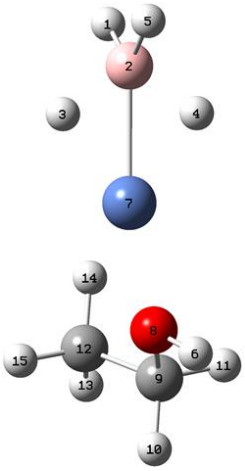
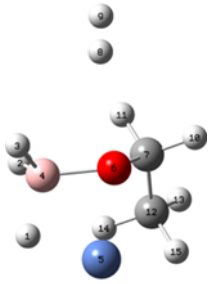
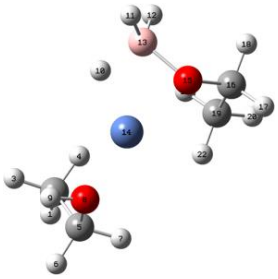
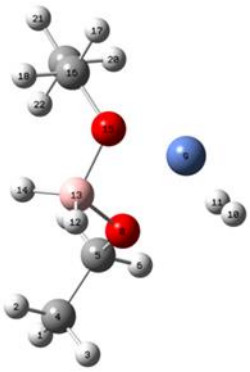
Acronym	Geom.	Energy (a.u.)
TS-4T-4T(2)		E_0 = –446.208863 E_G = –446.250313
INT-4T(2)		E_0 = –446.208258 E_G = –446.249167
INT-5T(2)		E_0 = –446.216400 E_G = –446.259017
INT-5T(3)		E_0 = –446.218152 E_G = –446.257297

Table S6. Second order perturbation analysis for the 'donor-acceptor' (bond-antibond) interactions between the coordinated B species and the Ni center in the NBO basis.

Geom.	*α* orbitals			*β* orbitals		
	Donor	**Acceptor**	**Δ*E* (kcal/mol)**	**Donor**	**Acceptor**	**Δ*E* (kcal/mol)**
 INT-1D	BD (1) H1 - B3	LP* (8) Ni6	0.28	BD (1) H1 - B3	LP* (7) Ni6	0.31
	BD (1) H1 - B3	LP* (9) Ni6	0.05	BD (1) H1 - B3	LP* (8) Ni6	0.06
	BD (1) H1 - B3	RY* (1) Ni6	0.05	BD (1) H1 - B3	RY* (2) Ni6	0.08
	BD (1) H1 - B3	RY* (9) Ni6	0.04	BD (1) H1 - B3	RY* (4) Ni6	0.04
	BD (1) H2 - B3	LP* (6) Ni6	14.95	BD (1) H2 - B3	LP* (5) Ni6	9.4
	BD (1) H2 - B3	LP* (7) Ni6	1.32	BD (1) H2 - B3	LP* (6) Ni6	16.07
	BD (1) H2 - B3	LP* (8) Ni6	1.47	BD (1) H2 - B3	LP* (7) Ni6	1.52
	BD (1) H2 - B3	RY* (1) Ni6	1.37	BD (1) H2 - B3	LP* (9) Ni6	0.25
	BD (1) H2 - B3	RY* (2) Ni6	0.04	BD (1) H2 - B3	RY* (2) Ni6	1.94
	BD (1) H2 - B3	RY* (3) Ni6	0.59	BD (1) H2 - B3	RY* (4) Ni6	2.06
	BD (1) H2 - B3	RY* (5) Ni6	0.05	BD (1) H2 - B3	RY* (8) Ni6	0.25
	BD (1) H2 - B3	RY* (8) Ni6	0.52	BD (1) H2 - B3	RY* (9) Ni6	0.13
	BD (1) H2 - B3	RY* (9) Ni6	0.8	BD (1) B3 - H4	LP* (5) Ni6	9.4
	BD (1) B3 - H4	LP* (6) Ni6	14.95	BD (1) B3 - H4	LP* (6) Ni6	16.07
	BD (1) B3 - H4	LP* (7) Ni6	1.31	BD (1) B3 - H4	LP* (7) Ni6	1.52
	BD (1) B3 - H4	LP* (8) Ni6	1.47	BD (1) B3 - H4	LP* (9) Ni6	0.25
	BD (1) B3 - H4	RY* (1) Ni6	1.37	BD (1) B3 - H4	RY* (2) Ni6	1.94
	BD (1) B3 - H4	RY* (2) Ni6	0.04	BD (1) B3 - H4	RY* (4) Ni6	2.06
	BD (1) B3 - H4	RY* (3) Ni6	0.59	BD (1) B3 - H4	RY* (8) Ni6	0.25
	BD (1) B3 - H4	RY* (5) Ni6	0.05	BD (1) B3 - H4	RY* (9) Ni6	0.13
	BD (1) B3 - H4	RY* (8) Ni6	0.52	BD (1) B3 - H5	LP* (7) Ni6	0.31
	BD (1) B3 - H4	RY* (9) Ni6	0.8	BD (1) B3 - H5	LP* (8) Ni6	0.06
	BD (1) B3 - H5	LP* (8) Ni6	0.28	BD (1) B3 - H5	RY* (2) Ni6	0.08
	BD (1) B3 - H5	LP* (9) Ni6	0.05	BD (1) B3 - H5	RY* (4) Ni6	0.04
	BD (1) B3 - H5	RY* (1) Ni6	0.05	CR (1) B3	LP* (6) Ni6	0.65
	BD (1) B3 - H5	RY* (9) Ni6	0.04	CR (1) B3	LP* (7) Ni6	0.88
	CR (1) B3	LP* (6) Ni6	0.62			
	CR (1) B3	LP* (8) Ni6	0.86			
	CR (1) B3	RY* (9) Ni6	0.03			
 INT-1D$_{1ET}$	BD (1) H1 - B2	LP* (7) Ni7	0.12	BD (1) H1 - B2	LP* (7) Ni7	0.71
	BD (1) H1 - B2	LP* (8) Ni7	0.63	BD (1) H1 - B2	LP* (8) Ni7	0.03
	BD (1) H1 - B2	LP* (9) Ni7	0.25	BD (1) H1 - B2	LP* (9) Ni7	0.25
	BD (1) H1 - B2	RY* (1) Ni7	0.05	BD (1) H1 - B2	RY* (1) Ni7	0.04
	BD (1) H1 - B2	RY* (3) Ni7	0.03	BD (1) H1 - B2	RY* (2) Ni7	0.06
	BD (1) B2 - H3	LP* (6) Ni7	21.07	BD (1) B2 - H3	LP* (5) Ni7	32.05
	BD (1) B2 - H3	LP* (7) Ni7	0.33	BD (1) B2 - H3	LP* (6) Ni7	5.06
	BD (1) B2 - H3	LP* (8) Ni7	10.01	BD (1) B2 - H3	LP* (7) Ni7	8.61
	BD (1) B2 - H3	LP* (9) Ni7	0.05	BD (1) B2 - H3	LP* (8) Ni7	0.78
	BD (1) B2 - H3	RY* (1) Ni7	0.93	BD (1) B2 - H3	LP* (9) Ni7	0.04
	BD (1) B2 - H3	RY* (2) Ni7	0.65	BD (1) B2 - H3	RY* (1) Ni7	0.6
	BD (1) B2 - H3	RY* (3) Ni7	1.86	BD (1) B2 - H3	RY* (2) Ni7	2.46
	BD (1) B2 - H3	RY* (4) Ni7	0.91	BD (1) B2 - H3	RY* (3) Ni7	1.43
	BD (1) B2 - H3	RY* (5) Ni7	0.61	BD (1) B2 - H3	RY* (4) Ni7	0.33
	BD (1) B2 - H3	RY* (6) Ni7	0.1	BD (1) B2 - H3	RY* (5) Ni7	0.25
	BD (1) B2 - H3	RY* (8) Ni7	0.08	BD (1) B2 - H3	RY* (6) Ni7	0.05
	BD (1) B2 - H3	RY* (9) Ni7	1.89	BD (1) B2 - H3	RY* (7) Ni7	0.04
	BD (1) B2 - H4	LP* (6) Ni7	18.08	BD (1) B2 - H3	RY* (8) Ni7	0.1
	BD (1) B2 - H4	LP* (7) Ni7	6.13	BD (1) B2 - H3	RY* (9) Ni7	1.32
	BD (1) B2 - H4	LP* (8) Ni7	4.95	BD (1) B2 - H4	LP* (5) Ni7	0.56
	BD (1) B2 - H4	LP* (9) Ni7	0.04	BD (1) B2 - H4	LP* (6) Ni7	30.69
	BD (1) B2 - H4	RY* (1) Ni7	0.69	BD (1) B2 - H4	LP* (7) Ni7	6.12
	BD (1) B2 - H4	RY* (2) Ni7	0.17	BD (1) B2 - H4	LP* (8) Ni7	0.51
	BD (1) B2 - H4	RY* (3) Ni7	2.2	BD (1) B2 - H4	LP* (9) Ni7	0.03
	BD (1) B2 - H4	RY* (4) Ni7	0.43	BD (1) B2 - H4	RY* (1) Ni7	0.52
	BD (1) B2 - H4	RY* (5) Ni7	0.16	BD (1) B2 - H4	RY* (2) Ni7	2.14

	BD (1) B2 - H4	RY* (6) Ni7	0.03	BD (1) B2 - H4	RY* (3) Ni7	1.22
	BD (1) B2 - H4	RY* (7) Ni7	0.03	BD (1) B2 - H4	RY* (4) Ni7	0.19
	BD (1) B2 - H4	RY* (9) Ni7	1.23	BD (1) B2 - H4	RY* (6) Ni7	0.04
	BD (1) B2 - H5	LP* (7) Ni7	0.11	BD (1) B2 - H4	RY* (7) Ni7	0.13
	BD (1) B2 - H5	LP* (8) Ni7	0.6	BD (1) B2 - H4	RY* (8) Ni7	0.05
	BD (1) B2 - H5	LP* (9) Ni7	0.13	BD (1) B2 - H4	RY* (9) Ni7	0.77
	BD (1) B2 - H5	RY* (2) Ni7	0.03	BD (1) B2 - H5	LP* (7) Ni7	0.68
	BD (1) B2 - H5	RY* (3) Ni7	0.03	BD (1) B2 - H5	LP* (8) Ni7	0.03
	CR (1) B2	LP* (6) Ni7	0.45	BD (1) B2 - H5	LP* (9) Ni7	0.14
	CR (1) B2	LP* (7) Ni7	0.26	BD (1) B2 - H5	RY* (2) Ni7	0.05
	CR (1) B2	LP* (8) Ni7	2.14	CR (1) B2	LP* (5) Ni7	0.17
	CR (1) B2	RY* (4) Ni7	0.04	CR (1) B2	LP* (6) Ni7	0.4
				CR (1) B2	LP* (7) Ni7	2.31
				CR (1) B2	LP* (8) Ni7	0.03
				CR (1) B2	RY* (4) Ni7	0.03
 INT-2D$_{1ET}$	BD (1) H1 - B4	LP* (6) Ni5	10.19	BD (1) H1 - B4	LP* (5) Ni5	9.51
	BD (1) H1 - B4	LP* (7) Ni5	1.79	BD (1) H1 - B4	LP* (6) Ni5	9.55
	BD (1) H1 - B4	LP* (8) Ni5	0.43	BD (1) H1 - B4	LP* (7) Ni5	0.07
	BD (1) H1 - B4	LP* (9) Ni5	0.31	BD (1) H1 - B4	LP* (8) Ni5	1.45
	BD (1) H1 - B4	RY* (1) Ni5	1.5	BD (1) H1 - B4	LP* (9) Ni5	0.05
	BD (1) H1 - B4	RY* (2) Ni5	0.03	BD (1) H1 - B4	RY* (1) Ni5	0.74
	BD (1) H1 - B4	RY* (3) Ni5	0.32	BD (1) H1 - B4	RY* (2) Ni5	0.17
	BD (1) H1 - B4	RY* (4) Ni5	0.39	BD (1) H1 - B4	RY* (3) Ni5	0.41
	BD (1) H1 - B4	RY* (5) Ni5	0.04	BD (1) H1 - B4	RY* (4) Ni5	0.52
	BD (1) H1 - B4	RY* (6) Ni5	0.07	BD (1) H1 - B4	RY* (5) Ni5	0.08
	BD (1) H1 - B4	RY* (7) Ni5	0.16	BD (1) H1 - B4	RY* (6) Ni5	0.24
	BD (1) H1 - B4	RY* (9) Ni5	0.08	BD (1) H1 - B4	RY* (8) Ni5	0.33
	BD (1) H2 - B4	LP* (6) Ni5	0.13	BD (1) H1 - B4	RY* (9) Ni5	0.12
	BD (1) H2 - B4	LP* (7) Ni5	0.22	BD (1) H2 - B4	LP* (5) Ni5	0.11
	BD (1) H2 - B4	LP* (8) Ni5	0.25	BD (1) H2 - B4	LP* (6) Ni5	0.16
	BD (1) H2 - B4	LP* (9) Ni5	0.15	BD (1) H2 - B4	LP* (7) Ni5	0.34
	BD (1) H3 - B4	LP* (6) Ni5	0.18	BD (1) H2 - B4	LP* (9) Ni5	0.22
	BD (1) H3 - B4	LP* (7) Ni 5	0.07	BD (1) H3 - B4	LP* (5) Ni5	0.03
	BD (1) H3 - B4	LP* (8) Ni5	0.4	BD (1) H3 - B4	LP* (6) Ni5	0.19
	BD (1) H3 - B4	RY* (1) Ni5	0.03	BD (1) H3 - B4	LP* (7) Ni5	0.45
	BD (1) B4 - O6	LP* (6) Ni5	2.26	BD (1) H3 - B4	RY* (1) Ni5	0.04
	BD (1) B4 - O6	LP* (7) Ni5	0.65	BD (1) B4 - O6	LP* (5) Ni5	2.01
	BD (1) B4 - O6	LP* (8) Ni5	0.57	BD (1) B4 - O6	LP* (6) Ni5	3.16
	BD (1) B4 - O6	LP* (9) Ni5	0.33	BD (1) B4 - O6	LP* (7) Ni5	0.6
	BD (1) B4 - O6	RY* (1) Ni5	0.06	BD (1) B4 - O6	LP* (8) Ni5	0.18
	BD (1) O6 - C7	LP* (6) Ni5	0.26	BD (1) B4 - O6	LP* (9) Ni5	0.21
	BD (1) O6 - C7	LP* (7) Ni5	0.21	BD (1) B4 - O6	RY* (1) Ni5	0.05
	BD (1) O6 - C7	LP* (8) Ni5	0.16	BD (1) B4 - O6	RY* (3) Ni5	0.05
	BD (1) O6 - C7	LP* (9) Ni5	0.08	BD (1) O6 - C7	LP* (5) Ni5	0.2
	BD (1) O6 - C7	RY* (1) Ni5	0.05	BD (1) O6 - C7	LP* (6) Ni5	0.29
	BD (1) O6 - C7	RY* (4) Ni5	0.05	BD (1) O6 - C7	LP* (7) Ni5	0.23
	BD (1) C7 - H10	LP* (6) Ni5	0.06	BD (1) O6 - C7	LP* (9) Ni5	0.14
	BD (1) C7 - H10	LP* (7) Ni5	0.04	BD (1) O6 - C7	RY* (4) Ni5	0.06
	BD (1) C7 - H11	LP* (6) Ni5	0.33	BD (1) C7 - H10	LP* (6) Ni5	0.06
	BD (1) C7 - H11	LP* (7) Ni5	0.18	BD (1) C7 - H10	LP* (9) Ni5	0.03
	BD (1) C7 - H11	LP* (8) Ni5	0.04	BD (1) C7 - H11	LP* (5) Ni5	0.04
	BD (1) C7 - H11	LP* (9) Ni5	0.06	BD (1) C7 - H11	LP* (6) Ni5	0.35
	BD (1) C12 - H13	LP* (6) Ni5	0.03	BD (1) C7 - H11	LP* (7) Ni5	0.1
	BD (1) C12 - H14	LP* (6) Ni5	0.06	BD (1) C7 - H11	LP* (9) Ni5	0.13
	BD (1) C12 - H14	LP* (9) Ni5	0.06	BD (1) C12 - H13	LP* (6) Ni5	0.03
	BD (1) C12 - H15	LP* (6) Ni5	0.21	BD (1) C12 - H14	LP* (6) Ni5	0.06
	BD (1) C12 - H15	LP* (7) Ni5	0.09	BD (1) C12 - H14	LP* (9) Ni5	0.06
	BD (1) C12 - H15	LP* (8) Ni5	0.25	BD (1) C12 - H15	LP* (6) Ni5	0.22
	BD (1) C12 - H15	LP* (9) Ni5	0.03	BD (1) C12 - H15	LP* (7) Ni5	0.13
	CR (1) B4	LP* (6) Ni5	0.58	BD (1) C12 - H15	LP* (8) Ni5	0.09
	CR (1) B4	LP* (8) Ni5	0.5	BD (1) C12 - H15	LP* (9) Ni5	0.13

	CR (1) B4	LP* (9) Ni5	0.22	CR (1) B4	LP* (6) Ni5	0.58
	CR (1) O6	LP* (6) Ni5	0.35	CR (1) B4	LP* (7) Ni5	0.43
	CR (1) O6	LP* (7) Ni5	0.26	CR (1) B4	LP* (8) Ni5	0.19
	CR (1) O6	LP* (8) Ni5	0.15	CR (1) B4	LP* (9) Ni5	0.11
	CR (1) O6	LP* (9) Ni5	0.09	CR (1) O6	LP* (5) Ni5	0.25
	CR (1) C7	LP* (6) Ni5	0.05	CR (1) O6	LP* (6) Ni5	0.41
	CR (1) C7	LP* (7) Ni5	0.05	CR (1) O6	LP* (7) Ni5	0.21
	CR (1) C7	LP* (9) Ni5	0.03	CR (1) O6	LP* (9) Ni5	0.12
	CR (1) C12	LP* (9) Ni5	0.03	CR (1) C7	LP* (6) Ni5	0.06
	LP (1) O6	LP* (6) Ni5	1.01	CR (1) C7	LP* (9) Ni5	0.05
	LP (1) O6	LP* (7) Ni5	1.1	CR (1) C12	LP* (9) Ni5	0.04
	LP (1) O6	LP* (8) Ni5	0.43	LP (1) O6	LP* (5) Ni5	1.21
	LP (1) O6	RY* (1) Ni5	0.1	LP (1) O6	LP* (6) Ni5	1.22
	LP (2) O6	LP* (6) Ni5	6.66	LP (1) O6	LP* (7) Ni5	0.86
	LP (2) O6	LP* (7) Ni5	1.83	LP (1) O6	LP* (8) Ni5	0.1
	LP (2) O6	LP* (8) Ni5	0.08	LP (1) O6	LP* (9) Ni5	0.13
	LP (2) O6	LP* (9) Ni5	0.09	LP (1) O6	RY* (1) Ni5	0.04
	LP (2) O6	RY* (1) Ni5	0.68	LP (1) O6	LP* (5) Ni5	10.09
	LP (2) O6	RY* (2) Ni5	0.03	LP (2) O6	LP* (6) Ni5	7.64
	LP (2) O6	RY* (3) Ni5	0.13	LP (2) O6	LP* (7) Ni5	0.08
	LP (2) O6	RY* (4) Ni5	0.12	LP (2) O6	LP* (8) Ni5	0.05
	LP (2) O6	RY* (6) Ni5	0.09	LP (2) O6	RY* (1) Ni5	0.39
	LP (2) O6	RY* (9) Ni5	0.04	LP (2) O6	RY* (2) Ni5	0.04
				LP (2) O6	RY* (3) Ni5	0.25
				LP (2) O6	RY* (4) Ni5	0.13
				LP (2) O6	RY* (5) Ni5	0.05
				LP (2) O6	RY* (6) Ni5	0.1
				LP (2) O6	RY* (8) Ni5	0.1
 INT-3D	BD (1) H10 - B13	LP* (6) Ni14	12.27	BD (1) H10 - B13	LP* (5) Ni14	6.27
	BD (1) H10 - B13	LP* (7) Ni14	2.07	BD (1) H10 - B13	LP* (6) Ni14	19.47
	BD (1) H10 - B13	LP* (8) Ni14	6.67	BD (1) H10 - B13	LP* (7) Ni14	3.01
	BD (1) H10 - B13	RY* (1) Ni14	1.58	BD (1) H10 - B13	LP* (8) Ni14	1.94
	BD (1) H10 - B13	RY* (2) Ni14	1.74	BD (1) H10 - B13	LP* (9) Ni14	0.06
	BD (1) H10 - B13	RY* (3) Ni14	0.11	BD (1) H10 - B13	RY* (2) Ni14	2.19
	BD (1) H10 - B13	RY* (4) Ni14	0.21	BD (1) H10 - B13	RY* (4) Ni14	0.11
	BD (1) H10 - B13	RY* (7) Ni14	0.87	BD (1) H10 - B13	RY* (5) Ni14	0.1
	BD (1) H10 - B13	RY* (9) Ni14	0.35	BD (1) H10 - B13	RY* (6) Ni14	0.17
	BD (1) H11 - B13	LP* (6) Ni14	0.16	BD (1) H10 - B13	RY* (7) Ni14	0.86
	BD (1) H11 - B13	LP* (7) Ni14	0.13	BD (1) H10 - B13	RY* (9) Ni14	0.24
	BD (1) H11 - B13	LP* (8) Ni14	1.05	BD (1) H11 - B13	LP* (5) Ni14	0.03
	BD (1) H11 - B13	LP* (9) Ni14	0.15	BD (1) H11 - B13	LP* (6) Ni14	0.15
	BD (1) H12 - B13	LP* (6) Ni14	0.06	BD (1) H11 - B13	LP* (7) Ni14	1.09
	BD (1) H12 - B13	LP* (7) Ni14	0.32	BD (1) H11 - B13	LP* (8) Ni14	0.04
	BD (1) H12 - B13	LP* (8) Ni14	1.03	BD (1) H11 - B13	LP* (9) Ni14	0.21
	BD (1) H12 - B13	LP* (9) Ni14	0.05	BD (1) H12 - B13	LP* (5) Ni14	0.08
	BD (1) B13 - O15	LP* (6) Ni14	3.05	BD (1) H12 - B13	LP* (6) Ni14	0.04
	BD (1) B13 - O15	LP* (7) Ni14	1.87	BD (1) H12 - B13	LP* (7) Ni14	1.28
	BD (1) B13 - O15	LP* (8) Ni14	3.88	BD (1) H12 - B13	LP* (8) Ni14	0.05
	BD (1) B13 - O15	RY* (1) Ni14	0.06	BD (1) H12 - B13	LP* (9) Ni14	0.04
	BD (1) B13 - O15	RY* (2) Ni14	0.07	BD (1) B13 - O15	LP* (5) Ni14	3.33
	BD (1) B13 - O15	RY* (9) Ni14	0.03	BD (1) B13 - O15	LP* (6) Ni14	2.53
	CR (1) B13	LP* (6) Ni14	0.31	BD (1) B13 - O15	LP* (7) Ni14	5.63
	CR (1) B13	LP* (7) Ni14	0.06	BD (1) B13 - O15	LP* (8) Ni14	0.04
	CR (1) B13	LP* (8) Ni14	1.98	BD (1) B13 - O15	RY* (2) Ni14	0.11
	CR (1) O15	LP* (6) Ni14	0.33	CR (1) B13	LP* (6) Ni14	0.38
	CR (1) O15	LP* (7) Ni14	0.68	CR (1) B13	LP* (7) Ni14	1.78
	CR (1) O15	LP* (8) Ni14	0.89	CR (1) B13	LP* (8) Ni14	0.19
	LP (1) O15	LP* (6) Ni14	0.25	CR (1) O15	LP* (5) Ni14	0.41
	LP (1) O15	LP* (7) Ni14	1.86	CR (1) O15	LP* (6) Ni14	0.18
	LP (1) O15	LP* (8) Ni14	0.9	CR (1) O15	LP* (7) Ni14	1.47
	LP (1) O15	LP* (9) Ni14	0.25	LP (1) O15	LP* (5) Ni14	1.42

	LP (1) O15	RY* (1) Ni14	0.29	LP (1) O15	LP* (6) Ni14	0.21
	LP (1) O15	RY* (2) Ni14	0.39	LP (1) O15	LP* (7) Ni14	2.66
	LP (1) O15	RY* (5) Ni14	0.03	LP (1) O15	LP* (8) Ni14	0.39
	LP (1) O15	RY* (7) Ni14	0.12	LP (1) O15	LP* (9) Ni14	0.13
	LP (1) O15	RY* (9) Ni14	0.08	LP (1) O15	RY* (2) Ni14	0.32
	LP (2) O15	LP* (6) Ni14	10.65	LP (1) O15	RY* (6) Ni14	0.05
	LP (2) O15	LP* (7) Ni14	4.52	LP (1) O15	RY* (7) Ni14	0.09
	LP (2) O15	LP* (8) Ni14	2.03	LP (1) O15	RY* (9) Ni14	0.04
	LP (2) O15	RY* (1) Ni14	0.79	LP (2) O15	LP* (5) Ni14	16.32
	LP (2) O15	RY* (2) Ni14	0.76	LP (2) O15	LP* (6) Ni14	5.75
	LP (2) O15	RY* (5) Ni14	0.03	LP (2) O15	LP* (7) Ni14	3.41
	LP (2) O15	RY* (7) Ni14	0.51	LP (2) O15	LP* (8) Ni14	0.04
	LP (2) O15	RY* (9) Ni14	0.22	LP (2) O15	RY* (2) Ni14	0.96
				LP (2) O15	RY* (5) Ni14	0.03
				LP (2) O15	RY* (6) Ni14	0.13
				LP (2) O15	RY* (7) Ni14	0.38
				LP (2) O15	RY* (9) Ni14	0.09
	BD (1) O8 - B13	LP* (6) Ni9	1.23	BD (1) O8 - B13	LP* (5) Ni9	0.64
	BD (1) O8 - B13	LP* (7) Ni9	0.75	BD (1) O8 - B13	LP* (6) Ni9	2.13
	BD (1) O8 - B13	LP* (8) Ni9	0.06	BD (1) O8 - B13	LP* (7) Ni9	0.34
	BD (1) O8 - B13	LP* (9) Ni9	0.38	BD (1) O8 - B13	LP* (8) Ni9	0.18
	BD (1) H12 - B13	LP* (6) Ni9	0.56	BD (1) O8 - B13	LP* (9) Ni9	0.27
	BD (1) H12 - B13	LP* (8) Ni9	0.03	BD (1) H12 - B13	LP* (5) Ni9	0.03
	BD (1) H12 - B13	LP* (9) Ni9	0.1	BD (1) H12 - B13	LP* (6) Ni9	0.54
	BD (1) B13 - H14	LP* (6) Ni9	0.78	BD (1) H12 - B13	LP* (7) Ni9	0.05
	BD (1) B13 - H14	LP* (8) Ni9	0.06	BD (1) H12 - B13	LP* (9) Ni9	0.12
	BD (1) B13 - H14	LP* (9) Ni9	0.1	BD (1) B13 - H14	LP* (5) Ni9	0.04
	BD (1) B13 - O15	LP* (6) Ni9	1.5	BD (1) B13 - H14	LP* (6) Ni9	0.73
	BD (1) B13 - O15	LP* (7) Ni9	0.24	BD (1) B13 - H14	LP* (7) Ni9	0.08
	BD (1) B13 - O15	LP* (8) Ni9	0.21	BD (1) B13 - H14	LP* (9) Ni9	0.12
	BD (1) B13 - O15	LP* (9) Ni9	0.46	BD (1) B13 - H14	RY* (2) Ni9	0.04
	CR (1) O8	LP* (6) Ni9	0.36	BD (1) B13 - O15	LP* (5) Ni9	1.68
	CR (1) O8	LP* (7) Ni9	0.29	BD (1) B13 - O15	LP* (6) Ni9	1.27
	CR (1) O8	LP* (9) Ni9	0.18	BD (1) B13 - O15	LP* (7) Ni9	0.06
	CR (1) B13	LP* (6) Ni9	0.61	BD (1) B13 - O15	LP* (8) Ni9	0.12
	CR (1) B13	LP* (8) Ni9	0.07	BD (1) B13 - O15	LP* (9) Ni9	0.55
	CR (1) B13	LP* (9) Ni9	0.35	CR (1) O8	LP* (5) Ni9	0.12
	CR (1) O15	LP* (6) Ni9	0.47	CR (1) O8	LP* (6) Ni9	0.49
	CR (1) O15	LP* (7) Ni9	0.12	CR (1) O8	LP* (7) Ni9	0.15
	CR (1) O15	LP* (8) Ni9	0.06	CR (1) O8	LP* (8) Ni9	0.1
	CR (1) O15	LP* (9) Ni9	0.19	CR (1) O8	LP* (9) Ni9	0.12
	LP (1) O8	LP* (6) Ni9	0.82	CR (1) B13	LP* (6) Ni9	0.56
	LP (1) O8	LP* (7) Ni9	1.59	CR (1) B13	LP* (7) Ni9	0.11
	LP (1) O8	LP* (8) Ni9	0.38	CR (1) B13	LP* (9) Ni9	0.35
	LP (1) O8	LP* (9) Ni9	0.3	CR (1) O15	LP* (5) Ni9	0.33
	LP (1) O8	RY* (1) Ni9	0.15	CR (1) O15	LP* (6) Ni9	0.32
	LP (1) O8	RY* (4) Ni9	0.06	CR (1) O15	LP* (8) Ni9	0.07
	LP (1) O8	RY* (9) Ni9	0.03	CR (1) O15	LP* (9) Ni9	0.26
	LP (1) O8	LP* (6) Ni9	7.61	LP (1) O8	LP* (5) Ni9	0.65
	LP (1) O8	LP* (7) Ni9	2.26	LP (1) O8	LP* (6) Ni9	1.03
	LP (1) O8	LP* (8) Ni9	0.72	LP (1) O8	LP* (7) Ni9	1.35
	LP (1) O8	LP* (9) Ni9	1.21	LP (1) O8	LP* (8) Ni9	0.29
	LP (1) O8	RY* (1) Ni9	3.27	LP (1) O8	LP* (9) Ni9	0.2
	LP (1) O8	RY* (3) Ni9	0.61	LP (1) O8	RY* (1) Ni9	0.19
	LP (1) O8	RY* (4) Ni9	1.86	LP (1) O8	RY* (3) Ni9	0.13
	LP (1) O8	RY* (6) Ni9	0.37	LP (1) O8	RY* (9) Ni9	0.04
	LP (1) O8	RY* (7) Ni9	0.32	LP (2) O8	LP* (5) Ni9	6.66
	LP (1) O8	RY* (8) Ni9	0.96	LP (2) O8	LP* (6) Ni9	11.57
	LP (1) O8	RY* (9) Ni9	0.52	LP (2) O8	LP* (7) Ni9	0.31
	LP (1) O15	LP* (6) Ni9	1.17	LP (2) O8	LP* (8) Ni9	0.06
	LP (1) O15	LP* (7) Ni9	0.54	LP (2) O8	LP* (9) Ni9	0.98

INT-6D

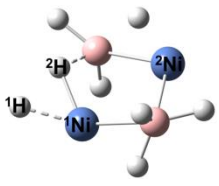
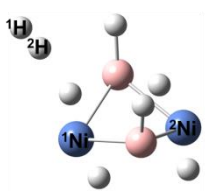
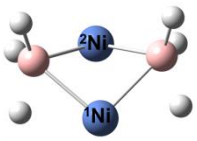
	LP (1) O15	LP* (8) Ni9	0.76	LP (2) O8	RY* (1) Ni9	2.98
	LP (1) O15	LP* (9) Ni9	0.19	LP (2) O8	RY* (2) Ni9	0.38
	LP (1) O15	RY* (1) Ni9	0.05	LP (2) O8	RY* (3) Ni9	2.22
	LP (1) O15	LP* (6) Ni9	9.43	LP (2) O8	RY* (5) Ni9	0.38
	LP (1) O15	LP* (7) Ni9	1.04	LP (2) O8	RY* (6) Ni9	0.04
	LP (1) O15	LP* (8) Ni9	0.2	LP (2) O8	RY* (7) Ni9	0.6
	LP (1) O15	LP* (9) Ni9	0.82	LP (2) O8	RY* (8) Ni9	0.72
	LP (1) O15	RY* (1) Ni9	2.9	LP (2) O8	RY* (9) Ni9	0.43
	LP (1) O15	RY* (2) Ni9	0.22	LP (1) O15	LP* (5) Ni9	1.37
	LP (1) O15	RY* (3) Ni9	0.16	LP (1) O15	LP* (6) Ni9	0.56
	LP (1) O15	RY* (4) Ni9	1.63	LP (1) O15	LP* (7) Ni9	0.26
	LP (1) O15	RY* (6) Ni9	0.4	LP (1) O15	LP* (8) Ni9	0.71
	LP (1) O15	RY* (7) Ni9	0.32	LP (1) O15	LP* (9) Ni9	0.37
	LP (1) O15	RY* (8) Ni9	0.73	LP (1) O15	RY* (1) Ni9	0.1
	LP (1) O15	RY* (9) Ni9	0.43	LP (1) O15	RY* (3) Ni9	0.03
				LP (2) O15	LP* (5) Ni9	13.14
				LP (2) O15	LP* (6) Ni9	6.53
				LP (2) O15	LP* (7) Ni9	0.64
				LP (2) O15	LP* (8) Ni9	0.36
				LP (2) O15	LP* (9) Ni9	0.6
				LP (2) O15	RY* (1) Ni9	2.85
				LP (2) O15	RY* (2) Ni9	0.35
				LP (2) O15	RY* (3) Ni9	1.74
				LP (2) O15	RY* (5) Ni9	0.17
				LP (2) O15	RY* (7) Ni9	0.5
				LP (2) O15	RY* (8) Ni9	0.76
				LP (2) O15	RY* (9) Ni9	0.41

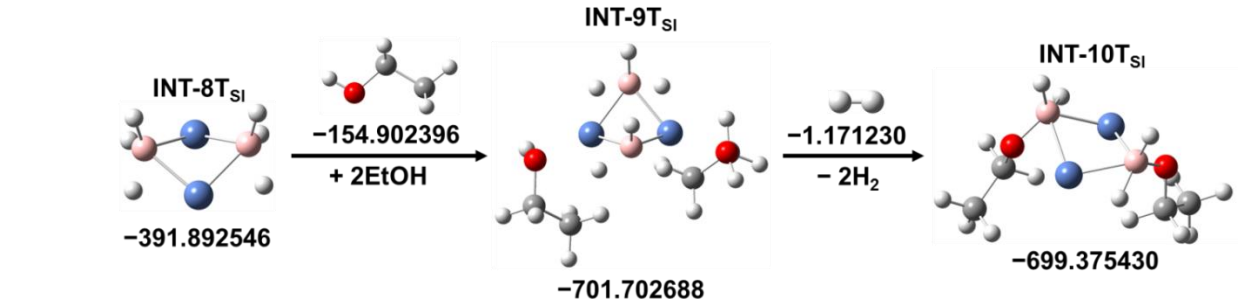
Table S7. Population analysis by matching up the α and β orbitals for NiH.

Geom.	Energy (a.u.)	[a] Occ.	Overlap	Contributions of relevant atoms
	E_0 = −169.876691	$\alpha\beta$	1.000	Ni_p = 1.00
	E_G = −169.896234	$\alpha\beta$	1.000	Ni_p = 1.00
		$\alpha\beta$	1.000	H_s = 0.51, and Ni_s = 0.44
		$\alpha\beta$	1.000	Ni_d = 1.00
		$\alpha\beta$	1.000	Ni_d = 1.00
		$\alpha\beta$	1.000	Ni_d = 1.00
		$\alpha\beta$	0.999	Ni_d = 0.91
		α	1.000	Ni_d = 1.00

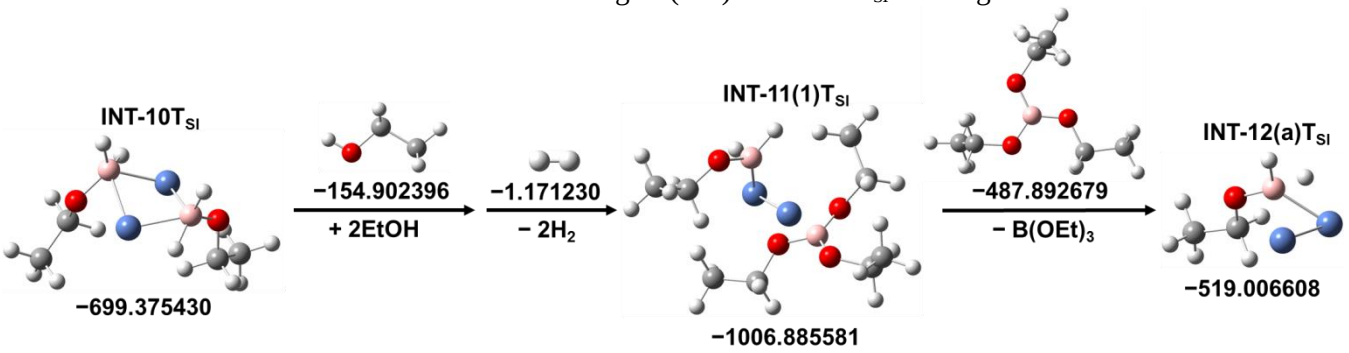
[a] Occ., occupied patterns of the highest several orbitals.

Table S8. INTs and TS in the dehydrogenation of $Ni_2(BH_4)_2$.

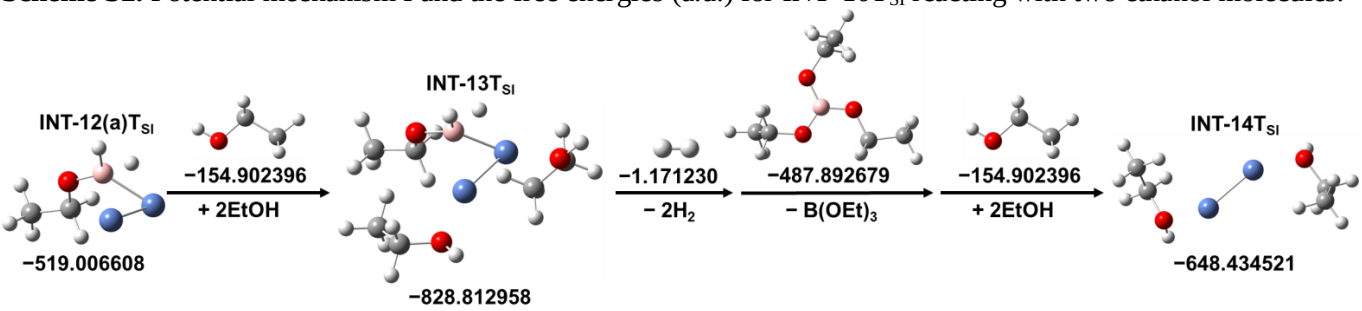
Acronym	INT-6T$_{SI}$	TS-6T$_{SI}$-7T$_{SI}$	INT-7T$_{SI}$	INT-8T$_{SI}$
Geom.				
E_0 (a.u.)	−393.023633	−392.972035	−393.021536	−391.861400
E_G (a.u.)	−393.057369	−393.004808	−393.056254	−391.892546



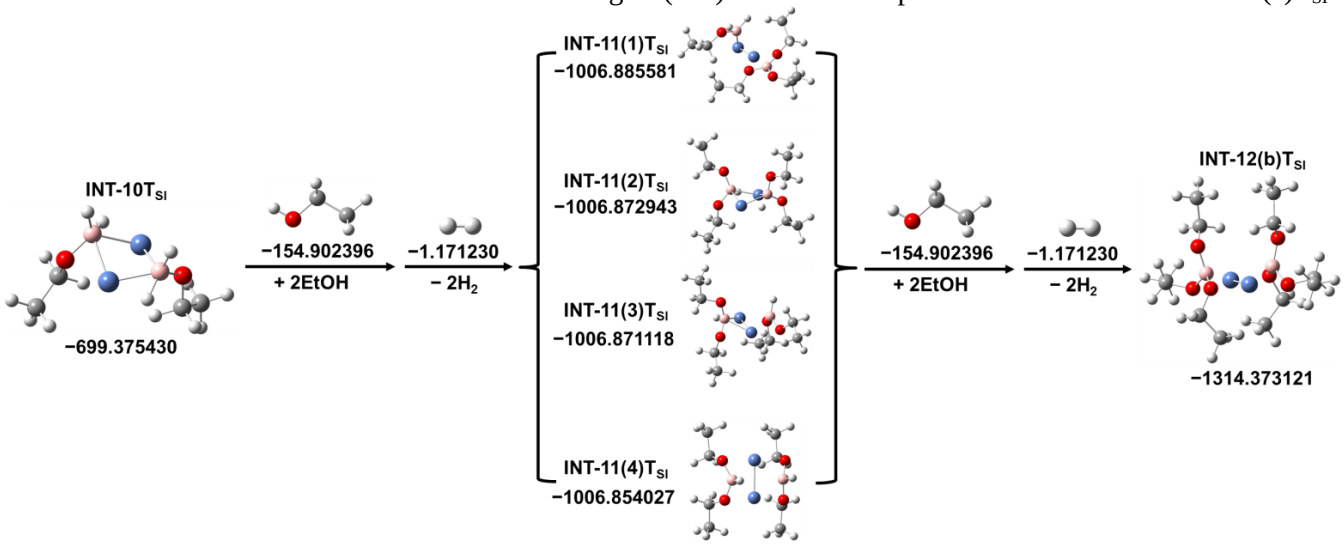
Scheme S1. Potential mechanism and the free energies (a.u.) for INT-8T$_{SI}$ reacting with two ethanol molecules.



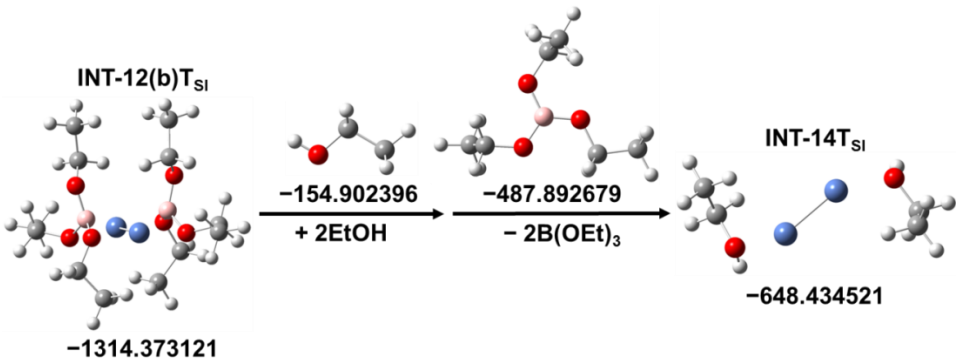
Scheme S2. Potential mechanism I and the free energies (a.u.) for INT-10T$_{SI}$ reacting with two ethanol molecules.



Scheme S3. Potential mechanism and the free energies (a.u.) for the last step of Ni formation after INT-12(a)T$_{SI}$.



Scheme S4. Potential mechanism II and the free energies (a.u.) for INT-10T$_{SI}$ reacting with 4 ethanol molecules.



Scheme S5. The last step and free energies (a.u.) for Ni formation after INT-12(b)T_{SI}.

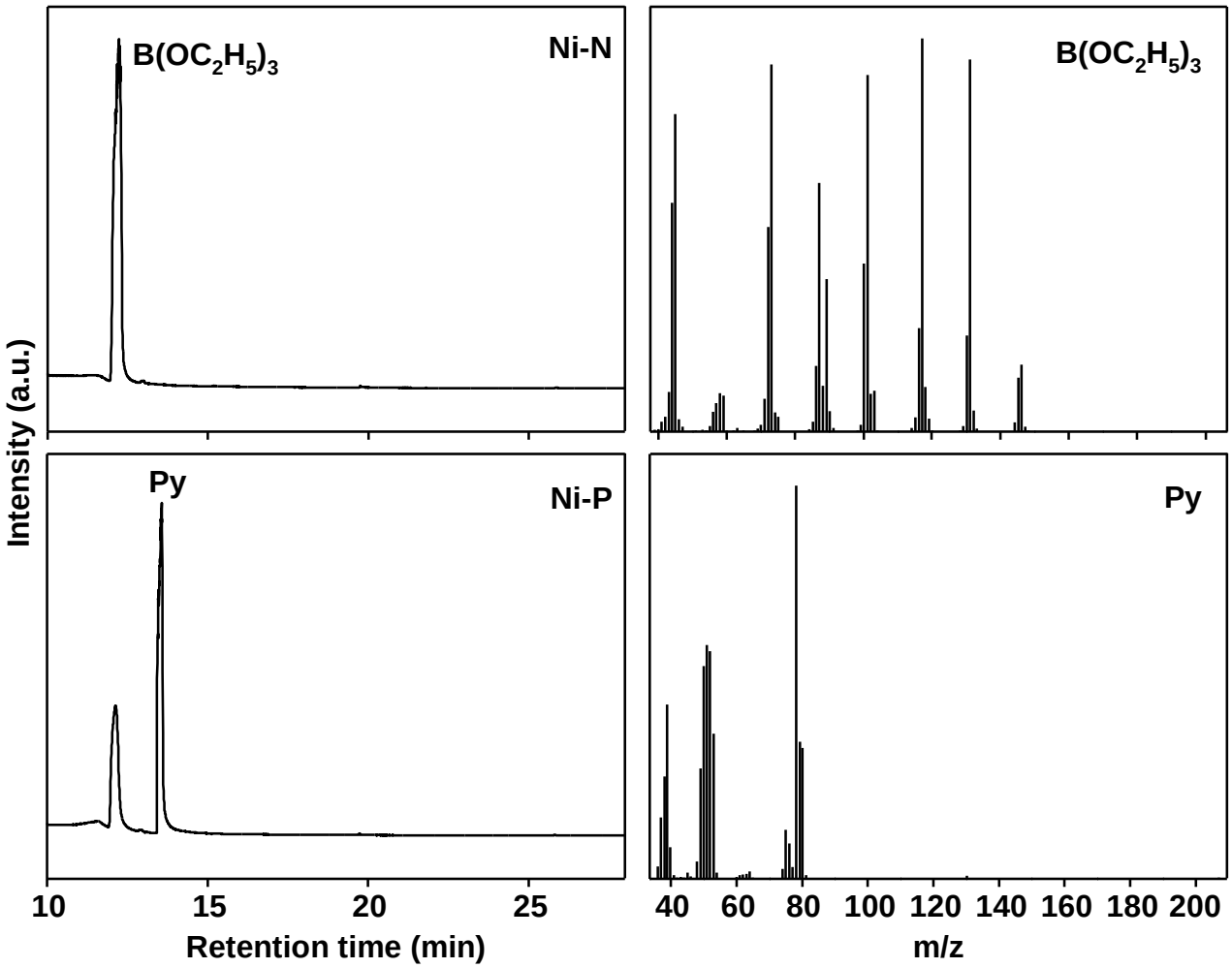
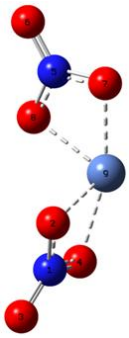


Fig. S7 The total chromatograms of the filtrates from Ni-N and Ni-P preparation and the mass spectra of $B(OEt)_3$ and Py.

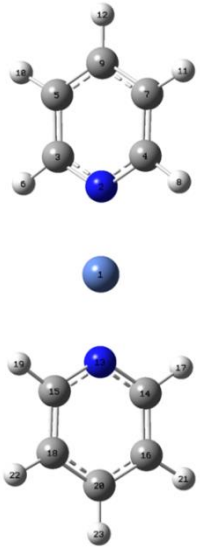
Table S9. Second order perturbation analysis for the 'donor-acceptor' (bond-antibond) interactions between the NO_3^- and the Ni center of $Ni(NO_3)_2$ in the NBO basis.

Geom.	*α* orbitals			*β* orbitals		
	Donor	**Acceptor**	**Δ*E* (kcal/mol)**	**Donor**	**Acceptor**	**Δ*E* (kcal/mol)**
 $Ni(NO_3)_2$	**$^1NO_3^-$**	**Ni**		**$^1NO_3^-$**	**Ni**	
	BD (1) N1-O2	LP* (6) Ni9	0.49	BD (1) N1-O2	LP (5) Ni9	0.39
	BD (1) N1-O2	LP* (7) Ni9	0.56	BD (2) N1-O2	LP (4) Ni9	0.37
	BD (1) N1-O2	LP* (8) Ni9	0.35	BD (2) N1-O2	LP (5) Ni9	0.38
	BD (1) N1-O2	LP* (9) Ni9	0.37	BD* (1) O3-O4	LP (4) Ni9	0.64
	BD (1) N1-O3	LP* (9) Ni9	0.03	BD* (1) O3-O4	LP (5) Ni9	0.61
	BD (2) N1-O3	LP* (6) Ni9	0.39	CR (1) O2	LP (4) Ni9	0.51
	BD (2) N1-O3	LP* (7) Ni9	0.71	CR (1) O2	LP (5) Ni9	0.5
	BD (2) N1-O3	LP* (8) Ni9	0.03	LP (1) O2	LP (4) Ni9	2.36
	BD (2) N1-O3	LP* (9) Ni9	0.14	LP (1) O2	LP (5) Ni9	2.09
	BD (1) N1-O4	LP* (6) Ni9	0.31			
	BD (1) N1-O4	LP* (7) Ni9	1.41			
	CR (1) N1	LP* (6) Ni9	0.11			
	CR (1) N1	LP* (7) Ni9	0.55			
	CR (1) N1	LP* (9) Ni9	0.12			
	CR (1) O2	LP* (6) Ni9	0.57			
	CR (1) O2	LP* (7) Ni9	0.39			
	CR (1) O2	LP* (8) Ni9	0.51			
	CR (1) O2	LP* (9) Ni9	0.54			
	CR (1) O4	LP* (6) Ni9	0.35			
	CR (1) O4	LP* (7) Ni9	1.6			
	CR (1) O4	LP* (8) Ni9	0.08			
	LP (1) O2	LP* (6) Ni9	2.35			
	LP (1) O2	LP* (7) Ni9	0.85			
	LP (1) O2	LP* (8) Ni9	2.01			
	LP (1) O2	LP* (9) Ni9	1.91			
	LP (2) O2	LP* (6) Ni9	13.23			
	LP (2) O2	LP* (7) Ni9	1.23			
	LP (2) O2	LP* (8) Ni9	3.41			
	LP (2) O2	LP* (9) Ni9	1.62			
	LP (2) O2	RY* (3) Ni9	0.03			
	LP (2) O2	RY* (4) Ni9	0.06			
	LP (2) O2	RY* (8) Ni9	0.11			
	LP (3) O2	LP* (6) Ni9	0.03			
	LP (3) O2	LP* (7) Ni9	0.08			
	LP (3) O2	LP* (8) Ni9	0.49			
	LP (3) O2	LP* (9) Ni9	0.61			
	LP (3) O2	RY* (2) Ni9	0.05			
	LP (1) O3	LP* (6) Ni9	0.03			
	LP (1) O4	LP* (6) Ni9	1.36			
	LP (1) O4	LP* (7) Ni9	5.27			
	LP (1) O4	LP* (8) Ni9	0.53			
	LP (2) O4	LP* (6) Ni9	10.95			
	LP (2) O4	LP* (7) Ni9	7.25			
	LP (2) O4	LP* (8) Ni9	0.76			
	LP (2) O4	LP* (9) Ni9	0.39			
	LP (2) O4	RY* (2) Ni9	0.04			
	LP (2) O4	RY* (4) Ni9	0.05			
	LP (2) O4	RY* (5) Ni9	0.09			
	LP (2) O4	RY* (8) Ni9	0.23			
	LP (3) O4	LP* (6) Ni9	0.06			
	LP (3) O4	LP* (7) Ni9	0.07			
	LP (3) O4	LP* (8) Ni9	0.55			
	LP (3) O4	LP* (9) Ni9	0.6			
	$^5NO_3^-$	**Ni**		**$^5NO_3^-$**	**Ni**	

BD (1) N5-O6	LP* (9) Ni9	0.03	BD (1) N5-O8	LP (4) Ni9	0.43
BD (2) N5-O6	LP* (6) Ni9	0.39	BD (1) N5-O8	LP (5) Ni9	0.39
BD (2) N5-O6	LP* (7) Ni9	0.71	BD (1) O7-O8	LP (4) Ni9	1.14
BD (2) N5-O6	LP* (8) Ni9	0.03	BD (1) O7-O8	LP (5) Ni9	1.11
BD (2) N5-O6	LP* (9) Ni9	0.14	CR (1) O8	LP (4) Ni9	0.51
BD (1) N5-O7	LP* (6) Ni9	0.31	CR (1) O8	LP (5) Ni9	0.5
BD (1) N5-O7	LP* (7) Ni9	1.41	LP (1) O8	LP (4) Ni9	2.36
BD (1) N5-O8	LP* (6) Ni9	0.49	LP (1) O8	LP (5) Ni9	2.09
BD (1) N5-O8	LP* (7) Ni9	0.56			
BD (1) N5-O8	LP* (8) Ni9	0.35			
BD (1) N5-O8	LP* (9) Ni9	0.37			
CR (1) N5	LP* (6) Ni9	0.11			
CR (1) N5	LP* (7) Ni9	0.55			
CR (1) N5	LP* (9) Ni9	0.12			
CR (1) O7	LP* (6) Ni9	0.35			
CR (1) O7	LP* (7) Ni9	1.6			
CR (1) O7	LP* (8) Ni9	0.08			
CR (1) O8	LP* (6) Ni9	0.57			
CR (1) O8	LP* (7) Ni9	0.39			
CR (1) O8	LP* (8) Ni9	0.51			
CR (1) O8	LP* (9) Ni9	0.54			
LP (1) O6	LP* (6) Ni9	0.03			
LP (1) O7	LP* (6) Ni9	1.36			
LP (1) O7	LP* (7) Ni9	5.27			
LP (1) O7	LP* (8) Ni9	0.53			
LP (2) O7	LP* (6) Ni9	10.95			
LP (2) O7	LP* (7) Ni9	7.25			
LP (2) O7	LP* (8) Ni9	0.76			
LP (2) O7	LP* (9) Ni9	0.39			
LP (2) O7	RY* (2) Ni9	0.04			
LP (2) O7	RY* (4) Ni9	0.05			
LP (2) O7	RY* (5) Ni9	0.09			
LP (2) O7	RY* (8) Ni9	0.23			
LP (3) O7	LP* (6) Ni9	0.06			
LP (3) O7	LP* (7) Ni9	0.07			
LP (3) O7	LP* (8) Ni9	0.55			
LP (3) O7	LP* (9) Ni9	0.6			
LP (1) O8	LP* (6) Ni9	2.35			
LP (1) O8	LP* (7) Ni9	0.85			
LP (1) O8	LP* (8) Ni9	2			
LP (1) O8	LP* (9) Ni9	1.91			
LP (2) O8	LP* (6) Ni9	13.23			
LP (2) O8	LP* (7) Ni9	1.23			
LP (2) O8	LP* (8) Ni9	3.41			
LP (2) O8	LP* (9) Ni9	1.62			
LP (2) O8	RY* (3) Ni9	0.03			
LP (2) O8	RY* (4) Ni9	0.06			
LP (2) O8	RY* (8) Ni9	0.11			
LP (3) O8	LP* (6) Ni9	0.03			
LP (3) O8	LP* (7) Ni9	0.08			
LP (3) O8	LP* (8) Ni9	0.49			
LP (3) O8	LP* (9) Ni9	0.61			
LP (3) O8	RY* (2) Ni9	0.05			

Table S10. Second order perturbation analysis for the 'donor-acceptor' (bond-antibond) interactions between the Py and the Ni center of $[NiPy_2]^{2+}$ in the NBO basis.

Geom.	*α* orbitals			*β* orbitals		
	Donor	**Acceptor**	**Δ*E* (kcal/mol)**	**Donor**	**Acceptor**	**Δ*E* (kcal/mol)**
	$^2NC_5H_5$	**Ni**		**$^2NC_5H_5$**	**Ni**	
	BD (1) N2-C3	LP* (6) Ni1	0.56	BD (1) N2-C3	LP* (4) Ni1	0.48
	BD (1) N2-C3	LP* (7) Ni1	0.77	BD (1) N2-C3	LP* (5) Ni1	0.74
	BD (1) N2-C3	LP* (8) Ni1	0.06	BD (1) N2-C3	LP* (6) Ni1	0.25
	BD (1) N2-C4	LP* (6) Ni1	0.56	BD (1) N2-C3	LP* (8) Ni1	0.05
	BD (1) N2-C4	LP* (7) Ni1	0.77	BD (1) N2-C4	LP* (4) Ni1	0.48
	BD (1) N2-C4	LP* (8) Ni1	0.06	BD (1) N2-C4	LP* (5) Ni1	0.74
	BD (2) N2-C4	LP* (8) Ni1	0.11	BD (1) N2-C4	LP* (6) Ni1	0.25
	BD (2) N2-C4	LP* (9) Ni1	0.28	BD (1) N2-C4	LP* (8) Ni1	0.05
	BD (1) C3-C5	LP* (6) Ni1	0.12	BD (2) N2-C4	LP* (7) Ni1	0.32
	BD (1) C3-C5	LP* (7) Ni1	0.53	BD (2) N2-C4	LP* (8) Ni1	0.12
	BD (1) C3-C5	RY* (1) Ni1	0.05	BD (1) C3-C5	LP* (4) Ni1	0.06
	BD (1) C3-C5	RY* (8) Ni1	0.08	BD (1) C3-C5	LP* (5) Ni1	0.53
	BD (1) C3-H6	LP* (6) Ni1	0.12	BD (1) C3-C5	LP* (6) Ni1	0.06
	BD (1) C3-H6	LP* (7) Ni1	0.05	BD (1) C3-C5	RY* (4) Ni1	0.08
	BD (1) C3-H6	LP* (8) Ni1	0.06	BD (1) C3-C5	RY* (8) Ni1	0.07
	BD (1) C3-H6	RY* (1) Ni1	0.03	BD (1) C3-H6	LP* (5) Ni1	0.05
	BD (1) C3-H6	RY* (8) Ni1	0.05	BD (1) C3-H6	LP* (6) Ni1	0.17
	BD (1) C4-C7	LP* (6) Ni1	0.12	BD (1) C3-H6	LP* (7) Ni1	0.03
	BD (1) C4-C7	LP* (7) Ni1	0.53	BD (1) C3-H6	LP* (8) Ni1	0.07
	BD (1) C4-C7	RY* (1) Ni1	0.05	BD (1) C3-H6	RY* (4) Ni1	0.03
	BD (1) C4-C7	RY* (8) Ni1	0.08	BD (1) C3-H6	RY* (8) Ni1	0.06
	BD (1) C4-H8	LP* (6) Ni1	0.12	BD (1) C4-C7	LP* (4) Ni1	0.06
	BD (1) C4-H8	LP* (7) Ni1	0.05	BD (1) C4-C7	LP* (5) Ni1	0.53
	BD (1) C4-H8	LP* (8) Ni1	0.06	BD (1) C4-C7	LP* (6) Ni1	0.06
	BD (1) C4-H8	RY* (1) Ni1	0.03	BD (1) C4-C7	RY* (4) Ni1	0.08
	BD (1) C4-H8	RY* (8) Ni1	0.05	BD (1) C4-C7	RY* (8) Ni1	0.07
	BD (1) C5-H10	LP* (7) Ni1	0.05	BD (1) C4-H8	LP* (5) Ni1	0.05
	BD (1) C7-H11	LP* (7) Ni1	0.05	BD (1) C4-H8	LP* (6) Ni1	0.17
	BD (1) C9-H12	LP* (7) Ni1	0.04	BD (1) C4-H8	LP* (7) Ni1	0.03
	CR (1) N2	LP* (6) Ni1	0.33	BD (1) C4-H8	LP* (8) Ni1	0.07
	CR (1) N2	LP* (7) Ni1	1.28	BD (1) C4-H8	RY* (4) Ni1	0.03
	CR (1) C3	LP* (7) Ni1	0.21	BD (1) C4-H8	RY* (8) Ni1	0.06
	CR (1) C4	LP* (7) Ni1	0.21	BD (1) C5-H10	LP* (5) Ni1	0.05
	LP (1) N2	LP* (6) Ni1	17.7	BD (1) C7-H11	LP* (5) Ni1	0.05
	LP (1) N2	LP* (7) Ni1	4.29	BD (1) C9-H12	LP* (5) Ni1	0.04
	LP (1) N2	RY* (1) Ni1	0.96	CR (1) N2	LP* (4) Ni1	0.32
	LP (1) N2	RY* (5) Ni1	0.59	CR (1) N2	LP* (5) Ni1	1.26
	LP (1) N2	RY* (8) Ni1	1.64	CR (1) N2	LP* (6) Ni1	0.11
	BD* (2) N2-C4	LP* (8) Ni1	0.07	CR (1) C3	LP* (5) Ni1	0.21
	BD* (2) N2-C4	LP* (9) Ni1	0.19	CR (1) C4	LP* (5) Ni1	0.21
				LP (1) N2	LP* (4) Ni1	33.83
				LP (1) N2	LP* (5) Ni1	4.23
				LP (1) N2	LP* (6) Ni1	4.66
				LP (1) N2	LP* (9) Ni1	0.11
				LP (1) N2	RY* (4) Ni1	0.93
				LP (1) N2	RY* (8) Ni1	1.36
				BD* (2) N2-C4	LP* (7) Ni1	0.26
				BD* (2) N2-C4	LP* (8) Ni1	0.1
	$^{13}NC_5H_5$	**Ni**		**$^{13}NC_5H_5$**	**Ni**	
	BD (1) N13-C14	LP* (6) Ni1	0.56	BD (1) N13-C14	LP* (4) Ni1	0.48
	BD (1) N13-C14	LP* (7) Ni1	0.77	BD (1) N13-C14	LP* (5) Ni1	0.74
	BD (1) N13-C14	LP* (8) Ni1	0.06	BD (1) N13-C14	LP* (6) Ni1	0.25
	BD (2) N13-C14	LP* (8) Ni1	0.11	BD (1) N13-C14	LP* (8) Ni1	0.05

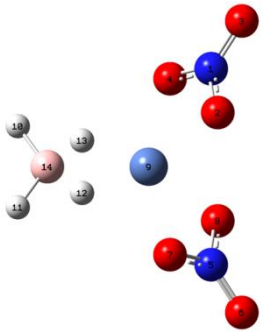


$[NiPy_2]^{2+}$

	BD (2) N13-C14	LP* (9) Ni1	0.28	BD (2) N13-C14	LP* (7) Ni1	0.32
	BD (1) N13-C15	LP* (6) Ni1	0.56	BD (2) N13-C14	LP* (8) Ni1	0.12
	BD (1) N13-C15	LP* (7) Ni1	0.77	BD (1) N13-C15	LP* (4) Ni1	0.48
	BD (1) N13-C15	LP* (8) Ni1	0.06	BD (1) N13-C15	LP* (5) Ni1	0.74
	BD (1) C14-C16	LP* (6) Ni1	0.12	BD (1) N13-C15	LP* (6) Ni1	0.25
	BD (1) C14-C16	LP* (7) Ni1	0.53	BD (1) N13-C15	LP* (8) Ni1	0.05
	BD (1) C14-C16	RY* (1) Ni1	0.05	BD (1) C14-C16	LP* (4) Ni1	0.06
	BD (1) C14-C16	RY* (8) Ni1	0.08	BD (1) C14-C16	LP* (5) Ni1	0.53
	BD (1) C14-H17	LP* (6) Ni1	0.12	BD (1) C14-C16	LP* (6) Ni1	0.06
	BD (1) C14-H17	LP* (7) Ni1	0.05	BD (1) C14-C16	RY* (4) Ni1	0.08
	BD (1) C14-H17	LP* (8) Ni1	0.06	BD (1) C14-C16	RY* (8) Ni1	0.07
	BD (1) C14-H17	RY* (1) Ni1	0.03	BD (1) C14-H17	LP* (5) Ni1	0.05
	BD (1) C14-H17	RY* (8) Ni1	0.05	BD (1) C14-H17	LP* (6) Ni1	0.17
	BD (1) C15-C18	LP* (6) Ni1	0.12	BD (1) C14-H17	LP* (7) Ni1	0.03
	BD (1) C15-C18	LP* (7) Ni1	0.53	BD (1) C14-H17	LP* (8) Ni1	0.07
	BD (1) C15-C18	RY* (1) Ni1	0.05	BD (1) C14-H17	RY* (4) Ni1	0.03
	BD (1) C15-C18	RY* (8) Ni1	0.08	BD (1) C14-H17	RY* (8) Ni1	0.06
	BD (1) C15-H19	LP* (6) Ni1	0.12	BD (1) C15-C18	LP* (4) Ni1	0.06
	BD (1) C15-H19	LP* (7) Ni1	0.05	BD (1) C15-C18	LP* (5) Ni1	0.53
	BD (1) C15-H19	LP* (8) Ni1	0.06	BD (1) C15-C18	LP* (6) Ni1	0.06
	BD (1) C15-H19	RY* (1) Ni1	0.03	BD (1) C15-C18	RY* (4) Ni1	0.08
	BD (1) C15-H19	RY* (8) Ni1	0.05	BD (1) C15-C18	RY* (8) Ni1	0.07
	BD (1) C16-H21	LP* (7) Ni1	0.05	BD (1) C15-H19	LP* (5) Ni1	0.05
	BD (1) C18-H22	LP* (7) Ni1	0.05	BD (1) C15-H19	LP* (6) Ni1	0.17
	BD (1) C20-H23	LP* (7) Ni1	0.04	BD (1) C15-H19	LP* (7) Ni1	0.03
	CR (1) N13	LP* (6) Ni1	0.33	BD (1) C15-H19	LP* (8) Ni1	0.07
	CR (1) N13	LP* (7) Ni1	1.28	BD (1) C15-H19	RY* (4) Ni1	0.03
	CR (1) C14	LP* (7) Ni1	0.21	BD (1) C15-H19	RY* (8) Ni1	0.06
	CR (1) C15	LP* (7) Ni1	0.21	BD (1) C16-H21	LP* (5) Ni1	0.05
	LP (1) N13	LP* (6) Ni1	17.7	BD (1) C18-H22	LP* (5) Ni1	0.05
	LP (1) N13	LP* (7) Ni1	4.29	BD (1) C20-H23	LP* (5) Ni1	0.04
	LP (1) N13	RY* (1) Ni1	0.96	CR (1) N13	LP* (4) Ni1	0.32
	LP (1) N13	RY* (5) Ni1	0.59	CR (1) N13	LP* (5) Ni1	1.26
	LP (1) N13	RY* (8) Ni1	1.64	CR (1) N13	LP* (6) Ni1	0.11
	BD* (2) N13-C14	LP* (8) Ni1	0.07	CR (1) C14	LP* (5) Ni1	0.21
	BD* (2) N13-C14	LP* (9) Ni1	0.19	CR (1) C15	LP* (5) Ni1	0.21
				LP (1) N13	LP* (4) Ni1	33.83
				LP (1) N13	LP* (5) Ni1	4.23
				LP (1) N13	LP* (6) Ni1	4.66
				LP (1) N13	LP* (9) Ni1	0.11
				LP (1) N13	RY* (4) Ni1	0.93
				LP (1) N13	RY* (8) Ni1	1.36
				BD* (2) N13-C14	LP* (7) Ni1	0.26
				BD* (2) N13-C14	LP* (8) Ni1	0.1

Table S11. Second order perturbation analysis for the 'donor-acceptor' (bond-antibond) interactions between the NO_3^- and the Ni center of $[(NO_3)_2NiBH_4]^-$ in the NBO basis.

Geom.	*α* orbitals			*β* orbitals		
	Donor	Acceptor	Δ*E* (kcal/mol)	Donor	Acceptor	Δ*E* (kcal/mol)
	$^1NO_3^-$	Ni		$^1NO_3^-$	Ni	
	BD (1) N1-O2	LP* (6) Ni9	1.08	BD (1) N1-O2	LP* (4) Ni9	0.03
	BD (1) N1-O2	LP* (7) Ni9	1.69	BD (1) N1-O2	LP* (6) Ni9	1.24
	BD (1) N1-O2	LP* (8) Ni9	2.52	BD (1) N1-O2	LP* (7) Ni9	2.6
	BD (1) N1-O2	RY* (1) Ni9	0.03	BD (1) N1-O2	LP* (8) Ni9	1.57
	BD (1) N1-O2	RY* (4) Ni9	0.04	BD (1) N1-O2	LP* (9) Ni9	0.04
	BD (1) N1-O3	LP* (7) Ni9	0.07	BD (1) N1-O2	RY* (2) Ni9	0.03
	BD (2) N1-O3	LP* (6) Ni9	0.41	BD (1) N1-O2	RY* (3) Ni9	0.05
	BD (2) N1-O3	LP* (7) Ni9	0.38	BD (1) N1-O3	LP* (8) Ni9	0.08
	BD (2) N1-O3	LP* (8) Ni9	1.01	BD (2) N1-O3	LP* (6) Ni9	0.46
	BD (2) N1-O3	LP* (9) Ni9	0.11	BD (2) N1-O3	LP* (7) Ni9	1.04
	BD (1) N1-O4	LP* (6) Ni9	1.05	BD (2) N1-O3	LP* (8) Ni9	0.34
	BD (1) N1-O4	LP* (7) Ni9	0.39	BD (2) N1-O3	LP* (9) Ni9	0.06
	BD (1) N1-O4	LP* (8) Ni9	2.61	BD (1) N1-O4	LP* (5) Ni9	0.06
	BD (1) N1-O4	LP* (9) Ni9	1.19	BD (1) N1-O4	LP* (6) Ni9	1.23
	BD (1) N1-O4	RY* (2) Ni9	0.05	BD (1) N1-O4	LP* (7) Ni9	2.91
	CR (1) N1	LP* (6) Ni9	0.17	BD (1) N1-O4	LP* (8) Ni9	0.3
	CR (1) N1	LP* (7) Ni9	0.35	BD (1) N1-O4	LP* (9) Ni9	0.93
	CR (1) N1	LP* (8) Ni9	0.89	BD (1) N1-O4	RY* (1) Ni9	0.06
	CR (1) N1	LP* (9) Ni9	0.09	BD (1) N1-O4	RY* (7) Ni9	0.03
	CR (1) O2	LP* (6) Ni9	0.7	CR (1) N1	LP* (6) Ni9	0.2
	CR (1) O2	LP* (7) Ni9	1.47	CR (1) N1	LP* (7) Ni9	0.93
	CR (1) O2	LP* (8) Ni9	1.4	CR (1) N1	LP* (8) Ni9	0.32
	CR (1) O2	LP* (9) Ni9	0.17	CR (1) N1	LP* (9) Ni9	0.05
	CR (1) O4	LP* (6) Ni9	0.57	CR (1) O2	LP* (6) Ni9	0.77
	CR (1) O4	LP* (7) Ni9	0.07	CR (1) O2	LP* (7) Ni9	1.37
	CR (1) O4	LP* (8) Ni9	1.58	CR (1) O2	LP* (8) Ni9	1.41
	CR (1) O4	LP* (9) Ni9	1.37	CR (1) O2	LP* (9) Ni9	0.27
	LP (1) O2	LP* (6) Ni9	1.44	CR (1) O4	LP* (5) Ni9	0.05
	LP (1) O2	LP* (7) Ni9	4.02	CR (1) O4	LP* (6) Ni9	0.66
	LP (1) O2	LP* (8) Ni9	3.21	CR (1) O4	LP* (7) Ni9	1.79
	LP (1) O2	LP* (9) Ni9	0.93	CR (1) O4	LP* (8) Ni9	0.04
	LP (2) O2	LP* (6) Ni9	15.27	CR (1) O4	LP* (9) Ni9	1.16
	LP (2) O2	LP* (7) Ni9	6.24	LP (1) O2	LP* (4) Ni9	0.04
	LP (2) O2	LP* (8) Ni9	7.29	LP (1) O2	LP* (5) Ni9	0.09
	LP (2) O2	LP* (9) Ni9	1.92	LP (1) O2	LP* (6) Ni9	3.31
	LP (2) O2	RY* (1) Ni9	0.04	LP (1) O2	LP* (7) Ni9	4.22
	LP (2) O2	RY* (3) Ni9	0.03	LP (1) O2	LP* (8) Ni9	4.98
	LP (2) O2	RY* (4) Ni9	0.09	LP (1) O2	LP* (9) Ni9	1.74
	LP (2) O2	RY* (6) Ni9	0.18	LP (2) O2	LP* (4) Ni9	6.29
	LP (2) O2	RY* (7) Ni9	0.06	LP (2) O2	LP* (5) Ni9	4.45
	LP (2) O2	RY* (9) Ni9	0.05	LP (2) O2	LP* (6) Ni9	16.4
	LP (3) O2	LP* (7) Ni9	0.81	LP (2) O2	LP* (7) Ni9	6.59
	LP (3) O2	LP* (8) Ni9	0.78	LP (2) O2	LP* (8) Ni9	4.69
	LP (3) O2	LP* (9) Ni9	0.33	LP (2) O2	LP* (9) Ni9	2.82
	LP (1) O3	LP* (6) Ni9	0.1	LP (2) O2	RY* (1) Ni9	0.08
	LP (1) O3	LP* (8) Ni9	0.06	LP (2) O2	RY* (3) Ni9	0.07
	LP (1) O4	LP* (6) Ni9	1.34	LP (2) O2	RY* (5) Ni9	0.18
	LP (1) O4	LP* (7) Ni9	0.04	LP (2) O2	RY* (9) Ni9	0.04
	LP (1) O4	LP* (8) Ni9	3.9	LP (3) O2	LP* (4) Ni9	0.06
	LP (1) O4	LP* (9) Ni9	4.57	LP (3) O2	LP* (7) Ni9	0.7
	LP (2) O4	LP* (6) Ni9	12.68	LP (3) O2	LP* (8) Ni9	0.88
	LP (2) O4	LP* (8) Ni9	8.49	LP (3) O2	LP* (9) Ni9	0.41
	LP (2) O4	LP* (9) Ni9	10.35	LP (1) O3	LP* (6) Ni9	0.1
	LP (2) O4	RY* (2) Ni9	0.03	LP (1) O3	LP* (7) Ni9	0.06



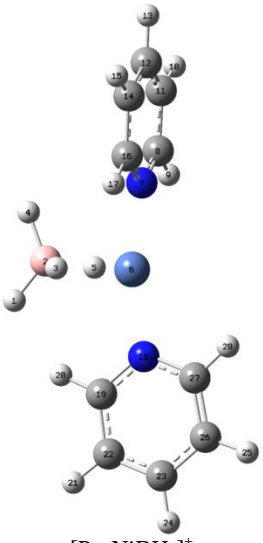
$[(NO_3)_2NiBH_4]^-$

	LP (2) O4	RY* (4) Ni9	0.05	LP (2) O3	LP* (5) Ni9	0.03
	LP (2) O4	RY* (6) Ni9	0.07	LP (1) O4	LP* (5) Ni9	0.17
	LP (2) O4	RY* (7) Ni9	0.15	LP (1) O4	LP* (6) Ni9	2.93
	LP (2) O4	RY* (9) Ni9	0.03	LP (1) O4	LP* (7) Ni9	6.06
	LP (3) O4	LP* (6) Ni9	0.03	LP (1) O4	LP* (9) Ni9	5.34
	LP (3) O4	LP* (7) Ni9	0.68	LP (2) O4	LP* (5) Ni9	6.78
	LP (3) O4	LP* (8) Ni9	0.58	LP (2) O4	LP* (6) Ni9	16.8
	LP (3) O4	LP* (9) Ni9	0.35	LP (2) O4	LP* (7) Ni9	8.12
				LP (2) O4	LP* (8) Ni9	0.1
				LP (2) O4	LP* (9) Ni9	7.77
				LP (2) O4	RY* (3) Ni9	0.07
				LP (2) O4	RY* (5) Ni9	0.13
				LP (2) O4	RY* (9) Ni9	0.03
				LP (3) O4	LP* (4) Ni9	0.05
				LP (3) O4	LP* (5) Ni9	0.03
				LP (3) O4	LP* (7) Ni9	0.72
				LP (3) O4	LP* (8) Ni9	0.74
				LP (3) O4	LP* (9) Ni9	0.3
				BD* (1) N1-O2	RY* (4) Ni9	0.06
				BD* (1) N1-O3	LP* (5) Ni9	0.06
				BD* (1) N1-O4	RY* (2) Ni9	0.06
				BD* (1) N1-O4	RY* (4) Ni9	0.03
	$^{5}NO_3^-$	**Ni**		**$^{5}NO_3^-$**	**Ni**	
	BD (1) N5-O6	LP* (7) Ni9	0.07	BD (1) N5-O6	LP* (8) Ni9	0.08
	BD (2) N5-O6	LP* (6) Ni9	0.41	BD (2) N5-O6	LP* (6) Ni9	0.46
	BD (2) N5-O6	LP* (7) Ni9	0.38	BD (2) N5-O6	LP* (7) Ni9	1.04
	BD (2) N5-O6	LP* (8) Ni9	1.01	BD (2) N5-O6	LP* (8) Ni9	0.34
	BD (2) N5-O6	LP* (9) Ni9	0.11	BD (2) N5-O6	LP* (9) Ni9	0.06
	BD (1) N5-O7	LP* (6) Ni9	1.05	BD (1) N5-O7	LP* (5) Ni9	0.06
	BD (1) N5-O7	LP* (7) Ni9	0.39	BD (1) N5-O7	LP* (6) Ni9	1.23
	BD (1) N5-O7	LP* (8) Ni9	2.61	BD (1) N5-O7	LP* (7) Ni9	2.91
	BD (1) N5-O7	LP* (9) Ni9	1.19	BD (1) N5-O7	LP* (8) Ni9	0.3
	BD (1) N5-O7	RY* (2) Ni9	0.05	BD (1) N5-O7	LP* (9) Ni9	0.93
	BD (1) N5-O8	LP* (6) Ni9	1.08	BD (1) N5-O7	RY* (1) Ni9	0.06
	BD (1) N5-O8	LP* (7) Ni9	1.69	BD (1) N5-O7	RY* (7) Ni9	0.03
	BD (1) N5-O8	LP* (8) Ni9	2.52	BD (1) N5-O8	LP* (4) Ni9	0.03
	BD (1) N5-O8	RY* (1) Ni9	0.03	BD (1) N5-O8	LP* (6) Ni9	1.24
	BD (1) N5-O8	RY* (4) Ni9	0.04	BD (1) N5-O8	LP* (7) Ni9	2.6
	CR (1) N5	LP* (6) Ni9	0.17	BD (1) N5-O8	LP* (8) Ni9	1.57
	CR (1) N5	LP* (7) Ni9	0.35	BD (1) N5-O8	LP* (9) Ni9	0.04
	CR (1) N5	LP* (8) Ni9	0.89	BD (1) N5-O8	RY* (2) Ni9	0.03
	CR (1) N5	LP* (9) Ni9	0.09	BD (1) N5-O8	RY* (3) Ni9	0.05
	CR (1) O7	LP* (6) Ni9	0.57	CR (1) N5	LP* (6) Ni9	0.2
	CR (1) O7	LP* (7) Ni9	0.07	CR (1) N5	LP* (7) Ni9	0.93
	CR (1) O7	LP* (8) Ni9	1.58	CR (1) N5	LP* (8) Ni9	0.32
	CR (1) O7	LP* (9) Ni9	1.37	CR (1) N5	LP* (9) Ni9	0.05
	CR (1) O8	LP* (6) Ni9	0.7	CR (1) O7	LP* (5) Ni9	0.05
	CR (1) O8	LP* (7) Ni9	1.47	CR (1) O7	LP* (6) Ni9	0.66
	CR (1) O8	LP* (8) Ni9	1.4	CR (1) O7	LP* (7) Ni9	1.79
	CR (1) O8	LP* (9) Ni9	0.17	CR (1) O7	LP* (8) Ni9	0.04
	LP (1) O6	LP* (6) Ni9	0.1	CR (1) O7	LP* (9) Ni9	1.16
	LP (1) O6	LP* (8) Ni9	0.06	CR (1) O8	LP* (6) Ni9	0.77
	LP (1) O7	LP* (6) Ni9	1.34	CR (1) O8	LP* (7) Ni9	1.37
	LP (1) O7	LP* (7) Ni9	0.04	CR (1) O8	LP* (8) Ni9	1.41
	LP (1) O7	LP* (8) Ni9	3.9	CR (1) O8	LP* (9) Ni9	0.27
	LP (1) O7	LP* (9) Ni9	4.57	LP (1) O6	LP* (6) Ni9	0.1
	LP (2) O7	LP* (6) Ni9	12.67	LP (1) O6	LP* (7) Ni9	0.06
	LP (2) O7	LP* (8) Ni9	8.49	LP (2) O6	LP* (5) Ni9	0.03
	LP (2) O7	LP* (9) Ni9	10.35	LP (1) O7	LP* (5) Ni9	0.17
	LP (2) O7	RY* (2) Ni9	0.03	LP (1) O7	LP* (6) Ni9	2.93
	LP (2) O7	RY* (4) Ni9	0.05	LP (1) O7	LP* (7) Ni9	6.06

	LP (2) O7	RY* (6) Ni9	0.07	LP (1) O7	LP* (9) Ni9	5.34
	LP (2) O7	RY* (7) Ni9	0.15	LP (2) O7	LP* (5) Ni9	6.78
	LP (2) O7	RY* (9) Ni9	0.03	LP (2) O7	LP* (6) Ni9	16.8
	LP (3) O7	LP* (6) Ni9	0.03	LP (2) O7	LP* (7) Ni9	8.12
	LP (3) O7	LP* (7) Ni9	0.68	LP (2) O7	LP* (8) Ni9	0.1
	LP (3) O7	LP* (8) Ni9	0.58	LP (2) O7	LP* (9) Ni9	7.77
	LP (3) O7	LP* (9) Ni9	0.35	LP (2) O7	RY* (3) Ni9	0.07
	LP (1) O8	LP* (6) Ni9	1.44	LP (2) O7	RY* (5) Ni9	0.13
	LP (1) O8	LP* (7) Ni9	4.02	LP (2) O7	RY* (9) Ni9	0.03
	LP (1) O8	LP* (8) Ni9	3.21	LP (3) O7	LP* (4) Ni9	0.05
	LP (1) O8	LP* (9) Ni9	0.93	LP (3) O7	LP* (5) Ni9	0.03
	LP (2) O8	LP* (6) Ni9	15.27	LP (3) O7	LP* (7) Ni9	0.72
	LP (2) O8	LP* (7) Ni9	6.24	LP (3) O7	LP* (8) Ni9	0.74
	LP (2) O8	LP* (8) Ni9	7.29	LP (3) O7	LP* (9) Ni9	0.3
	LP (2) O8	LP* (9) Ni9	1.92	LP (1) O8	LP* (4) Ni9	0.04
	LP (2) O8	RY* (1) Ni9	0.04	LP (1) O8	LP* (5) Ni9	0.09
	LP (2) O8	RY* (3) Ni9	0.03	LP (1) O8	LP* (6) Ni9	3.31
	LP (2) O8	RY* (4) Ni9	0.09	LP (1) O8	LP* (7) Ni9	4.23
	LP (2) O8	RY* (6) Ni9	0.18	LP (1) O8	LP* (8) Ni9	4.98
	LP (2) O8	RY* (7) Ni9	0.06	LP (1) O8	LP* (9) Ni9	1.74
	LP (2) O8	RY* (9) Ni9	0.05	LP (2) O8	LP* (4) Ni9	6.29
	LP (3) O8	LP* (7) Ni9	0.81	LP (2) O8	LP* (5) Ni9	4.45
	LP (3) O8	LP* (8) Ni9	0.78	LP (2) O8	LP* (6) Ni9	16.4
	LP (3) O8	LP* (9) Ni9	0.33	LP (2) O8	LP* (7) Ni9	6.6
				LP (2) O8	LP* (8) Ni9	4.68
				LP (2) O8	LP* (9) Ni9	2.82
				LP (2) O8	RY* (1) Ni9	0.08
				LP (2) O8	RY* (3) Ni9	0.07
				LP (2) O8	RY* (5) Ni9	0.18
				LP (2) O8	RY* (9) Ni9	0.04
				LP (3) O8	LP* (4) Ni9	0.06
				LP (3) O8	LP* (7) Ni9	0.7
				LP (3) O8	LP* (8) Ni9	0.88
				LP (3) O8	LP* (9) Ni9	0.41
				BD* (1) N5-O6	LP* (5) Ni9	0.06
				BD* (1) N5-O7	RY* (2) Ni9	0.06
				BD* (1) N5-O7	RY* (4) Ni9	0.03
				BD* (1) N5-O8	RY* (4) Ni9	0.06

Table S12. Second order perturbation analysis for the 'donor-acceptor' (bond-antibond) interactions between the Py and the Ni center of $[Py_2NiBH_4]^+$ in the NBO basis.

Geom.	*α* orbitals			*β* orbitals		
	Donor	**Acceptor**	**Δ*E*** **(kcal/mol)**	**Donor**	**Acceptor**	**Δ*E*** **(kcal/mol)**
	$^7NC_5H_5$	**Ni**		**$^7NC_5H_5$**	**Ni**	
	BD (1) N7-C8	LP* (6) Ni6	1.16	BD (1) N7-C8	LP* (4) Ni6	0.49
	BD (1) N7-C8	LP* (7) Ni6	3.42	BD (1) N7-C8	LP* (6) Ni6	0.77
	BD (1) N7-C8	RY* (1) Ni6	0.03	BD (1) N7-C8	LP* (7) Ni6	3.3
	BD (1) N7-C8	RY* (3) Ni6	0.03	BD (1) N7-C8	LP* (8) Ni6	0.13
	BD (1) N7-C8	RY* (4) Ni6	0.16	BD (1) N7-C8	RY* (2) Ni6	0.03
	BD (1) N7-C8	RY* (6) Ni6	0.03	BD (1) N7-C8	RY* (4) Ni6	0.16
	BD (2) N7-C8	LP* (8) Ni6	0.26	BD (1) N7-C16	LP* (4) Ni6	0.46
	BD (1) N7-C16	LP* (6) Ni6	1.21	BD (1) N7-C16	LP* (6) Ni6	0.84
	BD (1) N7-C16	LP* (7) Ni6	3.41	BD (1) N7-C16	LP* (7) Ni6	3.32
	BD (1) N7-C16	RY* (1) Ni6	0.03	BD (1) N7-C16	LP* (8) Ni6	0.1
	BD (1) N7-C16	RY* (3) Ni6	0.06	BD (1) N7-C16	RY* (2) Ni6	0.03
	BD (1) N7-C16	RY* (4) Ni6	0.16	BD (1) N7-C16	RY* (4) Ni6	0.17
	BD (1) N7-C16	RY* (6) Ni6	0.04	BD (2) N7-C16	LP* (4) Ni6	0.28
	BD (1) C8-H9	LP* (6) Ni6	0.26	BD (2) N7-C16	LP* (7) Ni6	0.03
	BD (1) C8-H9	LP* (7) Ni6	0.46	BD (2) N7-C16	LP* (8) Ni6	0.5
	BD (1) C8-H9	LP* (9) Ni6	0.25	BD (1) C8-H9	LP* (5) Ni6	0.04
	BD (1) C8-H9	RY* (4) Ni6	0.11	BD (1) C8-H9	LP* (6) Ni6	0.23
	BD (1) C8-C11	LP* (6) Ni6	0.1	BD (1) C8-H9	LP* (7) Ni6	0.46
	BD (1) C8-C11	LP* (7) Ni6	0.81	BD (1) C8-H9	LP* (9) Ni6	0.27
	BD (1) C8-C11	RY* (4) Ni6	0.08	BD (1) C8-H9	RY* (4) Ni6	0.11
	BD (1) H10-C11	LP* (7) Ni6	0.05	BD (1) C8-C11	LP* (4) Ni6	0.05
	BD (1) C12-H13	LP* (7) Ni6	0.03	BD (1) C8-C11	LP* (6) Ni6	0.06
	BD (1) C14-H15	LP* (7) Ni6	0.05	BD (1) C8-C11	LP* (7) Ni6	0.77
	BD (1) C14-C16	LP* (6) Ni6	0.09	BD (1) C8-C11	LP* (8) Ni6	0.04
	BD (1) C14-C16	LP* (7) Ni6	0.81	BD (1) C8-C11	RY* (4) Ni6	0.08
	BD (1) C14-C16	LP* (9) Ni6	0.03	BD (1) H10-C11	LP* (7) Ni6	0.05
	BD (1) C14-C16	RY* (4) Ni6	0.08	BD (1) C12-H13	LP* (7) Ni6	0.03
	BD (1) C16-H17	LP* (6) Ni6	0.27	BD (1) C14-H15	LP* (7) Ni6	0.05
	BD (1) C16-H17	LP* (7) Ni6	0.42	BD (1) C14-C16	LP* (4) Ni6	0.05
	BD (1) C16-H17	LP* (9) Ni6	0.33	BD (1) C14-C16	LP* (6) Ni6	0.04
	BD (1) C16-H17	RY* (4) Ni6	0.09	BD (1) C14-C16	LP* (7) Ni6	0.77
	CR (1) N7	LP* (6) Ni6	0.51	BD (1) C14-C16	LP* (8) Ni6	0.06
	CR (1) N7	LP* (7) Ni6	2.86	BD (1) C14-C16	RY* (4) Ni6	0.09
	CR (1) C8	LP* (6) Ni6	0.04	BD (1) C16-H17	LP* (5) Ni6	0.03
	CR (1) C8	LP* (7) Ni6	0.4	BD (1) C16-H17	LP* (6) Ni6	0.22
	CR (1) C16	LP* (6) Ni6	0.04	BD (1) C16-H17	LP* (7) Ni6	0.43
	CR (1) C16	LP* (7) Ni6	0.41	BD (1) C16-H17	LP* (8) Ni6	0.07
	LP (1) N7	LP* (6) Ni6	17.89	BD (1) C16-H17	LP* (9) Ni6	0.34
	LP (1) N7	LP* (7) Ni6	13.61	BD (1) C16-H17	RY* (4) Ni6	0.1
	LP (1) N7	RY* (1) Ni6	0.16	CR (1) N7	LP* (4) Ni6	0.28
	LP (1) N7	RY* (3) Ni6	0.1	CR (1) N7	LP* (6) Ni6	0.33
	LP (1) N7	RY* (4) Ni6	0.61	CR (1) N7	LP* (7) Ni6	2.83
	LP (1) N7	RY* (6) Ni6	0.15	CR (1) N7	LP* (8) Ni6	0.04
	BD* (2) N7-C8	LP* (8) Ni6	0.14	CR (1) C8	LP* (6) Ni6	0.03
				CR (1) C8	LP* (7) Ni6	0.4
				CR (1) C16	LP* (6) Ni6	0.03
				CR (1) C16	LP* (7) Ni6	0.41
				LP (1) N7	LP* (4) Ni6	27.52
				LP (1) N7	LP* (6) Ni6	11.16
				LP (1) N7	LP* (7) Ni6	13.17
				LP (1) N7	LP* (8) Ni6	0.31
				LP (1) N7	RY* (1) Ni6	0.07
				LP (1) N7	RY* (4) Ni6	0.41
				LP (1) N7	RY* (9) Ni6	0.04

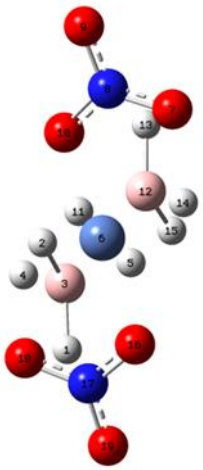


$[Py_2NiBH_4]^+$

			BD* (2) N7-C16	LP* (8) Ni6	0.28
$^{18}NC_5H_5$	**Ni**		**$^{18}NC_5H_5$**	**Ni**	
BD (1) N18-C19	LP* (6) Ni6	1.13	BD (1) N18-C19	LP* (4) Ni6	0.51
BD (1) N18-C19	LP* (7) Ni6	2.7	BD (1) N18-C19	LP* (6) Ni6	0.79
BD (1) N18-C19	LP* (8) Ni6	0.41	BD (1) N18-C19	LP* (7) Ni6	2.83
BD (1) N18-C19	RY* (4) Ni6	0.14	BD (1) N18-C19	LP* (8) Ni6	0.25
BD (2) N18-C19	LP* (9) Ni6	0.63	BD (1) N18-C19	RY* (4) Ni6	0.13
BD (1) N18-C27	LP* (6) Ni6	2.08	BD (2) N18-C19	LP* (9) Ni6	0.77
BD (1) N18-C27	LP* (7) Ni6	2.55	BD (1) N18-C27	LP* (4) Ni6	0.27
BD (1) N18-C27	RY* (1) Ni6	0.06	BD (1) N18-C27	LP* (6) Ni6	1.89
BD (1) N18-C27	RY* (3) Ni6	0.09	BD (1) N18-C27	LP* (7) Ni6	2.45
BD (1) N18-C27	RY* (4) Ni6	0.3	BD (1) N18-C27	RY* (1) Ni6	0.04
BD (1) N18-C27	RY* (6) Ni6	0.06	BD (1) N18-C27	RY* (2) Ni6	0.05
BD (1) C19-H20	LP* (6) Ni6	0.27	BD (1) N18-C27	RY* (4) Ni6	0.33
BD (1) C19-H20	LP* (7) Ni6	0.49	BD (1) C19-H20	LP* (6) Ni6	0.32
BD (1) C19-H20	LP* (8) Ni6	0.05	BD (1) C19-H20	LP* (7) Ni6	0.42
BD (1) C19-H20	RY* (3) Ni6	0.03	BD (1) C19-H20	LP* (8) Ni6	0.05
BD (1) C19-H20	RY* (4) Ni6	0.15	BD (1) C19-H20	RY* (4) Ni6	0.15
BD (1) C19-C22	LP* (6) Ni6	0.17	BD (1) C19-C22	LP* (6) Ni6	0.15
BD (1) C19-C22	LP* (7) Ni6	0.73	BD (1) C19-C22	LP* (7) Ni6	0.72
BD (1) C19-C22	RY* (3) Ni6	0.04	BD (1) C19-C22	RY* (2) Ni6	0.03
BD (1) C19-C22	RY* (4) Ni6	0.08	BD (1) C19-C22	RY* (4) Ni6	0.09
BD (1) C19-C22	RY* (6) Ni6	0.03	BD (1) H21-C22	LP* (7) Ni6	0.05
BD (1) H21-C22	LP* (7) Ni6	0.05	BD (1) C23-H24	LP* (7) Ni6	0.03
BD (1) C23-H24	LP* (7) Ni6	0.03	BD (1) C23-C26	LP* (8) Ni6	0.04
BD (1) C23-C26	LP* (8) Ni6	0.04	BD (1) H25-C26	LP* (7) Ni6	0.05
BD (1) H25-C26	LP* (7) Ni6	0.04	BD (1) H25-C26	LP* (8) Ni6	0.04
BD (1) H25-C26	LP* (8) Ni6	0.04	BD (1) C26-C27	LP* (4) Ni6	0.07
BD (1) C26-C27	LP* (6) Ni6	0.06	BD (1) C26-C27	LP* (7) Ni6	0.8
BD (1) C26-C27	LP* (7) Ni6	0.69	BD (1) C26-C27	LP* (8) Ni6	0.19
BD (1) C26-C27	LP* (8) Ni6	0.31	BD (1) C26-C27	RY* (4) Ni6	0.1
BD (1) C26-C27	RY* (4) Ni6	0.1	BD (1) C27-H28	LP* (6) Ni6	0.31
BD (1) C27-H28	LP* (6) Ni6	0.43	BD (1) C27-H28	LP* (7) Ni6	0.24
BD (1) C27-H28	LP* (7) Ni6	0.19	BD (1) C27-H28	LP* (8) Ni6	0.44
BD (1) C27-H28	LP* (8) Ni6	0.26	BD (1) C27-H28	RY* (4) Ni6	0.12
BD (1) C27-H28	RY* (1) Ni6	0.03	CR (1) N18	LP* (4) Ni6	0.23
BD (1) C27-H28	RY* (4) Ni6	0.11	CR (1) N18	LP* (6) Ni6	0.51
BD (1) C27-H28	RY* (6) Ni6	0.04	CR (1) N18	LP* (7) Ni6	2.53
CR (1) N18	LP* (6) Ni6	0.65	CR (1) N18	LP* (8) Ni6	0.06
CR (1) N18	LP* (7) Ni6	2.43	CR (1) C19	LP* (6) Ni6	0.07
CR (1) N18	LP* (8) Ni6	0.16	CR (1) C19	LP* (7) Ni6	0.35
CR (1) C19	LP* (6) Ni6	0.07	CR (1) C27	LP* (6) Ni6	0.03
CR (1) C19	LP* (7) Ni6	0.35	CR (1) C27	LP* (7) Ni6	0.34
CR (1) C27	LP* (6) Ni6	0.04	CR (1) C27	LP* (8) Ni6	0.05
CR (1) C27	LP* (7) Ni6	0.31	LP (1) N18	LP* (4) Ni6	24.59
CR (1) C27	LP* (8) Ni6	0.07	LP (1) N18	LP* (6) Ni6	13.46
LP (1) N18	LP* (6) Ni6	19.46	LP (1) N18	LP* (7) Ni6	10.28
LP (1) N18	LP* (7) Ni6	9.87	LP (1) N18	LP* (8) Ni6	0.29
LP (1) N18	LP* (8) Ni6	0.78	LP (1) N18	RY* (4) Ni6	0.35
LP (1) N18	RY* (1) Ni6	0.06	LP (1) N18	RY* (9) Ni6	0.03
LP (1) N18	RY* (3) Ni6	0.08	BD* (2) N18-C19	LP* (9) Ni6	0.74
LP (1) N18	RY* (4) Ni6	0.55	BD* (2) C26-C27	LP* (9) Ni6	0.08
LP (1) N18	RY* (6) Ni6	0.11			
BD* (2) N18-C19	LP* (9) Ni6	0.41			
BD* (2) C26-C27	LP* (9) Ni6	0.03			

Table S13. Second order perturbation analysis for the 'donor-acceptor' (bond-antibond) interactions between the NO_3^- and the Ni center of $[(NO_3)_2Ni(BH_4)_2]^{2-}$ in the NBO basis.

Geom.	*α* orbitals			*β* orbitals		
	Donor	**Acceptor**	**Δ*E* (kcal/mol)**	**Donor**	**Acceptor**	**Δ*E* (kcal/mol)**
	$^8NO_3^-$	**Ni**		**$^8NO_3^-$**	**Ni**	
	BD (1) O7-N8	LP* (6) Ni6	0.29	BD (1) O7-N8	LP* (6) Ni6	0.28
	BD (1) O7-N8	LP* (7) Ni6	1	BD (1) O7-N8	LP* (7) Ni6	0.96
	BD (1) N8-O9	LP* (6) Ni6	0.24	BD (1) O7-N8	LP* (8) Ni6	0.05
	BD (1) N8-O9	LP* (7) Ni6	0.93	BD (1) N8-O9	LP* (6) Ni6	0.24
	BD (1) N8-O9	RY* (1) Ni6	0.03	BD (1) N8-O9	LP* (7) Ni6	0.83
	BD (1) N8-O10	LP* (6) Ni6	0.67	BD (1) N8-O9	LP* (8) Ni6	0.11
	BD (1) N8-O10	LP* (7) Ni6	3.46	BD (1) N8-O9	RY* (1) Ni6	0.03
	BD (1) N8-O10	LP* (8) Ni6	0.54	BD (1) N8-O10	LP* (6) Ni6	0.68
	BD (1) N8-O10	RY* (1) Ni6	0.09	BD (1) N8-O10	LP* (7) Ni6	2.48
	BD (1) N8-O10	RY* (8) Ni6	0.04	BD (1) N8-O10	LP* (8) Ni6	1.44
	CR (1) O7	LP* (6) Ni6	0.07	BD (1) N8-O10	RY* (1) Ni6	0.06
	CR (1) O7	LP* (7) Ni6	0.33	BD (1) N8-O10	RY* (2) Ni6	0.08
	CR (1) O7	LP* (8) Ni6	0.05	CR (1) O7	LP* (6) Ni6	0.06
	CR (1) N8	LP* (6) Ni6	0.09	CR (1) O7	LP* (7) Ni6	0.38
	CR (1) N8	LP* (7) Ni6	0.5	CR (1) N8	LP* (6) Ni6	0.09
	CR (1) O10	LP* (6) Ni6	0.79	CR (1) N8	LP* (7) Ni6	0.43
	CR (1) O10	LP* (7) Ni6	3.19	CR (1) N8	LP* (8) Ni6	0.08
	CR (1) O10	LP* (8) Ni6	0.68	CR (1) O10	LP* (4) Ni6	0.04
	LP (1) O7	LP* (6) Ni6	0.68	CR (1) O10	LP* (6) Ni6	0.89
	LP (1) O7	LP* (7) Ni6	2.02	CR (1) O10	LP* (7) Ni6	2.21
	LP (1) O7	LP* (8) Ni6	0.46	CR (1) O10	LP* (8) Ni6	1.63
	LP (1) O7	RY* (4) Ni6	0.04	LP (1) O7	LP* (6) Ni6	0.65
	LP (2) O7	LP* (6) Ni6	0.48	LP (1) O7	LP* (7) Ni6	2.41
	LP (2) O7	LP* (7) Ni6	2.04	LP (1) O7	LP* (8) Ni6	0.06
	LP (2) O7	LP* (8) Ni6	0.91	LP (1) O7	RY* (4) Ni6	0.04
	LP (2) O7	RY* (2) Ni6	0.03	LP (2) O7	LP* (6) Ni6	0.48
	LP (3) O7	LP* (9) Ni6	0.13	LP (2) O7	LP* (7) Ni6	2.73
	LP* (1) N8	LP* (9) Ni6	0.17	LP (2) O7	LP* (8) Ni6	0.25
	LP (1) O9	LP* (6) Ni6	0.05	LP (2) O7	RY* (2) Ni6	0.05
	LP (1) O9	LP* (7) Ni6	0.07	LP (1) O9	LP* (6) Ni6	0.06
	LP (2) O9	LP* (6) Ni6	0.05	LP (1) O9	LP* (7) Ni6	0.06
	LP (2) O9	RY* (1) Ni6	0.08	LP (2) O9	LP* (6) Ni6	0.05
	LP (2) O9	RY* (4) Ni6	0.03	LP (2) O9	RY* (1) Ni6	0.05
	LP (1) O10	LP* (6) Ni6	0.79	LP (2) O9	RY* (4) Ni6	0.05
	LP (1) O10	LP* (7) Ni6	5.6	LP (1) O10	LP* (4) Ni6	0.12
	LP (1) O10	LP* (8) Ni6	3.52	LP (1) O10	LP* (6) Ni6	3.25
	LP (1) O10	RY* (1) Ni6	0.33	LP (1) O10	LP* (7) Ni6	6.39
	LP (2) O10	LP* (6) Ni6	14.16	LP (1) O10	LP* (8) Ni6	8.94
	LP (2) O10	LP* (7) Ni6	22.21	LP (1) O10	RY* (1) Ni6	0.12
	LP (2) O10	LP* (8) Ni6	4.36	LP (2) O10	LP* (4) Ni6	6.31
	LP (2) O10	RY* (1) Ni6	0.7	LP (2) O10	LP* (6) Ni6	19.34
	LP (2) O10	RY* (4) Ni6	0.34	LP (2) O10	LP* (7) Ni6	14.96
	LP (2) O10	RY* (5) Ni6	0.03	LP (2) O10	LP* (8) Ni6	8.22
	LP (2) O10	RY* (8) Ni6	0.03	LP (2) O10	RY* (1) Ni6	0.64
	LP (3) O10	LP* (9) Ni6	1.26	LP (2) O10	RY* (4) Ni6	0.27
	BD* (1) N8-O10	RY* (1) Ni6	0.09	LP (3) O10	LP* (9) Ni6	1.36
				BD* (2) O7-N8	LP* (9) Ni6	0.23
				BD* (1) N8-O9	RY* (1) Ni6	0.03
				BD* (1) N8-O10	RY* (1) Ni6	0.07
	$^{17}NO_3^-$	**Ni**		**$^{17}NO_3^-$**	**Ni**	
	BD (1) O16-N17	LP* (6) Ni6	0.74	BD (1) O16-N17	LP* (6) Ni6	0.75
	BD (1) O16-N17	LP* (7) Ni6	3.64	BD (1) O16-N17	LP* (7) Ni6	2.71
	BD (1) O16-N17	LP* (8) Ni6	0.36	BD (1) O16-N17	LP* (8) Ni6	1.23



$[(NO_3)_2Ni(BH_4)_2]^{2-}$

	BD (1) O16-N17	RY* (1) Ni6	0.1	BD (1) O16-N17	RY* (1) Ni6	0.06
	BD (1) O16-N17	RY* (8) Ni6	0.05	BD (1) O16-N17	RY* (2) Ni6	0.08
	BD (1) N17-O18	LP* (6) Ni6	0.33	BD (1) N17-O18	LP* (6) Ni6	0.32
	BD (1) N17-O18	LP* (7) Ni6	1.07	BD (1) N17-O18	LP* (7) Ni6	1.06
	BD (1) N17-O19	LP* (6) Ni6	0.24	BD (1) N17-O19	LP* (6) Ni6	0.25
	BD (1) N17-O19	LP* (7) Ni6	0.95	BD (1) N17-O19	LP* (7) Ni6	0.86
	BD (1) N17-O19	RY* (1) Ni6	0.03	BD (1) N17-O19	LP* (8) Ni6	0.09
	CR (1) O16	LP* (6) Ni6	0.82	BD (1) N17-O19	RY* (1) Ni6	0.04
	CR (1) O16	LP* (7) Ni6	3.29	CR (1) O16	LP* (4) Ni6	0.04
	CR (1) O16	LP* (8) Ni6	0.53	CR (1) O16	LP* (6) Ni6	0.92
	CR (1) N17	LP* (6) Ni6	0.09	CR (1) O16	LP* (7) Ni6	2.32
	CR (1) N17	LP* (7) Ni6	0.53	CR (1) O16	LP* (8) Ni6	1.49
	CR (1) O18	LP* (6) Ni6	0.08	CR (1) N17	LP* (6) Ni6	0.09
	CR (1) O18	LP* (7) Ni6	0.36	CR (1) N17	LP* (7) Ni6	0.47
	CR (1) O18	LP* (8) Ni6	0.08	CR (1) N17	LP* (8) Ni6	0.07
	LP (1) O16	LP* (6) Ni6	0.87	CR (1) O18	LP* (6) Ni6	0.08
	LP (1) O16	LP* (7) Ni6	6.07	CR (1) O18	LP* (7) Ni6	0.42
	LP (1) O16	LP* (8) Ni6	3.01	LP (1) O16	LP* (4) Ni6	0.11
	LP (1) O16	RY* (1) Ni6	0.32	LP (1) O16	LP* (6) Ni6	3.23
	LP (1) O16	RY* (2) Ni6	0.03	LP (1) O16	LP* (7) Ni6	6.8
	LP (2) O16	LP* (6) Ni6	14.44	LP (1) O16	LP* (8) Ni6	8.24
	LP (2) O16	LP* (7) Ni6	22.63	LP (1) O16	RY* (1) Ni6	0.13
	LP (2) O16	LP* (8) Ni6	3.44	LP (2) O16	LP* (4) Ni6	6.24
	LP (2) O16	RY* (1) Ni6	0.7	LP (2) O16	LP* (6) Ni6	19.54
	LP (2) O16	RY* (4) Ni6	0.35	LP (2) O16	LP* (7) Ni6	14.95
	LP (2) O16	RY* (8) Ni6	0.03	LP (2) O16	LP* (8) Ni6	7.97
	LP (3) O16	LP* (9) Ni6	1.25	LP (2) O16	RY* (1) Ni6	0.62
	LP* (1) N17	LP* (9) Ni6	0.17	LP (2) O16	RY* (3) Ni6	0.04
	LP (1) O18	LP* (6) Ni6	0.7	LP (2) O16	RY* (4) Ni6	0.26
	LP (1) O18	LP* (7) Ni6	2.05	LP (3) O16	LP* (4) Ni6	0.11
	LP (1) O18	LP* (8) Ni6	0.64	LP (3) O16	LP* (6) Ni6	0.18
	LP (1) O18	RY* (4) Ni6	0.04	LP (3) O16	LP* (7) Ni6	0.1
	LP (2) O18	LP* (6) Ni6	0.59	LP (3) O16	LP* (8) Ni6	0.08
	LP (2) O18	LP* (7) Ni6	2.07	LP (3) O16	LP* (9) Ni6	1.34
	LP (2) O18	LP* (8) Ni6	1.26	LP (1) O18	LP* (6) Ni6	0.72
	LP (2) O18	RY* (2) Ni6	0.03	LP (1) O18	LP* (7) Ni6	2.51
	LP (3) O18	LP* (9) Ni6	0.14	LP (1) O18	LP* (8) Ni6	0.12
	LP (1) O19	LP* (6) Ni6	0.06	LP (1) O18	RY* (4) Ni6	0.04
	LP (1) O19	LP* (7) Ni6	0.07	LP (2) O18	LP* (6) Ni6	0.63
	LP (2) O19	LP* (6) Ni6	0.04	LP (2) O18	LP* (7) Ni6	2.89
	LP (2) O19	RY* (1) Ni6	0.08	LP (2) O18	LP* (8) Ni6	0.41
	LP (2) O19	RY* (4) Ni6	0.03	LP (2) O18	RY* (2) Ni6	0.05
	BD* (1) O16-N17	RY* (1) Ni6	0.1	LP (1) O19	LP* (6) Ni6	0.06
				LP (1) O19	LP* (7) Ni6	0.06
				LP (2) O19	LP* (6) Ni6	0.05
				LP (2) O19	RY* (1) Ni6	0.05
				LP (2) O19	RY* (4) Ni6	0.05
				BD* (1) O16-N17	RY* (1) Ni6	0.08
				BD* (2) N17-O18	LP* (9) Ni6	0.24
				BD* (1) N17-O19	RY* (1) Ni6	0.03

Table S14. Second order perturbation analysis for the 'donor-acceptor' (bond-antibond) interactions between the Py and the Ni center of $Py_2Ni(BH_4)_2$ in the NBO basis.

Geom.	*α* orbitals			*β* orbitals		
	Donor	**Acceptor**	**Δ*E* (kcal/mol)**	**Donor**	**Acceptor**	**Δ*E* (kcal/mol)**
	$^{7}NC_5H_5$	**Ni**		**$^{7}NC_5H_5$**	**Ni**	
	BD (1) N7-C8	LP* (6) Ni6	1.71	BD (1) N7-C8	LP* (4) Ni6	0.09
	BD (1) N7-C8	LP* (8) Ni6	5.43	BD (1) N7-C8	LP* (6) Ni6	1.83
	BD (1) N7-C8	RY* (1) Ni6	0.03	BD (1) N7-C8	LP* (8) Ni6	5.46
	BD (1) N7-C8	RY* (3) Ni6	0.03	BD (1) N7-C8	RY* (2) Ni6	0.03
	BD (1) N7-C8	RY* (4) Ni6	0.09	BD (1) N7-C8	RY* (3) Ni6	0.2
	BD (1) N7-C8	RY* (5) Ni6	0.17	BD (1) N7-C8	RY* (7) Ni6	0.04
	BD (2) N7-C8	LP* (7) Ni6	0.1	BD (2) N7-C8	LP* (9) Ni6	0.12
	BD (1) N7-C16	LP* (6) Ni6	1.71	BD (1) N7-C16	LP* (4) Ni6	0.09
	BD (1) N7-C16	LP* (8) Ni6	5.43	BD (1) N7-C16	LP* (6) Ni6	1.83
	BD (1) N7-C16	RY* (1) Ni6	0.03	BD (1) N7-C16	LP* (8) Ni6	5.46
	BD (1) N7-C16	RY* (3) Ni6	0.03	BD (1) N7-C16	RY* (2) Ni6	0.03
	BD (1) N7-C16	RY* (4) Ni6	0.09	BD (1) N7-C16	RY* (3) Ni6	0.2
	BD (1) N7-C16	RY* (5) Ni6	0.17	BD (1) N7-C16	RY* (7) Ni6	0.04
	BD (1) C8-H9	LP* (6) Ni6	0.54	BD (1) C8-H9	LP* (6) Ni6	0.53
	BD (1) C8-H9	LP* (8) Ni6	0.78	BD (1) C8-H9	LP* (7) Ni6	0.45
	BD (1) C8-H9	LP* (9) Ni6	0.44	BD (1) C8-H9	LP* (8) Ni6	0.78
	BD (1) C8-H9	RY* (1) Ni6	0.06	BD (1) C8-H9	RY* (3) Ni6	0.14
	BD (1) C8-H9	RY* (4) Ni6	0.05	BD (1) C8-H9	RY* (7) Ni6	0.03
	BD (1) C8-H9	RY* (5) Ni6	0.11	BD (1) C8-C11	LP* (6) Ni6	0.18
	BD (1) C8-C11	LP* (6) Ni6	0.17	BD (1) C8-C11	LP* (8) Ni6	0.91
	BD (1) C8-C11	LP* (8) Ni6	0.9	BD (1) C8-C11	RY* (1) Ni6	0.03
	BD (1) C8-C11	RY* (1) Ni6	0.05	BD (1) C8-C11	RY* (3) Ni6	0.07
	BD (1) C8-C11	RY* (5) Ni6	0.06	BD (1) H10-C11	LP* (8) Ni6	0.05
	BD (1) H10-C11	LP* (8) Ni6	0.05	BD (1) C14-H15	LP* (8) Ni6	0.05
	BD (1) C14-H15	LP* (8) Ni6	0.05	BD (1) C14-C16	LP* (6) Ni6	0.18
	BD (1) C14-C16	LP* (6) Ni6	0.17	BD (1) C14-C16	LP* (8) Ni6	0.91
	BD (1) C14-C16	LP* (8) Ni6	0.9	BD (1) C14-C16	RY* (1) Ni6	0.03
	BD (1) C14-C16	RY* (1) Ni6	0.05	BD (1) C14-C16	RY* (3) Ni6	0.07
	BD (1) C14-C16	RY* (5) Ni6	0.06	BD (2) C14-C16	LP* (9) Ni6	0.04
	BD (2) C14-C16	LP* (7) Ni6	0.04	BD (1) C16-H17	LP* (6) Ni6	0.53
	BD (1) C16-H17	LP* (6) Ni6	0.54	BD (1) C16-H17	LP* (7) Ni6	0.45
	BD (1) C16-H17	LP* (8) Ni6	0.78	BD (1) C16-H17	LP* (8) Ni6	0.78
	BD (1) C16-H17	LP* (9) Ni6	0.44	BD (1) C16-H17	RY* (3) Ni6	0.14
	BD (1) C16-H17	RY* (1) Ni6	0.06	BD (1) C16-H17	RY* (7) Ni6	0.03
	BD (1) C16-H17	RY* (4) Ni6	0.05	CR (1) N7	LP* (4) Ni6	0.08
	BD (1) C16-H17	RY* (5) Ni6	0.11	CR (1) N7	LP* (6) Ni6	0.71
	CR (1) N7	LP* (6) Ni6	0.67	CR (1) N7	LP* (8) Ni6	3.74
	CR (1) N7	LP* (8) Ni6	3.77	CR (1) C8	LP* (6) Ni6	0.1
	CR (1) C8	LP* (6) Ni6	0.1	CR (1) C8	LP* (8) Ni6	0.48
$Py_2Ni(BH_4)_2$	CR (1) C8	LP* (8) Ni6	0.48	CR (1) C16	LP* (6) Ni6	0.1
	CR (1) C16	LP* (6) Ni6	0.1	CR (1) C16	LP* (8) Ni6	0.48
	CR (1) C16	LP* (8) Ni6	0.48	LP (1) N7	LP* (4) Ni6	15.38
	LP (1) N7	LP* (6) Ni6	14.87	LP (1) N7	LP* (6) Ni6	17.83
	LP (1) N7	LP* (8) Ni6	21	LP (1) N7	LP* (8) Ni6	21.17
	LP (1) N7	RY* (1) Ni6	0.15	LP (1) N7	RY* (1) Ni6	0.03
	LP (1) N7	RY* (4) Ni6	0.14	LP (1) N7	RY* (3) Ni6	0.13
	LP (1) N7	RY* (5) Ni6	0.27	LP (1) N7	RY* (4) Ni6	0.03
	LP (1) N7	RY* (6) Ni6	0.06	LP (1) N7	RY* (7) Ni6	0.04
	BD* (2) N7-C8	LP* (7) Ni6	0.1	BD* (2) N7-C8	LP* (9) Ni6	0.12
	$^{18}NC_5H_5$	**Ni**		**$^{18}NC_5H_5$**	**Ni**	
	BD (1) N18-C19	LP* (6) Ni6	1.73	BD (1) N18-C19	LP* (4) Ni6	0.09
	BD (1) N18-C19	LP* (8) Ni6	5.37	BD (1) N18-C19	LP* (6) Ni6	1.84
	BD (1) N18-C19	RY* (1) Ni6	0.03	BD (1) N18-C19	LP* (8) Ni6	5.4

	BD (1) N18-C19	RY* (3) Ni6	0.03	BD (1) N18-C19	RY* (2) Ni6	0.03
	BD (1) N18-C19	RY* (4) Ni6	0.09	BD (1) N18-C19	RY* (3) Ni6	0.2
	BD (1) N18-C19	RY* (5) Ni6	0.16	BD (1) N18-C19	RY* (7) Ni6	0.04
	BD (2) N18-C19	LP* (7) Ni6	0.09	BD (2) N18-C19	LP* (9) Ni6	0.13
	BD (2) N18-C19	LP* (9) Ni6	0.03	BD (1) N18-C27	LP* (4) Ni6	0.09
	BD (1) N18-C27	LP* (6) Ni6	1.73	BD (1) N18-C27	LP* (6) Ni6	1.84
	BD (1) N18-C27	LP* (8) Ni6	5.38	BD (1) N18-C27	LP* (8) Ni6	5.4
	BD (1) N18-C27	RY* (1) Ni6	0.03	BD (1) N18-C27	RY* (2) Ni6	0.03
	BD (1) N18-C27	RY* (3) Ni6	0.03	BD (1) N18-C27	RY* (3) Ni6	0.2
	BD (1) N18-C27	RY* (4) Ni6	0.09	BD (1) N18-C27	RY* (7) Ni6	0.04
	BD (1) N18-C27	RY* (5) Ni6	0.16	BD (1) C19-H20	LP* (6) Ni6	0.53
	BD (1) C19-H20	LP* (6) Ni6	0.53	BD (1) C19-H20	LP* (7) Ni6	0.44
	BD (1) C19-H20	LP* (8) Ni6	0.77	BD (1) C19-H20	LP* (8) Ni6	0.77
	BD (1) C19-H20	LP* (9) Ni6	0.42	BD (1) C19-H20	RY* (3) Ni6	0.14
	BD (1) C19-H20	RY* (1) Ni6	0.06	BD (1) C19-H20	RY* (7) Ni6	0.03
	BD (1) C19-H20	RY* (4) Ni6	0.04	BD (1) C19-C22	LP* (6) Ni6	0.18
	BD (1) C19-H20	RY* (5) Ni6	0.11	BD (1) C19-C22	LP* (8) Ni6	0.9
	BD (1) C19-C22	LP* (6) Ni6	0.17	BD (1) C19-C22	RY* (1) Ni6	0.03
	BD (1) C19-C22	LP* (8) Ni6	0.9	BD (1) C19-C22	RY* (3) Ni6	0.06
	BD (1) C19-C22	RY* (1) Ni6	0.05	BD (1) H21-C22	LP* (8) Ni6	0.05
	BD (1) C19-C22	RY* (5) Ni6	0.06	BD (1) H25-C26	LP* (8) Ni6	0.05
	BD (1) H21-C22	LP* (8) Ni6	0.05	BD (1) C26-C27	LP* (6) Ni6	0.18
	BD (1) H25-C26	LP* (8) Ni6	0.05	BD (1) C26-C27	LP* (8) Ni6	0.9
	BD (1) C26-C27	LP* (6) Ni6	0.17	BD (1) C26-C27	RY* (1) Ni6	0.03
	BD (1) C26-C27	LP* (8) Ni6	0.9	BD (1) C26-C27	RY* (3) Ni6	0.06
	BD (1) C26-C27	RY* (1) Ni6	0.05	BD (2) C26-C27	LP* (9) Ni6	0.04
	BD (1) C26-C27	RY* (5) Ni6	0.06	BD (1) C27-H28	LP* (6) Ni6	0.53
	BD (2) C26-C27	LP* (7) Ni6	0.04	BD (1) C27-H28	LP* (7) Ni6	0.44
	BD (1) C27-H28	LP* (6) Ni6	0.53	BD (1) C27-H28	LP* (8) Ni6	0.77
	BD (1) C27-H28	LP* (8) Ni6	0.77	BD (1) C27-H28	RY* (3) Ni6	0.14
	BD (1) C27-H28	LP* (9) Ni6	0.42	BD (1) C27-H28	RY* (7) Ni6	0.03
	BD (1) C27-H28	RY* (1) Ni6	0.06	CR (1) N18	LP* (4) Ni6	0.08
	BD (1) C27-H28	RY* (4) Ni6	0.04	CR (1) N18	LP* (6) Ni6	0.72
	BD (1) C27-H28	RY* (5) Ni6	0.11	CR (1) N18	LP* (8) Ni6	3.72
	CR (1) N18	LP* (6) Ni6	0.68	CR (1) C19	LP* (6) Ni6	0.1
	CR (1) N18	LP* (8) Ni6	3.75	CR (1) C19	LP* (8) Ni6	0.48
	CR (1) C19	LP* (6) Ni6	0.1	CR (1) C27	LP* (6) Ni6	0.1
	CR (1) C19	LP* (8) Ni6	0.48	CR (1) C27	LP* (8) Ni6	0.48
	CR (1) C27	LP* (6) Ni6	0.1	LP (1) N18	LP* (4) Ni6	15.26
	CR (1) C27	LP* (8) Ni6	0.48	LP (1) N18	LP* (6) Ni6	17.96
	LP (1) N18	LP* (6) Ni6	14.96	LP (1) N18	LP* (8) Ni6	20.99
	LP (1) N18	LP* (8) Ni6	20.81	LP (1) N18	RY* (1) Ni6	0.03
	LP (1) N18	RY* (1) Ni6	0.16	LP (1) N18	RY* (3) Ni6	0.13
	LP (1) N18	RY* (4) Ni6	0.14	LP (1) N18	RY* (7) Ni6	0.04
	LP (1) N18	RY* (5) Ni6	0.27	BD* (2) N18-C19	LP* (9) Ni6	0.12
	BD* (2) N18-C19	LP* (7) Ni6	0.1			

Table S15. E_0s and E_Gs of H_4BNiPy_2 and its potential products HNiPy and H_3BPy.

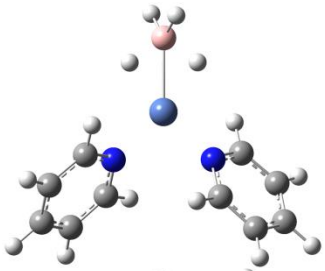
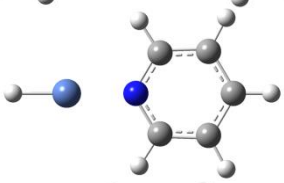
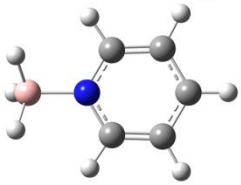
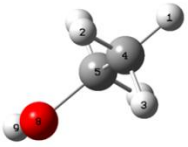
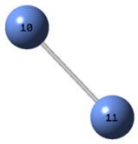
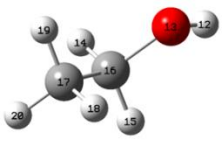
Acronym	Geom.	Energy (a.u.)
H_4BNiPy_2		E_0 = –692.612472 E_G = –692.658824
HNiPy		E_0 = –417.933269 E_G = –417.965682
H_3BPy		E_0 = –274.640415 E_G = –274.672136

Table S16. Second order perturbation analysis for the 'donor-acceptor' (bond-antibond) interactions between the EtOH and the Ni center of $Ni_2(EtOH)_2$ in the NBO basis.

Geom.	*α* orbitals			*β* orbitals		
	Donor	Acceptor	Δ*E* (kcal/mol)	Donor	Acceptor	Δ*E* (kcal/mol)
	Et-^{8}OH	**Ni**		**Et-^{8}OH**	**Ni**	
	BD (1) H1-C4	LP* (6) Ni10	0.1	BD (1) H1-C4	LP* (6) Ni10	0.1
	BD (1) H2-C4	LP* (6) Ni10	0.04	BD (1) H2-C4	LP* (6) Ni10	0.03
		BD* (1)			BD* (1)	
	BD (1) H2-C4	Ni10-Ni11	0.06	BD (1) H2-C4	Ni10-Ni11	0.07
	BD (1) H3-C4	LP* (6) Ni10	0.13	BD (1) H3-C4	LP* (6) Ni10	0.11
	BD (1) H3-C4	LP* (7) Ni10	0.03	BD (1) H3-C4	LP* (7) Ni10	0.1
	BD (1) H3-C4	LP* (8) Ni10	0.08	BD (1) H3-C4	LP* (8) Ni10	0.05
	BD (1) H3-C4	LP* (6) Ni11	0.05	BD (1) H3-C4	LP* (6) Ni11	0.09
	BD (1) H3-C4	LP* (8) Ni11	0.05	BD (1) H3-C4	LP* (8) Ni11	0.03
		BD* (1)			BD* (1)	
	BD (1) H3-C4	Ni10-Ni11	0.16	BD (1) H3-C4	Ni10-Ni11	0.17
	BD (1) C4-C5	LP* (8) Ni10	0.07	BD (1) C4-C5	LP* (5) Ni10	0.03
	BD (1) C4-C5	LP* (8) Ni11	0.04	BD (1) C4-C5	LP* (8) Ni10	0.05
		BD* (1)				
	BD (1) C4-C5	Ni10-Ni11	0.13	BD (1) C4-C5	LP* (8) Ni11	0.03
					BD* (1)	
	BD (1) C5-H6	LP* (6) Ni10	0.43	BD (1) C4-C5	Ni10-Ni11	0.13
		BD* (1)				
	BD (1) C5-H6	Ni10-Ni11	0.1	BD (1) C5-H6	LP* (5) Ni10	0.07
	BD (1) C5-H7	LP* (6) Ni10	0.33	BD (1) C5-H6	LP* (6) Ni10	0.41
$Ni_2(EtOH)_2$					BD* (1)	
	BD (1) C5-H7	LP* (6) Ni11	0.03	BD (1) C5-H6	Ni10-Ni11	0.1
	BD (1) C5-H7	LP* (8) Ni11	0.05	BD (1) C5-H7	LP* (5) Ni10	0.05

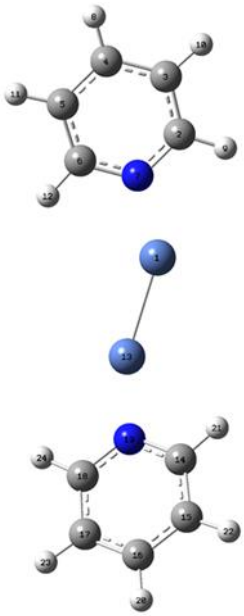
	BD* (1)				
BD (1) C5-H7	Ni10-Ni11	0.06	BD (1) C5-H7	LP* (6) Ni10	0.31
BD (1) C5-O8	LP* (6) Ni10	0.93	BD (1) C5-H7	LP* (6) Ni11	0.03
BD (1) C5-O8	LP* (7) Ni10	0.06	BD (1) C5-H7	LP* (7) Ni11	0.05
BD (1) C5-O8	LP* (8) Ni10	0.09	BD (1) C5-H7	LP* (8) Ni11	0.03
				BD* (1)	
BD (1) C5-O8	LP* (6) Ni11	0.06	BD (1) C5-H7	Ni10-Ni11	0.06
	BD* (1)				
BD (1) C5-O8	Ni10-Ni11	0.14	BD (1) C5-O8	LP* (5) Ni10	0.63
BD (1) O8-H9	LP* (6) Ni10	1.12	BD (1) C5-O8	LP* (6) Ni10	0.54
BD (1) O8-H9	LP* (7) Ni11	0.03	BD (1) C5-O8	LP* (7) Ni10	0.1
BD (1) O8-H9	RY* (1) Ni10	0.2	BD (1) C5-O8	LP* (8) Ni10	0.14
BD (1) O8-H9	RY* (1) Ni11	0.04	BD (1) C5-O8	LP* (6) Ni11	0.06
	BD* (1)				
BD (1) O8-H9	Ni10-Ni11	0.44	BD (1) C5-O8	LP* (7) Ni11	0.03
				BD* (1)	
CR (1) C4	LP* (6) Ni10	0.04	BD (1) C5-O8	Ni10-Ni11	0.13
CR (1) C5	LP* (6) Ni10	0.18	BD (1) O8-H9	LP* (5) Ni10	0.5
	BD* (1)				
CR (1) C5	Ni10-Ni11	0.05	BD (1) O8-H9	LP* (6) Ni10	0.84
CR (1) O8	LP* (6) Ni10	0.97	BD (1) O8-H9	LP* (7) Ni10	0.03
	BD* (1)				
CR (1) O8	Ni10-Ni11	0.22	BD (1) O8-H9	LP* (8) Ni10	0.09
LP (1) O8	LP* (6) Ni10	1.29	BD (1) O8-H9	RY* (1) Ni10	0.16
LP (1) O8	LP* (7) Ni10	0.48	BD (1) O8-H9	RY* (1) Ni11	0.04
				BD* (1)	
LP (1) O8	RY* (1) Ni10	0.05	BD (1) O8-H9	Ni10-Ni11	0.41
LP (1) O8	RY* (1) Ni11	0.03	CR (1) C4	LP* (6) Ni10	0.04
LP (1) O8	RY* (4) Ni11	0.03	CR (1) C5	LP* (6) Ni10	0.17
	BD* (1)			BD* (1)	
LP (1) O8	Ni10-Ni11	0.1	CR (1) C5	Ni10-Ni11	0.05
LP (2) O8	LP* (6) Ni10	5.14	CR (1) O8	LP* (5) Ni10	0.34
LP (2) O8	LP* (8) Ni10	0.08	CR (1) O8	LP* (6) Ni10	0.69
LP (2) O8	LP* (6) Ni11	0.07	CR (1) O8	LP* (8) Ni10	0.03
				BD* (1)	
LP (2) O8	LP* (8) Ni11	0.05	CR (1) O8	Ni10-Ni11	0.2
LP (2) O8	RY* (1) Ni10	0.2	LP (1) O8	LP* (5) Ni10	0.65
LP (2) O8	RY* (4) Ni10	0.15	LP (1) O8	LP* (6) Ni10	1.33
LP (2) O8	RY* (1) Ni11	0.12	LP (1) O8	LP* (7) Ni10	0.84
LP (2) O8	RY* (2) Ni11	0.03	LP (1) O8	LP* (8) Ni10	0.15
				BD* (1)	
LP (2) O8	RY* (4) Ni11	0.1	LP (1) O8	Ni10-Ni11	0.41
	BD* (1)				
LP (2) O8	Ni10-Ni11	4.44	LP (2) O8	LP* (5) Ni10	9.54
			LP (2) O8	LP* (6) Ni10	2.79
			LP (2) O8	LP* (7) Ni10	0.05
			LP (2) O8	LP* (6) Ni11	0.04
			LP (2) O8	LP* (8) Ni11	0.04
			LP (2) O8	RY* (1) Ni10	0.2
			LP (2) O8	RY* (3) Ni10	0.03
			LP (2) O8	RY* (4) Ni10	0.08
			LP (2) O8	RY* (6) Ni10	0.03
			LP (2) O8	RY* (1) Ni11	0.13
			LP (2) O8	RY* (2) Ni11	0.11
			LP (2) O8	RY* (3) Ni11	0.07
			LP (2) O8	RY* (4) Ni11	0.06
			LP (2) O8	RY* (5) Ni11	0.08
				BD* (1)	
			LP (2) O8	Ni10-Ni11	3.65
Et-^{13}OH	**Ni**		**Et-^{13}OH**	**Ni**	
BD (1) H12-O13	LP* (6) Ni11	1.07	BD (1) H12-O13	LP* (5) Ni11	0.48

BD (1) H12-O13	RY* (1) Ni10	0.04	BD (1) H12-O13	LP* (6) Ni11	0.78
BD (1) H12-O13	RY* (1) Ni11 BD* (1)	0.19	BD (1) H12-O13	LP* (7) Ni11	0.03
BD (1) H12-O13	Ni10-Ni11	0.5	BD (1) H12-O13	LP* (8) Ni11	0.08
BD (1) O13-C16	LP* (6) Ni10	0.07	BD (1) H12-O13	RY* (1) Ni10	0.04
BD (1) O13-C16	LP* (6) Ni11	0.96	BD (1) H12-O13	RY* (1) Ni11	0.15
BD (1) O13-C16	LP* (7) Ni11	0.08	BD (1) H12-O13	RY* (3) Ni11 BD* (1)	0.03
BD (1) O13-C16	LP* (8) Ni11 BD* (1)	0.09	BD (1) H12-O13	Ni10-Ni11	0.47
BD (1) O13-C16	Ni10-Ni11	0.11	BD (1) O13-C16	LP* (6) Ni10	0.06
BD (1) H14-C16	LP* (6) Ni10	0.03	BD (1) O13-C16	LP* (7) Ni10	0.03
BD (1) H14-C16	LP* (7) Ni10	0.03	BD (1) O13-C16	LP* (5) Ni11	0.69
BD (1) H14-C16	LP* (8) Ni10	0.07	BD (1) O13-C16	LP* (6) Ni11	0.53
BD (1) H14-C16	LP* (6) Ni11 BD* (1)	0.32	BD (1) O13-C16	LP* (7) Ni11	0.12
BD (1) H14-C16	Ni10-Ni11	0.05	BD (1) O13-C16	LP* (8) Ni11 BD* (1)	0.15
BD (1) H15-C16	LP* (6) Ni11 BD* (1)	0.42	BD (1) O13-C16	Ni10-Ni11	0.09
BD (1) H15-C16	Ni10-Ni11	0.11	BD (1) H14-C16	LP* (6) Ni10	0.03
BD (1) C16-C17	LP* (8) Ni10	0.04	BD (1) H14-C16	LP* (7) Ni10	0.06
BD (1) C16-C17	LP* (8) Ni11 BD* (1)	0.07	BD (1) H14-C16	LP* (8) Ni10	0.05
BD (1) C16-C17	Ni10-Ni11	0.1	BD (1) H14-C16	LP* (5) Ni11	0.06
BD (1) C17-H18	LP* (6) Ni11 BD* (1)	0.04	BD (1) H14-C16	LP* (6) Ni11 BD* (1)	0.29
BD (1) C17-H18	Ni10-Ni11	0.05	BD (1) H14-C16	Ni10-Ni11	0.05
BD (1) C17-H19	LP* (6) Ni10	0.05	BD (1) H15-C16	LP* (5) Ni11	0.06
BD (1) C17-H19	LP* (8) Ni10	0.07	BD (1) H15-C16	LP* (6) Ni11 BD* (1)	0.4
BD (1) C17-H19	LP* (6) Ni11	0.13	BD (1) H15-C16	Ni10-Ni11	0.11
BD (1) C17-H19	LP* (8) Ni11 BD* (1)	0.07	BD (1) C16-C17	LP* (5) Ni11	0.03
BD (1) C17-H19	Ni10-Ni11	0.11	BD (1) C16-C17	LP* (8) Ni11 BD* (1)	0.05
BD (1) C17-H20	LP* (6) Ni11	0.09	BD (1) C16-C17	Ni10-Ni11	0.1
CR (1) O13	LP* (6) Ni11 BD* (1)	0.96	BD (1) C17-H18	LP* (6) Ni11 BD* (1)	0.03
CR (1) O13	Ni10-Ni11	0.22	BD (1) C17-H18	Ni10-Ni11	0.05
CR (1) C16	LP* (6) Ni11 BD* (1)	0.17	BD (1) C17-H19	LP* (6) Ni10	0.09
CR (1) C16	Ni10-Ni11	0.05	BD (1) C17-H19	LP* (8) Ni10	0.04
CR (1) C17	LP* (6) Ni11	0.04	BD (1) C17-H19	LP* (6) Ni11	0.12
LP (1) O13	LP* (6) Ni11	1.3	BD (1) C17-H19	LP* (7) Ni11	0.07
LP (1) O13	LP* (7) Ni11	0.49	BD (1) C17-H19	LP* (8) Ni11 BD* (1)	0.04
LP (1) O13	RY* (1) Ni10	0.03	BD (1) C17-H19	Ni10-Ni11	0.11
LP (1) O13	RY* (2) Ni10	0.04	BD (1) C17-H20	LP* (6) Ni11	0.09
LP (1) O13	RY* (1) Ni11 BD* (1)	0.04	CR (1) O13	LP* (5) Ni11	0.36
LP (1) O13	Ni10-Ni11	0.11	CR (1) O13	LP* (6) Ni11	0.67
LP (2) O13	LP* (6) Ni10	0.07	CR (1) O13	LP* (8) Ni11 BD* (1)	0.03
LP (2) O13	LP* (8) Ni10	0.05	CR (1) O13	Ni10-Ni11	0.2
LP (2) O13	LP* (6) Ni11	5.13	CR (1) C16	LP* (6) Ni11 BD* (1)	0.16
LP (2) O13	LP* (8) Ni11	0.06	CR (1) C16	Ni10-Ni11	0.05
LP (2) O13	RY* (1) Ni10	0.1	CR (1) C17	LP* (6) Ni11	0.04
LP (2) O13	RY* (2) Ni10	0.07	LP (1) O13	LP* (5) Ni11	0.69
LP (2) O13	RY* (4) Ni10	0.1	LP (1) O13	LP* (6) Ni11	1.3
LP (2) O13	RY* (9) Ni10	0.05	LP (1) O13	LP* (7) Ni11	0.84

	LP (2) O13	RY* (1) Ni11	0.19	LP (1) O13	LP* (8) Ni11	0.09
	LP (2) O13	RY* (4) Ni11	0.14	LP (1) O13	RY* (2) Ni10	0.03
	LP (2) O13	BD* (1) Ni10-Ni11	4.45	LP (1) O13	RY* (2) Ni11	0.03
					BD* (1)	
				LP (1) O13	Ni10-Ni11	0.39
				LP (2) O13	LP* (6) Ni10	0.04
				LP (2) O13	LP* (8) Ni10	0.03
				LP (2) O13	LP* (5) Ni11	9.94
				LP (2) O13	LP* (6) Ni11	2.69
				LP (2) O13	LP* (7) Ni11	0.04
				LP (2) O13	RY* (1) Ni10	0.1
				LP (2) O13	RY* (2) Ni10	0.18
				LP (2) O13	RY* (4) Ni10	0.08
				LP (2) O13	RY* (1) Ni11	0.17
				LP (2) O13	RY* (2) Ni11	0.07
				LP (2) O13	RY* (4) Ni11	0.08
				LP (2) O13	RY* (6) Ni11	0.03
					BD* (1)	
				LP (2) O13	Ni10-Ni11	3.6

Table S17. Second order perturbation analysis for the 'donor-acceptor' (bond-antibond) interactions between the Py and the Ni center of Ni_2Py_2 in the NBO basis.

Geom.	***α* orbitals**			***β* orbitals**		
	Donor	**Acceptor**	**Δ*E*** **(kcal/mol)**	**Donor**	**Acceptor**	**Δ*E*** **(kcal/mol)**
	$^7NC_5H_5$	**Ni**		**$^7NC_5H_5$**	**Ni**	
	BD (1) C2-C3	LP* (6) Ni1	0.94	BD (1) C2-C3	LP* (5) Ni1	0.31
	BD (1) C2-C3	LP* (6) Ni13	0.03	BD (1) C2-C3	LP* (6) Ni1	0.52
	BD (1) C2-C3	RY* (2) Ni1	0.08	BD (1) C2-C3	LP* (7) Ni1	0.25
	BD (1) C2-C3	RY* (2) Ni13	0.03	BD (1) C2-C3	LP* (8) Ni1	0.04
	BD (2) C2-C3	LP* (8) Ni1	0.03	BD (1) C2-C3	RY* (4) Ni1	0.06
	BD (1) C2-N7	LP* (6) Ni1	0.27	BD (1) C2-C3	RY* (4) Ni13	0.03
	BD (1) C2-N7	LP* (7) Ni1	0.46	BD (2) C2-C3	LP* (8) Ni1	0.03
	BD (1) C2-N7	LP* (6) Ni13	0.24	BD (1) C2-N7	LP* (5) Ni1	0.63
	BD (1) C2-N7	RY* (2) Ni1	0.1	BD (1) C2-N7	LP* (6) Ni1	0.3
	BD (1) C2-N7	RY* (4) Ni1	0.05	BD (1) C2-N7	LP* (7) Ni1	0.24
	BD (1) C2-N7	RY* (2) Ni13	0.12	BD (1) C2-N7	LP* (6) Ni13	0.16
	BD (1) C2-N7	RY* (4) Ni13	0.05	BD (1) C2-N7	LP* (7) Ni13	0.14
	BD (1) C2-N7	BD* (1) Ni1-Ni13	2.26	BD (1) C2-N7	LP* (8) Ni13	0.03
	BD (1) C2-H9	LP* (6) Ni1	0.03	BD (1) C2-N7	RY* (4) Ni1	0.11
	BD (1) C2-H9	LP* (6) Ni13	0.1	BD (1) C2-N7	RY* (4) Ni13	0.1
	BD (1) C2-H9	RY* (2) Ni1	0.06	BD (1) C2-N7	RY* (6) Ni13	0.03
	BD (1) C2-H9	RY* (4) Ni1	0.04	BD (1) C2-N7	RY* (8) Ni13	0.03
	BD (1) C2-H9	RY* (6) Ni1	0.03	BD (1) C2-N7	BD* (1) Ni1-Ni13	2.18
	BD (1) C2-H9	RY* (1) Ni13	0.03	BD (1) C2-H9	LP* (5) Ni1	0.04
	BD (1) C2-H9	RY* (2) Ni13	0.03	BD (1) C2-H9	LP* (6) Ni13	0.06
	BD (1) C2-H9	BD* (1) Ni1-Ni13	0.64	BD (1) C2-H9	LP* (7) Ni13	0.06
	BD (1) C3-C4	LP* (6) Ni1	0.03	BD (1) C2-H9	RY* (1) Ni1	0.03
	BD (1) C3-H10	LP* (6) Ni1	0.1	BD (1) C2-H9	RY* (4) Ni1	0.05
	BD (1) C4-C5	LP* (6) Ni1	0.03	BD (1) C2-H9	RY* (6) Ni1	0.05
	BD (1) C4-H8	LP* (6) Ni1	0.06	BD (1) C2-H9	RY* (8) Ni1	0.03



Ni_2Py_2

BD (1) C5-C6	LP* (6) Ni1	0.54	BD (1) C2-H9	RY* (4) Ni13	0.03
BD (1) C5-C6	LP* (7) Ni1	0.1	BD (1) C2-H9	BD* (1) Ni1-Ni13	0.67
BD (1) C5-C6	BD* (1) Ni1-Ni13	0.13	BD (1) C3-H10	LP* (6) Ni1	0.06
BD (1) C5-H11	LP* (6) Ni1	0.07	BD (1) C3-H10	LP* (7) Ni1	0.04
BD (1) C6-N7	LP* (6) Ni1	1.63	BD (1) C4-C5	LP* (6) Ni1	0.03
BD (1) C6-N7	LP* (7) Ni1	0.11	BD (1) C4-H8	LP* (6) Ni1	0.05
BD (1) C6-N7	LP* (8) Ni13	0.05	BD (1) C5-C6	LP* (5) Ni1	0.17
BD (1) C6-N7	BD* (1) Ni1-Ni13	0.25	BD (1) C5-C6	LP* (6) Ni1	0.52
BD (2) C6-N7	LP* (8) Ni1	0.13	BD (1) C5-C6	BD* (1) Ni1-Ni13	0.14
BD (2) C6-N7	LP* (7) Ni13	0.05	BD (1) C5-H11	LP* (6) Ni1	0.08
BD (2) C6-N7	LP* (8) Ni13	0.04	BD (1) C6-N7	LP* (5) Ni1	1.5
BD (2) C6-N7	BD* (1) Ni1-Ni13	0.12	BD (1) C6-N7	LP* (6) Ni1	0.43
BD (1) C6-H12	LP* (6) Ni1	0.19	BD (1) C6-N7	LP* (7) Ni1	0.47
BD (1) C6-H12	LP* (7) Ni13	0.03	BD (1) C6-N7	LP* (8) Ni1	0.03
BD (1) C6-H12	LP* (8) Ni13	0.07	BD (1) C6-N7	LP* (6) Ni13	0.04
BD (1) C6-H12	BD* (1) Ni1-Ni13	0.11	BD (1) C6-N7	LP* (8) Ni13	0.05
CR (1) C2	LP* (6) Ni1	0.25	BD (1) C6-N7	BD* (1) Ni1-Ni13	0.21
CR (1) C6	LP* (6) Ni1	0.24	BD (2) C6-N7	LP* (8) Ni1	0.12
CR (1) C6	BD* (1) Ni1-Ni13	0.04	BD (2) C6-N7	LP* (7) Ni13	0.03
CR (1) N7	LP* (6) Ni1	1.44	BD (2) C6-N7	LP* (8) Ni13	0.05
CR (1) N7	BD* (1) Ni1-Ni13	0.2	BD (2) C6-N7	BD* (1) Ni1-Ni13	0.16
LP (1) N7	LP* (6) Ni1	6.79	BD (1) C6-H12	LP* (5) Ni1	0.07
LP (1) N7	LP* (7) Ni1	0.13	BD (1) C6-H12	LP* (6) Ni1	0.14
LP (1) N7	LP* (8) Ni1	0.03	BD (1) C6-H12	LP* (8) Ni1	0.03
LP (1) N7	LP* (6) Ni13	0.18	BD (1) C6-H12	LP* (7) Ni13	0.03
LP (1) N7	LP* (7) Ni13	0.09	BD (1) C6-H12	LP* (8) Ni13	0.05
LP (1) N7	RY* (1) Ni1	0.36	BD (1) C6-H12	RY* (1) Ni1	0.03
LP (1) N7	RY* (2) Ni1	0.47	BD (1) C6-H12	BD* (1) Ni1-Ni13	0.12
LP (1) N7	RY* (4) Ni1	0.34	CR (1) C2	LP* (5) Ni1	0.06
LP (1) N7	RY* (5) Ni1	0.06	CR (1) C2	LP* (6) Ni1	0.15
LP (1) N7	RY* (6) Ni1	0.22	CR (1) C2	LP* (7) Ni1	0.04
LP (1) N7	RY* (7) Ni1	0.24	CR (1) C6	LP* (5) Ni1	0.04
LP (1) N7	RY* (8) Ni1	0.04	CR (1) C6	LP* (6) Ni1	0.19
LP (1) N7	RY* (1) Ni13	0.24	CR (1) C6	BD* (1) Ni1-Ni13	0.05
LP (1) N7	RY* (2) Ni13	0.26	CR (1) N7	LP* (5) Ni1	0.85
LP (1) N7	RY* (6) Ni13	0.08	CR (1) N7	LP* (6) Ni1	0.72
LP (1) N7	RY* (8) Ni13	0.06	CR (1) N7	LP* (7) Ni1	0.07
LP (1) N7	RY* (9) Ni13	0.03	CR (1) N7	BD* (1) Ni1-Ni13	0.16
LP (1) N7	BD* (1) Ni1-Ni13	6.13	LP (1) N7	LP* (5) Ni1	23.37
BD* (2) C6-N7	LP* (8) Ni1	0.19	LP (1) N7	LP* (6) Ni1	1.77
			LP (1) N7	LP* (6) Ni13	0.04
			LP (1) N7	LP* (7) Ni13	0.19

			LP (1) N7	RY* (1) Ni1	0.35
			LP (1) N7	RY* (3) Ni1	0.04
			LP (1) N7	RY* (4) Ni1	0.28
			LP (1) N7	RY* (6) Ni1	0.27
			LP (1) N7	RY* (8) Ni1	0.18
			LP (1) N7	RY* (1) Ni13	0.18
			LP (1) N7	RY* (2) Ni13	0.12
			LP (1) N7	RY* (4) Ni13	0.22
			LP (1) N7	RY* (7) Ni13	0.04
			LP (1) N7	BD* (1) Ni1-Ni13	4.19
			BD* (2) C6-N7	LP* (8) Ni1	0.18
$^{19}NC_5H_5$	**Ni**		**$^{19}NC_5H_5$**	**Ni**	
BD (1) C14-C15	LP* (6) Ni13	0.54	BD (1) C14-C15	LP* (5) Ni13	0.17
BD (1) C14-C15	LP* (7) Ni13	0.1	BD (1) C14-C15	LP* (6) Ni13	0.52
BD (1) C14-C15	BD* (1) Ni1-Ni13	0.13	BD (1) C14-C15	BD* (1) Ni1-Ni13	0.14
BD (2) C14-C15	LP* (8) Ni13	0.03	BD (2) C14-C15	LP* (8) Ni13	0.03
BD (1) C14-N19	LP* (8) Ni1	0.05	BD (1) C14-N19	LP* (6) Ni1	0.04
BD (1) C14-N19	LP* (6) Ni13	1.63	BD (1) C14-N19	LP* (8) Ni1	0.05
BD (1) C14-N19	LP* (7) Ni13	0.11	BD (1) C14-N19	LP* (5) Ni13	1.5
BD (1) C14-N19	BD* (1) Ni1-Ni13	0.25	BD (1) C14-N19	LP* (6) Ni13	0.43
BD (1) C14-H21	LP* (7) Ni1	0.03	BD (1) C14-N19	LP* (7) Ni13	0.47
BD (1) C14-H21	LP* (8) Ni1	0.07	BD (1) C14-N19	LP* (8) Ni13	0.03
BD (1) C14-H21	LP* (6) Ni13	0.19	BD (1) C14-N19	BD* (1) Ni1-Ni13	0.21
BD (1) C14-H21	BD* (1) Ni1-Ni13	0.11	BD (1) C14-H21	LP* (7) Ni1	0.03
BD (1) C15-C16	LP* (6) Ni13	0.03	BD (1) C14-H21	LP* (8) Ni1	0.05
BD (1) C15-H22	LP* (6) Ni13	0.07	BD (1) C14-H21	LP* (5) Ni13	0.07
BD (1) C16-C17	LP* (6) Ni13	0.03	BD (1) C14-H21	LP* (6) Ni13	0.14
BD (1) C16-H20	LP* (6) Ni13	0.06	BD (1) C14-H21	LP* (8) Ni13	0.03
BD (1) C17-C18	LP* (6) Ni1	0.03	BD (1) C14-H21	RY* (1) Ni13	0.03
BD (1) C17-C18	LP* (6) Ni13	0.94	BD (1) C14-H21	BD* (1) Ni1-Ni13	0.12
BD (1) C17-C18	RY* (2) Ni1	0.03	BD (1) C15-C16	LP* (6) Ni13	0.03
BD (1) C17-C18	RY* (2) Ni13	0.08	BD (1) C15-H22	LP* (6) Ni13	0.08
BD (1) C17-H23	LP* (6) Ni13	0.1	BD (1) C16-H20	LP* (6) Ni13	0.05
BD (1) C18-N19	LP* (6) Ni1	0.24	BD (1) C17-C18	LP* (5) Ni13	0.31
BD (1) C18-N19	LP* (6) Ni13	0.27	BD (1) C17-C18	LP* (6) Ni13	0.52
BD (1) C18-N19	LP* (7) Ni13	0.46	BD (1) C17-C18	LP* (7) Ni13	0.25
BD (1) C18-N19	RY* (2) Ni1	0.12	BD (1) C17-C18	LP* (8) Ni13	0.04
BD (1) C18-N19	RY* (4) Ni1	0.05	BD (1) C17-C18	RY* (4) Ni1	0.03
BD (1) C18-N19	RY* (2) Ni13	0.1	BD (1) C17-C18	RY* (4) Ni13	0.06
BD (1) C18-N19	RY* (4) Ni13	0.05	BD (1) C17-H23	LP* (6) Ni13	0.06
BD (1) C18-N19	BD* (1) Ni1-Ni13	2.26	BD (1) C17-H23	LP* (7) Ni13	0.04
BD (2) C18-N19	LP* (7) Ni1	0.05	BD (1) C18-N19	LP* (6) Ni1	0.16
BD (2) C18-N19	LP* (8) Ni13	0.11	BD (1) C18-N19	LP* (7) Ni1	0.14
BD (2) C18-N19	BD* (1) Ni1-Ni13	0.11	BD (1) C18-N19	LP* (8) Ni1	0.03
BD (1) C18-H24	LP* (6) Ni1	0.1	BD (1) C18-N19	LP* (5) Ni13	0.63
BD (1) C18-H24	LP* (6) Ni13	0.03	BD (1) C18-N19	LP* (6) Ni13	0.3
BD (1) C18-H24	RY* (1) Ni1	0.03	BD (1) C18-N19	LP* (7) Ni13	0.24
BD (1) C18-H24	RY* (2) Ni1	0.03	BD (1) C18-N19	RY* (4) Ni1	0.1
BD (1) C18-H24	RY* (2) Ni13	0.06	BD (1) C18-N19	RY* (6) Ni1	0.03
BD (1) C18-H24	RY* (4) Ni13	0.04	BD (1) C18-N19	RY* (8) Ni1	0.03
BD (1) C18-H24	RY* (6) Ni13	0.03	BD (1) C18-N19	RY* (4) Ni13	0.11

	BD* (1) Ni1-Ni13			BD* (1) Ni1-Ni13	
BD (1) C18-H24		0.64	BD (1) C18-N19		2.18
CR (1) C14	LP* (6) Ni13	0.24	BD (2) C18-N19	LP* (7) Ni1	0.03
	BD* (1) Ni1-Ni13				
CR (1) C14		0.04	BD (2) C18-N19	LP* (8) Ni1	0.03
CR (1) C18	LP* (6) Ni13	0.25	BD (2) C18-N19	LP* (8) Ni13	0.11
				BD* (1) Ni1-Ni13	
CR (1) N19	LP* (6) Ni13	1.44	BD (2) C18-N19		0.15
	BD* (1) Ni1-Ni13				
CR (1) N19		0.2	BD (1) C18-H24	LP* (6) Ni1	0.06
LP (1) N19	LP* (6) Ni1	0.18	BD (1) C18-H24	LP* (7) Ni1	0.06
LP (1) N19	LP* (7) Ni1	0.09	BD (1) C18-H24	LP* (5) Ni13	0.04
LP (1) N19	LP* (6) Ni13	6.79	BD (1) C18-H24	RY* (4) Ni1	0.03
LP (1) N19	LP* (7) Ni13	0.13	BD (1) C18-H24	RY* (1) Ni13	0.03
LP (1) N19	LP* (8) Ni13	0.03	BD (1) C18-H24	RY* (4) Ni13	0.05
LP (1) N19	RY* (1) Ni1	0.24	BD (1) C18-H24	RY* (6) Ni13	0.05
LP (1) N19	RY* (2) Ni1	0.26	BD (1) C18-H24	RY* (8) Ni13	0.03
				BD* (1) Ni1-Ni13	
LP (1) N19	RY* (6) Ni1	0.08	BD (1) C18-H24		0.67
LP (1) N19	RY* (8) Ni1	0.06	CR (1) C14	LP* (5) Ni13	0.04
LP (1) N19	RY* (9) Ni1	0.03	CR (1) C14	LP* (6) Ni13	0.19
				BD* (1) Ni1-Ni13	
LP (1) N19	RY* (1) Ni13	0.36	CR (1) C14		0.05
LP (1) N19	RY* (2) Ni13	0.47	CR (1) C18	LP* (5) Ni13	0.06
LP (1) N19	RY* (4) Ni13	0.34	CR (1) C18	LP* (6) Ni13	0.15
LP (1) N19	RY* (5) Ni13	0.06	CR (1) C18	LP* (7) Ni13	0.04
LP (1) N19	RY* (6) Ni13	0.22	CR (1) N19	LP* (5) Ni13	0.85
LP (1) N19	RY* (7) Ni13	0.24	CR (1) N19	LP* (6) Ni13	0.72
LP (1) N19	RY* (8) Ni13	0.04	CR (1) N19	LP* (7) Ni13	0.07
	BD* (1) Ni1-Ni13			BD* (1) Ni1-Ni13	
LP (1) N19		6.13	CR (1) N19		0.16
BD* (2) C18-N19	LP* (8) Ni13	0.22	LP (1) N19	LP* (6) Ni1	0.04
			LP (1) N19	LP* (7) Ni1	0.19
			LP (1) N19	LP* (5) Ni13	23.37
			LP (1) N19	LP* (6) Ni13	1.77
			LP (1) N19	RY* (1) Ni1	0.18
			LP (1) N19	RY* (2) Ni1	0.12
			LP (1) N19	RY* (4) Ni1	0.22
			LP (1) N19	RY* (7) Ni1	0.04
			LP (1) N19	RY* (1) Ni13	0.35
			LP (1) N19	RY* (3) Ni13	0.04
			LP (1) N19	RY* (4) Ni13	0.28
			LP (1) N19	RY* (6) Ni13	0.27
			LP (1) N19	RY* (8) Ni13	0.18
				BD* (1) Ni1-Ni13	
			LP (1) N19		4.19
			BD* (2) C18-N19	LP* (8) Ni13	0.19
				BD* (1) Ni1-Ni13	
			BD* (2) C18-N19		0.03

Atomic Coordinates For All Molecules, INTs, And TSs Involved In This Paper

Phenol
(E = −307.27305898)
0, 1

C	-1.18635000	-1.15927400	0.00000000
C	-1.20303500	0.23328500	0.00000000
C	0.00000000	0.93762200	0.00000000
C	1.21463900	0.25320500	0.00000000
C	1.21736900	-1.13608300	0.00000000
C	0.02042000	-1.85180700	0.00000000
H	-2.12839700	-1.70283000	0.00000000
H	-2.14961000	0.77373000	0.00000000
H	2.13828900	0.82607300	0.00000000
H	2.16708300	-1.66616800	0.00000000
H	0.02970500	-2.93847200	0.00000000
O	0.05083800	2.29814400	0.00000000
H	-0.84204100	2.66084000	0.00000000

p-Cresol
(E = −346.560116105)
0, 1

C	-0.64352000	1.19864500	-0.00000100
C	0.75045900	1.19239600	0.00000000
C	1.43561800	-0.01852400	0.00000000
C	0.72366900	-1.21763300	0.00000000
C	-0.66346700	-1.19122200	-0.00000100
C	-1.37651500	0.01344100	-0.00000100
H	-1.16947200	2.15265600	-0.00000100
H	1.30260800	2.13229500	0.00000000
H	1.27469700	-2.15465900	0.00000000
H	-1.21232200	-2.13286600	-0.00000100
O	2.79657300	-0.09669600	0.00000100
H	3.17523000	0.78938900	0.00000100
C	-2.87731700	0.01454200	0.00000100
H	-3.28032400	-0.49884200	-0.88200400
H	-3.28032200	-0.49880100	0.88203100
H	-3.27624100	1.03453100	-0.00002200

2,4-Dimethylphenol
(E = −385.848306027)
0, 1

C	-0.59495400	1.04655600	-0.00599600
C	0.76288400	0.71890700	-0.00003200
C	1.10952900	-0.63652000	0.00307000
C	0.12528800	-1.62132800	-0.00171900
C	-1.21479600	-1.26076900	-0.00757200
C	-1.60155800	0.08243400	-0.00747000
H	-0.87155200	2.10232100	-0.01087700
H	0.43357300	-2.66390600	-0.00379400
H	-1.97833400	-2.03812700	-0.01385300

O	2.40799300	-1.05861900	0.00637400
H	3.00642900	-0.30352600	0.00822600
C	-3.05224200	0.46707000	0.00933100
H	-3.63235800	-0.12220600	-0.71083500
H	-3.50166300	0.30086100	0.99704300
H	-3.18900500	1.52534000	-0.23840000
C	1.82413800	1.77893800	-0.00166300
H	2.47006600	1.72213800	0.88669700
H	2.47253700	1.71696700	-0.88787400
H	1.37663100	2.77735900	-0.00502200

2,3,5-Trimethylphenol
(E = −425.135885441)
0, 1

C	1.73023400	0.03584900	-0.01144200
C	1.06898800	-1.18752700	-0.01058700
C	-0.32161200	-1.22868600	-0.00110200
C	-1.09634700	-0.06127000	0.00459200
C	-0.42774000	1.17416000	-0.00098300
C	0.96731600	1.20518800	-0.00996300
H	1.61746500	-2.12781800	-0.01825800
H	1.47418800	2.17067500	-0.01791900
O	-0.89084500	-2.46850400	-0.00175200
H	-1.85173900	-2.39730500	-0.00349100
C	-2.59427200	-0.17659200	0.00913800
H	-2.97112500	-0.70270100	-0.88089500
H	-2.96417900	-0.71628300	0.89382900
H	-3.08132100	0.80105600	0.01866700
C	-1.18980100	2.46910600	-0.00179900
H	-1.83871600	2.56419200	-0.88197800
H	-1.83048600	2.56975600	0.88377600
H	-0.50282600	3.32115300	-0.00754300
C	3.22885600	0.09332900	0.01355000
H	3.60219000	1.01638900	-0.44332500
H	3.60797000	0.06222000	1.04331300
H	3.67161100	-0.75466100	-0.52058300

p-Propylphenol
(E = −425.128332713)
0, 1

C	-0.32989800	-1.19028700	-0.29815300
C	-1.68989800	-1.21891700	-0.01918600
C	-2.38651200	-0.02103500	0.12799300
C	-1.71648500	1.19287200	-0.00517200
C	-0.35266800	1.20100400	-0.28553500
C	0.36529000	0.01493900	-0.43827700
H	0.21009100	-2.13036200	-0.41424500
H	-2.23033200	-2.15640000	0.08418100
H	-2.26037000	2.13110800	0.10583900
H	0.16466300	2.15493800	-0.39010800
O	-3.72048700	-0.09919600	0.39738600

H	-4.09204100	0.78680400	0.47141000
C	1.84755000	0.02901000	-0.68156500
H	2.13246000	-0.83069500	-1.30758500
H	2.12570300	0.92960600	-1.25037300
C	2.65902800	-0.01049900	0.61348000
H	2.37267500	0.84846400	1.23887800
H	2.37365000	-0.90632600	1.18530300
C	4.15683200	-0.00251500	0.35940100
H	4.45894400	0.89835800	-0.19041500
H	4.72989800	-0.03001300	1.29260400
H	4.45912100	-0.86935100	-0.24249300

o-Methoxyphenol
(E = −421.743790978)
0, 1

C	-0.00563900	-1.38904100	0.00000000
C	0.44341400	-0.07514600	0.00000000
C	-0.47586900	0.98653700	0.00000000
C	-1.83603100	0.72075900	0.00000000
C	-2.28802500	-0.59901500	0.00000000
C	-1.37896400	-1.64901900	0.00000000
H	0.70090700	-2.21452100	-0.00000100
H	-2.52565900	1.56099900	0.00000000
H	-3.35615500	-0.80024000	0.00000000
H	-1.72689300	-2.67862800	0.00000000
O	-0.03734700	2.26922100	0.00000000
H	0.93051500	2.25801000	0.00000000
O	1.75139200	0.32381200	-0.00000100
C	2.74392500	-0.67702400	0.00000100
H	2.67109400	-1.30837200	-0.89619600
H	3.70587700	-0.16144700	0.00000100
H	2.67109200	-1.30837100	0.89619800

o-Ethoxyphenol
(E = −461.032827319)
0, 1

C	0.48474200	-1.39410500	0.00000000
C	0.01877900	-0.08558500	0.00000000
C	0.92665300	0.98629800	0.00000000
C	2.28999500	0.73717500	0.00000000
C	2.75785800	-0.57701100	0.00000000
C	1.86104400	-1.63745800	0.00000000
H	-0.21080500	-2.22868000	0.00000000
H	2.96939500	1.58573600	0.00000000
H	3.82831000	-0.76561700	0.00000000
H	2.22112800	-2.66293200	0.00000000
O	0.47261700	2.26389200	0.00000000
H	-0.49507200	2.23944700	0.00000000
O	-1.29286600	0.29768500	0.00000000
C	-2.28750800	-0.71468900	0.00000000
H	-2.16015400	-1.35064300	0.89027200

H	-2.16015300	-1.35064300	-0.89027200
C	-3.63393800	-0.03972000	0.00000000
H	-3.75174300	0.58967900	-0.88815300
H	-4.43292900	-0.78808000	-0.00000100
H	-3.75174300	0.58967900	0.88815300

Syringol
(E = −536.207032306)
0, 1

C	-1.23597000	1.38547500	0.00000100
C	-1.22271000	-0.01164000	0.00000100
C	0.00147600	-0.68995400	0.00000000
C	1.19387800	0.03926500	0.00000000
C	1.18667200	1.43243300	0.00000000
C	-0.03763600	2.09339600	0.00000000
H	-2.17773100	1.92507400	0.00000100
H	2.11382500	1.99719700	-0.00000100
H	-0.05928900	3.17998500	0.00000000
O	0.01445300	-2.04377200	0.00000000
H	0.93995100	-2.32674100	0.00000000
O	-2.32629900	-0.79764500	0.00000100
C	-3.58171300	-0.16248900	-0.00000100
H	-3.71973800	0.45987700	-0.89580700
H	-4.32761300	-0.95953600	-0.00000200
H	-3.71974100	0.45987700	0.89580400
O	2.31212200	-0.74870900	-0.00000100
C	3.56825800	-0.10956400	0.00000000
H	3.69757900	0.51260600	0.89613200
H	4.31944000	-0.90146800	0.00000000
H	3.69758000	0.51260600	-0.89613100

Catechol
(E = −382.474597246)
0, 1

C	1.37745600	0.69459300	0.00000000
C	0.00000000	0.85662800	0.00000000
C	-0.84640000	-0.25795700	0.00000000
C	-0.29717600	-1.53304000	0.00000000
C	1.08660500	-1.69792800	0.00000000
C	1.92534900	-0.58824100	0.00000000
H	2.02194600	1.57350900	0.00000000
H	-0.97301000	-2.38441900	0.00000000
H	1.50681200	-2.70024700	0.00000000
H	3.00487200	-0.71232500	0.00000000
O	-2.19351900	-0.10217400	0.00000000
H	-2.39699400	0.84348700	0.00000000
O	-0.63683200	2.07048600	0.00000000
H	0.00417300	2.78916900	0.00000000

Orcinol
(E = −421.762651586)

0, 1

C	0.83328100	-1.13206100	0.00070700
C	1.43178700	0.12317700	0.00637700
C	0.61690300	1.25342900	0.00088800
C	-0.76984200	1.13490600	-0.00925500
C	-1.36114300	-0.13308600	-0.01178300
C	-0.55559800	-1.26749500	-0.00989500
H	2.51338200	0.24535200	0.01012900
H	-1.39551300	2.02861000	-0.01654700
H	-0.98668800	-2.26594600	-0.01702500
O	1.24456300	2.46049300	0.00243400
H	0.58883600	3.16691500	-0.00285000
O	1.56640700	-2.27703700	0.00176500
H	2.50646800	-2.06409000	0.00439200
C	-2.85529900	-0.26182000	0.00994700
H	-3.17675100	-1.25206400	-0.32851300
H	-3.24611000	-0.11778300	1.02534500
H	-3.33192200	0.48905000	-0.63044200

Pyrogallol
(E = −457.676585396)
0, 1

C	-1.24824900	-1.37507900	0.00000000
C	-1.22098700	0.01707700	0.00000000
C	0.00000000	0.68930700	0.00000000
C	1.18979500	-0.03156100	0.00000000
C	1.17427500	-1.42194800	0.00000000
C	-0.05239100	-2.08443000	0.00000000
H	-2.21169300	-1.87664600	0.00000000
H	2.11161900	-1.97591400	0.00000000
H	-0.07245100	-3.17089100	0.00000000
O	-0.03053700	2.05440700	0.00000000
H	0.87604800	2.38988600	0.00000000
O	2.32548200	0.73419200	0.00000000
H	3.10866000	0.17366900	0.00000000
O	-2.38131200	0.71615300	0.00000000
H	-2.17590900	1.66166700	0.00000000

p-Hydroxybenzaldehyde
(E = −420.550280625)
0, 1

C	-0.17920900	1.33958400	0.00000000
C	1.19982800	1.21251800	0.00000000
C	1.76441600	-0.06452400	0.00000000
C	0.95127800	-1.20424000	0.00000000
C	-0.42534200	-1.06336800	0.00000000
C	-1.00493400	0.21037600	0.00000000
H	-0.63250400	2.33064300	0.00000000
H	1.85833000	2.07658900	0.00000000
H	1.40690200	-2.19408700	0.00000000
H	-1.07922800	-1.93268700	0.00000000

O	3.11520100	-0.14220400	0.00000000
H	3.39878500	-1.06413200	0.00000000
C	-2.46305900	0.37103700	0.00000000
O	-3.26547600	-0.53997800	0.00000000
H	-2.80795300	1.43283300	0.00000000

Vanillin
(E = −535.020800820)
0, 1

C	-0.20392400	-0.88805500	0.00000000
C	0.99371900	-0.19567000	0.00000000
C	0.98842300	1.21230700	0.00000000
C	-0.21519400	1.90963200	0.00000000
C	-1.41557600	1.21477800	-0.00000100
C	-1.41634000	-0.18122800	-0.00000100
H	-0.22645700	-1.97661400	0.00000000
H	-0.18001900	2.99573300	0.00000000
H	-2.36915000	1.73673700	-0.00000100
O	2.15183500	1.89111400	0.00000000
H	2.88096300	1.25280900	0.00000100
C	-2.67587500	-0.93333800	-0.00000100
O	-3.78566600	-0.44205700	0.00000100
H	-2.54690000	-2.04324800	0.00000200
O	2.24358700	-0.74242400	0.00000100
C	2.34447500	-2.15065500	0.00000000
H	1.87770000	-2.57975700	-0.89683400
H	3.40986500	-2.38559500	-0.00000100
H	1.87770000	-2.57975900	0.89683200

Syringaldehyde
(E = −649.485774207)
0, 1

C	-1.02034100	1.12778600	0.00000000
C	-1.40634300	-0.21030700	0.00000000
C	-0.41689000	-1.20364300	0.00000000
C	0.94140100	-0.84455800	0.00000000
C	1.32751300	0.48460900	0.00000000
C	0.33502500	1.46870800	0.00000000
H	-1.76196400	1.92346300	0.00000000
H	2.36802200	0.79697100	0.00000100
O	-0.78190700	-2.49807200	0.00000000
H	0.02561200	-3.03397700	0.00000000
O	-2.68232700	-0.65741400	0.00000000
C	-3.71181500	0.30433300	0.00000000
H	-3.66960100	0.93887900	-0.89653000
H	-4.64989800	-0.25313700	0.00000000
H	-3.66960100	0.93887900	0.89653000
O	1.77989500	-1.91929300	0.00000000
C	3.17038900	-1.66434800	-0.00000100
H	3.46766900	-1.10397600	0.89592400
H	3.66267200	-2.63795600	-0.00000100

H	3.46766800	-1.10397600	-0.89592600
C	0.71139100	2.88581700	0.00000000
O	1.85086100	3.30656600	0.00000000
H	-0.15473900	3.59015300	-0.00000100

BH_4^-

(E = −27.32866810)

−1, 1

H	0.71453700	0.71453700	0.71453700
H	-0.71453700	-0.71453700	0.71453700
H	-0.71453700	0.71453700	-0.71453700
H	0.71453700	-0.71453700	-0.71453700
B	0.00000000	0.00000000	0.00000000

Ni^{2+}

(E = −168.94240487)

(2, 3)

Ni	0.00000000	0.00000000	0.00000000

$[NiBH_4]^+$

(E = −196.30281822)

1, 1

Ni	0.45935200	0.00592100	-0.00143600
H	-1.65428500	1.21816300	-0.08828900
H	-0.59688000	-0.34141200	0.99676400
H	-0.62056800	-0.54418600	-0.89360100
B	-1.51137000	0.04011100	-0.00554500
H	-2.43326300	-0.69891900	0.05304900

$[NiBH_4]^+$

(E = −196.34237619)

1, 3

H	2.66350900	-0.02574300	0.00127500
H	0.99498700	1.08690700	-0.43443900
H	0.95967400	-0.90970800	-0.71654500
H	0.96962900	-0.15602400	1.15122400
B	1.47890000	0.00139300	-0.00004600
Ni	-0.46365300	-0.00008600	-0.00004600

$Ni(BH_4)_2$

(E = −223.73740774)

0, 1

H	-2.83200900	0.83426500	0.10698400
H	-1.15163800	0.08085900	1.04007500
B	-1.99986700	-0.01440300	-0.00196800
H	-2.36993800	-1.14415900	-0.14726000
H	-1.15047900	0.34753800	-0.98401700
Ni	0.00000000	0.00000000	0.00000000
H	1.15163800	-0.08085900	-1.04007500
H	1.15047800	-0.34753800	0.98401700
H	2.36993800	1.14415800	0.14726000

B	1.99986700	0.01440300	0.00196800
H	2.83200900	-0.83426500	-0.10698400

$Ni(BH_4)_2$
(E = −223.74888145)
0, 3

Ni	0.00000000	0.00000000	0.00000000
H	3.12860500	-0.00644000	0.00092300
H	1.42449300	-0.88968900	0.73973700
H	1.43391700	1.08911300	0.40215600
H	1.42862400	-0.19090900	-1.14063000
H	-1.42862400	0.19090900	1.14063000
H	-1.42449300	0.88968900	-0.73973700
H	-1.43391700	-1.08911300	-0.40215600
H	-3.12860500	0.00644000	-0.00092300
B	-1.94155700	-0.00073900	-0.00129500
B	1.94155700	0.00073900	0.00129500

$Ni_2(BH_4)_4$-S1
(E = −447.50327492)
0, 5

H	0.93554800	3.14550400	0.06077000
B	1.36873900	2.03996200	0.04088600
H	0.65309800	1.20088300	0.66271600
H	1.48482900	1.55719400	-1.12591000
H	2.51899300	1.92512900	0.55782700
Ni	2.07667300	0.23344700	-0.00089400
H	3.53677000	-0.71734900	-0.61026900
H	2.61358300	-1.10680900	1.12836000
H	1.67064000	-1.45137100	-0.60788400
B	2.79607400	-1.56872200	-0.03834800
H	3.23127200	-2.67320200	-0.05326400
H	-0.93554400	-3.14550300	0.06077000
H	-1.48484500	-1.55719900	-1.12591000
H	-2.51898600	-1.92512800	0.55784200
H	-0.65309300	-1.20087800	0.66270600
B	-1.36873900	-2.03996200	0.04088700
Ni	-2.07667400	-0.23344700	-0.00089500
H	-2.61354800	1.10682200	1.12836000
H	-3.53678500	0.71734300	-0.61023700
B	-2.79607200	1.56872300	-0.03834700
H	-3.23127100	2.67320200	-0.05326300
H	-1.67065400	1.45136600	-0.60791300

$Ni_2(BH_4)_4$-S2
(E = −447.50014157)
0, 5

H	2.88394600	1.32187400	2.40779100
H	1.27068300	0.60990400	1.34222400
H	3.02724300	-0.34514000	1.20521400
B	2.53095400	0.80407300	1.40108500

H	2.79700300	1.46102800	0.35291900
Ni	1.91514900	-0.06432400	-0.22547100
H	0.63557200	-1.37278700	-2.60269700
H	0.99482100	-1.52443700	-0.62316900
H	0.83268600	0.33462300	-1.57273800
B	0.42555400	-0.86185200	-1.53870600
H	-0.78700800	-0.90383000	-1.32215600
Ni	-1.59263300	0.03493500	-0.03085100
H	-2.49811500	1.14156000	-1.19792100
H	-2.64812500	1.32251600	0.79772000
B	-2.18374300	1.89981700	-0.23158300
H	-0.93142000	1.79421300	-0.12699200
H	-2.56252700	3.01879700	-0.36999900
H	-0.86462900	-0.81343700	1.30302700
H	-1.21473700	-2.75840400	0.97560300
H	-2.46361600	-1.65620200	2.19766800
H	-2.50245000	-1.43558600	0.19382100
B	-1.77272000	-1.71639800	1.21254000

$Ni_2(BH_4)_4$-S3

(E = −447.49887403)

0, 5

H	3.28263200	0.91201500	0.26947500
H	4.65171500	-0.56942200	0.70810900
H	3.07260000	-0.89852600	-0.57155700
B	3.51703400	-0.31917200	0.45918200
H	2.71030600	-0.66131100	1.37987100
Ni	1.63056400	0.06725500	0.08575800
H	0.50404000	1.28015300	0.82775100
H	0.46760500	2.87534400	-0.39822200
H	-0.96719300	1.55720900	-0.55896800
B	0.24894100	1.69890500	-0.32934900
H	0.88234300	1.07406500	-1.21541400
H	0.82404300	-1.66688300	-1.57523200
H	0.34382300	-1.09105100	0.36468600
H	-0.47913200	-2.67427500	-0.35645100
B	-0.02371000	-1.61853700	-0.71559200
H	-0.91137400	-0.91912900	-1.28700300
Ni	-1.86325800	0.09476400	-0.29279400
H	-1.72216000	-0.32912700	1.47035000
H	-3.18096700	0.86214200	0.79183000
B	-2.97931100	-0.29203400	1.26650100
H	-3.16454500	-1.09417300	0.30422900
H	-3.61306900	-0.53937400	2.23984400

$[Ni(BH_4)_3]^-$

(E = −251.11914952)

−1, 3

H	-2.72011400	-1.12951700	-0.60473000
H	-1.37235900	-0.75345400	0.84306700
B	-2.18057200	-0.23247800	0.00077700

H	-1.50435400	0.45623700	-0.83700300
H	-2.90614900	0.52350400	0.60440700
Ni	-0.00130400	-0.00003500	-0.00098100
H	2.34085100	-1.78715300	-0.60446600
H	1.34116300	-0.80692300	0.84147300
B	1.29406200	-1.76859700	0.00090700
H	1.00275000	-2.77450500	0.60560400
H	0.36048900	-1.52912600	-0.83794000
H	1.13751000	1.07594700	-0.84602600
H	0.02714000	1.56493500	0.83633000
B	0.89125000	2.00087800	0.00113600
H	1.91015200	2.23415400	0.60933300
H	0.39574000	2.92785600	-0.59669100

$[Ni_2(BH_4)_3]^+$-case1
(E = −420.08794327)
1, 5

H	-0.40078300	-2.87961400	-0.49646300
H	0.66580600	-1.64277600	0.69585800
B	-0.36811300	-1.80023900	0.00438900
H	-0.39743800	-0.97981200	-0.98878200
H	-1.35430400	-1.62548800	0.75831600
Ni	1.02067100	-0.01896900	0.00747600
H	3.60049300	0.96786300	-0.62211700
H	2.36547200	0.48348100	0.92145300
B	3.14705900	0.03572900	-0.01834300
H	3.87626100	-0.76207000	0.49807200
H	2.37187300	-0.61867300	-0.83464900
H	0.69218100	1.64547400	-0.67529200
H	-0.39675200	0.97673000	0.98653300
B	-0.34860400	1.80035800	-0.00203900
H	-0.39590900	2.87421800	0.51017400
H	-1.32591500	1.62765300	-0.77128000
Ni	-1.78683900	0.01017500	-0.00397100

$[Ni_2(BH_4)_3]^+$-case2
(E = −420.09893707)
1, 5

H	0.91488200	2.85961100	-0.38186200
H	-0.40592100	1.47702800	0.21367600
B	0.78885500	1.72290600	-0.03724600
H	1.41680700	1.48073700	1.02166500
H	1.18787800	1.00530100	-0.99940900
Ni	1.94072400	-0.09407000	0.17294900
H	1.58707000	-1.55087500	-0.89917500
B	0.50032300	-1.63567200	-0.26504600
H	0.23901400	-2.76494200	0.01916200
H	0.56900500	-0.99825100	0.82837800
H	-0.33827300	-1.13511200	-1.03700300
Ni	-1.41573900	0.13537500	-0.32804900
H	-2.96093100	-0.94538300	-0.23249800

H	-1.81127500	-0.42523200	1.33422600
B	-2.95992200	-0.22655300	0.80752800
H	-2.89925000	0.96754700	0.37917300
H	-3.84484300	-0.43036700	1.57027900

$[Ni_2(BH_4)_3]^+$-case3
(E = −420.10794503)
1, 5

H	1.01475100	-2.71877900	0.00001100
H	-0.47446600	-1.41975200	0.00002200
B	0.74652000	-1.55339700	0.00001300
H	1.21628100	-1.00950000	1.04485200
H	1.21626400	-1.00950300	-1.04483500
Ni	2.21249700	0.02214900	-0.00000600
H	1.31670100	1.48846500	0.00001100
H	-0.38393600	1.10829400	1.04466600
B	0.06975300	1.63055100	0.00001000
H	-0.09283200	2.81568900	0.00001400
H	-0.38393500	1.10830000	-1.04465000
Ni	-1.42360900	0.05718400	0.00000200
H	-3.08035600	0.90749400	-0.00001700
H	-2.69161400	-0.78614200	-1.00279800
B	-3.33063800	-0.33695200	-0.00001100
H	-2.69163100	-0.78612900	1.00279300
H	-4.48227700	-0.62076100	-0.00002000

$[Ni_2(BH_4)_3]^+$-case4
(E = −420.09995804)
1, 5

H	-4.37492600	1.20869600	-0.08674800
B	-3.28930100	0.73737400	-0.05001100
H	-2.55794200	1.02632500	-1.04579100
H	-2.59759900	1.07982500	0.95722600
H	-3.26785800	-0.53854300	-0.01201700
Ni	-1.51755500	-0.03999700	0.01085000
H	-0.58266400	-1.14055300	1.09374900
H	-0.58276900	-1.19061000	-1.00046500
H	-0.38642500	-2.87495400	0.08212700
B	-0.14654000	-1.70551600	0.05907300
H	1.09770200	-1.62936100	0.05773400
Ni	2.01324800	-0.19178600	-0.03532100
H	1.20736200	1.22597000	-0.90624300
H	3.03367600	1.36568200	-0.08296500
H	1.42258500	1.12530200	1.09574200
B	1.83881700	1.74996000	0.06795900
H	1.69458900	2.92303800	0.14773400

$[Ni_2(BH_4)_3]^+$-case5
(E = −420.10044098)
1, 5

H	-2.76780300	2.71320600	-0.28716500

H	-1.06224200	1.57017300	-0.11017300
H	-2.64170900	0.81556900	-1.08185600
B	-2.33294500	1.62002900	-0.15049600
H	-2.70307300	1.03812900	0.91485300
Ni	-1.65494000	-0.18572300	0.06478600
H	-0.37887100	-2.92495100	0.38318900
H	-0.55025500	-1.34326400	-0.83417100
H	-0.68391400	-1.12075600	1.24574800
B	-0.16153400	-1.75470000	0.29388000
H	1.07355200	-1.62221900	0.42801900
Ni	1.59387400	-0.13976200	-0.29211700
H	3.14018100	0.02631600	0.61884900
H	2.50132900	1.43803100	-0.66318900
B	2.67827600	1.21701100	0.56922900
H	1.50584500	1.10599900	1.05397800
H	3.35782700	2.00563200	1.13410600

$[Ni_2(BH_4)_3]^+$-TS1,2
(E = −420.08790091)
1, 5

H	-0.60555200	-2.89025600	-0.48531000
H	0.55283900	-1.66790100	0.61295100
B	-0.52751700	-1.80001000	-0.01429700
H	-0.59321800	-0.99832600	-1.01573900
H	-1.47581400	-1.58829800	0.78518200
Ni	1.02955600	-0.06757100	-0.04807000
H	3.45227100	1.05916100	-0.49591000
H	2.27176600	0.38167800	1.02561600
B	3.12632200	0.06459800	0.09243400
H	3.94762500	-0.62425800	0.62276800
H	2.45503400	-0.69078900	-0.73222500
H	0.69620500	1.64679300	-0.72117000
H	-0.36165800	0.97653200	0.95693400
B	-0.32708700	1.80032800	-0.03588300
H	-0.37236300	2.86412200	0.49733600
H	-1.32252800	1.62456100	-0.78421600
Ni	-1.74395600	0.05265700	0.03101700

$[Ni_2(BH_4)_3]^+$-TS2,3
(E = −420.09312350)
1, 5

H	-0.64257000	-2.56624300	-1.00868700
H	0.39107000	-0.86455600	-1.21026300
B	-0.61404900	-1.40481500	-0.73016300
H	-0.66988600	-1.28509900	0.52491400
H	-1.55309600	-0.79194900	-1.30606400
Ni	-2.04346500	-0.12492300	0.28251900
H	-0.88397800	1.60673500	-1.31059400
B	-0.50004600	1.84662600	-0.19828700
H	-0.63519400	2.97967000	0.18521400
H	-1.05288100	1.19246100	0.73926900

H	0.72288900	1.62238100	-0.01344100
Ni	1.50052700	0.14209000	-0.30156700
H	3.01983000	0.67959600	0.63320700
H	1.60854000	-0.53406200	1.37925500
B	2.81916900	-0.52326400	0.97663600
H	2.79373100	-1.17476800	-0.10895400
H	3.57845900	-0.93758900	1.78854900

$[Ni_2(BH_4)_3]^+$-TS3,4
(E = −420.09775085)
1, 5

H	-4.65176800	0.69989100	-0.24164900
B	-3.49871100	0.45534000	-0.12492100
H	-2.75889100	0.97387700	-1.01480300
H	-2.98349800	0.81347200	0.97372000
H	-3.22625500	-0.79418600	-0.19849300
Ni	-1.62280600	-0.00190400	0.03893700
H	-0.63013500	-1.04201800	1.10526700
H	-0.48230100	-0.95783700	-0.98034300
H	-0.37624900	-2.72164800	-0.00442200
B	-0.12964500	-1.55448100	0.06993800
H	1.10281100	-1.46068400	0.21644000
Ni	2.26470800	-0.19167400	-0.05082800
H	1.35131400	0.99372000	-0.93593700
H	2.65761700	2.28326000	-0.06213800
H	1.64998900	0.95649800	1.09649400
B	1.58357100	1.75159400	0.08245200
H	0.59802200	2.41355600	0.24147500

$[Ni_2(BH_4)_3]^+$-TS4,5
(E = −420.09310354)
1, 5

H	-3.09947200	2.43525500	-0.25582100
B	-3.06757200	1.24126800	-0.19512700
H	-2.26327700	0.83460800	-1.12091000
H	-2.50718000	0.93754200	0.93075500
H	-4.09084800	0.61511900	-0.28167500
Ni	-1.52883700	-0.18482600	0.06063700
H	-0.64810900	-1.24019300	1.25486500
H	-0.34874700	-1.36260100	-0.81433700
H	-0.10573500	-2.96042500	0.35886600
B	0.00043400	-1.77266500	0.32178700
H	1.19692100	-1.51736100	0.58051800
Ni	1.75060700	-0.12718800	-0.26254400
H	2.51088100	1.48619400	-0.75512000
H	2.92437100	0.51451100	0.95631200
H	1.10910900	1.31174200	0.68641700
B	2.34750600	1.55520400	0.49591700
H	2.71068600	2.56295700	1.00062600

2Et.-$[Ni_2(BH_4)_3]^+$-case1

(E = −730.06747368)

1, 5

H	4.85413500	-0.08311500	1.58672800
H	5.15868700	-0.30131700	-0.45327700
B	4.41006800	-0.18831100	0.47759500
H	3.61452600	-1.21645900	0.46692100
H	3.65765500	0.85134000	0.26764800
Ni	2.30864700	-0.18054800	0.09731800
H	1.64587300	-0.34124500	1.79980800
H	0.57522000	-2.03753100	2.08792000
H	0.89190800	-1.49446500	0.22592400
B	0.69070100	-1.05748000	1.41982200
H	-0.37018200	-0.38472100	1.44998400
Ni	-0.35296600	-0.12796100	-0.36001500
H	0.26081400	0.07907400	-2.03894000
H	2.28353400	0.07990600	-1.74122400
H	1.32798000	1.75209500	-2.35585200
B	1.24854400	0.77557800	-1.67724800
H	1.06844800	1.21319400	-0.47949600
H	-0.74452800	2.11908500	1.78550800
H	-1.65778600	3.62637400	1.76448500
H	-2.52860800	2.08246700	1.79543100
C	-1.64953700	2.59704400	1.39309000
C	-1.68097000	2.61549100	-0.10890500
H	-0.77901900	3.06721000	-0.54067400
H	-2.55511800	3.15679100	-0.48337600
O	-1.79933000	1.24715900	-0.60461100
H	-2.10518200	1.27660900	-1.52363800
H	-1.49322100	-1.97842500	-1.67476000
O	-1.58581400	-1.66982000	-0.76141600
C	-2.98408800	-1.74110700	-0.36330700
H	-3.54200200	-0.95723700	-0.88825800
H	-3.35212100	-2.71758300	-0.69479600
C	-3.07147300	-1.59541300	1.12832400
H	-2.74958200	-0.59980100	1.45509800
H	-4.11047700	-1.72635100	1.44513700
H	-2.45902500	-2.35138200	1.63137200

2Et.-$[Ni_2(BH_4)_3]^+$-case2

(E = −730.07138504)

1, 5

H	5.51909000	-1.28981100	-0.20084500
H	4.26062000	-0.01191900	-1.23583800
H	4.40853800	0.16898200	0.75768200
B	4.50605000	-0.67262100	-0.18457500
H	3.48309400	-1.42721200	-0.03491500
Ni	2.77093400	0.21901400	-0.13093000
H	1.93551700	0.40348200	1.41262300
H	1.29257200	-1.04731800	2.64269500
H	0.76109600	-1.17698200	0.74495800
B	1.01034300	-0.38707700	1.68553200

H	0.03031500	0.35853700	1.92949100
Ni	-0.59326200	-0.06045400	0.20482000
H	0.45064800	1.23435600	-0.56221000
H	0.51775800	1.14244600	-2.54415600
H	1.72951300	-0.08537100	-1.52633900
B	0.61883300	0.48039000	-1.55202200
H	-0.21733300	-0.45723100	-1.55914900
H	-2.17079600	-1.68943500	-1.73800400
H	-2.91051500	-3.29509400	-1.69849000
H	-3.75626600	-1.91755100	-0.96242500
C	-2.77363400	-2.37188900	-1.12734200
C	-2.10013200	-2.68429200	0.17948400
H	-1.11170100	-3.14079100	0.03577200
H	-2.70799700	-3.35205500	0.79776900
H	-1.78117800	-1.64063500	1.85531200
O	-1.93010100	-1.44176300	0.91947300
H	-3.00131900	0.72960700	0.16342400
O	-2.24050900	0.98352600	-0.38080900
C	-2.23263500	2.41690800	-0.58886400
H	-3.18890100	2.68317800	-1.05178400
H	-1.44336500	2.59146000	-1.32643700
C	-1.99209900	3.17420300	0.69110100
H	-2.00405800	4.25099900	0.49282700
H	-2.77197000	2.95931100	1.43058900
H	-1.01843000	2.92222800	1.12826200

2Et.-$[Ni_2(BH_4)_3]^+$-case3
(E = −730.07619062)
1, 5

H	6.08162300	0.03756500	0.60610300
H	4.64305700	-0.21688600	-0.86354100
H	4.31134400	1.08975700	0.62385900
H	4.27887400	-0.87328000	0.99935500
B	4.92272800	0.00777400	0.35263200
Ni	3.00250500	-0.01627800	0.00475700
H	2.05541200	0.27589200	1.45940200
H	0.57535100	0.40896000	2.75460400
B	0.82782200	0.23870200	1.59520100
H	0.40574500	-0.89469600	1.22713500
H	0.31931800	1.17153600	0.90581500
H	1.98794500	0.86216000	-1.18928800
H	1.74485400	-0.44244200	-2.72111600
H	1.94924800	-1.20260600	-0.85677600
B	1.52963500	-0.24884300	-1.55917300
H	0.28815700	-0.19048800	-1.45082000
Ni	-0.63051300	-0.06169600	0.02161800
H	-1.35532100	-2.09823100	-1.40189700
O	-1.59624700	-1.75299500	-0.53085800
C	-2.99883800	-2.01697700	-0.25965000
H	-3.18216900	-3.06221900	-0.52890600
H	-3.61058000	-1.37738200	-0.90789600

C	-3.27085100	-1.77988900	1.20146900
H	-2.57494200	-2.35432500	1.82229500
H	-4.28884400	-2.10463600	1.43757200
H	-3.20341500	-0.71895100	1.47991000
H	-2.44293300	1.83026600	1.55793600
H	-3.24242100	3.32972600	1.09284700
H	-1.52479300	3.11555800	0.71774300
C	-2.48981700	2.60074500	0.77694800
C	-2.88462700	2.03503900	-0.55797300
H	-3.80655700	1.44505500	-0.49275500
H	-3.02578300	2.82846700	-1.29935200
O	-1.81637400	1.18261500	-1.05381300
H	-2.03411500	0.86585100	-1.94143400

2Et.-$[Ni_2(BH_4)_3]^+$-case4
(E = −730.06776586)
1, 5

H	-4.82689800	-1.07178900	1.52019300
B	-3.92512600	-0.83601800	0.78897800
H	-3.41118300	0.31476200	0.94783100
H	-2.94936500	-1.64211000	0.88212000
H	-4.22926000	-0.87130900	-0.44719800
Ni	-2.45514400	-0.44494900	-0.40901000
H	-1.53422200	-1.27070800	-1.72820500
H	-2.06925500	0.71844200	-1.76691200
H	-0.65100800	-0.00424300	-3.03119800
B	-1.12671400	-0.09795300	-1.94365200
H	-0.28892500	0.19078300	-1.06062900
Ni	0.62864200	-0.30418900	0.43671100
H	-0.05075500	-1.90101100	1.22532700
H	1.40547600	-0.78210600	2.02003800
H	-0.04682400	-1.54773600	3.25732800
B	0.18375300	-1.11036200	2.17722000
H	-0.45784600	-0.04200000	1.92045000
H	-1.19237200	2.24050500	0.61731700
H	-0.16177800	3.37937700	1.51291800
H	-1.00288000	3.90811600	0.04583600
C	-0.47863700	3.06699800	0.51106700
C	0.70378100	2.67167600	-0.33422900
H	0.40794800	2.32663400	-1.32974500
H	1.41178800	3.49721200	-0.46276300
O	1.44073700	1.56345600	0.24675800
H	1.84085500	1.86086900	1.07746300
H	3.59179500	-0.39112900	1.13073400
H	5.05539000	-0.84216900	0.25211600
H	3.83345400	-2.07801600	0.61649800
C	3.98032700	-1.03106900	0.33023500
C	3.32390200	-0.74072100	-0.99025700
H	3.38720400	0.32100300	-1.25622900
H	3.77168900	-1.33517500	-1.79371000

O	1.92457800	-1.11962300	-0.91336100
H	1.55071600	-1.13264600	-1.80600200

2Et.-$[Ni_2(BH_4)_3]^+$-case5
(E = −730.07202078)
1, 5

H	-1.53613600	-1.23224800	3.32640900
H	-0.16410600	-1.24715800	1.78937100
H	-1.67924500	0.06852100	1.74942100
B	-1.35350300	-1.08686400	2.16192700
H	-2.03503700	-1.88436300	1.44324600
Ni	-1.20335700	-0.81684500	0.21809800
H	-0.45017200	-0.46069300	-2.74126300
H	-0.25686100	0.27328000	-0.89165000
H	-0.55980100	-1.77062000	-1.19475300
B	-0.04105100	-0.71764800	-1.64765200
H	1.18599900	-0.94496800	-1.75760800
Ni	2.03733000	-0.55740500	-0.28493300
H	3.59904000	-1.37659500	-0.65300300
H	2.18299200	-2.24182600	0.47761200
H	4.16830600	-2.46019400	0.99457000
B	3.34157200	-1.73665700	0.54773000
H	3.20741500	-0.63981100	1.16734200
H	2.85761200	1.51278200	-1.49792400
O	2.19571300	1.38301100	-0.80357200
C	2.35438500	2.39561300	0.22821100
H	3.23557200	2.14873600	0.83364300
H	2.53345200	3.34748400	-0.28157200
C	1.09459900	2.44126200	1.04906300
H	1.17139500	3.24159000	1.79144700
H	0.22500000	2.64343700	0.41313500
H	0.92297000	1.50529400	1.59613300
H	-2.60904900	1.89200900	0.52604300
H	-3.20447500	2.21721200	-1.11938700
C	-3.47658400	1.81010500	-0.13999300
H	-4.27743100	2.42520200	0.28190200
C	-3.94430900	0.38644300	-0.26705600
H	-4.19459500	-0.05582600	0.70627900
H	-4.82126600	0.31142800	-0.91840000
O	-2.88367600	-0.39252000	-0.87932000
H	-3.25275700	-1.21228600	-1.23784900

INT-1Q
(E = −447.43841021)
0, 5

H	-0.32574700	3.24890500	-0.69213400
H	-0.81473600	1.44246200	-1.41004000
B	-1.13459100	2.36685200	-0.56515900
H	-2.29947800	2.64250100	-0.73303600
H	-0.98440400	1.89432800	0.62212000
Ni	-1.04352700	0.31351500	-0.10222100

H	-2.87405400	-0.53230500	0.31458900
H	-1.98793500	-2.26386400	0.85380500
H	-1.15369100	-0.51629200	1.52175800
B	-2.25991500	-1.01526000	1.25680300
H	-0.71125200	-1.02209300	-1.31245100
H	-2.86107900	-1.24819500	2.27036600
H	-1.13447000	-2.38759100	0.16173000
H	-0.28746400	-2.95479400	-1.59431200
H	0.82035700	-2.00589600	-0.18055700
B	-0.25111600	-2.05488400	-0.80759600
Ni	1.43527900	-0.35042100	-0.20212400
H	1.64701800	0.03703700	1.50304500
H	2.05011400	1.26007600	-0.13128100
B	2.45946400	0.92439300	1.04386800
H	3.56416900	0.43492900	0.95786900
H	2.31439300	1.89866100	1.73060900

TS-1Q-2Q
(E = −447.43408113)
0, 5

H	-0.32158900	3.33205600	-0.52493900
H	-0.68709600	1.54012900	-1.34275200
B	-1.07864700	2.40003200	-0.46226100
H	-2.25553000	2.61236400	-0.64660700
H	-0.92230600	1.87260300	0.70031400
Ni	-0.98599000	0.34293400	-0.12230300
H	-2.91850700	-0.40723800	0.17997000
H	-2.33670600	-2.26745600	0.78382200
H	-1.26561700	-0.58252700	1.46088100
B	-2.38611700	-0.97755500	1.11434100
H	-0.69255100	-0.94355200	-1.33058600
H	-3.05749900	-1.13691100	2.09666800
H	-1.59428300	-2.12264300	0.24148800
H	-0.13234600	-2.86508200	-1.54347200
H	0.49948000	-1.94388700	0.19356200
B	-0.26070000	-1.96366400	-0.77798400
Ni	1.39514300	-0.43736100	-0.14854900
H	1.72806300	0.12298400	1.45309600
H	2.24642400	1.04988600	-0.34696800
B	2.56618600	0.92962200	0.89401400
H	3.66746200	0.43748500	0.96674800
H	2.38268900	2.00356000	1.40207600

INT-2Q
(E = −447.46521050)
0, 5

H	-0.31946900	3.31631000	-0.21802500
H	-0.59594800	1.63571600	-1.26313900
B	-1.02555900	2.34436000	-0.28557400
H	-2.21648200	2.52984400	-0.42750300
H	-0.83356200	1.66941300	0.78951200

Ni	-0.98223600	0.25053000	-0.23220100
H	-3.16279800	-0.02282300	0.28017600
H	-3.24548600	-2.05248100	1.01427400
H	-1.52641200	-0.90618800	1.26771000
B	-2.72660100	-0.79220900	1.09936100
H	-1.07444700	-1.08320700	-1.50604600
H	-3.34076700	-0.78251700	2.12695600
H	-2.93434900	-1.87320500	0.26515000
H	0.99829100	-1.28439000	-1.70114800
H	-0.05382200	-2.54366200	-0.39715900
B	-0.01792700	-1.53828500	-1.05008300
Ni	1.40574400	-0.42397300	0.02529700
H	1.85909700	0.50875900	1.54281700
H	2.31494600	1.13836200	-0.30890200
B	2.83985400	0.70395600	0.76332400
H	3.27739400	-0.43787400	0.47840300
H	3.64676700	1.45523100	1.21507300

H_2
(E = −1.16983358)
0, 1

H	0.00000000	0.00000000	0.37150500
H	0.00000000	0.00000000	-0.37150500

INT-3Q
(E = −446.31045661)
0, 5

H	1.35831000	2.47382500	0.77800500
H	1.25925100	0.51985800	1.27198200
B	2.00612600	1.49338200	1.01460200
H	2.81094400	1.53463300	1.90688500
H	2.90319800	1.42848500	0.03735500
Ni	0.96419700	-0.55730600	-0.07111400
H	2.79778300	-0.56342600	-0.49415400
H	1.38045000	0.73780400	-1.29046100
B	2.54996500	0.59316300	-0.87368000
H	0.48477700	-1.91663600	1.10222200
H	3.30993900	0.93237900	-1.73236200
H	-1.56677500	-1.51866900	1.11070800
H	-0.73584500	-2.64743900	-0.44913400
B	-0.57713300	-1.88430900	0.46247000
Ni	-1.46794000	-0.06723700	-0.06435500
H	-1.37991900	1.47359100	-1.07726700
H	-1.61772900	1.47099900	0.91865000
B	-2.21741600	1.75210500	-0.16638000
H	-3.13268100	0.90146200	-0.27126000
H	-2.57460600	2.88863400	-0.20308400

TS-3Q-4T
(E = −446.33693941)
0, 3

H	1.03578800	2.32515200	0.93540600
H	1.24930200	0.34655800	1.33650700
B	1.83019400	1.45205200	1.15020200
H	2.57033700	1.57959100	2.09137800
H	2.79274100	1.57394600	0.24841900
Ni	1.21708700	-0.56652900	-0.12998200
H	3.07081000	-0.23807900	-0.67657900
H	1.38544700	0.85387900	-1.22015600
B	2.57067000	0.88031800	-0.82616300
H	0.67447000	-2.07171000	0.90682100
H	3.18364700	1.55958700	-1.59854600
H	-1.35586400	-1.69058700	1.20216800
H	-0.50123100	-1.45282100	-0.74461100
B	-0.37581100	-1.61755700	0.49480500
Ni	-1.67034200	-0.19824700	-0.03783900
H	-1.51607200	1.22918400	-1.00894700
H	-2.26003900	1.12446500	0.92794900
B	-2.41498300	1.68671200	-0.21440200
H	-3.51078600	1.41092900	-0.66151400
H	-2.17776200	2.85600300	-0.06151200

TS-4T
(E = −446.34762780)
0, 3

H	-3.46801300	-1.91350900	0.77472900
H	-1.49556900	-1.61188900	0.69598200
B	-2.60255700	-1.17275300	0.41321900
H	-2.80986000	-0.80114300	-0.74596000
H	-3.02836800	-0.15486600	1.17583900
H	-2.72677200	1.69658600	1.45146900
H	-1.29892100	0.39427400	2.23518300
B	-2.09061800	0.68841400	1.40236000
H	-1.31104900	1.17841200	0.26120800
Ni	-0.99980000	-0.24678700	-0.63774700
H	-0.44832800	2.72771200	-0.65924400
H	0.66416600	1.70614500	0.70395300
B	-0.07939000	1.66350200	-0.28160800
H	0.27433600	0.92735200	-1.26750800
Ni	1.46898800	0.25582600	0.05444200
H	2.19204600	-1.16262600	-0.58453700
H	4.05765500	-0.79919700	0.11038700
H	2.49541400	-0.33056800	1.32132100
B	2.94790400	-1.14987400	0.45079300
H	2.88930900	-2.25623700	0.93590000

INT-2T
(E = −447.51418276)
0, 3

H	-0.86594500	2.22333300	1.08092800
H	1.06724500	1.73447500	0.93038800
B	0.02034900	2.05407100	0.28624600

H	0.25656900	2.95659200	-0.47859600
H	-0.33686800	1.08959700	-0.55239900
Ni	1.26736300	0.42364100	-0.17201000
H	2.97516400	-0.22377800	0.18116600
H	2.92745600	-2.32040400	-0.28083700
H	1.69053000	-0.96453900	-1.35702500
B	2.72015700	-1.04520800	-0.69545500
H	-0.76941200	-0.16028900	1.93001200
H	3.67352900	-1.27862600	-1.37438000
H	2.28941700	-2.02841000	0.16747700
H	1.03753000	-1.08041600	2.23479600
H	-0.18992900	-1.80878600	0.70912100
B	0.07796000	-0.96275000	1.54579000
Ni	-1.28916900	-0.26379700	0.18900300
H	-1.85522800	-0.60168700	-1.42530000
H	-3.05578900	-0.08982700	0.20717000
B	-3.04255800	-0.31289200	-1.04675900
H	-3.73229000	-1.28419300	-1.26789100
H	-3.38093300	0.69520200	-1.62955000

INT-3T
(E = −446.33045065)
0, 3

H	0.24836900	2.93817600	1.00502100
H	1.41198100	1.30225500	1.18475800
B	0.74419600	2.04149400	0.39838400
H	-0.23131900	1.33049800	-0.11464500
H	1.45221600	2.31763000	-0.57247100
Ni	1.36926900	0.27484700	-0.25054300
H	2.53863800	-1.06148000	0.07690500
H	1.17850500	-0.97384600	-1.58490900
B	1.84121700	-1.60907000	-0.77244200
H	1.93504600	-2.77375700	-0.91745200
H	0.98423500	-1.57055200	2.09237600
H	-0.64147900	-0.36050800	1.89386900
B	0.08836400	-1.22470400	1.40106200
H	-0.27946900	-1.91064500	0.45632500
Ni	-1.20080600	-0.14664700	0.23248200
H	-1.80980200	-0.06894500	-1.39174200
H	-2.92781500	0.17011700	0.36229300
B	-2.98292700	0.12746600	-0.91243500
H	-3.67295600	-0.81108600	-1.24328100
H	-3.35737300	1.20659100	-1.31417500

TS-3T-4T
(E = −446.32981854)
0, 3

H	2.94181300	1.77409700	0.22483500
H	3.27954300	0.80567600	-1.58228000
H	1.37230500	1.22586800	-1.00137100
B	2.58964700	1.01527900	-0.62852400

H	2.63837600	-0.27090000	0.06561300
H	2.56160600	-1.27019200	1.91774500
H	2.92614300	-2.33442000	0.17233700
B	2.25376800	-1.57699100	0.80522300
H	1.01423800	-1.74845700	0.64204700
Ni	0.97961700	-0.22072600	-0.20717000
H	0.38485000	2.69506000	0.91230700
B	-0.29702900	1.78394200	0.61085900
H	-0.98711100	1.89824000	-0.40061500
H	-0.50528500	0.91370900	1.46291100
Ni	-1.50702700	0.26208000	0.12422800
H	-3.47914800	-0.39011300	-0.09475200
H	-1.89725400	-0.68913100	-1.33318200
B	-2.64790800	-1.23372800	-0.45347100
H	-1.88427000	-1.45060200	0.54331100
H	-3.09072500	-2.25926800	-0.87698800

TS-4T-5T

(E = −446.34676971)

0, 3

H	-3.44114900	-2.10438000	0.28668100
H	-1.53368500	-1.66485200	0.62633700
B	-2.60492200	-1.25409300	0.20038300
H	-2.67153900	-0.77204100	-0.93776100
H	-3.22962800	-0.46105800	1.03739200
H	-3.11971500	1.48757200	0.94527900
B	-2.43841700	0.55045700	1.20879000
H	-1.79684300	0.45410500	2.20130800
H	-1.24382900	1.23634800	0.28467200
Ni	-0.95783700	-0.17268400	-0.53775100
H	0.35544500	1.00850900	-1.18924400
H	-0.30446200	2.79704600	-0.51999200
B	-0.02685400	1.69234300	-0.17345300
H	0.70234600	1.65850400	0.82888100
Ni	1.49789100	0.24926500	0.07432200
H	4.06339200	-0.80694200	0.02869500
H	2.18679000	-1.14748800	-0.65691500
B	2.96395500	-1.19735600	0.36029700
H	2.51457900	-0.45063900	1.29408600
H	2.92797500	-2.33573100	0.76649300

INT-5T

(E = −446.38618271)

0, 3

H	2.32679100	2.53753500	-0.92811000
H	1.25574000	0.83404800	-1.17274100
B	2.14059000	1.42577300	-0.56788700
H	3.29402600	0.78902900	-0.59269800
H	2.01428000	1.48144200	0.74743400
B	2.93224300	0.53024400	0.64828400
H	3.81879800	0.86165000	1.35863200

H	2.52852900	-0.61484400	0.79557800
Ni	0.94861800	-0.57034400	-0.10288800
H	0.39050400	-2.00539000	0.70010300
H	-0.60904400	-1.21317200	-1.00600700
H	-0.94298400	-3.05176800	-0.35489100
B	-0.69235300	-1.95239500	0.05315000
H	-1.59319600	-1.56466000	0.83304900
Ni	-1.56239500	-0.00845900	0.00070700
H	-2.82081100	2.78712200	-0.02608000
H	-1.59896700	1.47073300	-0.89877700
B	-1.90525000	2.03069800	0.20782700
H	-2.34173400	1.15808500	1.03150000
H	-0.91232900	2.56507000	0.66719900

INT-1D

(E = −196.54186054)

0, 2

H	-2.20461700	0.00015900	-1.02243400
H	-0.83592900	-1.06980500	-0.00012600
B	-1.55317900	-0.00001500	-0.00000200
H	-0.83593600	1.06981100	0.00013000
H	-2.20459700	-0.00010900	1.02244600
Ni	0.49453500	0.00000100	0.00000000

B_2H_6

(E = −53.24082695)

0, 1

H	-1.45263500	1.03717600	0.00001500
H	-1.45266800	-1.03715500	-0.00001500
B	-0.86854600	0.00000200	0.00000000
H	0.00000000	0.00000300	-0.98634700
H	0.00000000	-0.00006000	0.98634700
H	1.45267400	-1.03715100	-0.00001500
B	0.86854400	0.00000200	0.00000000
H	1.45264100	1.03717200	0.00001500

TS-4T-4T(2)

(E = −446.34665038)

0, 3

H	-2.74085800	-0.89781400	-0.89190800
H	-3.70567600	-1.85207100	0.56477100
H	-1.78362100	-1.47766300	0.91258900
B	-2.79760700	-1.11452600	0.31783400
H	-3.36082700	-0.10055600	0.94526700
H	-3.19263700	1.73871000	0.20392800
B	-2.61685200	0.94840700	0.87995600
H	-2.23972800	1.17352200	1.98465400
H	-1.27915400	1.13607900	0.21831500
Ni	-0.95439700	-0.37918600	-0.42293900
H	0.31225300	0.75668200	-1.25268600
H	-0.40424600	2.60195900	-0.83767700

B	-0.05330000	1.57774600	-0.34715000
H	0.66146900	1.70243600	0.65360100
Ni	1.55376300	0.27234400	0.04411100
H	4.21279300	-0.56926600	-0.00652600
H	2.34467800	-1.12958500	-0.54844200
B	3.16145100	-0.98731200	0.42932600
H	2.69520100	-0.15267900	1.27751600
H	3.22966000	-2.05975700	0.98395700

INT-4T(2)
(E = −446.34712355)
0, 3

H	-3.73738300	-1.78830400	0.68973300
H	-1.77089700	-1.52333200	0.90642600
B	-2.80341800	-1.11553500	0.36810800
H	-2.79344900	-0.91852500	-0.83969400
H	-3.18414500	-0.06698700	1.11210300
B	-2.65476200	1.02612300	0.70366400
H	-3.16446300	1.53764600	-0.23693200
H	-2.50930500	1.59475000	1.74204100
H	-1.21577100	1.05368000	0.42070800
Ni	-0.94036300	-0.42335500	-0.39279200
H	0.25608800	0.73941300	-1.21452700
H	-0.52095500	2.56029400	-0.78661100
B	-0.09118800	1.56542500	-0.30146300
H	0.68512600	1.74054300	0.64367400
Ni	1.55819200	0.29444900	0.04174100
H	2.30545300	-1.13359000	-0.53596400
H	4.22865100	-0.67881600	-0.12028300
H	2.81893900	-0.02697200	1.17860700
B	3.17221300	-0.97308600	0.39515100
H	3.18867100	-1.99506000	1.04284700

INT-5T(2)
(E = −446.35765355)
0, 3

H	-1.43075900	-2.91821400	1.27485000
H	-1.20523900	-0.91910100	1.23037800
B	-1.99337000	-1.89887000	0.94525500
H	-2.23571200	-1.95648100	-0.31325900
H	-3.03934700	-1.67263300	1.51000700
Ni	-1.13078500	-0.64118400	-0.47440000
H	-2.28597100	2.94705200	-0.66177500
H	-1.39868400	3.67490500	1.08822200
B	-1.45860300	2.91207800	0.18477300
H	-1.42244800	1.66314600	0.69138300
H	-0.25751600	2.85579300	-0.40793800
H	0.59304400	1.62498500	0.98322200
B	-0.26728800	1.66891900	0.11144300
H	-0.21990700	0.91948400	-0.89103900
Ni	1.30033100	0.24370900	0.09553000

H	1.92961100	-1.12404800	-0.71622100
H	3.84479700	-0.46535400	-0.72933800
H	2.74814600	-0.15427500	0.95827700
B	2.99234600	-0.94680400	-0.01530200
H	3.26726000	-2.02257200	0.46073600

INT-5T(3)
(E = −446.36081007)
0, 3

H	-3.23323500	1.48307100	1.33128100
H	-1.56214400	0.38754200	1.52689100
B	-2.43143800	0.79488600	0.76564800
H	-3.02898400	-0.03109100	0.05794700
H	-2.00294300	1.78380500	-0.01854000
H	-1.24449000	2.14785900	-1.70856800
H	-0.02142600	2.01373100	-0.09878200
B	-0.96634000	1.51463500	-0.73063800
H	-0.74245300	0.33573000	-1.18862300
Ni	-1.40282400	-0.90575200	0.00210500
H	1.38873300	-1.17450700	-0.48715900
H	3.26870100	-1.21357100	-1.24107900
B	2.60324200	-1.34079700	-0.24768500
H	2.67644900	-2.40566300	0.31692800
Ni	0.82628500	0.45108200	-0.18691100
H	1.68856700	0.43589500	1.54458100
H	3.21578900	-0.66074800	0.69460900
H	2.58006800	1.16539300	-0.20512200
B	2.70354100	0.52704900	0.84632700
H	3.61542400	0.98446000	1.48196200

C_2H_5OH
(E = −154.95648438)
0, 1

C	1.21681000	-0.22112000	0.00000300
H	1.28916900	-0.85909300	-0.88806700
H	1.28916900	-0.85908400	0.88807800
H	2.07004200	0.46520000	-0.00000200
C	-0.08082600	0.54575300	-0.00000200
H	-0.14313000	1.19380700	0.88755200
H	-0.14312300	1.19380500	-0.88755900
O	-1.14900100	-0.39559500	-0.00000500
H	-1.98602000	0.08233000	0.00003700

INT-$1D_{1ET}$
(E = −351.52653315)
0, 2

H	-2.88148200	1.72654800	0.54847800
B	-2.68877000	0.56021200	0.27469900
H	-2.14609600	0.52737000	-0.88750700
H	-1.91797400	0.05967900	1.16263200
H	-3.69306500	-0.11861600	0.22580400

H	1.08431600	-1.88176200	0.08173700
Ni	-0.79493500	-0.17860100	-0.12747600
O	1.01082200	-0.93998900	-0.11857400
C	2.17036900	-0.22541800	0.37032100
H	3.06295600	-0.74508500	0.00480200
H	2.16744900	-0.25731800	1.46664700
C	2.10566700	1.18570000	-0.14431600
H	2.98311900	1.74525800	0.19503500
H	1.21191200	1.70013000	0.23019200
H	2.08811500	1.20178500	-1.23943300

TS-1D_{1ET}-2D_{1ET}
(E = −351.44935605)
0, 2

H	2.95263500	1.52070600	1.03873000
B	2.15916200	0.75019700	0.60928500
H	2.42517600	0.22924400	-0.46014000
H	1.34850700	0.31185700	1.41387100
H	1.29484500	2.41430700	0.04304500
H	0.81668500	1.93321800	-0.30750300
Ni	0.73697600	-0.60571000	-0.10336700
O	-0.61620900	0.39425400	-0.92208600
C	-1.65094500	0.80332700	-0.08656000
H	-2.39549600	1.37564700	-0.67354900
H	-1.28414900	1.50749900	0.69569700
C	-2.35896300	-0.35020400	0.60698400
H	-3.18374200	-0.00181600	1.24328800
H	-1.65038400	-0.90360300	1.24199800
H	-2.76609200	-1.05091700	-0.13343400

INT-2D_{1ET}
(E = −351.50054448)
0, 2

H	1.07778000	0.65010300	1.27450200
H	-0.78733700	1.09938400	1.84150400
H	0.27360000	2.42911300	0.71628100
B	-0.02710800	1.26188300	0.90193500
Ni	1.29282800	-0.21208600	-0.15050200
O	-0.52903600	0.63477600	-0.36835900
C	-1.70680600	-0.15389000	-0.30847600
H	-1.92830600	2.63128500	-0.76820900
H	-2.44233600	3.15022700	-0.92196000
H	-2.06541800	-0.27375200	-1.34050900
H	-2.47643500	0.40855400	0.24494100
C	-1.48929400	-1.50790700	0.33065000
H	-2.41522900	-2.09483300	0.31266400
H	-1.16999500	-1.40642700	1.37480100
H	-0.72107500	-2.07209600	-0.21579100

INT-1D_{2ET}
(E = −506.48730472)

0, 2

H	2.88576200	-2.00226400	1.54212000
C	2.41177900	-1.07866100	1.19239200
H	2.90418200	-0.23405200	1.68970200
H	1.35875700	-1.09242800	1.50215100
C	2.52970700	-0.96889800	-0.30769400
H	3.57479600	-1.00305600	-0.63771600
H	1.99254000	-1.77878000	-0.81286900
O	1.93412600	0.24386800	-0.81184900
H	2.47407200	0.99991900	-0.54514500
H	0.42007000	3.29923500	1.28050200
B	-0.32036900	2.43820400	0.83909100
H	-0.16975200	2.42180100	-0.41580700
H	-0.00371700	1.34393600	1.37411200
H	-1.50523200	2.66110200	1.08216300
H	-2.36099400	1.11453500	0.12542200
Ni	-0.03633200	0.58263800	-0.35755900
O	-2.08398900	0.29042700	-0.31027200
C	-2.48029500	-0.83250600	0.49586300
H	-3.57608100	-0.86644800	0.54013000
H	-2.09484300	-0.69864900	1.51777600
C	-1.92078200	-2.07762200	-0.13909800
H	-2.20564300	-2.96258300	0.43854400
H	-0.82255200	-2.04011300	-0.17517200
H	-2.29577400	-2.19526900	-1.16152300

TS-1D_{2ET}-2D_{2ET}

(E = −506.42912658)

0, 2

H	-3.09131800	1.96170100	1.20222000
C	-2.63617900	0.98034100	1.03074600
H	-3.28017700	0.22507400	1.49701500
H	-1.66082100	0.96142100	1.53269100
C	-2.48395100	0.72674700	-0.44805700
H	-3.45048600	0.74565000	-0.96604300
H	-1.83231200	1.47046700	-0.92110300
O	-1.84877900	-0.53974300	-0.71417300
H	-2.39337900	-1.25460800	-0.35966100
H	0.65618300	-3.05719000	1.86395800
B	0.48132400	-2.14995400	1.11609300
H	0.28038200	-2.45586100	-0.04864000
H	0.23796300	-1.06337600	1.59759200
H	2.49624700	-2.12148000	1.16664500
H	2.40885100	-1.62269400	0.59498600
Ni	0.16630100	-0.62029100	-0.33416900
O	1.91363100	-0.00846300	-0.69406700
C	2.39737200	0.99197400	0.13962800
H	3.37122200	1.35730200	-0.24290100
H	2.61034000	0.60068200	1.16246300
C	1.46049100	2.18375600	0.28056200
H	1.90478800	2.98238700	0.89028900

H	0.51830600	1.87926300	0.76230000
H	1.21594300	2.59793100	-0.70690800

INT-2D$_{2ET}$
(E = −506.48479214)
0, 2

H	-3.46059200	1.75484900	1.07936500
C	-2.81991600	0.87196400	0.97923800
H	-3.19932000	0.09849300	1.65709600
H	-1.80545800	1.14601200	1.29608600
C	-2.82288500	0.39361800	-0.45034100
H	-3.83263800	0.15517100	-0.80294100
H	-2.39648900	1.14182400	-1.12633800
O	-1.99917200	-0.78265500	-0.63018700
H	-2.44957900	-1.55898900	-0.27284300
H	0.45909400	-0.83071500	1.48862100
H	2.22868000	-0.05088500	2.00791400
H	2.12889000	-1.97345400	1.33369300
B	1.72807400	-0.82712700	1.20962800
Ni	-0.08435500	-0.65407700	-0.14935700
O	1.89283900	-0.37522300	-0.21693400
C	2.36432600	0.94287800	-0.45209700
H	4.20294000	-1.20517400	-0.12528300
H	4.93688300	-1.34095200	-0.14229400
H	2.61881500	1.00553800	-1.51941800
H	3.29618200	1.08467000	0.11930800
C	1.36482900	2.02139300	-0.08971100
H	1.77051200	3.01182100	-0.32861900
H	1.12586800	1.99979500	0.98036300
H	0.43031800	1.89569900	-0.65641700

INT-1D$_{3ET}$
(E = −661.44939569)
0, 2

H	-4.01309700	-1.20955000	-1.64716100
C	-3.32946200	-1.13547600	-0.79454500
H	-3.85317000	-1.50763300	0.09424800
H	-3.09062000	-0.07648300	-0.63425800
C	-2.07709300	-1.93268200	-1.06023400
H	-2.29865100	-2.98878200	-1.25436000
H	-1.52480000	-1.54182500	-1.92161500
O	-1.14637700	-1.85962600	0.04026600
H	-1.51043500	-2.33165900	0.80125400
H	-1.54493100	0.20180100	3.57308000
B	-0.94270100	0.66971600	2.62472100
H	0.00669300	-0.11597000	2.35360600
H	-1.75951700	0.78631500	1.67090000
H	-0.47143400	1.78076100	2.86596000
H	0.56294100	2.08817900	1.26758900
Ni	-0.47816000	0.00495200	0.55328700
O	0.56427000	1.80601200	0.33448100

C	-0.12484800	2.79097900	-0.46506200
H	0.47712400	3.70724600	-0.48267600
H	-1.09082100	3.01357800	0.00910200
C	-0.30732500	2.22220100	-1.84603900
H	-0.81441300	2.94629600	-2.49111000
H	-0.92291200	1.31216400	-1.81548100
H	0.65790100	1.97471800	-2.30233900
O	2.62702000	0.13325300	-0.80308700
H	2.04188600	0.83125900	-0.46623700
C	2.72951800	-0.87460200	0.19239200
H	2.99731100	-0.42802600	1.16419600
H	1.75562300	-1.38092000	0.32956100
C	3.77655400	-1.87141700	-0.23662200
H	4.75205000	-1.38372700	-0.34670700
H	3.87376800	-2.67339300	0.50302300
H	3.50810900	-2.32271600	-1.19885100

TS-1D_{3ET}-2D_{3ET}
(E = −661.39838836)
0, 2

H	-4.91742900	1.17222300	0.55855300
C	-4.19056400	0.35296500	0.55480400
H	-4.68632200	-0.53878100	0.95653300
H	-3.36582500	0.62271500	1.22584600
C	-3.68625700	0.10902900	-0.84527200
H	-4.50040500	-0.14899500	-1.53304900
H	-3.16886700	0.98720800	-1.24812700
O	-2.70475900	-0.94649800	-0.88659300
H	-3.11156700	-1.77650400	-0.60523600
H	-0.34536300	-2.57412600	2.42876300
B	-0.51439400	-1.79832900	1.54510800
H	-0.35403900	-2.22751300	0.41510100
H	-1.07652500	-0.75653500	1.81752200
H	1.38267300	-1.30125600	2.02297500
H	1.30518700	-0.88175800	1.39227600
Ni	-0.86723600	-0.50016000	-0.10905900
O	0.75137500	0.48375800	-0.24710300
C	0.84524700	1.66818100	0.48274200
H	1.76680200	2.20873000	0.18948800
H	0.95321100	1.45990600	1.57126700
C	-0.34715100	2.58846900	0.28456300
H	-0.22001200	3.53966500	0.81799200
H	-1.26581800	2.11355800	0.66094300
H	-0.49009500	2.80515000	-0.78229000
O	3.16701600	-0.37903300	-0.97375700
H	2.24303500	-0.07631000	-0.76919000
C	4.02032500	0.13533900	0.02467700
H	4.12860100	1.23043900	-0.07849400
H	3.59583400	-0.04476600	1.02915400
C	5.37563700	-0.52198600	-0.08822600

H	5.80851400	-0.34021700	-1.07932600
H	6.06770700	-0.12819500	0.66471300
H	5.29281500	-1.60631600	0.05259000

INT-2D$_{3ET}$
(E = −661.44990808)
0, 2

H	4.80110600	-0.52152800	0.53856100
C	3.87630600	-0.61110400	-0.04168300
H	4.13581800	-0.98195100	-1.04003100
H	3.43750700	0.38960400	-0.14476900
C	2.91942300	-1.54315700	0.65607300
H	3.34861200	-2.54013300	0.80473000
H	2.61936700	-1.15464200	1.63459200
O	1.68159100	-1.69699000	-0.07964900
H	1.81401500	-2.28482300	-0.83503300
H	-0.86052200	1.55854600	-2.45393500
B	-0.11580600	1.80381400	-1.51775800
H	0.96485600	1.10724400	-1.68096200
H	0.24530800	2.96549600	-1.46720700
H	-3.62948800	2.69054400	-0.75620600
H	-2.95068200	2.38040700	-0.74100800
Ni	0.62044900	-0.07890200	-0.45812200
O	-0.77112700	1.34693000	-0.23496500
C	-0.70638600	2.18407800	0.91434700
H	-1.41622400	1.77113300	1.64525100
H	-1.06429800	3.18589800	0.62933200
C	0.68057000	2.27113800	1.51179400
H	0.66859600	2.90583100	2.40556400
H	1.39392600	2.70031100	0.79802300
H	1.04295800	1.27685000	1.81057900
O	-2.68434000	-0.61259600	-0.81694800
H	-2.11025100	0.17441000	-0.81599500
C	-2.83716100	-0.98696700	0.54131200
H	-1.84737600	-1.13785000	1.00882800
H	-3.33983800	-0.18201400	1.10603600
C	-3.64750500	-2.25753600	0.60943600
H	-3.14344500	-3.06607700	0.06712600
H	-3.78793100	-2.57542100	1.64823700
H	-4.63603900	-2.10910100	0.15930800

INT-3D
(E = −505.31284795)
0, 2

H	-3.24796800	1.84836500	1.18716200
C	-2.65928000	0.93760700	1.03223400
H	-3.08760500	0.14575400	1.65762600
H	-1.63278800	1.13100800	1.36891000
C	-2.68025600	0.55342200	-0.42508500
H	-3.69974300	0.40205600	-0.79687800

H	-2.20229700	1.31534100	-1.04932200
O	-1.92999800	-0.65879200	-0.67679500
H	-2.43861900	-1.42863900	-0.39056200
H	0.51427900	-0.98997700	1.45398100
H	2.18199200	-2.12748900	1.30673100
H	2.27893000	-0.21208600	2.00018200
B	1.78746200	-0.97873600	1.18778100
Ni	-0.02265200	-0.68855900	-0.16116000
O	1.96144800	-0.50892600	-0.23088200
C	2.51337200	0.77972100	-0.45187700
H	2.77079300	0.83931600	-1.51844100
H	3.45151800	0.85811500	0.11995600
C	1.58097900	1.91366900	-0.07879900
H	2.05091600	2.88047100	-0.29609500
H	1.33081000	1.88828900	0.98875300
H	0.64623600	1.85801700	-0.65586400

TS-3D-4D
(E = −505.28725229)
0, 2

H	-2.48585800	2.49139500	0.99141400
C	-1.92360500	1.92101200	0.24416200
H	-0.85942400	1.97436800	0.49719400
H	-2.07235500	2.39116800	-0.73447500
C	-2.39409500	0.49024400	0.22411100
H	-2.25842100	0.00957900	1.20418000
H	-3.45748800	0.43104100	-0.03623700
O	-1.63438200	-0.24177000	-0.75982400
H	-2.19638800	-0.92208900	-1.15008400
Ni	0.07760400	-1.36327400	-0.17098700
H	-0.09336500	-2.87334800	-0.49833800
H	-0.05113000	-0.18858600	2.48304600
H	2.04338400	0.02786600	2.58737800
B	1.01050700	0.04341800	1.98620300
O	0.99677600	0.37326600	0.66520900
C	2.21594200	0.75481400	-0.02172400
H	2.80602900	-0.15651000	-0.18470300
H	2.78068900	1.42221200	0.63893200
C	1.84484400	1.42102900	-1.31842300
H	2.74915500	1.72105900	-1.85736600
H	1.23751000	2.31474700	-1.13731200
H	1.27454900	0.73713000	-1.95884900

INT-4D
(E = −505.28930336)
0, 2

H	-2.33174100	2.51044000	1.20075800
C	-1.70179600	2.01420600	0.45531100
H	-0.70254100	1.88703200	0.88930000
H	-1.60970600	2.66925800	-0.41806600
C	-2.29630200	0.68484800	0.07060200

H	-2.40836400	0.02876400	0.94738800
H	-3.28753200	0.81837800	-0.37865700
O	-1.42842800	0.04397000	-0.88381100
H	-1.96213300	-0.50945900	-1.46729800
Ni	-0.14847000	-1.47790700	-0.01621700
H	-0.81520100	-2.86758300	-0.22983000
H	0.37875600	0.12088000	2.56851700
H	2.07347200	1.30113700	2.13898200
B	1.24492800	0.49280100	1.83643000
O	1.26137500	-0.04112700	0.59296200
C	2.24506800	0.37277500	-0.38957700
H	2.45680900	-0.51745300	-0.99104200
H	3.15762500	0.66020800	0.14618700
C	1.69434800	1.49997600	-1.22144600
H	2.40754900	1.76645800	-2.00826600
H	1.51806600	2.38885300	-0.60271600
H	0.74596000	1.20691700	-1.68589500

TS-4D-5D
(E = −505.25995266)
0, 2

H	-3.13772500	1.76940400	1.54315000
C	-2.46775600	1.39530900	0.75890000
H	-1.44559400	1.37915600	1.16483400
H	-2.48662200	2.10577600	-0.07729900
C	-2.87790400	0.01308800	0.28937600
H	-2.81794200	-0.69427000	1.14139000
H	-3.93433900	0.02709900	-0.02845800
O	-2.07720300	-0.43938900	-0.77552500
H	-1.55966600	-1.58753700	-0.49527200
H	-0.85837900	-2.22672200	-0.21225600
H	1.78574300	-2.12076100	1.54040300
H	3.56257900	-0.99434500	1.42156900
B	2.43521700	-1.22349600	1.10550000
Ni	-0.12975300	-0.61315900	-0.26246200
O	1.83029500	-0.42156100	0.19037800
C	2.52174100	0.69592300	-0.43239500
H	2.60551400	0.45152400	-1.49634500
H	3.52699100	0.74393400	0.00019700
C	1.74591200	1.96591800	-0.20540400
H	2.28921200	2.80970200	-0.64284300
H	1.61273000	2.15934800	0.86465700
H	0.75780000	1.92980800	-0.68396800

INT-5D
(E = −505.28372568)
0, 2

H	-3.08996200	2.42028200	-0.10855100
C	-2.33739100	1.64094200	0.07393100
H	-1.97773700	1.74440900	1.10670000
H	-1.48517600	1.82091200	-0.59834100

C	-2.91124800	0.25199100	-0.15266600
H	-3.80567100	0.13485400	0.48948300
H	-3.28143400	0.19026800	-1.19538700
O	-2.02461700	-0.79469000	0.10890600
Ni	-0.24584400	-0.58146200	-0.03739400
H	-0.50103800	-3.10603700	0.67883200
H	-0.44602100	-3.82102200	0.89023600
H	2.10777900	-2.41248100	0.39733400
H	3.74350100	-1.11835500	0.08067200
B	2.57634700	-1.36204600	0.09701000
O	1.69978400	-0.37679100	-0.25228900
C	2.17367900	0.96211300	-0.60064300
H	1.51152500	1.30994900	-1.39935900
H	3.18807100	0.85422000	-0.99916800
C	2.12423100	1.84712500	0.61369600
H	2.45138800	2.85763700	0.34871100
H	2.78571700	1.46654400	1.40042600
H	1.10397900	1.90881600	1.01155600

TS-5D-6D
(E = −505.26983938)
0, 2

H	3.32780300	-2.18775400	0.01061200
C	2.75272800	-1.39429900	0.50616900
H	3.42977100	-0.83987100	1.16856700
H	1.98201700	-1.86433500	1.13195000
C	2.11340200	-0.45489200	-0.50245100
H	2.90538100	-0.04754900	-1.16357900
H	1.45447200	-1.04867900	-1.16933200
O	1.42410800	0.57814200	0.13505500
H	0.31994700	3.18432000	0.94559600
H	0.46025000	3.85618500	1.24096000
H	-0.36409000	1.05543700	2.18431400
H	-0.25820200	-1.04014400	1.99844800
B	-0.64038900	0.03387400	1.63371100
Ni	-0.24215800	1.09159200	-0.53890000
O	-1.65065200	0.10383100	0.68998000
C	-2.24722100	-1.11441800	0.18896600
H	-3.19319400	-0.81212000	-0.27093800
H	-2.47454300	-1.75442600	1.05002500
C	-1.35369400	-1.81784700	-0.79916900
H	-1.86133300	-2.70352900	-1.19631000
H	-0.41699800	-2.14090000	-0.32870600
H	-1.10784400	-1.15762300	-1.64235600

INT-6D
(E = −505.30702990)
0, 2

H	3.90930200	-1.32021400	-0.70217900
H	3.00159900	-1.58121500	0.80272600
H	3.78285400	-0.01470900	0.49808500

C	3.24293800	-0.84451800	0.02705800
C	1.98241800	-0.34573700	-0.64453000
H	2.23084400	0.38756300	-1.42484800
H	1.45277400	-1.18129100	-1.13507800
O	1.12149600	0.29434900	0.28282800
Ni	-0.51719900	1.23381800	-0.44381900
H	-0.24487200	2.98427200	2.24045600
H	-0.27423100	2.49270600	1.67645200
H	0.55235300	-0.26011100	2.37483900
B	0.30300800	-0.56982100	1.21285000
H	0.48825400	-1.76108500	0.98768200
O	-1.11909200	-0.17446400	0.88817500
C	-2.03166500	-1.18611600	0.49614900
H	-3.04393100	-0.77173900	0.60228300
H	-1.95196300	-2.02926100	1.19950100
C	-1.80978500	-1.66475900	-0.92267500
H	-1.89681000	-0.82681300	-1.62821800
H	-2.55138700	-2.42391400	-1.19912300
H	-0.81093100	-2.10428900	-1.03394000

INT-7D

(E = −504.13474361)

0, 2

H	-0.60499900	-0.94733700	-2.20445200
H	-0.43056600	-1.91668000	-0.41422500
B	-0.30925400	-0.85307500	-1.01525000
Ni	0.48030700	1.35519500	0.07607200
H	-2.97966900	-1.75931900	-0.40225100
C	-3.25621600	-0.83633000	0.12152500
H	-3.78094200	-0.18437100	-0.58683200
H	-3.94948300	-1.09585600	0.93025500
C	-2.02731900	-0.14475300	0.66976300
H	-2.31225900	0.77170900	1.20549900
H	-1.50665400	-0.80025200	1.39007200
O	-1.13817200	0.22894600	-0.36886100
H	2.16097200	-0.24809000	1.61980200
C	2.01725100	-1.24279800	1.17610200
H	2.79311000	-1.90928300	1.57188200
H	1.03945100	-1.62421400	1.49574400
C	2.09051500	-1.16318800	-0.33380400
H	3.06839800	-0.77123600	-0.64677100
H	1.98880500	-2.16668800	-0.77489500
O	1.09643900	-0.31720100	-0.88602900

TS-7D-8D

(E = −504.12394200)

0, 2

H	0.60877200	0.09566000	1.77476400
H	0.07797200	-1.87441300	1.44192800
B	-0.03056200	-0.70911900	1.05123400
Ni	0.32566100	1.33693300	-0.02125200

H	2.88318300	-0.72253400	1.11120300
C	2.94305300	-0.62337400	0.02159800
H	3.00729300	0.44672700	-0.22134700
H	3.86879600	-1.10344300	-0.31665700
C	1.74490800	-1.24932000	-0.66158600
H	1.87410200	-1.21588400	-1.75238100
H	1.65469200	-2.30972300	-0.37284100
O	0.52056100	-0.60669100	-0.36578700
H	-3.12197900	0.80407800	-0.77751000
C	-2.73456700	-0.19605200	-1.00984500
H	-3.51386300	-0.74562800	-1.55222300
H	-1.86443500	-0.08242000	-1.66753500
C	-2.34183600	-0.91563800	0.26422900
H	-3.23208100	-1.06052300	0.89763200
H	-1.94865800	-1.91912000	0.02730200
O	-1.38666700	-0.18018600	0.99830800

INT-8D
(E = −504.13326470)
0, 2

H	-0.45948600	-1.20699800	1.09683200
H	0.57597800	0.46514900	1.65779800
B	0.41234000	-0.28714200	0.70157500
Ni	-1.50696400	-1.07334500	-0.20478500
H	-1.72084900	1.58147400	1.55792800
C	-1.86274200	1.96644100	0.54086100
H	-2.69997200	1.42534100	0.07949400
H	-2.14218300	3.02444400	0.61158900
C	-0.60299700	1.80251600	-0.28230200
H	-0.74612700	2.22755200	-1.28527600
H	0.23066800	2.34745600	0.19086200
O	-0.21837200	0.44869600	-0.45353000
H	2.93376800	0.24197300	-1.63709800
C	3.04405100	0.67893700	-0.63707500
H	4.05053900	1.10743100	-0.55558300
H	2.31679100	1.49510400	-0.54584800
C	2.82115600	-0.37365000	0.43257200
H	3.60424000	-1.14293300	0.36390200
H	2.91162800	0.09096900	1.43175800
O	1.57855900	-1.02532600	0.32045700

TS-8D-9D
(E = −504.12862784)
0, 2

H	-2.98777400	2.42081100	0.84013600
H	-1.79664000	1.36807000	1.62983400
H	-3.03458800	0.67075100	0.55843600
C	-2.36574800	1.52826100	0.70691600
C	-1.44968000	1.71377400	-0.47998800
H	-2.02893800	1.89935900	-1.39181700
H	-0.78640200	2.57660700	-0.32724300

O	-0.64041700	0.56291100	-0.75087500
Ni	-1.18155000	-1.29073400	0.04848000
H	0.01390500	-1.22564700	1.05113400
H	0.63856700	0.99475600	1.06108800
B	0.50215300	0.32612300	0.06674100
O	1.59907100	-0.15206000	-0.62280000
C	2.76751800	-0.45131800	0.12446500
H	2.48619500	-0.89632000	1.09284100
H	3.31635300	-1.22051400	-0.43383500
H	3.93122500	1.20039300	-0.63617500
C	3.63342700	0.77254500	0.32796500
H	4.54189300	0.51265400	0.88343500
H	3.09650300	1.54265200	0.89426400

INT-9D

(E = −504.14867157)

0, 2

H	-1.81413000	-2.78838600	0.21875500
Ni	-1.26658000	-1.38666500	-0.01204600
B	0.72565700	0.86548000	-0.01604600
H	1.06638200	2.00984800	-0.09526500
H	-1.61271700	2.40103100	1.29714000
C	-2.28951100	1.95188900	0.56058000
H	-2.78591500	1.09113500	1.02406900
H	-3.05290900	2.69197000	0.29898800
C	-1.53303000	1.52769200	-0.67062100
H	-2.19175700	1.07965800	-1.42198700
H	-1.00252200	2.36697200	-1.13538500
O	-0.56325500	0.50945700	-0.33269500
H	3.66316200	-0.97003900	-1.00850000
C	3.76585900	0.02790300	-0.56875300
H	4.82185800	0.19249100	-0.32951500
H	3.46602400	0.76933800	-1.31949800
C	2.92062700	0.15467900	0.67436100
H	3.22363200	-0.56789400	1.43916200
H	3.00369800	1.15990100	1.10948900
O	1.54668900	-0.12318100	0.37852800

NiH

(E = −169.88082173)

0, 2

Ni	0.00000000	0.00000000	0.05172100
H	0.00000000	0.00000000	-1.44820200

H_2BOEt

(E = −180.42155528)

0, 1

H	2.48428300	-0.23723100	0.39702800
H	1.20373800	-1.45641600	0.23120500
H	1.69655800	-0.48604300	-1.17491500
C	1.53072500	-0.46093600	-0.09253200

C	0.49968000	0.57863100	0.26773100
H	0.82098200	1.58147300	-0.03311300
H	0.30714500	0.58976600	1.34913800
O	-0.72745500	0.31649900	-0.42604200
B	-1.71599400	-0.37657700	0.15770000
H	-2.69729100	-0.58645200	-0.49112100
H	-1.59823700	-0.76037800	1.29042700

$HB(OEt)_2$-case1
(E = −334.24837600)
0, 1

H	2.14525400	1.75473100	0.33681200
H	3.83809600	1.22060500	0.37933300
H	2.93326100	1.18042400	-1.14880100
C	2.85727200	1.02461200	-0.06710100
H	3.12590400	-1.11871400	-0.13968000
H	2.31613600	-0.53690000	1.32455500
C	2.40800200	-0.38327100	0.24002200
O	1.15980900	-0.66472000	-0.39237400
H	0.00000000	0.00829100	1.38922700
B	0.00000000	-0.41383100	0.26185200
O	-1.15980900	-0.66472000	-0.39237400
H	-3.12590400	-1.11871400	-0.13968000
H	-2.31613600	-0.53690000	1.32455500
C	-2.40800200	-0.38327100	0.24002200
C	-2.85727200	1.02461200	-0.06710000
H	-2.14525300	1.75473100	0.33681300
H	-2.93326100	1.18042400	-1.14880100
H	-3.83809600	1.22060500	0.37933300

$HB(OEt)_2$-case2
(E = −334.24143821)
0, 1

H	-3.36973600	-0.24232700	1.02954300
C	-3.05272700	-0.67902100	0.07627700
H	-3.34527400	-1.73414000	0.06578200
H	-3.58401800	-0.16568000	-0.73245900
C	-1.56112200	-0.54773700	-0.10016400
H	-1.03133300	-1.06614100	0.70903200
H	-1.24634000	-0.99309600	-1.05342600
O	-1.22424000	0.83956800	-0.09612500
B	0.00000000	1.41550800	0.00000000
H	0.00000100	2.61324200	0.00000100
O	1.22423800	0.83956600	0.09612500
C	1.56112300	-0.54773800	0.10016500
H	1.03133400	-1.06614500	-0.70903000
H	1.24634400	-0.99309700	1.05342800
C	3.05272800	-0.67901900	-0.07627800
H	3.58401900	-0.16567600	0.73245700
H	3.34527800	-1.73413700	-0.06578200
H	3.36973400	-0.24232400	-1.02954500

$B(OEt)_3$-case1
(E = −488.06942534)
0, 1

H	-2.63400000	-0.12692400	1.23602200
H	-3.92950900	-1.24675500	0.76850200
C	-2.84467100	-1.14269500	0.88123000
H	-2.50976600	-1.85341100	1.64506100
C	-2.14963100	-1.40610400	-0.43427300
H	-2.48432400	-0.69629200	-1.20178500
H	-2.37107900	-2.41737100	-0.79458000
O	-0.73319000	-1.33287200	-0.29160900
B	-0.08125500	-0.13368700	-0.34787600
H	1.61303000	-1.75591400	1.02216900
C	2.00648800	-1.27725900	0.11465000
H	1.86720900	-1.98631900	-0.71322300
H	4.05261800	-1.82109900	0.48651700
H	3.59906700	-0.22313400	1.11343700
C	3.46211300	-0.92206600	0.28081200
H	3.85453200	-0.45414400	-0.62892100
O	1.26996400	-0.08678600	-0.15088000
O	-0.77721100	1.01040900	-0.61605600
C	-0.14179000	2.28537800	-0.60826100
H	0.86872600	2.20294300	-1.02878900
H	-0.72980100	2.92771600	-1.27406100
C	-0.09948600	2.85849900	0.78913800
H	-1.11003900	2.92984300	1.20752100
H	0.50507900	2.22668200	1.45005400
H	0.33988300	3.86209100	0.78004400

$B(OEt)_3$-case2
(E = −488.06948949)
0, 1

H	3.65709200	0.91011000	1.18239400
H	4.60595600	-0.22102400	0.19629000
C	3.70568500	0.40229400	0.21269100
H	3.80074800	1.16359600	-0.56959200
C	2.47798900	-0.44363800	-0.01018400
H	2.38643400	-1.21510000	0.76693300
H	2.52813400	-0.96147000	-0.97805900
O	1.32797900	0.39745700	0.01879200
B	0.07940700	-0.12376200	-0.16996400
H	-0.36175600	2.27294700	1.02864000
C	-0.85863300	2.09992900	0.06393500
H	-0.20796900	2.51815800	-0.71658800
H	-2.13095000	3.82738900	0.19431500
H	-2.86298400	2.33611200	0.82051200
C	-2.21957600	2.74757700	0.03486900
H	-2.70842100	2.58208800	-0.93166900
O	-1.01110800	0.69866100	-0.14577000
O	-0.07119400	-1.46305600	-0.38986400

C	-1.36050100	-2.04483200	-0.56578300
H	-2.00695200	-1.35667900	-1.12547000
H	-1.21335700	-2.94023400	-1.18083200
C	-1.98176200	-2.40551100	0.76320400
H	-1.33382600	-3.09171000	1.31994200
H	-2.14371600	-1.50947700	1.37315100
H	-2.95010400	-2.89530600	0.61219400

$B(OEt)_3$-case3

(E = −488.06948949)

0, 1

H	-3.80073700	1.16361200	-0.56956600
H	-4.60595800	-0.22102400	0.19627400
C	-3.70568400	0.40228800	0.21269800
H	-3.65709500	0.91007900	1.18241400
C	-2.47798900	-0.44364100	-0.01019300
H	-2.52813500	-0.96145700	-0.97807600
H	-2.38643100	-1.21511500	0.76691000
O	-1.32797900	0.39745500	0.01879500
B	-0.07940600	-0.12376100	-0.16996100
H	0.20798000	2.51815200	-0.71662000
C	0.85862800	2.09993400	0.06392300
H	0.36173200	2.27296500	1.02861500
H	2.13094200	3.82739500	0.19431400
H	2.70843400	2.58208900	-0.93165300
C	2.21957100	2.74758300	0.03487500
H	2.86296600	2.33612200	0.82053200
O	1.01110700	0.69866400	-0.14576100
O	0.07119800	-1.46305500	-0.38986400
C	1.36050400	-2.04483000	-0.56578400
H	1.21336200	-2.94023000	-1.18083700
H	2.00695700	-1.35667500	-1.12546600
C	1.98176200	-2.40551700	0.76320200
H	2.14371400	-1.50948900	1.37315700
H	1.33382500	-3.09172100	1.31993300
H	2.95010400	-2.89531300	0.61219200

INT-10D

(E = −339.80762283)

0, 3

H	0.92248900	2.42381000	0.00000000
Ni	0.00315500	-1.25566600	0.00000000
H	-1.09917600	-0.07455000	0.00000000
Ni	0.00315500	1.17176300	0.00000000

TS-10D-11D

(E = −339.75677260)

0, 3

H	-1.62039100	1.36330700	-0.00195400
Ni	1.20556500	-0.00151700	-0.00003500
H	-0.51297100	1.24692300	0.00219000

Ni	-1.12937300	-0.09170500	0.00002700

INT-11D
(E = −339.75449755)
0, 3

Ni	0.11507900	-1.04244000	0.00000000
H	-2.84824100	-0.00299400	0.00000000
Ni	0.11507900	1.04290400	0.00000000
H	-3.59615600	-0.00999000	0.00000000

INT-11D’
(E = −339.77979692)
0, 3

H	-2.92718300	0.43066600	0.14603400
Ni	1.24747500	0.00282500	0.01044000
H	-2.95034400	-0.33096900	0.20492900
Ni	-1.03756300	-0.00638500	-0.02297400

INT-10D_{1ET}
(E = −494.77045915)
0, 3

Ni	-0.03923400	-0.43190700	-0.36157600
H	-1.31652100	-1.36827700	-0.22061900
O	1.53108100	0.72180700	-0.65369400
H	1.27967900	1.61721000	-0.91563300
C	2.61823300	0.77223500	0.29890800
H	3.44089000	1.33093400	-0.16198600
H	2.28466300	1.31088400	1.19437800
C	3.03102400	-0.63750000	0.62382200
H	3.90459900	-0.62486200	1.28335900
H	2.23170700	-1.18152200	1.14232600
H	3.29766400	-1.18493400	-0.28683000
Ni	-2.05770800	0.14492200	0.25471300
H	-2.55251400	1.55326400	0.65035200

TS-10D_{1ET}-11D_{1ET}
(E = −494.72648191)
0, 3

Ni	0.02091200	-0.52645600	-0.17028800
H	2.20571100	-0.87636700	-0.59116200
O	-2.02969300	-0.90854900	-0.00787000
H	-2.22485400	-1.73720500	0.44909200
C	-2.84497500	0.15140200	0.53237100
H	-3.88691100	-0.18945200	0.56518100
H	-2.51805300	0.36799100	1.55890300
C	-2.68916000	1.35793300	-0.35484400
H	-3.30009900	2.18542500	0.02087200
H	-1.63922100	1.68000600	-0.37730000
H	-3.00334700	1.13030200	-1.37938400
Ni	2.14252800	0.39071200	0.14122700
H	3.23282800	-0.54749200	-0.43470900

INT-11D$_{1ET}$
(E = −494.75476315)
0, 3

Ni	0.05938700	0.61241300	0.12016100
H	2.51575800	2.42904700	0.81980100
O	-1.94816700	0.90976400	-0.25543200
H	-2.11304900	1.54900300	-0.96089000
C	-2.69991600	-0.29474400	-0.51361700
H	-3.75144800	-0.02381100	-0.66799300
H	-2.32109200	-0.76290100	-1.43299100
C	-2.53261300	-1.21017100	0.66960400
H	-3.10134700	-2.13324100	0.51646500
H	-1.47286800	-1.47116500	0.79967600
H	-2.88883200	-0.72988400	1.58752600
Ni	1.98504900	-0.61814200	-0.14092300
H	2.86917900	3.05476200	1.02727200

INT-11D'$_{1ET}$
(E = −494.75137242)
0, 3

Ni	-0.04260200	-0.41459700	-0.10352300
H	4.12063200	1.05693200	0.35029800
O	-2.08404300	-0.89571300	-0.13815000
H	-2.29379800	-1.78206700	0.18243400
C	-3.01775900	0.05579700	0.40604500
H	-4.03607800	-0.26345800	0.15057100
H	-2.92397800	0.06960800	1.50035900
C	-2.70491300	1.40647900	-0.18159100
H	-3.40534900	2.15641900	0.20039300
H	-1.68408700	1.71324900	0.08470400
H	-2.78289700	1.38266600	-1.27431300
Ni	2.17533300	0.18804000	0.05148300
H	4.29746300	0.40228600	0.02115300

Ni-Ni
(E = −338.53231782)
0, 1

Ni	0.00000000	0.00000000	1.03432100
Ni	0.00000000	0.00000000	-1.03432100

Ni-Ni
(E = −338.58050909)
0, 3

Ni	0.00000000	0.00000000	1.04129100
Ni	0.00000000	0.00000000	-1.04129100

Ni-Ni
(E = −338.52888300)
0, 5

Ni	0.00000000	0.00000000	1.14085900

Ni	0.00000000	0.00000000	-1.14085900

INT-6T_{SI}

(E = −393.10227498)

0, 3

H	1.57241900	-1.06181000	0.54409100
H	1.57242000	1.06183300	0.54405700
H	3.14622600	0.00000900	0.31468500
B	1.99076500	0.00000200	-0.03597400
H	1.87947000	-0.00001500	-1.24663100
Ni	0.00000400	-1.11005400	0.00000000
H	-1.57242700	1.06181700	-0.54406600
H	-3.14622600	-0.00001800	-0.31468100
B	-1.99076500	-0.00001100	0.03597500
H	-1.87946600	-0.00001900	1.24663200
H	-1.57241300	-1.06182500	-0.54408300
Ni	-0.00000400	1.11005700	0.00000000

TS-6T_{SI}-7T_{SI}

(E = −393.04386965)

0, 3

H	1.12684100	-1.84972900	-0.29308800
H	-0.86330500	-1.51511900	-0.84652200
H	-0.38029400	-2.19449700	1.09906800
B	-0.03511000	-1.61823800	0.10788300
Ni	1.27393000	-0.09225300	-0.00291900
H	-2.20899400	0.95796700	0.66930300
H	-0.84557800	1.21107100	0.73817300
Ni	-1.26546200	-0.02698900	-0.05428000
H	0.04306500	1.90566100	-1.18471600
B	0.30566900	1.74132700	-0.01676400
H	1.53042900	1.54708100	0.25541100
H	0.00794200	2.66090200	0.70835200

INT-7T_{SI}

(E = −393.09246503)

0, 3

H	1.09751500	-1.82415800	-0.01102300
H	-0.94654900	-1.80872400	-0.30654900
H	-0.18314400	-1.73531500	1.61653400
B	-0.01009700	-1.45811000	0.45944400
Ni	1.32007200	0.00000400	-0.01764100
H	-2.85757000	0.00006500	2.54416300
H	-2.33687100	0.00004600	2.00850600
Ni	-1.12864800	-0.00000900	-0.40181500
H	-0.94655400	1.80869900	-0.30660200
B	-0.01010700	1.45811200	0.45941500
H	1.09750600	1.82417000	-0.01104500
H	-0.18316900	1.73534300	1.61649700

INT-8T_{SI}

(E = −391.92016264)

0, 3

H	0.38099200	2.05399300	-0.06584300
H	1.96311600	0.73017200	-0.08154100
H	1.11809900	1.30722300	1.71849300
B	0.94032000	1.10573100	0.54676300
Ni	-0.94032000	0.80476400	-0.15374700
H	-1.96311600	-0.73017200	-0.08154100
H	-1.11809900	-1.30722300	1.71849300
B	-0.94032000	-1.10573100	0.54676300
H	-0.38099200	-2.05399300	-0.06584300
Ni	0.94032000	-0.80476400	-0.15374700

INT-9T_{SI}

(E = −701.87882171)

0, 3

H	2.34295600	3.03349200	1.27263100
H	1.91725200	2.76119800	-0.42862200
H	1.18631000	1.75284200	0.84384600
C	2.10761800	2.26325400	0.53001500
C	3.24778600	1.28065900	0.41636800
H	4.18776900	1.77454500	0.14373600
H	3.40958800	0.74441200	1.35762700
O	2.97616700	0.25042300	-0.55667500
H	3.04496200	0.62491000	-1.44470300
H	0.62838000	-0.98547900	-1.98200100
H	-0.32376600	-2.77517700	-1.58713300
H	-1.38613400	-1.00728400	-1.56000900
B	-0.28873300	-1.59274800	-1.36068500
Ni	1.21103100	-0.75809300	-0.26394200
H	1.38613400	-1.00728400	1.56000900
B	0.28873300	-1.59274700	1.36068500
H	0.32376500	-2.77517600	1.58713300
H	-0.62838000	-0.98547800	1.98200100
Ni	-1.21103100	-0.75809200	0.26394200
H	-3.04496300	0.62491000	1.44470300
O	-2.97616800	0.25042300	0.55667500
H	-3.40958800	0.74441200	-1.35762700
H	-4.18776800	1.77454500	-0.14373600
C	-3.24778600	1.28066000	-0.41636800
C	-2.10761800	2.26325400	-0.53001500
H	-1.91725200	2.76119800	0.42862300
H	-1.18630900	1.75284200	-0.84384600
H	-2.34295500	3.03349300	-1.27263000

INT-10T_{SI}

(E = −699.51792714)

0, 3

H	3.31487100	2.87859900	-0.00412000
H	2.72804700	1.81371800	1.29070600
H	4.20818000	1.39680800	0.39887100

C	3.20755200	1.83296100	0.30356200
C	2.38322200	1.06703000	-0.69874100
H	2.84116700	1.08982900	-1.69903100
H	1.37118600	1.50095800	-0.78921100
O	2.27792300	-0.29310100	-0.28472400
Ni	0.66533400	-0.53795700	1.02646400
B	1.28260800	-1.13726700	-0.92303600
H	1.58508300	-2.30279800	-0.96903000
H	0.79651000	-0.68304700	-2.01562700
Ni	-0.66533100	-0.53795900	-1.02646300
B	-1.28260500	-1.13726800	0.92303800
H	-0.79650800	-0.68304600	2.01562700
H	-1.58507700	-2.30279900	0.96903300
O	-2.27792100	-0.29310500	0.28472300
H	-2.84116500	1.08982600	1.69902800
H	-1.37118900	1.50096100	0.78920400
C	-2.38322300	1.06702800	0.69873700
C	-3.20756200	1.83295700	-0.30356200
H	-2.72806300	1.81371800	-1.29070800
H	-4.20818900	1.39680000	-0.39886600
H	-3.31488500	2.87859500	0.00412100

INT-11(1)T_{SI}
(E = −1007.13956204)
0, 3

H	-5.42646200	0.04231700	-1.13049800
H	-4.80194700	-1.59379800	-1.42662500
H	-5.51297500	-1.18732200	0.14817200
C	-4.89780200	-0.80222200	-0.67379300
C	-3.53763100	-0.37560900	-0.17277300
H	-3.63882700	0.43931400	0.57019400
H	-2.92664600	0.04080000	-1.00062700
O	-2.86841400	-1.46729700	0.39831700
B	-1.58025300	-1.24090300	0.97503400
H	-1.64759200	-0.31384000	1.93086500
H	-1.13577500	-2.24686600	1.49766800
Ni	-0.23083700	-0.99456800	-0.78929400
Ni	-0.64083700	0.57699700	1.00436900
H	-1.76277400	2.78958800	-0.14180300
H	-1.33347600	4.01261400	-1.35544900
C	-0.94833200	3.42680300	-0.51435500
H	-0.65381600	4.11740600	0.28320600
H	1.03143300	3.19867600	-1.36511000
H	-0.08550700	1.86019100	-1.72697700
C	0.21738900	2.58524800	-0.96009000
O	0.73512100	1.87401100	0.18410300
B	1.64389500	0.81890900	0.02795200
O	2.40486800	0.55200400	1.12164800
H	1.06346100	-1.06993500	2.74131300
H	2.47268800	-0.39864900	3.59841700
C	2.15808900	-1.10922900	2.82626600

H	2.44785100	-2.11721300	3.14292900
C	2.79080100	-0.77004100	1.49842600
H	3.88647000	-0.79858600	1.55600300
H	2.47176600	-1.49214100	0.73210400
O	1.75248600	0.21918200	-1.20895900
C	2.96509100	-0.35557200	-1.72044500
H	3.71786000	-0.41593500	-0.92454800
H	3.34616700	0.33555100	-2.48192900
C	2.67894200	-1.70899600	-2.31901200
H	3.57978200	-2.10976100	-2.79515400
H	2.35059700	-2.42352800	-1.55385800
H	1.89461500	-1.63242500	-3.08155400

INT-11(2)T_{SI}
(E = −1007.12431513)
0, 3

H	3.10192900	-3.76586000	-1.29127600
H	1.93931300	-2.76640100	-2.18553000
H	3.64361100	-2.27055400	-2.08277800
C	2.81931700	-2.73498100	-1.53017200
C	2.51582600	-1.96422500	-0.27101800
H	3.37863400	-1.95362100	0.41288500
H	1.67045800	-2.42175800	0.27043200
O	2.19885800	-0.61348900	-0.60359500
Ni	0.21615000	-0.39796200	-1.20227300
Ni	-0.21614500	-0.39796300	1.20226700
H	1.48006000	-0.34440700	1.56845100
B	1.52079300	0.21938100	0.38637000
O	1.92009400	1.56473600	0.40316100
H	3.38337200	1.37783600	1.85253200
H	3.95989600	1.27863600	0.17821100
C	3.24816900	1.80017500	0.83967700
C	3.52467500	3.28394000	0.84724500
H	4.54704800	3.48602400	1.18556600
H	2.83083300	3.80373800	1.51790900
H	3.40622500	3.70310400	-0.15857300
H	-2.83087400	3.80368600	-1.51799400
H	-4.54707300	3.48600300	-1.18554100
H	-3.40617600	3.70314100	0.15852500
C	-3.52468300	3.28392800	-0.84726500
H	-3.95988900	1.27866100	-0.17811000
H	-3.38344500	1.37777100	-1.85246300
C	-3.24819000	1.80016100	-0.83963600
O	-1.92009600	1.56473300	-0.40317100
H	-1.48006100	-0.34441600	-1.56845100
B	-1.52079100	0.21937900	-0.38637500
O	-2.19884700	-0.61348900	0.60359800
H	-3.37864400	-1.95361000	-0.41287100
H	-1.67047100	-2.42176000	-0.27043900
C	-2.51582800	-1.96422300	0.27102100
C	-2.81931100	-2.73497800	1.53017700

H	-1.93930100	-2.76640400	2.18552700
H	-3.64359800	-2.27054900	2.08279200
H	-3.10193100	-3.76585600	1.29128100

INT-11(3)T_{SI}
(E = −1007.12515147)
0, 3

H	3.44723200	-3.41435200	0.59613300
H	1.80082700	-3.39240200	-0.06353300
H	3.20013300	-3.35953100	-1.16247300
C	2.81819300	-3.00173400	-0.19988300
C	2.82206400	-1.49571300	-0.14516400
H	3.83959400	-1.09020600	-0.22173400
H	2.39061100	-1.13757100	0.80345700
O	2.05406100	-0.98496400	-1.24162400
B	1.56191700	0.36661800	-1.20194700
H	1.31124900	0.82818800	-2.28690800
Ni	0.04203200	-1.22199700	-0.87561500
Ni	0.18443400	0.76393500	0.51803100
O	2.09519400	1.25503900	-0.21284700
C	2.27565500	2.62829900	-0.57867400
H	1.40002600	2.96949900	-1.15196400
H	3.15236500	2.69574600	-1.23788800
C	2.46063200	3.45426300	0.66787600
H	2.63311500	4.50402100	0.40789800
H	1.56802000	3.40549500	1.30449800
H	3.31889000	3.09757300	1.24804900
H	-0.30830000	0.12458400	3.57439200
H	-2.03742100	-0.04848400	3.94560300
H	-0.91698500	-1.38480000	4.28751600
C	-1.15036700	-0.57971100	3.58220500
C	-1.38295600	-1.13075600	2.19785800
H	-0.47900800	-1.65518900	1.83562200
H	-2.20748000	-1.86162000	2.18751500
O	-1.70683500	-0.06719800	1.31417800
B	-1.56557600	-0.27905600	-0.11970400
H	-1.55898500	-1.57155200	-0.42831600
O	-2.46828800	0.46274300	-0.91041600
C	-3.83284000	0.10789700	-0.78655200
H	-4.16907600	0.25080200	0.25396500
H	-3.95766200	-0.96667100	-1.01754500
C	-4.66335700	0.94716400	-1.72774800
H	-5.72458900	0.68545900	-1.64947500
H	-4.55411000	2.01231900	-1.49214400
H	-4.34641200	0.79340500	-2.76588900

INT-11(4)T_{SI}
(E = −1007.11017837)
0, 3

H	-1.74566600	3.89015800	2.12583600
H	-0.37095200	3.58316500	1.04553800

H	-1.86623500	4.29511300	0.39928700
C	-1.46684400	3.56957600	1.11634600
C	-2.00199500	2.18780500	0.83478000
H	-3.09679800	2.16372600	0.92767000
H	-1.58220100	1.46166300	1.54955400
O	-1.64290900	1.82187100	-0.49643600
Ni	0.32947000	1.10111900	-0.54277700
B	-1.75151800	0.51176100	-1.08259500
H	-1.79924100	0.56894700	-2.28860100
Ni	-0.36591000	-1.22175900	-0.67867800
O	-2.53360400	-0.56711000	-0.57570200
H	-3.62708100	-0.10838500	1.12000600
C	-2.85852200	-0.81955900	0.78616700
H	-1.96133600	-0.66757100	1.41412800
C	-3.34993100	-2.24043000	0.91433400
H	-4.21972400	-2.41119800	0.27034200
H	-2.56374700	-2.95066400	0.62566600
H	-3.63808300	-2.45418700	1.94926100
H	0.49706200	-3.68230800	0.91529800
C	1.53661000	-3.49697700	1.21694300
H	1.62535600	-3.72242000	2.28527000
H	2.18288400	-4.18689400	0.66302700
C	1.92531900	-2.06420000	0.94670000
H	1.23873400	-1.37553500	1.47377000
H	2.94454400	-1.86391400	1.30625900
O	1.85520000	-1.81961500	-0.45212400
B	1.74568600	-0.54544200	-1.07882600
H	1.80050200	-0.63463300	-2.28311400
O	2.36266000	0.66996500	-0.60540300
C	2.96949900	0.86377000	0.67101800
H	3.86156900	0.22555900	0.74283100
H	2.27139200	0.56462700	1.46933300
C	3.33084500	2.32098400	0.81179700
H	2.43197600	2.94629200	0.73292700
H	3.79490700	2.51082300	1.78545100
H	4.03095100	2.62724700	0.02693400

INT-12(a)T_{SI}
(E = −519.06133299)
0, 3

Ni	0.99159000	1.18908200	-0.12813600
Ni	1.21266700	-1.14371100	-0.17937300
B	-0.15602700	0.01327600	1.11620700
H	-0.01180100	1.30089500	1.25463200
H	0.28568900	-0.53581000	2.11025000
O	-1.49451600	-0.35308400	0.81561900
H	-2.10165100	1.37176100	-0.13934200
H	-1.53466500	0.06895000	-1.19641900
C	-2.11612400	0.27371600	-0.27479600
C	-3.53660600	-0.21966500	-0.41850600
H	-3.55495200	-1.30432100	-0.57791600

H	-4.11880600	0.00171600	0.48388000
H	-4.03036500	0.26040800	-1.27100100

INT-12(b)T_{SI}
(E = −1314.74188685)
0, 3

H	-1.35233300	-3.76222400	2.68200700
H	-0.69466100	-2.96443000	1.23465700
H	0.03791400	-2.67046000	2.83237000
C	-0.91061200	-2.83311100	2.30268300
C	-1.85239600	-1.67052200	2.52197900
H	-2.09698900	-1.57264500	3.58765000
H	-2.79313800	-1.82912400	1.97781800
O	-1.27431500	-0.42799900	2.12160300
Ni	0.53819000	-0.43906800	1.08798400
Ni	-0.53817300	-0.43904600	-1.08807400
H	-3.45414100	-1.43213100	-2.35063300
H	-4.80684000	-0.28072000	-2.33029100
H	-3.13928800	0.31257600	-2.48558000
C	-3.77403600	-0.44217400	-2.00255700
C	-3.66301000	-0.35183800	-0.50033500
H	-4.32832200	-1.08160400	-0.01520100
H	-3.94789600	0.64387900	-0.13426100
O	-2.32640900	-0.65300900	-0.09804300
B	-1.55859700	0.16665400	0.82390200
O	-1.88658400	1.52733200	0.96200600
C	-1.81890400	2.39460500	-0.14903400
H	-0.89530400	2.18400400	-0.72014600
H	-2.66253900	2.21270400	-0.83768800
C	-1.84761800	3.82691300	0.32961700
H	-1.80243500	4.51975500	-0.51867900
H	-0.99311000	4.03126300	0.98702400
H	-2.76648900	4.03116400	0.89188800
H	0.99286800	4.03130700	-0.98702800
H	1.80209600	4.51985400	0.51870900
H	2.76624400	4.03133800	-0.89182000
C	1.84736500	3.82701700	-0.32958800
H	2.66235300	2.21286800	0.83775300
H	0.89512600	2.18403100	0.72012300
C	1.81873800	2.39470500	0.14905800
O	1.88654100	1.52744100	-0.96198200
B	1.55862600	0.16674300	-0.82391800
O	1.27441900	-0.42790100	-2.12163100
H	0.69494000	-2.96434200	-1.23457000
H	-0.03774200	-2.67043900	-2.83224600
H	1.35256300	-3.76213700	-2.68194200
C	0.91082200	-2.83303700	-2.30261100
C	1.85253900	-1.67040800	-2.52199100
H	2.79331600	-1.82894500	-1.97787400
H	2.09707200	-1.57255500	-3.58767900
O	2.32645600	-0.65289900	0.09803500

C	3.66300700	-0.35164100	0.50042900
H	3.94783300	0.64412100	0.13443100
H	4.32840700	-1.08132400	0.01529100
C	3.77394900	-0.44206000	2.00265200
H	4.80672100	-0.28054800	2.33045800
H	3.13911600	0.31261400	2.48568300
H	3.45410700	-1.43206200	2.35064900

INT-13T_{SI}
(E = −829.01420335)
0, 3

H	0.78140000	4.08438800	1.31825500
C	1.15196800	3.60499700	0.40476000
H	2.20033600	3.32351600	0.56637300
H	1.11959100	4.34205100	-0.40670200
C	0.32442500	2.38807300	0.05979300
H	-0.73902100	2.67027100	-0.07265800
H	0.34314900	1.65566900	0.89341300
O	0.81247800	1.78595500	-1.10576000
H	-1.12661100	0.82636800	-1.80132900
B	0.15093500	0.59411700	-1.55782400
H	0.65958900	0.17266200	-2.58924000
Ni	-1.37359100	-0.36940000	-0.64554400
Ni	0.89070700	-1.02044400	-0.29082700
H	2.61195200	-2.80734400	0.67471900
O	2.48963800	-1.85017000	0.70358900
C	3.76516200	-1.17720600	0.66073900
H	4.24287700	-1.37303400	-0.30808400
H	4.40165100	-1.59070700	1.45243300
C	3.52349500	0.29550500	0.86396600
H	4.47373300	0.83919400	0.83556700
H	2.86918000	0.70056900	0.07787300
H	3.04883500	0.48052300	1.83529200
H	-2.71414700	-0.40673500	2.47067800
C	-3.20756400	0.37610600	1.88353500
H	-3.83543200	0.97010200	2.55563300
H	-2.43504500	1.03321700	1.46331500
C	-4.04834700	-0.22545200	0.78996400
H	-4.83423200	-0.87099400	1.20061200
H	-4.52098600	0.55282900	0.17669000
O	-3.19211500	-1.02978400	-0.04646000
H	-3.71559100	-1.47763700	-0.72282900

INT-14T_{SI}
(E = −648.55173871)
0, 3

H	-4.39623800	-1.82982300	-0.36205700
H	-4.34385200	-0.28940700	-1.24888800
H	-2.84033700	-1.19963800	-0.95710600
C	-3.81172900	-0.91859300	-0.52693100
C	-3.60806300	-0.18678600	0.77322300

H	-4.56461200	0.09848600	1.22835500
H	-3.05200800	-0.80705000	1.49139400
O	-2.85035200	1.00775100	0.49679200
H	-2.80692000	1.55048100	1.29504800
Ni	-0.92852100	0.60633000	-0.26439700
Ni	0.95832700	-0.73676000	-0.20789300
H	2.96099800	-1.43941600	1.32178200
O	2.92929100	-0.91462700	0.51099800
H	2.96052300	0.93749300	1.45506900
H	4.55279900	0.18137200	1.19084800
C	3.56647500	0.35723100	0.74382200
C	3.67863000	1.07163500	-0.57687500
H	4.26147700	0.48026400	-1.29159800
H	2.67837300	1.24319800	-0.99800000
H	4.17184200	2.04017500	-0.44249100

$Ni(NO_3)_2$

(E = −729.75252771)

0, 3

N	-2.13285200	0.38712300	0.06679100
O	-1.19744500	0.58074400	0.91425000
O	-3.17375000	0.99280900	0.08864900
O	-1.86253300	-0.50325400	-0.80574800
N	2.13285100	0.38712800	-0.06678500
O	3.17375300	0.99280800	-0.08863400
O	1.86254000	-0.50328200	0.80572200
O	1.19743300	0.58078900	-0.91422200
Ni	0.00000100	-0.80516600	-0.00000600

Py

(E = −248.11480877)

0, 1

C	1.14173400	-0.72018100	0.00000600
C	1.19642300	0.67100200	-0.00000200
C	-0.00001800	1.38086400	-0.00000100
C	-1.19644100	0.67097100	0.00000300
C	-1.14171500	-0.72021100	-0.00001000
N	0.00001900	-1.41675600	0.00000100
H	-0.00003200	2.46802800	0.00000300
H	2.06271400	-1.30291800	-0.00000100
H	2.15604200	1.18027000	-0.00000600
H	-2.15607400	1.18021300	0.00001300
H	-2.06267900	-1.30297200	0.00001200

$[NiPy_2]^{2+}$

(E = −665.24640802)

2, 3

Ni	0.00000000	0.00000100	0.00000000
N	-1.96751300	0.00000100	0.00000000
C	-2.64463500	-0.98956500	-0.61064700
C	-2.64463600	0.98956500	0.61064700

C	-4.02899200	-1.02181400	-0.63095500
H	-2.04948000	-1.76539100	-1.08663000
C	-4.02899300	1.02181300	0.63095500
H	-2.04948200	1.76539200	1.08662900
C	-4.73213400	-0.00000100	0.00000000
H	-4.53986300	-1.83630500	-1.13336300
H	-4.53986500	1.83630300	1.13336400
H	-5.81844500	-0.00000200	0.00000000
N	1.96751300	0.00000100	0.00000000
C	2.64463600	0.98956500	-0.61064700
C	2.64463400	-0.98956500	0.61064700
C	4.02899300	1.02181300	-0.63095400
H	2.04948200	1.76539200	-1.08663000
C	4.02899200	-1.02181400	0.63095500
H	2.04947900	-1.76539100	1.08662900
C	4.73213400	-0.00000100	0.00000100
H	4.53986500	1.83630300	-1.13336300
H	4.53986300	-1.83630500	1.13336400
H	5.81844500	-0.00000100	0.00000100

$[(NO_3)_2NiBH_4]^-$
(E = −757.13969582)
−1, 3

N	2.09645700	-0.70662600	0.07020200
O	1.15957200	-0.84683200	0.91880400
O	3.11746900	-1.36056400	0.11300800
O	1.88193400	0.17189200	-0.82262700
N	-2.09645500	-0.70663100	-0.07020300
O	-3.11747000	-1.36056600	-0.11303000
O	-1.88195100	0.17189200	0.82262600
O	-1.15955100	-0.84684700	-0.91878400
Ni	0.00000000	0.62696900	0.00000500
H	0.86765900	3.42240700	-0.55408300
H	-0.86765300	3.42242600	0.55404900
H	-0.56115500	2.04998500	-0.87987300
H	0.56111700	2.04998200	0.87987700
B	-0.00000100	2.79221200	-0.00001600

$[(NO_3)_2Ni(BH_4)_2]^{2-}$
(E = −784.48818991)
−2, 3

H	0.91464400	2.89835300	-0.42138400
H	-1.05227400	2.84350600	0.18134500
B	-0.04275900	2.23006400	-0.09427500
H	0.28919300	1.53346300	0.91108200
H	-0.31722200	1.44851700	-1.05830500
Ni	0.00968300	0.01320500	-0.04083700
O	-2.75724000	-0.01581500	-1.19622700
N	-2.91361000	-0.01867200	0.03132300
O	-4.03657700	-0.02780400	0.55425100
O	-1.89450000	-0.01209300	0.79892900

H	0.32208300	-1.50194200	0.90556500
B	0.01393300	-2.20396300	-0.10340600
H	-0.97576900	-2.85009600	0.16884700
H	-0.28539200	-1.42700600	-1.06339100
H	0.99254300	-2.84035000	-0.43219300
O	1.95679300	0.03469600	-0.78121500
N	2.91254300	-0.00173500	0.06402400
O	2.65791100	0.00210300	1.27571000
O	4.07269700	-0.03881700	-0.36734300

$[Py_2NiBH_4]^+$
(E = −692.64637819)
1, 3

H	-0.64871000	3.12949600	0.17790800
B	0.23703600	2.31364100	0.11661300
H	0.07845000	1.50471000	1.10247600
H	1.37167300	2.71660000	0.13220100
H	0.05527800	1.63852200	-0.96200800
Ni	-0.00866700	0.14129000	-0.02113400
N	1.97205100	-0.17652100	-0.02694200
C	2.68942600	-0.01398000	-1.15031600
H	2.13252100	0.22535000	-2.05333900
H	4.61380300	0.00742000	-2.09318400
C	4.07059400	-0.13159600	-1.16410600
C	4.72944100	-0.41950400	0.02739900
H	5.81176200	-0.51207200	0.04919400
C	3.98491400	-0.57939900	1.19215400
H	4.45989500	-0.79798900	2.14303000
C	2.60629700	-0.44724100	1.12524800
H	1.98481900	-0.55572000	2.01199500
N	-2.01829100	-0.09433000	-0.01897100
C	-2.85067600	0.94711900	0.14905900
H	-2.38467100	1.92208700	0.27222300
H	-4.86278000	1.66440900	0.30242100
C	-4.22875900	0.79484100	0.16279700
C	-4.76712400	-0.47697500	-0.00435000
H	-5.84334000	-0.62595200	0.00177000
H	-4.28036300	-2.56554000	-0.31355200
C	-3.90625700	-1.55576000	-0.17949600
C	-2.53991700	-1.32386500	-0.17975600
H	-1.83478600	-2.14151800	-0.31287100

$Py_2Ni(BH_4)_2$
(E = −720.03080724)
0, 3

H	1.02201300	1.21665800	2.59346300
B	-0.00488400	0.94095300	2.01267400
H	-0.00455800	1.56106400	0.89715300
H	-1.03691100	1.20874100	2.58815500
H	0.00044000	-0.31166300	1.77455400
Ni	0.00022600	-0.00006100	0.00001200

N	-2.08869300	0.00001900	-0.00007900
C	-2.76668900	-1.06085800	0.45269100
H	-2.17103800	-1.89943200	0.81116800
H	-4.66491900	-1.98432400	0.84593900
C	-4.15449300	-1.10285600	0.47040300
C	-4.86058500	0.00019900	-0.00005000
H	-5.94736800	0.00027200	-0.00003400
C	-4.15436000	1.10315900	-0.47052600
H	-4.66468000	1.98469200	-0.84605200
C	-2.76656000	1.06098000	-0.45284300
H	-2.17081100	1.89947600	-0.81134100
N	2.09016200	0.00003800	0.00000700
C	2.76855200	1.09891400	-0.35065600
H	2.17294900	1.96854200	-0.62494800
H	4.66661300	2.05516600	-0.65638200
C	4.15631600	1.14236400	-0.36488600
C	4.86258500	0.00019300	-0.00002500
H	5.94936900	0.00025300	-0.00004100
H	4.66685900	-2.05480000	0.65634400
C	4.15645200	-1.14205600	0.36485800
C	2.76868300	-1.09876200	0.35066300
H	2.17318200	-1.96845300	0.62497400
H	-1.03682900	-1.20985000	-2.58774600
H	-0.00449600	-1.56147900	-0.89659600
B	-0.00480800	-0.94181400	-2.01236700
H	1.02209300	-1.21778700	-2.59302400
H	0.00052700	0.31086100	-1.77473700

$Ni_2(EtOH)_2$
(E = −648.55173871)
0, 3

H	-4.39623800	-1.82982300	-0.36205700
H	-4.34385200	-0.28940700	-1.24888800
H	-2.84033700	-1.19963800	-0.95710600
C	-3.81172900	-0.91859300	-0.52693100
C	-3.60806300	-0.18678600	0.77322300
H	-4.56461200	0.09848600	1.22835500
H	-3.05200800	-0.80705000	1.49139400
O	-2.85035200	1.00775100	0.49679200
H	-2.80692000	1.55048100	1.29504800
Ni	-0.92852100	0.60633000	-0.26439700
Ni	0.95832700	-0.73676000	-0.20789300
H	2.96099800	-1.43941600	1.32178200
O	2.92929100	-0.91462700	0.51099800
H	2.96052300	0.93749300	1.45506900
H	4.55279900	0.18137200	1.19084800
C	3.56647500	0.35723100	0.74382200
C	3.67863000	1.07163500	-0.57687500
H	4.26147700	0.48026400	-1.29159800
H	2.67837300	1.24319800	-0.99800000
H	4.17184200	2.04017500	-0.44249100

Ni_2Py_2

(E = −834.87908829)

0, 3

Ni	-1.10482500	0.38454100	-0.74159500
C	-3.82590100	1.16030400	0.14582300
C	-5.12254100	0.97468700	0.60605100
C	-5.53097700	-0.30982000	0.95453100
C	-4.62583200	-1.36027800	0.82998000
C	-3.34816000	-1.08682100	0.36088400
N	-2.95048200	0.15005300	0.02447100
H	-6.53893200	-0.48894300	1.31973100
H	-3.46130300	2.14713500	-0.13578800
H	-5.79504500	1.82337200	0.68820800
H	-4.90164900	-2.37775300	1.09085900
H	-2.59913100	-1.87100200	0.24665400
Ni	1.10482700	-0.38457200	-0.74158700
C	3.34815100	1.08683100	0.36085900
C	4.62582200	1.36031000	0.82994700
C	5.53097500	0.30986100	0.95452300
C	5.12254700	-0.97465800	0.60607500
C	3.82590800	-1.16029400	0.14585300
N	2.95048200	-0.15005300	0.02447700
H	6.53892800	0.48900000	1.31971700
H	2.59911700	1.87100500	0.24661000
H	4.90163200	2.37779300	1.09080100
H	5.79505700	-1.82333500	0.68825300
H	3.46131700	-2.14713500	-0.13573300

H_4BNiPy_2

(E = −692.83065334)

0, 2

H	0.04978200	4.24075200	1.01539000
H	1.05057000	2.85985600	-0.05007100
B	-0.00000500	3.57016300	0.00000200
H	-1.05057800	2.85985200	0.05006800
H	-0.04979500	4.24076000	-1.01538100
Ni	-0.00000200	1.42858200	-0.00000100
C	2.59796500	0.21538400	-0.68904700
C	3.67572500	-0.65933900	-0.64818600
C	3.62177000	-1.74726000	0.21787300
C	2.48877700	-1.91925200	1.00705600
C	1.45166900	-1.00272100	0.89437200
N	1.49796500	0.05070100	0.06319400
H	4.45011500	-2.44832000	0.27808100
H	2.60505700	1.08715400	-1.34133400
H	4.53900200	-0.48336600	-1.28288700
H	2.40238000	-2.75065100	1.70018400
H	0.54378000	-1.10660700	1.48635600
C	-1.45165800	-1.00273800	-0.89435600

C	-2.48876300	-1.91927200	-1.00703900
C	-3.62176600	-1.74727000	-0.21787200
C	-3.67573300	-0.65933600	0.64817100
C	-2.59797400	0.21538900	0.68903200
N	-1.49796400	0.05069600	-0.06319400
H	-4.45011000	-2.44833100	-0.27808000
H	-0.54376100	-1.10663100	-1.48632800
H	-2.40235700	-2.75068100	-1.70015400
H	-4.53901700	-0.48335500	1.28285900
H	-2.60507400	1.08716800	1.34130600

HNiPy
(E = −418.02909913)
0, 2

H	-3.51298000	-0.00004300	-0.00007100
Ni	-1.98130900	0.00000100	-0.00001200
C	0.68585000	1.15395000	0.00001800
C	2.07310300	1.19773300	0.00000100
C	2.78130700	0.00000100	-0.00000600
C	2.07310900	-1.19773200	0.00000300
C	0.68585800	-1.15395000	0.00001900
N	-0.00422500	-0.00000100	0.00002500
H	3.86808200	0.00000300	-0.00001900
H	0.09572400	2.06776600	0.00002700
H	2.58214100	2.15662700	-0.00000500
H	2.58215000	-2.15662600	-0.00000100
H	0.09573500	-2.06776900	0.00002900

H_3BPy
(E = −274.76109811)
0, 1

B	-0.05640400	2.50495700	0.00000000
H	-1.24070600	2.79973600	0.00000000
H	0.50214300	2.87869100	1.01413500
H	0.50214300	2.87869100	-1.01413500
N	0.01050700	0.89636800	0.00000000
C	0.01207700	0.21553400	-1.15902400
C	0.01207700	0.21553400	1.15902400
C	0.01207700	-1.16830400	-1.19795500
H	0.01514400	0.82137100	-2.06030900
C	0.01207700	-1.16830400	1.19795500
H	0.01514400	0.82137100	2.06030900
C	0.01287700	-1.87533100	0.00000000
H	0.01538100	-1.67627700	-2.15655200
H	0.01538100	-1.67627700	2.15655200
H	0.01672500	-2.96145100	0.00000000