Electronic Supplementary Material (ESI) for ChemComm.

Electronic Supplementary Information

Insertion of Phenyl Isothiocyanate into a P−P Bond of a Nickel-substituted Bicyclo[1.1.0]tetraphosphabutane

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The supporting information contains:

(S1) Experimental Section

General procedures and starting materials.

All experiments were performed under an atmosphere of dry argon using standard Schlenk techniques or an MBraun UniLab glovebox. Solvents were dried and degassed with an MBraun SPS800 solvent purification system. Tetrahydrofuran and toluene were stored over molecular sieves (3 Å). Diethyl ether and *n*-hexane were stored over a potassium mirror. NMR spectra were recorded on Bruker Avance 300 and Avance 400 spectrometers at 300 K and internally referenced to residual solvent resonances. Melting points were measured on samples in sealed capillaries on a Stuart SMP10 melting point apparatus. UV/Vis spectra were recorded on a Varian Cary 50 spectrophotometer. Infrared spectra were recorded at ambient temperature (~5wt% THF solutions) using a Bruker ALPHA with a Platinum-ATR unit. Elemental analyses were determined by the analytical department of Regensburg University. Phenyl isothiocyanate was purchased from ALFA Aesar and used as received.

Synthesis of $\mathbf{1^{Mes}}$.

P_4 (310.4 mg, 2.505 mmol, 1.0 eq) was added in one portion at −60 °C to a solution of CpNi(IMes) (2.165 g, 5.053 mmol, 2.0 eq). The solution turned immediately dark red. After stirring the solution for 19 h, the solvent was removed in vacuum, and the residue was extracted with toluene (50 mL). Subsequently, the solution was filtered and reduced in volume (45 mL). Dark red crystals of $\mathbf{1^{Mes}}$ formed upon storing the solution at −16 °C for one day. The isolated compound contains one equivalent of toluene per formula unit after drying in high vacuum. Yield 1.932 g (71%); m.p. >158 °C (slow decomp. to a black oil); UV/Vis (THF, λ_{max} /nm, (ε_{max} /L·mol^{-1}·cm^{-1})): 354 (15100), 421 (9600), 515 (9200); elemental analysis calcd. for $C_{54}H_{66}N_4Ni_2P_4 \cdot C_7H_8$ (M = 1104.55): C 66.33, H 6.75, N 5.07, found: C 66.35, H 6.15, N 5.12; ^{1}H NMR ([D$_8$]THF, 300 K, 400.13 MHz) δ /ppm = 2.19 (s, 24H, *ortho*-C*H*$_3$), 2.41 (s, 12H, *para*-C*H*$_3$), 4.31 (s, 10H, Cp), 7.04 (s, 8H, *meta*-CH$_{Dipp}$), 7.10 (s, 4H, NC-H); ^{13}C{^{1}H} NMR ([D$_8$]THF, 300 K, 100.61 MHz) δ /ppm =19.6 (*ortho*-*C*H$_3$), 21.2 (*para*-*C*H$_3$), 90.6 (Cp), 124.3 (NCH), 129.7 (*meta*-C$_{Dipp}$), 136.7 (C$_{Dipp}$), 138.3 (C$_{Dipp}$), 138.8 (C$_{Dipp}$), 182.8 (C$_{Carbene}$); ^{31}P{^{1}H} NMR ([D$_8$]THF, 193 K, 100.61 MHz) δ /ppm = −320.4 (t, $^1J_{PP}$ = −190.5 Hz, 2P), −56.0 (t, $^1J_{PP}$ = −190.5 Hz, 2P).

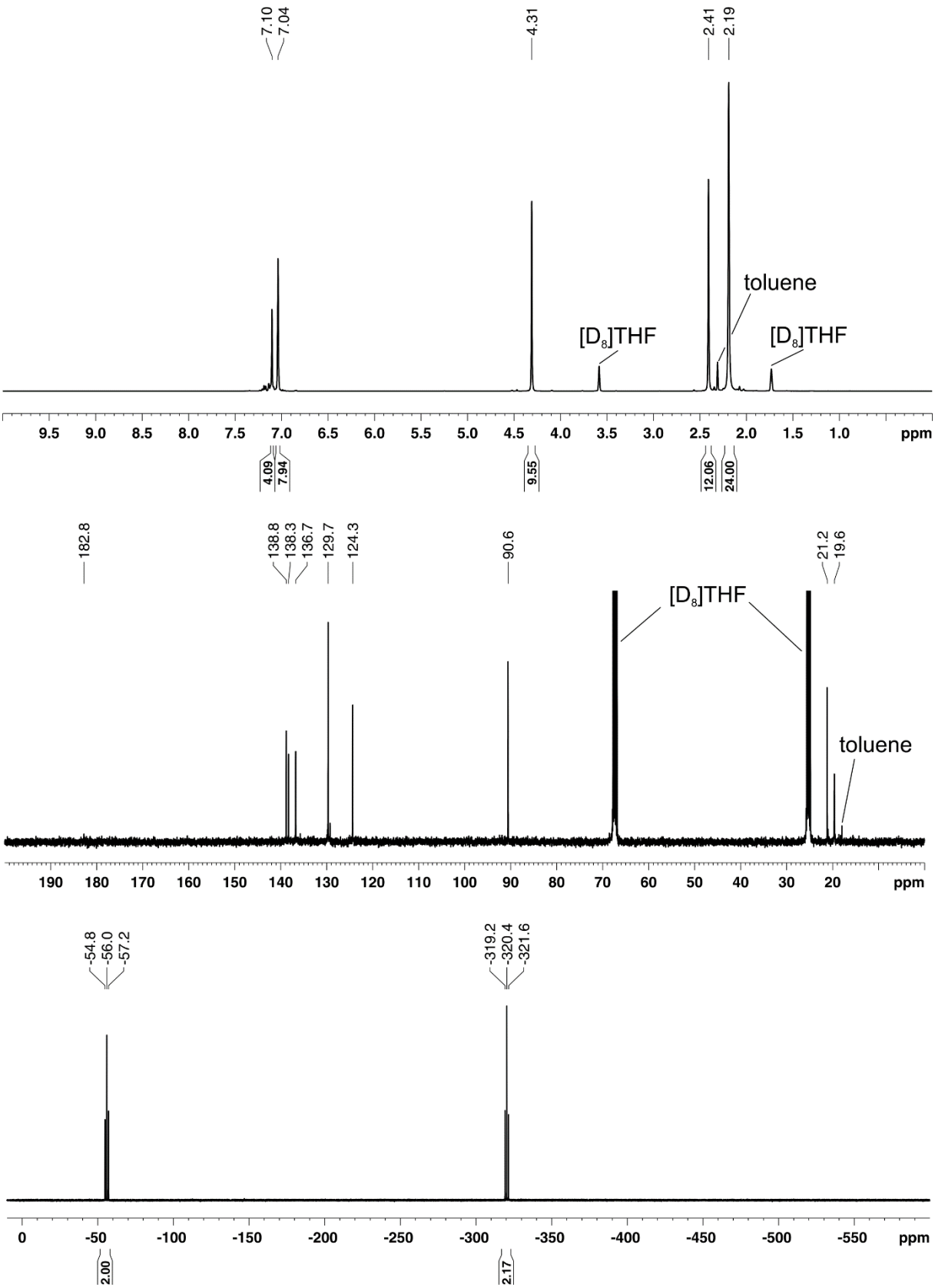

Fig. S1. ^{1}H (top), ^{13}C{^{1}H} (middle), and ^{31}P{^{1}H} NMR spectrum (bottom) of **1**$^{\mathbf{Mes}}$ (400.16/100.61/161.98 MHz, [D$_8$]THF, 300 K).

Synthesis of 2a.

A solution of phenyl isothiocyanate (122 mg, 0.900 mmol, 7.0 eq) in tetrahydrofuran (1.5 mL) was added to a solution of **1^{Mes}** (139 mg, 0.129 mmol, 1.0 eq) in tetrahydrofuran (2 mL) at room temperature. After stirring this solution for 4.5 hours the solvent was removed in *vacuo*, and the residue was washed with *n*-hexane (2 mL). The residue was extracted with toluene (1.5 mL) and layered with *n*-hexane (1 mL). Dark brown crystals formed during storage at room temperature after one day. X-ray quality crystals of **2a** were obtained by recrystallization of the crude product from toluene (2 mL) and diffusing *n*-hexane into this solution. The isolated compound contains two equivalents of toluene per formula unit after drying in high vacuum. Yield 54 mg (31%); m.p. >150 °C (slow decomp. to a black solid); UV/Vis (THF, λ_{max} /nm, (ε_{max} /L·mol^{-1}·cm^{-1})): 353sh (21500), 403 (13700), 490 (8000), 565sh (4800); elemental analysis calcd. for $C_{61}H_{71}N_5Ni_2P_4S{\cdot}2C_7H_8$ (M = 1331.90): C 67.63, H 6.58, N 5.26, found: C 67.65, H 5.85, N 5.38; ^{1}H NMR ([D$_8$]THF, 300 K, 400.13 MHz) δ /ppm = 2.12 (s, 6H, *para*-CH$_3$), 2.21 (s, 6H, *para*-CH$_3$), 2.30 (s, 12H, *ortho*-CH$_3$), 2.36 (s, 6H, *ortho*-CH$_3$), 4.29 (s, 5H, Cp), 4.62 (s, 5H, Cp), 6.65 (m, 2H, *meta*-CH$_{Ph}$), 6.92 (m, 1H, *para*-CH$_{Ph}$), 6.97−7.01 (m, 5H, CH$_{Ph/Dipp}$), 7.07−7.14 (m, 3H, CH$_{Ph/Dipp}$), 7.17−7.22 (m, 6H, CH$_{Ph/Dipp}$); ^{1}H NMR ([D$_8$]THF, 193 K, 400.13 MHz) δ /ppm = 1.98 (s, 3H, CH$_3$), 1.99 (s, 3H, CH$_3$), 2.03 (s, 3H, CH$_3$), 2.23 (s, 3H, CH$_3$), 2.24 (s, 3H, CH$_3$), 2.27 (s, 3H, CH$_3$), 2.30 (s, 3H, CH$_3$), 2.39 (s, 6H, CH$_3$), 2.42 (s, 3H, CH$_3$), 2.50 (s, 3H, CH$_3$), 2.61 (s, 3H, CH$_3$), 4.19 (s, 5H, Cp), 4.49 (s, 5H, Cp), 6.65 (s, 1H, CH$_{Ph/Dipp}$), 6.67 (s, 1H, CH$_{Ph/Dipp}$), 6.80 (s, 1H, CH$_{Ph/Dipp}$), 6.98 (t, $^3J_{HH}$ = 7.4 Hz, 1H, CH$_{Ph/Dipp}$), 7.02 (s, 1H, CH$_{Ph/Dipp}$), 7.13 (s, 1H, CH$_{Ph/Dipp}$), 7.15 (m, 2H, CH$_{Ph/Dipp}$), 7.22 (m, 6H, CH$_{Ph/Dipp}$), 7.30 (s, 1H, CH$_{Ph/Dipp}$), 7.39 (s, 1H, CH$_{Ph/Dipp}$), 7.44 (s, 1H, CH$_{Ph/Dipp}$), 7.47 (s, 1H, CH$_{Ph/Dipp}$), 7.51 (s, 1H, CH$_{Ph/Dipp}$), 7.53 (s, 1H, CH$_{Ph/Dipp}$); ^{13}C{^{1}H} NMR ([D$_8$]THF, 300 K, 100.61 MHz) δ /ppm = 19.4 (*ortho*-CH$_3$), 19.4 (*ortho*-CH$_3$), 21.3 (*para*-CH$_3$), 21.4 (*para*-CH$_3$), 91.1 (Cp), 91.6 (Cp), 120.5, 122.6, 124.9, 128.8, 129.7, 129.9, 130.1, 136.5, 138.0, 138.9, 155.8, 156.0, 179.3 (C$_{Carbene}$), 179.4 (C$_{Carbene}$); ^{31}P{^{1}H} NMR ([D$_8$]THF, 300 K, 100.61 MHz) δ /ppm = −150.1 (m, 1P), −96.4 (m, 1P), −75.0 (m, 1P), 32.1 (m, 1P); ^{31}P{^{1}H} NMR ([D$_8$]THF, 193 K, 100.61 MHz) δ /ppm = −151.8 (m, 1P), −105.5 (m, 1P), −78.0 (m, 1P), 27.8 (m, 1P).

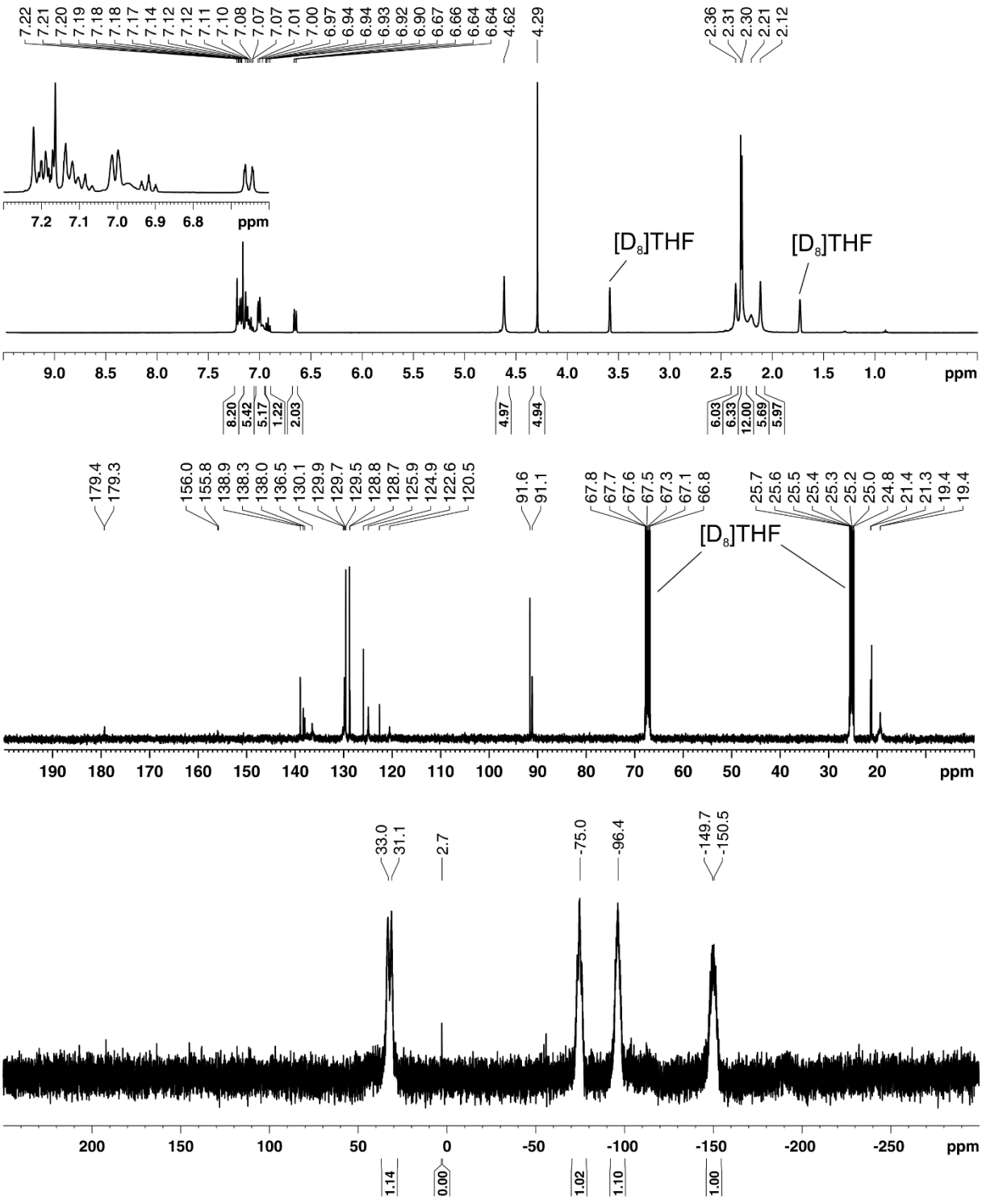

Fig. S2. ^{1}H (top), $^{13}C\{^{1}H\}$ (middle), and $^{31}P\{^{1}H\}$ NMR spectrum (bottom) of **2a** (400.16/100.61/161.98 MHz, $[D_8]THF$, 300 K).

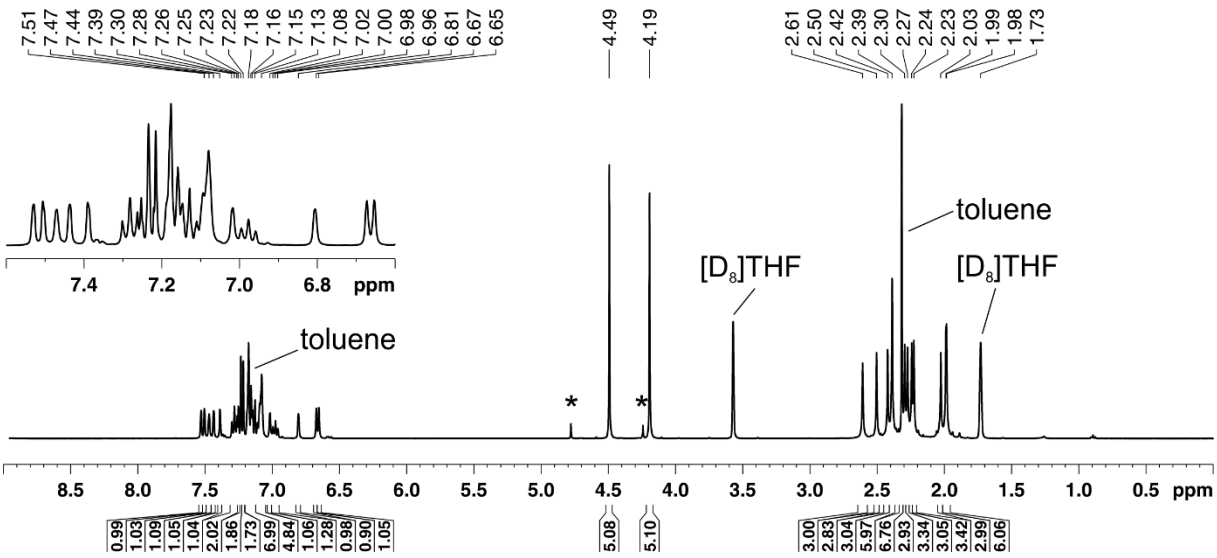

Fig. S3. ^{1}H NMR spectrum of **2a** (400.16 MHz, [D_8]THF, 193 K). The signals assigned to **2b** are labeled with an asterisk.

Synthesis of 2b.

A solution of phenyl isothiocyanate (176 mg, 1.30 mmol, 7.0 eq) in tetrahydrofuran (3 mL) was added to a solution of **1**$^{\mathbf{Mes}}$ (201 mg, 0.186 mmol, 1.0 eq) in tetrahydrofuran (2 mL) at room temperature. After stirring this solution for 25 hours the solvent was removed in vacuum, and the residue was washed with *n*-hexane (5 mL). The residue was extracted with diethyl ether (8 mL) and after filtration reduced in volume to 3 mL. Dark yellow crystals formed upon storing this solution at −35 °C for one day. X-ray quality crystals of **2b** were obtained by recrystallizing from toluene (1.5 mL) and diffusing *n*-hexane into this solution. Yield 34 mg (16%); m.p. >170 °C (slow decomp. to a black solid); UV/Vis (THF, λ_{max} /nm, (ε_{max} /L·mol^{-1}·cm^{-1})): 348 (22600), 400 (14400), 503 (7400), 586sh (4600); elemental analysis calcd. for $C_{61}H_{71}N_5NiP_4S$ (M = 1147.62): C 63.84, H 6.24, N 6.10, found: C 63.95, H 6.24, N 6.08; ^{1}H NMR ([D$_8$]THF, 300 K, 400.13 MHz) δ /ppm = 2.13 (s, 6H, *para*-CH$_3$), 2.20 (s, 12H, *ortho*-CH$_3$), 2.30 (s, 6H, *para*-CH$_3$), 2.38 (s, 6H, *ortho*-CH$_3$), 4.18 (s, 5H, Cp), 4.65 (s, 5H, Cp), 6.84 (s, 2H, CH$_{Ph/Dipp}$), 6.97 (s, 2H, CH$_{Ph/Dipp}$), 7.00 (m, 1H, *para*-CH$_{Ph}$), 7.02 (m, 3H, CH$_{Ph/Dipp}$), 7.09 (s, 2H, CH$_{Ph/Dipp}$), 7.14−7.16 (m, 3H, CH$_{Ph/Dipp}$), 7.24−7.27 (m, 4H, CH$_{Ph/Dipp}$); ^{1}H NMR ([D$_8$]THF, 193 K, 400.13 MHz) δ /ppm = 1.90 (s, 3H, CH$_3$), 1.97 (s, 3H, CH$_3$), 2.17 (s, 3H, CH$_3$), 2.23 (s, 9H, CH$_3$), 2.24 (s, 3H, CH$_3$), 2.27 (s, 3H, CH$_3$), 2.36 (s, 3H, CH$_3$), 2.51 (s, 3H, CH$_3$), 2.54 (s, 6H, CH$_3$), 4.10 (s, 5H, Cp), 4.58 (s, 5H, Cp), 6.59 (s, 1H, CH$_{Ph/Dipp}$), 6.73 (s, 1H, CH$_{Ph/Dipp}$), 6.94 (s, 1H, CH$_{Ph/Dipp}$), 6.96 (s, 1H, CH$_{Ph/Dipp}$), 6.99 (s, 2H, NCH), 7.06 (s, 1H, CH$_{Ph/Dipp}$), 7.11 (s, 1H, CH$_{Ph/Dipp}$), 7.22 (d, $^3J_{HH}$ = 7.5 Hz, 1H, CH$_{Ph/Dipp}$), 7.30−7.36 (m, 5H, CH$_{Ph/Dipp}$), 7.41 (s, 1H, CH$_{Ph/Dipp}$), 7.49 (s, 1H, CH$_{Ph/Dipp}$), 7.55 (s, 1H, CH$_{Ph/Dipp}$); ^{13}C{^{1}H} NMR ([D$_8$]THF, 300 K, 100.61 MHz) δ /ppm = 19.4 (*ortho*-CH$_3$), 19.7 (*ortho*-CH$_3$), 21.2 (*para*-CH$_3$), 21.2 (*para*-CH$_3$), 90.9 (Cp), 92.5 (Cp), 125.0, 125.3, 126.3, 128.7, 129.7, 129.9, 136.5, 137.1, 137.8, 138.2, 138.9, 139.0, 146.8, 146.9, 178.0 (C$_{Carbene}$), 178.1 (C$_{Carbene}$), 178.6 (NCS); ^{31}P{^{1}H} NMR ([D$_8$]THF, 300 K, 100.61 MHz) δ /ppm = −182.1 (m, 1P), −104.5 (m, 1P), 4.5 (m, 1P), 50.1 (m, 1P); ^{31}P{^{1}H} NMR ([D$_8$]THF, 193 K, 100.61 MHz) δ /ppm = −180.5 (m, 1P), −109.1 (m, 1P), 1.2 (m, 1P), 48.2 (m, 1P).

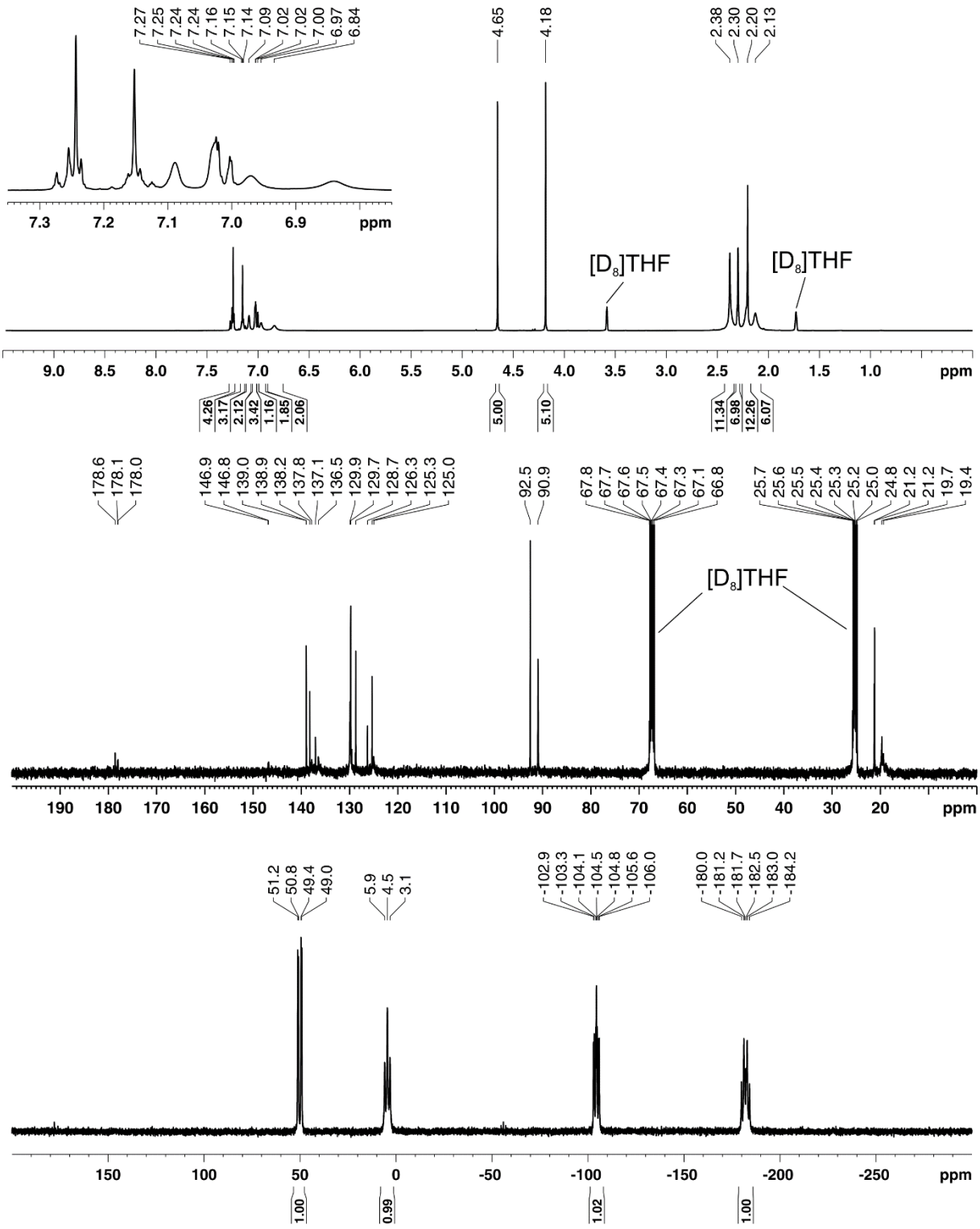

Fig. S4. ^{1}H (top), $^{13}C\{^{1}H\}$ (middle), and $^{31}P\{^{1}H\}$ NMR spectrum (bottom) of **2b** (400.16/100.61/161.98 MHz, [D_8]THF, 300 K).

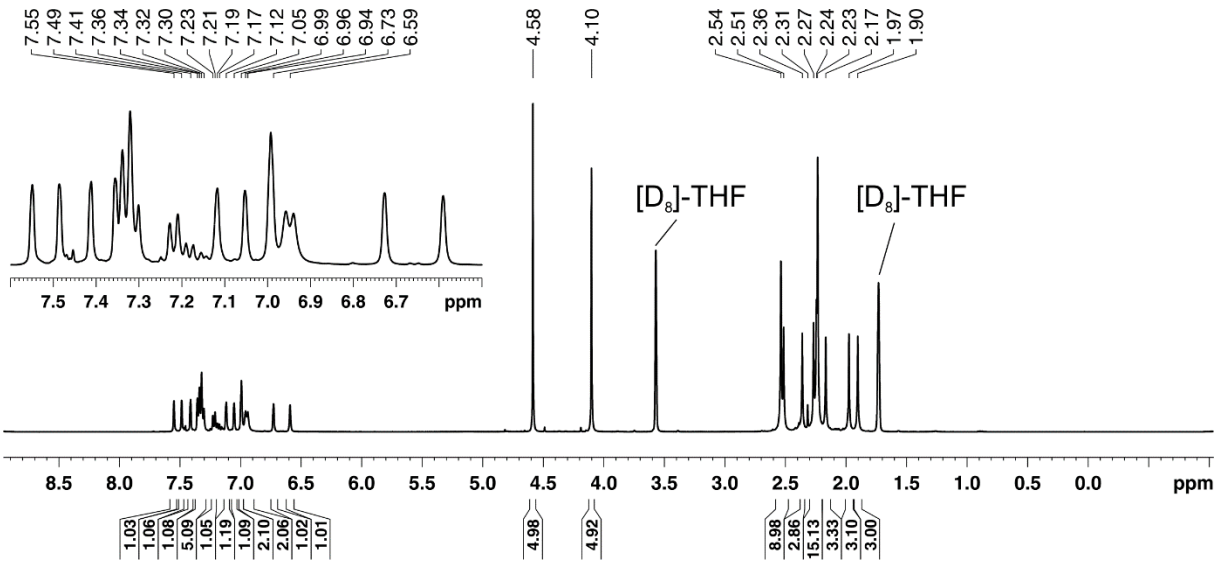

Fig. S5. ^{1}H NMR spectrum of **2b** (400.16 MHz, [D_8]THF, 193 K).

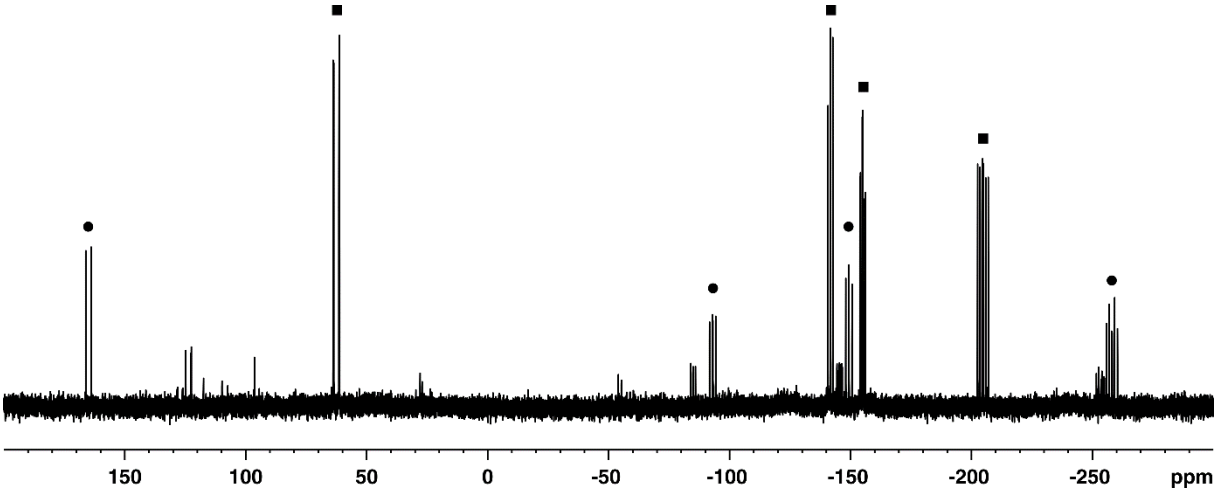

Fig. S6. ^{31}P{^{1}H} NMR spectrum (161.98 MHz, THF/C_6D_6-capillary) of the reaction of CS_2 and **1**^{Mes} (10:1) after one hour; ■ = major species, ● = minor species.

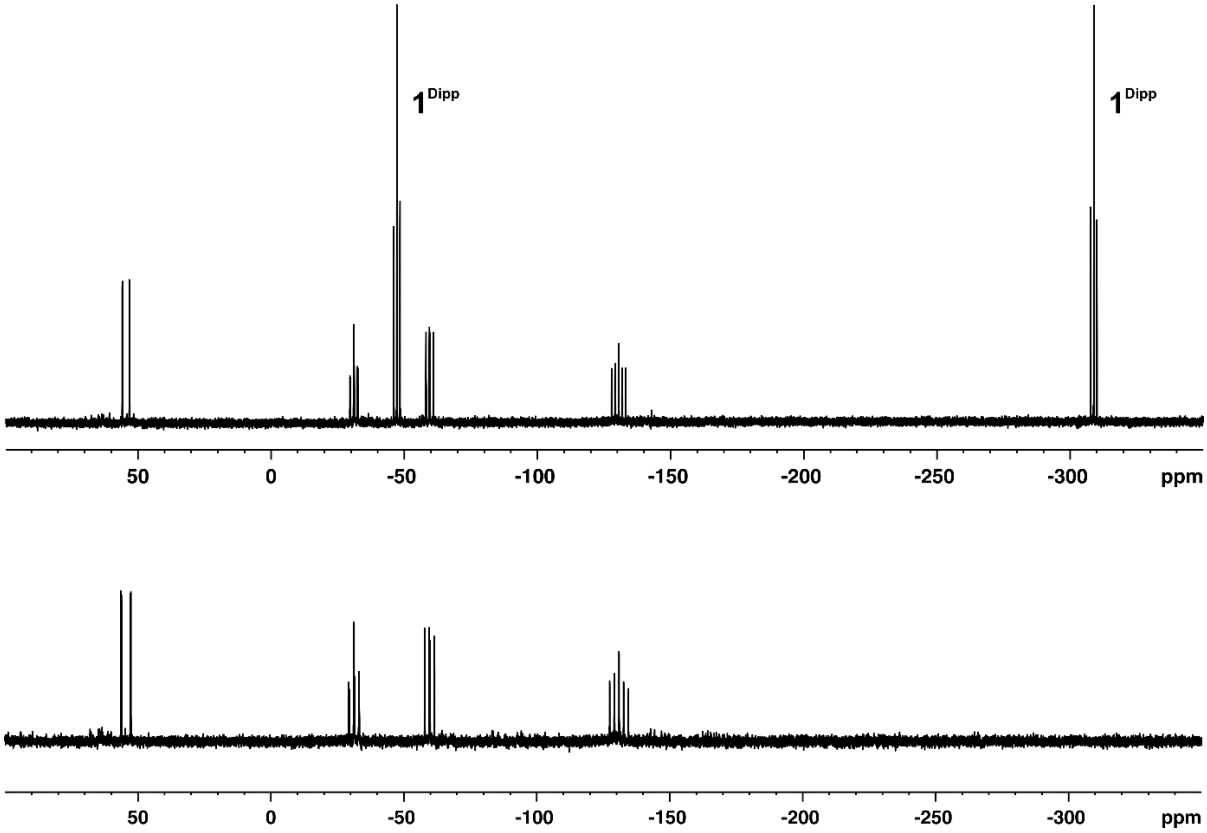

Fig. S7. $^{31}P\{^{1}H\}$ NMR spectra (161.98 MHz, THF/C_6D_6-capillary) of the reaction of CS_2 and **1^{Dipp}** (10:1) after 1.5 hours (top) and after one day (bottom, 121.49 MHz) .

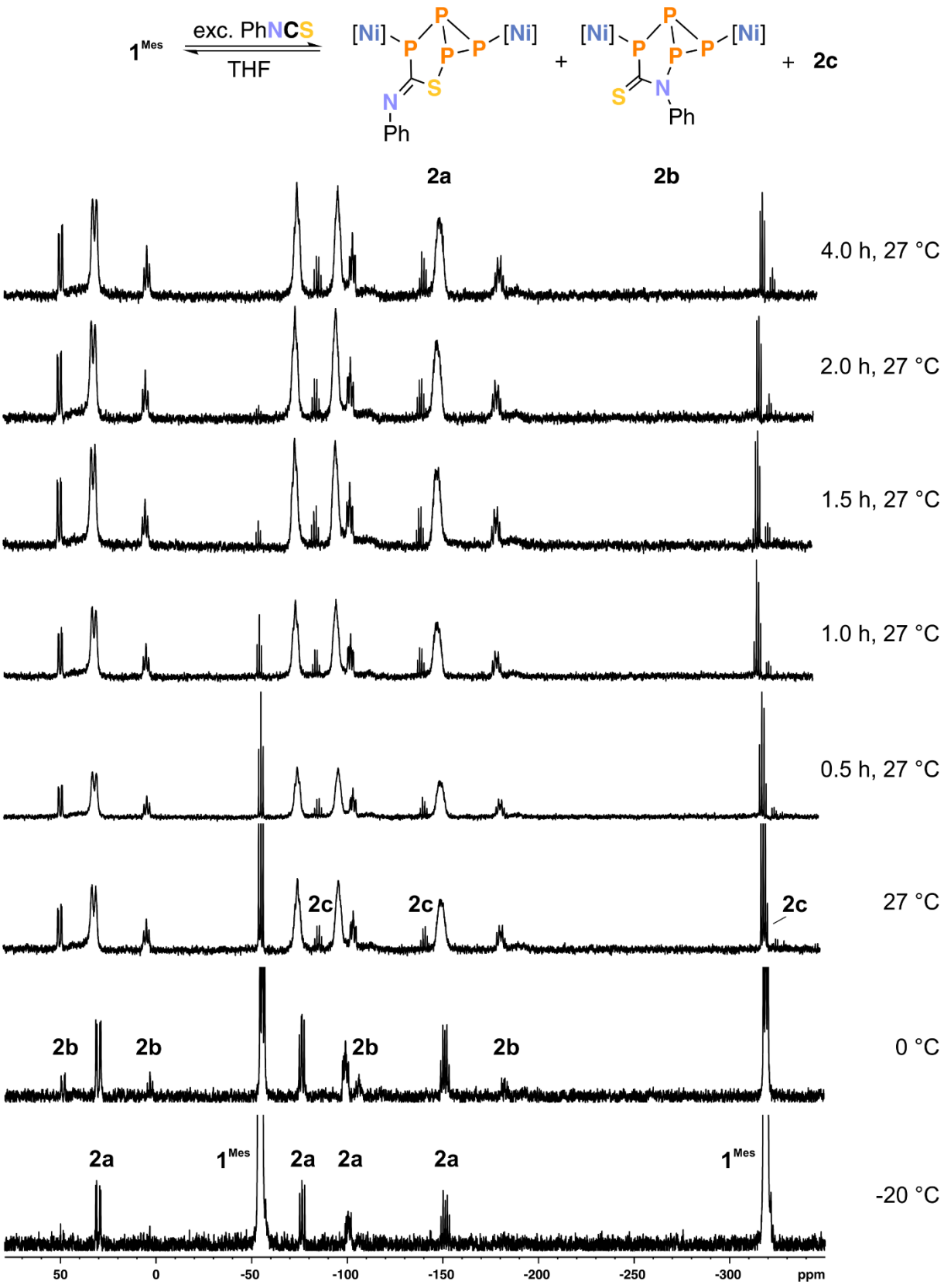

Fig. S8. $^{31}P\{^{1}H\}$ NMR monitoring (161.98 MHz, [D8]THF) of the reaction of PhNCS and **1**^{Mes} (7:1) at variable temperatures.

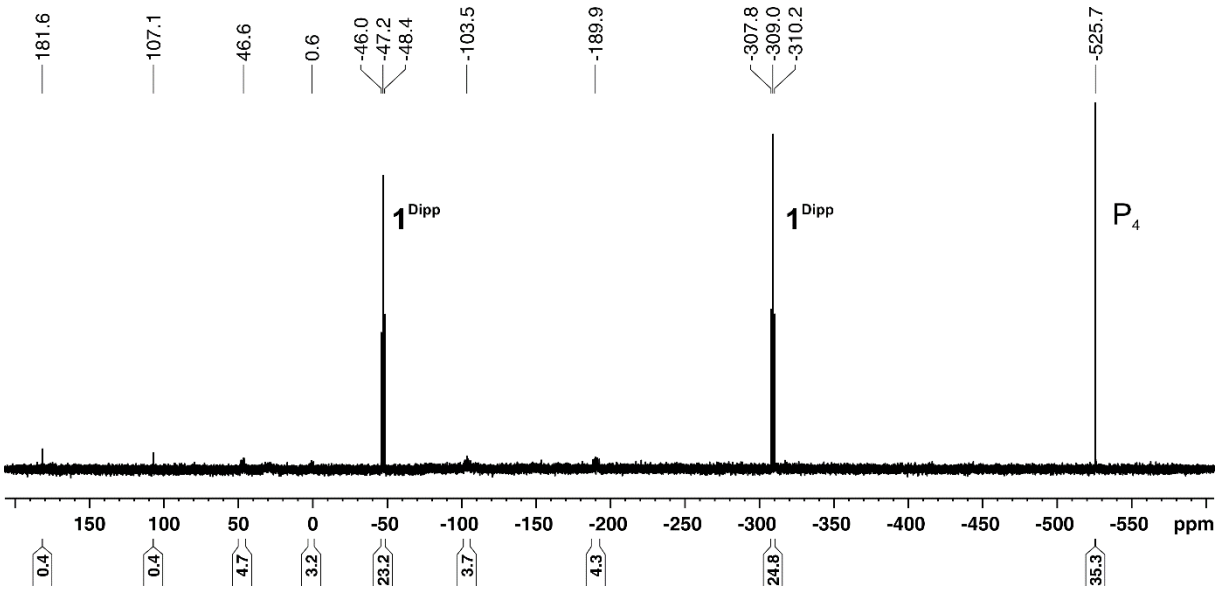

Fig. S9. $^{31}P\{^{1}H\}$ NMR spectrum (161.98 MHz, THF/C_6D_6-capillary) of the reaction of PhNCS and $\mathbf{1^{Dipp}}$ (29:1) after two days.

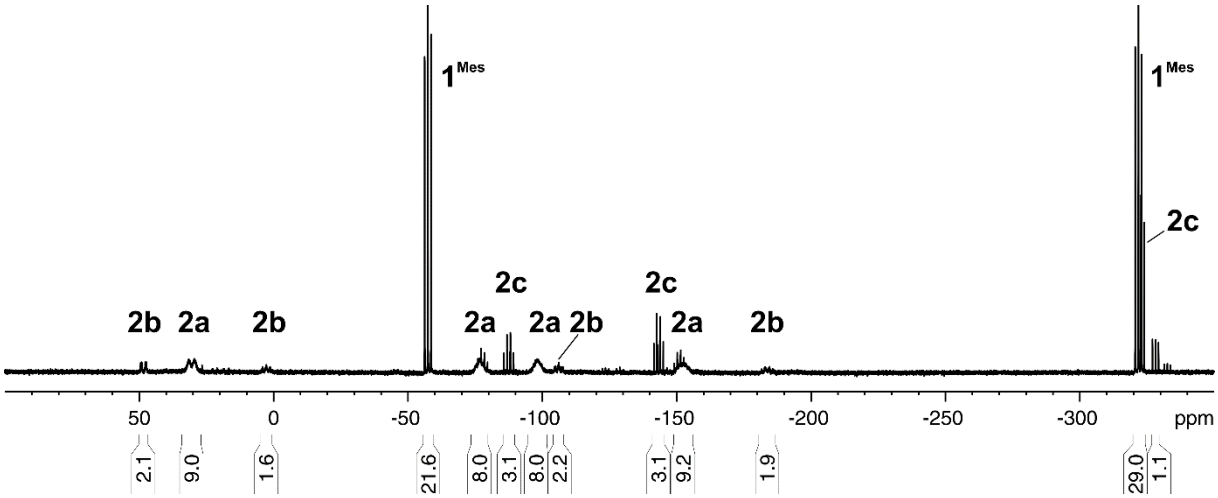

Fig. S10. $^{31}P\{^{1}H\}$ NMR spectrum (161.98 MHz, THF/C_6D_6-capillary) of the reaction of PhNCS and $\mathbf{1^{Mes}}$ (1:1) after one day.

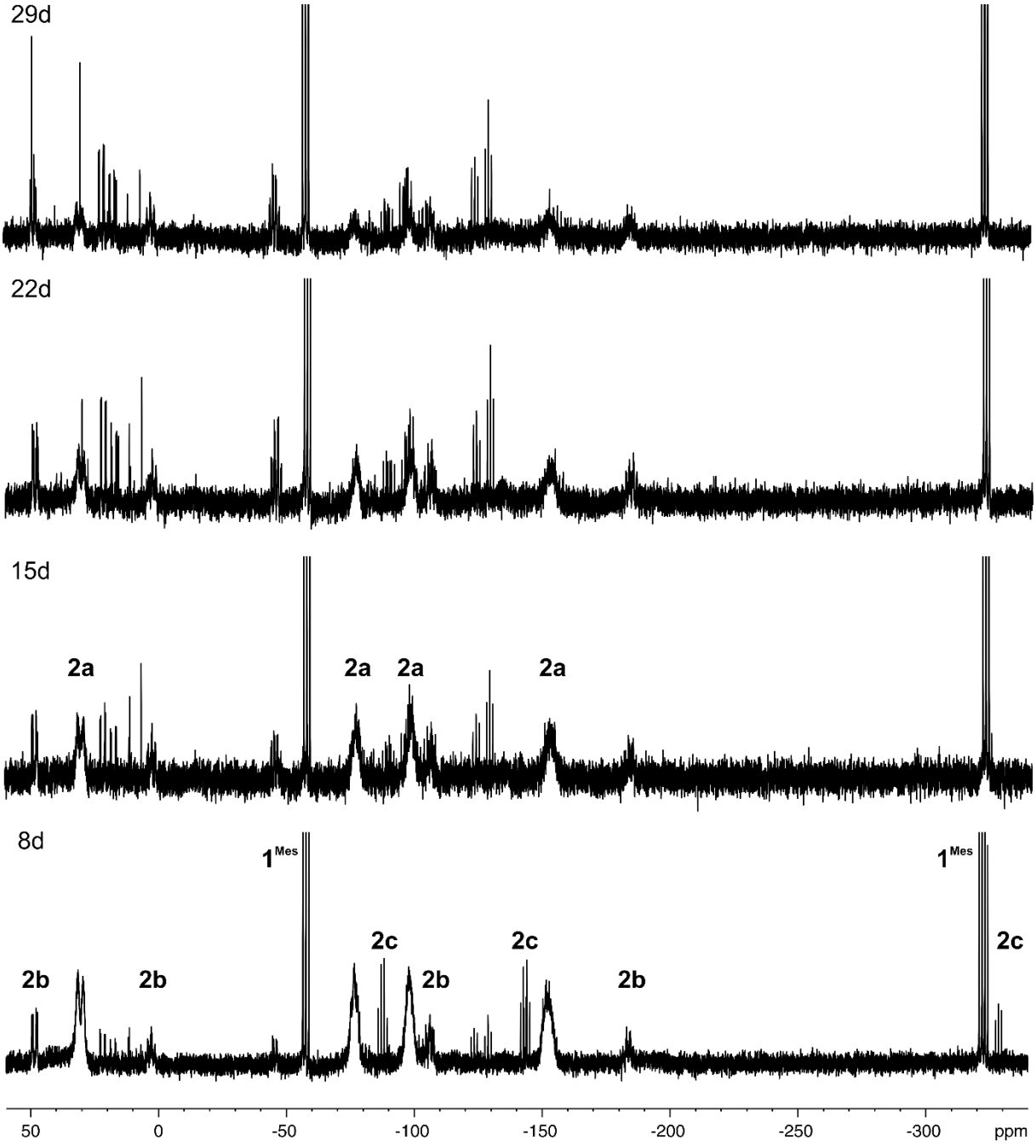

Fig. S11. $^{31}P\{^{1}H\}$ NMR monitoring (161.98 MHz, $[D_8]$THF) of a solution of **2a**.

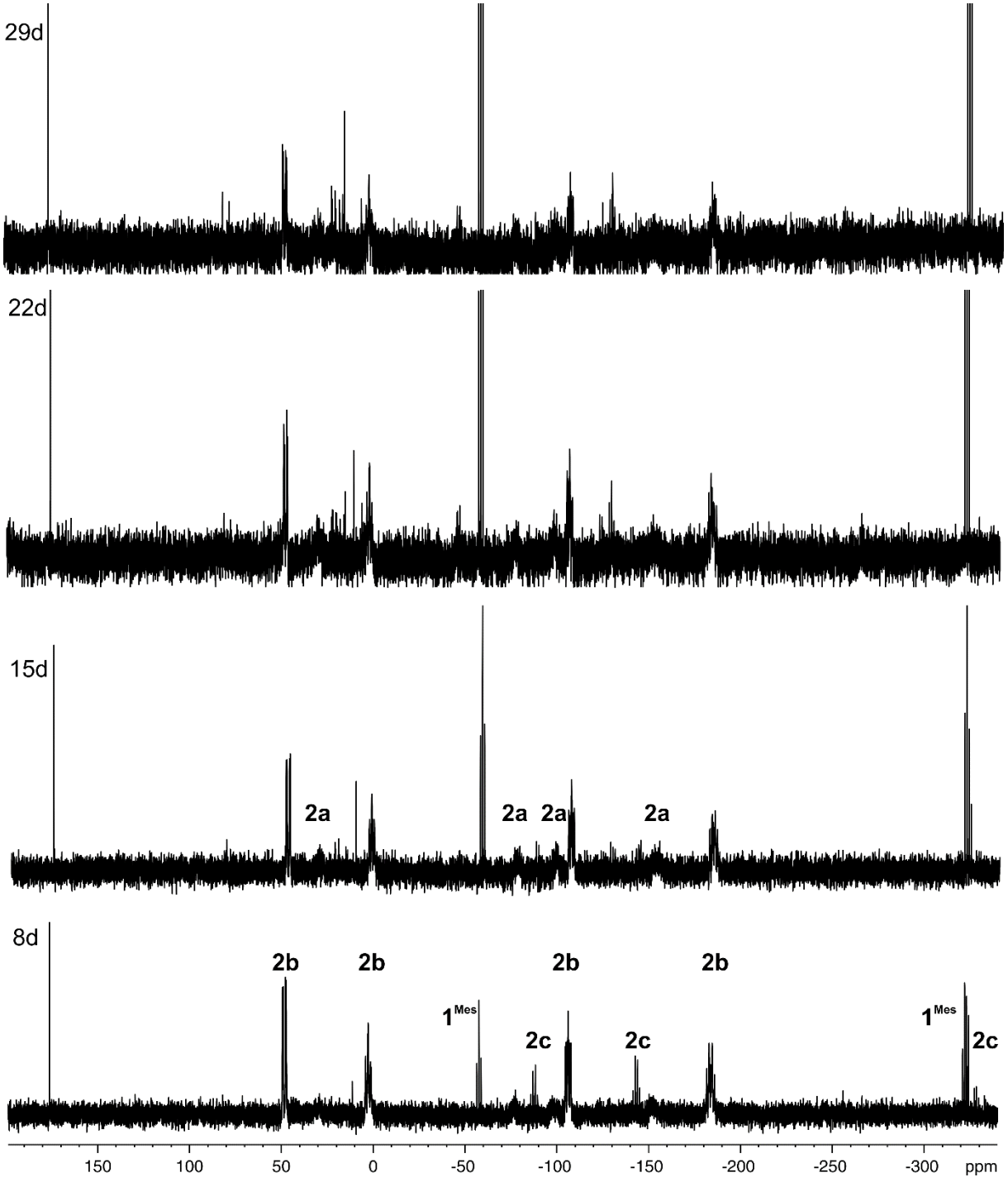

Fig. S12. $^{31}P\{^{1}H\}$ NMR monitoring (161.98 MHz, $[D_8]$THF) of a solution of **2b**.

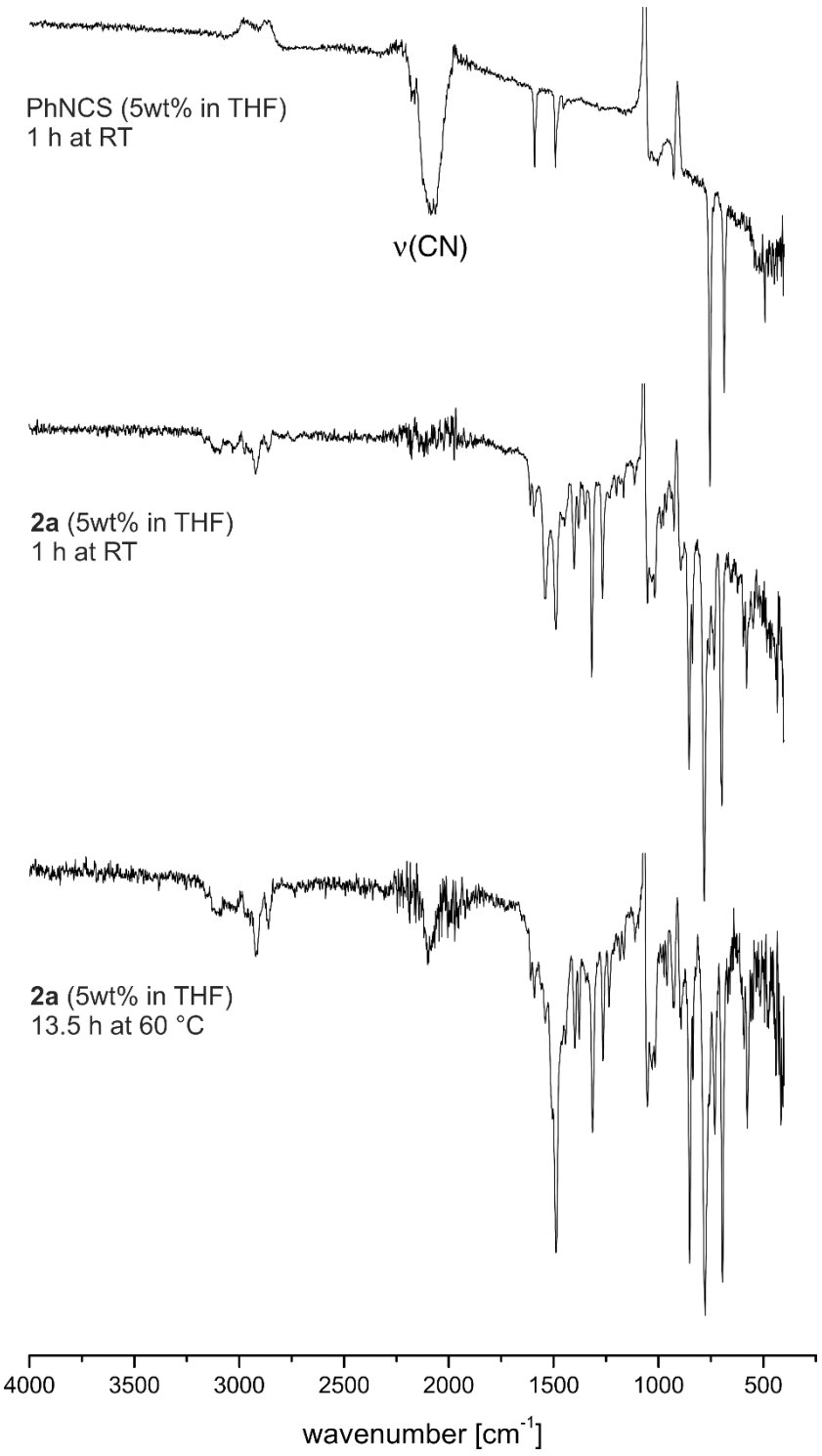

Fig. S13. IR spectra of THF solutions (5wt%) of PhNCS (top, measured one hour after preparation), **2a** (centre, measured one hour after preparation) and **2a** (bottom, measured after heating the solution for 13.5 h at 60 °C).

(S2) X-ray crystallography

The single crystal X-ray diffraction data were recorded on an Agilent Technologies Gemini Ultra R diffractometer and an Agilent Technologies SuperNova in case of **2b** with Cu K_α radiation (λ = 1.54184 Å). Semi-empirical multi-scan absorption corrections[1] and analytical ones[2] were applied to the data. The structures were solved with SHELXT[3] and least-square refinements on F^2 were carried out with SHELXL.[4]

CCDC 1446071-1446073 contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

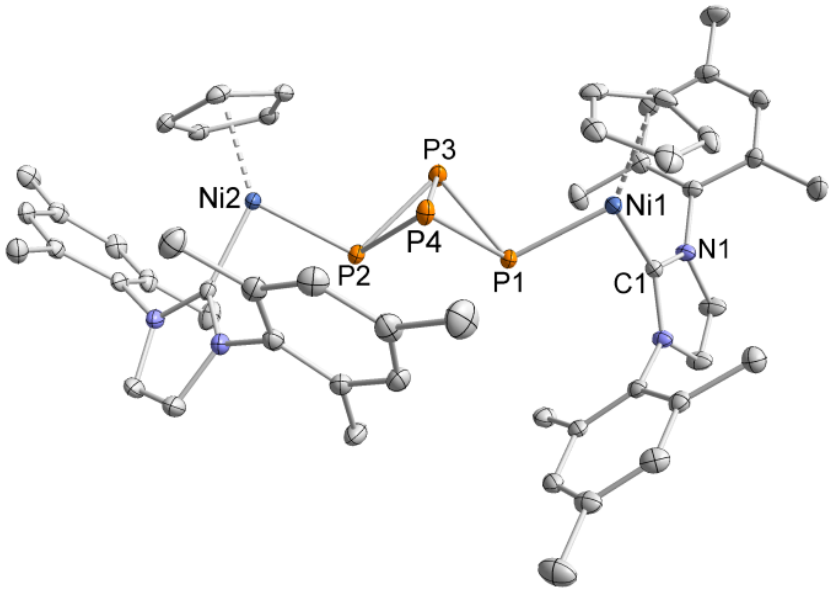

Fig. S14. Solid-state molecular structure of [{CpNi(IMes)}$_2$(μ-η^1:η^1-P_4)] (**1^{Mes}**). The hydrogen atoms are omitted for clarity. Thermal ellipsoids are drawn at 40% level. Selected bond lengths [Å] and angles [°]: Ni1–P1 2.2207(6), Ni2–P2 2.2177(6), P1–P3 2.2239(7), P1–P4 2.2233(7), P3–P4 2.1681(8), P1–P2 2.9288(7), fold angle (of the planes P1–P3–P4 and P2–P3–P4) 98.07(3), P4–P1–P3 58.36(2), P1–P3–P4 60.81(2), P1–P4–P3 60.83(2).

Table S1. Crystallographic data of **1**, **2**, and **3**

Compound	**1**	**2a**	**2b**
Empirical formula	$C_{62.5}H_{70}N_4Ni_2P_4$	$C_{76.5}H_{83}N_5Ni_2P_4S$	$C_{73}H_{79}N_5Ni_2P_4S$
Formula weight	1118.52	1345.83	1299.77
Temperature/K	123(1)	123(1)	123(1)
Crystal system	triclinic	triclinic	triclinic
Space group	*P*-1	*P*-1	*P*-1
a/Å	12.4093(4)	13.6251(4)	12.4533(2)
b/Å	13.1987(2)	14.0607(3)	15.5940(3)
c/Å	18.3557(4)	19.7007(5)	19.3068(3)
α/°	79.4323(17)	99.8667(19)	104.2274(14)
β/°	76.229(2)	99.819(2)	103.1281(14)
γ/°	84.6926(19)	98.0922(19)	106.3708(16)
Volume/Å^3	2866.71(12)	3607.32(16)	3305.17(10)
Z	2	2	2
ρ_{calc}g/cm^3	1.296	1.239	1.306
μ/mm^{-1}	2.190	2.096	2.269
F(000)	1178.0	1418.0	1368.0
Crystal size/mm^3	0.332 × 0.182 × 0.168	0.267 × 0.187 × 0.178	0.161 × 0.099 × 0.072
Radiation	CuKα (λ = 1.54184)	CuKα (λ = 1.54184)	CuKα (λ = 1.54184)
2Θ range for data collection/°	9.13 to 133.45	7.34 to 133.25	6.58 to 146.95
Index ranges	-14 ≤ h ≤ 14, -14 ≤ k ≤ 15, -21 ≤ l ≤ 19	-16 ≤ h ≤ 16, -16 ≤ k ≤ 16, -23 ≤ l ≤ 23	-15 ≤ h ≤ 15, -18 ≤ k ≤ 19, -23 ≤ l ≤ 23
Reflections collected	25046	65571	31085
Independent reflections	10078 [R_{int} = 0.0256, R_{sigma} = 0.0285]	12645 [R_{int} = 0.0489, R_{sigma} = 0.0324]	12849 [R_{int} = 0.0374, R_{sigma} = 0.0442]
Data/restraints/parameters	10078/0/652	12645/4/754	12849/2/742
Goodness-of-fit on F^2	1.030	1.050	1.032
Final R indexes [I>=2σ (I)]	R_1 = 0.0379, wR_2 = 0.0966	R_1 = 0.0753, wR_2 = 0.2095	R_1 = 0.0574, wR_2 = 0.1646
Final R indexes [all data]	R_1 = 0.0426, wR_2 = 0.1006	R_1 = 0.0845, wR_2 = 0.2185	R_1 = 0.0721, wR_2 = 0.1791
Largest diff. peak/hole / e Å^{-3}	1.14/-0.61	1.49/-0.91	1.05/-0.90

(S3) Computational Details

Density functional calculations were performed using Gaussian09, revision D.01[5] at the ωB97X-D level of theory.[6] Geometry optimizations were performed using the 6-311G(d,p)[7] basis set for all atoms. The nature of each stationary point was validated by frequency calculations.

The *Synchronous Transit-Guided Quasi-Newton* (STQN) Method was used for the transition state search.[8] The geometry optimizations of the starting materials and QST2 optimizations were performed at the ωB97X-D[6] level of theory using LANL2DZ[9] for Ni and the 6-31G(d,p)[7] basis set for the C, H, N, P, and S atoms. One imaginary frequency was found for each transition state structure which corresponds to the nuclear motion along the reaction coordinate. Moreover, intrinsic reaction coordinate (IRC) calculations were conducted to confirm the transition states.

The optimized structures of $\mathbf{1}^{\mathbf{Ph}}$, $\mathbf{2a}^{\mathbf{Ph}}$ and $\mathbf{2b}^{\mathbf{Ph}}$ and the five possible geometries for **2c** are illustrated in Fig. S14. The NMR spectroscopically detected species **2c** gives rise to an A_2MX spin system in the $^{31}P\{^1H\}$ NMR spectrum (see manuscript page 2, left column, paragraph 3) indicative of an unsymmetrically-substituted "P_4 butterfly" fragment.[10] It is conceivable that adduct complexes $\mathbf{2c}^{\mathbf{Add1}}$ and $\mathbf{2c}^{\mathbf{Add2}}$ (Fig. S14) represent intermediates on the reaction coordinate from $\mathbf{1}^{\mathbf{Mes}}$ and PhNCS to **2a** and **2b**, respectively. However, the transition states connecting $\mathbf{2c}^{\mathbf{Add1}}$ with $\mathbf{2a}^{\mathbf{Ph}}$, and $\mathbf{2c}^{\mathbf{Add2}}$ with $\mathbf{2b}^{\mathbf{Ph}}$ possess unrealistically high energies (~50 kcal mol^{-1}), thus indicating that a direct interconversion between these species is unlikely to occur under the reaction conditions (*vide supra*). The energies found for the Ni−P insertion products (*E*)-$\mathbf{2c}^{\mathbf{Ins1}}$, (*Z*)-$\mathbf{2c}^{\mathbf{Ins1}}$ and $\mathbf{2c}^{\mathbf{Ins2}}$ are significantly higher than those of $\mathbf{2a}^{\mathbf{Ph}}$ and $\mathbf{2b}^{\mathbf{Ph}}$ (Fig. S14).

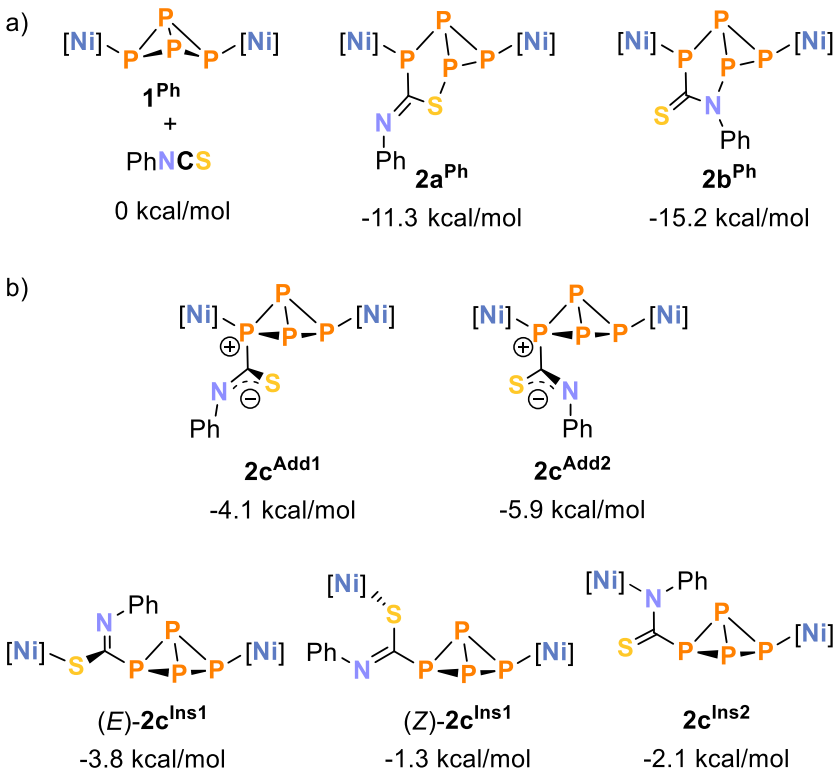

Fig. S15. a) Calculated, relative Gibbs free energies (kcal/mol) of $\mathbf{1}^{Ph}$, $\mathbf{2a}^{Ph}$ and $\mathbf{2b}^{Ph}$; b) optimized structures of further isomers which potentially correspond to **2c**, including their relative Gibbs free energies referring to $\mathbf{1}^{Ph}$ + PhNCS (kcal/mol).

$\mathbf{1}^{Ph}$:

electronic energy *E*/ a.u.	−6145.58651995
thermal enthalpy *H*/ a.u.	−6144.889305
total free Gibbs energy at 298 K *G*/ a.u.	−6145.019660

Cartesian Coordinates:

Ni	-3.37594200	-0.31682500	0.57778400
P	-1.47982800	-0.16526700	-0.57429600
C	-4.04439200	1.08664200	-0.45300200
C	-3.29108600	-2.30390200	1.26078200
H	-2.64675500	-3.04865300	0.81808600
C	-5.04243100	-0.92882200	1.70212100
H	-6.01634000	-0.46174800	1.65640100
C	-4.62930700	-2.04827500	0.92617900
H	-5.20617800	-2.53414800	0.15320800
C	-2.90819700	-1.41047700	2.32570100
H	-1.93887700	-1.38794700	2.80113700
C	-4.00824500	-0.60105900	2.63187600

H	-4.04946600	0.16222000	3.39384500
Ni	3.37647200	0.31719400	0.57834200
P	1.48019300	0.16725200	-0.57365900
C	4.04362500	-1.08698300	-0.45245600
C	2.90944300	1.41261400	2.32473700
H	1.94026900	1.39134000	2.80052200
C	4.00909400	0.60289400	2.63180600
H	4.04984300	-0.15979500	3.39439600
C	5.04351300	0.92927700	1.70187700
H	6.01722800	0.46174300	1.65673400
C	3.29297700	2.30501400	1.25921000
H	2.64917600	3.04980400	0.81580600
C	4.63105400	2.04833500	0.92495200
H	5.20833800	2.53341800	0.15180400
P	0.12837300	-1.08060800	0.67051700
P	-0.12824000	1.08039800	0.67246600
N	3.85909400	-2.43185100	-0.39219200
C	3.01427800	-3.10905700	0.53765300
C	4.56960100	-3.08740700	-1.38697400
N	-3.86051300	2.43160400	-0.39290800
C	-3.01560300	3.10920900	0.53657400
C	-4.57132500	3.08665700	-1.38779200
N	4.88870800	-0.92800900	-1.50451900
C	5.35255200	0.34119100	-1.96696100
C	5.22145900	-2.14012800	-2.08579300
N	-4.88937100	0.92708000	-1.50501800
C	-5.35264700	-0.34251100	-1.96695700
C	-5.22276900	2.13895600	-2.08644600
C	-4.44410300	-1.24193100	-2.50771900
C	-6.69583300	-0.66329800	-1.84067500
C	-4.89462700	-2.48787600	-2.91948600
C	3.16750100	-2.88696100	1.89763400
C	2.04774400	-3.98379800	0.05995600
C	-7.13953800	-1.91046100	-2.26282700
C	4.44446700	1.24078400	-2.50821100
C	6.69589200	0.66136800	-1.84079600
C	2.32752800	-3.53811300	2.78965000
C	4.89563500	2.48629100	-2.92060000
H	-4.18979900	-3.20021200	-3.33146500
C	-6.23883600	-2.82369100	-2.79722500
C	-3.16926600	2.88822100	1.89668100
C	-2.04858200	3.98315000	0.05842800
C	1.22295800	-4.64306600	0.96064700
H	5.87605400	-2.20480200	-2.93734700
H	0.45721900	-5.31564700	0.59285800
C	1.35809600	-4.41757900	2.32463300
H	4.55026100	-4.15837600	-1.48816800
H	-8.18629000	-2.17128200	-2.16011700
H	-5.87741600	2.20317600	-2.93799300
H	4.19116400	3.19876700	-3.33295000
C	6.24000700	2.82150100	-2.79845700
H	-4.55246400	4.15761700	-1.48920200
C	-2.32924700	3.53968700	2.78841900
C	7.14023700	1.90809500	-2.26356100
C	-1.22375300	4.64277300	0.95883100
H	2.43312100	-3.35634000	3.85256600

C	-1.35934200	4.41839900	2.32295800
H	8.18711500	2.16844300	-2.16093400
H	-2.43516500	3.35875300	3.85144500
H	-0.45764000	5.31475200	0.59072200
H	0.69963000	-4.91889200	3.02406900
H	1.91802100	-4.11274700	-1.00822200
H	3.92928100	-2.20017400	2.24030400
H	3.39803300	0.96530800	-2.58002300
H	7.37845900	-0.05314400	-1.39508600
H	6.58670200	3.79725800	-3.11888000
H	-7.37877000	0.05109300	-1.39534100
H	-6.58501900	-3.79979200	-3.11715500
H	-3.39782600	-0.96592600	-2.57970100
H	-0.70084200	4.91998900	3.02216300
H	-3.93140600	2.20197900	2.23963800
H	-1.91858500	4.11124300	-1.00981900

PhNCS:

electronic energy *E*/ a.u.	−722.64982621
thermal enthalpy *H*/ a.u.	−722.539229
total free Gibbs energy at 298 K *G*/ a.u.	−722.581603

Cartesian Coordinates:

C	2.05512100	-0.18514500	-0.00017900
S	3.60154000	0.14662000	0.00002500
N	0.91282700	-0.49904900	-0.00034300
C	-0.44436400	-0.22268900	-0.00013100
C	-0.89051000	1.09996800	-0.00012500
C	-1.35399500	-1.27757400	0.00004700
H	-0.16800100	1.90721900	-0.00027700
C	-2.25288600	1.35708900	0.00008000
H	-2.60172400	2.38320000	0.00009000
C	-3.16721900	0.30944800	0.00027400
H	-0.98338600	-2.29506200	0.00002600
C	-2.71401300	-1.00459300	0.00025500
H	-4.23070500	0.51676400	0.00044000
H	-3.42341600	-1.82372800	0.00040000

$2a^{Ph}$:

electronic energy *E*/ a.u.	−6868.28335893
thermal enthalpy *H*/ a.u.	−6867.472885
total free Gibbs energy at 298 K *G*/ a.u.	−6867.619246

Cartesian Coordinates:

Ni	-3.78067500	-0.50899400	0.59109300

P	-1.84788500	0.20373200	-0.25684900
C	-4.61599600	0.79515100	-0.44845300
C	-3.41071700	-2.51307100	1.12957900
H	-2.60935900	-3.08751200	0.69076300
C	-3.26566600	-1.65314300	2.27911700
H	-2.35195900	-1.52270600	2.83995100
Ni	3.22953200	-0.84436700	0.93690700
P	1.50866700	-0.39555100	-0.43309700
C	3.78242700	-2.14329800	-0.28060100
C	2.73637500	0.24185700	2.64698400
H	1.75795600	0.65555300	2.83512900
C	3.20613300	-1.01521800	3.07996800
C	4.50888500	-1.16287100	2.54616500
C	3.81018400	0.93768100	1.98945500
P	-0.22509700	-0.84325800	0.83099300
C	1.55554200	1.45185700	-0.47718700
S	0.57602000	2.48092200	0.64118600
P	-0.90398600	1.17174000	1.47950100
N	3.21220700	-3.34222600	-0.55748700
C	2.01379100	-3.82375300	0.05176600
C	3.88945100	-4.00296500	-1.57064100
N	-4.69546800	2.13820300	-0.28561600
C	-4.07830100	2.86593400	0.77863300
C	-5.38731400	2.73531200	-1.32769500
N	4.83651900	-2.07854300	-1.12932000
C	5.72756300	-0.96469100	-1.21920900
C	4.91680400	-3.20920300	-1.92710600
N	-5.28182200	0.56852400	-1.60884000
C	-5.41160000	-0.72216300	-2.20571000
C	-5.76158600	1.74568600	-2.16054100
N	2.38363500	1.97667800	-1.28605600
C	2.57716700	3.36155200	-1.38904000
C	-4.27111500	-1.37817500	-2.64921600
C	-6.66406200	-1.30869800	-2.30489000
C	-4.39316700	-2.64847200	-3.19284000
C	1.97262800	-4.02841000	1.42353900
C	0.90189300	-4.06824900	-0.74287800
C	-6.77795600	-2.57857300	-2.85757800
C	5.22960500	0.27866100	-1.58205700
C	7.07052000	-1.14711400	-0.92070000
C	0.79754700	-4.47979500	2.00656900
C	6.09984200	1.35911700	-1.63776200
H	-3.50711700	-3.16887400	-3.53657300
C	-5.64314200	-3.24969400	-3.29675700
C	-4.73637400	-2.44232500	0.69041600
C	-4.45018600	2.61244400	2.09045100
C	-3.10204400	3.80418800	0.47587800
C	-5.39187400	-1.46737300	1.50439600
H	-6.42258700	-1.15928800	1.39819000
C	-4.50806600	-1.06289800	2.54815600
H	-5.16338200	-2.94500800	-0.16476000
C	-0.26331800	-4.53966100	-0.15281300
H	5.68393200	-3.32712800	-2.67227600
H	2.63811500	-1.75524000	3.62258000
H	-1.13803700	-4.72473700	-0.76566700
C	-0.31783100	-4.74205800	1.22035800

H	3.58008100	-4.97041600	-1.92581100
H	5.14437500	-2.03130200	2.64907500
C	4.90524300	0.07993500	1.93496100
H	-7.75206300	-3.04681600	-2.93460400
H	-6.30503900	1.76186700	-3.08909300
H	5.71272800	2.33231000	-1.91613300
C	7.44763200	1.19261500	-1.33911500
H	-5.54978900	3.79827400	-1.36683300
C	-3.82662500	3.30868800	3.11593500
H	-4.73030100	-0.37211300	3.34688100
C	7.93389400	-0.06057300	-0.98465600
C	-2.49172100	4.50483200	1.50768300
C	3.66085100	3.96826400	-0.75138600
C	1.73655400	4.13563800	-2.19176800
H	0.75209400	-4.62662100	3.07899000
H	3.73877800	1.93346200	1.57987700
H	5.85800900	0.27587000	1.46560700
C	-2.85170100	4.25583600	2.82614400
H	8.98331300	-0.19325500	-0.74892700
H	-4.09914700	3.10708700	4.14502100
H	-1.71139700	5.22019900	1.27815300
H	4.31553500	3.36113000	-0.13640500
C	3.89176700	5.32865700	-0.90732000
H	4.73398500	5.78876300	-0.40188100
C	3.05309800	6.09822300	-1.70439500
H	0.89903700	3.65575500	-2.68483100
C	1.97628300	5.49332100	-2.34423900
H	3.23765500	7.15893300	-1.82932900
H	1.31694500	6.08507900	-2.97015500
H	-2.79305900	3.94896800	-0.55267800
H	-2.35939600	4.78888500	3.63082900
H	7.42700300	-2.12574500	-0.61940300
H	4.17674200	0.41694900	-1.80158500
H	-3.30590000	-0.89456300	-2.55314200
H	-5.73376300	-4.24234300	-3.72236900
H	-7.53481000	-0.78249000	-1.93090100
H	-1.23595900	-5.08746400	1.68103900
H	2.85336100	-3.82135000	2.01758900
H	0.94728200	-3.85923100	-1.80509600
H	8.12166400	2.04048100	-1.38256100
H	-5.20871800	1.86755400	2.29375600

2b^{Ph}:

electronic energy *E*/ a.u.	−6868.29212478
thermal enthalpy *H*/ a.u.	−6867.481530
total free Gibbs energy at 298 K *G*/ a.u.	−6867.625484

Cartesian Coordinates:

Ni	-3.43422700	-0.96413000	0.56412300
P	-1.69137700	-0.20843500	-0.60927500

C	-4.51440900	0.31980900	-0.26405600
C	-2.83481600	-2.93944800	0.95960300
H	-2.04872600	-3.41944700	0.39766500
C	-2.62458300	-2.12749700	2.13356500
H	-1.66235200	-1.93552200	2.58452600
Ni	3.44814700	-0.22513500	0.66506700
P	1.76185500	-0.34119500	-0.83522300
C	4.20337100	-1.75476000	-0.09835400
C	2.76079800	1.22733900	2.00075200
H	1.73317700	1.55136400	2.05621200
C	3.34059200	0.20220500	2.77299200
C	4.67616200	0.06530700	2.31888000
C	3.78250600	1.83222500	1.18500700
P	0.10399600	-0.83743000	0.53549700
C	1.40459900	1.43650900	-1.11260500
S	2.29849400	2.25830500	-2.26492700
P	-0.68408600	1.20462600	0.75301800
N	3.79133800	-3.04499300	-0.03221700
C	2.62716800	-3.49401300	0.66229100
C	4.61463500	-3.87820000	-0.77424900
N	-4.70274900	1.64088200	-0.01967500
C	-4.02124100	2.40487600	0.97636500
C	-5.61398200	2.19480200	-0.90582100
N	5.30576500	-1.80440700	-0.88536900
C	6.07773500	-0.65765000	-1.24688400
C	5.57209300	-3.09636200	-1.30750600
N	-5.33318600	0.06635200	-1.31728000
C	-5.46994200	-1.21523600	-1.93377800
C	-6.01490100	1.20198300	-1.72114400
N	0.44250500	2.02815200	-0.35830800
C	0.17547000	3.42898500	-0.50867400
C	-4.39152500	-1.76607900	-2.61203200
C	-6.67266200	-1.89611600	-1.81848800
C	-4.52360300	-3.02809500	-3.17378900
C	2.51550800	-3.28667000	2.02952200
C	1.62393900	-4.13860500	-0.04862600
C	-6.79864800	-3.15551200	-2.39109400
C	5.46654300	0.37723600	-1.93822400
C	7.40851900	-0.58278100	-0.85945500
C	1.37537500	-3.72162700	2.69008900
C	6.19917800	1.51949600	-2.22597600
H	-3.68325600	-3.46921800	-3.69631800
C	-5.72316900	-3.72324100	-3.06370400
C	-4.20748400	-2.98104200	0.68744000
C	-4.01342400	1.97549700	2.29476900
C	-3.37121100	3.57094000	0.59925500
C	-4.83794500	-2.10439200	1.61872300
H	-5.89650000	-1.88823400	1.65503100
C	-3.86942600	-1.66416500	2.57235300
H	-4.68874000	-3.48413800	-0.13799200
C	0.49790500	-4.59034500	0.62579200
H	6.40186700	-3.32593500	-1.95293300
H	2.82928600	-0.42171700	3.48990800
H	-0.29033700	-5.09232300	0.07684600
C	0.36864900	-4.37730000	1.99224100
H	4.44250400	-4.93830400	-0.83911400

H	5.39492300	-0.66252500	2.66849100
C	4.96611700	1.13148100	1.39605600
H	-7.73357300	-3.69578500	-2.30077300
H	-6.70515700	1.19098100	-2.54651000
H	5.71280900	2.33790800	-2.74304300
C	7.53210400	1.61201700	-1.84151600
H	-5.89295400	3.23274000	-0.85709100
C	-3.31772100	2.71371700	3.24137800
H	-4.05606200	-1.04380400	3.43549900
C	8.13889900	0.55845100	-1.16639300
C	-2.68952800	4.31096600	1.55455600
C	-0.66652000	3.86786400	-1.52257300
C	0.73961900	4.33361200	0.38037700
H	1.27268400	-3.54695400	3.75447500
H	3.62852900	2.63823100	0.48241300
H	5.91051300	1.29930400	0.90004600
C	-2.65533900	3.87875100	2.87385700
H	9.17684100	0.63095700	-0.86304300
H	-3.29249400	2.37461100	4.27034500
H	-2.15601800	5.20355800	1.25177900
H	-1.08154300	3.13913700	-2.20928000
C	-0.93703400	5.22293100	-1.65087700
H	-1.58255500	5.56977400	-2.45029100
C	-0.37106500	6.13609200	-0.76649200
H	1.39817100	3.96883400	1.16047300
C	0.46768700	5.68934400	0.24801500
H	-0.57562800	7.19528900	-0.87553900
H	0.91537200	6.39766800	0.93595100
H	-3.35702000	3.87443500	-0.44042600
H	-2.10341500	4.44561000	3.61430800
H	7.85488400	-1.39791800	-0.30100400
H	4.42494300	0.30852900	-2.22929400
H	-3.46064100	-1.21434200	-2.67774100
H	-5.82062400	-4.70881500	-3.50394700
H	-7.49196700	-1.44882600	-1.26739700
H	-0.52666200	-4.70498100	2.50745100
H	3.31242200	-2.77777100	2.55618000
H	1.71930000	-4.25823400	-1.12143500
H	8.09911000	2.50840800	-2.06510000
H	-4.53825100	1.06882800	2.56245500

2c^{Add1}:

electronic energy *E*/ a.u.	−6868.27270590
thermal enthalpy *H*/ a.u.	−6867.461964
total free Gibbs energy at 298 K *G*/ a.u.	−6867.607822

Cartesian Coordinates:

Ni	-3.65574100	-0.88429700	-0.84699800
P	-1.66471200	-0.20921400	-0.15391700
C	-4.20924800	-0.67710200	0.92603800

C	-3.79421700	-0.39327700	-2.90317300
H	-3.22571400	0.39710500	-3.37005700
C	-3.33813100	-1.75129400	-2.72694000
H	-2.38631800	-2.13681800	-3.06247100
Ni	3.26260300	-0.98553000	-1.09687600
P	1.27979400	-0.51747200	-0.36345100
C	3.87350400	0.75928200	-0.73861200
C	2.91292800	-2.71288000	-2.24467000
H	1.95922000	-2.95649700	-2.68953800
C	3.95800500	-2.00847800	-2.85114400
C	4.97359800	-1.84569200	-1.85754900
C	3.32877800	-3.08761200	-0.91019700
P	-0.26358600	-0.15779600	-1.87812000
C	1.16274100	0.51236800	1.18026200
S	1.23427900	-0.38351200	2.63506400
P	-0.34639100	-1.95207000	-0.53448000
N	3.52366700	1.93875300	-1.30244500
C	2.55566400	2.11916900	-2.33856900
C	4.19893000	2.99361600	-0.71643200
N	-3.92872200	-1.43368400	2.01165000
C	-3.06932500	-2.57858500	1.99410700
C	-4.48782600	-0.89861800	3.16005600
N	4.79330500	1.09701900	0.19452600
C	5.48815200	0.16529000	1.03143600
C	5.00460500	2.46336400	0.22337000
N	-4.96813300	0.33351300	1.41662100
C	-5.43838100	1.42128600	0.62027900
C	-5.14915100	0.21382000	2.78574900
N	1.13125600	1.77067300	0.92384200
C	0.93386100	2.70890400	1.94587400
C	-4.51411100	2.29815600	0.06825300
C	-6.79734100	1.56502100	0.38613900
C	-4.96361200	3.32771900	-0.74518200
C	2.74494200	1.50733300	-3.56912300
C	1.45351600	2.92619100	-2.09336000
C	-7.23969600	2.60435400	-0.42315700
C	4.82785300	-0.42516800	2.09689500
C	6.81298700	-0.13179200	0.74073300
C	1.80707900	1.70339200	-4.57379200
C	5.51273200	-1.35033500	2.87486000
H	-4.24847800	4.01271000	-1.18465700
C	-6.32374400	3.48097400	-0.99231100
C	-5.07749500	-0.28962500	-2.36006000
C	-3.47793400	-3.73308700	1.34152500
C	-1.82667700	-2.48914600	2.60207900
C	-5.39061100	-1.55988100	-1.77974800
H	-6.30785300	-1.79635800	-1.25912200
C	-4.35792700	-2.48581800	-2.10219200
H	-5.68447900	0.60189600	-2.30285300
C	0.53082000	3.12795300	-3.11096300
H	5.69237900	2.91676100	0.91539600
H	3.96420800	-1.59660700	-3.84834400
H	-0.34091500	3.74388600	-2.92448100
C	0.70489800	2.51880300	-4.34791200
H	4.03709300	4.01135400	-1.02506900
H	5.90742800	-1.31991100	-1.99555600

C	4.62273700	-2.60771000	-0.69971900
H	-8.29931900	2.72247100	-0.61647900
H	-5.71323900	0.93337400	3.35301000
H	4.99969800	-1.82354800	3.70368600
C	6.83716400	-1.66510800	2.59361600
H	-4.35886400	-1.36196800	4.12243800
C	-2.62257600	-4.82557800	1.30757800
H	-4.32417200	-3.53142300	-1.83775500
C	7.48986300	-1.05273700	1.52860000
C	-0.97877900	-3.58865100	2.56476800
C	1.91492600	3.65593700	2.23635600
C	-0.29750000	2.78110100	2.60618700
H	1.94065600	1.22105800	-5.53473700
H	2.72392800	-3.63678300	-0.20428900
H	5.20646300	-2.69457300	0.20382200
C	-1.37733100	-4.75462900	1.92354800
H	8.52283000	-1.29502300	1.30832900
H	-2.92686800	-5.73099500	0.79572200
H	0.00636000	-3.50368400	3.00671900
H	2.86750700	3.59265700	1.72282900
C	1.67531500	4.65026700	3.17754800
H	2.45132300	5.37489300	3.40189300
C	0.45108800	4.72195000	3.82917900
H	-1.05049600	2.03776800	2.36862300
C	-0.53303400	3.78142500	3.53539600
H	0.26400400	5.50031100	4.56035000
H	-1.49245400	3.82669900	4.04035700
H	-1.49224200	-1.55670800	3.04283700
H	-0.70769600	-5.60621200	1.88601800
H	7.29702800	0.34423200	-0.10475100
H	3.78639700	-0.19078600	2.30217600
H	-3.45811000	2.15572800	0.26856500
H	-6.67058900	4.28524500	-1.63069600
H	-7.49451100	0.85458300	0.81521200
H	-0.02757600	2.66723400	-5.13276400
H	3.61693700	0.88504200	-3.72641500
H	1.29992300	3.32606100	-1.09893900
H	7.36487900	-2.38761500	3.20571500
H	-4.44738700	-3.75905700	0.85913000

2c^{Add2}:

electronic energy *E*/ a.u.	−6868.27571923
thermal enthalpy *H*/ a.u.	−6867.465505
total free Gibbs energy at 298 K *G*/ a.u.	−6867.610695

Cartesian Coordinates:

Ni	3.64477900	0.54681800	-1.12046200
P	1.48815300	0.76933500	-0.75352700
C	3.83750600	0.57796700	0.74317000
C	3.88197000	-0.41904400	-2.99786700

H	3.17120400	-1.11850600	-3.41340900
C	3.81900300	1.01616800	-3.14020600
H	3.06343000	1.55477700	-3.69195700
Ni	-2.93813100	-1.66114900	-1.03363700
P	-1.20769000	-0.39768700	-0.72409900
C	-3.34462100	-1.69728500	0.80310500
C	-2.59050200	-2.50116800	-2.93851500
H	-1.60947300	-2.66585400	-3.35895000
C	-3.34844400	-3.41546400	-2.20204300
C	-4.53386500	-2.72908100	-1.78410100
C	-3.35274900	-1.27855600	-3.06422500
P	0.74610400	-1.30340100	-0.47486000
C	-1.44815200	1.14474500	0.29997400
S	-1.35003700	0.92460900	1.99667100
P	0.25728000	-0.17446500	-2.34555400
N	-2.72539600	-2.31621500	1.83567400
C	-1.50524400	-3.05328700	1.75884500
C	-3.37052200	-2.05445200	3.03176500
N	3.48955700	1.55158300	1.62203000
C	2.95504500	2.83080200	1.25300900
C	3.71355700	1.15753500	2.92866500
N	-4.40397700	-1.07799800	1.37227900
C	-5.34130100	-0.26191600	0.66240800
C	-4.43045600	-1.27882100	2.73964800
N	4.30402600	-0.42205600	1.53357500
C	4.82814900	-1.65722600	1.04024800
C	4.23316700	-0.08450700	2.87599500
N	-1.72686900	2.12904100	-0.47955200
C	-1.96354600	3.44397100	-0.06604200
C	3.95982100	-2.66361200	0.64514200
C	6.20307200	-1.81992800	0.94760000
C	4.47874900	-3.84245700	0.12757900
C	-1.41107500	-4.15112200	0.91605100
C	-0.43235000	-2.65994900	2.54886200
C	6.71593200	-3.00539900	0.43711600
C	-4.93917900	0.97845100	0.19133300
C	-6.62761900	-0.73542800	0.44524500
C	-0.22168600	-4.86559300	0.86160100
C	-5.83771800	1.75091000	-0.53104700
H	3.80156800	-4.62088700	-0.20440900
C	5.85420800	-4.01440200	0.02170700
C	5.00383200	-0.73231800	-2.22818900
C	3.73358900	3.68637500	0.48778600
C	1.66436300	3.16856800	1.63532100
C	5.60295400	0.50700700	-1.83334100
H	6.48421700	0.60262200	-1.21502200
C	4.93069900	1.57663100	-2.48701800
H	5.31782900	-1.71656600	-1.91428400
C	0.74521400	-3.39398900	2.50245400
H	-5.18458600	-0.83564100	3.36556500
H	-3.07059400	-4.42591700	-1.94538600
H	1.58999800	-3.08676400	3.10822300
C	0.85319000	-4.49411600	1.66013800
H	-3.01166200	-2.44740400	3.96634400
H	-5.31825700	-3.15096500	-1.17223400
C	-4.57820100	-1.44888900	-2.41323300

H	7.78809100	-3.13549700	0.35032100
H	4.55519800	-0.75863500	3.65031200
H	-5.51986900	2.71550100	-0.90846700
C	-7.12671600	1.28542000	-0.76556200
H	3.48563500	1.80144600	3.75997100
C	3.20137200	4.90476500	0.08759100
H	5.17119000	2.62625500	-2.41609900
C	-7.52344800	0.04646100	-0.27308400
C	1.14693000	4.39495600	1.24204900
C	-1.57522600	4.43816900	-0.97416800
C	-2.57543700	3.83689800	1.13183600
H	-0.13986300	-5.71884300	0.19864900
H	-3.01889000	-0.38992100	-3.57862100
H	-5.35936100	-0.71223100	-2.30401200
C	1.91074200	5.25751800	0.46524200
H	-8.52811300	-0.31677300	-0.45494900
H	3.79555800	5.57534100	-0.52246200
H	0.12799700	4.65281900	1.50587000
H	-1.11360200	4.11795400	-1.90083100
C	-1.75074500	5.78051300	-0.68322500
H	-1.42551900	6.53180600	-1.39512600
C	-2.34984200	6.16443800	0.51407200
H	-2.87049600	3.08632900	1.85151300
C	-2.76921200	5.18645600	1.40723400
H	-2.49546000	7.21448900	0.74223300
H	-3.24328800	5.47318600	2.34010900
H	1.04226500	2.45730000	2.16885800
H	1.48656600	6.20075800	0.14073000
H	-6.91220300	-1.71178000	0.82105300
H	-3.93001800	1.32123000	0.37287800
H	2.88986900	-2.51003800	0.71158800
H	6.25653000	-4.93281600	-0.38977100
H	6.85810800	-1.01241500	1.25344700
H	1.78027700	-5.05491200	1.62061600
H	-2.26483900	-4.43531800	0.31493800
H	-0.51289400	-1.75810600	3.14335300
H	-7.82520200	1.88936900	-1.33322700
H	4.73274400	3.38463800	0.19768600

(*E*)-2c^{Ins1}:

electronic energy *E*/ a.u.	−6868.27175336
thermal enthalpy *H*/ a.u.	−6867.461189
total free Gibbs energy at 298 K *G*/ a.u.	−6867.607389

Cartesian Coordinates:

Ni	-4.29601900	0.13388600	-0.68372200
P	-2.80699400	0.91889900	0.77604700
C	-5.05453200	-0.85530400	0.71467500
C	-4.43577700	1.62664600	-2.18545400
H	-4.19267900	2.66492100	-2.01711800

C	-3.49306500	0.60428300	-2.56935600
H	-2.44236600	0.76843700	-2.75734700
Ni	4.30255300	-1.38179200	0.60868400
P	0.03759800	1.12241100	1.52202600
C	4.38987700	-0.25181300	-0.87201400
C	4.49011400	-3.11002300	1.79102300
H	3.64094700	-3.62463900	2.21636700
C	5.08585400	-3.37970500	0.54878400
C	6.08489200	-2.38472000	0.36144700
C	5.23480100	-2.06133500	2.44658800
P	-1.03424700	1.65782200	-0.36536000
C	1.75850900	0.73388700	0.82897900
S	2.24494400	-0.89406800	1.23412800
P	-1.08267100	-0.40344200	0.37698900
N	3.68397800	-0.33596000	-2.02019900
C	2.68545700	-1.32354300	-2.28285000
C	4.00868500	0.69475700	-2.88663700
N	-4.67604800	-2.01950600	1.30032400
C	-3.50919800	-2.76800800	0.95515700
C	-5.54675100	-2.38395200	2.31548300
N	5.20038900	0.81566900	-1.05456600
C	6.09547500	1.31886600	-0.06449700
C	4.96607800	1.42009700	-2.27712300
N	-6.18304800	-0.50979700	1.38571900
C	-6.94048300	0.66913000	1.10778700
C	-6.50010100	-1.43472500	2.36646700
N	2.49803700	1.56029500	0.19342200
C	2.15089000	2.90588300	0.02089700
C	-6.36099400	1.91303000	1.31476700
C	-8.22564400	0.54764900	0.60056100
C	-7.08146000	3.05370400	0.99159000
C	3.07197800	-2.63852800	-2.49802600
C	1.35064800	-0.95141800	-2.30793800
C	-8.94344900	1.69558300	0.28844400
C	5.59174300	1.71837900	1.16578700
C	7.45437500	1.37374800	-0.33928800
C	2.10034700	-3.59860000	-2.74115900
C	6.47172700	2.17284700	2.13695500
H	-6.63185900	4.02817700	1.13945100
C	-8.36915400	2.94687600	0.47706500
C	-5.69627900	1.03561500	-2.06665500
C	-3.34811300	-3.22339400	-0.34446500
C	-2.54314100	-3.00476000	1.92332700
C	-5.52561700	-0.36590300	-2.29477800
H	-6.31422900	-1.10416500	-2.25436100
C	-4.18408400	-0.60774200	-2.70976800
H	-6.61183300	1.52323500	-1.76675800
C	0.38353000	-1.91708800	-2.55145100
H	5.48325700	2.31371100	-2.57955000
H	4.76676000	-4.11690600	-0.17158600
H	-0.66369900	-1.63940400	-2.52881600
C	0.75822600	-3.23626200	-2.77186200
H	3.53457800	0.80241800	-3.84648800
H	6.71627200	-2.28036500	-0.50963400
C	6.23868400	-1.64154200	1.58420300
H	-9.94472000	1.60979900	-0.11688300

H	-7.35797900	-1.31885600	3.00556300
H	6.08699500	2.48361800	3.10115100
C	7.83691700	2.23051900	1.87730800
H	-5.40557100	-3.28425200	2.88757000
C	-2.18644300	-3.90252100	-0.68345100
H	-3.76062300	-1.55633500	-3.00241500
C	8.32727700	1.83550600	0.63825100
C	-1.38655700	-3.68989000	1.57541600
C	2.00469300	3.42450500	-1.26780500
C	2.03529600	3.76891300	1.11397600
H	2.39078300	-4.62927000	-2.90919800
H	5.00555600	-1.64859400	3.41719400
H	6.94615700	-0.84346200	1.75221400
C	-1.20264700	-4.12952100	0.27069600
H	9.39090400	1.87671100	0.43466300
H	-2.04895800	-4.24979300	-1.70081900
H	-0.61021300	-3.84024000	2.31529400
H	2.10911500	2.75266300	-2.11171700
C	1.71461600	4.76708700	-1.45529600
H	1.58482300	5.15180900	-2.46112500
C	1.58796100	5.62057500	-0.36393600
H	2.17093700	3.37368700	2.11491900
C	1.75370200	5.11424400	0.91892800
H	1.36740100	6.67108900	-0.51381700
H	1.66281800	5.77039400	1.77766200
H	-2.67292300	-2.60424300	2.92204800
H	-0.28191200	-4.62807500	-0.00731700
H	7.82312200	1.03706300	-1.30173700
H	4.52311700	1.66089400	1.33161200
H	-5.35388700	1.97474100	1.71083200
H	-8.92558900	3.84134900	0.22213600
H	-8.64629900	-0.43686500	0.43092900
H	0.00201700	-3.98934600	-2.96230500
H	4.12367200	-2.89531800	-2.46353100
H	1.07348700	0.07366100	-2.09011800
H	8.52047100	2.58403100	2.64064300
H	-4.12153900	-3.02828500	-1.07558200

(*Z*)-2c^{Ins1}:

electronic energy *E*/ a.u.	−6868.27110289
thermal enthalpy *H*/ a.u.	−6867.460233
total free Gibbs energy at 298 K *G*/ a.u.	−6867.603407

Cartesian Coordinates:

Ni	-3.83961900	-0.12536400	0.66984900
P	-2.63099800	-0.73992200	-1.10118900
C	-4.77282800	1.14874700	-0.32810300
C	-3.12293800	-1.57978800	1.96353800
H	-2.35223300	-2.28694000	1.69576800
C	-2.89607200	-0.32035800	2.60261500

H	-1.93276800	0.10310200	2.84760500
Ni	2.50350900	0.40879300	1.04354100
P	0.06307300	-0.83018600	-2.33921000
C	3.71438800	-1.00169700	0.76981700
C	0.83340700	1.33518900	2.01887700
H	-0.09987700	1.48647200	1.49965800
C	1.19483200	0.20956000	2.75287500
C	2.58051300	0.36602100	3.09005200
C	1.95592000	2.24269000	1.99059300
P	-0.60182800	-0.95008100	-0.23182900
C	1.83775900	-0.26331400	-2.09253500
S	2.25497400	1.12293500	-1.05819200
P	-1.05604200	0.83890900	-1.36111000
N	3.51306100	-2.33501100	0.65080200
C	2.24357100	-2.99879900	0.62616300
C	4.71226600	-3.03087800	0.65497000
N	-4.51350500	2.45066500	-0.62437100
C	-3.30757300	3.15692700	-0.32569500
C	-5.55828000	3.02471900	-1.33417400
N	5.06350600	-0.88083800	0.83533100
C	5.75401000	0.36048800	0.99148700
C	5.68894600	-2.11176000	0.77115300
N	-5.99959000	0.93400700	-0.87358900
C	-6.70883800	-0.30496100	-0.80818900
C	-6.49491700	2.07213600	-1.48769600
N	2.64790300	-0.92836600	-2.82138900
C	4.01579700	-0.62619500	-2.90291200
C	-6.17801300	-1.43585800	-1.41239500
C	-7.92010500	-0.35369000	-0.13215800
C	-6.86717000	-2.63677700	-1.31792900
C	1.56337600	-3.19426800	1.82030100
C	1.74927900	-3.48751500	-0.57318600
C	-8.60806100	-1.55754400	-0.05234800
C	5.65461700	1.32409400	0.00011500
C	6.49370300	0.58062600	2.14545300
C	0.35883500	-3.88187600	1.81032500
C	6.29873500	2.53968100	0.18177800
H	-6.45194200	-3.52506200	-1.77892600
C	-8.07897700	-2.70040300	-0.63959000
C	-4.52726500	-1.80386400	1.86295000
C	-2.75853400	3.10379700	0.94673600
C	-2.68955300	3.88270500	-1.33671700
C	-5.15606900	-0.62721100	2.28436700
H	-6.21946100	-0.43776200	2.28335200
C	-4.14755500	0.28718600	2.75493100
H	-5.00788400	-2.67329900	1.44090200
C	0.54628800	-4.18307400	-0.57339100
H	6.76044500	-2.20757600	0.78348100
H	0.58839700	-0.66786600	2.91477700
H	0.13813400	-4.54261500	-1.50989700
C	-0.14782100	-4.37810400	0.61365600
H	4.74575700	-4.10228800	0.56152900
H	3.17466200	-0.34354900	3.64943400
C	3.00538000	1.68221600	2.72085600
H	-9.55181500	-1.60374600	0.47814400
H	-7.45227200	2.08610900	-1.97857800

H	6.21845300	3.30107100	-0.58488100
C	7.03946000	2.77886600	1.33368800
H	-5.53670100	4.05437200	-1.64505800
C	-1.56532200	3.76678400	1.20001300
H	-4.34690800	1.25692800	3.18726100
C	7.14250000	1.79722400	2.31289500
C	-1.50205700	4.54867000	-1.07216500
C	4.95128200	-1.56511000	-2.47383600
C	4.46793100	0.56019100	-3.48935400
H	-0.18538700	-4.02763000	2.73616400
H	1.96979400	3.19053400	1.47276200
H	3.99067500	2.09934000	2.86508000
C	-0.93246300	4.48292800	0.19266100
H	7.71566200	1.98176700	3.21395500
H	-1.12390100	3.71275900	2.18818400
H	-1.00444200	5.09069300	-1.86707900
H	4.60134100	-2.49796700	-2.04833700
C	6.31143900	-1.30546400	-2.58125300
H	7.02470100	-2.04289900	-2.22837500
C	6.75871900	-0.12006600	-3.14962500
H	3.74168400	1.28408000	-3.83776600
C	5.82726500	0.80413100	-3.61362700
H	7.82017000	0.07804000	-3.24219700
H	6.16304000	1.72882900	-4.07042000
H	-3.10937800	3.88261000	-2.33586300
H	0.00803100	4.98313400	0.39024600
H	6.53913400	-0.18600200	2.91083500
H	5.06076000	1.12721300	-0.88358700
H	-5.22756100	-1.37556400	-1.92993000
H	-8.61129900	-3.64177900	-0.56832200
H	-8.30631300	0.54123800	0.34277100
H	-1.09412000	-4.90642800	0.60503700
H	1.97949600	-2.80179500	2.74028900
H	2.27551500	-3.28372300	-1.49863200
H	7.53802400	3.73170800	1.47001200
H	-3.25969000	2.54554200	1.72343000

2c^{Ins2}:

electronic energy *E*/ a.u.	−6868.26931825
thermal enthalpy *H*/ a.u.	−6867.458543
total free Gibbs energy at 298 K *G*/ a.u.	−6867.604613

Cartesian Coordinates:

Ni	4.58429300	0.41151500	-1.01595200
P	2.88055500	-0.48946400	0.09621400
C	5.36949700	0.79508200	0.63563900
C	4.53312900	-0.55958500	-2.89429600
H	4.05769600	-1.51566600	-3.05353900
C	3.86926400	0.71965300	-2.97110500
H	2.82716800	0.86890300	-3.21242000

Ni	-4.49419500	-0.78717100	-0.54625000
P	0.01505300	-0.57331000	0.59779700
C	-4.84483600	0.51949900	0.75902000
C	-4.98459500	-2.73095900	-1.41323100
H	-4.37866800	-3.61544300	-1.28675900
C	-6.04381400	-2.33484400	-0.60862700
C	-6.46027900	-1.04294400	-1.07997300
C	-4.79193900	-1.73372900	-2.44025400
P	1.16123100	-0.69687600	-1.30152300
C	-1.69573400	0.02069200	0.03500500
S	-2.00701700	1.67845700	0.19454400
P	1.31598300	1.09532300	-0.05354200
N	-4.59859100	0.46223600	2.08661800
C	-3.97146500	-0.62501500	2.77048600
C	-4.98543500	1.62990900	2.72216200
N	5.10584400	1.76302800	1.54911700
C	4.08717700	2.75533800	1.41716800
C	5.93484000	1.65784300	2.65504600
N	-5.45395700	1.71719200	0.58557500
C	-5.88605700	2.24996300	-0.66880600
C	-5.52739300	2.41917900	1.77640500
N	6.38518600	0.09095500	1.19756400
C	6.99425500	-1.04701700	0.58638600
C	6.74505200	0.60602600	2.43194400
N	-2.58319400	-0.90250600	-0.28657900
C	-2.11349600	-2.24385600	-0.46753300
C	6.24614000	-2.20081600	0.39780200
C	8.31179000	-0.96456700	0.16116000
C	6.83221700	-3.28656800	-0.23669200
C	-4.69630100	-1.78087400	3.02619200
C	-2.66181700	-0.48516600	3.20691400
C	8.89300500	-2.05900100	-0.46661800
C	-4.95344000	2.51385500	-1.66182300
C	-7.23836800	2.49599800	-0.86568500
C	-4.09696800	-2.81418000	3.73515100
C	-5.39309800	3.02675400	-2.87489900
H	6.25349400	-4.18826000	-0.39721500
C	8.15237500	-3.21718100	-0.66960800
C	5.87894900	-0.33853400	-2.58361500
C	4.10168000	3.60763700	0.32385600
C	3.09295600	2.84133800	2.38170200
C	6.03248300	1.06542300	-2.37373500
H	6.95466700	1.55704300	-2.09675000
C	4.81344300	1.72232700	-2.71745300
H	6.63886200	-1.09070800	-2.43253900
C	-2.06778200	-1.52534000	3.90956600
H	-5.94366200	3.40986500	1.82794300
H	-6.42422000	-2.84967800	0.26026400
H	-1.03566500	-1.43357000	4.22483600
C	-2.78558700	-2.68471100	4.18038900
H	-4.83994400	1.77704300	3.77779000
H	-7.26184800	-0.45274500	-0.66053400
C	-5.76794200	-0.74540000	-2.29060600
H	9.91933900	-2.00015000	-0.80932000
H	7.52793000	0.16921000	3.02705600
H	-4.67130300	3.23417900	-3.65628400

C	-6.74477800	3.27267500	-3.08863200
H	5.87350600	2.34841400	3.47788700
C	3.09231000	4.54994600	0.18657400
H	4.63115900	2.78590200	-2.71305300
C	-7.66744700	3.00980200	-2.08283300
C	2.09295300	3.79379900	2.24116500
C	-1.60866800	-2.64053900	-1.70284300
C	-2.23761700	-3.17709800	0.55571700
H	-4.65298500	-3.72251500	3.93557100
H	-4.03548600	-1.77773000	-3.20896300
H	-5.89990000	0.13707500	-2.89666700
C	2.08939700	4.64452600	1.14296700
H	-8.72230400	3.19591400	-2.24688500
H	3.08679400	5.20821800	-0.67403500
H	1.29747800	3.84785700	2.97422800
H	-1.51958600	-1.90390700	-2.49273800
C	-1.23004200	-3.95942800	-1.91027000
H	-0.83265800	-4.25779900	-2.87388800
C	-1.35636300	-4.89277900	-0.88760900
H	-2.64415500	-2.86074300	1.50575600
C	-1.85844900	-4.49523900	0.34657000
H	-1.06381400	-5.92362600	-1.05162500
H	-1.95565900	-5.21503600	1.15192600
H	3.08052600	2.13615100	3.20463100
H	1.29304600	5.36910000	1.02385200
H	-7.94697000	2.26925800	-0.07658300
H	-3.90632200	2.30653000	-1.46564800
H	5.21510100	-2.22922100	0.73162700
H	8.60390700	-4.06739000	-1.16751100
H	8.86280700	-0.04160800	0.30098300
H	-2.31685100	-3.49622800	4.72477400
H	-5.71369400	-1.86271600	2.66333400
H	-2.11582200	0.41822700	2.96032700
H	-7.08096200	3.67099600	-4.03910900
H	4.88992700	3.51512400	-0.41150100

TS 2c^{Add1} → 2a^{Ph}:

electronic energy *E*/ a.u.	−4189.65803101
thermal enthalpy *H*/ a.u.	−4188.844993
total free Gibbs energy at 298 K *G*/ a.u.	−4188.989059

Cartesian Coordinates:

Ni	-3.64408300	-0.74265300	-0.15846800
P	-1.96837900	0.47471800	-1.04612500
C	-4.27243400	0.85754500	0.61589000
C	-4.44414200	-2.31755400	-1.53818100
H	-4.50923000	-2.18251900	-2.60850400
C	-3.26856900	-2.71592600	-0.80931500
H	-2.33473500	-3.03891000	-1.24885200
Ni	2.90111000	-0.76740000	0.66285900

P	1.57875200	0.02391500	-0.98971000
C	3.54686500	-2.12827900	-0.47995400
C	2.40571100	0.43746700	2.35814300
H	1.47859800	0.98756300	2.42696000
C	2.64879700	-0.86336800	2.84703400
C	3.96401300	-1.20502300	2.43985800
C	3.63766500	0.97804500	1.83190100
P	-0.40637800	-1.09429200	-1.36308300
C	1.56829200	1.85629500	-0.73603400
S	0.35314300	2.47846700	0.35905400
P	-0.45450500	0.03370100	0.47954400
N	3.00463100	-3.32808700	-0.81794400
C	1.75513800	-3.83607000	-0.34955300
C	3.80932300	-4.00211400	-1.72744000
N	-3.87761000	1.50785600	1.74138200
C	-2.84943700	1.07176700	2.63278300
C	-4.60613200	2.67331900	1.93436900
N	4.70056100	-2.07166500	-1.19153800
C	5.62888700	-0.98194500	-1.17403800
C	4.87660500	-3.21191400	-1.96036600
N	-5.26969700	1.63786400	0.12000300
C	-6.03729100	1.32837300	-1.04471500
C	-5.48731300	2.75242400	0.91633600
N	2.55774200	2.46147300	-1.28933900
C	2.77722600	3.83105100	-1.07509100
C	-5.40334400	1.16391800	-2.27135600
C	-7.41440400	1.17552500	-0.91854000
C	-6.16490800	0.81914400	-3.38255200
C	1.40927200	-3.70315100	0.98991700
C	0.89648200	-4.46166800	-1.24926000
C	-8.16887600	0.84101600	-2.03920200
C	5.21769500	0.29166600	-1.55082100
C	6.93674500	-1.22999300	-0.76756200
C	0.18090300	-4.18557600	1.42726900
C	6.13825300	1.33357600	-1.50898100
H	-5.67604400	0.68183200	-4.34127800
C	-7.54371100	0.65543900	-3.26941200
C	-5.43363200	-2.01833000	-0.60389200
C	-2.87597900	-0.22466300	3.13749900
C	-1.84305300	1.96231000	2.99133600
C	-4.89444100	-2.27090500	0.71388600
H	-5.43916100	-2.14712400	1.64139200
C	-3.59283400	-2.79475400	0.57408400
H	-6.41540700	-1.61578100	-0.81410800
C	-0.31646300	-4.96709300	-0.79552000
H	5.73449900	-3.34034600	-2.59940600
H	1.91866700	-1.51426400	3.30719300
H	-0.99141300	-5.44946600	-1.49475800
C	-0.67929300	-4.82686800	0.54108900
H	3.55697100	-4.98079300	-2.09992800
H	4.46048100	-2.15160400	2.61340300
C	4.59969100	-0.02293700	1.88904700
H	-9.24226700	0.71356200	-1.94571200
H	-6.22991100	3.49312100	0.67012400
H	5.81519100	2.32763400	-1.79951400
C	7.44949000	1.10231000	-1.10032800

H	-4.43142900	3.32010700	2.77805400
C	-1.86493000	-0.63724500	3.99669300
H	-2.91491400	-3.07514200	1.36776000
C	7.84985300	-0.18064600	-0.73296500
C	-0.84287000	1.54247300	3.86254200
C	3.97650500	4.24210200	-0.48141800
C	1.86196400	4.80278000	-1.49734500
H	-0.09666200	-4.06441100	2.46929300
H	3.74123900	1.96213400	1.39683200
H	5.61234700	0.03153800	1.51437600
C	-0.84862200	0.24319800	4.36104400
H	8.86992900	-0.36511500	-0.41231100
H	-1.87493900	-1.65010500	4.38647000
H	-0.04435900	2.22804300	4.12499400
H	4.68784900	3.48628300	-0.16149800
C	4.24582200	5.59397500	-0.29554600
H	5.17535300	5.89519400	0.17904500
C	3.33319700	6.55691400	-0.71803100
H	0.93410600	4.48405700	-1.95983800
C	2.14442700	6.15237600	-1.32187800
H	3.54526000	7.61233100	-0.57835700
H	1.42554600	6.89493700	-1.65584800
H	-1.81519000	2.95582400	2.55587900
H	-0.05706700	-0.08294300	5.02796400
H	7.22557800	-2.23148500	-0.46310300
H	4.19301500	0.48612000	-1.84932800
H	-4.32874200	1.29341100	-2.34333600
H	-8.13128300	0.38559500	-4.14101000
H	-7.88287200	1.29518600	0.05341000
H	-1.63610400	-5.20643200	0.88377700
H	2.09310400	-3.21145000	1.66929200
H	1.15632000	-4.52000800	-2.30099900
H	8.16182700	1.92048900	-1.07000400
H	-3.66981200	-0.89770300	2.83779200

TS 2c^{Add2} → 2b^{Ph}:

electronic energy *E*/ a.u.	− 4189.66462650
thermal enthalpy *H*/ a.u.	− 4188.844993
total free Gibbs energy at 298 K *G*/ a.u.	− 4188.989059

Cartesian Coordinates:

Ni	-3.25989000	-0.61145000	0.57323400
P	-1.67892600	0.54096700	-0.54874200
C	-4.35966700	-0.46805600	-0.93253600
C	-2.32914200	-1.44389000	2.29841600
H	-1.25751600	-1.54466400	2.39239600
C	-3.10052900	-0.31066200	2.75012900
H	-2.69004000	0.58907000	3.18675400
Ni	3.44054700	0.05284400	0.79123300
P	1.75842900	0.32262300	-0.67205300

C	3.99718000	-1.57756300	-0.00680600
C	3.43101200	0.72066200	2.87622300
H	2.74757500	0.30581000	3.60342000
C	4.69298000	0.20993300	2.50501200
C	5.27092400	1.08863600	1.49978000
C	3.14411800	1.77321200	1.96945600
P	-0.11158600	-1.04780700	-0.47833100
C	1.44473300	2.13512100	-0.90967600
S	2.34773000	3.00164800	-2.03849700
P	-0.01297300	0.65313000	0.88717400
N	3.49991900	-2.83791900	0.10751100
C	2.36921100	-3.21486100	0.89460100
C	4.20722500	-3.72827000	-0.68984700
N	-5.03495600	0.61135900	-1.39274900
C	-4.93890000	1.90685400	-0.78517700
C	-5.78156600	0.29704500	-2.51820000
N	5.02106900	-1.70235900	-0.88888400
C	5.86080000	-0.62693800	-1.32206000
C	5.16517400	-3.01336400	-1.31434300
N	-4.70011500	-1.46662300	-1.78606600
C	-4.18714400	-2.79545700	-1.67186200
C	-5.57477600	-1.01585200	-2.76513100
N	0.54261800	2.50681200	-0.00833400
C	-0.07757900	3.75209700	0.16685900
C	-2.82573500	-3.00905900	-1.85396200
C	-5.04211900	-3.83970100	-1.33728900
C	-2.30973900	-4.28776900	-1.67884300
C	2.20224100	-2.68671900	2.17009600
C	1.43780800	-4.10244300	0.36277500
C	-4.51875600	-5.11917400	-1.17270000
C	5.29575000	0.50744000	-1.89306900
C	7.23516000	-0.73214000	-1.12916300
C	1.07746600	-3.03670500	2.90799100
C	6.12364100	1.56603600	-2.24959700
H	-1.24481300	-4.45013600	-1.80848800
C	-3.15345200	-5.34253800	-1.33696700
C	-3.21470600	-2.42893500	1.80667600
C	-5.69176300	2.18468400	0.34953600
C	-4.04602500	2.83557100	-1.30799300
C	-4.50766700	-1.84429700	1.80403000
H	-5.41163700	-2.31617400	1.44057600
C	-4.44283300	-0.56444900	2.46312600
H	-2.94343100	-3.38399000	1.37760000
C	0.32532300	-4.45963600	1.11665400
H	5.92275900	-3.30266800	-2.02367800
H	5.20157300	-0.63240900	2.95671700
H	-0.41367500	-5.13496100	0.69776000
C	0.13977300	-3.92447000	2.38751600
H	3.97676600	-4.78009600	-0.71804900
H	6.24060400	0.96112100	1.03878200
C	4.32471200	2.05527300	1.18628700
H	-5.17772600	-5.93836600	-0.90442600
H	-5.94480800	-1.66409000	-3.54230600
H	5.67337700	2.45842500	-2.67115900
C	7.50036000	1.47830000	-2.05809900
H	-6.37949900	1.03353900	-3.02912700

C	-5.53527000	3.41433200	0.98092700
H	-5.27393500	0.10546600	2.63046600
C	8.05659800	0.32614300	-1.50628400
C	-3.88684200	4.05716800	-0.66400800
C	-0.14261000	4.76635200	-0.79982700
C	-0.70011800	3.96001000	1.40751400
H	0.93328900	-2.60909200	3.89474200
H	2.22989200	2.35015100	1.93255400
H	4.38888000	2.80702200	0.41197800
C	-4.62681200	4.34358500	0.47941900
H	9.12856100	0.25365500	-1.35436800
H	-6.11074100	3.63860700	1.87329300
H	-3.15460400	4.76818900	-1.02945700
H	0.33572000	4.61673000	-1.75846100
C	-0.78703100	5.96422900	-0.50534900
H	-0.81161900	6.74779200	-1.25723400
C	-1.38926600	6.17074900	0.73407000
H	-0.65820900	3.17235400	2.15393400
C	-1.34865100	5.15537600	1.68705800
H	-1.88069200	7.11353100	0.95503400
H	-1.81742400	5.29614200	2.65646200
H	-3.44686500	2.57868300	-2.17419100
H	-4.47818600	5.29098700	0.98706800
H	7.65049200	-1.62160400	-0.66514000
H	4.22313900	0.58810600	-2.03425700
H	-2.17882500	-2.17626100	-2.10686600
H	-2.74842500	-6.34056200	-1.20131900
H	-6.09887300	-3.64363500	-1.18543500
H	-0.74348400	-4.18172100	2.96282400
H	2.93740300	-1.99453400	2.56111200
H	1.55882300	-4.47464200	-0.64945100
H	8.14196700	2.30763900	-2.33801700
H	-6.37271700	1.43341800	0.73552100

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