Supplementary Material (ESI) for Chemical Communications

1-Phosphabarrelene Complexes of Palladium and their use in Suzuki- Miyaura Coupling Reactions.

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Contents

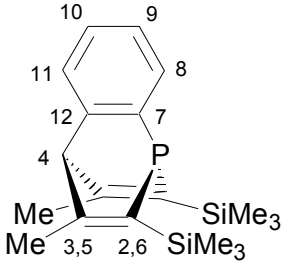
Experimental Section

General: All experiments were performed under an atmosphere of dry nitrogen or argon using standard schlenk and glove box techniques. Solvents were freshly distilled under nitrogen from Na (toluene), Na/benzophenone (THF, diethylether, hexanes), P_2O_5 (dichloromethane) and calcium hydride (acetonitrile). Nuclear magnetic resonance spectra were recorded on a Bruker Avance 300 spectrometer operating at 300 MHz for 1H, 75.5 MHz for 13C and 121.5 MHz for 31P. 1H and 13C chemical shifts are reported in ppm relative to Me_4Si as external standard. 31P shifts are relative to a 85% H_3PO_4 external reference. Coupling constants are given in hertz. The following abbreviations are used: br, broad; s, singlet; d, doublet; dd, doublet of doublets; t, triplet; m, multiplet; v, virtual. Elemental analyses were performed by the "Service d'analyse du CNRS", at Gif sur Yvette, France**.** High resolution mass spectra (EI-MS) were recorded with a JEOL GCmate instrument. $[Pd(allyl)Cl]_2$ was purchased from Strem. Phosphinine **1** and $[(COD)PdCl_2]$ were prepared according to the following literature procedures:

N. Avarvari, P. Le Floch and F. Mathey, *J. Am. Chem. Soc.* 1996, **118**, 11978

D. Drew, J. R. Doyle, in Inorganic Syntheses, Vol. 28 (Ed. R. J. Angelici), John Wiley and Sons, Inc, New Tork, 1990, 110.

Synthesis and characterization of Phosphabarrelene 2:



2-Bromofluorobenzene (0.57 mL, 5.21 mmol) was slowly added to a mixture of Phosphinine **1** (1.00 g, 3.72 mmol) and Magnesium turnings (135.7 mg, 5.58 mmol) in THF (20 mL) at room temperature. The reaction mixture is stirred during 4 h at room temperature. The solvent was evaporated and H_2O was added to the residue and extracted with CH_2Cl_2 (3 x 100 mL). After evaporation of the solvent the title compound was obtained as an off-white crystalline solid after recrystallization from MeOH.

Yield: 960.2 mg (2.79 mmol, 75 %),

Elemental composition (Found: C 66.4; H, 8.5. Calc. for $C_{19}H_{29}PSi_2$: C: 66.2; H: 8.5 %.)

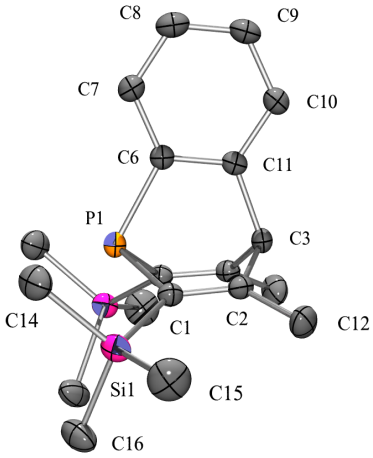
^{1}H NMR($CDCl_3$): δ 0.20(s, 18 H, $SiMe_3$), 2.20(s, 6H, Me), 4.95(s, 1H, C_4H), 7.05(t, $^3J_{HH}$= 7.0 Hz, 1H C_9H), 7.13(t, $^3J_{HH}$=7.2 Hz, 1H, C_{10}H), 7.36(d, $^3J_{HH}$= 7.2 Hz, 1H, C_{11}H), 7.60(t, $^3J_{HH}$=7.2 Hz, 1H C_8H).

^{13}C NMR($CDCl_3$): δ 0.5 (d+ sat $^3J_{PC}$=7.3 Hz, $^1J_{SiC}$=52.8 Hz, $SiMe_3$), 24.2 (d, $^3J_{PC}$= 2.9 Hz, Me), 71.5 (d, $^3J_{PC}$= 9.4 Hz, C_4H), 123.7 (d, $^3J_{PC}$= 0.9 Hz, C_{11}H), 124.4 (d, $^4J_{PC}$=11.5 Hz, C_{10}H), 126.4 (d, $^3J_{PC}$=1.5 Hz, C_9H), 129.8 (d, $^2J_{PC}$= 36.1 Hz, C_8H), 135.9 (d, $^1J_{PC}$=46.2 Hz, C_2,C_6), 143.1 (d, $^2J_{PC}$=20.3 Hz, C_{12}), 148.3(d, $^1J_{PC}$=3.6 Hz, C_7), 167.3 (d, $^2J_{PC}$=4.4 Hz, C_3,C_5)

^{31}P NMR($CDCl_3$): δ -60.1(s).

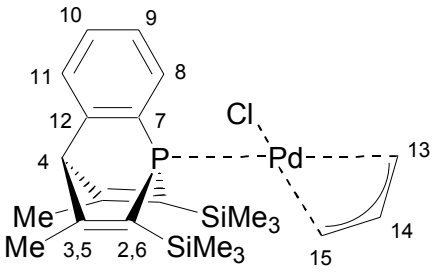
HRMS EI$^+$: 344.1551 (calcd 344.1545 for $C_{19}H_{29}PSi_2$)

Single crystals were grown by recrystallization of **2** from methanol.



ORTEP-plot (50 % thermal ellipsoids) of the X-Ray-crystal structure of **2** (hydrogen atoms were omitted for clarity). Selected bond lengths [Å] and angles [°]:P1-C1: 1.863(2), P1-C6: 1.835(2) C1-C2: 1.342(2), C6-C11:1.400(3), Σ(CPC): 287.7

Synthesis and Characterization of Pd-complex 3:



A mixture of ligand **2** (34.5 mg, 0.10 mmol) and $[Pd(C_3H_5)Cl]_2$ (18.3 mg, 0.05 mmol) in CH_2Cl_2 (10 mL) was stirred for 15 min at room temperature . The color of the solution turned from light green to pale yellow. The title compound was obtained as an off-white solid after evaporation of the solvent.

Yield: 51.6 mg (0.098 mmol, 98 %).

Elemental composition (Found: C 49.95; H, 6.5. Calc. for $C_{22}H_{34}PSi_2PdCl$: C: 50.1; H: 6.5 %.)

^{1}H NMR($CDCl_3$): δ 0.22-0.34 (m, 18H, $SiMe_3$), 2.27 (s, 6H, Me), 2.98 (d, $^3J_{HH}$= 11.4 Hz, 1H, $C_{15}H_2$), 3.87 (dd, $^3J_{HH}$= 10.6 Hz, $^2J_{PH}$=13.3 Hz, 1H, $C_{13}H_2$), 4.40 (d, $^3J_{HH}$=5.3 Hz, 1H, $C_{15}H_2$), 4.87 (br, 2H, $C_{13}H_2$ and C_4H) 5.43-5.60 (m, $C_{14}H$), 7.13 (m, 2H,C_9H and $C_{10}H$), 7.30 (m, 1H, $C_{11}H$), 7.77 (m, 1H, C_8H),

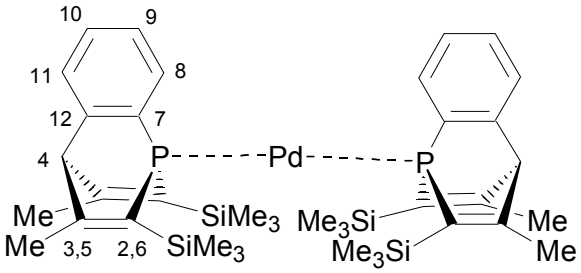
^{13}C NMR($CDCl_3$): δ 2.53 (s, $SiMe_3$), 26.1 (d, $^3J_{PC}$= 9.1 Hz, Me), 51.6 (d, $^2J_{PC}$= 2.5 Hz, $C_{15}H_2$ of allyl), 70.1 (d, $^2J_{PC}$= 27.4 Hz, $C_{14}H$ of allyl), 79.8 (d, $^2J_{PC}$= 32.4 Hz, $C_{13}H_2$ of allyl), 115.6 (d, $^3J_{PC}$= 5.7 Hz, C_4), 124.3(d, $^3J_{PC}$=3.2 Hz, $C_{11}H$), 125.3(d, $^4J_{PC}$=11.9 Hz, $C_{10}H$), 127.5 (d, $^3J_{PC}$= 2.0 Hz, C_9H), 129.5 (d, $^2J_{PC}$= 19.4 Hz, C_8H), 133.2 (dd, J_{PC}= 8.1 Hz, $^1J_{PC}$=54.1 Hz, C_2,C_6), 139.2 (d, $^2J_{PC}$= 27.3Hz, C_{12}), 146.9 (d, $^1J_{PC}$= 2.7 Hz, C_7), 169.9 (dd, $^1J_{PC}$=6.6 Hz, $^1J_{PC}$=11.1 Hz, C_3,C_5).

^{31}P NMR($CDCl_3$): δ -6.1 (s)

HRMS EI$^+$: 526.0653 (calcd 526.0660 for $C_{22}H_{34}PSi_2PdCl$)

Single crystals were grown by slow evaporation of a solution of **3** in toluene.

Synthesis and Characterization of Pd-complex 4:



To a mixture of ligand **2** (69.0 mg, 0.20 mmol) and [(COD)$PdCl_2$] (28.5 mg, 0.10 mmol) in acetonitrile (10 mL) cobaltocene (37.8 mg, 0.20 mmol) was added as a solid. The reaction mixture was stirred for 24 h at r.t.. The resulting dark-green suspension was taken to dryness and the residue was extracted with hexanes (10 mL). The product was isolated as a pale yellow solid after the evaporation of the solvent.

Yield: 71.6mg (0.09 mmol, 90 %)

Elemental composition (Found: C, 57.35; H, 6.4. Calc. for $C_{38}H_{58}P_2Si_4Pd$: C, 57.4; H, 6.5 %.)

^{1}H NMR(C_6D_6): δ 0.65(s, 18H, $SiMe_3$); 2.03(s, 6H, Me); 4.61(s, 1H, C_4H); 6.94(t, $^3J_{HH}$=7.3 Hz , 1H, $C_{10}H$), 7.05(t, $^3J_{HH}$=7.3 Hz , 1H, C_9H), 7.12(d, $^3J_{HH}$=7.3 Hz, 1H, $C_{11}H$), 8.85(*pseudo*-q, $^3J_{HH}$=7.5 Hz , 1H, C_8H).

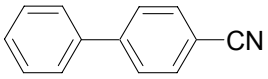
^{13}C NMR(C_6D_6): δ 2.0(*pseudo*-t, ΣJ_{PC}= 6.3 Hz, $SiMe_3$); 24.0(*pseudo*-t, ΣJ_{PC}= 7.5 Hz, CH_3); 70.3(*pseudo*-t, ΣJ_{PC}= 22.7 Hz, C_4) 123.2(s, $C_{11}H$), 124.3(*pseudo*-t, ΣJ_{PC}= 13.3 Hz, C_9H), 126.8(s, $C_{10}H$), 133.2(*pseudo*-t, ΣJ_{PC}=30.2 Hz, C_8H), 135.7(*pseudo*-t, ΣJ_{PC}= 15.8 Hz, C_2,C_6), 142.1(*pseudo*-t, ΣJ_{PC}= 20.7 Hz, C_{12}), 146.5(s, C_7) 166.9(*pseudo*-t, ΣJ_{PC}= 6.5 Hz, C_3,C_5).

^{31}P -NMR: δ -28.8 (s)

Single crystals were grown from a concentrated solution of **4** in hexanes at -20 °C.

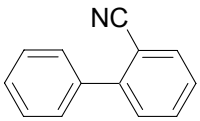
Literature references for known biaryls:

4-Cyano-biphenyl, CAS-Registry-Nr. : 2920-38-9



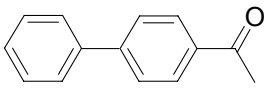
Liu, L.; Zhang, Y.; Xin, B. *J. Org. Chem.* 2006, **71**, 3994-3997.

2-Cyano-biphenyl, CAS-Registry-Nr. : 24973-49-7



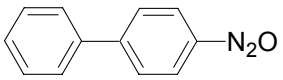
Zapf, A.; Beller, M.; *Chem Eur. J.* **2000**, *6*, 1830-1833

4-Acetyl-biphenyl CAS-Registry-Nr. : 92-91-1



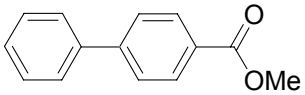
Liang, L-C.; Chien, PS.; Huang, M-H. *Organometallics* **2005**, *24*, 353-357.

4-Nitro-biphenyl CAS-Registry-Nr. : 86-00-0



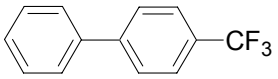
Liu, L.; Zhang, Y.; Xin, B. *J. Org. Chem.* **2006**, 71, 3994-3997.

Methyl 4-biphenylcarboxylate, CAS-Registry-Nr. : 720-75-2



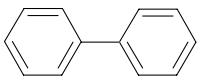
Zhang, C.; Huang, J.; Trudell, M. L.; Nolan, S. P.; *J. Org. Chem.* **1999**, *64*, 3804-3805.

4-Trifluoromethyl-biphenyl CAS-Registry-Nr. : 398-36-7



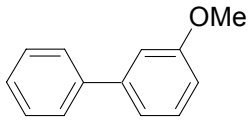
Liu, L.; Zhang, Y.; Xin, B. *J. Org. Chem.* 2006, **71**, 3994-3997.

Biphenyl, CAS-Registry-Nr. : 92-52-4



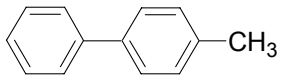
Pickett, T. E.; Richards, *Tetrahedron Lett.* 2001, **42**, 3767-3769.

3-Methoxy-biphenyl CAS-Registry-Nr. : 2113-56-6



Zapf. A.; Ehrentraut, A.; Beller, M. *Angew. Chem., Int. Ed.* 2000, **39**, 4153-4155.

4-Methyl-biphenyl CAS-Registry-Nr. : 92-91-1



Liu, L.; Zhang, Y.; Xin, B. *J. Org. Chem.* 2006, **71**, 3994-3997.

DFT Data

CDA calculations

Description of the method.
In the CDA method the (canonical, natural, or Kohn Sham) molecular orbitals of the complex are expressed in terms of MOs of appropriately chosen fragments. In the cases studied, the Kohn-Sham orbitals of the calculations are formed in the CDA procedure as a linear combination of the MOs of the phosphine ligand and those of the remaining [$Ni(CO)_3$] fragment. In all cases, the ligands and the metal fragments were computed in the geometry of the complex. The orbital contributions are divided in four parts: (i) the mixing of the occupied MOs of the ligand and the unoccupied MOs of the metal fragment. This value (noted d) represents the L→M donation; (ii) the mixing of the unoccupied MOs of the ligand and the occupied MOs of the metal fragment. This value (noted b) accounts for the M→L back donation; (iii) the mixing of the occupied MOs of the ligand and the occupied MOs of the metal fragment. This term (noted r), which describes the repulsive polarization between the ligand and metal fragment, is negative because electronic charge is removed from the overlapping area of the occupied orbitals; (iv) the residual term (Δ) which results from the mixing of the unoccupied MOs of the two respective fragments. Usually this term is very close to zero for closed-shell interactions. This value constitutes an important probe to determine whether the bonding studied can be really classified as a donor-acceptor interaction following the Dewar-Chatt-Duncansson model. Important deviations from Δ = 0 imply that the bond studied is more conventionally described as a normal covalent bond between two open shell fragments. A more detailed presentation of the CDA method and the interpretation of the results can be found in the literature. Compositions of molecular orbitals, overlap populations between molecular fragments, bond orders and density-of-states spectra were calculated using the AOMix program developed by I. Gorelski (version 6.23)[1]

Ligand	d	b	d/b	b/(d+b)	r	Δ
PPh_3	0,643	0,073	8,81	10,20	-0,142	-0,026
2	0,810	0,135	6,00	14,29	-0,141	-0,041
PF_3	0,721	0,136	5,30	15,87	-0,081	-0,051

Structure optimization: Gaussian03[2], B3PW91[3]/6-31G* (P, C, H, F, O) Ni: Hay Wadt-ECP[4] with an additional f-polarization function[5];

References

1 Gorelsky, S. I. *AOMIX: Program for Molecular Orbital Analysis,* http://www.sgchem.*net/* York University: Toronto, Canada, 1997; Gorelsky, S. I. *J. Organomet. Chem.* 2001, **635**, 187.

2 Gaussian 03, Revision C.02, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, r., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I.

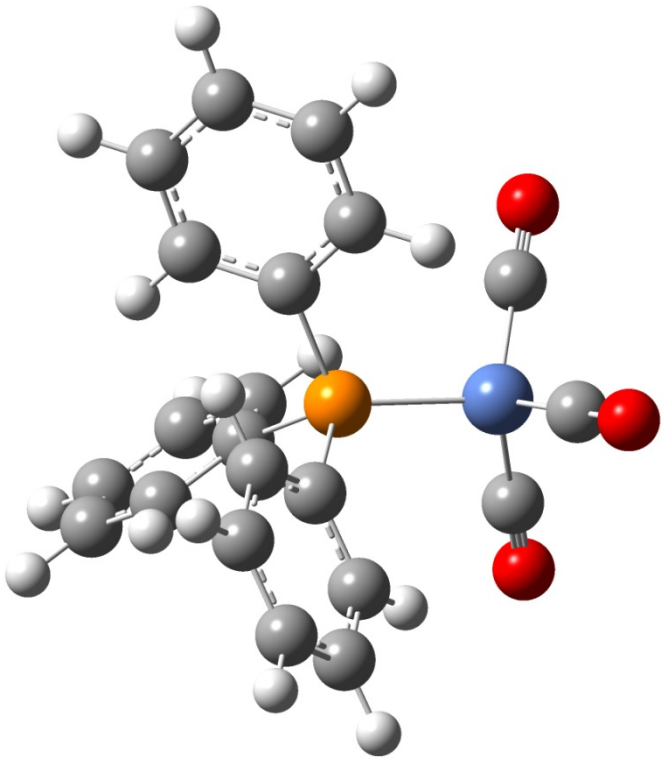
Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople, Gaussian, Inc., Wallingford CT, 2004.

3 Becke, A. D. *J. Chem. Phys.* 1993, **98**, 5648; Perdew, J. P.; Wang, Y. *Phys. Rev. B* 1992, **45**, 13244.

4 Hay, P. J.; Wadt, W. R. *J. Chem. Phys.* 1985, **82**, 299.

5 Ehlers, A. W.; Bohme, M.; Dapprich, S.; Gobbi, A.; Hollwarth, A.; Jonas, V.; Kohler, K. F.; Stegmann, R.; Veldkamp, A.; Frenking, G. *Chem. Phys. Lett.* 1993, **208**, 111.

Optimized geometry, three lower frequencies, thermochemistry and CDA calculations for $PPh_3Ni(CO)_3$



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5	6	0	1.188168	-.104966	3.949420
6	1	0	2.061712	-.100075	1.983591
7	6	0	-1.221135	-.016455	4.035159
8	1	0	-2.236888	.030925	2.140523
9	6	0	.007623	-.066231	4.691279
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14	6	0	-2.832868	-.389805	-.623898
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20	6	0	-4.332594	1.460597	-1.040049
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36	6	0	1.821787	2.611442	.093536
37	6	0	3.040249	.079226	-.885156
38	8	0	.749427	1.782503	-3.643691
39	8	0	1.981455	3.565020	.718095
40	8	0	3.978187	-.587745	-.885501
41	28	0	1.586824	1.132646	-.895722

	1	2	3
	A	A	A
Frequencies --	17.0483	18.7998	26.8268
Red. masses --	6.6078	5.3275	4.1505
Frc consts --	.0011	.0011	.0018
IR Inten --	.0564	.0894	.1331

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
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2	6	.00	.01	.03	.00	.00	.02	.02	.00	.02
3	6	.04	.01	-.02	-.03	-.03	.10	-.04	-.04	.14
4	6	-.04	.00	.09	.04	.03	-.04	.10	.04	-.10
5	6	.03	.01	-.01	-.03	-.02	.13	-.02	-.03	.15
6	1	.07	.02	-.07	-.06	-.05	.14	-.10	-.07	.24
7	6	-.04	.00	.11	.04	.03	-.01	.12	.05	-.09
8	1	-.07	-.01	.14	.07	.05	-.10	.15	.06	-.19
9	6	-.01	.01	.05	.01	.01	.07	.06	.01	.03
10	1	.06	.02	-.05	-.06	-.04	.19	-.07	-.06	.25
11	1	-.08	-.01	.16	.08	.05	-.05	.18	.08	-.18
12	1	-.01	.00	.06	.01	.01	.09	.07	.02	.04
13	6	.01	.03	-.01	-.01	.00	-.01	-.01	-.01	.02
14	6	.11	-.10	.00	-.12	.15	-.05	-.01	-.01	.02
15	6	-.07	.19	-.05	.09	-.15	.03	-.01	-.01	.01
16	6	.12	-.08	-.03	-.14	.16	-.05	-.01	-.01	.02
17	1	.16	-.23	.02	-.19	.27	-.08	-.01	-.01	.02
18	6	-.05	.22	-.07	.07	-.14	.03	-.01	-.01	.02
19	1	-.14	.30	-.06	.17	-.27	.06	-.01	-.01	.01
20	6	.04	.08	-.07	-.04	.02	-.01	-.01	-.01	.02
21	1	.20	-.19	-.03	-.23	.28	-.08	-.01	-.01	.02
22	1	-.11	.35	-.10	.15	-.26	.07	-.01	-.01	.02
23	1	.05	.10	-.09	-.06	.02	.00	-.01	-.01	.02
24	6	-.01	-.02	.00	.01	-.03	-.02	-.01	.00	.02
25	6	.02	.01	.02	-.02	-.07	-.07	.08	.10	.12
26	6	-.05	-.05	-.03	.05	-.01	.03	-.13	-.09	-.10
27	6	.00	-.01	.01	-.02	-.09	-.08	.06	.10	.11
28	1	.05	.04	.05	-.05	-.09	-.10	.17	.18	.21
29	6	-.06	-.07	-.04	.05	-.03	.02	-.16	-.09	-.11
30	1	-.07	-.07	-.04	.08	.03	.07	-.20	-.17	-.18
31	6	-.03	-.04	-.02	.02	-.07	-.03	-.07	.01	-.01
32	1	.03	.01	.03	-.05	-.13	-.12	.13	.18	.19
33	1	-.09	-.10	-.06	.08	-.01	.05	-.26	-.16	-.21
34	1	-.04	-.06	-.03	.02	-.09	-.04	-.09	.01	-.02
35	6	-.03	-.05	.13	.03	.00	.10	.02	.00	-.04
36	6	.00	-.13	-.10	-.01	-.04	-.07	-.05	.00	-.03
37	6	.03	.12	-.04	-.02	.12	-.04	.04	.00	-.03
38	8	-.05	-.08	.20	.05	-.01	.18	.03	.01	-.05
39	8	.00	-.21	-.18	-.02	-.08	-.11	-.09	.01	-.03
40	8	.04	.20	-.07	-.03	.20	-.05	.08	.02	-.05
41	28	.00	-.01	.01	.00	.01	-.01	.00	-.01	-.02

HF=-1546.8856093

Sum of electronic and zero-point Energies= -1546.585086

```
Sum of electronic and thermal Energies=            -1546.559657
Sum of electronic and thermal Enthalpies=          -1546.558713
Sum of electronic and thermal Free Energies=       -1546.645668
```

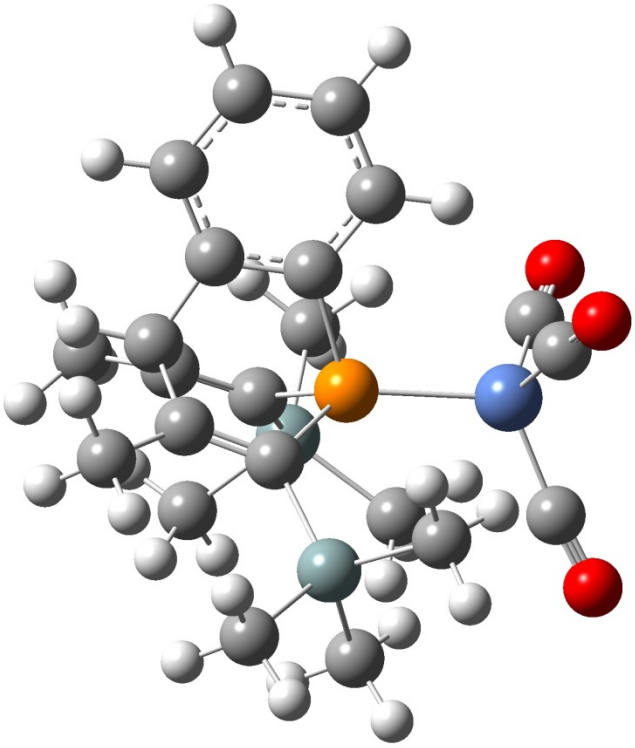
Electron donation between fragments (<0.001e for any omitted MO)

Alpha-spin MO	1->2	2->1
HOMO -69 (# 30)	0.000	-0.004
HOMO -66 (# 33)	-0.001	-0.002
HOMO -62 (# 37)	-0.011	0.000
HOMO -59 (# 40)	0.014	0.000
HOMO -58 (# 41)	0.002	0.000
HOMO -57 (# 42)	0.002	0.000
HOMO -53 (# 46)	0.023	-0.001
HOMO -52 (# 47)	0.001	0.000
HOMO -51 (# 48)	0.002	0.000
HOMO -47 (# 52)	0.008	-0.006
HOMO -46 (# 53)	0.006	-0.001
HOMO -45 (# 54)	0.000	0.002
HOMO -44 (# 55)	0.000	0.002
HOMO -43 (# 56)	0.004	0.000
HOMO -42 (# 57)	0.004	0.000
HOMO -41 (# 58)	0.009	0.000
HOMO -40 (# 59)	0.003	-0.001
HOMO -37 (# 62)	-0.008	-0.013
HOMO -34 (# 65)	0.006	0.001
HOMO -31 (# 68)	-0.008	-0.003
HOMO -30 (# 69)	0.001	-0.001
HOMO -29 (# 70)	0.001	-0.001
HOMO -27 (# 72)	0.004	-0.003
HOMO -26 (# 73)	0.004	-0.003
HOMO -25 (# 74)	0.002	0.000
HOMO -24 (# 75)	-0.001	-0.003
HOMO -23 (# 76)	-0.001	-0.003
HOMO -20 (# 79)	0.021	0.003
HOMO -19 (# 80)	0.004	0.000
HOMO -18 (# 81)	0.004	0.000
HOMO -17 (# 82)	0.006	0.000
HOMO -16 (# 83)	0.004	0.000
HOMO -15 (# 84)	0.001	0.000
HOMO -14 (# 85)	0.001	0.000
HOMO -13 (# 86)	0.001	0.001
HOMO -12 (# 87)	0.002	0.001
HOMO -11 (# 88)	0.080	0.012
HOMO -10 (# 89)	-0.001	0.008
HOMO -9 (# 90)	0.000	0.008
HOMO -8 (# 91)	0.003	-0.001
HOMO -7 (# 92)	0.003	-0.001
HOMO -6 (# 93)	0.001	0.000
HOMO -5 (# 94)	-0.006	-0.002
HOMO -4 (# 95)	0.002	0.000
HOMO -3 (# 96)	0.002	0.000
HOMO -2 (# 97)	-0.002	0.022
HOMO -1 (# 98)	-0.002	0.022
HOMO 0 (# 99)	0.130	0.007
Total over OMOs	0.321	0.036
TotalALPHA+BETA	0.643	0.073

Repulsion and residue (Delta) terms between fragments

Alpha-spin MO	1<->2	Delta
HOMO -69 (# 30)	-0.002	0.000
HOMO -66 (# 33)	-0.002	0.000
HOMO -62 (# 37)	0.000	0.000
HOMO -59 (# 40)	0.002	0.000
HOMO -58 (# 41)	0.000	0.000
HOMO -57 (# 42)	0.000	0.000
HOMO -53 (# 46)	0.006	-0.001
HOMO -52 (# 47)	0.001	0.000
HOMO -51 (# 48)	0.001	0.000
HOMO -47 (# 52)	0.022	0.000
HOMO -46 (# 53)	-0.013	0.000
HOMO -45 (# 54)	0.001	0.000
HOMO -44 (# 55)	0.001	0.000
HOMO -43 (# 56)	0.002	0.000
HOMO -42 (# 57)	0.002	0.000
HOMO -41 (# 58)	0.002	0.000
HOMO -40 (# 59)	0.039	0.000
HOMO -37 (# 62)	-0.021	-0.001
HOMO -34 (# 65)	-0.004	0.000
HOMO -31 (# 68)	-0.009	-0.001
HOMO -30 (# 69)	0.004	0.000
HOMO -29 (# 70)	0.004	0.000
HOMO -27 (# 72)	0.005	0.000
HOMO -26 (# 73)	0.004	0.000
HOMO -25 (# 74)	-0.007	0.000
HOMO -24 (# 75)	-0.004	0.000
HOMO -23 (# 76)	-0.006	0.000
HOMO -20 (# 79)	0.001	-0.002
HOMO -19 (# 80)	0.000	0.000
HOMO -18 (# 81)	0.000	0.000
HOMO -17 (# 82)	0.001	0.000
HOMO -16 (# 83)	0.002	0.000
HOMO -15 (# 84)	0.000	0.000
HOMO -14 (# 85)	0.000	0.000
HOMO -13 (# 86)	0.007	0.000
HOMO -12 (# 87)	0.006	0.000
HOMO -11 (# 88)	0.018	-0.009
HOMO -10 (# 89)	-0.005	0.000
HOMO -9 (# 90)	-0.005	0.000
HOMO -8 (# 91)	-0.002	-0.001
HOMO -7 (# 92)	-0.001	-0.001
HOMO -6 (# 93)	-0.001	-0.001
HOMO -5 (# 94)	-0.016	0.000
HOMO -4 (# 95)	0.001	0.000
HOMO -3 (# 96)	0.000	0.000
HOMO -2 (# 97)	-0.035	0.001
HOMO -1 (# 98)	-0.035	0.001
HOMO 0 (# 99)	-0.108	-0.007
Total over OMOs	-0.142	-0.026

Optimized geometry, three lower frequencies, thermochemistry and CDA calculations for $2Ni(CO)_3$



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	.711185	.258254	2.991561
2	6	0	3.037995	1.693896	2.394182
3	6	0	1.558012	.684792	4.019145
4	1	0	-.186290	-.305417	3.225226
5	6	0	2.713917	1.402141	3.722059
6	1	0	3.944156	2.248430	2.158729
7	1	0	1.310395	.453127	5.051764
8	1	0	3.370078	1.733974	4.522777
9	6	0	1.457521	-.683190	-.783809
10	6	0	.039512	1.751955	-.656452
11	6	0	2.540925	.123734	-.777544
12	6	0	1.275060	2.295115	-.680426
13	6	0	2.445776	1.494657	-.099026
14	1	0	3.380606	2.046710	-.239596
15	14	0	1.395399	-2.378531	-1.652047
16	14	0	-1.551826	2.379570	-1.483259
17	6	0	2.193576	1.265521	1.375204
18	6	0	1.026920	.554364	1.668761
19	15	0	.039582	.070484	.182220
20	6	0	2.168690	-3.694018	-.534970
21	1	0	3.204811	-3.447492	-.275000
22	1	0	1.609040	-3.803466	.400501
23	1	0	2.172696	-4.669757	-1.036885
24	6	0	2.316900	-2.333113	-3.315585
25	1	0	1.926417	-3.140125	-3.948630
26	1	0	2.146799	-1.390111	-3.847998
27	1	0	3.398452	-2.483791	-3.236682

28	6	0	-.366714	-2.881539	-2.091445
29	1	0	-1.001000	-3.018273	-1.213092
30	1	0	-.849324	-2.145497	-2.744567
31	1	0	-.333609	-3.833836	-2.636394
32	6	0	-1.422046	4.069612	-2.333866
33	1	0	-.672376	4.102431	-3.131780
34	1	0	-2.396950	4.263132	-2.801372
35	1	0	-1.233233	4.895846	-1.639270
36	6	0	-2.952560	2.540328	-.229896
37	1	0	-3.221024	1.579619	.216477
38	1	0	-2.679218	3.224442	.582249
39	1	0	-3.846031	2.945315	-.721798
40	6	0	-1.990029	1.150903	-2.852700
41	1	0	-2.950987	1.416235	-3.310865
42	1	0	-1.227872	1.169442	-3.641249
43	1	0	-2.071501	.122556	-2.490134
44	6	0	3.908951	-.183630	-1.315040
45	1	0	4.009185	-1.206330	-1.677119
46	1	0	4.174618	.499997	-2.133244
47	1	0	4.654368	-.031967	-.522319
48	6	0	1.689918	3.640717	-1.201814
49	1	0	.857039	4.248862	-1.547036
50	1	0	2.212681	4.195433	-.410310
51	1	0	2.405087	3.528863	-2.029002
52	28	0	-1.813591	-1.075185	.859244
53	6	0	-1.195867	-2.618620	1.532408
54	6	0	-2.592807	-.121028	2.170212
55	6	0	-3.035110	-1.375645	-.423420
56	8	0	-.841947	-3.614221	1.990903
57	8	0	-3.143946	.424273	3.021079
58	8	0	-3.877680	-1.607078	-1.172791

	1			2			3		
	A			A			A		
Frequencies --	3.1717			33.1211			37.4948		
Red. masses --	3.0205			4.7557			5.1727		
Frc consts --	.0000			.0031			.0043		
IR Inten --	.0106			.0289			.0063		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	.03	-.03	-.01	-.04	.12	.00	.01	-.02	-.03
2 6	.01	.01	-.02	-.02	.08	-.03	.03	-.05	-.04
3 6	.04	-.03	-.02	-.06	.17	.00	.03	-.05	-.03
4 1	.04	-.05	-.01	-.05	.14	.02	.01	-.01	-.03
5 6	.03	-.01	-.02	-.04	.15	-.02	.04	-.06	-.04
6 1	.00	.02	-.02	-.01	.06	-.04	.03	-.05	-.04
7 1	.05	-.05	-.02	-.08	.23	.01	.04	-.05	-.03
8 1	.03	-.01	-.02	-.06	.19	-.02	.05	-.08	-.04
9 6	.02	.02	-.02	.00	-.03	.03	-.02	.00	-.04
10 6	-.01	.00	.00	.03	-.01	-.04	-.01	.02	.00
11 6	.00	.04	-.03	.01	-.05	.03	-.02	.00	-.05
12 6	-.02	.02	.00	.04	-.04	-.07	-.01	.01	-.01
13 6	-.01	.03	-.01	.02	-.03	-.02	-.01	-.01	-.03
14 1	-.02	.04	-.02	.03	-.04	-.03	-.01	-.01	-.04
15 14	.02	.00	.02	-.02	-.03	.02	.00	-.04	.04
16 14	-.02	-.01	.01	.01	.04	.03	-.03	.07	.06
17 6	.01	.01	-.02	.00	.03	-.02	.01	-.02	-.03
18 6	.02	-.01	-.01	-.01	.06	-.01	.01	-.02	-.03
19 15	.01	.00	-.01	.00	.01	.00	-.01	.00	-.02
20 6	-.14	.00	.13	-.09	-.07	.01	.02	.03	.11
21 1	-.15	-.05	.18	-.09	-.11	.04	.02	.06	.10
22 1	-.21	.06	.10	-.11	-.07	.00	.02	.08	.12
23 1	-.16	-.02	.16	-.11	-.06	-.01	.03	.00	.17
24 6	.18	-.13	.10	.03	-.03	.05	.01	-.12	.04
25 1	.07	-.03	.04	.01	.01	.01	.00	-.14	.07
26 1	.45	-.08	.11	.10	-.01	.07	.05	-.14	.00

27	1	.14	-.38	.22	.02	-.09	.08	.01	-.15	.06
28	6	.02	.10	-.11	-.03	.04	-.05	.02	-.09	.06
29	1	-.06	.21	-.15	-.05	.01	-.07	.03	-.12	.06
30	1	.13	.09	-.19	.01	.08	-.02	-.02	-.11	.06
31	1	-.01	.06	-.04	-.03	.06	-.09	.04	-.09	.06
32	6	-.04	-.01	.01	-.02	.08	.11	-.04	.13	.19
33	1	-.03	.00	.01	-.10	.10	.04	-.08	.18	.15
34	1	-.04	-.03	.00	-.06	.15	.23	-.07	.18	.25
35	1	-.06	-.01	.00	.09	.03	.15	.00	.07	.24
36	6	-.02	-.02	.01	.07	.00	.10	-.02	-.01	.08
37	1	-.02	-.02	.01	.09	-.01	.09	-.11	-.06	-.07
38	1	-.02	-.01	.01	.11	-.02	.10	.03	-.17	.20
39	1	-.02	-.02	.01	.04	.01	.16	.02	.15	.14
40	6	-.01	-.01	.01	-.06	.10	-.01	-.05	.15	.00
41	1	-.02	-.03	.02	-.06	.14	.03	-.05	.18	.01
42	1	-.02	.00	.00	-.08	.11	-.03	-.05	.17	.00
43	1	.01	-.02	.01	-.07	.09	-.04	-.06	.13	-.05
44	6	.00	.07	-.05	.02	-.09	.06	-.02	.01	-.07
45	1	.00	.09	-.11	.01	-.11	.11	-.03	.02	-.09
46	1	.00	.12	-.01	.04	-.14	.04	-.03	.03	-.06
47	1	.00	.02	-.04	.01	-.07	.07	-.01	-.01	-.07
48	6	-.04	.03	.02	.07	-.08	-.14	.00	.01	.00
49	1	-.05	.03	.04	.10	-.09	-.22	.00	.02	.02
50	1	-.04	.03	.02	.06	-.03	-.17	.02	-.01	.00
51	1	-.05	.05	.01	.10	-.15	-.11	-.01	.01	-.01
52	28	.01	-.01	-.01	.02	-.02	-.01	.00	.00	-.03
53	6	-.04	-.03	-.02	.04	-.03	-.06	.01	.05	.07
54	6	.04	.00	.01	-.02	-.12	.03	-.05	.04	-.08
55	6	-.02	.03	.01	.02	.01	-.02	.07	-.08	-.08
56	8	-.09	-.04	-.02	.06	-.04	-.08	.02	.09	.15
57	8	.06	.00	.02	-.06	-.20	.06	-.08	.06	-.12
58	8	-.04	.05	.02	.02	.04	-.03	.13	-.14	-.13

HF=-2172.357671

Sum of electronic and zero-point Energies=	-2171.904992
Sum of electronic and thermal Energies=	-2171.867604
Sum of electronic and thermal Enthalpies=	-2171.866659
Sum of electronic and thermal Free Energies=	-2171.976100

Electron donation between fragments (<0.001e for any omitted MO)

Alpha-spin MO	1->2	2->1
HOMO -94 (# 29)	0.002	0.000
HOMO -88 (# 35)	0.000	-0.006
HOMO -79 (# 44)	-0.001	-0.002
HOMO -75 (# 48)	-0.003	0.000
HOMO -74 (# 49)	0.002	0.000
HOMO -73 (# 50)	0.001	0.000
HOMO -72 (# 51)	0.009	0.000
HOMO -70 (# 53)	0.017	0.000
HOMO -69 (# 54)	0.008	0.000
HOMO -68 (# 55)	0.008	0.000
HOMO -67 (# 56)	0.003	0.000
HOMO -66 (# 57)	0.001	0.000
HOMO -65 (# 58)	0.004	0.000
HOMO -64 (# 59)	0.001	0.000
HOMO -63 (# 60)	0.006	0.000
HOMO -62 (# 61)	0.005	0.000
HOMO -61 (# 62)	0.007	0.000
HOMO -60 (# 63)	0.010	-0.001
HOMO -59 (# 64)	0.008	-0.001
HOMO -58 (# 65)	0.005	-0.003

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 HOMO -57 (# 66) -0.001  0.003
 HOMO -56 (# 67) -0.002  0.002
 HOMO -55 (# 68)  0.002  0.000
 HOMO -54 (# 69)  0.002  0.000
 HOMO -53 (# 70)  0.001 -0.001
 HOMO -52 (# 71)  0.004 -0.001
 HOMO -51 (# 72)  0.002 -0.011
 HOMO -49 (# 74)  0.003  0.000
 HOMO -48 (# 75)  0.002 -0.001
 HOMO -47 (# 76)  0.000  0.003
 HOMO -45 (# 78)  0.000  0.001
 HOMO -44 (# 79)  0.001  0.002
 HOMO -43 (# 80) -0.001  0.001
 HOMO -42 (# 81)  0.002  0.001
 HOMO -40 (# 83)  0.004  0.001
 HOMO -39 (# 84)  0.001 -0.007
 HOMO -38 (# 85)  0.002 -0.003
 HOMO -36 (# 87)  0.002  0.000
 HOMO -35 (# 88)  0.003  0.000
 HOMO -34 (# 89)  0.003  0.001
 HOMO -33 (# 90)  0.002  0.000
 HOMO -32 (# 91)  0.001  0.000
 HOMO -31 (# 92)  0.002  0.000
 HOMO -30 (# 93)  0.005  0.001
 HOMO -29 (# 94)  0.005  0.000
 HOMO -28 (# 95)  0.003  0.000
 HOMO -27 (# 96)  0.008  0.000
 HOMO -26 (# 97)  0.001  0.000
 HOMO -25 (# 98)  0.002  0.000
 HOMO -24 (# 99)  0.003  0.000
 HOMO -21 (#102)  0.005  0.000
 HOMO -20 (#103)  0.003  0.000
 HOMO -18 (#105)  0.001  0.000
 HOMO -17 (#106)  0.011  0.001
 HOMO -15 (#108)  0.073  0.012
 HOMO -12 (#111)  0.005  0.000
 HOMO -11 (#112)  0.004  0.001
 HOMO -10 (#113)  0.004  0.000
 HOMO  -9 (#114)  0.003  0.001
 HOMO  -8 (#115) -0.003  0.006
 HOMO  -7 (#116) -0.004  0.004
 HOMO  -6 (#117)  0.001 -0.001
 HOMO  -4 (#119)  0.005  0.000
 HOMO  -3 (#120)  0.012  0.023
 HOMO  -2 (#121)  0.002  0.017
 HOMO  -1 (#122)  0.000  0.011
 HOMO   0 (#123)  0.124  0.012
 ----------------------------
 Total over OMOs  0.405  0.068
 ============================
 TotalALPHA+BETA  0.810  0.135
```

Repulsion and residue (Delta) terms between fragments

```
Alpha-spin MO    1<->2  Delta
 HOMO -94 (# 29)  0.000  0.000
 HOMO -88 (# 35) -0.002  0.000
 HOMO -79 (# 44) -0.003  0.000
 HOMO -75 (# 48)  0.000  0.000
 HOMO -74 (# 49)  0.000  0.000
```

HOMO	-73	(# 50)	0.000 0.000
HOMO	-72	(# 51)	0.002 0.000
HOMO	-70	(# 53)	0.002 0.000
HOMO	-69	(# 54)	0.001 0.000
HOMO	-68	(# 55)	0.000 0.000
HOMO	-67	(# 56)	0.001 0.000
HOMO	-66	(# 57)	0.000 0.000
HOMO	-65	(# 58)	0.001 0.000
HOMO	-64	(# 59)	0.000 0.000
HOMO	-63	(# 60)	0.001 0.000
HOMO	-62	(# 61)	0.001 0.000
HOMO	-61	(# 62)	0.002 0.000
HOMO	-60	(# 63)	0.016 0.000
HOMO	-59	(# 64)	0.011 0.000
HOMO	-58	(# 65)	-0.009 -0.001
HOMO	-57	(# 66)	0.001 0.000
HOMO	-56	(# 67)	0.001 -0.001
HOMO	-55	(# 68)	0.000 0.000
HOMO	-54	(# 69)	0.003 0.000
HOMO	-53	(# 70)	0.000 -0.001
HOMO	-52	(# 71)	0.014 0.000
HOMO	-51	(# 72)	0.018 0.000
HOMO	-49	(# 74)	0.008 0.000
HOMO	-48	(# 75)	0.000 0.000
HOMO	-47	(# 76)	0.014 0.000
HOMO	-45	(# 78)	0.008 0.000
HOMO	-44	(# 79)	0.018 0.000
HOMO	-43	(# 80)	0.004 0.000
HOMO	-42	(# 81)	0.000 0.000
HOMO	-40	(# 83)	-0.019 0.000
HOMO	-39	(# 84)	0.001 -0.001
HOMO	-38	(# 85)	-0.001 -0.001
HOMO	-36	(# 87)	-0.006 0.000
HOMO	-35	(# 88)	-0.008 0.000
HOMO	-34	(# 89)	-0.007 0.000
HOMO	-33	(# 90)	-0.004 0.000
HOMO	-32	(# 91)	-0.001 0.000
HOMO	-31	(# 92)	-0.002 0.000
HOMO	-30	(# 93)	-0.011 0.000
HOMO	-29	(# 94)	-0.014 0.000
HOMO	-28	(# 95)	-0.006 0.000
HOMO	-27	(# 96)	0.000 0.000
HOMO	-26	(# 97)	-0.002 0.000
HOMO	-25	(# 98)	-0.002 0.000
HOMO	-24	(# 99)	-0.003 0.000
HOMO	-21	(#102)	-0.006 0.000
HOMO	-20	(#103)	-0.003 0.000
HOMO	-18	(#105)	0.000 0.000
HOMO	-17	(#106)	0.002 -0.001
HOMO	-15	(#108)	0.025 -0.013
HOMO	-12	(#111)	0.007 -0.001
HOMO	-11	(#112)	0.005 0.000
HOMO	-10	(#113)	0.001 0.000
HOMO	-9	(#114)	0.007 0.000
HOMO	-8	(#115)	-0.016 0.000
HOMO	-7	(#116)	-0.013 -0.001
HOMO	-6	(#117)	-0.001 0.000
HOMO	-4	(#119)	0.000 0.000
HOMO	-3	(#120)	-0.043 -0.002
HOMO	-2	(#121)	-0.026 0.000

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HOMO  -1 (#122) -0.025  0.000
HOMO   0 (#123) -0.100 -0.009
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Total over OMOs -0.141 -0.041
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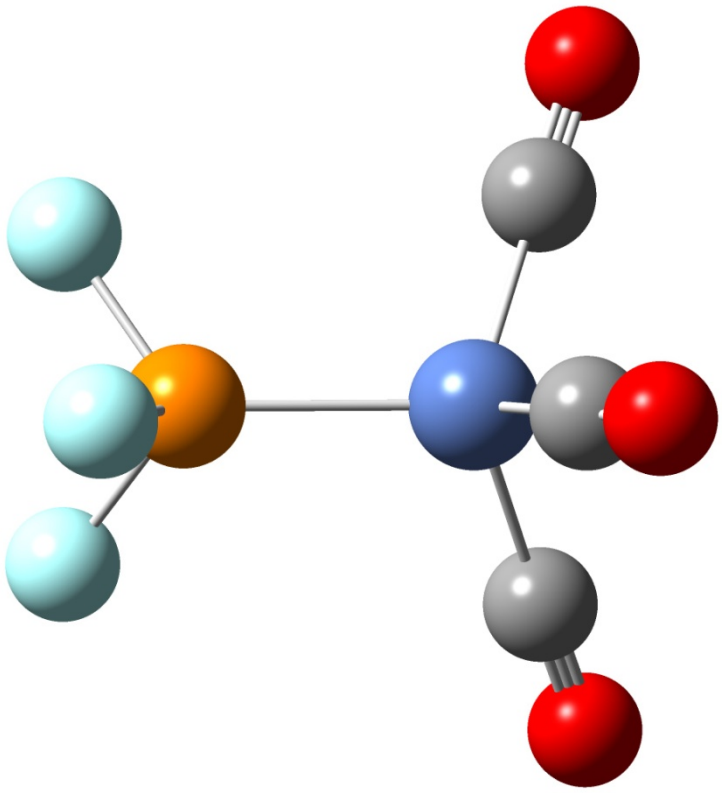
Optimized geometry, three lower frequencies, thermochemistry and CDA calculations for $PF_3Ni(CO)_3$



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-.627195	.429112	-1.224908
2	6	0	-.780673	.211253	1.974463
3	6	0	1.887648	.649491	.754303
4	6	0	.553923	-1.993336	.508218
5	8	0	-1.446989	.462528	2.871092
6	8	0	.721495	-3.125764	.483839
7	8	0	2.895633	1.176824	.884584
8	28	0	.295792	-.199391	.574051
9	9	0	-.917412	-.635726	-2.368628
10	9	0	.078317	1.528879	-2.128866
11	9	0	-2.072101	1.088305	-1.173374

	1			2			3		
	A			A			A		
Frequencies --	10.0805			58.4856			59.4638		
Red. masses --	18.0835			16.0158			15.9981		
Frc consts --	.0011			.0323			.0333		
IR Inten --	.0000			.0296			.0293		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 15	.00	.00	.00	.00	.01	-.06	.00	-.06	.00
2 6	.00	-.14	-.02	.25	.01	-.03	-.02	.17	.03
3 6	.00	.05	.13	-.11	.07	.14	.22	.00	.08
4 6	.00	.09	-.11	-.14	-.10	.11	-.21	.04	-.09
5 8	.00	-.23	-.03	.57	.04	-.15	-.04	.38	.06

6	8	.00	.15	-.19	-.31	-.25	.20	-.47	.03	-.24
7	8	.01	.08	.21	-.24	.18	.29	.50	-.06	.21
8	28	.00	.00	.00	.00	.00	.06	.00	.05	.00
9	9	.00	-.33	.39	.11	.01	-.16	.15	-.16	-.01
10	9	-.01	-.17	-.48	.07	.01	-.17	-.17	-.16	-.01
11	9	.00	.50	.09	-.19	.01	-.16	.02	-.17	-.01

HF=-1151.7102687

Sum of electronic and zero-point Energies= -1151.675873
Sum of electronic and thermal Energies= -1151.662699
Sum of electronic and thermal Enthalpies= -1151.661755
Sum of electronic and thermal Free Energies= -1151.719083

Electron donation between fragments (<0.001e for any omitted MO)

Alpha-spin MO	1->2	2->1
HOMO -40 (# 11)	0.001	0.000
HOMO -36 (# 15)	0.000	-0.003
HOMO -33 (# 18)	-0.001	-0.001
HOMO -32 (# 19)	0.047	-0.001
HOMO -31 (# 20)	0.005	0.000
HOMO -30 (# 21)	0.005	0.000
HOMO -26 (# 25)	0.036	-0.001
HOMO -25 (# 26)	0.001	-0.006
HOMO -22 (# 29)	0.004	0.000
HOMO -21 (# 30)	0.003	0.000
HOMO -20 (# 31)	0.012	0.000
HOMO -19 (# 32)	-0.004	-0.021
HOMO -18 (# 33)	0.004	-0.004
HOMO -17 (# 34)	0.004	-0.004
HOMO -14 (# 37)	-0.002	-0.003
HOMO -10 (# 41)	0.001	-0.001
HOMO -9 (# 42)	0.001	-0.001
HOMO -8 (# 43)	0.009	0.001
HOMO -7 (# 44)	0.009	0.001
HOMO -5 (# 46)	0.116	0.024
HOMO -4 (# 47)	-0.001	0.013
HOMO -3 (# 48)	-0.001	0.013
HOMO -2 (# 49)	-0.002	0.028
HOMO -1 (# 50)	-0.002	0.028
HOMO 0 (# 51)	0.114	0.008
Total over OMOs	0.360	0.068
TotalALPHA+BETA	0.721	0.136

Repulsion and residue (Delta) terms between fragments

Alpha-spin MO	1<->2	Delta
HOMO -40 (# 11)	0.000	0.000
HOMO -36 (# 15)	-0.001	0.000
HOMO -33 (# 18)	-0.002	0.000
HOMO -32 (# 19)	0.001	-0.002
HOMO -31 (# 20)	0.000	0.000
HOMO -30 (# 21)	0.000	0.000
HOMO -26 (# 25)	0.012	-0.001
HOMO -25 (# 26)	0.016	0.000
HOMO -22 (# 29)	0.002	0.000
HOMO -21 (# 30)	0.002	0.000

HOMO -20	(# 31)	0.013	0.000
HOMO -19	(# 32)	-0.026	-0.001
HOMO -18	(# 33)	0.000	-0.005
HOMO -17	(# 34)	0.000	-0.005
HOMO -14	(# 37)	-0.005	0.000
HOMO -10	(# 41)	0.004	0.000
HOMO -9	(# 42)	0.004	0.000
HOMO -8	(# 43)	-0.005	0.000
HOMO -7	(# 44)	-0.005	0.000
HOMO -5	(# 46)	0.031	-0.035
HOMO -4	(# 47)	-0.006	0.001
HOMO -3	(# 48)	-0.006	0.001
HOMO -2	(# 49)	-0.011	0.004
HOMO -1	(# 50)	-0.011	0.004
HOMO 0	(# 51)	-0.097	-0.010
Total over OMOs		-0.081	-0.051