Electronic Supplementary Material (ESI) for CrystEngComm.

ELECTRONIC SUPPLEMENTARY INFORMATION

Coordination polymers and polygons using di-pyridyl-thiadiazole spacers and substituted phosphorodithioato Ni^{II} complexes: potential and limitations for inorganic crystal engineering

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Figure S1 Numbering scheme adopted for $(\mathbf{1}\cdot\mathbf{L1})_{\infty}$: R1, R2 = OMe; $(\mathbf{2}\cdot\mathbf{L1})_{\infty}$: R1, R2 = OEt; $(\mathbf{3}\cdot\mathbf{L1})_{\infty}$: R1 = 4-$MeOC_6H_4$; R2 = OCH_3; and $(\mathbf{4}\cdot\mathbf{L1})_{\infty}$: R1, R2 = Ph.

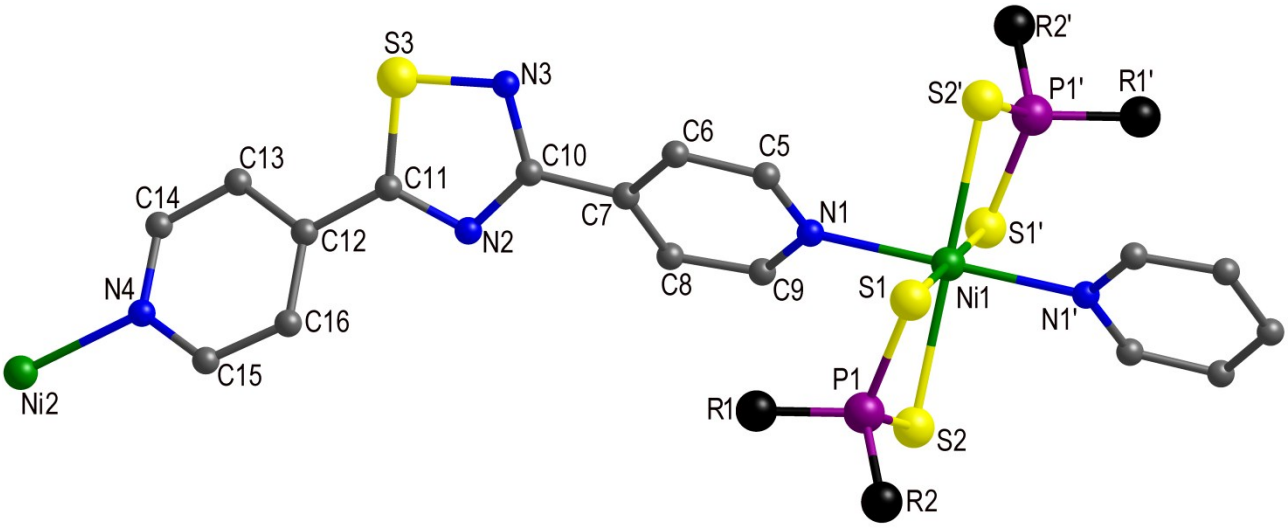


Figure S2 Asymmetric unit and original numbering scheme for $(\mathbf{1}\cdot\mathbf{L1})_{\infty}$.

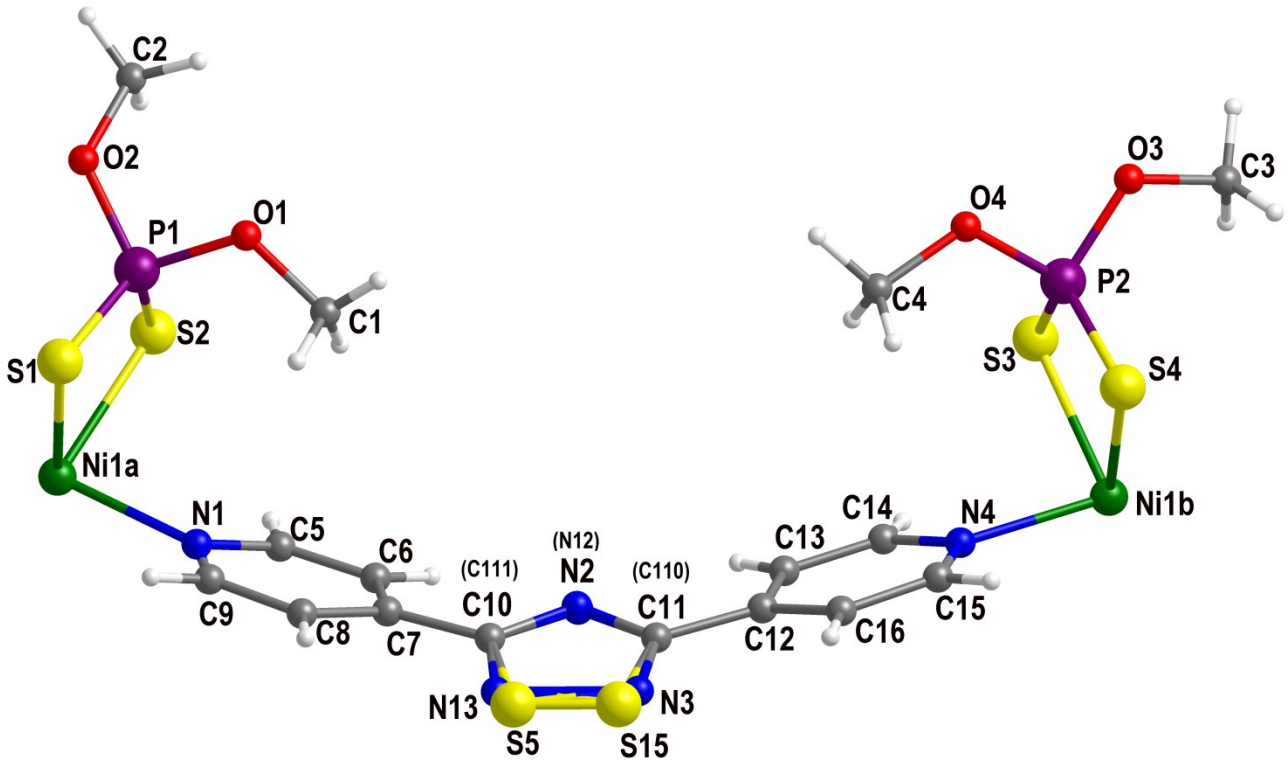


Figure S3: Packing views of $(\mathbf{1}\cdot\mathbf{L1})_{\infty}$ showing (a) view along the 001 direction with polymeric chains coloured in blue and yellow according to their orientation. The Ni^{II} ions and the O and H atoms involved in the described H-bonds (d, $C6^{ii}$–$H6^{ii}\cdots O3$ 2.37(4), 3.288(5), 155(3); e, $C5^{ii}$–$H5^{ii}\cdots O4$ 2.60(4) Å, 3.419(5) Å, 148(3)°; ^{ii} x, 1.5-y, 0.5+z) have been left of the conventional colours; (b) polymeric chains coloured in blue and yellow according to their orientation along the 2_1 screw axis depicted as black arrows, and void channels coloured in red. H-atoms not involved in showed interactions have been omitted for clarity. The labels used for the described interactions refer to the original numbering scheme (Fig. S1 in ESI)

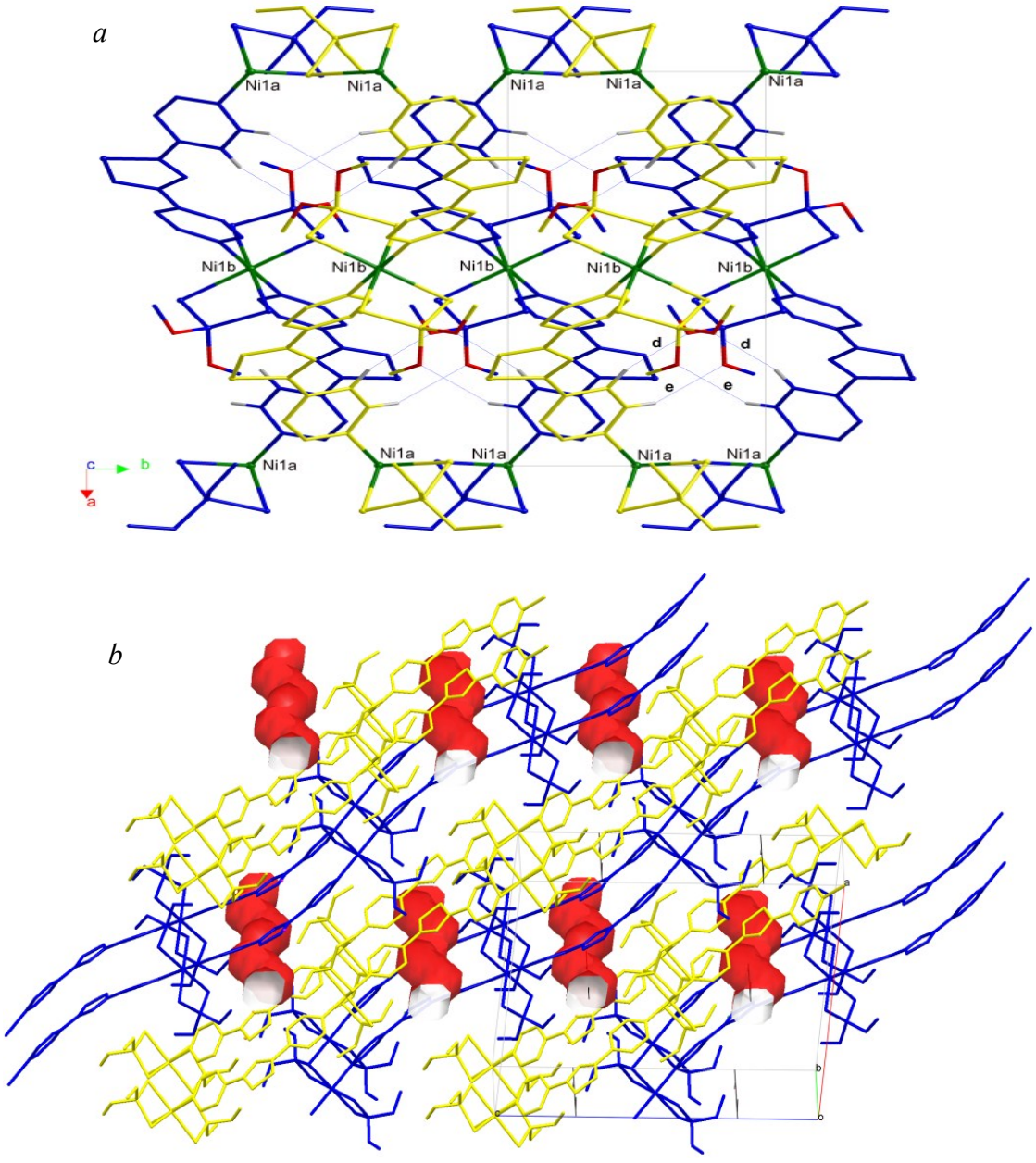


Figure S4 Original numbering scheme for (**2**·**L1**)$_\infty$.

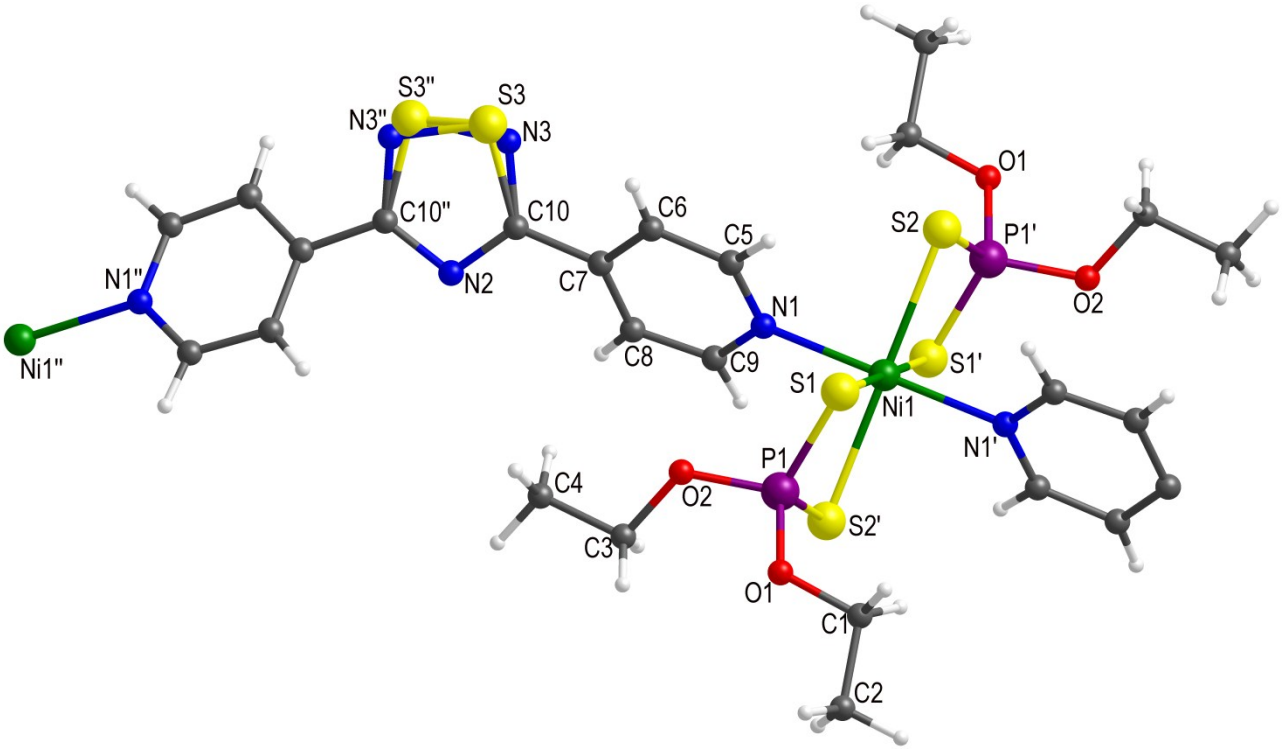


Figure S5 (a) Asymmetric unit and original numbering scheme for $(\mathbf{3}\cdot\mathbf{L1})_{\infty}$; (b) packing views of $(\mathbf{3}\cdot\mathbf{L1})_{\infty}$ showing interactions between the parallel layers showed in Fig. 5: **d**, C15–H15c···S3^{iii} 2.85, 3.608(3), 135; **e**, C8–H8b···S5b^{iv} 2.95, 3.449(7), 113; **f**, C16–H16b···S2^{v} 2.86, 3.560(4), 129; **g**, C6–H6···S2^{vi} 3.04 Å, 3.784(7) Å, 137°. Symmetry codes: ^{iii} x, 1+y, z; ^{iv} –1+x, y, z; ^{v} –x, –y, 1–z. H-atoms not involved in showed interactions have been omitted for clarity. The labels used for the described interactions refer to the original numbering scheme here reported.

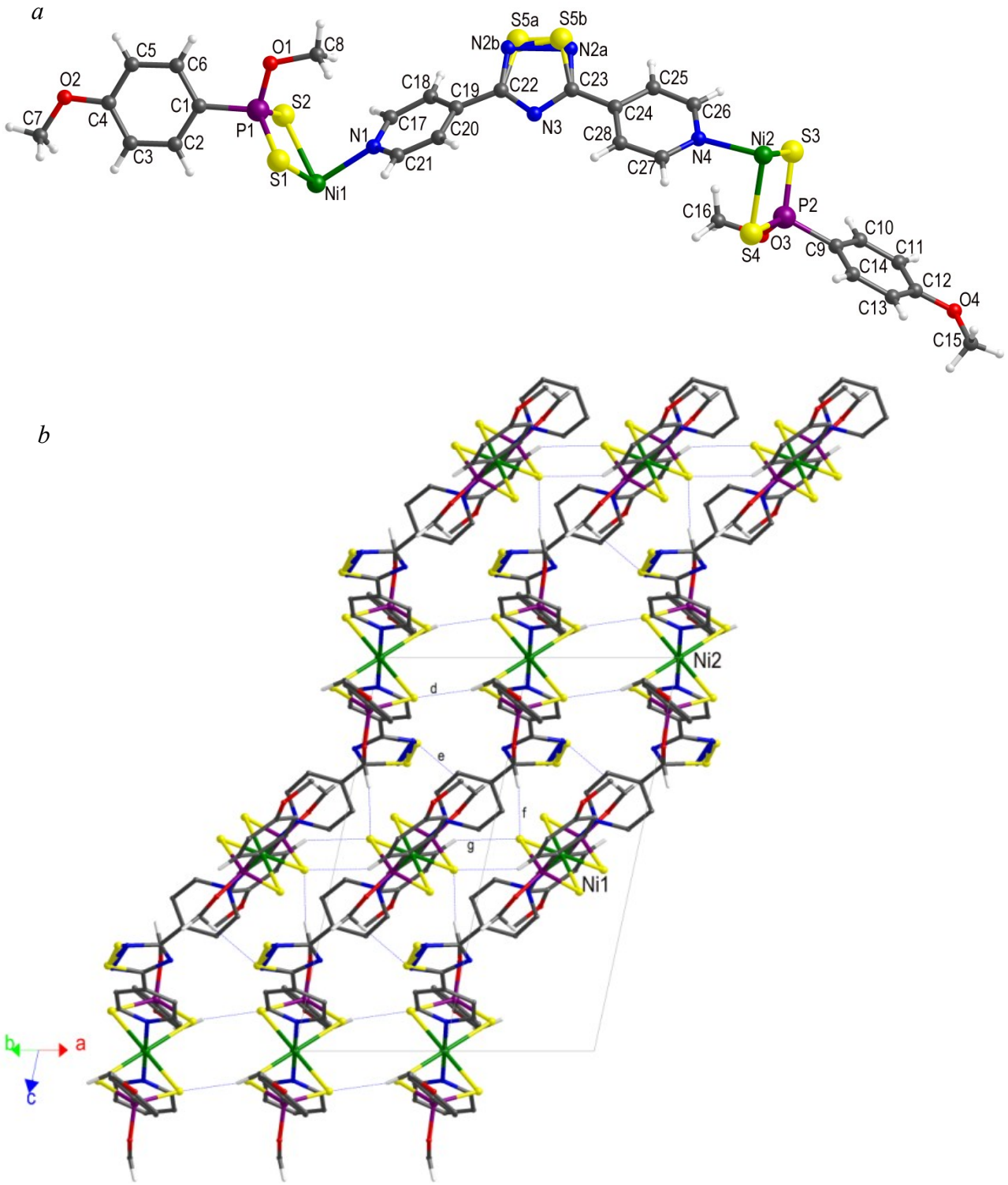
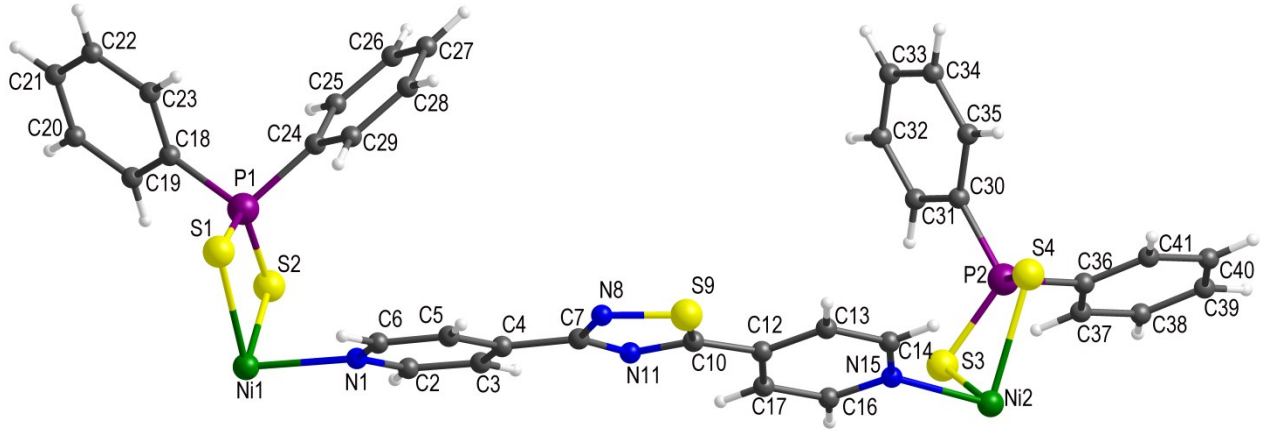


Figure S6 (a) Asymmetric unit and original numbering scheme for $(\mathbf{4}\cdot\mathbf{L1})_\infty$; (b) view of $(\mathbf{4}\cdot\mathbf{L1})_\infty$ showing the packing of layers showed in Fig. 6 through the C–H···S interactions h-j: **h**, C37–H37a···S4^{v} 2.84, 3.736(3), 158; **i**, C14–H14a···S3^{vi} 2.86, 3.788(2), 166; **j**, C5–H5a···S2^{vi} 3.02 Å, 3.571(2) Å, 119°. Symmetry codes: ^{v} –1+x, y, z; ^{vi} 1+x, y, z. H-atoms not involved in showed interactions have been omitted for clarity. The labels used for the described interactions refer to the original numbering scheme here reported.

a



b

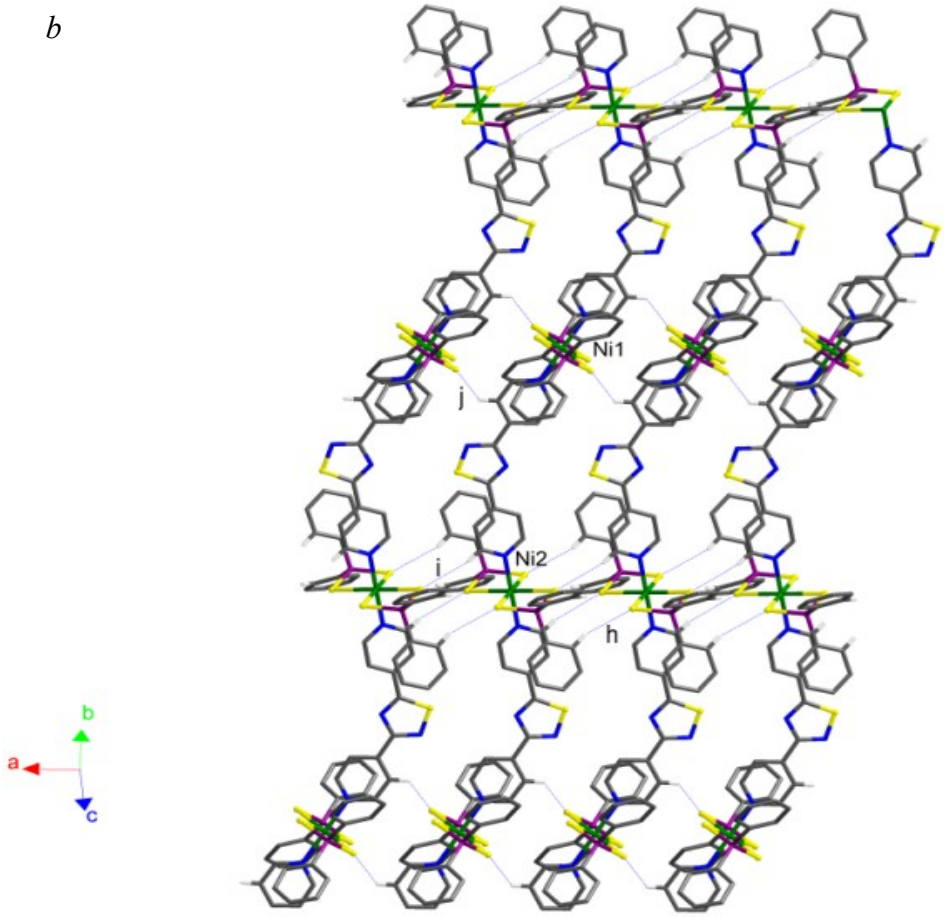


Figure S7 Numbering scheme adopted for $(\mathbf{1}\cdot\mathbf{L2})_{\infty}$: R1, R2 = OMe; $(\mathbf{2}\cdot\mathbf{L2})_{\infty}$: R1, R2 = OEt; $(\mathbf{3}\cdot\mathbf{L2})_{\infty}$: R1 = 4-$MeOC_6H_4$; R2 = OCH_3; and $(\mathbf{4}\cdot\mathbf{L2})_{\infty}$: R1, R2 = Ph.

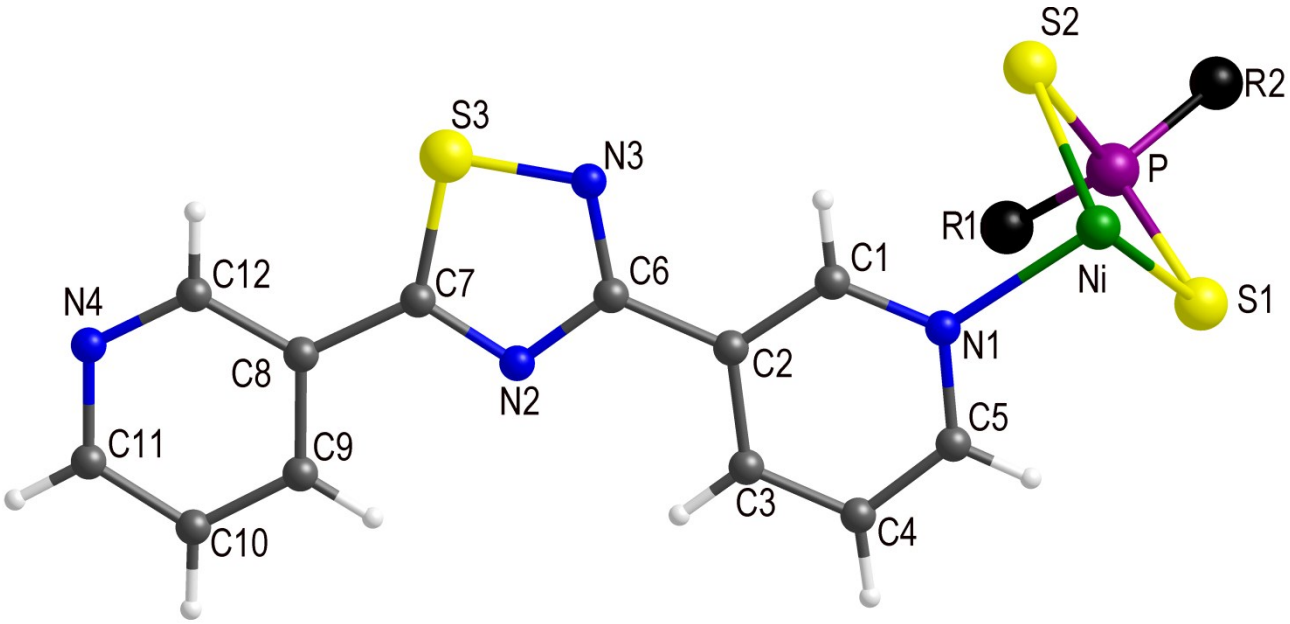


Figure S8 Asymmetric unit and original numbering scheme for $(\mathbf{1}\cdot\mathbf{L2})_2$.

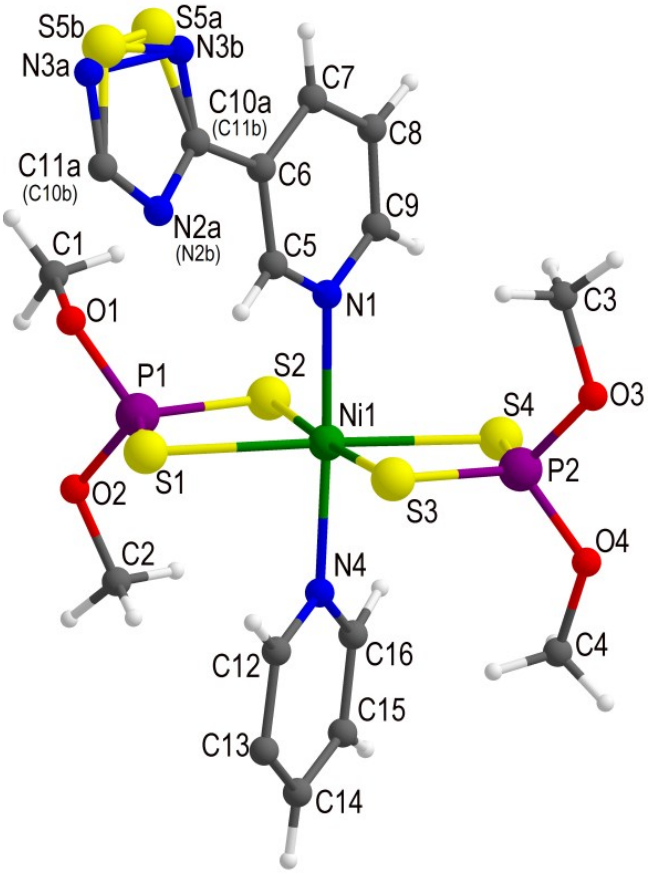


Figure S9 Asymmetric unit and original numbering scheme for $(\mathbf{2}\cdot\mathbf{L2})_2$.

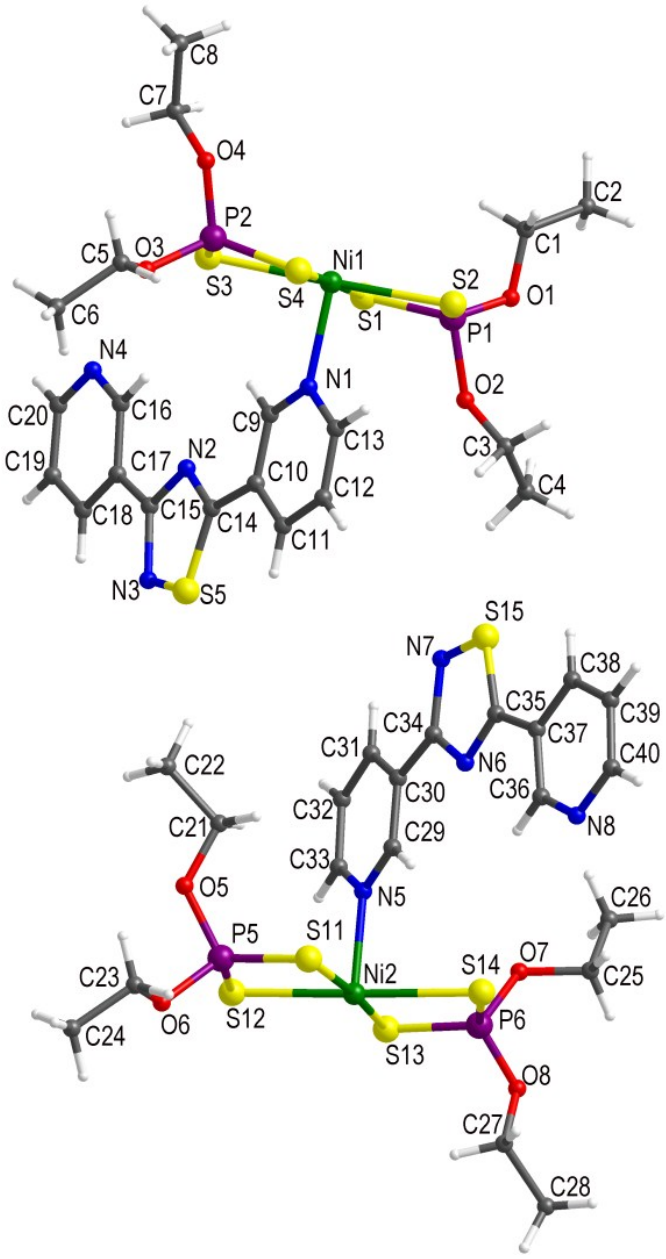


Figure S10 Asymmetric unit and original numbering scheme for $(\mathbf{3}\cdot\mathbf{L1})_{\infty}$.

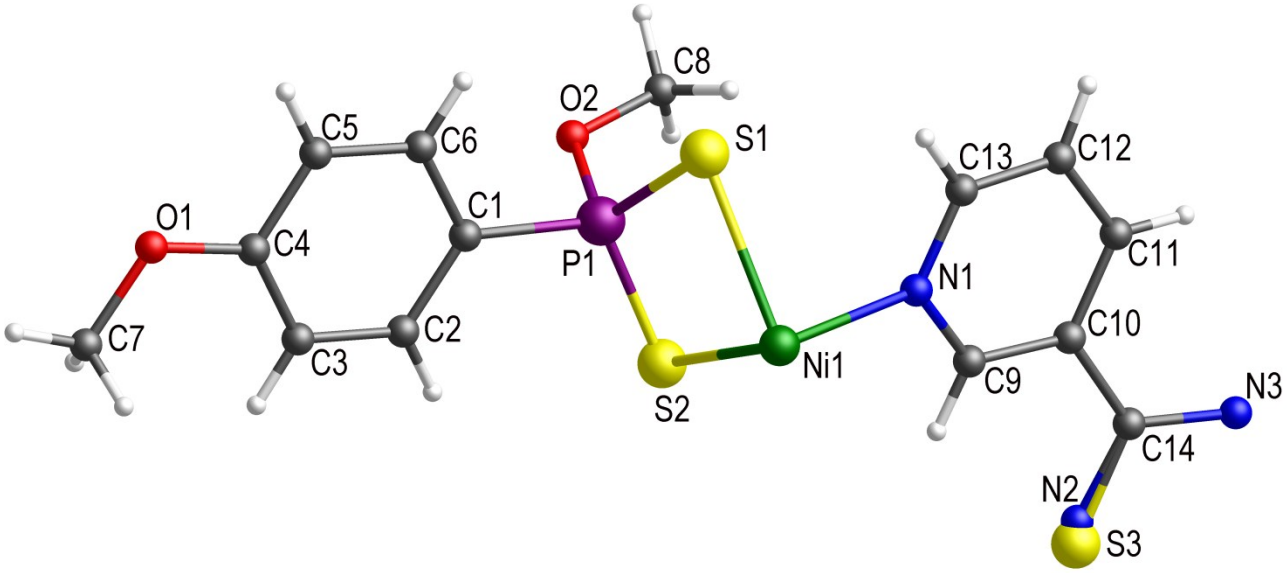


Figure S11 Asymmetric unit and original numbering scheme for (**4**·**L2**·2C_7H_8)$_\infty$.

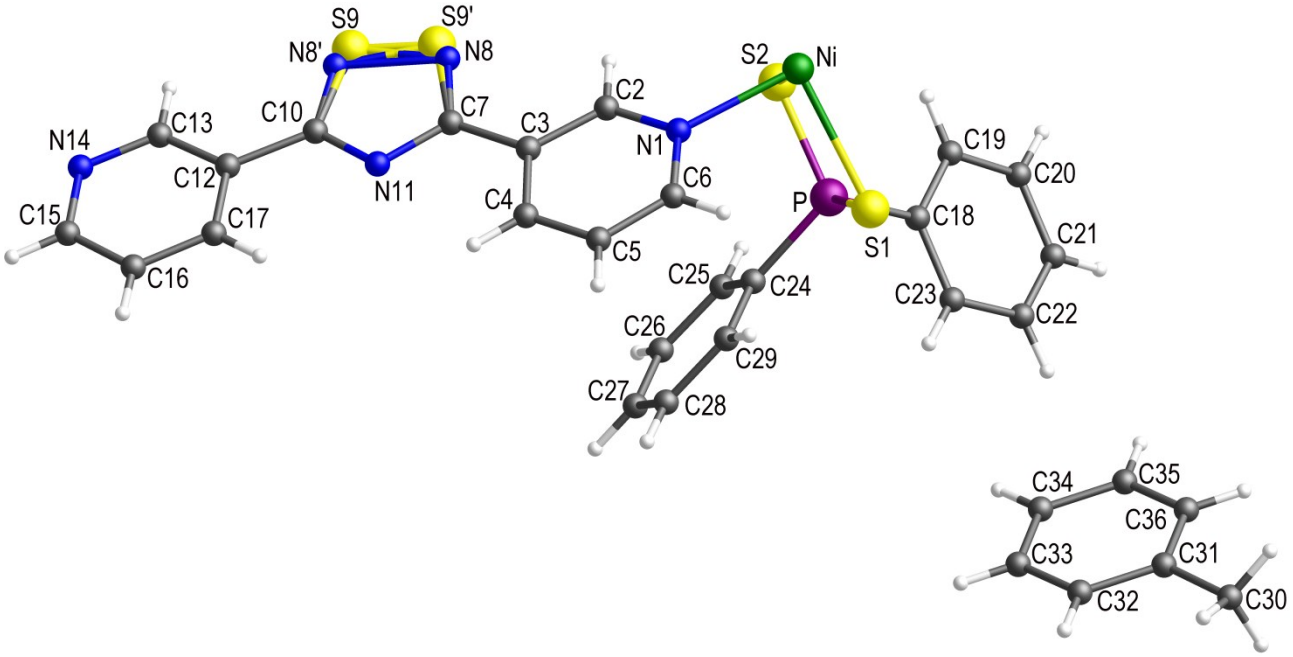
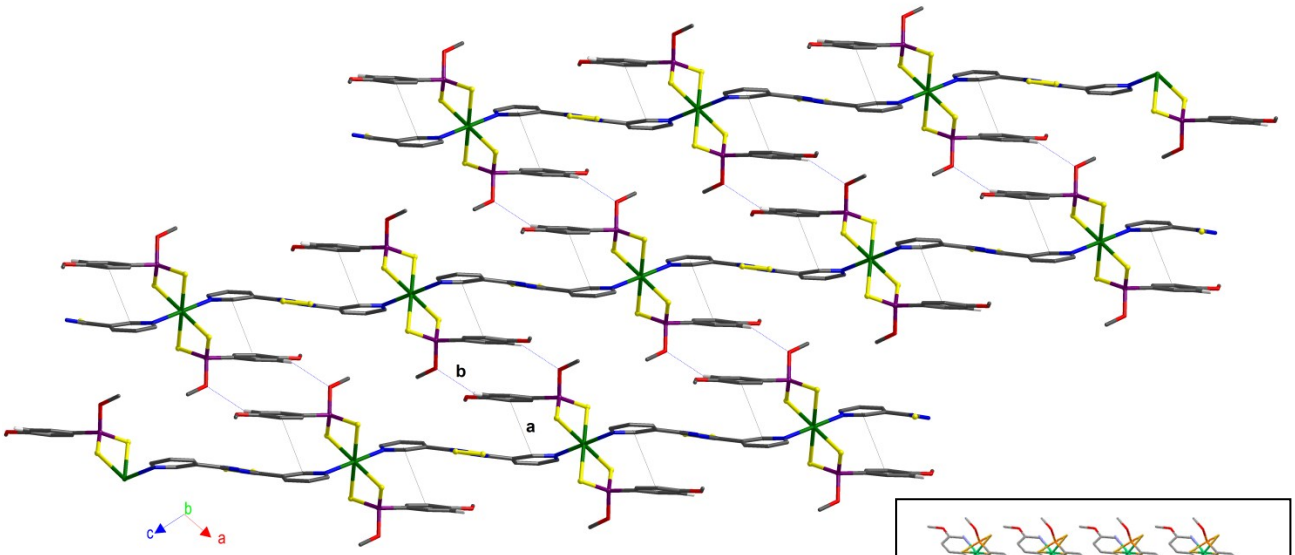
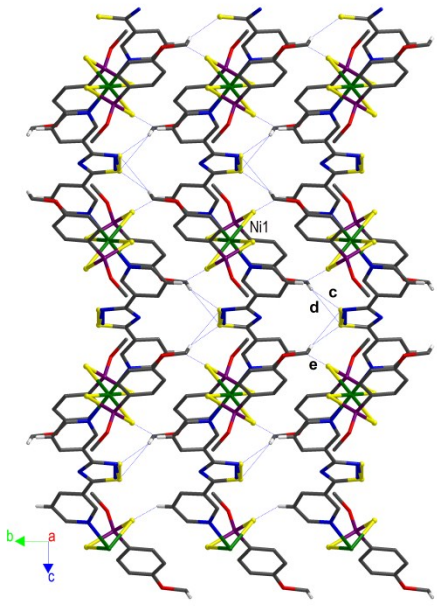


Figure S12 Packing views showing the (***a***) view along the 010 direction of the layers formed by interacting (**3**·**L2**)$_\infty$ chains and (***b***) packing of interacting parallel layers; in the inset the calculated voids intercalating the packing are evidenced in blue colour. All the hydrogen atoms with the exception of those involved in the showed interactions have been omitted. Interactions: a, $Cnt_{C_6H_4}\cdots Cnt_{Py^i}$ 3.72 Å, C_6H_4^Py^i 7.5°; b, C5–H5···O2^{ii} 2.66, 3.522(8), 151; c, C7–H7c···S3^{iii} 2.87, 3.789(8), 156; d, C7–H7c···S3^{iv} 2.85, 3.580(8), 132; e, C12–H12···S2^{v} 2.80 Å, 3.537(2) Å, 135°. Symmetry codes: ^{i} 1–x, –y, 1–z; ^{ii} –x, –y, 1–z; ^{iii} 1–x, –1–y, 1–z; ^{iv} –0.5+x, –1–y, 0.5+z; ^{v} x, 1+y, z.

a



b



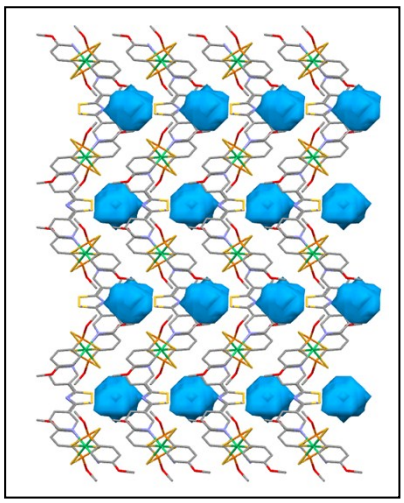


Table S1 Crystal data collections and refinement parameters for $(\mathbf{1}\cdot\mathbf{L1})_\infty$, $(\mathbf{2}\cdot\mathbf{L1})_\infty$, $(\mathbf{3}\cdot\mathbf{L1})_\infty$, and $(\mathbf{4}\cdot\mathbf{L1})_\infty$.

	$(\mathbf{1}\cdot\mathbf{L1})_\infty$	$(\mathbf{2}\cdot\mathbf{L1})_\infty$	$(\mathbf{3}\cdot\mathbf{L1})_\infty$	$(\mathbf{4}\cdot\mathbf{L1})_\infty$
Empirical formula	$C_{16}H_{20}N_4NiO_4P_2S_5$	$C_{20}H_{28}N_4NiO_4P_2S_5$	$C_{28}H_{28}N_4NiO_4P_2S_5$	$C_{36}H_{28}N_4NiP_2S_5$
Formula weight	613.34	669.41	765.52	797.57
Temperature (K)	120(2)	120(2)	120(2)	173(2)
Crystal system	Monoclinic	Orthorhombic	Triclinic	Triclinic
Space group	*P2(1)/c* (no. 14)	*Pbcn* (no. 60)	*P-1* (no. 2)	*P-1* (no. 2)
a (Å)	16.542(3)	11.6939(8)	9.7075(2)	6.8385(2)
b (Å)	7.489(2)	15.2594(14)	10.6736(2)	12.0415(3)
c (Å)	20.642(6)	15.9310(13)	17.4582(2)	22.6405(4)
α (°)	90	90	73.230(1)	101.922(2)
β (°)	94.29(2)	90	87.086(1)	97.350(2)
γ (°)	90	90	72.131(1)	93.086(2)
Volume (Å^3)	2550.0(11)	2842.8(4)	1647.02(4)	1802.94(8)
Z	4	4	2	2
D_{calc} (Mg/m^3)	1.598	1.564	1.544	1.469
μ(mm^{-1})	1.326	1.197	1.044	0.950
θ min-max (°)	2.9-27.5	3.1-27.5	3.2-27.5	3.7-32.4
Refl.col/unique/R_{int}	32091/5840/0.0707	21763/3263/0.0403	36271/7555/0.047	30395/11661/0.0447
Refl.obs (I>2σ(I))	4078	2733	6352	7622
R1/ *wR2* (I>2σ(I))	0.0492/0.1031	0.0331/0.0817	0.0361/0.0798	0.0407/0.1033
R1/*wR2* (all data)	0.0868/0.1164	0.0438/0.0903	0.0474/0.0850	0.0684/0.1140
GOF	1.051	0.860	1.038	0.964

Table S2 Crystal data collections and refinement parameters for $(\mathbf{1}\cdot\mathbf{L2})_2$, $(\mathbf{2}\cdot\mathbf{L2})_2$, $(\mathbf{3}\cdot\mathbf{L2})_\infty$, and $(\mathbf{4}\cdot\mathbf{L2}\cdot 2C_7H_8)_\infty$.

	$(\mathbf{1}\cdot\mathbf{L2})_2$	$(\mathbf{2}\cdot\mathbf{L2})_2$	$(\mathbf{3}\cdot\mathbf{L2})_\infty$	$(\mathbf{4}\cdot\mathbf{L2})_\infty\cdot 2(C_7H_8)$
Empirical formula	$C_{32}H_{40}N_8Ni_2O_8P_4S_{10}$	$C_{40}H_{56}N_8Ni_2O_8P_4S_{10}$	$C_{28}H_{28}N_4NiO_4P_2S_5$	$C_{36}H_{28}N_4NiP_2S_5\cdot 2(C_7H_8)$
Formula weight	1226.68	1338.89	765.81	981.84
Temperature (K)	120(2)	120(2)	120(2)	173(2)
Crystal system	Monoclinic	Triclinic	Monoclinic	Orthorhombic
Space group	P2(1)/c (no. 14)	*P-1* (no. 2)	*P2/n (No. 13)*	*Pnma(no. 62)*
a (Å)	14.0311(13)	11.728(2)	12.8213(3)	26.5284(2)
b (Å)	14.9236(13)	14.435(3)	7.2342(2)	25.8535(2)
c (Å)	12.8460(5)	18.657(4)	19.1246(3)	7.0091(1)
α (°)	90	104.40(3)	90	26.5284(2)
β (°)	113.786(5)	103.02(3)	106.1860(10)	25.8535(2)
γ (°)	90	101.92(3)	90	7.0091(1)
Volume (Å^3)	2461.4(3)	2862.9(13)	1703.53(7)	4807.17(9)
Z	2	2	2	4
D_{calc} (Mg/m^3)	1.655	1.553	1.493	1.357
μ(mm^{-1})	1.374	1.188	1.010	3.543
θ min-max (°)	3.1-27.5	2.4-27.5	3.0-27.5	3.3-71.4
Refl.col/unique/R_{int}	19049/5601/0.036	25481/2921/0.036	19777/3900/0.039	65823/4757/0.037
Refl.obs (I>2σ(I))	4837	9150	3388	4485
R1/ *wR2* (I>2σ(I))	0.0641/0.1917	0.0969/0.2663	0.0372/0.0741	0.0861/0.2236
R1/*wR2* (all data)	0.0739/0.1964	0.1277/0.2445	0.0459/0.0778	0.0886/0.2246
GOF	1.161	1.137	1.040	1.211

Table S3 - Crystal Data and Details of the Structure Determination

for: $(1 \cdot \mathbf{L1})_{\infty}$

Crystal Data			
Formula		C16 H20 N4 Ni O4 P2 S5	
Formula Weight			613.34
Crystal System			Monoclinic
Space group		P21/c	(No. 14)
a, b, c [Angstrom]	16.542(3)	7.489(2)	20.642(6)
alpha, beta, gamma [deg]	90	94.29(2)	90
V [Ang**3]			2550.0(11)
Z			4
D(calc) [g/cm**3]			1.598
Mu(MoKa) [/mm]			1.326
F(000)			1256
Crystal Size [mm]		0.04 x 0.04 x 0.10	
Data Collection			
Temperature (K)			120
Radiation [Angstrom]		MoKa	0.71073
Theta Min-Max [Deg]			3.0, 27.5
Dataset		-20: 21 ; -9: 9 ; -26: 26	
Tot., Uniq. Data, R(int)		32091, 5840, 0.071	
Observed data [I > 2.0 sigma(I)]			4078
Refinement			
Nref, Npar			5840, 400
R, wR2, S		0.0492, 0.1164, 1.05	
w = 1/[\s^2^(Fo^2^)+(0.0431P)^2^+4.9629P] where P=(Fo^2^+2Fc^2^)/3			
Max. and Av. Shift/Error			0.24, 0.01
Min. and Max. Resd. Dens. [e/Ang^3]			-0.54, 0.91

Table S4 - Final Coordinates and Equivalent Isotropic Displacement Parameters of the non-Hydrogen atoms

for: $(1 \cdot \mathbf{L1})_{\infty}$

Atom	x	y	z	U(eq) [Ang^2]
Ni1A	1	1	0	0.0176(2)
Ni1B	1/2	1	1/2	0.0165(2)
S1	1.11588(6)	1.06334(13)	0.08270(5)	0.0238(3)
S2	0.99157(6)	0.72574(12)	0.06498(4)	0.0218(3)
S3	0.58108(6)	0.72748(12)	0.49081(5)	0.0242(3)
S4	0.60842(5)	1.07063(13)	0.58668(4)	0.0231(3)
*S5	0.77885(17)	1.5711(3)	0.22598(12)	0.0242(6)
P1	1.08453(6)	0.83101(13)	0.11791(5)	0.0216(3)
P2	0.65075(6)	0.83463(14)	0.56278(5)	0.0248(3)
O1	1.06623(16)	0.8403(4)	0.19291(12)	0.0276(8)
O2	1.16132(15)	0.7033(3)	0.12483(13)	0.0260(8)
O3	0.66430(17)	0.7009(4)	0.62206(14)	0.0351(9)
O4	0.74383(15)	0.8425(4)	0.54871(14)	0.0322(9)
N1	0.91829(17)	1.1244(4)	0.05833(14)	0.0193(9)
*N2	0.732(4)	1.253(2)	0.238(3)	0.0230(11)
*N3	0.7199(7)	1.5303(13)	0.2851(5)	0.0248(14)
N4	0.56767(17)	1.1206(4)	0.42985(14)	0.0192(9)
C1	0.9971(3)	0.9411(8)	0.2113(2)	0.0420(16)
C2	1.1535(3)	0.5285(5)	0.1540(2)	0.0302(14)
C3	0.5953(3)	0.6267(9)	0.6508(3)	0.0520(19)
C4	0.7674(3)	0.9530(8)	0.4962(2)	0.0379(16)
C5	0.8520(2)	1.0419(5)	0.07790(19)	0.0241(12)
C6	0.8038(2)	1.1120(5)	0.12292(18)	0.0217(11)
C7	0.8230(2)	1.2785(5)	0.14897(17)	0.0194(10)
C8	0.8889(2)	1.3693(5)	0.12769(18)	0.0224(12)
C9	0.9344(2)	1.2874(5)	0.08300(17)	0.0205(11)

Table S4 - Final Coordinates and Equivalent Isotropic Displacement Parameters of the non-Hydrogen atoms (continued)

for: $(1 \cdot \mathbf{L1})_{\infty}$

Atom	x	y	z	U(eq) [Ang^2]
*C10	0.7772(2)	1.3547(5)	0.20150(17)	0.0223(8)
*C11	0.7017(2)	1.3568(5)	0.28326(18)	0.0241(8)
C12	0.6533(2)	1.2786(5)	0.33333(17)	0.0218(11)
C13	0.6211(2)	1.1090(5)	0.32516(18)	0.0234(11)
C14	0.5791(2)	1.0353(5)	0.37404(18)	0.0242(12)
C15	0.6000(2)	1.2830(5)	0.43755(18)	0.0220(11)
C16	0.6428(2)	1.3674(5)	0.39122(19)	0.0237(12)
*N13	0.7836(10)	1.5272(16)	0.2145(7)	0.0233(16)
*C110	0.7017(2)	1.3568(5)	0.28326(18)	0.0241(8)
*C111	0.7772(2)	1.3547(5)	0.20150(17)	0.0223(8)
*S15	0.7301(3)	1.5690(5)	0.2768(2)	0.0253(9)
*N12	0.729(6)	1.254(4)	0.237(4)	0.0228(12)

U(eq) = 1/3 of the trace of the orthogonalized U Tensor

Starred Atom sites have a S.O.F less than 1.0

Table S5 - Hydrogen Atom Positions and Isotropic Displacement Parameters

for: $(1 \cdot \mathbf{L1})_{\infty}$

Atom	x	y	z	U(iso) [Ang^2]
H2B	1.142(3)	0.545(6)	0.200(2)	0.037(12)
H2C	1.207(3)	0.469(7)	0.154(2)	0.061(16)
H1A	0.945(3)	0.884(7)	0.186(2)	0.053(14)
H1B	0.998(2)	0.937(5)	0.254(2)	0.021(10)
H1C	1.010(3)	1.072(8)	0.200(3)	0.073(18)
H4B	0.742(3)	0.919(6)	0.458(2)	0.037(13)
H4C	0.751(3)	1.069(7)	0.500(2)	0.039(13)
H5	0.842(2)	0.928(5)	0.0614(17)	0.016(9)
H6	0.757(2)	1.041(5)	0.1341(17)	0.021(10)
H8	0.902(2)	1.482(5)	0.1419(17)	0.016(9)
H9	0.980(2)	1.341(4)	0.0684(15)	0.006(8)
H13	0.628(2)	1.042(5)	0.2914(19)	0.024(11)
H14	0.552(2)	0.931(6)	0.3685(18)	0.022(10)
H2A	1.108(3)	0.460(7)	0.128(2)	0.056(15)
H15	0.591(2)	1.342(5)	0.4752(19)	0.024(10)
H16	0.661(2)	1.479(5)	0.3973(16)	0.009(9)
H3A	0.547(4)	0.586(9)	0.617(3)	0.09(2)
H3B	0.621(4)	0.524(9)	0.672(3)	0.08(2)
H3C	0.574(4)	0.716(8)	0.677(3)	0.072(19)
H4A	0.831(3)	0.927(7)	0.491(3)	0.070(16)

The Temperature Factor has the Form of Exp(-T) Where
T = 8*(Pi**2)*U*(Sin(Theta)/Lambda)**2 for Isotropic Atoms

Table S6 - (An)isotropic Displacement Parameters
for: $(1 \cdot \mathbf{L1})_{\infty}$

Atom	U(1,1) or U	U(2,2)	U(3,3)	U(2,3)	U(1,3)	U(1,2)
Ni1A	0.0202(3)	0.0143(3)	0.0189(3)	-0.0005(3)	0.0052(3)	-0.0036(3)
Ni1B	0.0194(3)	0.0130(3)	0.0175(3)	-0.0011(2)	0.0051(2)	0.0015(3)
S1	0.0265(5)	0.0190(5)	0.0257(5)	0.0003(4)	-0.0001(4)	-0.0064(4)
S2	0.0264(5)	0.0159(4)	0.0235(5)	0.0011(4)	0.0046(4)	-0.0051(4)
S3	0.0280(5)	0.0159(4)	0.0294(5)	-0.0020(4)	0.0067(4)	0.0042(4)
S4	0.0237(5)	0.0223(5)	0.0233(5)	-0.0031(4)	0.0018(4)	0.0014(4)
S5	0.0301(9)	0.0186(11)	0.0252(11)	-0.0002(7)	0.0106(7)	-0.0004(8)
P1	0.0256(5)	0.0191(5)	0.0203(5)	0.0004(4)	0.0035(4)	-0.0020(4)
P2	0.0235(5)	0.0238(5)	0.0273(5)	0.0023(4)	0.0034(4)	0.0067(4)
O1	0.0322(15)	0.0294(15)	0.0215(14)	0.0004(11)	0.0046(11)	0.0049(12)
O2	0.0263(14)	0.0212(14)	0.0311(15)	0.0036(11)	0.0054(11)	-0.0005(11)
O3	0.0336(16)	0.0367(17)	0.0346(16)	0.0124(13)	0.0005(13)	0.0095(13)
O4	0.0211(14)	0.0357(16)	0.0400(17)	0.0044(13)	0.0043(12)	0.0090(12)
N1	0.0218(15)	0.0177(16)	0.0189(15)	0.0006(12)	0.0058(12)	-0.0045(13)
N2	0.025(2)	0.0235(18)	0.021(2)	-0.0006(17)	0.0060(17)	-0.0021(17)
N3	0.030(2)	0.023(3)	0.023(2)	0.000(2)	0.012(2)	-0.003(2)
N4	0.0249(16)	0.0151(15)	0.0182(15)	-0.0011(12)	0.0047(12)	0.0017(13)
C1	0.053(3)	0.053(3)	0.021(2)	-0.001(2)	0.010(2)	0.018(3)
C2	0.032(2)	0.019(2)	0.040(3)	0.0031(18)	0.005(2)	0.0027(18)
C3	0.045(3)	0.065(4)	0.048(3)	0.031(3)	0.016(3)	0.017(3)
C4	0.031(2)	0.051(3)	0.033(3)	0.002(2)	0.011(2)	0.001(2)
C5	0.027(2)	0.018(2)	0.028(2)	-0.0047(16)	0.0066(16)	-0.0057(16)
C6	0.0197(18)	0.0201(19)	0.026(2)	0.0004(15)	0.0058(15)	-0.0079(16)
C7	0.0225(18)	0.0147(17)	0.0216(18)	0.0010(14)	0.0060(15)	0.0001(15)
C8	0.027(2)	0.019(2)	0.022(2)	-0.0005(16)	0.0062(16)	-0.0049(16)
C9	0.0223(19)	0.0163(18)	0.0234(19)	0.0012(15)	0.0060(15)	-0.0044(15)

Table S6 - (An)isotropic Displacement Parameters (continued)

for: $(1 \cdot \mathbf{L1})_{\infty}$

Atom	U(1,1) or U	U(2,2)	U(3,3)	U(2,3)	U(1,3)	U(1,2)
C10	0.0239(13)	0.0215(14)	0.0221(14)	0.0014(12)	0.0058(12)	-0.0011(12)
C11	0.0263(14)	0.0240(14)	0.0229(14)	0.0004(12)	0.0073(12)	-0.0012(13)
C12	0.0255(19)	0.0203(19)	0.0210(19)	0.0024(15)	0.0101(15)	0.0034(16)
C13	0.030(2)	0.023(2)	0.0182(19)	-0.0044(16)	0.0084(16)	-0.0028(17)
C14	0.028(2)	0.019(2)	0.027(2)	-0.0074(16)	0.0104(16)	-0.0069(17)
C15	0.0249(19)	0.0205(19)	0.0217(19)	-0.0047(16)	0.0083(15)	0.0005(16)
C16	0.027(2)	0.016(2)	0.029(2)	-0.0029(16)	0.0084(17)	-0.0051(17)
N13	0.028(2)	0.020(3)	0.023(3)	0.002(2)	0.010(2)	-0.002(2)
C110	0.0263(14)	0.0240(14)	0.0229(14)	0.0004(12)	0.0073(12)	-0.0012(13)
C111	0.0239(13)	0.0215(14)	0.0221(14)	0.0014(12)	0.0058(12)	-0.0011(12)
S15	0.0331(16)	0.0184(17)	0.0256(16)	-0.0002(12)	0.0108(12)	-0.0024(13)
N12	0.025(2)	0.023(2)	0.021(2)	0.000(2)	0.006(2)	-0.002(2)

==========

The Temperature Factor has the Form of Exp(-T) Where
T = 8*(Pi**2)*U*(Sin(Theta)/Lambda)**2 for Isotropic Atoms
T = 2*(Pi**2)*Sumij(h(i)*h(j)*U(i,j)*Astar(i)*Astar(j)), for
Anisotropic Atoms. Astar(i) are Reciprocal Axial Lengths and
h(i) are the Reflection Indices.

Table S7 - Bond Distances (Angstrom)
for: $(1 \cdot \mathbf{L1})_{\infty}$

Ni1A	-S1	2.5148(12)	N4	-C14	1.343(5)
Ni1A	-S2	2.4628(11)	N12	-C111	1.35(8)
Ni1A	-N1	2.095(3)	N12	-C110	1.33(7)
Ni1B	-S3	2.4573(12)	N13	-C111	1.322(13)
Ni1B	-S4	2.4935(11)	C5	-C6	1.373(5)
Ni1B	-N4	2.100(3)	C6	-C7	1.385(5)
S1	-P1	1.9700(15)	C7	-C10	1.483(5)
S2	-P1	1.9821(15)	C7	-C8	1.384(5)
S3	-P2	1.9807(15)	C7	-C111	1.483(5)
S4	-P2	1.9771(15)	C8	-C9	1.378(5)
S5	-N3	1.647(11)	C11	-C12	1.475(5)
S5	-C10	1.697(4)	C12	-C110	1.475(5)
S15	-N13	1.645(16)	C12	-C13	1.383(5)
S15	-C110	1.665(5)	C12	-C16	1.390(5)
P1	-O1	1.601(3)	C13	-C14	1.382(5)
P1	-O2	1.588(3)	C15	-C16	1.384(5)
P2	-O4	1.589(3)	C1	-H1A	1.06(5)
P2	-O3	1.584(3)	C1	-H1B	0.88(4)
O1	-C1	1.445(6)	C1	-H1C	1.03(6)
O2	-C2	1.451(5)	C2	-H2A	1.03(5)
O3	-C3	1.437(6)	C2	-H2B	0.99(4)
O4	-C4	1.440(6)	C2	-H2C	0.99(5)
N1	-C5	1.347(5)	C3	-H3A	1.07(6)
N1	-C9	1.342(5)	C3	-H3B	0.97(7)
N2	-C10	1.34(5)	C3	-H3C	0.94(6)
N2	-C11	1.34(5)	C4	-H4A	1.08(5)
N3	-C11	1.334(11)	C4	-H4B	0.90(4)
N4	-C15	1.333(5)	C4	-H4C	0.92(5)

Table S7 - Bond Distances (Angstrom) (continued)
for: $(1 \cdot \mathbf{L1})_{\infty}$

C5	-H5	0.93(4)	C13	-H13	0.87(4)
C6	-H6	0.98(3)	C14	-H14	0.90(4)
C8	-H8	0.91(4)	C15	-H15	0.92(4)
C9	-H9	0.92(3)	C16	-H16	0.89(4)

Table S8 - Bond Angles (Degrees)
for: $(1 \cdot \mathbf{L1})_{\infty}$

S1	-Ni1A	-S2	81.89(4)	S3_a	-Ni1B	-N4_a	88.96(9)
S1	-Ni1A	-N1	91.02(8)	S4_a	-Ni1B	-N4_a	90.67(8)
S1	-Ni1A	-S1_b	180.00	Ni1A	-S1	-P1	82.85(5)
S1	-Ni1A	-S2_b	98.11(4)	Ni1A	-S2	-P1	83.99(5)
S1	-Ni1A	-N1_b	88.98(8)	Ni1B	-S3	-P2	84.03(5)
S2	-Ni1A	-N1	89.58(9)	Ni1B	-S4	-P2	83.14(5)
S1_b	-Ni1A	-S2	98.11(4)	N3	-S5	-C10	92.7(4)
S2	-Ni1A	-S2_b	180.00	N13	-S15	-C110	93.0(5)
S2	-Ni1A	-N1_b	90.42(9)	S1	-P1	-S2	111.27(7)
S1_b	-Ni1A	-N1	88.98(8)	S1	-P1	-O1	113.10(12)
S2_b	-Ni1A	-N1	90.42(9)	S2	-P1	-O1	110.81(12)
N1	-Ni1A	-N1_b	180.00	S2	-P1	-O2	113.11(11)
S1_b	-Ni1A	-S2_b	81.89(4)	O1	-P1	-O2	98.45(15)
S1_b	-Ni1A	-N1_b	91.02(8)	S1	-P1	-O2	109.53(11)
S2_b	-Ni1A	-N1_b	89.58(9)	S3	-P2	-S4	110.63(6)
S3	-Ni1B	-S4	82.19(4)	S3	-P2	-O4	113.28(12)
S3	-Ni1B	-N4	88.96(9)	S4	-P2	-O3	113.87(12)
S3	-Ni1B	-S3_a	180.00	S3	-P2	-O3	111.35(12)
S3	-Ni1B	-S4_a	97.81(4)	O3	-P2	-O4	94.68(16)
S3	-Ni1B	-N4_a	91.04(9)	S4	-P2	-O4	112.24(13)
S4	-Ni1B	-N4	90.67(8)	P1	-O1	-C1	119.2(2)
S3_a	-Ni1B	-S4	97.81(4)	P1	-O2	-C2	119.0(3)
S4	-Ni1B	-S4_a	180.00	P2	-O3	-C3	119.5(3)
S4	-Ni1B	-N4_a	89.33(8)	P2	-O4	-C4	118.6(3)
S3_a	-Ni1B	-N4	91.04(9)	Ni1A	-N1	-C5	122.9(2)
S4_a	-Ni1B	-N4	89.33(8)	C5	-N1	-C9	116.5(3)
N4	-Ni1B	-N4_a	180.00	Ni1A	-N1	-C9	120.3(2)
S3_a	-Ni1B	-S4_a	82.19(4)	C10	-N2	-C11	108.4(12)

Table S8 - Bond Angles (Degrees) (continued)
for: $(1 \cdot \mathbf{L1})_{\infty}$

S5	-N3	-C11	107.7(7)	N4	-C15	-C16	123.7(3)
Ni1B	-N4	-C14	120.2(2)	C12	-C16	-C15	118.6(3)
Ni1B	-N4	-C15	122.7(2)	O1	-C1	-H1B	107(2)
C14	-N4	-C15	117.1(3)	O1	-C1	-H1C	105(3)
C110	-N12	-C111	108(2)	H1A	-C1	-H1B	115(3)
S15	-N13	-C111	107.8(9)	H1A	-C1	-H1C	116(4)
N1	-C5	-C6	123.7(3)	H1B	-C1	-H1C	106(4)
C5	-C6	-C7	118.6(3)	O1	-C1	-H1A	107(3)
C8	-C7	-C10	120.0(3)	O2	-C2	-H2A	109(3)
C8	-C7	-C111	120.0(3)	H2A	-C2	-H2B	112(4)
C6	-C7	-C10	121.0(3)	H2A	-C2	-H2C	113(4)
C6	-C7	-C111	121.0(3)	H2B	-C2	-H2C	107(4)
C6	-C7	-C8	118.8(3)	O2	-C2	-H2B	108(3)
C7	-C8	-C9	118.5(3)	O2	-C2	-H2C	107(3)
N1	-C9	-C8	123.8(3)	O3	-C3	-H3C	108(4)
N2	-C10	-C7	122.0(17)	O3	-C3	-H3A	115(4)
S5	-C10	-N2	111.9(17)	O3	-C3	-H3B	99(4)
S5	-C10	-C7	126.0(3)	H3A	-C3	-H3C	106(5)
N2	-C11	-C12	120.6(17)	H3B	-C3	-H3C	118(5)
N2	-C11	-N3	119.3(18)	H3A	-C3	-H3B	111(5)
N3	-C11	-C12	120.0(5)	O4	-C4	-H4A	107(3)
C11	-C12	-C13	120.2(3)	O4	-C4	-H4C	112(3)
C11	-C12	-C16	121.5(3)	H4A	-C4	-H4B	105(5)
C16	-C12	-C110	121.5(3)	O4	-C4	-H4B	111(3)
C13	-C12	-C16	118.2(3)	H4B	-C4	-H4C	103(4)
C13	-C12	-C110	120.2(3)	H4A	-C4	-H4C	118(4)
C12	-C13	-C14	119.2(3)	N1	-C5	-H5	116(2)
N4	-C14	-C13	123.2(3)	C6	-C5	-H5	120(2)

Table S8 - Bond Angles (Degrees) (continued)
for: $(1 \cdot \mathbf{L1})_{\infty}$

C7	-C6	-H6	124(2)	N12	-C111	-N13	118(2)
C5	-C6	-H6	117(2)	N12	-C111	-C7	122(2)
C7	-C8	-H8	122(2)	C12	-C13	-H13	124(2)
C9	-C8	-H8	120(2)	C14	-C13	-H13	117(2)
N1	-C9	-H9	114.5(19)	N4	-C14	-H14	115(2)
C8	-C9	-H9	121.7(19)	C13	-C14	-H14	122(2)
N12	-C110	-C12	120(3)	N4	-C15	-H15	117(2)
S15	-C110	-N12	112(3)	C16	-C15	-H15	119(2)
S15	-C110	-C12	127.3(3)	C12	-C16	-H16	120(2)
N13	-C111	-C7	119.1(7)	C15	-C16	-H16	121(2)

Table S9 - Torsion Angles (Degrees)
for: $(1 \cdot \mathbf{L1})_{\infty}$

S2	-Ni1A	-S1	-P1	-0.35(5)
N1	-Ni1A	-S1	-P1	89.07(9)
S2_b	-Ni1A	-S1	-P1	179.65(5)
N1_b	-Ni1A	-S1	-P1	-90.93(9)
S1_b	-Ni1A	-N1	-C5	56.0(3)
S2_b	-Ni1A	-N1	-C5	137.9(3)
S1	-Ni1A	-N1	-C9	49.7(3)
S1	-Ni1A	-S2	-P1	0.35(5)
N1	-Ni1A	-S2	-P1	-90.74(9)
S1_b	-Ni1A	-S2	-P1	-179.65(5)
N1_b	-Ni1A	-S2	-P1	89.26(9)
S1	-Ni1A	-N1	-C5	-124.0(3)
S2	-Ni1A	-N1	-C5	-42.1(3)
S2_b	-Ni1A	-N1	-C9	-48.4(3)
S2	-Ni1A	-N1	-C9	131.6(3)
S1_b	-Ni1A	-N1	-C9	-130.3(3)
S3	-Ni1B	-S4	-P2	-0.96(5)
N4_a	-Ni1B	-S3	-P2	-88.23(9)
S4	-Ni1B	-N4	-C14	131.3(3)
S3_a	-Ni1B	-N4	-C14	-130.8(3)
S3_a	-Ni1B	-N4	-C15	48.3(3)
N4_a	-Ni1B	-S4	-P2	90.18(9)
N4	-Ni1B	-S4	-P2	-89.82(9)
S3_a	-Ni1B	-S4	-P2	179.04(5)
S4	-Ni1B	-S3	-P2	0.96(5)
S3	-Ni1B	-N4	-C14	49.2(3)
S4_a	-Ni1B	-N4	-C15	130.4(3)
S4	-Ni1B	-N4	-C15	-49.6(3)

Table S9 - Torsion Angles (Degrees) (continued)
for: $(1 \cdot \mathbf{L1})_{\infty}$

N4	-Ni1B	-S3	-P2	91.77(9)
S4_a	-Ni1B	-S3	-P2	-179.04(5)
S4_a	-Ni1B	-N4	-C14	-48.7(3)
S3	-Ni1B	-N4	-C15	-131.7(3)
Ni1A	-S1	-P1	-O2	126.26(12)
Ni1A	-S1	-P1	-O1	-125.02(12)
Ni1A	-S1	-P1	-S2	0.47(6)
Ni1A	-S2	-P1	-O1	126.28(13)
Ni1A	-S2	-P1	-O2	-124.26(12)
Ni1A	-S2	-P1	-S1	-0.47(6)
Ni1B	-S3	-P2	-O3	126.41(13)
Ni1B	-S3	-P2	-O4	-128.31(13)
Ni1B	-S3	-P2	-S4	-1.28(6)
Ni1B	-S4	-P2	-S3	1.26(6)
Ni1B	-S4	-P2	-O4	128.87(13)
Ni1B	-S4	-P2	-O3	-125.03(13)
C10	-S5	-N3	-C11	-0.3(7)
N3	-S5	-C10	-N2	0(3)
N3	-S5	-C10	-C7	-176.4(5)
S2	-P1	-O1	-C1	-59.3(3)
O2	-P1	-O1	-C1	-178.0(3)
S1	-P1	-O2	-C2	175.9(2)
S2	-P1	-O2	-C2	-59.3(3)
S1	-P1	-O1	-C1	66.5(3)
O1	-P1	-O2	-C2	57.7(3)
S4	-P2	-O4	-C4	-61.6(3)
O4	-P2	-O3	-C3	-172.5(4)
S3	-P2	-O4	-C4	64.6(3)

Table S9 - Torsion Angles (Degrees) (continued)
for: $(1 \cdot \mathbf{L1})_{\infty}$

S3	-P2	-O3	-C3	-55.3(4)
O3	-P2	-O4	-C4	-179.8(3)
S4	-P2	-O3	-C3	70.6(4)
C9	-N1	-C5	-C6	-3.0(5)
Ni1A	-N1	-C5	-C6	171.0(3)
Ni1A	-N1	-C9	-C8	-172.1(3)
C5	-N1	-C9	-C8	2.1(5)
C10	-N2	-C11	-C12	-176(2)
C10	-N2	-C11	-N3	0(5)
C11	-N2	-C10	-C7	177(2)
C11	-N2	-C10	-S5	0(5)
S5	-N3	-C11	-C12	176.3(4)
S5	-N3	-C11	-N2	0(3)
C14	-N4	-C15	-C16	1.1(5)
C15	-N4	-C14	-C13	-0.9(5)
Ni1B	-N4	-C14	-C13	178.2(3)
Ni1B	-N4	-C15	-C16	-178.0(3)
N1	-C5	-C6	-C7	1.4(6)
C5	-C6	-C7	-C10	-175.1(3)
C5	-C6	-C7	-C8	1.3(5)
C6	-C7	-C8	-C9	-2.2(5)
C8	-C7	-C10	-N2	-158(3)
C8	-C7	-C10	-S5	18.5(5)
C6	-C7	-C10	-N2	19(3)
C10	-C7	-C8	-C9	174.3(3)
C6	-C7	-C10	-S5	-165.2(3)
C7	-C8	-C9	-N1	0.5(5)
N3	-C11	-C12	-C16	-16.3(7)

Table S9 - Torsion Angles (Degrees) (continued)

for: $(1 \cdot \mathbf{L1})_{\infty}$

N2	-C11	-C12	-C13	-17(3)
N2	-C11	-C12	-C16	160(3)
N3	-C11	-C12	-C13	167.6(6)
C11	-C12	-C16	-C15	-176.9(3)
C16	-C12	-C13	-C14	0.8(5)
C11	-C12	-C13	-C14	177.1(3)
C13	-C12	-C16	-C15	-0.7(5)
C12	-C13	-C14	-N4	0.0(5)
N4	-C15	-C16	-C12	-0.3(5)

Table S10 - Contact Distances(Angstrom)

for: $(1 \cdot \mathbf{L1})_{\infty}$

S1	.S15_d	3.715(5)	S4	.H15	3.07(4)
S2	.C8_e	3.466(4)	S4	.H14_a	2.87(3)
S2	.C9_e	3.444(4)	S4	.H4C	3.07(5)
S3	.C15_e	3.527(4)	S5	.H8	2.85(3)
S3	.C16_e	3.585(4)	S15	.H16	2.89(3)
S4	.C111_g	3.569(4)	O1	.S5_d	3.423(4)
S4	.C10_g	3.569(4)	O1	.C10_d	3.260(4)
S5	.O3_i	3.240(4)	O1	.C111_d	3.260(4)
S5	.O1_h	3.423(4)	O2	.C12_d	3.174(4)
S15	.S1_h	3.715(5)	O2	.C11_d	3.068(4)
S15	.C10	2.404(5)	O2	.C110_d	3.068(4)
S1	.H9	3.06(3)	O2	.C4_d	3.404(6)
S1	.H2A_c	3.12(5)	O2	.N2_d	3.24(6)
S1	.H5_b	3.11(3)	O3	.S5_g	3.240(4)
S1	.H1C	3.09(6)	O3	.C6_j	3.288(5)
S2	.H1A	2.92(4)	O4	.C5_j	3.419(5)
S2	.H5	2.90(3)	O1	.H2B	2.54(5)
S2	.H9_b	2.87(3)	O3	.H6_j	2.37(4)
S2	.H8_e	2.90(4)	O4	.H5_j	2.60(4)
S2	.H2A	3.00(5)	N2	.C2_h	3.28(5)
S2	.H4A_f	3.18(5)	N2	.O2_h	3.24(6)
S2	.H9_e	2.89(3)	N12	.C2_h	3.32(8)
S3	.H4B	3.14(5)	N13	.C11	2.401(15)
S3	.H3A	2.91(6)	N2	.H13	2.64(6)
S3	.H15_e	2.91(4)	N2	.H2B_h	2.83(7)
S3	.H14	2.96(4)	N2	.H6	2.72(6)
S3	.H15_a	3.03(3)	N3	.H16	2.61(3)
S3	.H16_e	3.05(3)	N12	.H2B_h	2.88(9)

Table S10 - Contact Distances(Angstrom) (continued)

for: $(1 \cdot \mathbf{L1})_{\infty}$

N12	.H13	2.62(9)	C110	.C10	2.173(5)
N12	.H6	2.72(8)	C111	.C11	2.173(5)
N13	.H8	2.58(4)	C111	.O1_h	3.260(4)
C1	.C5	3.595(6)	C111	.S4_i	3.569(4)
C2	.N2_d	3.28(6)	C13	.H2C_h	3.03(5)
C2	.C4_d	3.500(6)	C15	.H3A_a	2.78(7)
C2	.N12_d	3.32(8)	H1A	.C5	2.87(5)
C4	.C2_h	3.500(6)	H1A	.S2	2.92(4)
C4	.O2_h	3.404(6)	H1B	.C8_d	3.01(4)
C4	.C8_g	3.516(6)	H1C	.S1	3.09(6)
C5	.O4_f	3.419(5)	H1C	.C9	3.09(6)
C5	.C1	3.595(6)	H2A	.H9_e	2.53(6)
C6	.O3_f	3.288(5)	H2A	.S1_e	3.12(5)
C8	.C4_i	3.516(6)	H2A	.S2	3.00(5)
C8	.S2_c	3.466(4)	H2B	.N2_d	2.83(7)
C9	.S2_c	3.444(4)	H2B	.N12_d	2.88(9)
C10	.O1_h	3.260(4)	H2B	.O1	2.54(5)
C10	.S4_i	3.569(4)	H2C	.H4B_d	2.55(6)
C11	.O2_h	3.068(4)	H2C	.C13_d	3.03(5)
C12	.O2_h	3.174(4)	H3A	.C15_a	2.78(7)
C15	.S3_c	3.527(4)	H3A	.S3	2.91(6)
C16	.S3_c	3.585(4)	H3B	.H6_j	2.48(7)
C2	.H4B_d	3.10(5)	H3B	.H13_j	2.51(7)
C3	.H6_j	3.00(3)	H4A	.S2_j	3.18(5)
C5	.H1A	2.87(5)	H4B	.S3	3.14(5)
C8	.H1B_h	3.01(4)	H4B	.C2_h	3.10(4)
C9	.H1C	3.09(6)	H4B	.H2C_h	2.55(6)
C110	.O2_h	3.068(4)	H4C	.S4	3.07(5)

Table S10 - Contact Distances(Angstrom) (continued)

for: $(1 \cdot \mathbf{L1})_{\infty}$

H5	.O4_f	2.60(4)	H9	.S1	3.06(3)
H5	.S2	2.90(3)	H9	.S2_b	2.87(3)
H5	.S1_b	3.11(3)	H13	.H3B_f	2.51(7)
H6	.C3_f	3.00(3)	H13	.N12	2.62(9)
H6	.N2	2.72(6)	H13	.N2	2.64(6)
H6	.H3B_f	2.48(7)	H14	.S3	2.96(4)
H6	.O3_f	2.37(4)	H14	.S4_a	2.87(3)
H6	.N12	2.72(8)	H15	.S3_a	3.03(3)
H8	.S2_c	2.90(4)	H15	.S3_c	2.91(4)
H8	.N13	2.58(4)	H15	.S4	3.07(4)
H8	.S5	2.85(3)	H16	.N3	2.61(3)
H9	.S2_c	2.89(3)	H16	.S15	2.89(3)
H9	.H2A_c	2.53(6)	H16	.S3_c	3.05(3)

Table S11 - Hydrogen Bonds (Angstrom, Deg)

for: $(1 \cdot \mathbf{L1})_{\infty}$

C2	-- H2B	.. O1	0.99(4)	2.54(5)	2.891(5)	101(3)	.
C5	-- H5	.. O4	0.93(4)	2.60(4)	3.419(5)	148(3)	4_564
C6	-- H6	.. O3	0.98(3)	2.37(4)	3.288(5)	155(3)	4_564
C8	-- H8	.. S5	0.91(4)	2.85(3)	3.204(4)	104(2)	.
C9	-- H9	.. S2	0.92(3)	2.87(3)	3.376(4)	116(2)	3_775
C14	-- H14	.. S4	0.90(4)	2.87(3)	3.359(4)	115(3)	3_676

Translation of Symmetry Code to Equiv.Pos for $(1 \cdot \mathbf{L1})_{\infty}$

a =[3676.00] = 1-x,2-y,1-z
b =[3775.00] = 2-x,2-y,-z
c =[1565.00] = x,1+y,z
d =[2745.00] = 2-x,-1/2+y,1/2-z
e =[1545.00] = x,-1+y,z
f =[4564.00] = x,3/2-y,-1/2+z
g =[4575.00] = x,5/2-y,1/2+z
h =[2755.00] = 2-x,1/2+y,1/2-z
i =[4574.00] = x,5/2-y,-1/2+z
j =[4565.00] = x,3/2-y,1/2+z

Table S12 - Crystal Data and Details of the Structure Determination for: $(1 \cdot L2)_2$

Crystal Data			
Formula		C32 H40 N8 Ni2 O8 P4 S10	
Formula Weight			1226.68
Crystal System			Monoclinic
Space group		P21/c	(No. 14)
a, b, c [Angstrom]	14.0311(13)	14.9236(13)	12.8460(5)
alpha, beta, gamma [deg]	90	113.786(5)	90
V [Ang**3]			2461.4(3)
Z			2
D(calc) [g/cm**3]			1.655
Mu(MoKa) [/mm]			1.374
F(000)			1256
Crystal Size [mm]		0.04 x 0.22 x 0.32	
Data Collection			
Temperature (K)			120
Radiation [Angstrom]		MoKa	0.71073
Theta Min-Max [Deg]			3.1, 27.5
Dataset		-17: 18 ; -19: 17 ; -14: 16	
Tot., Uniq. Data, R(int)		19049, 5601, 0.036	
Observed data [I > 2.0 sigma(I)]			4837
Refinement			
Nref, Npar			5601, 330
R, wR2, S		0.0641, 0.1964, 1.16	
w = 1/[\S^2^(FO^2^)+(0.0617P)^2^+25.6697P] WHERE P=(FO^2^+2FC^2^)/			
Max. and Av. Shift/Error			2.30, 0.03
Min. and Max. Resd. Dens. [e/Ang^3]			-0.67, 1.85

Table S13 - Final Coordinates and Equivalent Isotropic Displacement Parameters of the non-Hydrogen atoms for: $(1 \cdot L2)_2$

Atom	x	y	z	U(eq) [Ang^2]
Ni1	0.23266(5)	0.54002(5)	0.41724(6)	0.0153(2)
S1	0.12323(12)	0.40826(10)	0.42612(12)	0.0210(4)
S2	0.30967(12)	0.42463(10)	0.33551(13)	0.0221(4)
S3	0.15626(12)	0.66268(10)	0.49039(12)	0.0202(4)
S4	0.35002(11)	0.66105(10)	0.41285(12)	0.0189(4)
*S5A	-0.2660(2)	0.54901(17)	-0.02445(19)	0.0197(7)
P1	0.20794(13)	0.34404(10)	0.35952(14)	0.0219(4)
P2	0.26650(12)	0.73593(10)	0.47290(13)	0.0190(4)
O1	0.1304(4)	0.2963(3)	0.2464(4)	0.0282(14)
O2	0.2654(4)	0.2590(3)	0.4316(4)	0.0297(14)
O3	0.2221(4)	0.8242(3)	0.4003(4)	0.0235(12)
O4	0.3377(4)	0.7865(3)	0.5853(4)	0.0252(12)
N1	0.1252(4)	0.5705(3)	0.2526(4)	0.0178(12)
*N2A	-0.1891(12)	0.5483(13)	0.1889(8)	0.0174(14)
*N3A	-0.3483(8)	0.5345(8)	0.0378(8)	0.0199(14)
N4	0.3310(4)	0.5082(3)	0.5857(4)	0.0179(12)
C1	0.1701(7)	0.2456(5)	0.1773(6)	0.038(2)
C2	0.3564(6)	0.2719(5)	0.5357(7)	0.041(2)
C3	0.1436(6)	0.8154(5)	0.2857(6)	0.0312(19)
C4	0.4073(5)	0.7346(5)	0.6801(5)	0.032(2)
C5	0.0236(5)	0.5633(4)	0.2287(5)	0.0190(17)
C6	-0.0537(4)	0.5742(4)	0.1208(5)	0.0177(17)
C7	-0.0240(5)	0.5981(4)	0.0337(5)	0.0212(17)
C8	0.0804(5)	0.6098(4)	0.0580(5)	0.0215(17)
C9	0.1525(5)	0.5940(4)	0.1677(5)	0.0197(17)
*C10A	-0.1625(4)	0.5594(4)	0.1020(4)	0.0180(9)

Table S13 - Final Coordinates and Equivalent Isotropic Displacement Parameters of the non-Hydrogen atoms (continued) for: $(1 \cdot L2)_2$

Atom	x	y	z	U(eq) [Ang^2]
*C11A	-0.2937(4)	0.5384(4)	0.1485(5)	0.0187(9)
C12	0.2894(4)	0.4971(4)	0.6627(5)	0.0166(17)
C13	0.3467(4)	0.4722(4)	0.7750(5)	0.0189(17)
C14	0.4532(5)	0.4567(5)	0.8099(6)	0.0271(19)
C15	0.4965(5)	0.4685(5)	0.7311(6)	0.0265(19)
C16	0.4340(5)	0.4948(4)	0.6217(5)	0.0217(17)
*N3B	-0.2356(12)	0.5639(16)	-0.0016(13)	0.0189(17)
*C10B	-0.2937(4)	0.5384(4)	0.1485(5)	0.0187(9)
*C11B	-0.1625(4)	0.5594(4)	0.1020(4)	0.0180(9)
*N2B	-0.191(2)	0.550(3)	0.1907(14)	0.0179(14)
*S5B	-0.3484(5)	0.5456(5)	0.0073(5)	0.0219(11)

U(eq) = 1/3 of the trace of the orthogonalized U Tensor

Starred Atom sites have a S.O.F less than 1.0

Table S14 - Hydrogen Atom Positions and Isotropic Displacement Parameters
for: $(1 \cdot L2)_2$

Atom	x	y	z	U(iso) [Ang^2]
H2C	0.41030	0.30280	0.51900	0.0620
H2A	0.38290	0.21360	0.57040	0.0620
H2B	0.33800	0.30820	0.58850	0.0620
H1B	0.21350	0.19640	0.22230	0.0570
H1C	0.21190	0.28470	0.15100	0.0570
H1A	0.11180	0.22100	0.11140	0.0570
H4C	0.36690	0.69210	0.70420	0.0470
H5	0.00330	0.55010	0.28920	0.0230
H4B	0.45610	0.70160	0.65720	0.0470
H7	-0.07490	0.60630	-0.04150	0.0260
H8	0.10240	0.62840	0.00040	0.0260
H9	0.22440	0.60010	0.18350	0.0240
H12	0.21670	0.50680	0.63880	0.0200
H14	0.494(7)	0.438(6)	0.886(7)	0.04(2)
H15	0.563(7)	0.459(5)	0.741(7)	0.04(2)
H16	0.459(6)	0.500(5)	0.561(6)	0.027(19)
H3A	0.12380	7/8	0.25170	0.0470
H3B	0.08220	0.78530	0.28760	0.0470
H3C	0.17140	0.77990	0.24010	0.0470
H4A	0.44620	0.77480	0.74340	0.0470

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The Temperature Factor has the Form of Exp(-T) Where
T = 8*(Pi**2)*U*(Sin(Theta)/Lambda)**2 for Isotropic Atoms

Table S15 - (An)isotropic Displacement Parameters
for: $(1 \cdot L2)_2$

Atom	U(1,1) or U	U(2,2)	U(3,3)	U(2,3)	U(1,3)	U(1,2)
Ni1	0.0162(4)	0.0189(4)	0.0125(4)	-0.0007(3)	0.0076(3)	-0.0022(3)
S1	0.0212(7)	0.0267(8)	0.0176(7)	-0.0001(6)	0.0103(6)	-0.0058(6)
S2	0.0258(8)	0.0198(7)	0.0272(8)	-0.0015(6)	0.0175(6)	-0.0016(6)
S3	0.0224(7)	0.0240(7)	0.0180(7)	-0.0008(5)	0.0122(6)	0.0013(5)
S4	0.0194(7)	0.0213(7)	0.0192(7)	-0.0036(5)	0.0112(6)	-0.0034(5)
S5A	0.0196(12)	0.0279(12)	0.0108(11)	-0.0001(8)	0.0053(8)	-0.0018(9)
P1	0.0269(8)	0.0183(7)	0.0229(8)	-0.0019(6)	0.0126(6)	-0.0050(6)
P2	0.0229(7)	0.0188(7)	0.0173(7)	-0.0027(6)	0.0101(6)	-0.0012(6)
O1	0.035(3)	0.028(2)	0.023(2)	-0.0069(19)	0.013(2)	-0.0062(19)
O2	0.035(3)	0.021(2)	0.030(2)	0.0024(19)	0.010(2)	-0.0035(19)
O3	0.033(2)	0.019(2)	0.019(2)	-0.0003(16)	0.0111(18)	-0.0003(17)
O4	0.031(2)	0.025(2)	0.018(2)	-0.0060(17)	0.0081(18)	-0.0025(18)
N1	0.020(2)	0.022(2)	0.014(2)	-0.0028(19)	0.0094(19)	-0.0022(19)
N2A	0.019(2)	0.021(3)	0.0136(19)	0.0021(18)	0.0079(17)	-0.0015(19)
N3A	0.020(2)	0.024(2)	0.014(3)	0.003(2)	0.005(2)	-0.003(2)
N4	0.019(2)	0.021(2)	0.016(2)	-0.0010(19)	0.0095(19)	-0.0026(19)
C1	0.071(5)	0.024(3)	0.022(3)	0.001(3)	0.022(3)	0.006(3)
C2	0.047(4)	0.025(4)	0.036(4)	0.010(3)	0.001(3)	-0.006(3)
C3	0.041(4)	0.025(3)	0.023(3)	0.002(3)	0.008(3)	0.004(3)
C4	0.033(4)	0.038(4)	0.016(3)	-0.008(3)	0.002(3)	0.000(3)
C5	0.021(3)	0.020(3)	0.018(3)	0.000(2)	0.010(2)	0.000(2)
C6	0.020(3)	0.019(3)	0.015(3)	-0.001(2)	0.008(2)	0.000(2)
C7	0.025(3)	0.023(3)	0.017(3)	0.003(2)	0.010(2)	0.001(2)
C8	0.028(3)	0.023(3)	0.018(3)	-0.001(2)	0.014(2)	-0.007(2)
C9	0.021(3)	0.021(3)	0.019(3)	0.000(2)	0.010(2)	-0.005(2)
C10A	0.0197(16)	0.0220(17)	0.0127(15)	0.0001(14)	0.0071(13)	-0.0022(14)

Table S15 - (An)isotropic Displacement Parameters (continued)
for: $(1 \cdot L2)_2$

Atom	U(1,1) or U	U(2,2)	U(3,3)	U(2,3)	U(1,3)	U(1,2)
C11A	0.0203(16)	0.0205(17)	0.0145(16)	0.0030(15)	0.0063(14)	-0.0018(14)
C12	0.020(3)	0.020(3)	0.013(3)	0.002(2)	0.010(2)	-0.001(2)
C13	0.017(3)	0.022(3)	0.016(3)	0.001(2)	0.005(2)	-0.004(2)
C14	0.021(3)	0.039(4)	0.020(3)	0.005(3)	0.007(2)	-0.001(3)
C15	0.013(3)	0.041(4)	0.025(3)	0.003(3)	0.007(2)	-0.002(2)
C16	0.018(3)	0.026(3)	0.026(3)	0.001(2)	0.014(2)	-0.002(2)
N3B	0.020(3)	0.024(3)	0.013(3)	0.000(3)	0.007(2)	-0.004(3)
C10B	0.0203(16)	0.0205(17)	0.0145(16)	0.0030(15)	0.0063(14)	-0.0018(14)
C11B	0.0197(16)	0.0220(17)	0.0127(15)	0.0001(14)	0.0071(13)	-0.0022(14)
N2B	0.020(2)	0.021(3)	0.013(2)	0.001(2)	0.007(2)	-0.002(2)
S5B	0.0216(17)	0.026(2)	0.014(2)	0.0018(18)	0.0030(17)	-0.0048(15)

==========

The Temperature Factor has the Form of Exp(-T) Where
T = 8*(Pi**2)*U*(Sin(Theta)/Lambda)**2 for Isotropic Atoms
T = 2*(Pi**2)*Sumij(h(i)*h(j)*U(i,j)*Astar(i)*Astar(j)), for
Anisotropic Atoms. Astar(i) are Reciprocal Axial Lengths and
h(i) are the Reflection Indices.

Table S16 - Bond Distances (Angstrom)
for: $(1 \cdot L2)_2$

Ni1	-S1	2.5255(18)	N3A	-C11A	1.317(11)
Ni1	-S2	2.4800(18)	N3B	-C11B	1.314(16)
Ni1	-S3	2.4891(18)	N4	-C12	1.346(8)
Ni1	-S4	2.4601(18)	N4	-C16	1.343(9)
Ni1	-N1	2.093(5)	C5	-C6	1.383(9)
Ni1	-N4	2.099(5)	C6	-C10A	1.463(9)
S1	-P1	1.971(2)	C6	-C11B	1.463(9)
S2	-P1	1.983(2)	C6	-C7	1.389(9)
S3	-P2	1.979(2)	C7	-C8	1.380(10)
S4	-P2	1.987(2)	C8	-C9	1.384(9)
S5A	-N3A	1.663(12)	C10B	-C13_a	1.461(9)
S5A	-C10A	1.694(6)	C11A	-C13_a	1.461(9)
S5B	-N3B	1.65(2)	C12	-C13	1.389(8)
S5B	-C10B	1.664(8)	C13	-C14	1.395(10)
P1	-O1	1.590(5)	C14	-C15	1.386(10)
P1	-O2	1.586(5)	C15	-C16	1.380(9)
P2	-O4	1.578(5)	C1	-H1A	0.9808
P2	-O3	1.589(5)	C1	-H1B	0.9799
O1	-C1	1.439(10)	C1	-H1C	0.9790
O2	-C2	1.442(10)	C2	-H2A	0.9799
O3	-C3	1.446(9)	C2	-H2B	0.9805
O4	-C4	1.441(8)	C2	-H2C	0.9806
N1	-C5	1.336(9)	C3	-H3A	0.9804
N1	-C9	1.340(8)	C3	-H3B	0.9806
N2A	-C10A	1.322(14)	C3	-H3C	0.9799
N2A	-C11A	1.353(18)	C4	-H4A	0.9803
N2B	-C11B	1.36(2)	C4	-H4B	0.9800
N2B	-C10B	1.33(3)	C4	-H4C	0.9803

Table S16 - Bond Distances (Angstrom) (continued)
for: 04slh021

C5	-H5	0.9500	C12	-H12	0.9503
C7	-H7	0.9496	C14	-H14	0.95(8)
C8	-H8	0.9508	C15	-H15	0.90(10)
C9	-H9	0.9498	C16	-H16	0.98(8)

Table S17 - Bond Angles (Degrees)
for: $(1 \cdot L2)_2$

S1	-Ni1	-S2	81.67(6)	S3	-P2	-O3	112.7(2)
S1	-Ni1	-S3	101.14(6)	S4	-P2	-O3	113.0(2)
S1	-Ni1	-S4	175.89(6)	S4	-P2	-O4	111.7(2)
S1	-Ni1	-N1	90.66(15)	O3	-P2	-O4	95.4(3)
S1	-Ni1	-N4	86.34(15)	S3	-P2	-O4	113.3(2)
S2	-Ni1	-S3	176.38(6)	P1	-O1	-C1	120.5(5)
S2	-Ni1	-S4	95.17(6)	P1	-O2	-C2	119.1(4)
S2	-Ni1	-N1	88.99(15)	P2	-O3	-C3	118.7(4)
S2	-Ni1	-N4	93.55(15)	P2	-O4	-C4	118.6(4)
S3	-Ni1	-S4	82.12(6)	Ni1	-N1	-C9	123.6(5)
S3	-Ni1	-N1	88.70(14)	C5	-N1	-C9	117.6(5)
S3	-Ni1	-N4	88.93(14)	Ni1	-N1	-C5	118.8(4)
S4	-Ni1	-N1	91.91(15)	C10A	-N2A	-C11A	108.8(8)
S4	-Ni1	-N4	91.26(15)	C10B	-N2B	-C11B	108.0(13)
N1	-Ni1	-N4	175.7(2)	S5A	-N3A	-C11A	107.4(8)
Ni1	-S1	-P1	82.81(8)	S5B	-N3B	-C11B	107.4(11)
Ni1	-S2	-P1	83.77(8)	Ni1	-N4	-C12	119.1(4)
Ni1	-S3	-P2	83.57(8)	Ni1	-N4	-C16	123.9(4)
Ni1	-S4	-P2	84.20(8)	C12	-N4	-C16	117.0(5)
N3A	-S5A	-C10A	92.5(4)	N1	-C5	-C6	123.6(6)
N3B	-S5B	-C10B	93.0(7)	C5	-C6	-C11B	119.5(5)
S1	-P1	-O1	107.7(2)	C7	-C6	-C11B	122.5(5)
S1	-P1	-O2	112.9(2)	C5	-C6	-C10A	119.5(5)
S2	-P1	-O1	113.6(2)	C7	-C6	-C10A	122.5(5)
S2	-P1	-O2	110.3(2)	C5	-C6	-C7	118.0(6)
O1	-P1	-O2	100.0(3)	C6	-C7	-C8	119.1(6)
S1	-P1	-S2	111.75(10)	C7	-C8	-C9	118.8(6)
S3	-P2	-S4	110.11(10)	N1	-C9	-C8	122.8(7)

Table S17 - Bond Angles (Degrees) (continued)
for: $(1 \cdot L2)_2$

N2A	-C10A	-C6	120.7(8)	H2A	-C2	-H2B	109.47
S5A	-C10A	-C6	127.3(4)	H2A	-C2	-H2C	109.42
S5A	-C10A	-N2A	111.9(8)	H2B	-C2	-H2C	109.45
N2B	-C10B	-C13_a	120.1(9)	O3	-C3	-H3A	109.50
S5B	-C10B	-C13_a	127.2(5)	O3	-C3	-H3B	109.42
S5B	-C10B	-N2B	112.5(9)	O3	-C3	-H3C	109.53
N3A	-C11A	-C13_a	119.3(7)	H3A	-C3	-H3B	109.44
N2A	-C11A	-C13_a	121.4(7)	H3A	-C3	-H3C	109.50
N2A	-C11A	-N3A	119.2(8)	H3B	-C3	-H3C	109.44
N2B	-C11B	-C6	121.2(11)	O4	-C4	-H4A	109.44
N2B	-C11B	-N3B	118.8(14)	O4	-C4	-H4B	109.50
N3B	-C11B	-C6	119.7(9)	O4	-C4	-H4C	109.48
N4	-C12	-C13	123.7(6)	H4A	-C4	-H4B	109.50
C11A_a	-C13	-C12	119.3(5)	H4A	-C4	-H4C	109.48
C11A_a	-C13	-C14	122.4(6)	H4B	-C4	-H4C	109.43
C12	-C13	-C14	118.3(6)	N1	-C5	-H5	118.22
C13	-C14	-C15	118.2(6)	C6	-C5	-H5	118.15
C14	-C15	-C16	119.6(7)	C6	-C7	-H7	120.38
N4	-C16	-C15	123.1(6)	C8	-C7	-H7	120.53
O1	-C1	-H1A	109.50	C7	-C8	-H8	120.60
O1	-C1	-H1B	109.47	C9	-C8	-H8	120.58
O1	-C1	-H1C	109.54	N1	-C9	-H9	118.60
H1A	-C1	-H1B	109.40	C8	-C9	-H9	118.59
H1A	-C1	-H1C	109.42	N4	-C12	-H12	118.09
H1B	-C1	-H1C	109.51	C13	-C12	-H12	118.19
O2	-C2	-H2A	109.57	C13	-C14	-H14	120(6)
O2	-C2	-H2B	109.49	C15	-C14	-H14	122(6)
O2	-C2	-H2C	109.42	C14	-C15	-H15	128(5)

Table S17 - Bond Angles (Degrees) (continued)
for: $(1 \cdot L2)_2$

C16	-C15	-H15	113(5)	C15	-C16	-H16	123(5)
N4	-C16	-H16	113(5)				

Table S18 - Torsion Angles (Degrees)
for: $(1 \cdot L2)_2$

S2	-Ni1	-S1	-P1	0.15(7)
S3	-Ni1	-S1	-P1	177.83(7)
N1	-Ni1	-S1	-P1	89.03(16)
N4	-Ni1	-S1	-P1	-93.98(16)
S2	-Ni1	-N4	-C12	-132.3(4)
S3	-Ni1	-N4	-C12	50.3(4)
S2	-Ni1	-S4	-P2	177.79(7)
S1	-Ni1	-S2	-P1	-0.15(7)
S4	-Ni1	-S2	-P1	177.21(7)
N1	-Ni1	-S2	-P1	-90.96(16)
N4	-Ni1	-S2	-P1	85.62(16)
S3	-Ni1	-N1	-C5	-61.0(4)
S4	-Ni1	-N1	-C5	-143.0(4)
S1	-Ni1	-N1	-C9	-137.3(4)
S1	-Ni1	-S3	-P2	177.27(7)
S4	-Ni1	-S3	-P2	-0.21(7)
N1	-Ni1	-S3	-P2	-92.32(16)
N4	-Ni1	-S3	-P2	91.21(16)
S1	-Ni1	-N4	-C12	-50.9(4)
S2	-Ni1	-N1	-C5	121.8(4)
S3	-Ni1	-N4	-C16	-132.2(4)
N4	-Ni1	-S4	-P2	-88.54(16)
S3	-Ni1	-S4	-P2	0.21(7)
N1	-Ni1	-S4	-P2	88.62(16)
S2	-Ni1	-N1	-C9	-55.7(4)
S4	-Ni1	-N4	-C16	-50.1(4)
S1	-Ni1	-N1	-C5	40.2(4)
S2	-Ni1	-N4	-C16	45.2(4)

Table S18 - Torsion Angles (Degrees) (continued)
for: $(1 \cdot L2)_2$

S3	-Ni1	-N1	-C9	121.5(4)
S4	-Ni1	-N1	-C9	39.4(4)
S4	-Ni1	-N4	-C12	132.4(4)
S1	-Ni1	-N4	-C16	126.6(4)
Ni1	-S1	-P1	-O2	124.9(2)
Ni1	-S1	-P1	-O1	-125.60(19)
Ni1	-S1	-P1	-S2	-0.20(9)
Ni1	-S2	-P1	-O1	122.3(2)
Ni1	-S2	-P1	-O2	-126.3(2)
Ni1	-S2	-P1	-S1	0.20(10)
Ni1	-S3	-P2	-O3	127.5(2)
Ni1	-S3	-P2	-O4	-125.6(2)
Ni1	-S3	-P2	-S4	0.27(9)
Ni1	-S4	-P2	-S3	-0.27(9)
Ni1	-S4	-P2	-O4	126.5(2)
Ni1	-S4	-P2	-O3	-127.2(2)
C10A	-S5A	-N3A	-C11A	0.1(8)
N3A	-S5A	-C10A	-N2A	2.6(11)
N3A	-S5A	-C10A	-C6	179.6(7)
S2	-P1	-O1	-C1	54.2(5)
O2	-P1	-O1	-C1	-63.3(5)
S1	-P1	-O2	-C2	-76.1(6)
S2	-P1	-O2	-C2	49.7(6)
S1	-P1	-O1	-C1	178.5(4)
O1	-P1	-O2	-C2	169.7(6)
S4	-P2	-O4	-C4	-56.0(5)
O4	-P2	-O3	-C3	-176.1(6)
S3	-P2	-O4	-C4	69.1(6)

Table S18 - Torsion Angles (Degrees) (continued)
for: $(1 \cdot L2)_2$

S3	-P2	-O3	-C3	-58.0(6)
O3	-P2	-O4	-C4	-173.4(5)
S4	-P2	-O3	-C3	67.6(6)
C9	-N1	-C5	-C6	3.4(9)
Ni1	-N1	-C5	-C6	-174.2(5)
Ni1	-N1	-C9	-C8	176.8(4)
C5	-N1	-C9	-C8	-0.7(8)
C10A	-N2A	-C11A	-C13_a	-178.0(8)
C10A	-N2A	-C11A	-N3A	4.9(18)
C11A	-N2A	-C10A	-C6	178.4(8)
C11A	-N2A	-C10A	-S5A	-4.4(16)
S5A	-N3A	-C11A	-C13_a	179.9(5)
S5A	-N3A	-C11A	-N2A	-2.9(14)
Ni1	-N4	-C16	-C15	-175.9(5)
C12	-N4	-C16	-C15	1.7(9)
Ni1	-N4	-C12	-C13	177.1(5)
C16	-N4	-C12	-C13	-0.6(8)
N1	-C5	-C6	-C7	-3.1(9)
N1	-C5	-C6	-C10A	176.2(5)
C5	-C6	-C10A	-S5A	-167.1(5)
C7	-C6	-C10A	-S5A	12.2(9)
C5	-C6	-C10A	-N2A	9.6(13)
C10A	-C6	-C7	-C8	-179.2(6)
C7	-C6	-C10A	-N2A	-171.1(11)
C5	-C6	-C7	-C8	0.1(9)
C6	-C7	-C8	-C9	2.4(9)
C7	-C8	-C9	-N1	-2.2(9)
N2A	-C11A	-C13_a	-C12_a	-17.9(13)

Table S18 - Torsion Angles (Degrees) (continued)
for: $(1 \cdot L2)_2$

N3A	-C11A	-C13_a	-C14_a	-21.9(11)
N2A	-C11A	-C13_a	-C14_a	161.0(11)
N3A	-C11A	-C13_a	-C12_a	159.2(8)
N4	-C12	-C13	-C11A_a	-179.7(6)
N4	-C12	-C13	-C14	-0.8(9)
C11A_a	-C13	-C14	-C15	180.0(6)
C12	-C13	-C14	-C15	1.1(10)
C13	-C14	-C15	-C16	-0.1(11)
C14	-C15	-C16	-N4	-1.4(10)

Table S19 - Contact Distances(Angstrom)
for: $(1 \cdot L2)_2$

S2	.C15_c	3.543(8)	S4	.H4A_d	3.1378
S2	.C16_c	3.618(8)	S4	.H9	2.9027
S5A	.C2_e	3.542(8)	S5A	.H2A_e	2.8794
S5A	.C8_f	3.673(7)	S5A	.H7	2.9056
S5A	.C9_f	3.583(7)	S5B	.H14_i	2.67(9)
S5A	.O2_e	3.352(5)	S5B	.H2A_e	2.6696
S5B	.O2_e	3.373(9)	S5B	.H14_a	2.89(10)
S5B	.C15_i	3.524(9)	P2	.H8_g	3.1909
S5B	.C10A	2.401(9)	O2	.N3B_h	3.12(2)
S5B	.C14_i	3.201(10)	O2	.C11B_h	3.262(8)
S5B	.C2_e	3.417(11)	O2	.S5A_h	3.352(5)
S1	.H5	2.8317	O2	.C10A_h	3.262(8)
S1	.H12	2.9080	O2	.S5B_h	3.373(9)
S1	.H1A_b	3.1176	O1	.H7_f	2.8274
S2	.H9	3.1965	O1	.H3B_h	2.8399
S2	.H2C	2.8584	O2	.H1B	2.6557
S2	.H15_c	2.93(9)	O3	.H8_g	2.5917
S2	.H16	3.02(7)	N2A	.C1_e	3.365(19)
S2	.H1C	3.0394	N2B	.C1_e	3.33(4)
S2	.H16_c	3.18(9)	N3A	.C14_i	3.331(13)
S3	.H5	3.1039	N3B	.O2_e	3.12(2)
S3	.H4C	3.1502	N3B	.C11A	2.407(18)
S3	.H3B	3.0052	N2A	.H5	2.4785
S3	.H12	2.9088	N2A	.H12_a	2.5331
S4	.H4B	2.9438	N2A	.H3A_h	2.7471
S4	.H3C	3.1409	N2A	.H1B_e	2.5726
S4	.H2C_c	3.1610	N2B	.H1B_e	2.5312
S4	.H16	3.06(7)	N2B	.H5	2.5002

Table S19 - Contact Distances(Angstrom) (continued)
for: $(1 \cdot L2)_2$

N2B	.H3A_h	2.7739	C14	.S5B_a	3.235(10)
N2B	.H12_a	2.5066	C14	.N3A_k	3.331(13)
N3A	.H14_i	2.70(9)	C15	.S2_c	3.543(8)
N3A	.H14_a	2.63(10)	C15	.S5B_k	3.524(9)
N3B	.H2A_e	2.9275	C16	.S2_c	3.618(8)
N3B	.H7	2.5845	C16	.C2	3.536(10)
C1	.N2A_h	3.365(19)	C1	.H7_f	2.7987
C1	.N2B_h	3.33(4)	C2	.H4A_j	3.0636
C1	.C7_f	3.537(10)	C2	.H1C_b	3.0725
C2	.C16	3.536(10)	C9	.H3C	2.9040
C2	.S5A_h	3.542(8)	C10B	.H1B_e	2.8415
C2	.S5B_h	3.417(11)	C11A	.H1B_e	2.8415
C6	.C8_f	3.502(8)	C12	.H4C	3.0770
C7	.C1_f	3.537(10)	C13	.H1B_b	3.0433
C7	.C8_f	3.300(8)	C15	.H4A_j	2.9829
C7	.C7_f	3.201(9)	C16	.H2B	3.0476
C8	.C7_f	3.300(8)	H1A	.S1_l	3.1176
C8	.C6_f	3.502(8)	H1B	.C11A_h	2.8415
C8	.S5A_f	3.673(7)	H1B	.O2	2.6557
C9	.S5A_f	3.583(7)	H1B	.N2A_h	2.5726
C10A	.O2_e	3.262(8)	H1B	.C13_l	3.0433
C10B	.C10A	2.175(9)	H1B	.N2B_h	2.5312
C11B	.C11A	2.175(9)	H1B	.C10B_h	2.8415
C11B	.O2_e	3.262(8)	H1C	.C2_l	3.0725
C12	.N2B_a	2.84(3)	H1C	.H7_f	2.4776
C13	.N2B_a	2.42(3)	H1C	.S2	3.0394
C13	.S5B_a	2.800(9)	H2A	.S5A_h	2.8794
C14	.S5B_k	3.201(10)	H2A	.S5B_h	2.6696

Table S19 - Contact Distances(Angstrom) (continued)
for: $(1 \cdot L2)_2$

H2A	.N3B_h	2.9275	H7	.H1C_f	2.4776
H2B	.C16	3.0476	H7	.C1_f	2.7987
H2C	.S4_c	3.1610	H7	.N3B	2.5845
H2C	.S2	2.8584	H7	.O1_f	2.8274
H3A	.N2B_e	2.7739	H8	.O3_d	2.5917
H3A	.N2A_e	2.7471	H8	.P2_d	3.1909
H3B	.O1_e	2.8399	H9	.S4	2.9027
H3B	.S3	3.0052	H9	.S2	3.1965
H3C	.C9	2.9040	H12	.S1	2.9080
H3C	.S4	3.1409	H12	.N2B_a	2.5066
H4A	.C15_m	2.9829	H12	.S3	2.9088
H4A	.S4_g	3.1378	H12	.N2A_a	2.5331
H4A	.C2_m	3.0636	H14	.N3A_k	2.70(9)
H4B	.S4	2.9438	H14	.N3A_a	2.63(10)
H4C	.C12	3.0770	H14	.S5B_a	2.89(10)
H4C	.S3	3.1502	H14	.S5B_k	2.67(9)
H5	.N2A	2.4785	H15	.S2_c	2.93(9)
H5	.S1	2.8317	H16	.S2_c	3.18(8)
H5	.N2B	2.5002	H16	.H16_c	2.29(12)
H5	.S3	3.1039	H16	.S2	3.02(7)
H7	.S5A	2.9056	H16	.S4	3.06(7)

Table S20 - Hydrogen Bonds (Angstrom, Deg)
for: $(1 \cdot L2)_2$

C1	-- H1B	.. N2A	0.9800	2.5700	3.365(19)	138.00	2_545
C2	-- H2C	.. S2	0.9800	2.8600	3.298(8)	108.00	.
C5	-- H5	.. S1	0.9500	2.8300	3.298(6)	111.00	.
C5	-- H5	.. N2A	0.9500	2.4800	2.826(19)	102.00	.
C8	-- H8	.. O3	0.9500	2.5900	3.504(9)	161.00	4_564
C12	-- H12	.. N2A	0.9500	2.5300	2.870(16)	101.00	3_566

Translation of Symmetry Code to Equiv.Pos for $(1 \cdot L2)_2$

a =[3566.00] = -x,1-y,1-z
b =[4555.00] = x,1/2-y,1/2+z
c =[3666.00] = 1-x,1-y,1-z
d =[4564.00] = x,3/2-y,-1/2+z
e =[2555.00] = -x,1/2+y,1/2-z
f =[3565.00] = -x,1-y,-z
g =[4565.00] = x,3/2-y,1/2+z
h =[2545.00] = -x,-1/2+y,1/2-z
i =[1454.00] = -1+x,y,-1+z
j =[2646.00] = 1-x,-1/2+y,3/2-z
k =[1656.00] = 1+x,y,1+z
l =[4554.00] = x,1/2-y,-1/2+z
m =[2656.00] = 1-x,1/2+y,3/2-z

Table S21 - Crystal Data and Details of the Structure Determination for: $(2 \cdot L1)_{\infty}$

Crystal Data			
Formula	C20 H28 N4 Ni O4 P2 S5		
Formula Weight	669.44		
Crystal System	Orthorhombic		
Space group	Pbcn	(No. 60)	
a, b, c [Angstrom]	11.6939(8)	15.2594(14)	15.9310(13)
V [Ang**3]	2842.8(4)		
Z	4		
D(calc) [g/cm**3]	1.564		
Mu(MoKa) [/mm]	1.197		
F(000)	1384		
Crystal Size [mm]	0.10 x	0.28 x	0.30
Data Collection			
Temperature (K)	120		
Radiation [Angstrom]	MoKa	0.71073	
Theta Min-Max [Deg]	3.1,	27.5	
Dataset	-15: 14 ; -18: 19 ; -20: 20		
Tot., Uniq. Data, R(int)	21763,	3263,	0.040
Observed data [I > 2.0 sigma(I)]	2733		
Refinement			
Nref, Npar	3263,	231	
R, wR2, S	0.0331,	0.0903,	0.86
w = 1/[\s^2^(Fo^2^)+(0.0576P)^2^+4.1336P] where P=(Fo^2^+2Fc^2^)/3			
Max. and Av. Shift/Error	0.04,	0.00	
Min. and Max. Resd. Dens. [e/Ang^3]	-0.49,	0.71	

Table S22 - Final Coordinates and Equivalent Isotropic Displacement Parameters of the non-Hydrogen atoms for: (2·L1)∞

Atom	x	y	z	U(eq) [Ang^2]
Ni1	0	0	1/2	0.0136(1)
S1	-0.11976(5)	0.01194(3)	0.62832(3)	0.0198(2)
S2	0.08302(4)	0.14869(3)	0.50288(3)	0.0187(2)
*S3	-0.4577(3)	0.2467(2)	0.2778(3)	0.0240(6)
P1	-0.18616(4)	-0.09683(4)	0.58302(3)	0.0187(2)
O1	-0.21806(13)	-0.16754(10)	0.65251(10)	0.0256(5)
O2	-0.30974(12)	-0.07657(10)	0.54748(11)	0.0243(5)
N1	-0.13802(14)	0.04577(11)	0.42748(10)	0.0164(5)
N2	-1/2	0.08843(17)	1/4	0.0190(7)
*N3	-0.4314(8)	0.2287(7)	0.2831(8)	0.022(2)
C1	-0.1281(2)	-0.20887(17)	0.70098(16)	0.0298(7)
C2	-0.1648(3)	-0.2993(2)	0.7249(3)	0.0484(10)
C3	-0.3763(2)	-0.14711(18)	0.5097(2)	0.0367(9)
C4	-0.4696(3)	-0.1091(2)	0.4575(2)	0.0435(10)
C5	-0.19276(17)	0.11889(14)	0.45002(13)	0.0190(6)
C6	-0.28608(18)	0.15175(14)	0.40744(14)	0.0206(6)
C7	-0.32794(16)	0.10532(13)	0.33875(13)	0.0176(6)
C8	-0.27327(17)	0.02882(14)	0.31555(13)	0.0178(6)
C9	-0.17814(18)	0.00214(13)	0.36048(13)	0.0177(6)
C10	-0.42541(17)	0.13973(14)	0.29042(13)	0.0190(6)

U(eq) = 1/3 of the trace of the orthogonalized U Tensor

Starred Atom sites have a S.O.F less than 1.0

Table S23 - Hydrogen Atom Positions and Isotropic Displacement Parameters
for: (2·L1)∞

Atom	x	y	z	U(iso) [Ang^2]
H1A	-0.055(2)	-0.2102(18)	0.6645(17)	0.031(7)
H1B	-0.114(3)	-0.174(2)	0.749(2)	0.045(8)
H2A	-0.234(3)	-0.294(2)	0.762(2)	0.067(11)
H2B	-0.177(2)	-0.3263(16)	0.6733(18)	0.020(7)
H2C	-0.098(3)	-0.328(3)	0.759(2)	0.071(11)
H3A	-0.397(3)	-0.189(2)	0.552(2)	0.054(10)
H3B	-0.333(4)	-0.169(3)	0.456(3)	0.085(13)
H4A	-0.435(3)	-0.074(3)	0.410(3)	0.073(12)
H4B	-0.518(3)	-0.161(3)	0.428(3)	0.082(13)
H4C	-0.524(3)	-0.072(2)	0.501(2)	0.057(10)
H5	-0.161(2)	0.1482(18)	0.4975(16)	0.027(7)
H6	-0.320(2)	0.2024(17)	0.4258(16)	0.022(6)
H8	-0.296(2)	-0.0041(15)	0.2668(17)	0.023(7)
H9	-0.135(2)	-0.0484(17)	0.3446(16)	0.027(7)

The Temperature Factor has the Form of Exp(-T) Where
T = 8*(Pi**2)*U*(Sin(Theta)/Lambda)**2 for Isotropic Atoms

Table S24 - (An)isotropic Displacement Parameters
for: (2·L1)∞

Atom	U(1,1) or U	U(2,2)	U(3,3)	U(2,3)	U(1,3)	U(1,2)
Ni1	0.0131(2)	0.0147(2)	0.0129(2)	-0.0013(1)	-0.0012(1)	-0.0005(1)
S1	0.0207(3)	0.0226(3)	0.0162(3)	-0.0030(2)	0.0026(2)	-0.0017(2)
S2	0.0187(3)	0.0160(3)	0.0214(3)	-0.0025(2)	-0.0004(2)	-0.0019(2)
S3	0.0185(13)	0.0199(10)	0.0337(8)	-0.0011(8)	-0.0100(9)	0.0000(8)
P1	0.0167(3)	0.0187(3)	0.0208(3)	0.0019(2)	0.0011(2)	-0.0010(2)
O1	0.0221(8)	0.0249(8)	0.0297(9)	0.0085(7)	0.0045(6)	-0.0005(6)
O2	0.0165(7)	0.0211(8)	0.0353(9)	0.0002(7)	-0.0026(6)	-0.0014(6)
N1	0.0161(8)	0.0181(9)	0.0149(8)	-0.0009(7)	-0.0009(6)	-0.0003(7)
N2	0.0159(12)	0.0230(13)	0.0180(12)	0	-0.0029(9)	0
N3	0.009(4)	0.032(5)	0.025(3)	-0.007(3)	-0.008(3)	0.002(3)
C1	0.0335(13)	0.0300(13)	0.0260(12)	0.0077(10)	0.0016(10)	0.0076(10)
C2	0.0405(16)	0.0368(16)	0.068(2)	0.0223(16)	0.0164(16)	0.0102(13)
C3	0.0234(12)	0.0247(13)	0.0621(19)	-0.0028(13)	-0.0099(12)	-0.0055(10)
C4	0.0379(15)	0.0465(18)	0.0462(18)	0.0029(14)	-0.0085(13)	-0.0141(13)
C5	0.0206(10)	0.0185(10)	0.0179(10)	-0.0034(8)	-0.0031(8)	0.0009(8)
C6	0.0203(10)	0.0200(11)	0.0216(10)	-0.0026(9)	-0.0005(8)	0.0036(8)
C7	0.0149(9)	0.0208(10)	0.0171(10)	0.0012(8)	-0.0012(8)	-0.0009(7)
C8	0.0181(10)	0.0202(10)	0.0150(9)	-0.0020(8)	-0.0016(8)	-0.0024(8)
C9	0.0195(10)	0.0167(10)	0.0169(10)	-0.0018(8)	0.0011(8)	-0.0005(8)
C10	0.0172(9)	0.0213(11)	0.0186(10)	-0.0017(8)	-0.0015(8)	0.0014(8)

==========

The Temperature Factor has the Form of Exp(-T) Where
T = 8*(Pi**2)*U*(Sin(Theta)/Lambda)**2 for Isotropic Atoms
T = 2*(Pi**2)*Sumij(h(i)*h(j)*U(i,j)*Astar(i)*Astar(j)), for Anisotropic Atoms. Astar(i) are Reciprocal Axial Lengths and h(i) are the Reflection Indices.

Table S25 - Bond Distances (Angstrom)
for: (2·L1)∞

Ni1	-S1	2.4847(6)	C6	-C7	1.393(3)
Ni1	-S2	2.4683(5)	C7	-C8	1.381(3)
Ni1	-P1	2.9447(6)	C7	-C10	1.472(3)
Ni1	-N1	2.1042(16)	C8	-C9	1.384(3)
S1	-P1	1.9694(8)	C1	-H1A	1.03(2)
S2	-P1_b	1.9884(7)	C1	-H1B	0.95(3)
S3	-N3	0.421(11)	C2	-H2A	1.01(3)
S3	-C10	1.687(4)	C2	-H2B	0.93(3)
P1	-O1	1.5903(17)	C2	-H2C	1.05(4)
P1	-O2	1.5826(15)	C3	-H3A	0.96(3)
O1	-C1	1.449(3)	C3	-H3B	1.05(5)
O2	-C3	1.458(3)	C4	-H4A	1.01(5)
N1	-C5	1.336(3)	C4	-H4B	1.08(4)
N1	-C9	1.343(3)	C4	-H4C	1.10(3)
N2	-C10	1.337(3)	C5	-H5	0.95(3)
N3	-C10	1.364(11)	C6	-H6	0.92(3)
C1	-C2	1.495(4)	C8	-H8	0.96(3)
C3	-C4	1.489(4)	C9	-H9	0.96(3)
C5	-C6	1.379(3)			

Table S26 - Bond Angles (Degrees)
for: (2·L1)∞

S1	-Ni1	-S2	97.99(2)	Ni1	-S1	-P1	81.89(2)
S1	-Ni1	-P1	41.46(2)	Ni1	-S2	-P1_b	81.95(2)
S1	-Ni1	-N1	89.72(5)	N3	-S3	-C10	35.0(14)
S1	-Ni1	-S1_b	180.00	Ni1	-P1	-S1	56.65(2)
S1	-Ni1	-S2_b	82.01(2)	Ni1	-P1	-O1	145.74(6)
S1	-Ni1	-P1_b	138.54(2)	Ni1	-P1	-O2	114.60(6)
S1	-Ni1	-N1_b	90.28(5)	Ni1	-P1	-S2_b	56.09(2)
S2	-Ni1	-P1	138.04(2)	S1	-P1	-O1	114.16(6)
S2	-Ni1	-N1	90.39(5)	S1	-P1	-O2	109.06(7)
S1_b	-Ni1	-S2	82.01(2)	S1	-P1	-S2_b	110.39(3)
S2	-Ni1	-S2_b	180.00	O1	-P1	-O2	99.64(8)
S2	-Ni1	-P1_b	41.96(2)	S2_b	-P1	-O1	110.57(7)
S2	-Ni1	-N1_b	89.61(5)	S2_b	-P1	-O2	112.67(7)
P1	-Ni1	-N1	81.15(5)	P1	-O1	-C1	119.73(14)
S1_b	-Ni1	-P1	138.54(2)	P1	-O2	-C3	119.40(14)
S2_b	-Ni1	-P1	41.96(2)	Ni1	-N1	-C5	119.82(13)
P1	-Ni1	-P1_b	180.00	Ni1	-N1	-C9	122.68(13)
P1	-Ni1	-N1_b	98.85(5)	C5	-N1	-C9	117.42(17)
S1_b	-Ni1	-N1	90.28(5)	C10	-N2	-C10_a	108.3(2)
S2_b	-Ni1	-N1	89.61(5)	S3	-N3	-C10	134.7(17)
P1_b	-Ni1	-N1	98.85(5)	O1	-C1	-C2	109.2(2)
N1	-Ni1	-N1_b	180.00	O2	-C3	-C4	109.5(2)
S1_b	-Ni1	-S2_b	97.99(2)	N1	-C5	-C6	123.42(19)
S1_b	-Ni1	-P1_b	41.46(2)	C5	-C6	-C7	118.66(19)
S1_b	-Ni1	-N1_b	89.72(5)	C6	-C7	-C8	118.53(18)
S2_b	-Ni1	-P1_b	138.04(2)	C6	-C7	-C10	120.11(18)
S2_b	-Ni1	-N1_b	90.39(5)	C8	-C7	-C10	121.32(18)
P1_b	-Ni1	-N1_b	81.15(5)	C7	-C8	-C9	118.83(19)

Table S26 - Bond Angles (Degrees) (continued)
for: (2·L1)∞

N1	-C9	-C8	123.10(19)	O2	-C3	-H3B	108(3)
S3	-C10	-N2	111.3(2)	C4	-C3	-H3A	118(2)
S3	-C10	-N3	10.2(4)	C4	-C3	-H3B	91(3)
S3	-C10	-C7	125.5(2)	H3A	-C3	-H3B	119(3)
N2	-C10	-N3	120.5(5)	C3	-C4	-H4A	109(2)
N2	-C10	-C7	123.23(19)	C3	-C4	-H4B	110(2)
N3	-C10	-C7	116.1(5)	C3	-C4	-H4C	105.8(17)
O1	-C1	-H1A	108.0(15)	H4A	-C4	-H4B	106(4)
O1	-C1	-H1B	108(2)	H4A	-C4	-H4C	116(3)
C2	-C1	-H1A	111.3(15)	H4B	-C4	-H4C	110(3)
C2	-C1	-H1B	111.3(19)	N1	-C5	-H5	114.7(15)
H1A	-C1	-H1B	109(3)	C6	-C5	-H5	121.8(15)
C1	-C2	-H2A	107.9(18)	C5	-C6	-H6	119.5(16)
C1	-C2	-H2B	103.2(16)	C7	-C6	-H6	121.8(15)
C1	-C2	-H2C	108(2)	C7	-C8	-H8	122.0(14)
H2A	-C2	-H2B	116(2)	C9	-C8	-H8	119.1(14)
H2A	-C2	-H2C	109(3)	N1	-C9	-H9	115.2(15)
H2B	-C2	-H2C	113(3)	C8	-C9	-H9	121.7(15)
O2	-C3	-H3A	109.7(19)				

Table S27 - Torsion Angles (Degrees)
for: (2·L1)∞

S2	-Ni1	-S1	-P1	167.24(2)
N1	-Ni1	-S1	-P1	76.89(5)
S2_b	-Ni1	-S1	-P1	-12.76(2)
P1_b	-Ni1	-S1	-P1	180.00(3)
N1_b	-Ni1	-S1	-P1	-103.11(5)
S1	-Ni1	-S2	-P1_b	167.37(2)
P1	-Ni1	-S2	-P1_b	-180.00(3)
N1	-Ni1	-S2	-P1_b	-102.86(5)
S2	-Ni1	-P1	-S1	-19.09(3)
N1	-Ni1	-P1	-S1	-99.71(5)
S1_b	-Ni1	-P1	-S1	-180.00(4)
S2_b	-Ni1	-P1	-S1	160.91(3)
N1_b	-Ni1	-P1	-S1	80.29(5)
S1	-Ni1	-P1	-O1	-84.49(11)
S2	-Ni1	-P1	-O1	-103.58(11)
N1	-Ni1	-P1	-O1	175.80(12)
S1_b	-Ni1	-P1	-O1	95.51(11)
S2_b	-Ni1	-P1	-O1	76.42(11)
N1_b	-Ni1	-P1	-O1	-4.20(12)
S1	-Ni1	-P1	-O2	97.38(7)
S2	-Ni1	-P1	-O2	78.29(7)
N1	-Ni1	-P1	-O2	-2.33(8)
S1_b	-Ni1	-P1	-O2	-82.62(7)
S2_b	-Ni1	-P1	-O2	-101.71(7)
N1_b	-Ni1	-P1	-O2	177.67(8)
S1	-Ni1	-P1	-S2_b	-160.91(3)
S2	-Ni1	-P1	-S2_b	-180.00(1)
N1	-Ni1	-P1	-S2_b	99.38(5)

Table S27 - Torsion Angles (Degrees) (continued)
for: (2·L1)∞

S2	-Ni1	-N1	-C5	-47.35(15)
P1	-Ni1	-N1	-C5	91.38(15)
S1_b	-Ni1	-N1	-C5	-129.36(15)
S2_b	-Ni1	-N1	-C5	132.65(15)
P1_b	-Ni1	-N1	-C5	-88.62(15)
S1	-Ni1	-N1	-C9	-126.12(15)
S2	-Ni1	-N1	-C9	135.89(15)
P1	-Ni1	-N1	-C9	-85.38(15)
S1_b	-Ni1	-N1	-C9	53.88(15)
S2_b	-Ni1	-N1	-C9	-44.11(15)
P1_b	-Ni1	-N1	-C9	94.62(15)
S1	-Ni1	-N1	-C5	50.64(15)
Ni1	-S1	-P1	-O1	142.12(7)
Ni1	-S1	-P1	-O2	-107.46(7)
Ni1	-S1	-P1	-S2_b	16.84(3)
Ni1	-S2_b	-P1	-O1	-144.24(6)
Ni1	-S2_b	-P1	-O2	105.24(7)
Ni1	-S2_b	-P1	-S1	-16.95(3)
N3	-S3	-C10	-N2	-156(3)
N3	-S3	-C10	-C7	24(3)
S1	-P1	-O2	-C3	179.48(17)
O1	-P1	-O2	-C3	-60.66(19)
Ni1	-P1	-O1	-C1	-0.7(2)
S1	-P1	-O1	-C1	-66.37(17)
S2_b	-P1	-O1	-C1	58.81(17)
Ni1	-P1	-O2	-C3	118.27(17)
S2_b	-P1	-O2	-C3	56.54(19)
O2	-P1	-O1	-C1	177.58(16)

Table S27 - Torsion Angles (Degrees) (continued)
for: (2·L1)∞

P1	-O1	-C1	-C2	-149.7(2)
P1	-O2	-C3	-C4	-161.95(19)
Ni1	-N1	-C5	-C6	-177.94(16)
Ni1	-N1	-C9	-C8	175.83(15)
C5	-N1	-C9	-C8	-1.0(3)
C9	-N1	-C5	-C6	-1.0(3)
C10_a	-N2	-C10	-C7	-177.32(18)
C10_a	-N2	-C10	-S3	2.3(2)
C10_a	-N2	-C10	-N3	-2.5(6)
S3	-N3	-C10	-C7	-159(3)
S3	-N3	-C10	-N2	26(3)
N1	-C5	-C6	-C7	1.9(3)
C5	-C6	-C7	-C10	-178.30(19)
C5	-C6	-C7	-C8	-0.8(3)
C10	-C7	-C8	-C9	176.41(19)
C6	-C7	-C10	-S3	29.8(3)
C8	-C7	-C10	-S3	-147.6(3)
C6	-C7	-C8	-C9	-1.1(3)
C8	-C7	-C10	-N2	31.9(3)
C8	-C7	-C10	-N3	-143.1(6)
C6	-C7	-C10	-N3	34.4(6)
C6	-C7	-C10	-N2	-150.63(18)
C7	-C8	-C9	-N1	2.0(3)

Table S28 - Contact Distances(Angstrom)
for: (2·L1)∞

S1	.C8_d	3.536(2)	C7	.O1_f	3.370(3)
S2	.C6_e	3.696(2)	C8	.O1_f	3.412(3)
S3	.C2_f	3.617(5)	C8	.S1_f	3.536(2)
S1	.H5	2.98(3)	C10	.O1_f	3.299(3)
S1	.H8_d	3.02(3)	C1	.H1A_g	3.03(3)
S1	.H9_b	3.06(2)	C1	.H1B_g	2.99(3)
S2	.H6_e	2.78(3)	C2	.H4B_h	3.04(4)
S2	.H1A_b	2.85(3)	C4	.H4C_i	2.84(3)
S2	.H3B_b	3.01(5)	C6	.H4C_i	2.92(3)
S2	.H9_b	2.94(3)	C7	.H1B_f	3.07(3)
S2	.H5	2.85(2)	C8	.H4A	2.88(4)
S3	.H6	2.93(3)	C8	.H1B_f	3.08(3)
S3	.H2A_f	2.73(3)	H1A	.H4B_h	2.49(5)
O1	.C10_d	3.299(3)	H1A	.C1_g	3.03(3)
O1	.C7_d	3.370(3)	H1A	.H1B_g	2.47(4)
O1	.C8_d	3.412(3)	H1A	.S2_b	2.85(3)
O1	.H3A	2.66(3)	H1B	.C1_g	2.99(3)
N3	.C2_f	3.426(10)	H1B	.H1A_g	2.47(4)
N2	.H8_a	2.78(2)	H1B	.C7_d	3.07(3)
N2	.H8	2.78(2)	H1B	.C8_d	3.08(3)
N3	.H6	2.65(3)	H2A	.S3_d	2.73(3)
N3	.H2A_f	2.54(4)	H2A	.N3_d	2.54(4)
C1	.C1_g	3.379(3)	H2B	.H4B_h	2.47(5)
C1	.C7_d	3.574(3)	H2C	.H2C_g	2.31(5)
C2	.S3_d	3.617(5)	H3A	.O1	2.66(3)
C2	.N3_d	3.426(10)	H3B	.S2_b	3.01(5)
C6	.S2_j	3.696(2)	H4A	.C8	2.88(4)
C7	.C1_f	3.574(3)	H4B	.C2_k	3.04(4)

Table S28 - Contact Distances(Angstrom) (continued)
for: (2·L1)∞

H4B	.H1A_k	2.49(5)	H6	.S3	2.93(3)
H4B	.H2B_k	2.47(5)	H6	.N3	2.65(3)
H4C	.C4_i	2.84(3)	H6	.S2_j	2.78(3)
H4C	.C6_i	2.92(3)	H8	.N2	2.78(2)
H4C	.H4C_i	2.27(4)	H8	.S1_f	3.02(3)
H5	.S1	2.98(3)	H9	.S1_b	3.06(2)
H5	.S2	2.85(2)	H9	.S2_b	2.94(3)

Table S29 - Hydrogen Bonds (Angstrom, Deg)
for: $(2{\cdot}L1)_{\infty}$

C1	-- H1A	.. S2	1.03(2)	2.85(3)	3.416(3)	115.2(17)	5_556
C2	-- H2A	.. S3	1.01(3)	2.73(3)	3.617(5)	148(2)	8_555
C2	-- H2A	.. N3	1.01(3)	2.54(4)	3.426(10)	147(2)	8_555
C5	-- H5	.. S2	0.95(3)	2.85(2)	3.364(2)	114.5(17)	.
C6	-- H6	.. S2	0.92(3)	2.78(3)	3.696(2)	174(2)	3_456

Translation of Symmetry Code to Equiv.Pos for $(2{\cdot}L1)_{\infty}$

a =[4455.00] = -1-x,y,1/2-z
b =[5556.00] = -x,-y,1-z
c =[8655.00] = 1+x,-y,1/2+z
d =[8555.00] = x,-y,1/2+z
e =[3556.00] = 1/2+x,1/2-y,1-z
f =[8554.00] = x,-y,-1/2+z
g =[4556.00] = -x,y,3/2-z
h =[3546.00] = 1/2+x,-1/2-y,1-z
i =[5456.00] = -1-x,-y,1-z
j =[3456.00] = -1/2+x,1/2-y,1-z
k =[3446.00] = -1/2+x,-1/2-y,1-z

Table S30 - Crystal Data and Details of the Structure Determination for: (2·L2)2

Crystal Data			
Formula		C40 H56 N8 Ni2 O8 P4 S10	
Formula Weight			1338.89
Crystal System			Triclinic
Space group		P-1	(No. 2)
a, b, c [Angstrom]	11.728(2)	14.435(3)	18.657(4)
alpha, beta, gamma [deg]	104.40(3)	103.02(3)	101.92(3)
V [Ang**3]			2862.9(13)
Z			2
D(calc) [g/cm**3]			1.553
Mu(X) [/mm]			0.000
F(000)			1384
Crystal Size [mm]		0.01 x 0.03 x 0.10	
Data Collection			
Temperature (K)			120
Radiation [Angstrom]		X	0.68930
Theta Min-Max [Deg]			2.4, 27.5
Dataset		-15: 15 ; -18: 18 ; -24: 24	
Tot., Uniq. Data, R(int)		25481, 12921, 0.036	
Observed data [I > 2.0 sigma(I)]			9150
Refinement			
Nref, Npar			12921, 657
R, wR2, S		0.0969, 0.2663, 1.14	
w = 1/[\S^2^(FO^2^)+(0.1059P)^2^+17.9696P] WHERE P=(FO^2^+2FC^2^)/			
Max. and Av. Shift/Error			0.01, 0.00
Min. and Max. Resd. Dens. [e/Ang^3]			-1.51, 3.19

Table S31 - Final Coordinates and Equivalent Isotropic Displacement Parameters of the non-Hydrogen atoms for: (2·L2)2

Atom	x	y	z	U(eq) [Ang^2]
Ni1	0.50499(8)	0.72745(6)	-0.06184(5)	0.0299(3)
S1	0.33627(19)	0.79909(15)	-0.04002(10)	0.0389(6)
S2	0.34956(18)	0.56838(14)	-0.09077(11)	0.0373(5)
S3	0.6629(2)	0.88629(15)	-0.03672(11)	0.0486(6)
S4	0.6759(2)	0.65461(17)	-0.08097(14)	0.0494(7)
S5	0.6519(2)	0.96999(17)	0.34056(12)	0.0468(7)
P1	0.2512(3)	0.6582(2)	-0.0604(2)	0.0633(10)
P2	0.7535(2)	0.7922(2)	-0.07437(12)	0.0515(7)
O1	0.1254(12)	0.6270(9)	-0.0981(7)	0.133(2)
O2	0.2270(13)	0.6537(9)	0.0246(8)	0.142(5)
O3	0.8851(6)	0.8403(7)	-0.0189(4)	0.087(3)
O4	0.7706(10)	0.7899(7)	-0.1561(4)	0.098(3)
N1	0.5590(6)	0.7405(4)	0.0568(3)	0.0336(17)
N2	0.5939(5)	1.0132(4)	0.2173(3)	0.0275(17)
N3	0.6397(4)	1.0731(4)	0.3552(3)	0.0205(7)
N4	0.5499(5)	1.2768(4)	0.1787(3)	0.0301(17)
C1	0.0906(10)	0.6176(11)	-0.1759(7)	0.095(2)
C2	-0.0508(10)	0.5922(10)	-0.2173(7)	0.083(2)
C3	0.2104(18)	0.5722(13)	0.0519(11)	0.142(4)
C4	0.1271(14)	0.5994(12)	0.1008(9)	0.106(3)
C5	0.9880(10)	0.8095(11)	-0.0270(8)	0.103(3)
C6	1.0958(10)	0.8743(9)	0.0446(7)	0.081(2)
C7	0.7670(19)	0.8656(11)	-0.1900(8)	0.139(4)
C8	0.7886(10)	0.8318(8)	-0.2691(6)	0.0687(17)
C9	0.5701(6)	0.8273(5)	0.1095(4)	0.0309(19)
C10	0.5995(6)	0.8396(5)	0.1884(4)	0.0300(19)

Table S31 - Final Coordinates and Equivalent Isotropic Displacement Parameters of the non-Hydrogen atoms (continued) for: (2·L2)2

Atom	x	y	z	U(eq) [Ang^2]
C11	0.6173(6)	0.7595(5)	0.2138(4)	0.032(2)
C12	0.6042(6)	0.6709(5)	0.1598(4)	0.034(2)
C13	0.5738(6)	0.6633(5)	0.0821(4)	0.033(2)
C14	0.6127(6)	0.9375(5)	0.2414(3)	0.0274(19)
C15	0.6083(6)	1.0931(5)	0.2793(4)	0.0272(17)
C16	0.5670(6)	1.1949(5)	0.1940(4)	0.0257(17)
C17	0.5911(6)	1.1858(5)	0.2685(4)	0.0274(17)
C18	0.5957(7)	1.2680(5)	0.3284(4)	0.0337(19)
C19	0.5814(7)	1.3534(5)	0.3131(4)	0.036(2)
C20	0.5577(6)	1.3563(5)	0.2372(4)	0.0301(17)
Ni2	1.00993(8)	0.26181(6)	0.60979(5)	0.0290(3)
S11	1.19048(15)	0.21060(12)	0.57210(9)	0.0293(5)
S12	1.16163(16)	0.42579(13)	0.66208(10)	0.0331(5)
S13	0.85133(19)	0.32668(19)	0.65326(13)	0.0534(7)
S14	0.83885(17)	0.10219(15)	0.55453(10)	0.0387(5)
S15	0.8613(2)	0.0515(2)	0.16462(12)	0.0569(8)
P5	1.26771(16)	0.35601(13)	0.61486(10)	0.0289(5)
P6	0.7510(2)	0.1883(2)	0.60592(15)	0.0700(9)
O5	1.3122(5)	0.4015(4)	0.5528(3)	0.0363(16)
O6	1.3962(4)	0.3892(4)	0.6798(3)	0.0316(14)
O7	0.6240(7)	0.2007(6)	0.5433(6)	0.099(4)
O8	0.6906(8)	0.1531(7)	0.6599(5)	0.106(4)
N5	0.9531(5)	0.2848(4)	0.5027(3)	0.0330(17)
N6	0.9168(5)	0.0593(4)	0.3041(3)	0.0305(17)
N7	0.8738(5)	0.1503(4)	0.2146(4)	0.0343(9)

Table S31 - Final Coordinates and Equivalent Isotropic Displacement Parameters of the non-Hydrogen atoms (continued) for: (2·L2)2

Atom	x	y	z	U(eq) [Ang^2]
N8	0.9361(5)	-0.2282(4)	0.2868(3)	0.0317(17)
C21	1.2378(7)	0.3797(6)	0.4754(4)	0.0404(11)
C22	1.3092(10)	0.4399(8)	0.4353(6)	0.0715(17)
C23	1.5002(6)	0.3616(6)	0.6613(4)	0.0385(10)
C24	1.6098(8)	0.4208(8)	0.7306(5)	0.0616(17)
C25	0.5251(10)	0.1153(9)	0.5128(8)	0.099(2)
C26	0.4344(8)	0.1464(7)	0.4598(5)	0.0540(17)
C27	0.7617(11)	0.1252(10)	0.7164(7)	0.084(2)
C28	0.6879(15)	0.0917(13)	0.7692(9)	0.116(3)
C29	0.9464(6)	0.2164(5)	0.4377(4)	0.0292(17)
C30	0.9125(6)	0.2290(5)	0.3647(4)	0.034(2)
C31	0.8851(6)	0.3171(6)	0.3598(4)	0.038(2)
C32	0.8910(7)	0.3868(6)	0.4271(5)	0.045(3)
C33	0.9241(6)	0.3691(6)	0.4968(5)	0.039(2)
C34	0.9021(6)	0.1484(5)	0.2964(4)	0.0325(19)
C35	0.8981(6)	-0.0025(6)	0.2350(4)	0.0328(19)
C36	0.9301(6)	-0.1366(5)	0.2902(4)	0.0319(19)
C37	0.9035(6)	-0.1061(6)	0.2245(4)	0.0330(19)
C38	0.8802(7)	-0.1751(6)	0.1523(4)	0.042(3)
C39	0.8844(7)	-0.2715(6)	0.1489(4)	0.039(2)
C40	0.9125(6)	-0.2953(6)	0.2167(4)	0.039(2)

U(eq) = 1/3 of the trace of the orthogonalized U Tensor

Table S32 - Hydrogen Atom Positions and Isotropic Displacement Parameters
for: (2·L2)2

Atom	x	y	z	U(iso) [Ang^2]
H1A	0.12180	0.56490	-0.20330	0.1140
H1B	0.13160	0.68080	-0.18260	0.1140
H2A	-0.09090	0.52390	-0.22080	0.1240
H2B	-0.06310	0.59840	-0.26950	0.1240
H2C	-0.08570	0.63860	-0.18730	0.1240
H3A	0.28820	0.56810	0.08350	0.1710
H3B	0.17040	0.50890	0.00930	0.1710
H4A	0.07350	0.63360	0.07610	0.1590
H4B	0.17650	0.64350	0.15240	0.1590
H4C	0.07750	0.53870	0.10530	0.1590
H5A	1.00580	0.81790	-0.07480	0.1240
H5B	0.97420	0.73830	-0.03040	0.1240
H6A	1.12610	0.93960	0.03860	0.1200
H6B	1.16120	0.84160	0.04960	0.1200
H6C	1.06830	0.88290	0.09110	0.1200
H7A	0.83080	0.92730	-0.15670	0.1670
H7B	0.68680	0.87940	-0.19620	0.1670
H8A	0.85640	0.80150	-0.26450	0.1030
H8B	0.80860	0.88930	-0.28750	0.1030
H8C	0.71480	0.78280	-0.30600	0.1030
H9	0.55730	0.88190	0.09220	0.0370
H11	0.63800	0.76600	0.26740	0.0380
H12	0.61600	0.61510	0.17570	0.0410
H13	0.56300	0.60100	0.04520	0.0400
H16	0.56270	1.13960	0.15230	0.0310
H18	0.60870	1.26460	0.37970	0.0400

Table S32 - Hydrogen Atom Positions and Isotropic Displacement Parameters (continued) for: (2·L2)2

Atom	x	y	z	U(iso) [Ang^2]
H19	0.58750	1.41050	0.35400	0.0420
H20	0.54700	1.41550	0.22670	0.0360
H21A	1.16100	0.39790	0.47570	0.0480
H21B	1.21730	0.30760	0.44770	0.0480
H22A	1.33770	0.51020	0.46660	0.1070
H22B	1.25650	0.43290	0.38430	0.1070
H22C	1.37940	0.41520	0.42920	0.1070
H23A	1.51120	0.37800	0.61440	0.0460
H23B	1.48900	0.28930	0.65190	0.0460
H24A	1.62570	0.49170	0.73540	0.0930
H24B	1.68120	0.39850	0.72360	0.0930
H24C	1.59340	0.41020	0.77760	0.0930
H25A	0.49310	0.09800	0.55400	0.1190
H25B	0.54750	0.05780	0.48390	0.1190
H26A	0.41610	0.20470	0.48960	0.0810
H26B	0.35930	0.09150	0.43540	0.0810
H26C	0.46840	0.16310	0.41970	0.0810
H27A	0.83350	0.18200	0.74810	0.1010
H27B	0.79140	0.06980	0.69140	0.1010
H28A	0.63370	0.13400	0.77800	0.1740
H28B	0.74410	0.09780	0.81890	0.1740
H28C	0.63930	0.02220	0.74420	0.1740
H29	0.96530	0.15650	0.44120	0.0350
H31	0.86290	0.32870	0.31130	0.0470
H32	0.87210	0.44720	0.42530	0.0550

Table S32 - Hydrogen Atom Positions and Isotropic Displacement Parameters (continued)
for: (2·L2)2

Atom	x	y	z	U(iso) [Ang^2]
H33	0.92660	0.41780	0.54240	0.0470
H36	0.94460	-0.08990	0.33950	0.0380
H38	0.86180	-0.15670	0.10640	0.0510
H39	0.86820	-0.32050	0.10040	0.0480
H40	0.91540	-0.36140	0.21400	0.0460

==========

The Temperature Factor has the Form of Exp(-T) Where
T = 8*(Pi**2)*U*(Sin(Theta)/Lambda)**2 for Isotropic Atoms

Table S33 - (An)isotropic Displacement Parameters
for: (2·L2)2

Atom	U(1,1) or U	U(2,2)	U(3,3)	U(2,3)	U(1,3)	U(1,2)
Ni1	0.0350(5)	0.0250(4)	0.0249(4)	0.0051(3)	0.0009(3)	0.0100(3)
S1	0.0511(11)	0.0397(10)	0.0305(9)	0.0098(7)	0.0103(8)	0.0255(9)
S2	0.0414(10)	0.0297(9)	0.0367(9)	0.0059(7)	0.0103(8)	0.0078(7)
S3	0.0573(13)	0.0362(10)	0.0330(10)	0.0094(8)	-0.0069(9)	-0.0042(9)
S4	0.0424(11)	0.0513(12)	0.0624(13)	0.0220(10)	0.0141(10)	0.0255(10)
S5	0.0505(12)	0.0518(12)	0.0423(11)	0.0204(9)	0.0136(9)	0.0160(10)
P1	0.0589(15)	0.0562(15)	0.101(2)	0.0347(15)	0.0501(16)	0.0292(13)
P2	0.0520(13)	0.0664(15)	0.0256(10)	0.0156(10)	0.0035(9)	0.0012(11)
O1	0.132(4)	0.132(4)	0.134(4)	0.0411(16)	0.0385(15)	0.0372(15)
O2	0.182(8)	0.114(7)	0.194(9)	0.054(6)	0.134(7)	0.080(6)
O3	0.052(4)	0.143(6)	0.049(4)	0.014(4)	0.024(3)	-0.001(4)
O4	0.174(8)	0.091(5)	0.053(4)	0.038(4)	0.049(5)	0.049(5)
N1	0.038(3)	0.029(3)	0.029(3)	0.008(2)	0.001(2)	0.010(2)
N2	0.029(3)	0.026(3)	0.027(3)	0.009(2)	0.008(2)	0.006(2)
N3	0.0183(12)	0.0228(13)	0.0182(13)	0.0013(9)	0.0066(9)	0.0057(9)
N4	0.027(3)	0.030(3)	0.025(3)	0.001(2)	0.002(2)	0.006(2)
C1	0.095(4)	0.095(4)	0.095(4)	0.0291(16)	0.0287(15)	0.0266(15)
C2	0.083(4)	0.083(4)	0.082(4)	0.023(2)	0.027(2)	0.020(2)
C3	0.142(7)	0.142(7)	0.142(7)	0.044(2)	0.042(2)	0.040(2)
C4	0.106(5)	0.107(5)	0.105(5)	0.034(2)	0.033(2)	0.028(2)
C5	0.103(5)	0.103(5)	0.103(5)	0.0318(17)	0.0302(16)	0.0290(16)
C6	0.077(4)	0.081(4)	0.083(4)	0.023(2)	0.024(2)	0.023(2)
C7	0.139(7)	0.140(7)	0.139(7)	0.043(2)	0.041(2)	0.039(2)
C8	0.069(3)	0.071(3)	0.065(3)	0.024(2)	0.019(2)	0.014(2)
C9	0.035(4)	0.026(3)	0.026(3)	0.006(3)	0.000(3)	0.009(3)
C10	0.029(3)	0.035(4)	0.026(3)	0.012(3)	0.004(3)	0.010(3)

Table S33 - (An)isotropic Displacement Parameters (continued)
for: (2·L2)2

Atom	U(1,1) or U	U(2,2)	U(3,3)	U(2,3)	U(1,3)	U(1,2)
C11	0.035(4)	0.034(4)	0.026(3)	0.010(3)	0.006(3)	0.010(3)
C12	0.036(4)	0.032(4)	0.038(4)	0.013(3)	0.009(3)	0.016(3)
C13	0.035(4)	0.029(4)	0.034(4)	0.009(3)	0.006(3)	0.011(3)
C14	0.026(3)	0.036(4)	0.017(3)	0.007(2)	0.004(2)	0.006(3)
C15	0.024(3)	0.031(3)	0.024(3)	0.007(3)	0.007(2)	0.004(3)
C16	0.024(3)	0.027(3)	0.023(3)	0.007(2)	0.003(2)	0.006(2)
C17	0.021(3)	0.031(3)	0.025(3)	0.004(3)	0.005(2)	0.004(2)
C18	0.039(4)	0.029(3)	0.026(3)	0.003(3)	0.009(3)	0.002(3)
C19	0.040(4)	0.028(3)	0.034(4)	0.002(3)	0.015(3)	0.004(3)
C20	0.028(3)	0.027(3)	0.029(3)	0.002(3)	0.007(3)	0.004(3)
Ni2	0.0246(4)	0.0295(5)	0.0259(4)	0.0029(3)	0.0014(3)	0.0064(3)
S11	0.0294(8)	0.0296(8)	0.0267(8)	0.0071(6)	0.0045(6)	0.0093(6)
S12	0.0292(8)	0.0285(8)	0.0328(9)	0.0033(7)	-0.0002(7)	0.0072(7)
S13	0.0354(10)	0.0680(15)	0.0457(12)	-0.0039(10)	0.0060(9)	0.0236(10)
S14	0.0328(9)	0.0403(10)	0.0309(9)	0.0073(7)	0.0018(7)	-0.0024(8)
S15	0.0535(13)	0.0726(16)	0.0337(11)	0.0173(10)	0.0067(9)	-0.0001(11)
P5	0.0274(8)	0.0302(9)	0.0241(8)	0.0078(7)	0.0014(6)	0.0047(7)
P6	0.0295(11)	0.095(2)	0.0501(14)	-0.0201(13)	0.0141(10)	-0.0081(12)
O5	0.040(3)	0.037(3)	0.027(2)	0.013(2)	0.004(2)	0.003(2)
O6	0.024(2)	0.040(3)	0.027(2)	0.008(2)	0.0035(18)	0.008(2)
O7	0.054(5)	0.093(6)	0.126(8)	-0.018(5)	0.041(5)	0.016(4)
O8	0.091(6)	0.121(8)	0.071(5)	0.005(5)	0.035(5)	-0.026(6)
N5	0.028(3)	0.029(3)	0.033(3)	0.008(2)	-0.004(2)	0.005(2)
N6	0.024(3)	0.036(3)	0.027(3)	0.011(2)	0.002(2)	0.003(2)
N7	0.0333(15)	0.0329(15)	0.0367(15)	0.0166(10)	0.0054(10)	0.0075(10)

Table S33 - (An)isotropic Displacement Parameters (continued)
for: (2·L2)2

Atom	U(1,1) or U	U(2,2)	U(3,3)	U(2,3)	U(1,3)	U(1,2)
N8	0.026(3)	0.038(3)	0.026(3)	0.005(2)	0.005(2)	0.007(2)
C21	0.0406(19)	0.0407(19)	0.0396(19)	0.0131(11)	0.0107(11)	0.0108(11)
C22	0.072(3)	0.073(3)	0.069(3)	0.026(2)	0.019(2)	0.016(2)
C23	0.0380(18)	0.0390(18)	0.0386(18)	0.0115(11)	0.0114(11)	0.0110(11)
C24	0.058(3)	0.065(3)	0.061(3)	0.0150(19)	0.019(2)	0.019(2)
C25	0.099(4)	0.099(4)	0.099(4)	0.0307(17)	0.0293(16)	0.0274(16)
C26	0.052(3)	0.055(3)	0.055(3)	0.0157(19)	0.0177(19)	0.0144(19)
C27	0.083(4)	0.084(4)	0.085(4)	0.0262(15)	0.0244(14)	0.0229(14)
C28	0.114(6)	0.118(6)	0.116(6)	0.036(3)	0.035(3)	0.031(2)
C29	0.022(3)	0.028(3)	0.028(3)	0.008(3)	-0.005(2)	0.001(2)
C30	0.027(3)	0.033(4)	0.035(4)	0.016(3)	-0.002(3)	-0.001(3)
C31	0.030(4)	0.038(4)	0.040(4)	0.019(3)	-0.006(3)	0.003(3)
C32	0.036(4)	0.027(4)	0.060(5)	0.014(3)	-0.008(4)	0.004(3)
C33	0.030(4)	0.032(4)	0.043(4)	0.007(3)	-0.004(3)	0.003(3)
C34	0.023(3)	0.041(4)	0.028(3)	0.015(3)	0.000(3)	0.000(3)
C35	0.025(3)	0.041(4)	0.026(3)	0.011(3)	0.001(3)	0.002(3)
C36	0.027(3)	0.036(4)	0.024(3)	0.004(3)	0.003(3)	0.002(3)
C37	0.026(3)	0.047(4)	0.022(3)	0.007(3)	0.007(3)	0.006(3)
C38	0.032(4)	0.057(5)	0.027(4)	0.005(3)	0.005(3)	0.003(3)
C39	0.039(4)	0.051(5)	0.024(3)	0.004(3)	0.010(3)	0.012(3)
C40	0.031(4)	0.048(4)	0.028(3)	0.001(3)	0.005(3)	0.008(3)

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The Temperature Factor has the Form of Exp(-T) Where
T = 8*(Pi**2)*U*(Sin(Theta)/Lambda)**2 for Isotropic Atoms
T = 2*(Pi**2)*Sumij(h(i)*h(j)*U(i,j)*Astar(i)*Astar(j)), for
Anisotropic Atoms. Astar(i) are Reciprocal Axial Lengths and
h(i) are the Reflection Indices.

Table S34 - Bond Distances (Angstrom)
for: (2·L2)2

Ni1	-S1	2.480(3)	P2	-O3	1.554(8)
Ni1	-S2	2.469(2)	P5	-O6	1.600(5)
Ni1	-S3	2.495(2)	P5	-O5	1.598(6)
Ni1	-S4	2.501(3)	P6	-O7	1.745(10)
Ni1	-P1	2.946(4)	P6	-O8	1.484(10)
Ni1	-N1	2.109(5)	O1	-C1	1.380(17)
Ni1	-N4_a	2.111(5)	O2	-C3	1.39(2)
Ni2	-S11	2.566(2)	O3	-C5	1.395(15)
Ni2	-S12	2.460(2)	O4	-C7	1.395(19)
Ni2	-S13	2.453(3)	O5	-C21	1.428(9)
Ni2	-S14	2.525(2)	O6	-C23	1.445(9)
Ni2	-N5	2.090(5)	O7	-C25	1.397(16)
Ni2	-N8_b	2.098(5)	O8	-C27	1.387(16)
S1	-P1	1.970(4)	N1	-C9	1.348(9)
S2	-P1	1.970(4)	N1	-C13	1.341(9)
S3	-P2	1.981(3)	N2	-C15	1.366(9)
S4	-P2	1.967(4)	N2	-C14	1.321(9)
S5	-N3	1.488(6)	N3	-C15	1.495(9)
S5	-C14	1.718(6)	N4	-C16	1.326(9)
S11	-P5	1.980(3)	N4	-C20	1.344(9)
S12	-P5	1.977(3)	N5	-C33	1.353(11)
S13	-P6	1.959(4)	N5	-C29	1.335(9)
S14	-P6	1.977(3)	N6	-C34	1.370(9)
S15	-N7	1.455(7)	N6	-C35	1.314(9)
S15	-C35	1.706(8)	N7	-C34	1.495(10)
P1	-O1	1.405(15)	N8	-C36	1.325(9)
P1	-O2	1.687(14)	N8	-C40	1.350(9)
P2	-O4	1.575(8)	C1	-C2	1.585(18)

Table S34 - Bond Distances (Angstrom) (continued)
for: (2·L2)2

C3	-C4	1.52(3)	C7	-H7A	0.9895
C5	-C6	1.545(18)	C7	-H7B	0.9887
C7	-C8	1.530(19)	C8	-H8A	0.9811
C9	-C10	1.390(10)	C8	-H8B	0.9795
C10	-C11	1.390(10)	C8	-H8C	0.9797
C10	-C14	1.464(10)	C9	-H9	0.9495
C11	-C12	1.372(10)	C11	-H11	0.9499
C12	-C13	1.383(10)	C12	-H12	0.9499
C15	-C17	1.449(10)	C13	-H13	0.9510
C16	-C17	1.399(10)	C16	-H16	0.9496
C17	-C18	1.395(10)	C18	-H18	0.9500
C18	-C19	1.367(11)	C19	-H19	0.9513
C19	-C20	1.393(10)	C20	-H20	0.9491
C1	-H1A	0.9898	C21	-C22	1.524(14)
C1	-H1B	0.9908	C23	-C24	1.517(12)
C2	-H2A	0.9798	C25	-C26	1.502(16)
C2	-H2B	0.9812	C27	-C28	1.55(2)
C2	-H2C	0.9795	C29	-C30	1.398(10)
C3	-H3B	0.9901	C30	-C31	1.394(11)
C3	-H3A	0.9904	C30	-C34	1.458(10)
C4	-H4B	0.9794	C31	-C32	1.377(11)
C4	-H4C	0.9804	C32	-C33	1.373(12)
C4	-H4A	0.9808	C35	-C37	1.476(12)
C5	-H5A	0.9904	C36	-C37	1.395(10)
C5	-H5B	0.9903	C37	-C38	1.391(10)
C6	-H6C	0.9804	C38	-C39	1.389(12)
C6	-H6A	0.9795	C39	-C40	1.379(11)
C6	-H6B	0.9793	C21	-H21A	0.9898

Table S34 - Bond Distances (Angstrom) (continued)
for: (2·L2)2

C21	-H21B	0.9906	C27	-H27A	0.9901
C22	-H22A	0.9796	C27	-H27B	0.9905
C22	-H22B	0.9793	C28	-H28A	0.9805
C22	-H22C	0.9804	C28	-H28B	0.9808
C23	-H23A	0.9898	C28	-H28C	0.9799
C23	-H23B	0.9895	C29	-H29	0.9496
C24	-H24A	0.9789	C31	-H31	0.9496
C24	-H24B	0.9806	C32	-H32	0.9495
C24	-H24C	0.9797	C33	-H33	0.9495
C25	-H25A	0.9904	C36	-H36	0.9503
C25	-H25B	0.9899	C38	-H38	0.9508
C26	-H26A	0.9793	C39	-H39	0.9507
C26	-H26B	0.9811	C40	-H40	0.9510
C26	-H26C	0.9804			

Table S35 - Bond Angles (Degrees)
for: (2·L2)2

S1	-Ni1	-S2	82.86(8)	S12	-Ni2	-S14	174.54(8)
S1	-Ni1	-S3	98.13(9)	S11	-Ni2	-S12	81.09(7)
S1	-Ni1	-S4	178.73(9)	S11	-Ni2	-S13	174.41(9)
S1	-Ni1	-P1	41.48(9)	S11	-Ni2	-S14	103.73(7)
S1	-Ni1	-N1	88.6(2)	S11	-Ni2	-N5	89.58(18)
S1	-Ni1	-N4_a	89.02(18)	S12	-Ni2	-N5	91.14(17)
S2	-Ni1	-S3	178.20(8)	S12	-Ni2	-N8_b	92.24(17)
S2	-Ni1	-S4	96.88(9)	S13	-Ni2	-S14	81.82(9)
S2	-Ni1	-P1	41.50(9)	Ni1	-S1	-P1	82.05(14)
S2	-Ni1	-N1	91.49(18)	Ni1	-S2	-P1	82.33(13)
S2	-Ni1	-N4_a	90.71(17)	Ni1	-S3	-P2	81.63(11)
S3	-Ni1	-S4	82.17(9)	Ni1	-S4	-P2	81.74(12)
S3	-Ni1	-P1	139.56(9)	N3	-S5	-C14	97.3(3)
S3	-Ni1	-N1	90.05(18)	Ni2	-S11	-P5	82.10(9)
S3	-Ni1	-N4_a	87.81(17)	Ni2	-S12	-P5	84.98(9)
S4	-Ni1	-P1	138.16(10)	Ni2	-S13	-P6	84.21(12)
S4	-Ni1	-N1	90.1(2)	Ni2	-S14	-P6	81.96(11)
S4	-Ni1	-N4_a	92.22(18)	N7	-S15	-C35	98.0(4)
P1	-Ni1	-N1	87.6(2)	S1	-P1	-O1	117.1(6)
P1	-Ni1	-N4_a	92.32(18)	S1	-P1	-O2	104.1(5)
N1	-Ni1	-N4_a	176.6(2)	S2	-P1	-O1	118.1(6)
S13	-Ni2	-N5	91.46(18)	S2	-P1	-O2	110.2(5)
S13	-Ni2	-N8_b	90.38(18)	O1	-P1	-O2	91.6(8)
S14	-Ni2	-N5	86.36(17)	Ni1	-P1	-O1	150.6(6)
S14	-Ni2	-N8_b	90.44(17)	Ni1	-P1	-S1	56.47(11)
N5	-Ni2	-N8_b	176.0(2)	Ni1	-P1	-S2	56.17(11)
S11	-Ni2	-N8_b	88.93(17)	Ni1	-P1	-O2	117.7(5)
S12	-Ni2	-S13	93.39(9)	S1	-P1	-S2	112.4(2)

Table S35 - Bond Angles (Degrees) (continued)
for: (2·L2)2

S3	-P2	-S4	112.55(16)	Ni1	-N1	-C13	122.5(5)
S3	-P2	-O4	114.0(4)	C14	-N2	-C15	109.7(5)
S4	-P2	-O3	116.4(4)	S5	-N3	-C15	108.3(4)
S3	-P2	-O3	103.5(3)	Ni1_a	-N4	-C16	118.4(4)
O3	-P2	-O4	103.1(5)	C16	-N4	-C20	119.1(6)
S4	-P2	-O4	107.2(4)	Ni1_a	-N4	-C20	122.2(5)
S11	-P5	-O5	112.2(2)	Ni2	-N5	-C29	120.3(5)
S11	-P5	-S12	111.36(12)	Ni2	-N5	-C33	121.7(5)
S12	-P5	-O5	112.9(2)	C29	-N5	-C33	117.9(6)
S12	-P5	-O6	106.2(2)	C34	-N6	-C35	108.6(6)
S11	-P5	-O6	115.2(2)	S15	-N7	-C34	108.2(5)
O5	-P5	-O6	98.3(3)	C36	-N8	-C40	118.5(6)
O7	-P6	-O8	98.5(5)	Ni2_b	-N8	-C36	119.0(4)
S14	-P6	-O8	117.1(4)	Ni2_b	-N8	-C40	122.4(5)
S13	-P6	-S14	111.86(16)	O1	-C1	-C2	117.2(11)
S13	-P6	-O7	102.0(3)	O2	-C3	-C4	99.3(15)
S13	-P6	-O8	111.3(4)	O3	-C5	-C6	107.6(11)
S14	-P6	-O7	114.4(4)	O4	-C7	-C8	108.4(12)
P1	-O1	-C1	116.7(11)	N1	-C9	-C10	122.2(7)
P1	-O2	-C3	128.0(12)	C9	-C10	-C11	118.9(7)
P2	-O3	-C5	126.1(8)	C11	-C10	-C14	122.8(6)
P2	-O4	-C7	126.2(10)	C9	-C10	-C14	118.3(6)
P5	-O5	-C21	123.2(5)	C10	-C11	-C12	118.6(6)
P5	-O6	-C23	120.6(4)	C11	-C12	-C13	119.6(7)
P6	-O7	-C25	114.4(8)	N1	-C13	-C12	122.5(7)
P6	-O8	-C27	116.5(9)	S5	-C14	-C10	126.1(5)
Ni1	-N1	-C9	119.2(5)	S5	-C14	-N2	111.1(5)
C9	-N1	-C13	118.1(6)	N2	-C14	-C10	122.8(5)

Table S35 - Bond Angles (Degrees) (continued)
for: (2·L2)2

N2	-C15	-N3	113.6(6)	H4A	-C4	-H4B	109.38
N2	-C15	-C17	120.7(6)	C3	-C4	-H4A	109.50
N3	-C15	-C17	125.7(6)	H4A	-C4	-H4C	109.39
N4	-C16	-C17	123.3(6)	H4B	-C4	-H4C	109.53
C16	-C17	-C18	116.9(7)	O3	-C5	-H5A	110.20
C15	-C17	-C18	123.9(6)	C6	-C5	-H5B	110.19
C15	-C17	-C16	119.2(6)	H5A	-C5	-H5B	108.37
C17	-C18	-C19	119.9(7)	O3	-C5	-H5B	110.26
C18	-C19	-C20	119.6(7)	C6	-C5	-H5A	110.17
N4	-C20	-C19	121.1(7)	C5	-C6	-H6A	109.47
O1	-C1	-H1A	108.03	H6A	-C6	-H6C	109.37
O1	-C1	-H1B	108.01	H6B	-C6	-H6C	109.49
C2	-C1	-H1A	108.04	C5	-C6	-H6C	109.44
C2	-C1	-H1B	108.01	H6A	-C6	-H6B	109.53
H1A	-C1	-H1B	107.17	C5	-C6	-H6B	109.52
H2A	-C2	-H2C	109.56	O4	-C7	-H7A	109.96
C1	-C2	-H2A	109.44	O4	-C7	-H7B	110.02
C1	-C2	-H2B	109.45	H7A	-C7	-H7B	108.47
H2B	-C2	-H2C	109.48	C8	-C7	-H7A	109.98
H2A	-C2	-H2B	109.45	C8	-C7	-H7B	109.98
C1	-C2	-H2C	109.45	H8A	-C8	-H8B	109.40
O2	-C3	-H3B	111.90	H8A	-C8	-H8C	109.43
O2	-C3	-H3A	111.88	H8B	-C8	-H8C	109.48
C4	-C3	-H3A	111.97	C7	-C8	-H8C	109.48
C4	-C3	-H3B	112.01	C7	-C8	-H8A	109.48
H3A	-C3	-H3B	109.55	C7	-C8	-H8B	109.56
C3	-C4	-H4B	109.49	N1	-C9	-H9	118.93
C3	-C4	-H4C	109.54	C10	-C9	-H9	118.85

Table S35 - Bond Angles (Degrees) (continued)
for: (2·L2)2

C10	-C11	-H11	120.67	S15	-C35	-N6	111.4(6)
C12	-C11	-H11	120.75	S15	-C35	-C37	127.4(5)
C13	-C12	-H12	120.18	N6	-C35	-C37	121.1(7)
C11	-C12	-H12	120.18	N8	-C36	-C37	122.7(7)
C12	-C13	-H13	118.77	C35	-C37	-C36	118.1(6)
N1	-C13	-H13	118.74	C35	-C37	-C38	123.1(7)
C17	-C16	-H16	118.28	C36	-C37	-C38	118.7(8)
N4	-C16	-H16	118.37	C37	-C38	-C39	118.4(7)
C17	-C18	-H18	120.06	C38	-C39	-C40	119.2(7)
C19	-C18	-H18	120.08	N8	-C40	-C39	122.4(8)
C20	-C19	-H19	120.18	O5	-C21	-H21A	110.15
C18	-C19	-H19	120.23	O5	-C21	-H21B	110.11
C19	-C20	-H20	119.39	C22	-C21	-H21A	110.14
N4	-C20	-H20	119.49	C22	-C21	-H21B	110.19
O5	-C21	-C22	107.8(7)	H21A	-C21	-H21B	108.41
O6	-C23	-C24	106.4(6)	C21	-C22	-H22A	109.50
O7	-C25	-C26	102.3(10)	C21	-C22	-H22B	109.46
O8	-C27	-C28	111.0(12)	C21	-C22	-H22C	109.44
N5	-C29	-C30	122.9(7)	H22A	-C22	-H22B	109.52
C29	-C30	-C31	118.4(6)	H22A	-C22	-H22C	109.48
C29	-C30	-C34	119.2(7)	H22B	-C22	-H22C	109.44
C31	-C30	-C34	122.3(6)	O6	-C23	-H23A	110.47
C30	-C31	-C32	118.3(7)	O6	-C23	-H23B	110.44
C31	-C32	-C33	120.1(8)	C24	-C23	-H23A	110.39
N5	-C33	-C32	122.3(8)	C24	-C23	-H23B	110.48
N6	-C34	-N7	113.6(6)	H23A	-C23	-H23B	108.69
N6	-C34	-C30	119.7(6)	C23	-C24	-H24A	109.55
N7	-C34	-C30	126.7(6)	C23	-C24	-H24B	109.44

Table S35 - Bond Angles (Degrees) (continued)
for: (2·L2)2

C23	-C24	-H24C	109.46	C27	-C28	-H28B	109.46
H24A	-C24	-H24B	109.51	C27	-C28	-H28C	109.54
H24A	-C24	-H24C	109.50	H28A	-C28	-H28B	109.47
H24B	-C24	-H24C	109.36	H28A	-C28	-H28C	109.49
O7	-C25	-H25A	111.34	H28B	-C28	-H28C	109.43
O7	-C25	-H25B	111.34	N5	-C29	-H29	118.53
C26	-C25	-H25A	111.28	C30	-C29	-H29	118.60
C26	-C25	-H25B	111.31	C30	-C31	-H31	120.81
H25A	-C25	-H25B	109.20	C32	-C31	-H31	120.92
C25	-C26	-H26A	109.52	C31	-C32	-H32	119.94
C25	-C26	-H26B	109.40	C33	-C32	-H32	119.92
C25	-C26	-H26C	109.53	N5	-C33	-H33	118.94
H26A	-C26	-H26B	109.45	C32	-C33	-H33	118.74
H26A	-C26	-H26C	109.48	N8	-C36	-H36	118.46
H26B	-C26	-H26C	109.45	C37	-C36	-H36	118.83
O8	-C27	-H27A	109.46	C37	-C38	-H38	120.79
O8	-C27	-H27B	109.36	C39	-C38	-H38	120.81
C28	-C27	-H27A	109.55	C38	-C39	-H39	120.39
C28	-C27	-H27B	109.44	C40	-C39	-H39	120.38
H27A	-C27	-H27B	108.02	N8	-C40	-H40	118.75
C27	-C28	-H28A	109.43	C39	-C40	-H40	118.84

Table S36 - Torsion Angles (Degrees)
for: (2·L2)2

S2	-Ni1	-S1	-P1	3.77(12)
S3	-Ni1	-S1	-P1	-177.75(12)
N1	-Ni1	-S1	-P1	-87.9(2)
N4_a	-Ni1	-S1	-P1	94.6(2)
S1	-Ni1	-S2	-P1	-3.77(12)
S4	-Ni1	-S2	-P1	174.97(13)
N1	-Ni1	-S2	-P1	84.7(2)
N4_a	-Ni1	-S2	-P1	-92.7(2)
S1	-Ni1	-S3	-P2	-172.31(10)
S4	-Ni1	-S3	-P2	8.93(10)
P1	-Ni1	-S3	-P2	-174.61(14)
N1	-Ni1	-S3	-P2	99.1(2)
N4_a	-Ni1	-S3	-P2	-83.61(19)
S2	-Ni1	-S4	-P2	169.46(10)
S3	-Ni1	-S4	-P2	-9.00(10)
P1	-Ni1	-S4	-P2	174.45(13)
N1	-Ni1	-S4	-P2	-99.02(19)
N4_a	-Ni1	-S4	-P2	78.48(19)
S2	-Ni1	-P1	-S1	-174.34(18)
S3	-Ni1	-P1	-S1	3.44(19)
S4	-Ni1	-P1	-S1	178.17(12)
N1	-Ni1	-P1	-S1	90.67(19)
N4_a	-Ni1	-P1	-S1	-85.90(19)
S1	-Ni1	-P1	-S2	174.34(18)
S3	-Ni1	-P1	-S2	177.78(12)
S4	-Ni1	-P1	-S2	-7.49(19)
N1	-Ni1	-P1	-S2	-95.0(2)
N4_a	-Ni1	-P1	-S2	88.44(19)

Table S36 - Torsion Angles (Degrees) (continued)
for: (2·L2)2

S1	-Ni1	-P1	-O1	86.3(12)
S2	-Ni1	-P1	-O1	-88.0(12)
S3	-Ni1	-P1	-O1	89.8(12)
S4	-Ni1	-P1	-O1	-95.5(12)
N1	-Ni1	-P1	-O1	177.0(12)
N4_a	-Ni1	-P1	-O1	0.4(12)
S1	-Ni1	-P1	-O2	-88.9(6)
S2	-Ni1	-P1	-O2	96.8(6)
S3	-Ni1	-P1	-O2	-85.5(6)
S4	-Ni1	-P1	-O2	89.3(6)
N1	-Ni1	-P1	-O2	1.8(6)
N4_a	-Ni1	-P1	-O2	-174.8(6)
S1	-Ni1	-N1	-C13	126.1(6)
S2	-Ni1	-N1	-C13	43.3(6)
S3	-Ni1	-N1	-C13	-135.7(6)
S4	-Ni1	-N1	-C13	-53.6(6)
P1	-Ni1	-N1	-C13	84.6(6)
S2_a	-Ni1_a	-N4	-C20	52.7(6)
S1_a	-Ni1_a	-N4	-C16	-50.3(5)
S2_a	-Ni1_a	-N4	-C16	-133.2(5)
S3_a	-Ni1_a	-N4	-C16	47.8(5)
S4_a	-Ni1_a	-N4	-C16	129.9(5)
P1_a	-Ni1_a	-N4	-C16	-91.7(5)
S1_a	-Ni1_a	-N4	-C20	135.5(6)
S1	-Ni1	-N1	-C9	-48.6(6)
S3_a	-Ni1_a	-N4	-C20	-126.3(6)
S4_a	-Ni1_a	-N4	-C20	-44.2(6)
P1_a	-Ni1_a	-N4	-C20	94.2(6)

Table S36 - Torsion Angles (Degrees) (continued)
for: (2·L2)2

P1	-Ni1	-N1	-C9	-90.1(6)
S2	-Ni1	-N1	-C9	-131.4(6)
S3	-Ni1	-N1	-C9	49.6(6)
S4	-Ni1	-N1	-C9	131.7(6)
N5	-Ni2	-S14	-P6	-94.49(19)
S11_b	-Ni2_b	-N8	-C36	59.1(5)
S11	-Ni2	-S12	-P5	4.49(8)
S14	-Ni2	-N5	-C33	124.9(6)
S13_b	-Ni2_b	-N8	-C40	50.4(6)
S14_b	-Ni2_b	-N8	-C40	132.3(6)
S12_b	-Ni2_b	-N8	-C36	140.1(5)
S13_b	-Ni2_b	-N8	-C36	-126.5(5)
S14_b	-Ni2_b	-N8	-C36	-44.6(5)
S11_b	-Ni2_b	-N8	-C40	-124.0(6)
S12_b	-Ni2_b	-N8	-C40	-43.0(6)
S13	-Ni2	-N5	-C33	43.2(6)
N8_b	-Ni2	-S14	-P6	87.84(19)
S13	-Ni2	-S14	-P6	-2.48(11)
S12	-Ni2	-S11	-P5	-4.51(8)
S14	-Ni2	-S11	-P5	172.86(9)
N5	-Ni2	-S11	-P5	86.72(18)
N8_b	-Ni2	-S11	-P5	-96.94(18)
S12	-Ni2	-N5	-C33	-50.2(6)
S13	-Ni2	-S12	-P5	-176.44(10)
S11	-Ni2	-N5	-C29	47.6(5)
S12	-Ni2	-N5	-C29	128.6(5)
S13	-Ni2	-N5	-C29	-137.9(5)
S14	-Ni2	-N5	-C29	-56.2(5)

Table S36 - Torsion Angles (Degrees) (continued)
for: (2·L2)2

S11	-Ni2	-N5	-C33	-131.3(6)
S14	-Ni2	-S13	-P6	2.49(11)
N8_b	-Ni2	-S13	-P6	-87.90(19)
S11	-Ni2	-S14	-P6	176.84(10)
S12	-Ni2	-S13	-P6	179.84(11)
N5	-Ni2	-S12	-P5	-84.90(18)
N8_b	-Ni2	-S12	-P5	93.05(18)
N5	-Ni2	-S13	-P6	88.60(19)
Ni1	-S1	-P1	-O2	114.2(6)
Ni1	-S1	-P1	-O1	-146.6(6)
Ni1	-S1	-P1	-S2	-5.08(16)
Ni1	-S2	-P1	-O2	-110.5(6)
Ni1	-S2	-P1	-S1	5.10(16)
Ni1	-S2	-P1	-O1	146.2(6)
Ni1	-S3	-P2	-O3	-138.7(4)
Ni1	-S3	-P2	-O4	110.1(4)
Ni1	-S3	-P2	-S4	-12.23(13)
Ni1	-S4	-P2	-O4	-113.9(5)
Ni1	-S4	-P2	-S3	12.20(13)
Ni1	-S4	-P2	-O3	131.4(3)
C14	-S5	-N3	-C15	-3.0(5)
N3	-S5	-C14	-C10	-176.3(6)
N3	-S5	-C14	-N2	3.1(6)
Ni2	-S11	-P5	-S12	5.95(11)
Ni2	-S11	-P5	-O5	-121.7(3)
Ni2	-S11	-P5	-O6	127.0(2)
Ni2	-S12	-P5	-O6	-132.3(2)
Ni2	-S12	-P5	-O5	121.1(2)

Table S36 - Torsion Angles (Degrees) (continued)
for: (2·L2)2

Ni2	-S12	-P5	-S11	-6.17(11)
Ni2	-S13	-P6	-O8	129.7(4)
Ni2	-S13	-P6	-S14	-3.40(15)
Ni2	-S13	-P6	-O7	-126.1(3)
Ni2	-S14	-P6	-O8	-126.9(4)
Ni2	-S14	-P6	-S13	3.32(15)
Ni2	-S14	-P6	-O7	118.6(4)
C35	-S15	-N7	-C34	-3.8(6)
N7	-S15	-C35	-N6	3.2(6)
N7	-S15	-C35	-C37	179.9(7)
Ni1	-P1	-O1	-C1	4(2)
S1	-P1	-O1	-C1	73.1(13)
S2	-P1	-O1	-C1	-66.2(13)
O2	-P1	-O1	-C1	179.8(12)
O1	-P1	-O2	-C3	86.1(18)
S2	-P1	-O2	-C3	-34.7(18)
Ni1	-P1	-O2	-C3	-96.2(17)
S1	-P1	-O2	-C3	-155.5(16)
O4	-P2	-O3	-C5	-52.3(12)
S4	-P2	-O3	-C5	64.7(11)
S3	-P2	-O4	-C7	22.9(15)
S4	-P2	-O4	-C7	148.1(13)
S3	-P2	-O3	-C5	-171.3(10)
O3	-P2	-O4	-C7	-88.5(14)
O6	-P5	-O5	-C21	169.0(6)
S11	-P5	-O6	-C23	64.1(6)
S12	-P5	-O5	-C21	-79.5(6)
O5	-P5	-O6	-C23	-55.2(6)

Table S36 - Torsion Angles (Degrees) (continued)
for: (2·L2)2

S12	-P5	-O6	-C23	-172.1(5)
S11	-P5	-O5	-C21	47.4(7)
O8	-P6	-O7	-C25	-53.6(10)
S13	-P6	-O8	-C27	-79.3(10)
S14	-P6	-O8	-C27	51.2(10)
O7	-P6	-O8	-C27	174.3(9)
S14	-P6	-O7	-C25	71.4(9)
S13	-P6	-O7	-C25	-167.6(8)
P1	-O1	-C1	-C2	-174.5(11)
P1	-O2	-C3	-C4	-149.4(13)
P2	-O3	-C5	-C6	-176.0(8)
P2	-O4	-C7	-C8	179.7(10)
P5	-O5	-C21	-C22	177.6(6)
P5	-O6	-C23	-C24	169.5(6)
P6	-O7	-C25	-C26	-177.6(7)
P6	-O8	-C27	-C28	179.1(10)
C9	-N1	-C13	-C12	-2.5(11)
Ni1	-N1	-C9	-C10	176.8(6)
C13	-N1	-C9	-C10	1.9(11)
Ni1	-N1	-C13	-C12	-177.2(6)
C14	-N2	-C15	-N3	-0.4(8)
C14	-N2	-C15	-C17	-179.2(7)
C15	-N2	-C14	-C10	177.6(7)
C15	-N2	-C14	-S5	-1.7(8)
S5	-N3	-C15	-N2	2.6(7)
S5	-N3	-C15	-C17	-178.6(6)
C20	-N4	-C16	-C17	1.1(11)
Ni1_a	-N4	-C16	-C17	-173.2(6)

Table S36 - Torsion Angles (Degrees) (continued)
for: (2·L2)2

Ni1_a	-N4	-C20	-C19	173.0(6)
C16	-N4	-C20	-C19	-1.0(11)
C29	-N5	-C33	-C32	-1.4(11)
C33	-N5	-C29	-C30	0.9(11)
Ni2	-N5	-C33	-C32	177.5(6)
Ni2	-N5	-C29	-C30	-178.1(6)
C35	-N6	-C34	-C30	177.2(7)
C35	-N6	-C34	-N7	-1.7(8)
C34	-N6	-C35	-C37	-177.9(7)
C34	-N6	-C35	-S15	-1.0(8)
S15	-N7	-C34	-N6	4.0(8)
S15	-N7	-C34	-C30	-174.8(6)
Ni2_b	-N8	-C36	-C37	175.3(6)
C40	-N8	-C36	-C37	-1.7(11)
Ni2_b	-N8	-C40	-C39	-175.9(6)
C36	-N8	-C40	-C39	1.1(11)
N1	-C9	-C10	-C14	178.4(7)
N1	-C9	-C10	-C11	-0.4(11)
C11	-C10	-C14	-S5	0.4(11)
C11	-C10	-C14	-N2	-178.9(7)
C9	-C10	-C11	-C12	-0.5(11)
C9	-C10	-C14	-S5	-178.4(6)
C9	-C10	-C14	-N2	2.3(11)
C14	-C10	-C11	-C12	-179.3(7)
C10	-C11	-C12	-C13	-0.1(11)
C11	-C12	-C13	-N1	1.6(12)
N3	-C15	-C17	-C16	177.3(7)
N2	-C15	-C17	-C16	-4.0(11)

Table S36 - Torsion Angles (Degrees) (continued)
for: (2·L2)2

N3	-C15	-C17	-C18	-3.5(12)
N2	-C15	-C17	-C18	175.2(7)
N4	-C16	-C17	-C18	0.6(11)
N4	-C16	-C17	-C15	179.9(7)
C15	-C17	-C18	-C19	178.4(8)
C16	-C17	-C18	-C19	-2.4(12)
C17	-C18	-C19	-C20	2.4(12)
C18	-C19	-C20	-N4	-0.7(12)
N5	-C29	-C30	-C31	0.3(11)
N5	-C29	-C30	-C34	-177.2(7)
C31	-C30	-C34	-N7	6.2(12)
C29	-C30	-C34	-N6	4.8(11)
C29	-C30	-C34	-N7	-176.4(7)
C34	-C30	-C31	-C32	176.4(7)
C29	-C30	-C31	-C32	-1.0(11)
C31	-C30	-C34	-N6	-172.6(7)
C30	-C31	-C32	-C33	0.5(12)
C31	-C32	-C33	-N5	0.7(13)
N6	-C35	-C37	-C38	177.7(7)
N6	-C35	-C37	-C36	-0.5(11)
S15	-C35	-C37	-C38	1.3(12)
S15	-C35	-C37	-C36	-177.0(6)
N8	-C36	-C37	-C38	1.2(12)
N8	-C36	-C37	-C35	179.5(7)
C36	-C37	-C38	-C39	0.0(12)
C35	-C37	-C38	-C39	-178.2(8)
C37	-C38	-C39	-C40	-0.6(12)
C38	-C39	-C40	-N8	0.1(12)

Table S37 - Contact Distances(Angstrom)
for: (2·L2)2

S2	.C13_d	3.669(8)	S12	.H40_b	2.9476
S2	.C12_d	3.572(8)	S12	.H32_i	2.7697
S5	.N6_f	3.393(7)	S13	.H2A_p	3.0403
S12	.C32_i	3.596(9)	S13	.H27A	3.0595
S15	.N2_r	3.471(7)	S13	.H33	2.9126
S1	.H6B_c	2.9908	S13	.H40_b	3.1036
S1	.H16_a	2.8605	S13	.H24B_q	2.8523
S1	.H1B	2.9873	S14	.H29	3.0069
S1	.H9	2.9336	S14	.H36_b	2.9135
S2	.H13	2.9968	S14	.H27B	2.8593
S2	.H13_d	3.0707	S15	.H38	2.9323
S2	.H12_d	2.8864	P2	.H38_f	3.1587
S2	.H1A	2.9851	O3	.C38_f	3.269(10)
S2	.H20_a	3.0855	O6	.C12_o	3.317(9)
S3	.H6A_e	3.1552	O6	.C11_o	3.270(9)
S3	.H9	2.9511	O1	.H5B_c	2.9151
S3	.H7B	3.0301	O3	.H38_f	2.4050
S3	.H16_a	2.9000	O4	.H5A	2.7244
S4	.H20_a	3.0962	O5	.H23A	2.4890
S4	.H13	3.1274	O5	.H19_s	2.6804
S5	.H11	2.8745	O6	.H11_o	2.6561
S5	.H25A_g	3.0827	O6	.H20_s	2.7729
S11	.H29	2.9735	O6	.H12_o	2.7470
S11	.H21B	3.0347	O8	.H25A	2.5093
S11	.H11_o	3.1031	N2	.S15_f	3.471(7)
S11	.H36_b	3.1196	N2	.C28_g	3.432(19)
S12	.H33	3.0926	N6	.S5_r	3.393(7)
S12	.H1A_p	2.9944	N6	.C14_r	3.419(9)

Table S37 - Contact Distances(Angstrom) (continued)
for: (2·L2)2

N2	.H16	2.4719	C14	.N6_f	3.419(9)
N2	.H9	2.4973	C14	.C35_f	3.317(11)
N3	.H26C_f	2.9261	C15	.C30_f	3.480(10)
N3	.H18	2.8007	C15	.C34_f	3.294(10)
N3	.H25B_f	2.8842	C17	.C31_f	3.381(11)
N5	.H21A	2.8605	C18	.C32_f	3.381(12)
N6	.H29	2.4626	C18	.C31_f	3.205(11)
N6	.H36	2.4661	C21	.C29	3.535(11)
N7	.H1B_d	2.6600	C23	.C11_o	3.586(11)
N7	.H31	2.7986	C25	.C25_t	3.151(19)
N8	.H27A_b	2.9042	C28	.N2_u	3.43(2)
C9	.C38_f	3.553(11)	C28	.C14_u	3.42(2)
C10	.C38_f	3.543(11)	C29	.C21	3.535(11)
C10	.C37_f	3.359(11)	C30	.C15_r	3.480(10)
C10	.C35_f	3.544(11)	C31	.C17_r	3.381(11)
C11	.C37_f	3.448(11)	C31	.C18_r	3.205(11)
C11	.O6_i	3.270(9)	C32	.C33_i	3.479(12)
C11	.C36_f	3.471(10)	C32	.C18_r	3.381(12)
C11	.C38_f	3.556(11)	C32	.S12_i	3.596(9)
C11	.C23_i	3.586(11)	C33	.C32_i	3.479(12)
C12	.S2_d	3.572(8)	C34	.C15_r	3.294(10)
C12	.O6_i	3.317(9)	C35	.C14_r	3.317(11)
C12	.C40_f	3.424(10)	C35	.C10_r	3.544(11)
C12	.C39_f	3.285(11)	C36	.C11_r	3.471(10)
C12	.C38_f	3.581(11)	C37	.C10_r	3.359(11)
C13	.S2_d	3.669(8)	C37	.C11_r	3.448(11)
C13	.C39_f	3.415(11)	C38	.C11_r	3.556(11)
C14	.C28_g	3.42(2)	C38	.C12_r	3.581(11)

Table S37 - Contact Distances(Angstrom) (continued)
for: (2·L2)2

C38	.C10_r	3.543(11)	H1A	.S12_j	2.9944
C38	.O3_r	3.269(10)	H1B	.H31_h	2.3871
C38	.C9_r	3.553(11)	H1B	.S1	2.9873
C39	.C13_r	3.415(11)	H1B	.N7_h	2.6600
C39	.C12_r	3.285(11)	H2A	.S13_j	3.0403
C40	.C12_r	3.424(10)	H2A	.H4C_k	2.5218
C1	.H31_h	2.9495	H3A	.H24C_i	2.5568
C6	.H28B_i	2.6826	H4C	.H2A_k	2.5218
C6	.H7A_e	2.9169	H5A	.O4	2.7244
C10	.H28A_g	3.0170	H5B	.O1_l	2.9151
C12	.H24C_i	2.9806	H6A	.S3_e	3.1552
C14	.H28A_g	2.7673	H6A	.H7A_e	2.4069
C15	.H28C_g	2.9089	H6B	.S1_l	2.9908
C16	.H7B_a	2.9614	H6B	.H28B_i	2.3068
C17	.H7B_a	3.0738	H6C	.C38_f	2.7783
C18	.H26C_f	2.9864	H6C	.H38_f	2.4687
C23	.H11_o	2.9574	H6C	.H28B_i	2.3638
C25	.H25B_t	2.4887	H6C	.H7A_e	2.5971
C25	.H25A_t	2.9629	H7A	.C6_e	2.9169
C29	.H21A	3.0413	H7A	.H6A_e	2.4069
C32	.H21A	3.0495	H7A	.H6C_e	2.5971
C32	.H33_i	3.0027	H7B	.S3	3.0301
C33	.H32_i	2.9591	H7B	.C16_a	2.9614
C33	.H21A	2.8538	H7B	.C17_a	3.0738
C34	.H8A_v	3.0044	H8A	.C34_m	3.0044
C38	.H6C_r	2.7783	H9	.N2	2.4973
C40	.H27A_b	2.9243	H9	.S1	2.9336
H1A	.S2	2.9851	H9	.S3	2.9511

Table S37 - Contact Distances(Angstrom) (continued)
for: (2·L2)2

H11	.S5	2.8745	H24C	.H3A_o	2.5568
H11	.S11_i	3.1031	H25A	.O8	2.5093
H11	.O6_i	2.6561	H25A	.S5_u	3.0827
H11	.C23_i	2.9574	H25A	.C25_t	2.9629
H11	.H23B_i	2.4979	H25A	.H25B_t	2.0975
H12	.O6_i	2.7470	H25B	.N3_r	2.8842
H12	.S2_d	2.8864	H25B	.C25_t	2.4887
H13	.S2	2.9968	H25B	.H25A_t	2.0975
H13	.S4	3.1274	H25B	.H25B_t	2.1021
H13	.S2_d	3.0707	H26C	.N3_r	2.9261
H16	.N2	2.4719	H26C	.C18_r	2.9864
H16	.S3_a	2.9000	H26C	.H18_r	2.3478
H16	.S1_a	2.8605	H27A	.S13	3.0595
H18	.N3	2.8007	H27A	.N8_b	2.9042
H18	.H26C_f	2.3478	H27A	.C40_b	2.9243
H19	.O5_n	2.6804	H27B	.S14	2.8593
H20	.S2_a	3.0855	H28A	.C10_u	3.0170
H20	.S4_a	3.0962	H28A	.C14_u	2.7673
H20	.O6_n	2.7729	H28B	.C6_o	2.6826
H21A	.N5	2.8605	H28B	.H6B_o	2.3068
H21A	.C29	3.0413	H28B	.H6C_o	2.3638
H21A	.C32	3.0495	H28C	.C15_u	2.9089
H21A	.C33	2.8538	H29	.S11	2.9735
H21B	.S11	3.0347	H29	.S14	3.0069
H23A	.O5	2.4890	H29	.N6	2.4626
H23B	.H11_o	2.4979	H31	.N7	2.7986
H24B	.S13_w	2.8523	H31	.C1_d	2.9495
H24C	.C12_o	2.9806	H31	.H1B_d	2.3871

Table S37 - Contact Distances(Angstrom) (continued)
for: (2·L2)2

H32	.S12_i	2.7697	H36	.S11_b	3.1196
H32	.C33_i	2.9591	H36	.S14_b	2.9135
H32	.H33_i	2.5707	H38	.S15	2.9323
H33	.S12	3.0926	H38	.P2_r	3.1587
H33	.S13	2.9126	H38	.O3_r	2.4050
H33	.C32_i	3.0027	H38	.H6C_r	2.4687
H33	.H32_i	2.5707	H40	.S12_b	2.9476
H36	.N6	2.4661	H40	.S13_b	3.1036

Table S38 - Hydrogen Bonds (Angstrom, Deg)
for: (2·L2)2

C9	-- H9 ..	N2	0.9500	2.5000	2.842(9)	101.00	.
C11	-- H11 ..	S5	0.9500	2.8700	3.236(8)	104.00	.
C16	-- H16 ..	N2	0.9500	2.4700	2.831(9)	102.00	.
C16	-- H16 ..	S1	0.9500	2.8600	3.332(7)	112.00	2_675
C23	-- H23A ..	O5	0.9900	2.4900	2.896(9)	104.00	.
C24	-- H24B ..	S13	0.9800	2.8500	3.796(10)	162.00	1_655
C27	-- H27B ..	S14	0.9900	2.8600	3.302(13)	108.00	.
C29	-- H29 ..	N6	0.9500	2.4600	2.819(9)	102.00	.
C32	-- H32 ..	S12	0.9500	2.7700	3.596(9)	146.00	2_766
C36	-- H36 ..	N6	0.9500	2.4700	2.815(9)	102.00	.
C38	-- H38 ..	O3	0.9500	2.4000	3.269(10)	151.00	1_545

Translation of Symmetry Code to Equiv.Pos for (2·L2)2

a =[2675.00] = 1-x,2-y,-z
b =[2756.00] = 2-x,-y,1-z
c =[1455.00] = -1+x,y,z
d =[2665.00] = 1-x,1-y,-z
e =[2775.00] = 2-x,2-y,-z
f =[1565.00] = x,1+y,z
g =[2666.00] = 1-x,1-y,1-z
h =[2665.00] = 1-x,1-y,-z
i =[2766.00] = 2-x,1-y,1-z
j =[1454.00] = -1+x,y,-1+z
k =[2565.00] = -x,1-y,-z
l =[1655.00] = 1+x,y,z
m =[2765.00] = 2-x,1-y,-z
n =[2776.00] = 2-x,2-y,1-z
p =[1656.00] = 1+x,y,1+z
q =[1455.00] = -1+x,y,z
r =[1545.00] = x,-1+y,z
s =[2776.00] = 2-x,2-y,1-z
t =[2656.00] = 1-x,-y,1-z
u =[2666.00] = 1-x,1-y,1-z
v =[2765.00] = 2-x,1-y,-z
w =[1655.00] = 1+x,y,z

Table S39 - Crystal Data and Details of the Structure Determination for: (3·L2)∞

Crystal Data			
Formula	C28 H28 N3.98 Ni O4 P2 S5.02		
Formula Weight	765.81		
Crystal System	Monoclinic		
Space group	P2/n	(No. 13)	
a, b, c [Angstrom]	12.8213(3)	7.2342(2)	19.1246(3)
alpha, beta, gamma [deg]	90	106.1860(10)	90
V [Ang**3]	1703.53(7)		
Z	2		
D(calc) [g/cm**3]	1.493		
Mu(MoKa) [/mm]	1.010		
F(000)	788		
Crystal Size [mm]	0.02 x	0.10 x	0.12
Data Collection			
Temperature (K)	120		
Radiation [Angstrom]	MoKa	0.71073	
Theta Min-Max [Deg]	3.0,	27.5	
Dataset	-16: 16 ;	-9: 9 ;	-24: 24
Tot., Uniq. Data, R(int)	19777,	3900,	0.039
Observed data [I > 2.0 sigma(I)]	3388		
Refinement			
Nref, Npar	3900,	213	
R, wR2, S	0.0372,	0.0778,	1.04
w = 1/[\s^2^(Fo^2^)+(0.0134P)^2^+2.6910P] where P=(Fo^2^+2Fc^2^)/3			
Max. and Av. Shift/Error	0.00,	0.00	
Min. and Max. Resd. Dens. [e/Ang^3]	-0.35,	0.33	

Table S40 - Final Coordinates and Equivalent Isotropic Displacement Parameters of the non-Hydrogen atoms for: (3·L2)∞

Atom	x	y	z	U(eq) [Ang^2]
Ni1	1/2	0	1/2	0.0185(1)
S1	0.33393(4)	0.18447(8)	0.49487(3)	0.0227(2)
S2	0.36728(5)	-0.18974(9)	0.40842(3)	0.0258(2)
*S3	0.7114(6)	-0.0848(11)	0.2741(4)	0.0244(7)
P1	0.26068(4)	-0.03953(9)	0.44239(3)	0.0215(2)
O1	0.03027(13)	-0.4386(2)	0.62679(9)	0.0288(5)
O2	0.15599(13)	0.0153(3)	0.37751(9)	0.0325(5)
N1	0.52769(14)	0.1718(3)	0.41452(10)	0.0206(5)
N3	3/4	0.2450(4)	1/4	0.0182(7)
C1	0.19495(17)	-0.1686(3)	0.49831(12)	0.0210(6)
C2	0.20254(18)	-0.3601(3)	0.50438(12)	0.0246(7)
C3	0.14948(18)	-0.4558(3)	0.54726(13)	0.0269(7)
C4	0.08672(17)	-0.3596(3)	0.58378(12)	0.0233(6)
C5	0.07885(17)	-0.1674(3)	0.57832(12)	0.0228(6)
C6	0.13312(17)	-0.0733(3)	0.53645(12)	0.0214(6)
C7	0.0378(2)	-0.6345(4)	0.63548(15)	0.0375(8)
C8	0.1674(2)	0.1405(6)	0.32131(16)	0.0582(13)
C9	0.58237(17)	0.1056(3)	0.36948(11)	0.0206(6)
C10	0.62095(17)	0.2162(3)	0.32289(11)	0.0208(6)
C11	0.59845(18)	0.4044(3)	0.32005(13)	0.0255(7)
C12	0.53789(19)	0.4728(3)	0.36383(13)	0.0283(7)
C13	0.50586(18)	0.3534(3)	0.41083(13)	0.0252(7)
C14	0.69101(17)	0.1376(3)	0.28138(11)	0.0203(6)
*N2	0.7005(18)	-0.052(3)	0.2749(12)	0.031(5)

U(eq) = 1/3 of the trace of the orthogonalized U Tensor

Starred Atom sites have a S.O.F less than 1.0

Table S41 - Hydrogen Atom Positions and Isotropic Displacement Parameters
for: (3·L2)∞

Atom	x	y	z	U(iso) [Ang^2]
H3	0.15600	-0.58640	0.55160	0.0320
H5	0.03620	-0.10160	0.60340	0.0270
H6	0.12850	0.05770	0.53350	0.0260
H7A	0.01160	-0.69400	0.58770	0.0560
H7B	-0.00670	-0.67460	0.66680	0.0560
H7C	0.11370	-0.66940	0.65780	0.0560
H2	0.24450	-0.42620	0.47890	0.0300
H8B	0.10240	0.21810	0.30560	0.0880
H8C	0.17620	0.06940	0.27970	0.0880
H9	0.59540	-0.02370	0.36950	0.0250
H11	0.62400	0.48390	0.28890	0.0310
H12	0.51840	0.59980	0.36180	0.0340
H13	0.46650	0.40290	0.44190	0.0300
H8A	0.23130	0.21900	0.34040	0.0880

==========

The Temperature Factor has the Form of Exp(-T) Where
T = 8*(Pi**2)*U*(Sin(Theta)/Lambda)**2 for Isotropic Atoms

Table S42 - (An)isotropic Displacement Parameters
for: (3·L2)∞

Atom	U(1,1) or U	U(2,2)	U(3,3)	U(2,3)	U(1,3)	U(1,2)
Ni1	0.0167(2)	0.0212(2)	0.0213(2)	0.0006(2)	0.0112(2)	0.0014(2)
S1	0.0207(3)	0.0213(3)	0.0309(3)	0.0008(2)	0.0153(2)	0.0023(2)
S2	0.0205(3)	0.0311(3)	0.0292(3)	-0.0079(2)	0.0125(2)	0.0013(2)
S3	0.0325(13)	0.0188(13)	0.0279(11)	-0.0035(7)	0.0185(10)	-0.0030(12)
P1	0.0160(3)	0.0275(3)	0.0232(3)	-0.0010(2)	0.0090(2)	0.0032(2)
O1	0.0268(9)	0.0286(9)	0.0325(9)	0.0058(7)	0.0108(7)	-0.0042(7)
O2	0.0217(8)	0.0502(12)	0.0267(8)	0.0050(8)	0.0084(7)	0.0049(8)
N1	0.0179(9)	0.0234(10)	0.0236(9)	0.0017(7)	0.0111(7)	-0.0002(8)
N3	0.0183(12)	0.0200(13)	0.0182(12)	0	0.0084(10)	0
C1	0.0146(10)	0.0261(12)	0.0225(11)	-0.0021(9)	0.0056(8)	-0.0007(9)
C2	0.0177(11)	0.0255(12)	0.0303(12)	-0.0063(10)	0.0061(9)	0.0027(9)
C3	0.0222(11)	0.0210(12)	0.0360(13)	-0.0006(10)	0.0056(10)	0.0007(9)
C4	0.0164(10)	0.0269(12)	0.0252(11)	0.0007(9)	0.0037(9)	-0.0037(9)
C5	0.0171(10)	0.0253(12)	0.0278(11)	-0.0027(9)	0.0091(9)	0.0002(9)
C6	0.0169(10)	0.0211(11)	0.0264(11)	-0.0027(9)	0.0066(9)	0.0007(9)
C7	0.0326(14)	0.0299(14)	0.0459(16)	0.0122(12)	0.0044(12)	-0.0032(11)
C8	0.0384(16)	0.101(3)	0.0373(16)	0.0330(18)	0.0138(13)	0.0121(18)
C9	0.0188(10)	0.0238(12)	0.0216(10)	-0.0009(9)	0.0095(8)	-0.0018(9)
C10	0.0156(10)	0.0298(12)	0.0189(10)	0.0012(9)	0.0079(8)	0.0010(9)
C11	0.0267(12)	0.0258(13)	0.0286(12)	0.0048(9)	0.0155(10)	0.0005(10)
C12	0.0301(12)	0.0226(12)	0.0381(13)	0.0053(10)	0.0191(11)	0.0029(10)
C13	0.0235(11)	0.0277(13)	0.0294(12)	-0.0004(10)	0.0154(10)	0.0022(10)
C14	0.0174(10)	0.0264(13)	0.0178(10)	0.0026(9)	0.0063(8)	-0.0001(9)
N2	0.035(6)	0.041(13)	0.029(5)	-0.002(6)	0.030(4)	-0.002(6)

==========

The Temperature Factor has the Form of Exp(-T) Where
T = 8*(Pi**2)*U*(Sin(Theta)/Lambda)**2 for Isotropic Atoms
T = 2*(Pi**2)*Sumij(h(i)*h(j)*U(i,j)*Astar(i)*Astar(j)), for
Anisotropic Atoms. Astar(i) are Reciprocal Axial Lengths and
h(i) are the Reflection Indices.

Table S43 - Bond Distances (Angstrom)
for: (3·L2)∞

Ni1	-S1	2.4915(6)	C5	-C6	1.378(3)
Ni1	-S2	2.4871(6)	C9	-C10	1.387(3)
Ni1	-N1	2.160(2)	C10	-C11	1.390(3)
S1	-P1	1.9974(8)	C10	-C14	1.469(3)
S2	-P1	1.9915(9)	C11	-C12	1.382(3)
S3	-C14	1.642(8)	C12	-C13	1.389(3)
S3	-S3_a	1.529(11)	C2	-H2	0.9496
P1	-O2	1.6031(18)	C3	-H3	0.9501
P1	-C1	1.797(2)	C5	-H5	0.9497
O1	-C4	1.363(3)	C6	-H6	0.9502
O1	-C7	1.427(3)	C7	-H7A	0.9808
O2	-C8	1.444(4)	C7	-H7B	0.9793
N1	-C9	1.341(3)	C7	-H7C	0.9805
N1	-C13	1.341(3)	C8	-H8A	0.9799
N2	-C14	1.39(2)	C8	-H8B	0.9800
N3	-C14	1.337(3)	C8	-H8C	0.9801
C1	-C2	1.391(3)	C9	-H9	0.9502
C1	-C6	1.399(3)	C11	-H11	0.9496
C2	-C3	1.388(3)	C12	-H12	0.9501
C3	-C4	1.390(3)	C13	-H13	0.9503
C4	-C5	1.396(3)			

Table S44 - Bond Angles (Degrees)
for: (3·L2)∞

S1	-Ni1	-S2	81.86(2)	C9	-N1	-C13	117.0(2)
S1	-Ni1	-N1	88.91(5)	C14	-N3	-C14_a	109.0(2)
S1	-Ni1	-S1_b	180.00	P1	-C1	-C2	122.25(17)
S1	-Ni1	-S2_b	98.14(2)	P1	-C1	-C6	118.82(16)
S1	-Ni1	-N1_b	91.09(5)	C2	-C1	-C6	118.9(2)
S2	-Ni1	-N1	90.52(5)	C1	-C2	-C3	120.8(2)
S1_b	-Ni1	-S2	98.14(2)	C2	-C3	-C4	119.7(2)
S2	-Ni1	-S2_b	180.00	O1	-C4	-C3	124.9(2)
S2	-Ni1	-N1_b	89.48(5)	O1	-C4	-C5	115.04(19)
S1_b	-Ni1	-N1	91.09(5)	C3	-C4	-C5	120.1(2)
S2_b	-Ni1	-N1	89.48(5)	C4	-C5	-C6	119.9(2)
N1	-Ni1	-N1_b	180.00	C1	-C6	-C5	120.7(2)
S1_b	-Ni1	-S2_b	81.86(2)	N1	-C9	-C10	123.4(2)
S1_b	-Ni1	-N1_b	88.91(5)	C9	-C10	-C11	118.9(2)
S2_b	-Ni1	-N1_b	90.52(5)	C9	-C10	-C14	120.3(2)
Ni1	-S1	-P1	82.08(3)	C11	-C10	-C14	120.6(2)
Ni1	-S2	-P1	82.31(3)	C10	-C11	-C12	118.2(2)
S3_a	-S3	-C14	101.3(5)	C11	-C12	-C13	119.1(2)
S1	-P1	-S2	109.71(4)	N1	-C13	-C12	123.3(2)
S1	-P1	-O2	111.29(9)	S3	-C14	-N3	114.1(3)
S1	-P1	-C1	110.82(8)	S3	-C14	-C10	124.1(3)
S2	-P1	-O2	112.66(7)	N3	-C14	-C10	121.7(2)
S2	-P1	-C1	112.90(8)	N2	-C14	-N3	117.4(10)
O2	-P1	-C1	99.14(10)	N2	-C14	-C10	120.9(10)
C4	-O1	-C7	117.16(18)	C1	-C2	-H2	119.67
P1	-O2	-C8	119.65(16)	C3	-C2	-H2	119.55
Ni1	-N1	-C9	120.40(16)	C2	-C3	-H3	120.14
Ni1	-N1	-C13	121.84(15)	C4	-C3	-H3	120.20

Table S44 - Bond Angles (Degrees) (continued)
for: (3·L2)∞

C4	-C5	-H5	120.09	O2	-C8	-H8C	109.49
C6	-C5	-H5	120.06	H8A	-C8	-H8B	109.48
C1	-C6	-H6	119.70	H8A	-C8	-H8C	109.46
C5	-C6	-H6	119.60	H8B	-C8	-H8C	109.40
O1	-C7	-H7A	109.44	N1	-C9	-H9	118.33
O1	-C7	-H7B	109.47	C10	-C9	-H9	118.29
O1	-C7	-H7C	109.46	C10	-C11	-H11	120.91
H7A	-C7	-H7B	109.46	C12	-C11	-H11	120.89
H7A	-C7	-H7C	109.46	C11	-C12	-H12	120.47
H7B	-C7	-H7C	109.52	C13	-C12	-H12	120.40
O2	-C8	-H8A	109.50	N1	-C13	-H13	118.40
O2	-C8	-H8B	109.49	C12	-C13	-H13	118.34

Table S45 - Torsion Angles (Degrees)
for: (3·L2)∞

S2	-Ni1	-S1	-P1	13.18(2)
N1	-Ni1	-S1	-P1	103.87(6)
S2_b	-Ni1	-S1	-P1	-166.82(2)
N1_b	-Ni1	-S1	-P1	-76.13(6)
S2	-Ni1	-N1	-C9	-71.31(16)
S1_b	-Ni1	-N1	-C9	26.84(16)
S2_b	-Ni1	-N1	-C9	108.69(16)
S1	-Ni1	-S2	-P1	-13.21(3)
N1	-Ni1	-S2	-P1	-102.04(6)
S1_b	-Ni1	-S2	-P1	166.79(3)
N1_b	-Ni1	-S2	-P1	77.96(6)
S1	-Ni1	-N1	-C9	-153.16(16)
S1	-Ni1	-N1	-C13	36.78(17)
S2	-Ni1	-N1	-C13	118.63(17)
S1_b	-Ni1	-N1	-C13	-143.22(17)
S2_b	-Ni1	-N1	-C13	-61.37(17)
Ni1	-S1	-P1	-O2	-142.79(7)
Ni1	-S1	-P1	-C1	107.91(8)
Ni1	-S1	-P1	-S2	-17.43(3)
Ni1	-S2	-P1	-O2	142.03(9)
Ni1	-S2	-P1	-C1	-106.68(8)
Ni1	-S2	-P1	-S1	17.45(3)
C14	-S3	-S3_a	-C14_a	4.6(6)
S3_a	-S3	-C14	-N3	-4.5(6)
S3_a	-S3	-C14	-C10	179.8(4)
S2	-P1	-O2	-C8	-67.1(2)
S1	-P1	-C1	-C2	-135.52(18)
C1	-P1	-O2	-C8	173.3(2)

Table S45 - Torsion Angles (Degrees) (continued)
for: (3·L2)∞

S1	-P1	-O2	-C8	56.6(2)
S1	-P1	-C1	-C6	45.1(2)
S2	-P1	-C1	-C6	168.67(16)
O2	-P1	-C1	-C6	-71.9(2)
S2	-P1	-C1	-C2	-12.0(2)
O2	-P1	-C1	-C2	107.4(2)
C7	-O1	-C4	-C3	0.9(3)
C7	-O1	-C4	-C5	-178.6(2)
Ni1	-N1	-C13	-C12	169.72(18)
C9	-N1	-C13	-C12	-0.7(3)
C13	-N1	-C9	-C10	3.2(3)
Ni1	-N1	-C9	-C10	-167.33(17)
C14_a	-N3	-C14	-S3	1.7(3)
C14_a	-N3	-C14	-C10	177.52(18)
P1	-C1	-C6	-C5	178.15(17)
C2	-C1	-C6	-C5	-1.2(3)
P1	-C1	-C2	-C3	-179.08(18)
C6	-C1	-C2	-C3	0.2(3)
C1	-C2	-C3	-C4	0.9(4)
C2	-C3	-C4	-C5	-1.2(3)
C2	-C3	-C4	-O1	179.4(2)
C3	-C4	-C5	-C6	0.2(3)
O1	-C4	-C5	-C6	179.7(2)
C4	-C5	-C6	-C1	1.0(3)
N1	-C9	-C10	-C11	-2.8(3)
N1	-C9	-C10	-C14	172.8(2)
C11	-C10	-C14	-N3	11.7(3)
C11	-C10	-C14	-S3	-173.0(4)

Table S45 - Torsion Angles (Degrees) (continued)
for: (3·L2)∞

C9	-C10	-C14	-S3	11.5(4)
C9	-C10	-C14	-N3	-163.84(18)
C14	-C10	-C11	-C12	-175.9(2)
C9	-C10	-C11	-C12	-0.3(3)
C10	-C11	-C12	-C13	2.6(3)
C11	-C12	-C13	-N1	-2.2(4)

Table S46 - Contact Distances(Angstrom)
for: (3·L2)∞

S1	.C12_e	3.698(2)	C3	.C11_b	3.529(3)
S2	.C12_f	3.537(2)	C4	.N3_b	3.386(2)
S3	.C7_h	3.580(8)	C4	.N3_b	3.386(2)
S1	.H2_d	3.0241	C5	.C6_i	3.451(3)
S1	.H6	3.0674	C5	.N3_b	3.449(2)
S1	.H8A	2.8903	C5	.C14_b	3.397(3)
S1	.H13	2.7152	C5	.N3_b	3.449(2)
S1	.H9_b	2.7553	C6	.C9_b	3.597(3)
S2	.H2	2.8990	C6	.C5_i	3.451(3)
S2	.H12_f	2.7982	C6	.C6_i	3.474(3)
S3	.H9	2.6924	C7	.S3_l	3.580(8)
S3	.H7C_g	2.8737	C7	.C2_k	3.472(4)
S3	.H7C_h	2.8504	C9	.C6_b	3.597(3)
P1	.C9_b	3.631(2)	C9	.P1_b	3.631(2)
O1	.H8B_i	2.8872	C9	.C1_b	3.275(3)
O2	.H5_i	2.6639	C10	.C2_b	3.599(3)
N2	.N2_a	1.79(3)	C10	.C1_b	3.589(3)
N3	.C4_j	3.386(2)	C11	.C3_b	3.529(3)
N3	.C4_b	3.386(2)	C12	.S1_e	3.698(2)
N3	.C5_b	3.449(2)	C12	.S2_d	3.537(2)
N3	.C5_j	3.449(2)	C14	.C5_b	3.397(3)
N2	.H9	2.5476	C1	.H7A_k	2.8772
N3	.H11_a	2.6115	C2	.H7A_k	2.8455
N3	.H11	2.6115	C3	.H7A	2.7304
C1	.C10_b	3.589(3)	C3	.H7A_k	3.0215
C1	.C9_b	3.275(3)	C3	.H7C	2.7583
C2	.C10_b	3.599(3)	C5	.H6_i	3.0168
C2	.C7_k	3.472(4)	C6	.H7A_k	3.0754

Table S46 - Contact Distances(Angstrom) (continued)
for: (3·L2)∞

C7	.H3	2.5192	H7C	.S3_g	2.8737
C7	.H11_c	3.0347	H7C	.S3_l	2.8504
H2	.S1_f	3.0241	H7C	.C3	2.7583
H2	.S2	2.8990	H7C	.H3	2.3225
H3	.H7A	2.2854	H8A	.S1	2.8903
H3	.C7	2.5192	H8B	.O1_i	2.8872
H3	.H7C	2.3225	H8C	.H8C_m	2.4638
H5	.O2_i	2.6639	H9	.S3	2.6924
H6	.S1	3.0674	H9	.S1_b	2.7553
H6	.C5_i	3.0168	H9	.N2	2.5476
H7A	.H3	2.2854	H11	.C7_j	3.0347
H7A	.C1_k	2.8772	H11	.N3	2.6115
H7A	.C3_k	3.0215	H12	.S2_d	2.7982
H7A	.C6_k	3.0754	H13	.H13_e	2.5663
H7A	.C2_k	2.8455	H13	.S1	2.7152
H7A	.C3	2.7304			

Table S47 - Hydrogen Bonds (Angstrom, Deg)
for: (3·L2)∞

C7	-- H7C	.. S3	0.9800	2.8700	3.789(8)	156.00	3_646
C7	-- H7C	.. S3	0.9800	2.8500	3.580(8)	132.00	4_445
C9	-- H9	.. S3	0.9500	2.6900	3.105(8)	107.00	.
C9	-- H9	.. S1	0.9500	2.7600	3.276(2)	115.00	3_656
C12	-- H12	.. S2	0.9500	2.8000	3.537(2)	135.00	1_565
C13	-- H13	.. S1	0.9500	2.7200	3.303(2)	121.00	.

Translation of Symmetry Code to Equiv.Pos for: (3·L2)∞

a =[2655.00] = 3/2-x,y,1/2-z
b =[3656.00] = 1-x,-y,1-z
c =[4455.00] = -1/2+x,-y,1/2+z
d =[1565.00] = x,1+y,z
e =[3666.00] = 1-x,1-y,1-z
f =[1545.00] = x,-1+y,z
g =[3646.00] = 1-x,-1-y,1-z
h =[4544.00] = 1/2+x,-1-y,-1/2+z
i =[3556.00] = -x,-y,1-z
j =[4554.00] = 1/2+x,-y,-1/2+z
k =[3546.00] = -x,-1-y,1-z
l =[4445.00] = -1/2+x,-1-y,1/2+z
m =[2555.00] = 1/2-x,y,1/2-z

Table S48 - Crystal Data and Details of the Structure Determination
for: (4·L1)∞

Crystal Data			
Formula			C36 H28 N4 Ni P2 S5
Formula Weight			797.57
Crystal System			Triclinic
Space group		P-1	(No. 2)
a, b, c [Angstrom]	6.8385(2)	12.0415(3)	22.6405(4)
alpha, beta, gamma [deg]	101.922(2)	97.350(2)	93.086(2)
V [Ang**3]			1802.95(8)
Z			2
D(calc) [g/cm**3]			1.469
Mu(MoKa) [/mm]			0.950
F(000)			820
Crystal Size [mm]		0.03 x 0.12 x 0.21	

Data Collection			
Temperature (K)			173
Radiation [Angstrom]		MoKa	0.71073
Theta Min-Max [Deg]			3.7, 32.4
Dataset		-10: 10 ; -18: 17 ; -33: 33	
Tot., Uniq. Data, R(int)		30395, 11661, 0.045	
Observed data [I > 2.0 sigma(I)]			7622

Refinement			
Nref, Npar			11661, 436
R, wR2, S		0.0407, 0.1140, 0.96	
w = 1/[\s^2^(Fo^2^)+(0.0651P)^2^]		where P=(Fo^2^+2Fc^2^)/3	
Max. and Av. Shift/Error			0.00, 0.00
Min. and Max. Resd. Dens. [e/Ang^3]			-0.89, 0.83

Table S49 - Final Coordinates and Equivalent Isotropic Displacement Parameters of the non-Hydrogen atoms for: (4·L1)∞

Atom	x	y	z	U(eq) [Ang^2]
Ni1	0	1	1/2	0.0192(1)
Ni2	1/2	1/2	1	0.0199(1)
S1	0.15509(8)	0.89579(5)	0.41352(2)	0.0257(1)
S2	-0.22510(8)	0.82348(5)	0.47711(2)	0.0255(1)
S3	0.15367(7)	0.42016(4)	0.95689(2)	0.0240(1)
S4	0.57586(7)	0.30334(5)	0.95116(2)	0.0251(1)
S9	0.83296(10)	0.70943(8)	0.73938(3)	0.0562(3)
P1	-0.05602(8)	0.77328(5)	0.41210(2)	0.0242(2)
P2	0.28260(8)	0.27351(5)	0.94590(2)	0.0222(1)
N1	0.1850(2)	0.92861(15)	0.56351(7)	0.0225(5)
N8	0.7480(3)	0.7671(2)	0.68585(8)	0.0374(7)
N11	0.4712(2)	0.73891(15)	0.73353(7)	0.0248(5)
N15	0.5277(2)	0.55499(15)	0.91881(7)	0.0231(5)
C2	0.1097(3)	0.88200(19)	0.60544(9)	0.0255(6)
C3	0.2231(3)	0.83383(19)	0.64696(9)	0.0261(6)
C4	0.4239(3)	0.83277(18)	0.64628(8)	0.0221(5)
C5	0.5029(3)	0.8808(2)	0.60306(10)	0.0361(7)
C6	0.3793(3)	0.9274(2)	0.56342(10)	0.0338(7)
C7	0.5502(3)	0.78011(19)	0.68940(9)	0.0258(6)
C10	0.6115(3)	0.69559(19)	0.76494(9)	0.0264(6)
C12	0.5812(3)	0.64396(19)	0.81700(9)	0.0250(6)
C13	0.7257(3)	0.58423(19)	0.84272(9)	0.0277(6)
C14	0.6932(3)	0.54155(19)	0.89305(9)	0.0256(6)
C16	0.3864(3)	0.61086(19)	0.89284(9)	0.0256(6)
C17	0.4071(3)	0.65553(19)	0.84248(9)	0.0275(6)
C18	-0.2085(4)	0.7332(2)	0.33800(10)	0.0375(7)

Table S49 - Final Coordinates and Equivalent Isotropic Displacement Parameters of the non-Hydrogen atoms (continued) for: (4·L1)∞

Atom	x	y	z	U(eq) [Ang^2]
C19	-0.4049(4)	0.7577(3)	0.33110(12)	0.0508(9)
C20	-0.5183(6)	0.7281(4)	0.27359(16)	0.0838(14)
C21	-0.4335(7)	0.6770(4)	0.22393(15)	0.0948(18)
C22	-0.2409(8)	0.6531(3)	0.23046(13)	0.0800(16)
C23	-0.1253(5)	0.6804(3)	0.28776(11)	0.0517(9)
C24	0.0536(4)	0.6426(2)	0.42081(11)	0.0349(7)
C25	-0.0699(5)	0.5447(2)	0.41569(15)	0.0590(11)
C26	0.0100(7)	0.4453(3)	0.42416(18)	0.0773(17)
C27	0.2088(8)	0.4419(3)	0.43612(19)	0.0849(18)
C28	0.3318(6)	0.5383(4)	0.4422(2)	0.0870(19)
C29	0.2555(5)	0.6408(3)	0.43456(16)	0.0600(11)
C30	0.1775(3)	0.17906(18)	0.87416(9)	0.0266(6)
C31	-0.0214(3)	0.1789(2)	0.85168(10)	0.0324(7)
C32	-0.1013(4)	0.1076(2)	0.79692(11)	0.0422(8)
C33	0.0176(5)	0.0361(3)	0.76397(12)	0.0516(9)
C34	0.2134(5)	0.0359(3)	0.78656(13)	0.0589(10)
C35	0.2949(4)	0.1065(2)	0.84129(12)	0.0438(8)
C36	0.2214(3)	0.19631(18)	1.00326(9)	0.0254(6)
C37	0.0370(4)	0.2018(2)	1.02216(11)	0.0398(8)
C38	-0.0138(4)	0.1421(3)	1.06459(12)	0.0479(9)
C39	0.1178(5)	0.0766(2)	1.08865(13)	0.0519(10)
C40	0.3013(5)	0.0694(3)	1.06990(15)	0.0591(11)
C41	0.3537(4)	0.1296(2)	1.02754(12)	0.0432(8)

U(eq) = 1/3 of the trace of the orthogonalized U Tensor

Table S50 - Hydrogen Atom Positions and Isotropic Displacement Parameters
for: (4·L1)∞

Atom	x	y	z	U(iso) [Ang^2]
H2A	-0.02860	0.88210	0.60670	0.0310
H3A	0.16280	0.80170	0.67580	0.0310
H5A	0.64070	0.88160	0.60080	0.0430
H6A	0.43620	0.96060	0.53430	0.0410
H13A	0.84520	0.57300	0.82590	0.0330
H14A	0.79280	0.50080	0.91020	0.0310
H16A	0.26720	0.61980	0.91010	0.0310
H17A	0.30350	0.69380	0.82540	0.0330
H19A	-0.46190	0.79440	0.36530	0.0610
H20A	-0.65370	0.74310	0.26870	0.1010
H21A	-0.51050	0.65820	0.18470	0.1140
H22A	-0.18460	0.61760	0.19580	0.0960
H23A	0.00900	0.66300	0.29230	0.0620
H25A	-0.20900	0.54620	0.40640	0.0710
H26A	-0.07490	0.37880	0.42160	0.0930
H27A	0.26280	0.37240	0.44030	0.1020
H28A	0.47070	0.53570	0.45170	0.1040
H29A	0.34110	0.70760	0.43880	0.0720
H31A	-0.10290	0.22810	0.87410	0.0390
H32A	-0.23750	0.10750	0.78180	0.0510
H33A	-0.03630	-0.01240	0.72600	0.0620
H34A	0.29450	-0.01360	0.76420	0.0710
H35A	0.43070	0.10540	0.85640	0.0530
H37A	-0.05590	0.24720	1.00570	0.0480
H38A	-0.14110	0.14670	1.07710	0.0570
H39A	0.08320	0.03620	1.11820	0.0620

Table S50 - Hydrogen Atom Positions and Isotropic Displacement Parameters (continued)
for: (4·L1)∞

Atom	x	y	z	U(iso) [Ang^2]
H40A	0.39260	0.02290	1.08610	0.0710
H41A	0.48120	0.12490	1.01520	0.0520

==========

The Temperature Factor has the Form of Exp(-T) Where
T = 8*(Pi**2)*U*(Sin(Theta)/Lambda)**2 for Isotropic Atoms

Table S51 - (An)isotropic Displacement Parameters
for: (4·L1)∞

Atom	U(1,1) or U	U(2,2)	U(3,3)	U(2,3)	U(1,3)	U(1,2)
Ni1	0.0206(2)	0.0227(2)	0.0160(2)	0.0090(1)	0.0018(1)	-0.0001(1)
Ni2	0.0231(2)	0.0243(2)	0.0148(2)	0.0091(1)	0.0022(1)	0.0064(1)
S1	0.0265(2)	0.0274(3)	0.0249(2)	0.0082(2)	0.0071(2)	-0.0005(2)
S2	0.0255(2)	0.0289(3)	0.0231(2)	0.0085(2)	0.0048(2)	-0.0026(2)
S3	0.0241(2)	0.0262(3)	0.0229(2)	0.0075(2)	0.0009(2)	0.0087(2)
S4	0.0231(2)	0.0298(3)	0.0240(2)	0.0075(2)	0.0044(2)	0.0079(2)
S9	0.0357(3)	0.0977(6)	0.0542(4)	0.0529(5)	0.0111(3)	0.0210(4)
P1	0.0283(3)	0.0247(3)	0.0199(2)	0.0065(2)	0.0032(2)	-0.0014(2)
P2	0.0242(2)	0.0249(3)	0.0188(2)	0.0068(2)	0.0029(2)	0.0070(2)
N1	0.0237(8)	0.0276(9)	0.0185(8)	0.0115(7)	0.0019(6)	0.0001(7)
N8	0.0209(8)	0.0768(16)	0.0248(9)	0.0340(10)	0.0073(7)	-0.0027(9)
N11	0.0278(9)	0.0312(9)	0.0201(8)	0.0148(7)	0.0054(6)	0.0042(7)
N15	0.0275(8)	0.0253(9)	0.0185(8)	0.0099(7)	0.0008(6)	0.0063(7)
C2	0.0227(9)	0.0348(11)	0.0223(9)	0.0140(9)	0.0036(7)	0.0011(9)
C3	0.0275(10)	0.0310(11)	0.0240(10)	0.0151(9)	0.0049(8)	0.0000(9)
C4	0.0258(9)	0.0257(10)	0.0168(8)	0.0097(8)	0.0028(7)	0.0005(8)
C5	0.0232(10)	0.0611(16)	0.0349(12)	0.0331(12)	0.0074(8)	0.0050(10)
C6	0.0250(10)	0.0535(15)	0.0325(11)	0.0295(11)	0.0073(8)	0.0032(10)
C7	0.0281(10)	0.0318(11)	0.0208(9)	0.0127(9)	0.0040(7)	0.0034(9)
C10	0.0259(10)	0.0369(12)	0.0193(9)	0.0127(9)	0.0030(7)	0.0031(9)
C12	0.0266(10)	0.0332(11)	0.0175(9)	0.0119(8)	0.0008(7)	0.0039(9)
C13	0.0278(10)	0.0364(12)	0.0233(10)	0.0137(9)	0.0063(8)	0.0068(9)
C14	0.0250(10)	0.0344(11)	0.0216(9)	0.0143(9)	0.0025(7)	0.0094(9)
C16	0.0258(10)	0.0322(11)	0.0237(10)	0.0153(9)	0.0042(7)	0.0078(9)
C17	0.0269(10)	0.0346(12)	0.0252(10)	0.0159(9)	0.0017(8)	0.0084(9)
C18	0.0505(14)	0.0381(13)	0.0209(10)	0.0082(10)	-0.0006(9)	-0.0163(11)

Table S51 - (An)isotropic Displacement Parameters (continued)
for: (4·L1)∞

Atom	U(1,1) or U	U(2,2)	U(3,3)	U(2,3)	U(1,3)	U(1,2)
C19	0.0431(14)	0.074(2)	0.0346(13)	0.0260(14)	-0.0120(11)	-0.0165(14)
C20	0.075(2)	0.118(3)	0.053(2)	0.047(2)	-0.0340(17)	-0.049(2)
C21	0.133(4)	0.103(3)	0.0330(18)	0.029(2)	-0.034(2)	-0.075(3)
C22	0.150(4)	0.055(2)	0.0228(14)	-0.0016(14)	0.0068(18)	-0.049(2)
C23	0.079(2)	0.0461(16)	0.0256(12)	0.0008(12)	0.0113(12)	-0.0167(15)
C24	0.0472(14)	0.0266(11)	0.0328(12)	0.0074(10)	0.0109(10)	0.0050(10)
C25	0.080(2)	0.0292(14)	0.066(2)	0.0078(14)	0.0118(17)	-0.0051(15)
C26	0.130(4)	0.0235(14)	0.080(3)	0.0093(16)	0.024(2)	0.0068(19)
C27	0.140(4)	0.045(2)	0.093(3)	0.036(2)	0.053(3)	0.046(2)
C28	0.082(3)	0.084(3)	0.128(4)	0.069(3)	0.044(2)	0.052(2)
C29	0.0570(18)	0.0576(19)	0.084(2)	0.0456(18)	0.0233(16)	0.0218(15)
C30	0.0335(11)	0.0252(10)	0.0210(9)	0.0049(8)	0.0035(8)	0.0038(9)
C31	0.0324(11)	0.0350(12)	0.0296(11)	0.0064(10)	0.0036(9)	0.0039(10)
C32	0.0435(14)	0.0426(15)	0.0349(13)	0.0053(12)	-0.0075(10)	-0.0027(12)
C33	0.0667(19)	0.0478(16)	0.0291(13)	-0.0077(12)	-0.0062(12)	-0.0020(15)
C34	0.0592(18)	0.061(2)	0.0433(16)	-0.0189(14)	0.0019(13)	0.0175(16)
C35	0.0446(14)	0.0454(15)	0.0350(13)	-0.0052(11)	-0.0002(10)	0.0142(12)
C36	0.0319(11)	0.0234(10)	0.0207(9)	0.0069(8)	-0.0001(8)	0.0025(8)
C37	0.0361(12)	0.0533(16)	0.0371(13)	0.0219(12)	0.0102(10)	0.0064(12)
C38	0.0482(15)	0.0565(18)	0.0429(14)	0.0178(14)	0.0140(12)	-0.0069(13)
C39	0.076(2)	0.0423(16)	0.0414(15)	0.0210(13)	0.0097(14)	-0.0087(15)
C40	0.068(2)	0.0523(18)	0.069(2)	0.0417(17)	0.0044(16)	0.0123(16)
C41	0.0448(14)	0.0402(14)	0.0544(16)	0.0277(13)	0.0105(12)	0.0143(12)

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The Temperature Factor has the Form of Exp(-T) Where
T = 8*(Pi**2)*U*(Sin(Theta)/Lambda)**2 for Isotropic Atoms
T = 2*(Pi**2)*Sumij(h(i)*h(j)*U(i,j)*Astar(i)*Astar(j)), for
Anisotropic Atoms. Astar(i) are Reciprocal Axial Lengths and
h(i) are the Reflection Indices.

Table S52 - Bond Distances (Angstrom)
for: (4·L1)∞

Ni1	-S1	2.4885(5)	C10	-C12	1.473(3)
Ni1	-S2	2.4788(6)	C12	-C13	1.391(3)
Ni1	-N1	2.1376(16)	C12	-C17	1.389(3)
Ni2	-S3	2.5024(5)	C13	-C14	1.381(3)
Ni2	-S4	2.5093(6)	C16	-C17	1.377(3)
Ni2	-N15	2.1052(16)	C18	-C19	1.387(4)
S1	-P1	2.0002(8)	C18	-C23	1.388(4)
S2	-P1	2.0029(7)	C19	-C20	1.394(5)
S3	-P2	2.0000(8)	C20	-C21	1.378(5)
S4	-P2	2.0022(7)	C21	-C22	1.359(7)
S9	-N8	1.581(2)	C22	-C23	1.396(4)
S9	-C10	1.701(2)	C24	-C25	1.388(4)
P1	-C18	1.816(2)	C24	-C29	1.378(4)
P1	-C24	1.815(3)	C25	-C26	1.381(5)
P2	-C30	1.816(2)	C26	-C27	1.356(7)
P2	-C36	1.823(2)	C27	-C28	1.369(6)
N1	-C2	1.340(3)	C28	-C29	1.400(6)
N1	-C6	1.330(2)	C30	-C31	1.390(3)
N8	-C7	1.381(3)	C30	-C35	1.386(3)
N11	-C7	1.360(3)	C31	-C32	1.382(3)
N11	-C10	1.316(3)	C32	-C33	1.387(4)
N15	-C14	1.340(2)	C33	-C34	1.371(5)
N15	-C16	1.349(3)	C34	-C35	1.381(4)
C2	-C3	1.382(3)	C36	-C37	1.383(3)
C3	-C4	1.376(3)	C36	-C41	1.378(3)
C4	-C5	1.385(3)	C37	-C38	1.380(4)
C4	-C7	1.483(3)	C38	-C39	1.363(4)
C5	-C6	1.378(3)	C39	-C40	1.377(5)

Table S52 - Bond Distances (Angstrom) (continued)
for: (4·L1)∞

C40	-C41	1.386(4)	C26	-H26A	0.9507
C2	-H2A	0.9499	C27	-H27A	0.9501
C3	-H3A	0.9498	C28	-H28A	0.9504
C5	-H5A	0.9499	C29	-H29A	0.9497
C6	-H6A	0.9506	C31	-H31A	0.9502
C13	-H13A	0.9494	C32	-H32A	0.9502
C14	-H14A	0.9500	C33	-H33A	0.9509
C16	-H16A	0.9499	C34	-H34A	0.9497
C17	-H17A	0.9500	C35	-H35A	0.9495
C19	-H19A	0.9493	C37	-H37A	0.9499
C20	-H20A	0.9499	C38	-H38A	0.9502
C21	-H21A	0.9496	C39	-H39A	0.9502
C22	-H22A	0.9504	C40	-H40A	0.9496
C23	-H23A	0.9505	C41	-H41A	0.9500
C25	-H25A	0.9495			

Table S53 - Bond Angles (Degrees)
for: (4·L1)∞

S1	-Ni1	-S2	82.95(2)	S3_b	-Ni2	-N15_b	89.58(4)
S1	-Ni1	-N1	91.22(4)	S4_b	-Ni2	-N15_b	90.33(5)
S1	-Ni1	-S1_a	180.00	Ni1	-S1	-P1	83.16(2)
S1	-Ni1	-S2_a	97.05(2)	Ni1	-S2	-P1	83.36(3)
S1	-Ni1	-N1_a	88.78(4)	Ni2	-S3	-P2	81.98(2)
S2	-Ni1	-N1	88.76(5)	Ni2	-S4	-P2	81.76(2)
S1_a	-Ni1	-S2	97.05(2)	N8	-S9	-C10	94.31(11)
S2	-Ni1	-S2_a	180.00	S1	-P1	-S2	110.53(3)
S2	-Ni1	-N1_a	91.24(5)	S1	-P1	-C18	111.35(8)
S1_a	-Ni1	-N1	88.78(4)	S1	-P1	-C24	110.29(9)
S2_a	-Ni1	-N1	91.24(5)	S2	-P1	-C18	110.05(9)
N1	-Ni1	-N1_a	180.00	S2	-P1	-C24	111.09(9)
S1_a	-Ni1	-S2_a	82.95(2)	C18	-P1	-C24	103.34(11)
S1_a	-Ni1	-N1_a	91.22(4)	S3	-P2	-S4	110.31(4)
S2_a	-Ni1	-N1_a	88.76(5)	S3	-P2	-C30	110.53(7)
S3	-Ni2	-S4	81.90(2)	S3	-P2	-C36	109.55(7)
S3	-Ni2	-N15	89.58(4)	S4	-P2	-C30	111.46(7)
S3	-Ni2	-S3_b	180.00	S4	-P2	-C36	111.05(7)
S3	-Ni2	-S4_b	98.10(2)	C30	-P2	-C36	103.76(10)
S3	-Ni2	-N15_b	90.42(4)	Ni1	-N1	-C2	121.27(12)
S4	-Ni2	-N15	90.33(5)	Ni1	-N1	-C6	122.16(14)
S3_b	-Ni2	-S4	98.10(2)	C2	-N1	-C6	116.57(18)
S4	-Ni2	-S4_b	180.00	S9	-N8	-C7	108.06(16)
S4	-Ni2	-N15_b	89.67(5)	C7	-N11	-C10	108.52(16)
S3_b	-Ni2	-N15	90.42(4)	Ni2	-N15	-C14	120.66(13)
S4_b	-Ni2	-N15	89.67(5)	Ni2	-N15	-C16	121.73(12)
N15	-Ni2	-N15_b	180.00	C14	-N15	-C16	117.48(17)
S3_b	-Ni2	-S4_b	81.90(2)	N1	-C2	-C3	123.30(19)

Table S53 - Bond Angles (Degrees) (continued)
for: (4·L1)∞

C2	-C3	-C4	119.58(19)	P1	-C24	-C29	120.9(2)
C3	-C4	-C5	117.47(19)	C25	-C24	-C29	120.1(3)
C3	-C4	-C7	121.20(18)	C24	-C25	-C26	119.9(3)
C5	-C4	-C7	121.32(19)	C25	-C26	-C27	120.4(4)
C4	-C5	-C6	119.25(19)	C26	-C27	-C28	120.2(4)
N1	-C6	-C5	123.8(2)	C27	-C28	-C29	120.8(4)
N8	-C7	-N11	117.12(18)	C24	-C29	-C28	118.5(3)
N8	-C7	-C4	122.61(19)	P2	-C30	-C31	120.30(16)
N11	-C7	-C4	120.24(18)	P2	-C30	-C35	120.33(17)
S9	-C10	-N11	111.91(15)	C31	-C30	-C35	119.4(2)
S9	-C10	-C12	124.12(16)	C30	-C31	-C32	120.4(2)
N11	-C10	-C12	123.96(18)	C31	-C32	-C33	119.9(2)
C10	-C12	-C13	121.48(19)	C32	-C33	-C34	119.5(3)
C10	-C12	-C17	120.44(19)	C33	-C34	-C35	121.1(3)
C13	-C12	-C17	118.08(19)	C30	-C35	-C34	119.7(3)
C12	-C13	-C14	119.16(19)	P2	-C36	-C37	119.92(17)
N15	-C14	-C13	123.0(2)	P2	-C36	-C41	121.42(17)
N15	-C16	-C17	123.00(19)	C37	-C36	-C41	118.6(2)
C12	-C17	-C16	119.2(2)	C36	-C37	-C38	120.8(2)
P1	-C18	-C19	120.53(19)	C37	-C38	-C39	120.3(3)
P1	-C18	-C23	119.4(2)	C38	-C39	-C40	119.6(3)
C19	-C18	-C23	120.1(2)	C39	-C40	-C41	120.4(3)
C18	-C19	-C20	119.6(3)	C36	-C41	-C40	120.2(3)
C19	-C20	-C21	119.8(4)	N1	-C2	-H2A	118.36
C20	-C21	-C22	120.8(3)	C3	-C2	-H2A	118.33
C21	-C22	-C23	120.4(3)	C2	-C3	-H3A	120.19
C18	-C23	-C22	119.3(3)	C4	-C3	-H3A	120.23
P1	-C24	-C25	118.9(2)	C4	-C5	-H5A	120.34

Table S53 - Bond Angles (Degrees) (continued)
for: (4·L1)∞

C6	-C5	-H5A	120.42	C28	-C27	-H27A	119.92
N1	-C6	-H6A	118.06	C27	-C28	-H28A	119.66
C5	-C6	-H6A	118.12	C29	-C28	-H28A	119.54
C12	-C13	-H13A	120.42	C24	-C29	-H29A	120.79
C14	-C13	-H13A	120.41	C28	-C29	-H29A	120.66
N15	-C14	-H14A	118.52	C30	-C31	-H31A	119.81
C13	-C14	-H14A	118.44	C32	-C31	-H31A	119.82
N15	-C16	-H16A	118.49	C31	-C32	-H32A	120.11
C17	-C16	-H16A	118.51	C33	-C32	-H32A	119.97
C12	-C17	-H17A	120.46	C32	-C33	-H33A	120.24
C16	-C17	-H17A	120.34	C34	-C33	-H33A	120.26
C18	-C19	-H19A	120.26	C33	-C34	-H34A	119.50
C20	-C19	-H19A	120.15	C35	-C34	-H34A	119.36
C19	-C20	-H20A	120.03	C30	-C35	-H35A	120.09
C21	-C20	-H20A	120.13	C34	-C35	-H35A	120.22
C20	-C21	-H21A	119.63	C36	-C37	-H37A	119.58
C22	-C21	-H21A	119.62	C38	-C37	-H37A	119.58
C21	-C22	-H22A	119.78	C37	-C38	-H38A	119.85
C23	-C22	-H22A	119.80	C39	-C38	-H38A	119.85
C18	-C23	-H23A	120.37	C38	-C39	-H39A	120.23
C22	-C23	-H23A	120.30	C40	-C39	-H39A	120.20
C24	-C25	-H25A	120.01	C39	-C40	-H40A	119.79
C26	-C25	-H25A	120.14	C41	-C40	-H40A	119.77
C25	-C26	-H26A	119.78	C36	-C41	-H41A	119.88
C27	-C26	-H26A	119.78	C40	-C41	-H41A	119.92
C26	-C27	-H27A	119.90				

Table S54 - Torsion Angles (Degrees)
for: (4·L1)∞

S2	-Ni1	-S1	-P1	-0.24(2)
N1	-Ni1	-S1	-P1	88.36(5)
S2_a	-Ni1	-S1	-P1	179.76(2)
N1_a	-Ni1	-S1	-P1	-91.64(5)
S1	-Ni1	-S2	-P1	0.24(2)
N1	-Ni1	-S2	-P1	-91.14(5)
S1_a	-Ni1	-S2	-P1	-179.76(2)
N1_a	-Ni1	-S2	-P1	88.86(5)
S1	-Ni1	-N1	-C2	-131.96(16)
S1	-Ni1	-N1	-C6	47.67(17)
S2	-Ni1	-N1	-C2	-49.04(16)
S2	-Ni1	-N1	-C6	130.58(17)
S1_a	-Ni1	-N1	-C2	48.04(16)
S1_a	-Ni1	-N1	-C6	-132.33(17)
S2_a	-Ni1	-N1	-C2	130.96(16)
S2_a	-Ni1	-N1	-C6	-49.42(17)
S4	-Ni2	-S3	-P2	13.16(2)
N15	-Ni2	-S3	-P2	103.56(5)
S4_b	-Ni2	-S3	-P2	-166.84(2)
N15_b	-Ni2	-S3	-P2	-76.44(5)
S3	-Ni2	-S4	-P2	-13.15(2)
N15	-Ni2	-S4	-P2	-102.69(4)
S3_b	-Ni2	-S4	-P2	166.85(2)
N15_b	-Ni2	-S4	-P2	77.31(4)
S3	-Ni2	-N15	-C14	-137.11(16)
S3	-Ni2	-N15	-C16	46.99(16)
S4	-Ni2	-N15	-C14	-55.22(16)
S4	-Ni2	-N15	-C16	128.89(16)

Table S54 - Torsion Angles (Degrees) (continued)
for: (4·L1)∞

S3_b	-Ni2	-N15	-C14	42.89(16)
S3_b	-Ni2	-N15	-C16	-133.01(16)
S4_b	-Ni2	-N15	-C14	124.78(16)
S4_b	-Ni2	-N15	-C16	-51.11(16)
Ni1	-S1	-P1	-S2	0.32(3)
Ni1	-S1	-P1	-C18	122.96(9)
Ni1	-S1	-P1	-C24	-122.92(8)
Ni1	-S2	-P1	-C18	-123.72(9)
Ni1	-S2	-P1	-C24	122.46(9)
Ni1	-S2	-P1	-S1	-0.32(3)
Ni2	-S3	-P2	-C36	105.00(7)
Ni2	-S3	-P2	-S4	-17.53(3)
Ni2	-S3	-P2	-C30	-141.26(8)
Ni2	-S4	-P2	-S3	17.49(3)
Ni2	-S4	-P2	-C30	140.68(8)
Ni2	-S4	-P2	-C36	-104.16(8)
N8	-S9	-C10	-N11	-2.10(18)
N8	-S9	-C10	-C12	179.4(2)
C10	-S9	-N8	-C7	2.55(18)
S2	-P1	-C18	-C23	-170.8(2)
C24	-P1	-C18	-C19	129.7(2)
S2	-P1	-C24	-C25	62.6(2)
S2	-P1	-C24	-C29	-115.0(2)
C18	-P1	-C24	-C25	-55.4(2)
C18	-P1	-C24	-C29	127.0(2)
C24	-P1	-C18	-C23	-52.1(3)
S1	-P1	-C24	-C25	-174.5(2)
S1	-P1	-C24	-C29	7.9(3)

Table S54 - Torsion Angles (Degrees) (continued)
for: (4·L1)∞

S1	-P1	-C18	-C19	-112.0(2)
S1	-P1	-C18	-C23	66.3(2)
S2	-P1	-C18	-C19	11.0(3)
S3	-P2	-C30	-C31	-34.1(2)
S3	-P2	-C30	-C35	145.91(17)
S4	-P2	-C30	-C31	-157.12(16)
S4	-P2	-C30	-C35	22.8(2)
C36	-P2	-C30	-C31	83.3(2)
C36	-P2	-C30	-C35	-96.7(2)
S3	-P2	-C36	-C37	35.1(2)
S3	-P2	-C36	-C41	-146.52(18)
S4	-P2	-C36	-C37	157.19(17)
S4	-P2	-C36	-C41	-24.4(2)
C30	-P2	-C36	-C37	-83.0(2)
C30	-P2	-C36	-C41	95.4(2)
Ni1	-N1	-C2	-C3	179.30(16)
C6	-N1	-C2	-C3	-0.3(3)
Ni1	-N1	-C6	-C5	-179.08(18)
C2	-N1	-C6	-C5	0.6(3)
S9	-N8	-C7	-N11	-2.7(3)
S9	-N8	-C7	-C4	179.39(17)
C10	-N11	-C7	-N8	1.2(3)
C10	-N11	-C7	-C4	179.14(19)
C7	-N11	-C10	-S9	0.8(2)
C7	-N11	-C10	-C12	179.4(2)
Ni2	-N15	-C14	-C13	-174.56(16)
C16	-N15	-C14	-C13	1.5(3)
Ni2	-N15	-C16	-C17	174.82(16)

Table S54 - Torsion Angles (Degrees) (continued)
for: (4·L1)∞

C14	-N15	-C16	-C17	-1.2(3)
N1	-C2	-C3	-C4	0.1(3)
C2	-C3	-C4	-C5	-0.1(3)
C2	-C3	-C4	-C7	-178.9(2)
C7	-C4	-C5	-C6	179.1(2)
C3	-C4	-C7	-N8	173.1(2)
C3	-C4	-C5	-C6	0.3(3)
C3	-C4	-C7	-N11	-4.7(3)
C5	-C4	-C7	-N8	-5.6(3)
C5	-C4	-C7	-N11	176.5(2)
C4	-C5	-C6	-N1	-0.6(4)
S9	-C10	-C12	-C13	-11.5(3)
S9	-C10	-C12	-C17	167.39(18)
N11	-C10	-C12	-C13	170.1(2)
N11	-C10	-C12	-C17	-11.0(3)
C17	-C12	-C13	-C14	-1.6(3)
C10	-C12	-C17	-C16	-177.1(2)
C13	-C12	-C17	-C16	1.9(3)
C10	-C12	-C13	-C14	177.3(2)
C12	-C13	-C14	-N15	-0.1(3)
N15	-C16	-C17	-C12	-0.5(3)
P1	-C18	-C19	-C20	178.8(3)
C19	-C18	-C23	-C22	0.4(5)
C23	-C18	-C19	-C20	0.6(5)
P1	-C18	-C23	-C22	-177.9(3)
C18	-C19	-C20	-C21	-1.4(6)
C19	-C20	-C21	-C22	1.2(7)
C20	-C21	-C22	-C23	-0.2(7)

Table S54 - Torsion Angles (Degrees) (continued)
for: (4·L1)∞

C21	-C22	-C23	-C18	-0.6(6)
C29	-C24	-C25	-C26	-0.3(5)
P1	-C24	-C29	-C28	178.5(3)
C25	-C24	-C29	-C28	1.0(5)
P1	-C24	-C25	-C26	-177.9(3)
C24	-C25	-C26	-C27	-1.5(6)
C25	-C26	-C27	-C28	2.5(6)
C26	-C27	-C28	-C29	-1.8(6)
C27	-C28	-C29	-C24	0.0(6)
P2	-C30	-C31	-C32	179.60(18)
C35	-C30	-C31	-C32	-0.4(3)
P2	-C30	-C35	-C34	-179.4(2)
C31	-C30	-C35	-C34	0.5(4)
C30	-C31	-C32	-C33	-0.3(4)
C31	-C32	-C33	-C34	0.8(5)
C32	-C33	-C34	-C35	-0.7(5)
C33	-C34	-C35	-C30	0.0(5)
C41	-C36	-C37	-C38	0.2(4)
P2	-C36	-C41	-C40	-178.3(2)
C37	-C36	-C41	-C40	0.1(4)
P2	-C36	-C37	-C38	178.6(2)
C36	-C37	-C38	-C39	0.1(4)
C37	-C38	-C39	-C40	-0.7(4)
C38	-C39	-C40	-C41	1.0(5)
C39	-C40	-C41	-C36	-0.7(4)

Table S55 - Contact Distances(Angstrom)
for: (4·L1)∞

S1	.C5_d	3.579(2)	S4	.H21A_g	3.1835
S1	.C6_d	3.651(2)	S9	.H3A_c	3.1010
S2	.C6_e	3.662(2)	S9	.H13A	2.8010
S2	.C5_e	3.571(2)	N8	.C27_i	3.386(5)
S3	.S3_f	3.4437(7)	N15	.C36_b	3.393(3)
S1	.H6A	3.0649	N8	.H5A	2.6441
S1	.H5A_d	3.0516	N8	.H33A_h	2.8792
S1	.H6A_d	3.1605	N8	.H3A_c	2.8894
S1	.H19A_c	3.1730	N11	.H3A	2.5695
S1	.H29A	2.7822	N11	.H17A	2.6356
S1	.H2A_a	2.9605	C3	.C34_j	3.579(4)
S2	.H5A_e	3.0152	C5	.S1_d	3.579(2)
S2	.H6A_e	3.1723	C5	.S2_c	3.571(2)
S2	.H2A	2.9909	C6	.S2_c	3.662(2)
S2	.H29A_e	3.1457	C6	.S1_d	3.651(2)
S2	.H6A_a	3.0817	C13	.C21_g	3.571(5)
S2	.H19A	2.7707	C14	.C21_g	3.537(5)
S3	.H14A_e	2.8575	C14	.C36_b	3.494(3)
S3	.H31A	2.9784	C14	.C37_b	3.559(3)
S3	.H37A	2.9407	C16	.C41_b	3.526(3)
S3	.H16A	2.9267	C21	.C14_g	3.537(5)
S3	.H14A_b	2.9312	C21	.C35_g	3.400(5)
S4	.H14A	3.0980	C21	.C13_g	3.571(5)
S4	.H31A_c	3.0385	C22	.C31_g	3.576(5)
S4	.H35A	2.8908	C22	.C30_g	3.468(4)
S4	.H37A_c	2.8383	C23	.C25	3.598(4)
S4	.H41A	2.9182	C25	.C23	3.598(4)
S4	.H16A_b	3.1152	C25	.C27_g	3.577(5)

Table S55 - Contact Distances(Angstrom) (continued)
for: (4·L1)∞

C25	.C26_g	3.573(5)	H2A	.S2	2.9909
C26	.C26_g	3.438(6)	H2A	.H5A_e	2.2479
C26	.C25_g	3.573(5)	H2A	.S1_a	2.9605
C27	.N8_i	3.386(5)	H3A	.S9_e	3.1010
C27	.C25_g	3.577(5)	H3A	.N8_e	2.8894
C28	.C28_i	3.561(6)	H3A	.N11	2.5695
C30	.C22_g	3.468(4)	H5A	.S2_c	3.0152
C31	.C22_g	3.576(5)	H5A	.N8	2.6441
C34	.C3_m	3.579(4)	H5A	.H2A_c	2.2479
C35	.C21_g	3.400(5)	H5A	.S1_d	3.0516
C36	.N15_b	3.393(3)	H6A	.S1	3.0649
C36	.C14_b	3.494(3)	H6A	.S2_c	3.1723
C37	.C14_b	3.559(3)	H6A	.S1_d	3.1605
C41	.C16_b	3.526(3)	H6A	.S2_a	3.0817
C2	.H26A_g	3.0629	H6A	.H6A_d	2.2227
C2	.H33A_j	3.0764	H13A	.S9	2.8010
C3	.H34A_j	2.8664	H14A	.S3_c	2.8575
C3	.H33A_j	3.0943	H14A	.S4	3.0980
C3	.H26A_g	2.7692	H14A	.S3_b	2.9312
C14	.H21A_g	2.7945	H16A	.S3	2.9267
C18	.H25A	2.9849	H16A	.S4_b	3.1152
C20	.H32A_k	3.0210	H17A	.N11	2.6356
C24	.H23A	2.9487	H19A	.S1_e	3.1730
C27	.H28A_i	3.0913	H19A	.S2	2.7707
C28	.H28A_i	2.9279	H20A	.C32_k	3.0062
C31	.H39A_l	2.8351	H20A	.H32A_k	2.4235
C32	.H39A_l	2.8361	H21A	.S4_g	3.1835
C32	.H20A_k	3.0062	H21A	.C14_g	2.7945

Table S55 - Contact Distances(Angstrom) (continued)
for: (4·L1)∞

H23A	.C24	2.9487	H32A	.H20A_k	2.4235
H25A	.C18	2.9849	H33A	.N8_n	2.8792
H25A	.H28A_e	2.5425	H33A	.C2_m	3.0764
H26A	.C2_g	3.0629	H33A	.C3_m	3.0943
H26A	.C3_g	2.7692	H34A	.C3_m	2.8664
H28A	.H25A_c	2.5425	H35A	.S4	2.8908
H28A	.C27_i	3.0913	H35A	.H40A_o	2.4842
H28A	.C28_i	2.9279	H37A	.S3	2.9407
H28A	.H28A_i	2.5046	H37A	.S4_e	2.8383
H29A	.S1	2.7822	H39A	.C31_l	2.8351
H29A	.S2_c	3.1457	H39A	.C32_l	2.8361
H31A	.S3	2.9784	H40A	.H35A_o	2.4842
H31A	.S4_e	3.0385	H41A	.S4	2.9182
H32A	.C20_k	3.0210			

Table S55 - Hydrogen Bonds (Angstrom, Deg)
for: (4·L1)∞

C13 -- H13A .. S9	0.9500	2.8000	3.172(2)	104.00	.
C14 -- H14A .. S3	0.9500	2.8600	3.788(2)	166.00	1_655
C19 -- H19A .. S2	0.9500	2.7700	3.292(3)	115.00	.
C29 -- H29A .. S1	0.9500	2.7800	3.298(4)	115.00	.
C37 -- H37A .. S4	0.9500	2.8400	3.735(3)	158.00	1_455

Translation of Symmetry Code to Equiv.Pos for (4·L1)∞

a =[2576.00] = -x,2-y,1-z
b =[2667.00] = 1-x,1-y,2-z
c =[1655.00] = 1+x,y,z
d =[2676.00] = 1-x,2-y,1-z
e =[1455.00] = -1+x,y,z
f =[2567.00] = -x,1-y,2-z
g =[2566.00] = -x,1-y,1-z
h =[1665.00] = 1+x,1+y,z
i =[2666.00] = 1-x,1-y,1-z
j =[1565.00] = x,1+y,z
k =[2466.00] = -1-x,1-y,1-z
l =[2557.00] = -x,-y,2-z
m =[1545.00] = x,-1+y,z
n =[1445.00] = -1+x,-1+y,z
o =[2657.00] = 1-x,-y,2-z

Table S56 - Crystal Data and Details of the Structure Determination
for: (4·L2)∞·2(C7H8)

Crystal Data			
Formula	C36 H28 N4 Ni P2 S5, 2(C7 H8)		
Formula Weight	981.84		
Crystal System	Orthorhombic		
Space group	Pnma	(No. 62)	
a, b, c [Angstrom]	26.5284(2)	25.8535(2)	7.0091(1)
V [Ang**3]	4807.17(9)		
Z	4		
D(calc) [g/cm**3]	1.357		
Mu(CuKa) [/mm]	3.543		
F(000)	2040		
Crystal Size [mm]	0.07 x	0.16 x	0.25
Data Collection			
Temperature (K)	173		
Radiation [Angstrom]	CuKa	1.54184	
Theta Min-Max [Deg]	3.3,	71.4	
Dataset	-31: 28 ; -31: 31 ;	-8:	8
Tot., Uniq. Data, R(int)	65823,	4757,	0.037
Observed data [I > 2.0 sigma(I)]	4485		
Refinement			
Nref, Npar	4757,	302	
R, wR2, S	0.0861,	0.2246,	1.21
w = 1/[\S^2^(FO^2^)+(0.0661P)^2^+25.4336P] WHERE P=(FO^2^+2FC^2^)/			
Max. and Av. Shift/Error	0.00,	0.00	
Min. and Max. Resd. Dens. [e/Ang^3]	-0.52,	1.31	

Table S57 - Final Coordinates and Equivalent Isotropic Displacement Parameters of the non-Hydrogen atoms for: (4·L2·2C7H8)∞

Atom	x	y	z	U(eq) [Ang^2]
Ni	0.66250(4)	1/4	0.76419(17)	0.0291(3)
S1	0.62930(5)	0.32160(5)	0.96355(19)	0.0367(4)
S2	0.69540(5)	0.32268(6)	0.5647(2)	0.0403(4)
*S9	0.93728(15)	1/4	0.6069(7)	0.0438(13)
P	0.66809(5)	0.36537(5)	0.7784(2)	0.0385(4)
N1	0.7313(2)	1/4	0.9206(8)	0.0327(19)
*N8	0.8775(7)	1/4	0.657(3)	0.055(6)
N11	0.9130(2)	1/4	0.9524(8)	0.0340(19)
N14	1.0943(2)	1/4	0.8967(9)	0.0333(19)
C2	0.7769(3)	1/4	0.8376(11)	0.035(2)
C3	0.8218(3)	1/4	0.9402(10)	0.036(2)
C4	0.8186(3)	1/4	1.1375(11)	0.048(3)
C5	0.7725(3)	1/4	1.2239(12)	0.054(3)
C6	0.7301(3)	1/4	1.1119(11)	0.043(3)
C7	0.8712(2)	1/4	0.8463(9)	0.035(2)
C10	0.9533(2)	1/4	0.8418(9)	0.031(2)
C12	1.0044(2)	1/4	0.9249(10)	0.032(2)
C13	1.0482(2)	1/4	0.8189(11)	0.033(2)
C15	1.0976(3)	1/4	1.0885(11)	0.043(3)
C16	1.0550(3)	1/4	1.2029(12)	0.049(3)
C17	1.0081(3)	1/4	1.1212(11)	0.041(3)
C18	0.6277(2)	0.4173(2)	0.6912(12)	0.055(2)
C19	0.6129(3)	0.4195(4)	0.4995(14)	0.079(3)
C20	0.5815(4)	0.4606(5)	0.446(2)	0.113(5)
C21	0.5652(4)	0.4968(5)	0.577(2)	0.118(6)
C22	0.5791(4)	0.4934(3)	0.758(2)	0.108(5)

Table S57 - Final Coordinates and Equivalent Isotropic Displacement Parameters of the non-Hydrogen atoms (continued) for: (4·L2·2C7H8)∞

Atom	x	y	z	U(eq) [Ang^2]
C23	0.6115(3)	0.4543(3)	0.8205(15)	0.076(3)
C24	0.7186(2)	0.3995(2)	0.8993(10)	0.0517(19)
C25	0.7471(4)	0.4339(4)	0.7974(15)	0.094(4)
C26	0.7873(4)	0.4592(5)	0.889(2)	0.119(5)
C27	0.7968(4)	0.4514(5)	1.0734(19)	0.111(5)
C28	0.7684(4)	0.4174(5)	1.1794(16)	0.109(5)
C29	0.7284(3)	0.3913(3)	1.0893(12)	0.072(3)
*S9'	0.8850(3)	1/4	0.6143(10)	0.048(2)
*N8'	0.9455(8)	1/4	0.653(3)	0.046(9)
*C30	0.4660(15)	0.610(2)	1.258(7)	0.22(2)
*C30'	0.6626(7)	0.6263(17)	1.004(5)	0.213(18)
*C30"	0.6403(11)	0.6173(18)	1.158(5)	0.206(17)
*C31	0.5102(9)	0.6157(13)	1.130(5)	0.074(10)
*C31'	0.6072(5)	0.6229(8)	1.021(3)	0.105(13)
*C31"	0.5972(7)	0.6229(9)	1.025(3)	0.26(4)
*C32	0.5585(12)	0.6117(12)	1.205(3)	0.14(2)
*C32'	0.5769(8)	0.6306(8)	0.861(2)	0.081(7)
*C32"	0.6051(8)	0.6343(9)	0.833(3)	0.095(8)
*C33	0.6002(8)	0.6184(11)	1.087(4)	0.046(7)
*C33'	0.5248(8)	0.6285(9)	0.879(3)	0.097(8)
*C33"	0.5644(10)	0.6376(10)	0.709(3)	0.139(14)
*C34	0.5934(8)	0.6289(11)	0.895(4)	0.063(9)
*C34'	0.5029(5)	0.6186(9)	1.055(4)	0.082(8)
*C34"	0.5157(9)	0.6296(12)	0.776(4)	0.177(18)
*C35	0.5451(11)	0.6329(12)	0.820(3)	0.064(8)

Table S57 - Final Coordinates and Equivalent Isotropic Displacement Parameters of the non-Hydrogen atoms (continued) for: (4·L2·2C7H8)∞

Atom	x	y	z	U(eq) [Ang^2]
*C35'	0.5332(8)	0.6109(9)	1.214(3)	0.128(12)
*C35"	0.5078(7)	0.6183(11)	0.968(5)	0.15(2)
*C36	0.5034(7)	0.6262(13)	0.938(5)	0.086(16)
*C36'	0.5853(7)	0.6130(8)	1.197(2)	0.079(7)
*C36"	0.5485(8)	0.6149(9)	1.092(3)	0.095(8)

U(eq) = 1/3 of the trace of the orthogonalized U Tensor

Starred Atom sites have a S.O.F less than 1.0

Table S58 - Hydrogen Atom Positions and Isotropic Displacement Parameters
for: (4·L2·2C7H8)∞

Atom	x	y	z	U(iso) [Ang^2]
H2A	0.77860	1/4	0.70220	0.0420
H6A	0.69820	1/4	1.17320	0.0510
H4A	0.84840	1/4	1.21250	0.0570
H5A	0.76980	1/4	1.35910	0.0650
H15A	1.12990	1/4	1.14680	0.0520
H16A	1.05830	1/4	1.33780	0.0580
H17A	0.97860	1/4	1.19840	0.0490
H19A	0.62370	0.39420	0.40980	0.0950
H20A	0.57110	0.46360	0.31700	0.1360
H21A	0.54400	0.52440	0.53740	0.1420
H13A	1.04550	1/4	0.68370	0.0390
H23A	0.62220	0.45300	0.94980	0.0910
H25A	0.73990	0.44050	0.66690	0.1120
H26A	0.80800	0.48220	0.81800	0.1430
H27A	0.82370	0.46970	1.13270	0.1330
H28A	0.77560	0.41160	1.31050	0.1310
H29A	0.70800	0.36790	1.16010	0.0870
H22A	0.56690	0.51800	0.84680	0.1300
*H30A	0.43940	0.59150	1.19040	0.3310
*H30B	0.45370	0.64480	1.29350	0.3310
*H30C	0.47530	0.59120	1.37370	0.3310
*H30D	0.67270	5/8	0.86920	0.3190
*H30E	0.67770	0.59720	1.07220	0.3190
*H30F	0.67410	0.65890	1.06030	0.3190
*H30G	0.62870	0.62690	1.28580	0.3100

Table S58 - Hydrogen Atom Positions and Isotropic Displacement Parameters (continued)
for: (4·L2·2C7H8)∞

Atom	x	y	z	U(iso) [Ang^2]
*H30H	0.66820	0.64000	1.11990	0.3100
*H30I	0.65180	0.58130	1.15840	0.3100
*H32A	0.56320	0.60450	1.33700	0.1620
*H32B	0.59190	0.63730	0.74080	0.0970
*H32C	0.63840	0.63970	0.78710	0.1140
*H33A	0.63320	0.61570	1.13850	0.0560
*H33B	0.50410	0.63370	0.76970	0.1160
*H33C	0.56980	0.64540	0.57800	0.1660
*H34A	0.62190	0.63350	0.81400	0.0750
*H34B	0.46720	0.61720	1.06680	0.0990
*H34C	0.48790	0.63190	0.69130	0.2130
*H35A	0.54050	0.64010	0.68800	0.0770
*H35B	0.51820	0.60420	1.33510	0.1540
*H35C	0.47450	0.61280	1.01370	0.1820
*H36A	0.47040	0.62890	0.88640	0.1030
*H36B	0.60600	0.60780	1.30620	0.0950
*H36C	0.54310	0.60720	1.22280	0.1140

==========

The Temperature Factor has the Form of Exp(-T) Where
T = 8*(Pi**2)*U*(Sin(Theta)/Lambda)**2 for Isotropic Atoms

Table S59 - (An)isotropic Displacement Parameters
for: (4·L2·2C7H8)∞

Atom	U(1,1) or U	U(2,2)	U(3,3)	U(2,3)	U(1,3)	U(1,2)
Ni	0.0131(5)	0.0437(7)	0.0304(6)	0	0.0007(4)	0
S1	0.0289(6)	0.0417(7)	0.0396(7)	-0.0002(5)	0.0071(5)	-0.0010(5)
S2	0.0309(7)	0.0534(8)	0.0365(7)	0.0052(6)	0.0046(5)	-0.0044(6)
S9	0.0173(16)	0.087(3)	0.027(2)	0	0.0064(15)	0
P	0.0277(6)	0.0408(7)	0.0469(8)	0.0036(6)	0.0021(6)	-0.0031(5)
N1	0.018(3)	0.051(4)	0.029(3)	0	0.002(2)	0
N11	0.016(3)	0.061(4)	0.025(3)	0	0.001(2)	0
N14	0.017(3)	0.050(4)	0.033(3)	0	-0.007(2)	0
C2	0.021(3)	0.049(4)	0.036(4)	0	-0.001(3)	0
C3	0.021(3)	0.053(4)	0.033(4)	0	0.001(3)	0
C4	0.015(3)	0.098(7)	0.030(4)	0	-0.006(3)	0
C5	0.023(4)	0.108(8)	0.032(4)	0	0.002(3)	0
C6	0.024(4)	0.070(5)	0.034(4)	0	0.003(3)	0
C7	0.022(3)	0.058(5)	0.026(4)	0	-0.001(3)	0
C10	0.013(3)	0.052(4)	0.028(4)	0	0.001(3)	0
C12	0.019(3)	0.044(4)	0.033(4)	0	-0.003(3)	0
C13	0.016(3)	0.049(4)	0.033(4)	0	0.001(3)	0
C15	0.012(3)	0.082(6)	0.035(4)	0	-0.001(3)	0
C16	0.020(4)	0.096(7)	0.030(4)	0	0.002(3)	0
C17	0.022(3)	0.074(6)	0.027(4)	0	0.001(3)	0
C18	0.029(3)	0.050(3)	0.087(5)	0.019(3)	0.011(3)	0.001(2)
C19	0.045(4)	0.088(6)	0.105(7)	0.037(5)	-0.006(4)	0.008(4)
C20	0.069(6)	0.118(9)	0.152(11)	0.067(9)	-0.011(7)	0.013(6)
C21	0.064(6)	0.087(7)	0.202(16)	0.063(9)	0.014(8)	0.021(5)
C22	0.062(5)	0.056(5)	0.207(14)	0.036(7)	0.031(7)	0.013(4)
C23	0.070(5)	0.046(4)	0.112(7)	0.013(4)	0.023(5)	0.007(3)

Table S59 - (An)isotropic Displacement Parameters (continued)
for: (4·L2·2C7H8)∞

Atom	U(1,1) or U	U(2,2)	U(3,3)	U(2,3)	U(1,3)	U(1,2)
C24	0.037(3)	0.052(3)	0.066(4)	-0.005(3)	-0.001(3)	-0.009(3)
C25	0.087(6)	0.099(7)	0.095(7)	0.011(6)	-0.007(5)	-0.055(5)
C26	0.081(7)	0.133(10)	0.144(11)	0.002(9)	-0.013(7)	-0.069(7)
C27	0.082(7)	0.120(9)	0.131(10)	-0.034(8)	-0.018(7)	-0.051(6)
C28	0.087(7)	0.150(10)	0.090(7)	-0.030(7)	-0.021(6)	-0.044(7)
C29	0.062(5)	0.088(6)	0.066(5)	-0.021(4)	-0.001(4)	-0.026(4)
S9'	0.022(3)	0.098(6)	0.024(3)	0	-0.008(2)	0

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The Temperature Factor has the Form of Exp(-T) Where
T = 8*(Pi**2)*U*(Sin(Theta)/Lambda)**2 for Isotropic Atoms
T = 2*(Pi**2)*Sumij(h(i)*h(j)*U(i,j)*Astar(i)*Astar(j)), for
Anisotropic Atoms. Astar(i) are Reciprocal Axial Lengths and
h(i) are the Reflection Indices.

Table S60 - Bond Distances (Angstrom)
for: (4·L2·2C7H8)∞

Ni	-S1	2.4809(15)	C16	-C17	1.370(11)
Ni	-S2	2.4995(17)	C18	-C23	1.386(11)
Ni	-N1	2.129(6)	C18	-C19	1.401(13)
S1	-P	2.0059(19)	C19	-C20	1.401(16)
S2	-P	1.997(2)	C20	-C21	1.381(19)
S9	-N8	1.624(19)	C21	-C22	1.324(19)
S9	-C10	1.700(8)	C22	-C23	1.397(13)
S9'	-C7	1.667(9)	C24	-C29	1.373(11)
S9'	-N8'	1.63(2)	C24	-C25	1.368(12)
P	-C24	1.814(6)	C25	-C26	1.406(16)
P	-C18	1.823(6)	C26	-C27	1.332(19)
N1	-C2	1.342(10)	C27	-C28	1.376(17)
N1	-C6	1.341(10)	C28	-C29	1.407(14)
N8	-C7	1.34(2)	C2	-H2A	0.9501
N8'	-C10	1.34(2)	C4	-H4A	0.9494
N11	-C7	1.335(8)	C5	-H5A	0.9503
N11	-C10	1.321(8)	C6	-H6A	0.9491
N14	-C13	1.339(8)	C13	-H13A	0.9503
N14	-C15	1.347(10)	C15	-H15A	0.9493
C2	-C3	1.391(11)	C16	-H16A	0.9496
C3	-C7	1.466(10)	C17	-H17A	0.9514
C3	-C4	1.385(10)	C19	-H19A	0.9514
C4	-C5	1.365(11)	C20	-H20A	0.9485
C5	-C6	1.372(11)	C21	-H21A	0.9500
C10	-C12	1.475(8)	C22	-H22A	0.9469
C12	-C13	1.379(8)	C23	-H23A	0.9503
C12	-C17	1.379(10)	C25	-H25A	0.9499
C15	-C16	1.386(11)	C26	-H26A	0.9502

Table S60 - Bond Distances (Angstrom) (continued)
for: (4·L2·2C7H8)∞

C27	-H27A	0.9518	C30	-H30A	0.9753
C28	-H28A	0.9504	C30	-H30B	0.9889
C29	-H29A	0.9514	C30	-H30C	0.9771
C30	-C31	1.48(5)	C30'	-H30D	0.9827
C30'	-C31'	1.48(2)	C30'	-H30E	0.9772
C30"	-C31"	1.48(4)	C30'	-H30F	0.9794
C31	-C32	1.3888	C30"	-H30G	0.9791
C31	-C36	1.3847	C30"	-H30H	0.9816
C31'	-C32'	1.3941	C30"	-H30I	0.9795
C31'	-C36'	1.3874	C32	-H32A	0.9519
C31"	-C32"	1.3935	C32'	-H32B	0.9477
C31"	-C36"	1.3901	C32"	-H32C	0.9505
C32	-C33	1.3921	C33	-H33A	0.9495
C32'	-C33'	1.3889	C33'	-H33B	0.9521
C32"	-C33"	1.3887	C33"	-H33C	0.9509
C33	-C34	1.3847	C34	-H34A	0.9529
C33'	-C34'	1.3874	C34'	-H34B	0.9514
C33"	-C34"	1.3901	C34"	-H34C	0.9486
C34	-C35	1.3888	C35	-H35A	0.9516
C34'	-C35'	1.3884	C35'	-H35B	0.9533
C34"	-C35"	1.3929	C35"	-H35C	0.9504
C35	-C36	1.3921	C36	-H36A	0.9498
C35'	-C36'	1.3883	C36'	-H36B	0.9516
C35"	-C36"	1.3888	C36"	-H36C	0.9490

Table S61 - Bond Angles (Degrees)
for: (4·L2·2C7H8)∞

S1	-Ni	-S2	83.00(5)	Ni_a	-N14	-C15	118.2(5)
S1	-Ni	-N1	90.82(11)	N1	-C2	-C3	123.2(7)
S1	-Ni	-S1_c	96.52(6)	C2	-C3	-C4	117.6(7)
S1	-Ni	-S2_c	179.49(6)	C4	-C3	-C7	120.2(7)
S2	-Ni	-N1	89.35(11)	C2	-C3	-C7	122.2(6)
S1_c	-Ni	-S2	179.49(6)	C3	-C4	-C5	119.9(7)
S2	-Ni	-S2_c	97.49(6)	C4	-C5	-C6	118.7(8)
S1_c	-Ni	-N1	90.82(11)	N1	-C6	-C5	123.6(7)
S2_c	-Ni	-N1	89.35(11)	N8	-C7	-C3	123.8(9)
S1_c	-Ni	-S2_c	83.00(5)	N8	-C7	-N11	116.7(9)
Ni	-S1	-P	82.79(6)	S9'	-C7	-C3	129.4(5)
Ni	-S2	-P	82.48(6)	S9'	-C7	-N11	111.2(5)
N8	-S9	-C10	92.0(8)	N11	-C7	-C3	119.5(6)
N8'	-S9'	-C7	93.1(8)	S9	-C10	-C12	127.7(5)
S1	-P	-S2	111.08(8)	N11	-C10	-C12	120.8(6)
S1	-P	-C24	110.6(2)	N8'	-C10	-C12	122.1(10)
S2	-P	-C18	111.6(3)	N8'	-C10	-N11	117.1(10)
S2	-P	-C24	110.6(2)	S9	-C10	-N11	111.5(4)
C18	-P	-C24	103.4(3)	C10	-C12	-C13	124.2(6)
S1	-P	-C18	109.3(2)	C13	-C12	-C17	118.5(6)
Ni	-N1	-C2	123.3(5)	C10	-C12	-C17	117.3(6)
Ni	-N1	-C6	119.6(5)	N14	-C13	-C12	123.4(7)
C2	-N1	-C6	117.0(6)	N14	-C15	-C16	121.6(7)
S9	-N8	-C7	109.7(13)	C15	-C16	-C17	119.9(8)
S9'	-N8'	-C10	108.5(14)	C12	-C17	-C16	118.8(7)
C7	-N11	-C10	110.2(5)	P	-C18	-C19	121.1(6)
Ni_a	-N14	-C13	124.0(5)	C19	-C18	-C23	120.8(7)
C13	-N14	-C15	117.8(6)	P	-C18	-C23	118.1(6)

Table S61 - Bond Angles (Degrees) (continued)
for: (4·L2·2C7H8)∞

C18	-C19	-C20	117.0(9)	C16	-C17	-H17A	120.62
C19	-C20	-C21	121.5(12)	C18	-C19	-H19A	121.43
C20	-C21	-C22	120.3(11)	C20	-C19	-H19A	121.57
C21	-C22	-C23	121.3(11)	C19	-C20	-H20A	119.34
C18	-C23	-C22	119.0(10)	C21	-C20	-H20A	119.17
P	-C24	-C25	118.7(6)	C20	-C21	-H21A	120.02
C25	-C24	-C29	120.1(7)	C22	-C21	-H21A	119.65
P	-C24	-C29	121.2(5)	C21	-C22	-H22A	119.34
C24	-C25	-C26	118.9(10)	C23	-C22	-H22A	119.35
C25	-C26	-C27	121.1(11)	C18	-C23	-H23A	120.43
C26	-C27	-C28	121.1(11)	C22	-C23	-H23A	120.55
C27	-C28	-C29	118.5(10)	C24	-C25	-H25A	120.55
C24	-C29	-C28	120.3(8)	C26	-C25	-H25A	120.57
N1	-C2	-H2A	118.40	C25	-C26	-H26A	119.36
C3	-C2	-H2A	118.40	C27	-C26	-H26A	119.57
C3	-C4	-H4A	120.11	C26	-C27	-H27A	119.36
C5	-C4	-H4A	120.03	C28	-C27	-H27A	119.50
C4	-C5	-H5A	120.67	C27	-C28	-H28A	120.86
C6	-C5	-H5A	120.59	C29	-C28	-H28A	120.65
N1	-C6	-H6A	118.28	C24	-C29	-H29A	119.75
C5	-C6	-H6A	118.17	C28	-C29	-H29A	119.99
N14	-C13	-H13A	118.35	C30	-C31	-C32	120(3)
C12	-C13	-H13A	118.27	C30	-C31	-C36	120(3)
N14	-C15	-H15A	119.22	C32	-C31	-C36	120.18
C16	-C15	-H15A	119.15	C30'	-C31'	-C32'	120(2)
C15	-C16	-H16A	120.07	C30'	-C31'	-C36'	120(2)
C17	-C16	-H16A	120.00	C32'	-C31'	-C36'	120.01
C12	-C17	-H17A	120.58	C30"	-C31"	-C32"	121(2)

Table S61 - Bond Angles (Degrees) (continued)
for: (4·L2·2C7H8)∞

C30"	-C31"	-C36"	119(2)	H30E	-C30'	-H30F	109.74
C32"	-C31"	-C36"	119.83	C31"	-C30"	-H30G	107.95
C31	-C32	-C33	119.93	C31"	-C30"	-H30H	110.62
C31'	-C32'	-C33'	119.68	C31"	-C30"	-H30I	109.56
C31"	-C32"	-C33"	120.03	H30G	-C30"	-H30H	109.53
C32	-C33	-C34	119.89	H30G	-C30"	-H30I	109.64
C32'	-C33'	-C34'	120.31	H30H	-C30"	-H30I	109.51
C32"	-C33"	-C34"	120.13	C31	-C32	-H32A	120.22
C33	-C34	-C35	120.18	C33	-C32	-H32A	119.85
C33'	-C34'	-C35'	119.85	C31'	-C32'	-H32B	119.94
C33"	-C34"	-C35"	119.83	C33'	-C32'	-H32B	120.38
C34	-C35	-C36	119.93	C31"	-C32"	-H32C	119.85
C34'	-C35'	-C36'	120.12	C33"	-C32"	-H32C	120.12
C34"	-C35"	-C36"	120.06	C32	-C33	-H33A	119.85
C31	-C36	-C35	119.89	C34	-C33	-H33A	120.27
C31'	-C36'	-C35'	120.03	C32'	-C33'	-H33B	119.69
C31"	-C36"	-C35"	120.11	C34'	-C33'	-H33B	120.00
C31	-C30	-H30A	109.07	C32"	-C33"	-H33C	120.01
C31	-C30	-H30B	108.82	C34"	-C33"	-H33C	119.85
C31	-C30	-H30C	110.59	C33	-C34	-H34A	120.01
H30A	-C30	-H30B	109.25	C35	-C34	-H34A	119.81
H30A	-C30	-H30C	110.00	C33'	-C34'	-H34B	120.08
H30B	-C30	-H30C	109.09	C35'	-C34'	-H34B	120.07
C31'	-C30'	-H30D	110.29	C33"	-C34"	-H34C	120.12
C31'	-C30'	-H30E	108.82	C35"	-C34"	-H34C	120.05
C31'	-C30'	-H30F	109.19	C34	-C35	-H35A	120.06
H30D	-C30'	-H30E	109.40	C36	-C35	-H35A	120.01
H30D	-C30'	-H30F	109.38	C34'	-C35'	-H35B	119.94

Table S61 - Bond Angles (Degrees) (continued)
for: (4·L2·2C7H8)∞

C36'	-C35'	-H35B	119.94	C31'	-C36'	-H36B	119.97
C34"	-C35"	-H35C	119.79	C35'	-C36'	-H36B	120.00
C36"	-C35"	-H35C	120.15	C31"	-C36"	-H36C	119.86
C31	-C36	-H36A	120.30	C35"	-C36"	-H36C	120.03
C35	-C36	-H36A	119.81				

Table S62 - Torsion Angles (Degrees)
for: (4·L2·2C7H8)∞

S2	-Ni	-S1	-P	-5.31(6)
N1	-Ni	-S1	-P	83.93(12)
S1_c	-Ni	-S1	-P	174.85(7)
S1	-Ni	-S2	-P	5.34(6)
N1	-Ni	-S2	-P	-85.56(13)
S2_c	-Ni	-S2	-P	-174.83(7)
S1	-Ni	-N1	-C2	-131.74(4)
S1	-Ni	-N1	-C6	48.26(4)
S2	-Ni	-N1	-C2	-48.75(4)
S2	-Ni	-N1	-C6	131.25(4)
Ni	-S1	-P	-S2	7.09(8)
Ni	-S1	-P	-C18	130.7(2)
Ni	-S1	-P	-C24	-116.04(19)
Ni	-S2	-P	-C18	-129.34(19)
Ni	-S2	-P	-C24	116.1(2)
Ni	-S2	-P	-S1	-7.04(8)
N8	-S9	-C10	-C12	180.00
C10	-S9	-N8	-C7	0.00
N8	-S9	-C10	-N11	0.00
S1	-P	-C18	-C19	-114.0(6)
S1	-P	-C18	-C23	65.2(5)
S2	-P	-C18	-C19	9.3(6)
S2	-P	-C18	-C23	-171.5(5)
C24	-P	-C18	-C19	128.2(6)
C24	-P	-C18	-C23	-52.6(6)
S1	-P	-C24	-C25	-175.8(6)
S1	-P	-C24	-C29	4.2(6)
S2	-P	-C24	-C25	60.7(6)

Table S62 - Torsion Angles (Degrees) (continued)
for: (4·L2·2C7H8)∞

S2	-P	-C24	-C29	-119.3(5)
C18	-P	-C24	-C25	-58.9(7)
C18	-P	-C24	-C29	121.1(6)
Ni	-N1	-C2	-C3	180.00
C6	-N1	-C2	-C3	0.00
Ni	-N1	-C6	-C5	180.00
C2	-N1	-C6	-C5	0.00
S9	-N8	-C7	-N11	0.00
S9	-N8	-C7	-C3	180.00
C10	-N11	-C7	-N8	0.00
C10	-N11	-C7	-C3	180.00
C7	-N11	-C10	-S9	0.00
C7	-N11	-C10	-C12	180.00
C15	-N14	-C13	-C12	0.00
C13	-N14	-C15	-C16	0.00
N1	-C2	-C3	-C4	0.00
N1	-C2	-C3	-C7	180.00
C2	-C3	-C7	-N8	0.00
C2	-C3	-C4	-C5	0.00
C7	-C3	-C4	-C5	180.00
C2	-C3	-C7	-N11	180.00
C4	-C3	-C7	-N8	180.00
C4	-C3	-C7	-N11	0.00
C3	-C4	-C5	-C6	0.00
C4	-C5	-C6	-N1	0.00
N11	-C10	-C12	-C13	180.00
N11	-C10	-C12	-C17	0.00
S9	-C10	-C12	-C17	180.00

Table S62 - Torsion Angles (Degrees) (continued)
for: (4·L2·2C7H8)∞

S9	-C10	-C12	-C13	0.00
C10	-C12	-C17	-C16	180.00
C10	-C12	-C13	-N14	180.00
C17	-C12	-C13	-N14	0.00
C13	-C12	-C17	-C16	0.00
N14	-C15	-C16	-C17	0.00
C15	-C16	-C17	-C12	0.00
P	-C18	-C19	-C20	179.5(7)
P	-C18	-C23	-C22	-177.8(6)
C19	-C18	-C23	-C22	1.5(11)
C23	-C18	-C19	-C20	0.3(12)
C18	-C19	-C20	-C21	-1.1(15)
C19	-C20	-C21	-C22	0.1(17)
C20	-C21	-C22	-C23	1.8(17)
C21	-C22	-C23	-C18	-2.5(14)
P	-C24	-C25	-C26	-178.0(8)
C25	-C24	-C29	-C28	-1.3(12)
C29	-C24	-C25	-C26	2.0(13)
P	-C24	-C29	-C28	178.7(7)
C24	-C25	-C26	-C27	-2.2(17)
C25	-C26	-C27	-C28	1.6(19)
C26	-C27	-C28	-C29	-0.8(18)
C27	-C28	-C29	-C24	0.6(15)

Table S63 - Contact Distances(Angstrom)
for: (4·L2·2C7H8)∞

Ni	.N14_d	2.132(6)	S9	.C32_k	3.64(3)
Ni	.C13_d	3.088(6)	S9	.C33_k	3.55(3)
Ni	.C15_d	3.013(8)	S9	.C34_k	3.56(3)
Ni	.C13_e	3.088(6)	S9	.C31"_l	3.46(2)
Ni	.C15_e	3.013(8)	S9	.C36"_l	3.51(2)
Ni	.N14_e	2.132(6)	S9	.C35_l	3.66(3)
Ni	.H13A_d	3.1252	S9	.C34_l	3.56(3)
Ni	.H15A_d	3.0077	S1	.H6A	2.9878
Ni	.H13A_e	3.1252	S1	.H16A_h	2.9854
Ni	.H15A_e	3.0077	S1	.H36A_g	3.1208
S1	.C30_g	3.45(5)	S1	.H13A_d	3.0715
S1	.C16_f	3.575(7)	S1	.H13A_e	3.0715
S1	.N14_d	3.266(5)	S1	.H16A_f	2.9854
S1	.C13_d	3.460(6)	S1	.H30A_g	3.0876
S1	.C16_h	3.575(7)	S1	.H29A	2.7730
S1	.N14_e	3.266(5)	S1	.H30B_g	2.9747
S1	.C13_e	3.460(6)	S1	.H34B_g	3.0170
S2	.C15_d	3.379(7)	S2	.H19A	2.8663
S2	.N14_d	3.286(5)	S2	.H5A_j	3.0827
S2	.N14_e	3.286(5)	S2	.H2A	3.0547
S2	.C15_e	3.379(7)	S2	.H5A_i	3.0827
S2	.C5_j	3.663(7)	S2	.H15A_d	2.9576
S2	.C5_i	3.663(7)	S2	.H29A_i	3.0856
S9	.C33_l	3.55(3)	S2	.H15A_e	2.9576
S9	.C35_k	3.66(3)	S9	.H17A_i	3.0659
S9	.C36"_k	3.51(2)	S9	.H13A	2.9209
S9	.C31"_k	3.46(2)	S9	.H17A_j	3.0659
S9	.C32_l	3.64(3)	S9'	.H4A_i	2.9789

Table S63 - Contact Distances(Angstrom) (continued)
for: (4·L2·2C7H8)∞

S9'	.H4A_j	2.9789	C27	.C25_u	3.552(16)
S9'	.H2A	2.8891	C28	.C30'_m	3.13(3)
P	.C30_g	3.62(4)	C30	.C18_w	2.61(4)
P	.H30A_g	3.0696	C30	.S1_w	3.45(5)
N8	.H2A	2.6427	C30	.C23_w	2.70(5)
N8'	.H13A	2.6616	C30	.P_w	3.62(4)
N11	.H33C_n	2.8803	C30	.C19_w	2.80(5)
N11	.H33C_m	2.8803	C30	.C20_w	3.04(5)
N11	.H17A	2.4498	C30	.C21_w	3.11(5)
N11	.H4A	2.5021	C30	.C22_w	2.93(5)
C5	.S2_o	3.663(7)	C30'	.C28_s	3.13(3)
C5	.S2_p	3.663(7)	C30'	.C25_u	3.52(3)
C16	.S1_q	3.575(7)	C30"	.C25_u	3.41(3)
C16	.S1_r	3.575(7)	C30"	.C26_u	3.20(4)
C17	.C34"_m	3.36(3)	C31"	.S9_x	3.46(2)
C17	.C33"_m	3.54(3)	C31"	.S9_u	3.46(2)
C17	.C34"_n	3.36(3)	C32	.S9_x	3.64(3)
C17	.C33"_n	3.54(3)	C32	.S9_u	3.64(3)
C18	.C30_g	2.61(4)	C33	.S9_x	3.55(3)
C19	.C30_g	2.80(5)	C33	.S9_u	3.55(3)
C20	.C30_g	3.04(5)	C33"	.C17_y	3.54(3)
C21	.C30_g	3.11(5)	C33"	.C17_s	3.54(3)
C22	.C30_g	2.93(5)	C34	.S9_u	3.56(3)
C23	.C30_g	2.70(5)	C34	.S9_x	3.56(3)
C25	.C27_s	3.552(16)	C34"	.C17_y	3.36(3)
C25	.C30"_k	3.41(3)	C34"	.C17_s	3.36(3)
C25	.C30'_k	3.52(3)	C35	.S9_u	3.66(3)
C26	.C30"_k	3.20(4)	C35	.S9_x	3.66(3)

Table S63 - Contact Distances(Angstrom) (continued)
for: (4·L2·2C7H8)∞

C36"	.S9_u	3.51(2)	C23	.H27A_s	2.9238
C36"	.S9_x	3.51(2)	C24	.H23A	2.9289
C12	.H30B_l	3.0791	C25	.H30I_k	2.8804
C12	.H30B_k	3.0791	C25	.H30E_k	2.6679
C13	.H30B_k	2.7261	C26	.H30I_k	2.5137
C13	.H30B_l	2.7261	C26	.H30E_k	2.8140
C17	.H34C_m	3.0944	C27	.H25A_u	3.0312
C17	.H34C_n	3.0944	C27	.H30D_m	2.9757
C18	.H25A	3.0411	C28	.H32C_m	2.9769
C18	.H30B_g	2.6930	C28	.H30D_m	2.3266
C18	.H30A_g	1.9771	C30'	.H28A_s	2.3425
C18	.H30C_g	2.7787	C31"	.H22A	3.0921
C19	.H30C_g	2.5182	C32'	.H22A	2.9249
C19	.H30B_g	2.8267	C33'	.H22A	3.0757
C19	.H30A_g	2.5942	C34	.H22A	2.9713
C20	.H30C_g	2.3793	C35	.H22A	3.0322
C20	.H30A_g	2.9354	C36"	.H22A	3.0770
C21	.H30C_g	2.5397	H2A	.S2	3.0547
C21	.H30A_g	2.8079	H2A	.H5A_j	2.4161
C21	.H21A_t	3.0554	H2A	.S2_c	3.0547
C21	.H27A_s	3.0966	H2A	.H5A_i	2.4161
C22	.H30A_g	2.2781	H2A	.S9'	2.8891
C22	.H27A_s	2.8862	H2A	.N8	2.6427
C22	.H30C_g	2.7782	H4A	.S9'_o	2.9789
C23	.H35C_g	3.0927	H4A	.N11	2.5021
C23	.H34B_g	2.8983	H4A	.S9'_p	2.9789
C23	.H30C_g	2.9221	H5A	.S2_o	3.0827
C23	.H30A_g	1.7976	H5A	.H2A_p	2.4161

Table S63 - Contact Distances(Angstrom) (continued)
for: (4·L2·2C7H8)∞

H5A	.H2A_o	2.4161	H22A	.C34	2.9713
H5A	.S2_p	3.0827	H22A	.C31"	3.0921
H6A	.H15A_h	2.2079	H22A	.C32'	2.9249
H6A	.S1_c	2.9878	H22A	.C33'	3.0757
H6A	.S1	2.9878	H22A	.C36"	3.0770
H6A	.H15A_f	2.2079	H23A	.C24	2.9289
H13A	.S9	2.9209	H23A	.H30A_g	2.2270
H13A	.H16A_i	2.4481	H25A	.H30E_k	2.4837
H13A	.N8'	2.6616	H25A	.C27_s	3.0312
H13A	.S1_a	3.0715	H25A	.C18	3.0411
H13A	.S1_b	3.0715	H26A	.H30I_k	2.2547
H13A	.H16A_j	2.4481	H27A	.C21_u	3.0966
H15A	.H6A_q	2.2079	H27A	.C23_u	2.9238
H15A	.S2_b	2.9576	H27A	.C22_u	2.8862
H15A	.S2_a	2.9576	H28A	.C30'_m	2.3425
H15A	.H6A_r	2.2079	H28A	.H30E_m	2.2251
H16A	.H13A_p	2.4481	H28A	.H30D_m	1.7163
H16A	.S1_r	2.9854	H29A	.S2_o	3.0856
H16A	.H13A_o	2.4481	H29A	.S1	2.7730
H16A	.S1_q	2.9854	H30A	.H36A	2.4802
H17A	.S9_p	3.0659	H30A	.S1_w	3.0876
H17A	.S9_o	3.0659	H30A	.P_w	3.0696
H17A	.N11	2.4498	H30A	.C18_w	1.9771
H19A	.S2	2.8663	H30A	.C19_w	2.5942
H21A	.H32A_v	2.5536	H30A	.C20_w	2.9354
H21A	.C21_t	3.0554	H30A	.C21_w	2.8079
H21A	.H35B_v	2.5953	H30A	.C22_w	2.2781
H22A	.C35	3.0322	H30A	.C23_w	1.7976

Table S63 - Contact Distances(Angstrom) (continued)
for: (4·L2·2C7H8)∞

H30A	.H23A_w	2.2270	H30E	.H28A_s	2.2251
H30B	.C12_u	3.0791	H30G	.H36C	2.3688
H30B	.C13_u	2.7261	H30H	.H32C	2.4630
H30B	.S1_w	2.9747	H30I	.C25_u	2.8804
H30B	.C18_w	2.6930	H30I	.C26_u	2.5137
H30B	.C19_w	2.8267	H30I	.H26A_u	2.2547
H30B	.C12_x	3.0791	H32A	.H21A_o	2.5536
H30B	.C13_x	2.7261	H32A	.H30C	2.3711
H30C	.H32A	2.3711	H32B	.H30D	2.3464
H30C	.C18_w	2.7787	H32C	.H30H	2.4630
H30C	.C19_w	2.5182	H32C	.C28_s	2.9769
H30C	.C20_w	2.3793	H33C	.N11_s	2.8803
H30C	.C21_w	2.5397	H33C	.N11_y	2.8803
H30C	.C22_w	2.7782	H34B	.S1_w	3.0170
H30C	.C23_w	2.9221	H34B	.C23_w	2.8983
H30D	.H32B	2.3464	H34C	.C17_s	3.0944
H30D	.C27_s	2.9757	H34C	.C17_y	3.0944
H30D	.C28_s	2.3266	H35B	.H21A_o	2.5953
H30D	.H28A_s	1.7163	H35C	.C23_w	3.0927
H30E	.H36B	2.5265	H36A	.H30A	2.4802
H30E	.C25_u	2.6679	H36A	.S1_w	3.1208
H30E	.C26_u	2.8140	H36B	.H30E	2.5265
H30E	.H25A_u	2.4837	H36C	.H30G	2.3688

Table S64 - Hydrogen Bonds (Angstrom, Deg)
for: (4·L2·2C7H8)∞

C17 -- H17A .. N11	0.9500	2.4500	2.787(10)	101.00	.
C19 -- H19A .. S2	0.9500	2.8700	3.356(10)	113.00	.
C29 -- H29A .. S1	0.9500	2.7700	3.307(8)	116.00	.

Translation of Symmetry Code to Equiv.Pos for (4·L2·2C7H8)∞

a =[3556.00] = 1/2+x,1/2-y,3/2-z
b =[6556.00] = 1/2+x,y,3/2-z
c =[8555.00] = x,1/2-y,z
d =[3456.00] = -1/2+x,1/2-y,3/2-z
e =[6456.00] = -1/2+x,y,3/2-z
f =[3457.00] = -1/2+x,1/2-y,5/2-z
g =[5667.00] = 1-x,1-y,2-z
h =[6457.00] = -1/2+x,y,5/2-z
i =[1554.00] = x,y,-1+z
j =[8554.00] = x,1/2-y,-1+z
k =[2664.00] = 3/2-x,1-y,-1/2+z
l =[7644.00] = 3/2-x,-1/2+y,-1/2+z
m =[2665.00] = 3/2-x,1-y,1/2+z
n =[7645.00] = 3/2-x,-1/2+y,1/2+z
o =[1556.00] = x,y,1+z
p =[8556.00] = x,1/2-y,1+z
q =[3557.00] = 1/2+x,1/2-y,5/2-z
r =[6557.00] = 1/2+x,y,5/2-z
s =[2664.00] = 3/2-x,1-y,-1/2+z
t =[5666.00] = 1-x,1-y,1-z
u =[2665.00] = 3/2-x,1-y,1/2+z
v =[1554.00] = x,y,-1+z
w =[5667.00] = 1-x,1-y,2-z
x =[7655.00] = 3/2-x,1/2+y,1/2+z
y =[7654.00] = 3/2-x,1/2+y,-1/2+z