Part 1:

Experimental Procedures: *General Considerations*: All operations were performed under a nitrogen atmosphere unless otherwise stated. Benzene, THF, and hexanes were distilled from dark purple solutions of benzophenone ketyl. Chlorobenzene was dried and distilled over CaH_2. Neutral silica and alumina were heated to 200°C under vacuum for two days and stored under nitrogen. Thiophene (99+%) was purchased from Aldrich Chemical Co. and purified as previously reported.[i] 5,5'-dimethyl-1-pyrroline N-oxide, cyclohexene sulfide, and sodium hydrosulfide hydrate was purchased from Aldrich Chemical Co. and used without further purification. A Siemens-SMART 3-Circle CCD diffractometer was used for X-ray crystal structure determination. Elemental analyses were obtained from Desert Analytics. All ^{1}H, ^{31}P and ^{13}C spectra were recorded on a Bruker AMX400 NMR spectrometer, and all ^{1}H chemical shifts are reported relative to the residual proton resonance in the deuterated solvent. UV-vis kinetics were carried out on an HP 8452 Diode Array spectophotometer using a constant temperature cell attached to a Haake recirculating bath. Temperatures inside the cell were measured directly with a thermocouple thermometer. $[(dcpe)NiH]_2$ and $[(dippe)NiH]_2$ were synthesized according to a previously published procedure.[ii] 3,4-dihydroisoquinoline N-oxide[iii] and $(dippe)Ni(SH)_2$[ii] were prepared according to literature procedures.

Preparation of (dcpe)Ni(Ph)(Cl): $[(dcpe)NiH]_2$ (680 mg, 0.70 mmol) was dissolved in 40 mL THF and 4 g of thiophene and stirred at room temperature for 2 hours to generate the labile $(dcpe)Ni(\eta^2\text{-C,S-thiophene})$.[ii] Chlorobenzene (2 g) was then added, and the solution was stirred at room temperature for 20 hours. The solvents were then concentrated to ca. 10 mL, and a yellow solid precipitated upon the addition of hexanes. The solid was collected by filtration and dried under vacuum. Yield: 786 mg (94 %). ^{1}H NMR (400 MHz, THF-d_8, 25°C): δ 7.39 (t, J =

6.7 Hz, 2H), 6.81 (dt, J = 7.3, 1.3 Hz, 2H), 6.65 (t, J = 7.0 Hz, 1H), 2.45 - 1.16 (m, 48 H). $^{31}P\{^{1}H\}$ (THF-d_8, 25°C, 162 MHz) δ 68.05 (d, J = 19.5 Hz), 66.03 (d, J = 20.0 Hz) Anal. Calcd (found) for $C_{32}H_{53}NiP_2Cl$: 64.72 (64.33) %C, 9.00 (8.82) %H.

Preparation of (dippe)Ni(Ph)(Cl): A similar procedure as above was followed using $[(dippe)NiH]_2$ as the nickel source. ^{1}H NMR (400 MHz, THF-d_8, 25°C): δ 7.40 (t, J = 7.1 Hz, 2H), 6.79 (dt, J = 7.8, 1.6 Hz, 2H), 6.64 (t, J = 7.4 Hz, 1H), 2.33 (oct, J = 7.1 Hz, 1H), 2.32 (oct, J = 7.3 Hz, 1H), 2.16 (oct, J = 7.1 Hz, 1H), 2.15 (oct, J = 7.1 Hz, 1H), 1.86 - 1.74 (m, 2H), 1.59 - 1.47 (m, 2H), 1.48 (dd, J = 14.6, 7.3 Hz, 6H), 1.29 (dd, J = 12.8, 7.1 Hz, 6H), 1.20 (dd, J = 14.1, 7.1 Hz, 6H), 1.04 (dd, J = 14.8, 7.3 Hz, 6H). $^{31}P\{^{1}H\}$ (THF-d_8, 25°C, 162 MHz) δ 76.08 (d, J = 20.1 Hz), 72.87 (d, J = 20.1 Hz). Anal. Calcd (found) for $C_{20}H_{37}NiP_2Cl$: 55.40 (55.18) %C, 8.60 (8.84) %H

Preparation of (dcpe)Ni(Ph)(SH): (dcpe)Ni(Ph)(Cl) (946 mg, 1.59 mmol) and $NaSH{\cdot}(H_2O)_x$ (946 mg, 16.89 mmol) were suspended in 100 mL THF and stirred at room temperature for 40 minutes. $MgSO_4$ was added to remove any residual water, and then the mixture was filtered. The solvents were removed under vacuum and the residue was extracted with benzene. The solvents were removed again, and the yellow solid was recrystallized from benzene/hexanes. Yield: 631 mg (67 %). ^{1}H NMR (400 MHz, THF-d_8, 25°C): δ 7.36 (t, J = 6.3 Hz, 2H), 6.80 (t, J = 6.9 Hz, 2H), 6.62 (t, J = 7.0 Hz, 1H), 2.35 - 0.70 (m, 48 H), -1.25 (dd, J = 25.3, 3.3 Hz, 1H). $^{31}P\{^{1}H\}$ (THF-d_8, 25°C, 162 MHz): 70.94 (d, J = 16.9 Hz), 65.11 (d, J = 17.7 Hz). Anal. Calcd (found) for $C_{32}H_{54}NiP_2S{\cdot}C_6H_6$: 68.16 (68.23) %C, 9.03 (8.86) %H.

Preparation of (dippe)Ni(Ph)(SH): A similar procedure as above was followed using (dippe)Ni(Ph)(Cl) as the nickel source. ^{1}H NMR (400 MHz, C_6D_6, 25°C): δ 7.38 (t, J = 6.4 Hz, 2H), 6.78 (dt, J = 7.3, 1.7 Hz, 2H), 6.60 (t, J = 7.0 Hz, 1H), 2.23 (oct, J = 7.1 Hz, 2H), 2.13 (oct,

J = 7.2 Hz, 1H), 2.12 (oct, J = 7.0 Hz, 1H), 1.84 - 1.59 (m, 4H), 1.43 (dd, J = 14.9, 7.3 Hz, 6H), 1.27 (dd, J = 13.0, 7.0 Hz, 6H), 1.15 (dd, J = 13.8, 7.0 Hz, 6H), 0.97 (dd, J = 14.6, 7.2 Hz, 6H), -1.23 (dd, J = 25.3, 3.5 Hz, 1H). $^{31}P\{^1H\}$ (THF-d_8, 25°C, 162 MHz) δ 78.06 (d, J = 17.8 Hz), 73.03 (d, J = 17.1 Hz) Anal. Calcd (found) for $C_{20}H_{38}NiP_2S$: 55.71 (55.23) %C, 8.98 (8.88) %H.

Preparation of [(dippe)Ni(μ-S)]$_2$ (2a): [(dippe)NiH]$_2$ (480 mg, 0.75 mmol) was added to a THF (60 mL) suspension of (dippe)Ni(SH)$_2$ (577 mg, 1.5 mmol) and stirred at room temperature for 24 h. The solution was then passed through a frit packed with a small amount of alumina. The solvent was removed on a vacuum line and the residue was recrystallized from THF-pentane to yield 335 mg (63 %) of brown product. ^1H NMR (400 MHz, C_6D_6, 25°C): δ 2.32 (oct, J = 5.9 Hz, 8H), 1.63 (dd, J = 14.5, 7.1 Hz, 24 H), 1.08 (dd, J = 12.2, 7.0 Hz, 24 Hz), 0.99 (d, J = 10.0 Hz, 8H). $^{13}C\{^1H\}$ NMR (C_6D_6, 25°C, 100 MHz): δ 25.85 - 25.57 (m), 22.11 (quin, J = 9.0 Hz), 20.29 (s), 18.73 (s). $^{31}P\{^1H\}$ (THF-d_8, 25°C, 162 MHz) δ 77.88 (s) Anal. Calcd (found) for $C_{28}H_{64}Ni_2P_4S_2$: 47.62 (47.36) %C, 9.13 (9.24) %H.

Alternative preparations of 2: (L_2)Ni(Ph)(SH) (75 mg) was heated in 2 mL of THF at 70 °C for 1.5 h upon which there was complete conversion to **2**. NMR spectrum of [(dcpe)Ni(μ-S)]$_2$: ^1H NMR (400 MHz, C_6D_6, 25°C): δ 2.51 - 1.18 (m, 48 H). $^{31}P\{^1H\}$ (THF-d_8, 25°C, 162 MHz) δ 69.80 (s).

Preparation of the nitrone adduct 7: 3,4-dihydroisoquinoline N-oxide (**6**) (416 mg, 2.8 mmol) and (dcpe)Ni(Ph)(SH) (81 mg, 0.1 mmol) were dissolved in 5.5 mL of THF and placed in a 36 °C oil bath for 17.5 h. The solvents were removed under vacuum leaving an oily residue. The residue was then passed through a silica gel column in the drybox using benzene:THF (95:5)

as an eluant. A golden band was collected and discarded. The column was then flushed with THF, and a bright red-orange band was collected. The solvents were removed under vacuum affording an orange solid. Isolated yield: 20 mg, 30 %. ^{1}H NMR (400 MHz, THF-d_8, 25°C): δ 7.12 (d, J = 6.5 Hz, 1H), 6.95-6.87 (m 3H), 3.28 (ddd, J = 3.9, 11.1, 12.7 Hz, 1H), 2.96 (ddd, J = 6.0, 12.7, 16.2 Hz, 1H), 2.60 (dd, J = 3.5, 16.2 Hz, 1H), 2.52 (dd, J = 5.7, 9.4 Hz, 1H) 2.39-1.17 (m, 48 H). ^{31}P{^{1}H} (THF-d_8, 25°C, 162 MHz): δ 79.77 (d, J = 30.9 Hz), 74.50 (d, J = 30.9 Hz). Anal. Calcd (found) for $C_{35}H_{57}NNiOP_2S$: 63.64 (63.41) %C, 8.70 (9.04) %H.

Monitoring the dimerization of the sulfido complex: Solutions of (dcpe)Ni(Ph)(SH) (0.012 and 0.037 M) in THF were kept at room temperature in an NMR tube, and the disappearance of the Ni-SH resonance was monitored over time relative to an internal standard (1 uL DME).

Reaction of [(dippe)NiH]$_2$ with cyclohexene sulfide: To [(dippe)NiH]$_2$ (20 mg, 0.03 mmol) was added cyclohexene sulfide (7 uL) in THF-d_8 (1 mL). Immediate inspection of the ^{31}P{^{1}H}spectrum showed a 4:1 ratio of [(dippe)Ni]$_2$(μ-S) to [(dippe)Ni(μ-S)]$_2$.

Trapping the sulfido complex with 5,5'-dimethyl-1-pyrroline N-oxide (4): 20 mg (0.034 mmol) of (dcpe)Ni(Ph)(SH) were dissolved in 1 mL THF-d_8 with 1 uL DME as an internal standard. **4** (39 mg, 10 equivalents, 0.34 M) was then added, and the disappearance of the Ni-SH resonance was monitored over time relative to the internal standard. The reaction was also performed with 30 equivalents of added **4** (1 M).

Kinetics of Conversion of 1b to 2b. A stock solution of 3.2 mg **1b** in 25.00 mL THF was prepared and stored in the refrigerator (-20 °C) in the dry box. 2.0 mL aliquots were placed into a 1 cm quartz UV cell attached to a Teflon stopcock and placed into the thermostated, stirred cell holder of the UV-vis spectrophotometer. The absorbance at 328-332 nm was recorded every 60-

120 s and data were treated as an exponential approach to equilibrium using the Solver algorithm in Microsoft Excel. Statistical errors (standard deviations) were determined using the SOLVERSTAT add-on supplied by E. Joseph Billo.[iv]

X-ray Structural Determination of [(dippe)Ni(μ-S)]$_2$ (2a). Slow evaporation of an isopropyl ether solution of **2a** containing a small amount of dibenzothiophene produced small, brown plates. A single crystal of dimensions 0.01 x 0.04 x 0.15 mm^3 was mounted on a glass fiber with oil. Data were collected at -80 °C on a Siemens SMART CCD area detector system employing a 3kW sealed tube X-ray source operating at 2.0 kW. 1.3 hemispheres of data were collected over 13 h, yielding 17708 total data after integration using SAINT (see Table 2). Laue symmetry revealed an monoclinic crystal system, and cell parameters were determined from 4165 unique reflections.[v] The space group was assigned as *Pn* on the basis of systematic absences using XPREP, and the structure solved using direct methods included in the SHELXTL 5.04 package. For a *Z* value of 2 there is one independent molecule and one dibenzothiophene molecule within the asymmetric unit. In the final model, non-hydrogen atoms other than those found in dibenzothiophene were refined anisotropically (full matrix on F^2), with hydrogens included in idealized locations. The structure refined with final residuals of $R_1 = 0.0741$ and $wR_2 = 0.1478$.[vi]

X-ray Structural Determination of 7. Slow cooling of a THF solution of **7** layered with hexanes produced small orange prisms. A single crystal of dimensions 0.20 x 0.20 x 0.30 mm^3 was mounted on a glass fiber with oil. Data were collected at -80 °C on a Siemens SMART CCD area detector system employing a 3kW sealed tube X-ray source operating at 2.0 kW. 1.3 hemispheres of data were collected over 27 h, yielding 38073 total data after integration using SAINT (see Table 2). Laue symmetry revealed an monoclinic crystal system, and cell parameters

were determined from 5841 unique reflections.[v] The space group was assigned as *Pbca* on the basis of systematic absences using XPREP, and the structure solved using direct methods included in the SHELXTL 5.04 package. For a *Z* value of 8 there is one independent molecule as well as one THF molecules disordered over two sites within the asymmetric unit. In the final model, non-hydrogen atoms other than those found in the THF molecules were refined anisotropically (full matrix on F^2), with hydrogens included in idealized locations. The structure refined with final residuals of $R_1 = 0.1328$ and $wR_2 = 0.3424$.[vi]

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[i] Spies, G. H. and Angelici, R.J. *Organometallics*, **1987**, *6*, 1897.

[ii] Vicic, D. A.; Jones, W. D. *J. Am. Chem. Soc.* **1997**, *119*, 10857.

[iii] Murahashi, S.-I.; Shiota, T. *Tetrahedron Lett.* **1987**, *28*, 2383.

[iv] Billo, E. J. "Excel for Chemists, A Comprehensive Guide," Wiley, New York (1997).

[v] It has been noted that the integration program SAINT produces cell constant errors that are unreasonably small, since systematic error is not included. More reasonable errors might be estimated at 10x the listed values.

[vi] Using the SHELXTL 5.04 package, $R_1 = (\Sigma \| F_o | - | F_c \|) / \Sigma | F_o |$, $wR_2 = [\Sigma[w(F_o^2 - F_c^2)^2] / \Sigma[w(F_o^2)^2] \}^{1/2}$, where $w = 1/[\sigma^2(F_o^2) + (a \cdot P)^2 + b \cdot P]$ and $P = [f \cdot (\text{Maximum of 0 or } F_o^2) + (1-f) \cdot F_c^2]$.

Part 2: Plots of kinetic data

Figure S-1. UV-vis changes upon conversion of (dcpe)Ni(Ph)SH to $[(dcpe)Ni(S)]_2$ in THF.

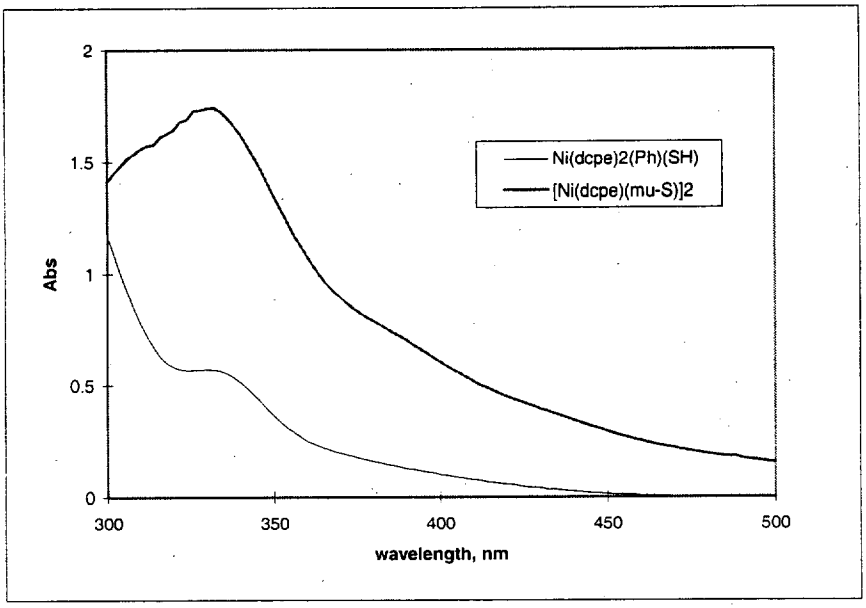


Figure S-2. Fit of 0.297 mM Ni(dcpe)(Ph)(SH) → $[Ni(dcpe)(S)]_2$ in THF at 30.4 °C. Monitored by UV-vis spectroscopy.

Solver Results
Ao= 0.728999
Ai= 1.68208
k= 1.940E-05 sec^{-1}
$t_{1/2}$= 35729.7 sec

Solver statistics:			
	Ao	Ai	k
	0.728999	1.68208	1.940E-05
σ =	0.000875	0.002921	1.189E-07
	0.999398	0.005254	

95%: ± 2.34E-07

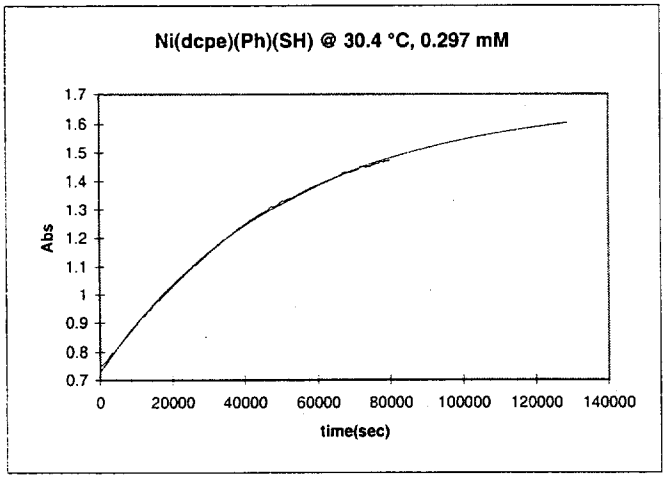


Figure S-3. Fit of 0.297 mM Ni(dcpe)(Ph)(SH) → $[Ni(dcpe)(S)]_2$ in THF at 37.9 °C. Monitored by UV-vis spectroscopy.

Solver Results
Ao= 0.6592947
Ai= 1.8039964
k= 4.663E-05 sec^{-1}
$t_{1/2}$= 14865.434 sec

Solver statistics:			
	Ao	Ai	k
	0.659295	1.803996	4.663E-05
σ =	0.000654	0.000976	1.050E-07
	0.99985	0.003527	

95%: ± 2.06E-07

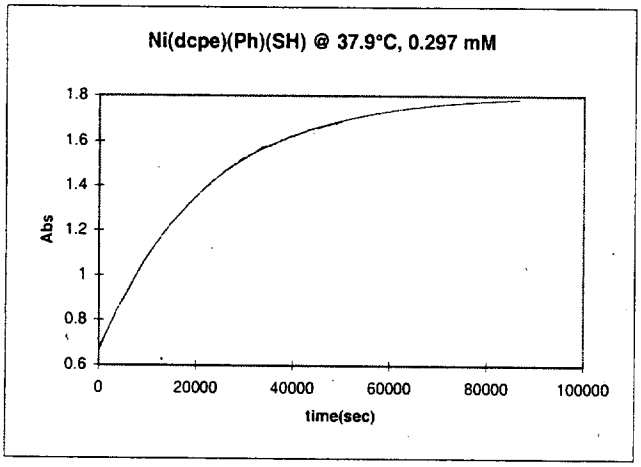


Figure S-4. Fit of 0.297 mM Ni(dcpe)(Ph)(SH) → $[Ni(dcpe)(S)]_2$ in THF at 48.0 °C. Monitored by UV-vis spectroscopy.

Solver Results
Ao= 0.6619469
Ai= 1.7406165
k= 0.0001564 sec^{-1}
$t_{1/2}$= 4431.9021 sec

Solver statistics:			
	Ao	Ai	k
	0.661947	1.740617	0.000156
σ =	0.000682	0.000404	2.36E-07
	0.999867	0.003201	

95%: ± 4.63E-07

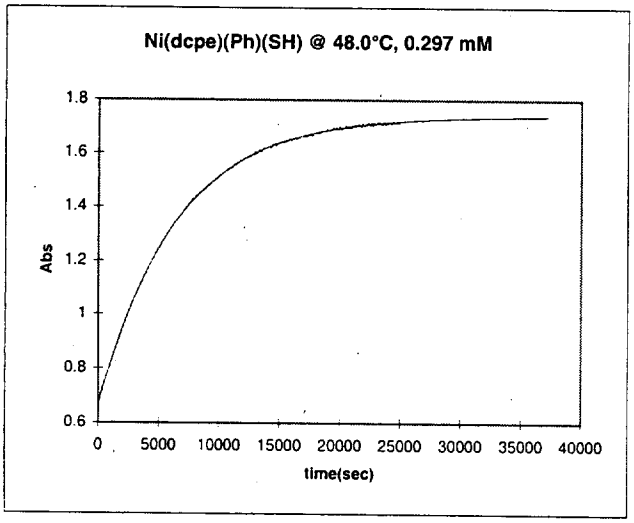


Figure S-5. Fit of 0.297 mM Ni(dcpe)(Ph)(SH) → $[Ni(dcpe)(S)]_2$ in THF at 56.1 °C. Monitored by UV-vis spectroscopy.

Solver Results
Ao= 0.6854708
Ai= 1.7150379
k= 0.0004064 sec^{-1}
$t_{1/2}$= 1705.7429 sec

Solver statistics:			
	Ao	Ai	k
	0.685471	1.715038	0.000406
σ =	0.000883	0.0005	8.15E-07
	0.999903	0.002637	

95%: ± 1.61E-06

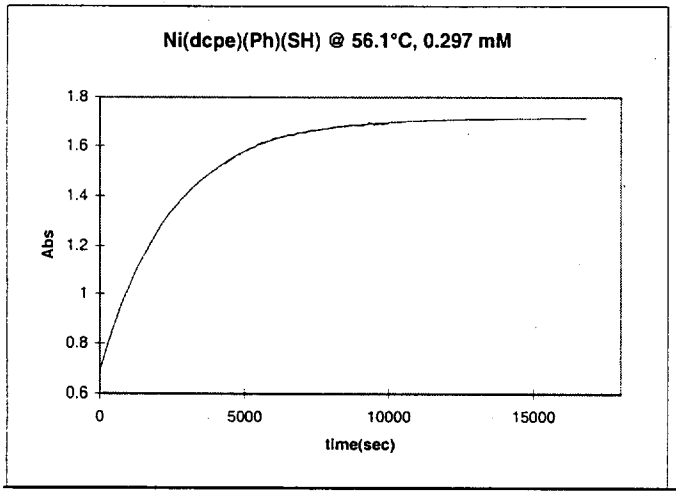


Figure S-6. Fit of 0.297 mM Ni(dcpe)(Ph)(SH) → $[Ni(dcpe)(S)]_2$ in THF at 64.8 °C. Monitored by UV-vis spectroscopy.

Solver Results
Ao= 0.6696443
Ai= 1.6987778
k= 0.001032 sec^{-1}
$t_{1/2}$= 671.65207 sec

Solver statistics:			
	Ao	Ai	k
	0.669644	1.698778	0.001032
σ =	0.002822	0.001623	6.7E-06
	0.999595	0.005537	

95%: ± 1.34E-05

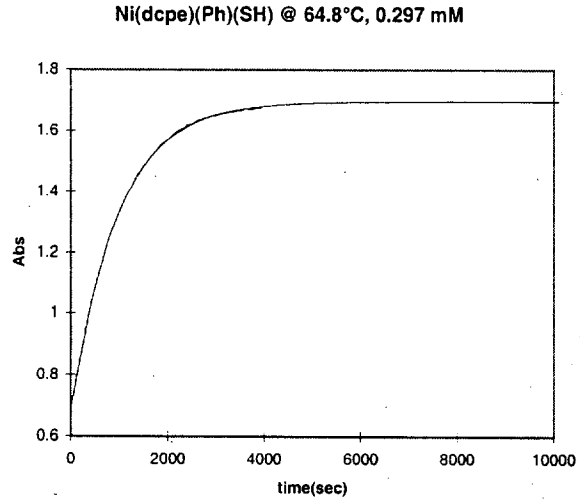


Figure S-7. Fit of 0.297 mM Ni(dcpe)(Ph)(SH) → $[Ni(dcpe)(S)]_2$ and Ni(dcpe)(Ph)(SD) → $[Ni(dcpe)(S)]_2$ in THF at 60.2 °C. Monitored by UV-vis spectroscopy.

Solver Results-NiSD
Ao= 1.0204245
Ai= 1.532703
k= 3.568E-04 sec^{-1}
$t_{1/2}$= 1942.7125 sec

Solver statistics-NiSD			
	Ao	Ai	k
	1.020425	1.532703	3.568E-04
σ =	0.000808	0.000832	1.790E-06
	0.99968	0.002399	

95%: ± 3.54E-06

Solver Results-NiSH
Ao= 0.7278359
Ai= 1.7849226
k= 5.141E-04 sec^{-1}
$t_{1/2}$= 1348.3894 sec

Solver statistics-NiSH			
	Ao	Ai	k
	0.727836	1.784923	5.141E-04
σ =	0.001543	0.001056	1.925E-06
	0.999789	0.004051	

95%: ± 3.81E-06

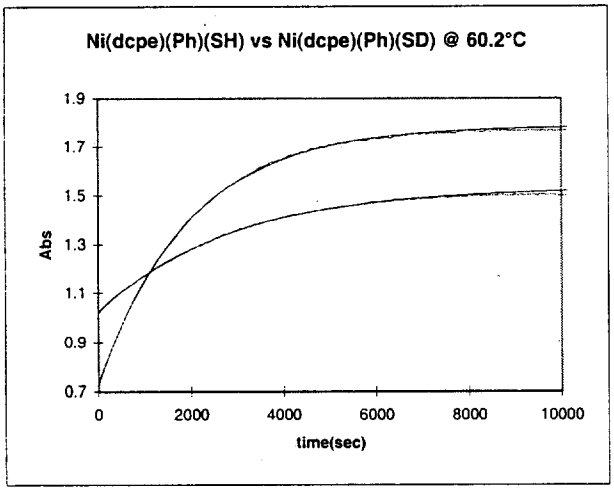


Figure S-8. Fit of 0.297 mM Ni(dcpe)(Ph)(SH) → $[Ni(dcpe)(S)]_2$ in THF at 60.2 °C with solid NaOH added. Monitored by UV-vis spectroscopy.

Solver Results-NiSH + NaOH
Ao= 0.668271
Ai= 1.758926
k= 4.943E-04 sec^{-1}
$t_{1/2}$= 1402.156 sec

Solver statistics-NiSH + NaOH		
Ao	Ai	k
0.668271	1.758926	4.943E-04
σ = 0.003265	0.001386	3.046E-06
0.998896	0.009141	

95%: ± 6.01E-06

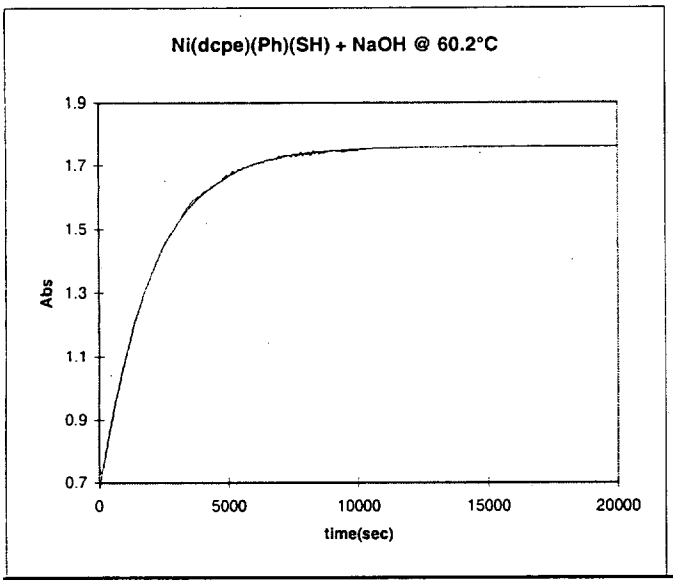


Figure S-9. Fit of 0.037 M Ni(dcpe)(Ph)(SH) → $[Ni(dcpe)(S)]_2$ in THF at 22 °C . Monitored by NMR spectroscopy.

linest stats:

k(s^{-1})= 4.960E-06 ± 7.87E-07

-4.960E-06 8.670E-01
3.327E-07 7.166E-02
0.96946518 0.133949
222.246516 7
3.98759197 0.125595

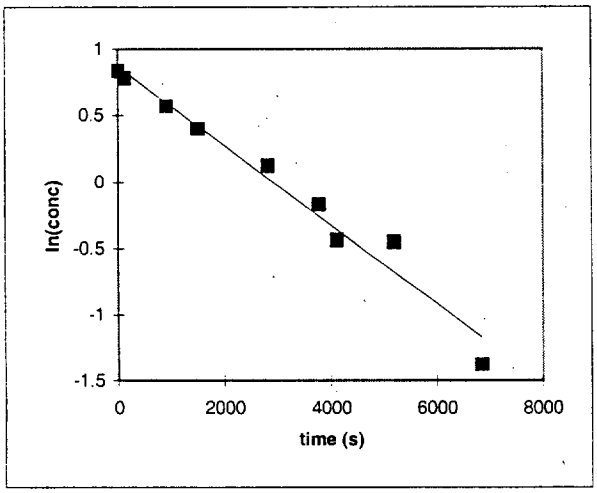


Figure S-10. Fit of 0.012 M Ni(dcpe)(Ph)(SH) → $[Ni(dcpe)(S)]_2$ in THF at 22 °C . Monitored by NMR spectroscopy.

linest stats:

$k(s^{-1})$= 4.764E-06 ± 9.77E-07

-4.764E-06	-1.109E-01
4.133E-07	8.901E-02
0.9499485	0.1663728
132.85602	7
3.6774429	0.1937594

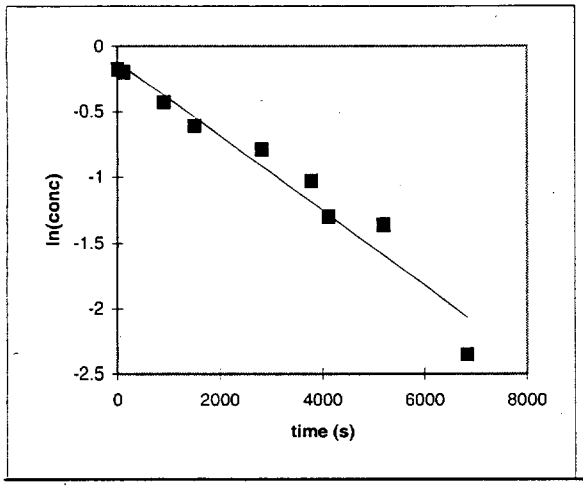


Figure S-11. Fit of 0.297 mM Ni(dcpe)(Ph)(SH) → $[Ni(dcpe)(S)]_2$ in THF at 60.2 °C with 0.34 nitrone trap added. Monitored by NMR spectroscopy.

linest stats:

$k(s^{-1})$= 5.023E-06 ± 4.45E-07

-5.023E-06	5.344E-01
2.058E-07	6.375E-02
0.9786301	0.10053
595.33113	13
6.0165408	0.131381

dimer:adduct = 1 : 0.2

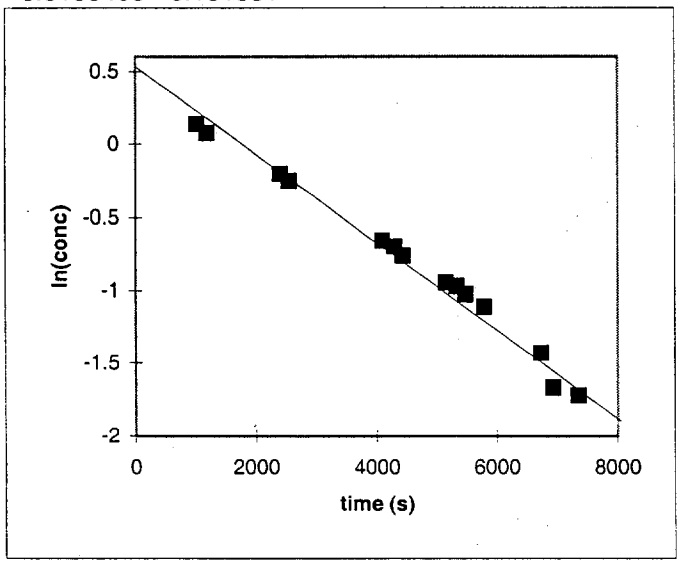


Figure S-12. Fit of 0.297 mM Ni(dcpe)(Ph)(SH) → $[Ni(dcpe)(S)]_2$ in THF at 60.2 °C with 1.0 M nitrone trap added. Monitored by NMR spectroscopy.

linest stats:

$k(s^{-1})$= 4.483E-06 ± 2.64E-07

-4.483E-06 2.155E-01
1.223E-07 3.746E-02
0.9904112 0.058639
1342.7451 13
4.6171258 0.044701

dimer:adduct = 1 : 1.14

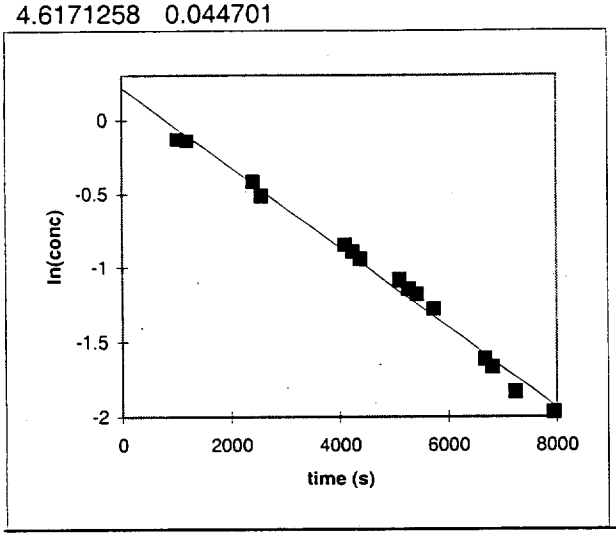


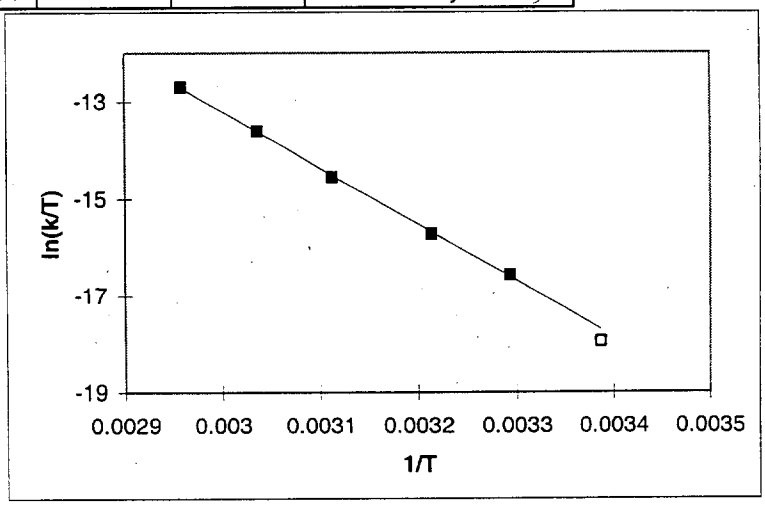
Figure S-13. Eyring plot of Ni(dcpe)(Ph)(SH) → $[Ni(dcpe)(S)]_2$ in THF.

Eyring Plot for Ni(dcpe)(Ph)(SH) ---> $[Ni(dcpe)(\mu\text{-}S)]_2$

T(°C)	$k(s^{-1})$	1/T	ln(k/T)	calc	$t_{1/2}$, hrs	measurement
22.0	4.83E-06	0.003386	-17.928	-17.6889	39.84	measured by nmr
30.4	1.940E-05	0.003293	-16.5663	-16.6016	9.92	measured by uv
37.9	4.66E-05	0.003213	-15.7137	-15.6803	4.13	measured by uv
48.0	0.000156	0.003112	-14.5355	-14.5076	1.23	measured by uv
56.1	0.000406	0.003036	-13.6055	-13.6191	0.47	measured by uv
64.8	0.001032	0.002958	-12.6996	-12.7122	0.19	measured by uv

95% confidence limits:

$\Delta H^{\ddagger}$= 23.07 ± 0.8 kcal/mol
$\Delta S^{\ddagger}$ = -4.2 ± 2.5 e.u.



Part 3:

Table S-1. Crystallographic Data for **2a** and **7**.

Crystal Parameters	**2a**	**7**
chemical formula	$C_{28}H_{64}Ni_2P_4S_2$·dibenzothiophene	$C_{35}H_{57}NNiOP_2S$·THF
formula weight	890.46	724.57
cryst syst	Monoclinic	Orthorhombic
space group	*Pn*	*Pbca*
Z	2	8
a, Å	11.2158(6)	15.8924(3)
b, Å	11.3846(7)	22.0377(5)
c, Å	18.1262(10)	29.3057(5)
β, deg	95.391(2)	90
vol., Å^3	2304.2(2)	10263.8(3)
ρ_{calc}, g cm^{-3}	1.283	0.938
cryst dimens, mm^3	0.01 x 0.04 x 0.15	0.30 x 0.20 x 0.20
temp, °C	-80	-80
Measurement of Intensity Data		
diffractometer	Siemens SMART	Siemens SMART
radiation	Mo, 0.71073 Å	Mo, 0.71073 Å
frame range/time, deg/sec	0.3/30	0.3/60
2θ range, deg	4.10-50	3.46-46.58
data collected	$-10 \le h \le 12$,	$-17 \le h \le 17$,
	$-12 \le k \le 11$,	$-24 \le k \le 23$,
	$-20 \le l \le 20$	$-32 \le l \le 21$
no. of data collected	9384	38073
no. of unique data	5464	7343
no. of obs data ($F_o>4\sigma(F_o)$)	4165	5841
agreement between equivalent data (R_{int})	0.0667	0.0809
no. of params varied	458	410
μ, mm^{-1}	1.118	0.512
abs cor	empirical (SADABS)	empirical (SADABS)
range of trans. factors	0.928 - 0.812	0.928 - 0.672
$R_1(F_o)$, $wR_2(F_o^2)$, ($F_o>4\sigma(F_o)$)	0.0741, 0.1478	0.1328, 0.3424
$R_1(F_o)$, $wR_2(F_o^2)$, (all data)	0.0994, 0.1626	0.1643, 0.3623
goodness of fit	1.053	1.256

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for 2a. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Ni(1)	2034(1)	2116(1)	4484(1)	26(1)
Ni(2)	218(1)	3968(1)	4544(1)	32(1)
P(1)	2574(3)	1160(3)	3552(2)	34(1)
P(2)	2617(3)	679(3)	5198(2)	30(1)
P(4)	-1111(3)	4240(3)	5310(2)	41(1)
P(3)	-871(4)	4913(3)	3708(2)	50(1)
S(2)	1428(3)	3138(3)	5413(2)	32(1)
S(1)	1532(3)	3591(3)	3747(2)	36(1)
S(3)	-437(5)	3467(5)	8316(3)	88(2)
C(1)	3607(11)	1918(13)	2958(7)	47(4)
C(2)	4054(16)	1129(14)	2360(9)	86(6)
C(3)	4651(14)	2485(15)	3437(10)	80(6)
C(4)	1397(12)	575(12)	2877(7)	49(4)
C(5)	910(12)	1486(13)	2282(7)	59(4)
C(6)	349(13)	127(13)	3279(8)	61(4)
C(7)	3973(11)	924(12)	5820(7)	40(3)
C(8)	3798(12)	1769(14)	6435(8)	60(5)
C(9)	4993(12)	1297(17)	5422(9)	77(5)
C(10)	1564(11)	31(11)	5811(7)	37(3)
C(11)	368(11)	-198(11)	5375(7)	39(3)
C(12)	2057(14)	-1052(13)	6215(8)	71(5)
C(13)	3004(11)	-584(11)	4634(7)	38(3)
C(14)	3416(12)	-166(10)	3882(7)	36(3)
C(15)	-285(20)	6370(14)	3435(10)	85(6)
C(16)	646(18)	6261(16)	2907(12)	100(7)
C(17)	303(31)	6977(17)	4140(12)	211(18)
C(18)	-1364(14)	4225(14)	2809(7)	57(4)
C(19)	-2243(15)	4972(18)	2325(8)	90(6)
C(20)	-1868(12)	3002(15)	2926(9)	73(6)
C(21)	-672(12)	4956(13)	6202(8)	57(4)
C(22)	108(15)	6051(12)	6105(10)	82(6)
C(23)	-1704(18)	5253(17)	6661(9)	101(7)
C(24)	-1980(11)	2931(13)	5560(7)	49(4)
C(25)	-1302(13)	2237(15)	6222(8)	63(4)
C(26)	-2227(12)	2148(13)	4872(8)	57(4)
C(27)	-2306(12)	5185(14)	4874(9)	65(5)
C(28)	-2377(16)	5250(18)	4066(9)	91(7)
C(29)	593(10)	2382(11)	8409(10)	48(4)
C(30)	1115(14)	1742(14)	7874(9)	61(4)
C(31)	1930(16)	894(16)	8083(12)	79(5)
C(32)	2237(16)	724(18)	8829(13)	82(6)
C(33)	1707(17)	1284(18)	9329(12)	84(6)
C(34)	906(15)	2131(14)	9148(9)	52(4)
C(35)	268(15)	2893(14)	9635(9)	54(4)
C(36)	387(12)	2883(13)	10374(10)	58(4)
C(37)	-229(18)	3648(18)	10800(10)	82(6)
C(38)	-1027(16)	4395(16)	10422(14)	90(7)
C(39)	-1125(15)	4424(16)	9642(14)	85(7)
C(40)	-502(16)	3654(17)	9289(8)	62(5)

Table S3. Bond lengths [A] and angles [deg] for 2a.

Ni(1)-P(1)	2.145(3)
Ni(1)-P(2)	2.149(3)
Ni(1)-S(1)	2.187(3)
Ni(1)-S(2)	2.206(3)
Ni(1)-Ni(2)	2.941(2)
Ni(2)-P(3)	2.144(4)
Ni(2)-P(4)	2.152(4)
Ni(2)-S(2)	2.194(3)
Ni(2)-S(1)	2.201(4)
P(1)-C(4)	1.839(13)
P(1)-C(14)	1.849(11)
P(1)-C(1)	1.866(12)
P(2)-C(7)	1.828(12)
P(2)-C(13)	1.839(12)
P(2)-C(10)	1.850(11)
P(4)-C(27)	1.838(13)
P(4)-C(21)	1.837(14)
P(4)-C(24)	1.860(14)
P(3)-C(18)	1.846(13)
P(3)-C(15)	1.87(2)
P(3)-C(28)	1.91(2)
S(3)-C(29)	1.689(14)
S(3)-C(40)	1.78(2)
C(1)-C(2)	1.53(2)
C(1)-C(3)	1.53(2)
C(4)-C(6)	1.53(2)
C(4)-C(5)	1.56(2)
C(7)-C(9)	1.47(2)
C(7)-C(8)	1.50(2)
C(10)-C(12)	1.51(2)
C(10)-C(11)	1.51(2)
C(13)-C(14)	1.55(2)
C(15)-C(16)	1.49(3)
C(15)-C(17)	1.54(2)
C(18)-C(19)	1.52(2)
C(18)-C(20)	1.52(2)
C(21)-C(23)	1.53(2)
C(21)-C(22)	1.54(2)
C(24)-C(26)	1.54(2)
C(24)-C(25)	1.57(2)
C(27)-C(28)	1.46(2)
C(29)-C(34)	1.38(2)
C(29)-C(30)	1.39(2)
C(30)-C(31)	1.36(2)
C(31)-C(32)	1.38(2)
C(32)-C(33)	1.30(2)
C(33)-C(34)	1.34(2)
C(34)-C(35)	1.47(2)
C(35)-C(40)	1.34(2)
C(35)-C(36)	1.33(2)
C(36)-C(37)	1.39(2)
C(37)-C(38)	1.37(2)
C(38)-C(39)	1.41(3)
C(39)-C(40)	1.32(2)

P(1)-Ni(1)-P(2)	89.73(13)
P(1)-Ni(1)-S(1)	89.07(13)
P(2)-Ni(1)-S(1)	177.2(2)
P(1)-Ni(1)-S(2)	177.73(14)
P(2)-Ni(1)-S(2)	92.33(13)
S(1)-Ni(1)-S(2)	88.90(13)
P(1)-Ni(1)-Ni(2)	129.85(11)
P(2)-Ni(1)-Ni(2)	134.13(11)
S(1)-Ni(1)-Ni(2)	48.11(10)
S(2)-Ni(1)-Ni(2)	47.88(9)
P(3)-Ni(2)-P(4)	90.0(2)
P(3)-Ni(2)-S(2)	175.0(2)
P(4)-Ni(2)-S(2)	91.05(13)
P(3)-Ni(2)-S(1)	90.33(14)
P(4)-Ni(2)-S(1)	176.8(2)
S(2)-Ni(2)-S(1)	88.87(13)
P(3)-Ni(2)-Ni(1)	133.16(12)
P(4)-Ni(2)-Ni(1)	130.64(12)
S(2)-Ni(2)-Ni(1)	48.24(9)
S(1)-Ni(2)-Ni(1)	47.71(9)
C(4)-P(1)-C(14)	103.5(6)
C(4)-P(1)-C(1)	103.2(6)
C(14)-P(1)-C(1)	103.8(6)
C(4)-P(1)-Ni(1)	118.0(4)
C(14)-P(1)-Ni(1)	109.4(4)
C(1)-P(1)-Ni(1)	117.2(5)
C(7)-P(2)-C(13)	103.7(6)
C(7)-P(2)-C(10)	103.4(6)
C(13)-P(2)-C(10)	102.7(6)
C(7)-P(2)-Ni(1)	116.3(4)
C(13)-P(2)-Ni(1)	109.6(4)
C(10)-P(2)-Ni(1)	119.3(4)
C(27)-P(4)-C(21)	104.1(7)
C(27)-P(4)-C(24)	101.3(7)
C(21)-P(4)-C(24)	104.1(7)
C(27)-P(4)-Ni(2)	109.2(5)
C(21)-P(4)-Ni(2)	119.1(5)
C(24)-P(4)-Ni(2)	116.9(4)
C(18)-P(3)-C(15)	103.1(8)
C(18)-P(3)-C(28)	100.6(8)
C(15)-P(3)-C(28)	104.8(10)
C(18)-P(3)-Ni(2)	121.0(5)
C(15)-P(3)-Ni(2)	116.2(6)
C(28)-P(3)-Ni(2)	109.0(5)
Ni(2)-S(2)-Ni(1)	83.89(11)
Ni(1)-S(1)-Ni(2)	84.17(12)
C(29)-S(3)-C(40)	94.6(9)
C(2)-C(1)-C(3)	111.4(12)
C(2)-C(1)-P(1)	113.6(10)
C(3)-C(1)-P(1)	110.5(9)
C(6)-C(4)-C(5)	108.5(11)
C(6)-C(4)-P(1)	109.9(9)
C(5)-C(4)-P(1)	113.8(9)
C(9)-C(7)-C(8)	110.0(12)
C(9)-C(7)-P(2)	112.4(10)
C(8)-C(7)-P(2)	113.4(9)
C(12)-C(10)-C(11)	112.2(11)
C(12)-C(10)-P(2)	113.0(9)
C(11)-C(10)-P(2)	109.8(8)
C(14)-C(13)-P(2)	110.7(8)

C(13)-C(14)-P(1)	110.4(8)
C(16)-C(15)-C(17)	107(2)
C(16)-C(15)-P(3)	112.4(12)
C(17)-C(15)-P(3)	108.2(13)
C(19)-C(18)-C(20)	111.3(13)
C(19)-C(18)-P(3)	113.4(11)
C(20)-C(18)-P(3)	110.4(10)
C(23)-C(21)-C(22)	110.5(13)
C(23)-C(21)-P(4)	115.1(11)
C(22)-C(21)-P(4)	111.5(11)
C(26)-C(24)-C(25)	111.4(12)
C(26)-C(24)-P(4)	109.0(9)
C(25)-C(24)-P(4)	111.2(9)
C(28)-C(27)-P(4)	115.4(10)
C(27)-C(28)-P(3)	111.4(11)
C(34)-C(29)-C(30)	118.9(14)
C(34)-C(29)-S(3)	110.9(13)
C(30)-C(29)-S(3)	130.2(14)
C(31)-C(30)-C(29)	120(2)
C(30)-C(31)-C(32)	118(2)
C(33)-C(32)-C(31)	122(2)
C(32)-C(33)-C(34)	122(2)
C(33)-C(34)-C(29)	119(2)
C(33)-C(34)-C(35)	129(2)
C(29)-C(34)-C(35)	111(2)
C(40)-C(35)-C(36)	118(2)
C(40)-C(35)-C(34)	116(2)
C(36)-C(35)-C(34)	126(2)
C(35)-C(36)-C(37)	123(2)
C(38)-C(37)-C(36)	116(2)
C(37)-C(38)-C(39)	120(2)
C(40)-C(39)-C(38)	118(2)
C(39)-C(40)-C(35)	123(2)
C(39)-C(40)-S(3)	129(2)
C(35)-C(40)-S(3)	108(2)

Table S4. Anisotropic displacement parameters (A^2 x 10^3) for 2a. The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Ni(1)	23(1)	24(1)	31(1)	2(1)	3(1)	3(1)
Ni(2)	33(1)	25(1)	35(1)	-6(1)	-7(1)	6(1)
P(1)	35(2)	34(2)	34(2)	4(2)	9(2)	12(2)
P(2)	26(2)	33(2)	31(2)	3(2)	4(1)	5(2)
P(4)	39(2)	43(2)	40(2)	-9(2)	-1(2)	13(2)
P(3)	61(3)	48(2)	39(2)	-12(2)	-11(2)	29(2)
S(2)	35(2)	34(2)	27(2)	-3(2)	-2(1)	7(2)
S(1)	45(2)	27(2)	36(2)	7(2)	3(2)	6(2)
S(3)	88(4)	98(4)	76(3)	16(3)	-12(3)	-5(3)
C(1)	37(8)	73(11)	34(8)	1`(7)	22(6)	9(8)
C(2)	113(15)	75(12)	82(13)	28(11)	69(11)	27(11)

C(3)	60(11)	82(13)	103(14)	48(11)	32(10)	11(10)
C(4)	56(10)	48(9)	44(8)	-13(7)	12(7)	4(7)
C(5)	49(10)	80(12)	44(9)	-2(8)	-17(7)	3(8)
C(6)	63(11)	63(11)	53(10)	15(8)	-19(8)	-5(8)
C(7)	30(8)	45(9)	43(8)	15(7)	0(6)	-1`(6)
C(8)	37(9)	85(13)	51(10)	-17(9)	-26(7)	-1(8)
C(9)	29(9)	127(16)	78(12)	-28(11)	17(8)	-15(9)
C(10)	34(8)	35(8)	45(8)	0(6)	23(6)	-9(6)
C(11)	44(8)	32(8)	44(8)	2(6)	21(7)	-8(6)
C(12)	91(12)	58(11)	69(11)	54(9)	28(9)	5(9)
C(13)	29(7)	38(8)	46(8)	6(6)	2(6)	16(6)
C(14)	54(9)	28(7)	29(7)	5(6)	13(6)	1`(6)
C(15)	132(17)	31(10)	85(14)	0(9)	-24(13)	14(10)
C(16)	110(17)	57(13)	126(19)	45(13)	-24(15)	-17(11)
C(17)	431(51)	46(13)	126(21)	2(13)	-122(28)	-61(21)
C(18)	51(10)	80(12)	37(8)	-8(8)	-13(7)	7(9)
C(19)	87(13)	153(18)	29(8)	-2(10)	-4(9)	25(13)
C(20)	34(9)	111(16)	71(12)	-42(11)	-2(8)	-17(9)
C(21)	54(10)	50(10)	66(10)	-21(8)	1(8)	32(8)
C(22)	87(13)	27(9)	129(17)	-30(10)	-6(12)	0(9)
C(23)	140(17)	106(15)	57(11)	-49(11)	5(11)	50(13)
C(24)	32(8)	69(10)	47(8)	-21(8)	14(6)	-18(7)
C(25)	56(10)	74(12)	61(10)	-3(9)	16(8)	4(9)
C(26)	50(9)	56(10)	65(10)	3(8)	13(7)	-6(8)
C(27)	33(9)	66(11)	97(13)	8(10)	14(8)	31(8)
C(28)	102(15)	120(16)	50(11)	-15(10)	4(10)	78(13)
C(29)	13(7)	37(9)	94(13)	4(8)	2(7)	-12(6)
C(30)	54(10)	63(12)	67(11)	-17(9)	4(9)	-21(9)
C(31)	73(13)	79(14)	90(15)	0(12)	37(11)	-5(11)
C(32)	60(13)	101(16)	91(16)	-16(13)	37(12)	-12(11)
C(33)	57(13)	83(15)	110(18)	28(13)	2(12)	-32(11)
C(34)	52(10)	42(10)	66(11)	-11(9)	26(9)	-32(8)
C(35)	53(10)	66(11)	43(10)	4(9)	1(8)	-44(9)
C(36)	29(8)	49(10)	96(14)	5(10)	6(9)	-1`(7)
C(37)	92(14)	101(16)	58(11)	13(11)	27(11)	-18(12)
C(38)	62(13)	75(14)	141(20)	0(14)	55(13)	32(10)
C(39)	53(11)	56(12)	144(21)	59(13)	-4(12)	12(9)
C(40)	56(11)	84(14)	45(10)	22(10)	-2(8)	-20(10)

Table S5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for 2a.

	x	y	z	U(eq)
H(1A)	3142(11)	2570(13)	2697(7)	56
H(2A)	4490(88)	1604(21)	2023(38)	129
H(2B)	3370(17)	750(77)	2079(40)	129
H(2C)	4589(80)	527(62)	2593(10)	129
H(3A)	5213(53)	2833(86)	3117(10)	120
H(3B)	5065(62)	1885(24)	3754(46)	120
H(3C)	4343(18)	3098(69)	3748(46)	120
H(4A)	1737(12)	-103(12)	2616(7)	59
H(5A)	337(61)	1101(22)	1918(28)	89
H(5B)	1577(16)	1803(59)	2031(35)	89

H(5C)	510(70)	2127(41)	2522(10)	89
H(6A)	-291(36)	-148(76)	2914(8)	92
H(6B)	46(54)	764(25)	3573(40)	92
H(6C)	620(23)	-524(53)	3607(39)	92
H(7A)	4196(11)	151(12)	6057(7)	47
H(8A)	4546(25)	1842(61)	6757(29)	89
H(8B)	3164(56)	1478(41)	6724(30)	89
H(8C)	3569(79)	2539(24)	6225(8)	89
H(9A)	5705(27)	1388(96)	5775(13)	116
H(9B)	4806(40)	2049(49)	5174(51)	116
H(9C)	5149(63)	703(47)	5051(43)	116
H(10A)	1426(11)	633(11)	6196(7)	44
H(11A)	-230(19)	-391(64)	5717(7)	59
H(11B)	446(20)	-857(43)	5035(30)	59
H(11C)	114(33)	505(24)	5090(32)	59
H(12A)	1472(41)	-1345(54)	6540(43)	107
H(12B)	2804(50)	-853(24)	6513(44)	107
H(12C)	2214(86)	-1660(34)	5854(9)	107
H(13A)	3654(11)	-1041(11)	4907(7)	45
H(13B)	2298(11)	-1104(11)	4542(7)	45
H(14A)	3281(12)	-801(10)	3510(7)	43
H(14B)	4283(12)	12(10)	3943(7)	43
H(15A)	-961(20)	6864(14)	3210(10)	102
H(16A)	1001(86)	7033(26)	2832(58)	150
H(16B)	280(29)	5960(112)	2432(26)	150
H(16C)	1271(63)	5717(93)	3109(36)	150
H(17A)	248(245)	7831(17)	4079(67)	316
H(17B)	1147(71)	6745(212)	4220(94)	316
H(17C)	-113(171)	6740(203)	4568(29)	316
H(18A)	-636(14)	4124(14)	2536(7)	69
H(19A)	-2224(83)	4740(76)	1805(11)	135
H(19B)	-2020(64)	5801(21)	2382(52)	135
H(19C)	-3052(21)	4856(83)	2474(45)	135
H(20A)	-1886(84)	2555(34)	2463(18)	109
H(20B)	-2682(37)	3070(16)	3076(54)	109
H(20C)	-1359(53)	2595(36)	3314(40)	109
H(21A)	-153(12)	4382(13)	6502(8)	68
H(22A)	308(83)	6423(57)	6588(14)	123
H(22B)	-336(42)	6608(45)	5771(51)	123
H(22C)	846(49)	5817(18)	5895(58)	123
H(23A)	-1399(26)	5335(120)	7183(14)	152
H(23B)	-2301(61)	4622(58)	6610(61)	152
H(23C)	-2076(79)	5992(63)	6484(50)	152
H(24A)	-2765(11)	3205(13)	5717(7)	58
H(25A)	-1776(42)	1550(47)	6339(35)	95
H(25B)	-1187(76)	2749(29)	6657(17)	95
H(25C)	-521(38)	1980(74)	6082(21)	95
H(26A)	-2589(75)	1408(34)	5014(12)	85
H(26B)	-1473(16)	1984(66)	4659(30)	85
H(26C)	-2777(64)	2553(35)	4504(21)	85
H(27A)	-3083(12)	4896(14)	5019(9)	77
H(27B)	-2187(12)	5990(14)	5075(9)	77
H(28A)	-2639(16)	6047(18)	3903(9)	109
H(28B)	-2982(16)	4682(18)	3851(9)	109
H(30A)	904(14)	1896(14)	7363(9)	74
H(31A)	2280(16)	431(16)	7724(12)	95
H(32A)	2853(16)	180(18)	8982(13)	99
H(33A)	1893(17)	1088(18)	9836(12)	101
H(36A)	917(12)	2329(13)	10620(10)	69
H(37A)	-104(18)	3653(18)	11326(10)	99
H(38A)	-1515(16)	4895(16)	10686(14)	108
H(39A)	-1627(15)	4983(16)	9375(14)	102

Table S-6. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for 7. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Ni(1)	937(1)	2328(1)	5473(1)	34(1)
S(1)	421(2)	1548(1)	5817(1)	43(1)
P(1)	2202(2)	1987(1)	5500(1)	36(1)
P(2)	1394(2)	3127(1)	5126(1)	36(1)
N(1)	-799(5)	2406(4)	5652(3)	41(2)
O(1)	-151(4)	2639(3)	5366(2)	39(2)
C(1)	-695(6)	1751(4)	5679(4)	38(2)
C(2)	-753(7)	2704(5)	6101(4)	46(3)
C(3)	-1532(7)	2512(5)	6368(4)	51(3)
C(4)	-1651(6)	1831(5)	6358(3)	45(3)
C(5)	-1276(6)	1471(5)	6027(3)	41(2)
C(6)	-1406(6)	858(5)	6023(4)	48(3)
C(7)	-1913(7)	588(6)	6357(4)	63(3)
C(8)	-2286(7)	934(6)	6685(4)	58(3)
C(9)	-2172(7)	1550(6)	6687(4)	60(3)
C(10)	2939(5)	2582(4)	5294(3)	37(2)
C(11)	2504(6)	3010(4)	4967(3)	40(2)
C(12)	2387(6)	1322(4)	5135(3)	38(2)
C(13)	3295(6)	1085(5)	5126(4)	46(3)
C(14)	3330(7)	502(4)	4840(4)	52(3)
C(15)	3058(7)	625(5)	4355(4)	54(3)
C(16)	2193(7)	878(5)	4339(4)	58(3)
C(17)	2106(7)	1449(5)	4645(4)	51(3)
C(18)	2666(6)	1760(4)	6049(3)	39(2)
C(19)	2389(7)	1138(5)	6223(4)	54(3)
C(20)	2870(8)	970(6)	6659(4)	66(3)
C(21)	2753(9)	1451(7)	7018(4)	78(4)
C(22)	3003(9)	2064(7)	6855(4)	74(4)
C(23)	2545(7)	2236(5)	6417(4)	54(3)
C(24)	1361(6)	3835(4)	5461(4)	43(2)
C(25)	1747(8)	3739(5)	5932(4)	62(3)
C(26)	1682(9)	4305(6)	6228(5)	79(4)
C(27)	784(9)	4530(6)	6270(5)	78(4)
C(28)	445(8)	4652(5)	5802(5)	70(4)
C(29)	466(7)	4084(5)	5497(4)	54(3)
C(30)	822(6)	3287(4)	4603(3)	36(2)
C(31)	1148(7)	3811(5)	4319(4)	47(3)
C(32)	591(8)	3923(5)	3903(4)	61(3)
C(33)	503(8)	3372(5)	3604(4)	61(3)
C(34)	200(7)	2831(5)	3891(4)	51(3)
C(35)	746(6)	2718(4)	4303(4)	43(2)
O(3S)	376(21)	-1127(14)	5570(11)	148(10)
O(2S)	50(33)	1048(25)	7284(19)	258(21)
C(83S)	1109(24)	-301(18)	5451(13)	110(12)
C(82S)	833(23)	-288(17)	5969(13)	106(11)
C(81S)	1190(25)	-854(18)	5406(12)	110(11)
C(80S)	301(32)	-840(23)	5973(17)	147(17)
C(93S)	326(40)	570(30)	6969(21)	188(22)
C(90S)	-117(38)	575(29)	7671(20)	181(21)
C(92S)	-135(37)	-1(27)	7060(20)	174(20)
C(91S)	-403(34)	147(25)	7452(20)	158(17)

Table S-7. Bond lengths [A] and angles [deg] for 7.

Ni(1)-O(1)	1.885(6)
Ni(1)-P(1)	2.148(3)
Ni(1)-S(1)	2.155(3)
Ni(1)-P(2)	2.159(3)
S(1)-C(1)	1.875(9)
P(1)-C(12)	1.837(9)
P(1)-C(18)	1.841(10)
P(1)-C(10)	1.859(9)
P(2)-C(30)	1.815(10)
P(2)-C(11)	1.843(9)
P(2)-C(24)	1.844(10)
N(1)-O(1)	1.424(10)
N(1)-C(1)	1.455(12)
N(1)-C(2)	1.470(13)
C(1)-C(5)	1.509(14)
C(2)-C(3)	1.525(14)
C(3)-C(4)	1.51(2)
C(4)-C(5)	1.387(14)
C(4)-C(9)	1.41(2)
C(5)-C(6)	1.366(14)
C(6)-C(7)	1.40(2)
C(7)-C(8)	1.36(2)
C(8)-C(9)	1.37(2)
C(10)-C(11)	1.512(13)
C(12)-C(17)	1.530(14)
C(12)-C(13)	1.536(12)
C(13)-C(14)	1.534(14)
C(14)-C(15)	1.51(2)
C(15)-C(16)	1.48(2)
C(16)-C(17)	1.551(14)
C(18)-C(23)	1.515(14)
C(18)-C(19)	1.526(14)
C(19)-C(20)	1.53(2)
C(20)-C(21)	1.50(2)
C(21)-C(22)	1.49(2)
C(22)-C(23)	1.52(2)
C(24)-C(25)	1.53(2)
C(24)-C(29)	1.528(14)
C(25)-C(26)	1.52(2)
C(26)-C(27)	1.52(2)
C(27)-C(28)	1.50(2)
C(28)-C(29)	1.54(2)
C(30)-C(31)	1.514(14)
C(30)-C(35)	1.537(13)
C(31)-C(32)	1.53(2)
C(32)-C(33)	1.50(2)
C(33)-C(34)	1.54(2)
C(34)-C(35)	1.51(2)
O(3S)-C(80S)	1.35(5)
O(3S)-C(81S)	1.51(5)
O(2S)-C(93S)	1.47(6)
O(2S)-C(90S)	1.56(6)
C(83S)-C(81S)	1.23(5)
C(83S)-C(82S)	1.58(5)
C(82S)-C(80S)	1.48(6)
C(93S)-C(92S)	1.48(7)
C(90S)-C(91S)	1.23(6)

C(92S)-C(91S)	1.27(6)
O(1)-Ni(1)-P(1)	172.5(2)
O(1)-Ni(1)-S(1)	91.1(2)
P(1)-Ni(1)-S(1)	93.44(10)
O(1)-Ni(1)-P(2)	86.2(2)
P(1)-Ni(1)-P(2)	89.29(10)
S(1)-Ni(1)-P(2)	177.27(11)
C(1)-S(1)-Ni(1)	93.9(3)
C(12)-P(1)-C(18)	103.2(4)
C(12)-P(1)-C(10)	105.8(4)
C(18)-P(1)-C(10)	102.9(4)
C(12)-P(1)-Ni(1)	114.0(3)
C(18)-P(1)-Ni(1)	120.1(3)
C(10)-P(1)-Ni(1)	109.4(3)
C(30)-P(2)-C(11)	107.0(4)
C(30)-P(2)-C(24)	105.7(4)
C(11)-P(2)-C(24)	106.2(4)
C(30)-P(2)-Ni(1)	112.8(3)
C(11)-P(2)-Ni(1)	109.1(3)
C(24)-P(2)-Ni(1)	115.4(3)
O(1)-N(1)-C(1)	107.9(7)
O(1)-N(1)-C(2)	109.2(7)
C(1)-N(1)-C(2)	112.9(8)
N(1)-O(1)-Ni(1)	115.8(5)
N(1)-C(1)-C(5)	111.9(8)
N(1)-C(1)-S(1)	110.8(6)
C(5)-C(1)-S(1)	109.6(7)
N(1)-C(2)-C(3)	107.1(8)
C(4)-C(3)-C(2)	111.5(9)
C(5)-C(4)-C(9)	118.6(10)
C(5)-C(4)-C(3)	121.8(9)
C(9)-C(4)-C(3)	119.7(10)
C(6)-C(5)-C(4)	120.5(10)
C(6)-C(5)-C(1)	119.3(9)
C(4)-C(5)-C(1)	120.1(9)
C(5)-C(6)-C(7)	120.0(11)
C(8)-C(7)-C(6)	120.4(12)
C(7)-C(8)-C(9)	120.0(11)
C(8)-C(9)-C(4)	120.5(11)
C(11)-C(10)-P(1)	110.9(6)
C(10)-C(11)-P(2)	111.4(7)
C(17)-C(12)-C(13)	108.7(8)
C(17)-C(12)-P(1)	110.8(6)
C(13)-C(12)-P(1)	115.6(7)
C(14)-C(13)-C(12)	109.1(8)
C(15)-C(14)-C(13)	110.8(8)
C(16)-C(15)-C(14)	111.4(9)
C(15)-C(16)-C(17)	111.6(9)
C(12)-C(17)-C(16)	111.7(8)
C(23)-C(18)-C(19)	110.4(8)
C(23)-C(18)-P(1)	112.5(7)
C(19)-C(18)-P(1)	114.8(7)
C(18)-C(19)-C(20)	110.5(10)
C(21)-C(20)-C(19)	110.6(10)
C(22)-C(21)-C(20)	112.3(11)
C(21)-C(22)-C(23)	111.7(11)
C(18)-C(23)-C(22)	111.5(9)
C(25)-C(24)-C(29)	111.1(9)
C(25)-C(24)-P(2)	110.8(7)
C(29)-C(24)-P(2)	111.5(7)

C(26)-C(25)-C(24)	112.0(9)
C(27)-C(26)-C(25)	112.3(11)
C(28)-C(27)-C(26)	108.8(11)
C(27)-C(28)-C(29)	112.2(10)
C(24)-C(29)-C(28)	110.7(9)
C(31)-C(30)-C(35)	109.6(8)
C(31)-C(30)-P(2)	116.2(7)
C(35)-C(30)-P(2)	111.3(6)
C(30)-C(31)-C(32)	111.3(9)
C(33)-C(32)-C(31)	113.0(9)
C(32)-C(33)-C(34)	109.7(10)
C(35)-C(34)-C(33)	112.7(9)
C(34)-C(35)-C(30)	111.7(8)
C(80S)-O(3S)-C(81S)	100(3)
C(93S)-O(2S)-C(90S)	92(5)
C(81S)-C(83S)-C(82S)	98(3)
C(80S)-C(82S)-C(83S)	99(3)
C(83S)-C(81S)-O(3S)	106(4)
O(3S)-C(80S)-C(82S)	109(4)
O(2S)-C(93S)-C(92S)	110(5)
C(91S)-C(90S)-O(2S)	101(5)
C(91S)-C(92S)-C(93S)	96(5)
C(90S)-C(91S)-C(92S)	123(7)

Table S-8. Anisotropic displacement parameters (A^2 x 10^3) for 7. The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Ni(1)	24(1)	31(1)	46(1)	1(1)	3(1)	-1(1)
S(1)	28(1)	39(1)	62(2)	11(1)	3(1)	0(1)
P(1)	28(1)	35(1)	45(2)	1(1)	1(1)	0(1)
P(2)	31(1)	29(1)	47(2)	-2(1)	4(1)	1(1)
N(1)	29(4)	44(5)	50(5)	5(4)	-1(4)	3(4)
O(1)	27(3)	44(4)	46(4)	5(3)	3(3)	4(3)
C(1)	27(5)	35(5)	52(6)	-4(5)	-2(4)	1(4)
C(2)	46(6)	44(6)	49(6)	-7(5)	2(5)	-5(5)
C(3)	49(7)	54(7)	51(7)	-3(5)	11(5)	4(5)
C(4)	33(5)	62(7)	39(6)	14(5)	1(5)	-5(5)
C(5)	23(5)	53(7)	48(6)	1(5)	1(4)	0(4)
C(6)	41(6)	42(6)	61(7)	-3(5)	-1(5)	-14(5)
C(7)	58(8)	64(8)	67(8)	14(7)	-4(6)	-24(6)
C(8)	53(7)	70(8)	52(7)	10(6)	0(6)	-22(6)
C(9)	43(6)	89(9)	48(7)	-5(7)	-3(5)	2(6)
C(10)	21(5)	41(5)	48(6)	-3(5)	1(4)	-1(4)
C(11)	29(5)	37(5)	53(6)	-9(5)	3(5)	-7(4)
C(12)	26(5)	38(5)	49(6)	-3(5)	4(4)	8(4)
C(13)	34(6)	48(6)	56(7)	-12(5)	-8(5)	14(5)
C(14)	43(6)	36(5)	77(8)	3(5)	5(6)	6(5)
C(15)	61(7)	43(6)	58(7)	-12(5)	2(6)	7(5)
C(16)	62(8)	54(7)	57(7)	-15(6)	-9(6)	6(6)
C(17)	47(6)	46(6)	60(7)	-2(5)	-8(5)	11(5)
C(18)	30(5)	47(6)	41(6)	3(5)	0(4)	7(4)
C(19)	55(7)	53(7)	54(7)	14(5)	-4(6)	4(5)
C(20)	71(8)	79(9)	48(7)	17(7)	-3(6)	20(7)
C(21)	83(10)	110(12)	40(7)	5(7)	-6(6)	29(9)
C(22)	75(9)	95(10)	51(8)	-12(7)	-4(7)	16(8)
C(23)	54(7)	56(7)	51(7)	-2(5)	5(5)	12(5)
C(24)	31(5)	32(5)	65(7)	-6(5)	10(5)	1(4)
C(25)	75(8)	49(7)	63(8)	-8(6)	-8(6)	7(6)
C(26)	100(11)	68(9)	70(9)	-27(7)	-22(8)	19(8)
C(27)	97(11)	58(8)	80(10)	-28(7)	15(8)	2(8)
C(28)	55(8)	48(7)	106(11)	-21(7)	4(7)	3(6)
C(29)	45(7)	47(6)	70(8)	-22(6)	14(6)	-2(5)
C(30)	34(5)	29(5)	45(6)	2(4)	7(4)	10(4)
C(31)	52(6)	37(6)	53(7)	-4(5)	0(5)	6(5)
C(32)	65(8)	47(7)	72(8)	14(6)	-1(6)	13(6)
C(33)	54(7)	61(8)	68(8)	7(6)	-12(6)	15(6)
C(34)	43(6)	51(7)	59(7)	-8(5)	-4(5)	8(5)
C(35)	39(6)	32(5)	57(7)	-1(5)	2(5)	3(4)

Table S-9. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for 7.

	x	y	z	U(eq)
H(1A)	-835(6)	1575(4)	5374(4)	45
H(2A)	-741(7)	3150(5)	6064(4)	56
H(2B)	-237(7)	2576(5)	6264(4)	56
H(3A)	-1478(7)	2649(5)	6688(4)	62
H(3B)	-2035(7)	2710(5)	6235(4)	62
H(6A)	-1152(6)	615(5)	5793(4)	58
H(7A)	-1998(7)	161(6)	6355(4)	76
H(8A)	-2626(7)	748(6)	6912(4)	70
H(9A)	-2445(7)	1790(6)	6912(4)	72
H(10A)	3158(5)	2814(4)	5557(3)	44
H(10B)	3422(5)	2387(4)	5138(3)	44
H(11A)	2533(6)	2841(4)	4654(3)	47
H(11B)	2800(6)	3405(4)	4967(3)	47
H(12A)	2025(6)	987(4)	5254(3)	45
H(13A)	3672(6)	1395(5)	4992(4)	55
H(13B)	3488(6)	999(5)	5441(4)	55
H(14A)	3911(7)	341(4)	4841(4)	62
H(14B)	2956(7)	193(4)	4977(4)	62
H(15A)	3454(7)	914(5)	4212(4)	65
H(15B)	3076(7)	242(5)	4179(4)	65
H(16A)	1788(7)	566(5)	4441(4)	70
H(16B)	2053(7)	986(5)	4020(4)	70
H(17A)	2452(7)	1781(5)	4516(4)	61
H(17B)	1512(7)	1584(5)	4645(4)	61
H(18A)	3286(6)	1731(4)	5997(3)	47
H(19A)	2497(7)	829(5)	5985(4)	65
H(19B)	1777(7)	1144(5)	6286(4)	65
H(20A)	2663(8)	576(6)	6776(4)	79
H(20B)	3476(8)	927(6)	6588(4)	79
H(21A)	2155(9)	1460(7)	7113(4)	93
H(21B)	3094(9)	1344(7)	7290(4)	93
H(22A)	3618(9)	2071(7)	6800(4)	89
H(22B)	2874(9)	2368(7)	7094(4)	89
H(23A)	1937(7)	2282(5)	6481(4)	64
H(23B)	2760(7)	2631(5)	6305(4)	64
H(24A)	1710(6)	4143(4)	5297(4)	51
H(25A)	1455(8)	3399(5)	6086(4)	75
H(25B)	2347(8)	3627(5)	5897(4)	75
H(26A)	1904(9)	4213(6)	6536(5)	95
H(26B)	2034(9)	4630(6)	6094(5)	95
H(27A)	434(9)	4221(6)	6425(5)	94
H(27B)	770(9)	4907(6)	6454(5)	94
H(28A)	781(8)	4977(5)	5657(5)	84
H(28B)	-142(8)	4798(5)	5828(5)	84
H(29A)	92(7)	3769(5)	5627(4)	65
H(29B)	256(7)	4188(5)	5189(4)	65
H(30A)	237(6)	3398(4)	4697(3)	43
H(31A)	1729(7)	3722(5)	4218(4)	57
H(31B)	1165(7)	4183(5)	4509(4)	57
H(32A)	26(8)	4051(5)	4007(4)	73
H(32B)	834(8)	4258(5)	3721(4)	73
H(33A)	1052(8)	3274(5)	3462(4)	73
H(33B)	94(8)	3455(5)	3357(4)	73
H(34A)	-384(7)	2908(5)	3993(4)	62
H(34B)	195(7)	2462(5)	3698(4)	62
H(35A)	1313(6)	2591(4)	4201(4)	52
H(35B)	502(6)	2383(4)	4485(4)	52