Electronic Supplementary Material (ESI) for Polymer Chemistry.

Supplementary data

Ethylene Polymerization Catalyzed by Dinickel Complex with a Double-Decker Structure

Daisuke Takeuchi, Yuriko Chiba, Shigenaga Takano,

Hideo Kurihara, Minoru Kobayashi and Kohtaro Osakada

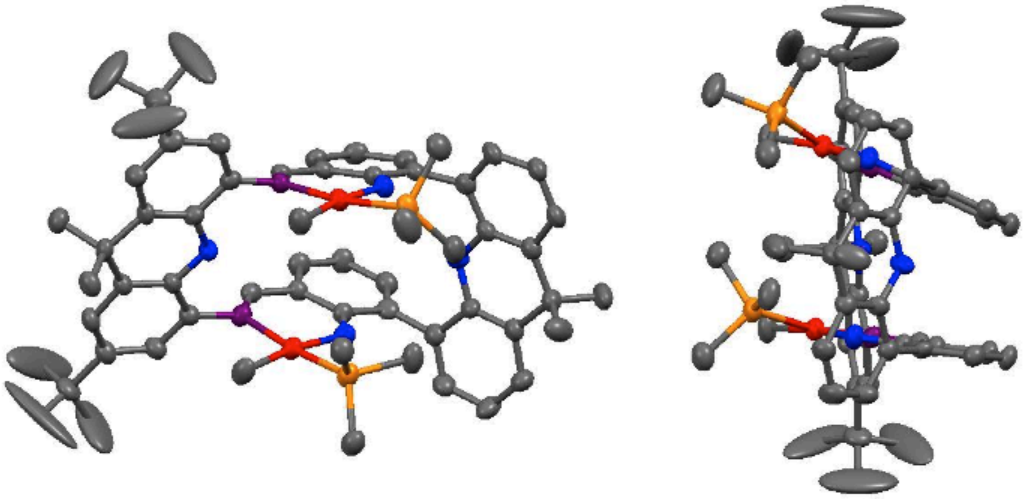

Figure S-1. Structure of $[Ni_2Me_2(PMe_3)_2(\mathbf{2})]$ determined by X-ray crystallography. Hydrogen atoms are omitted for clarity.

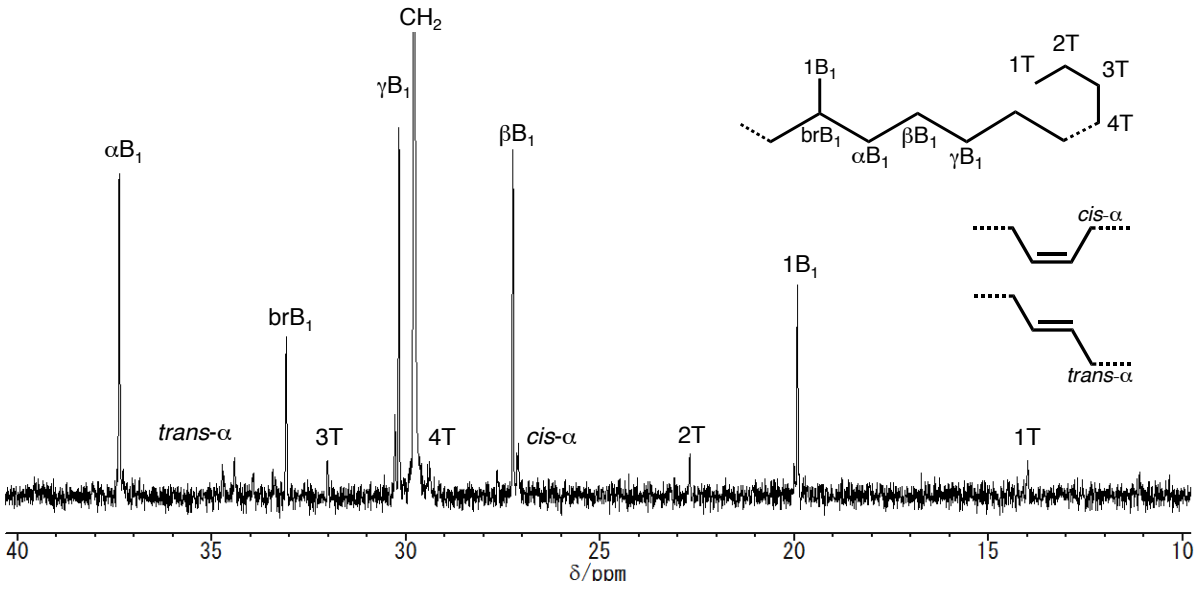

Figure S-2. $^{13}C\{^1H\}$ NMR spectrum of polyethylene obtained by $[Ni_2Me_2(PMe_3)_2(\mathbf{1})]/Ni(cod)_2$.

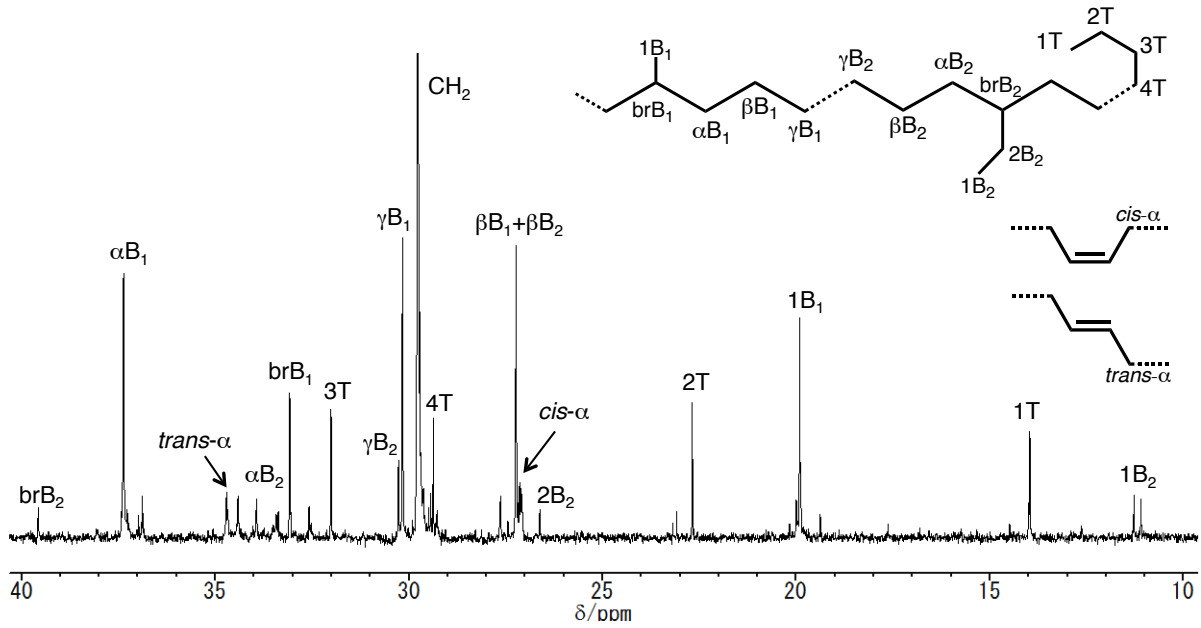

Figure S-3. $^{13}C\{^{1}H\}$ NMR spectrum of polyethylene obtained by $[Ni_2Me_2(PMe_3)_2(\mathbf{2})]/Ni(cod)_2$.

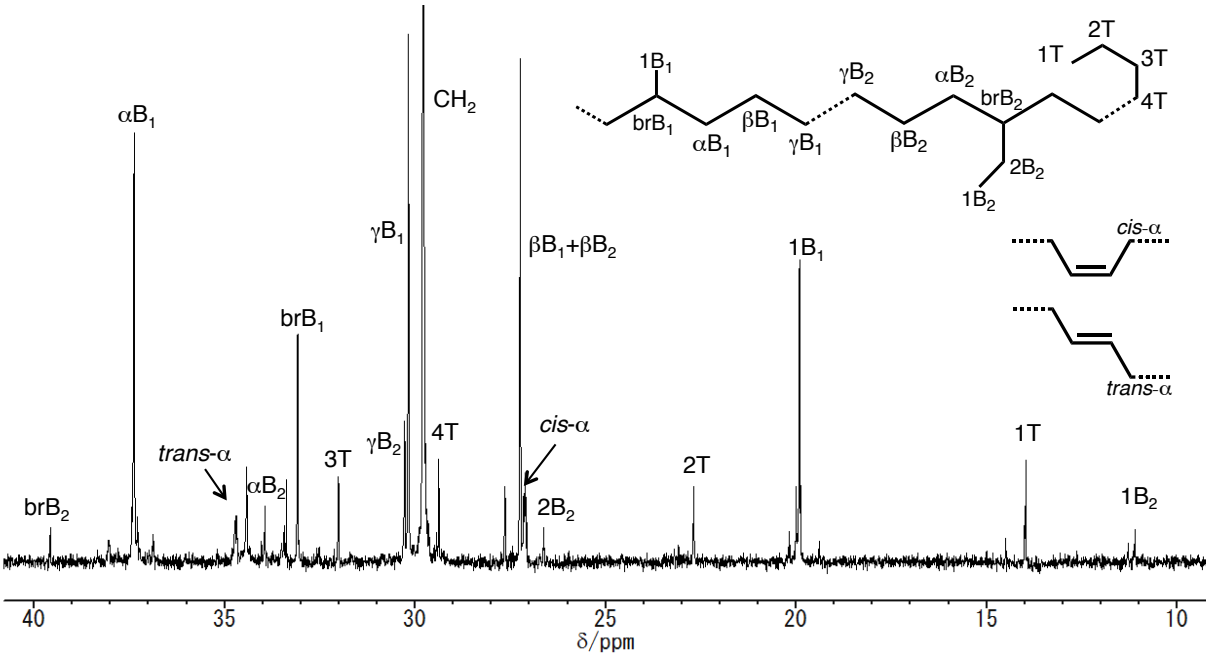

Figure S-4. $^{13}C\{^{1}H\}$ NMR spectrum of polyethylene obtained by $[NiMe(PMe_3)(\mathbf{1}\text{-H})]/Ni(cod)_2$.

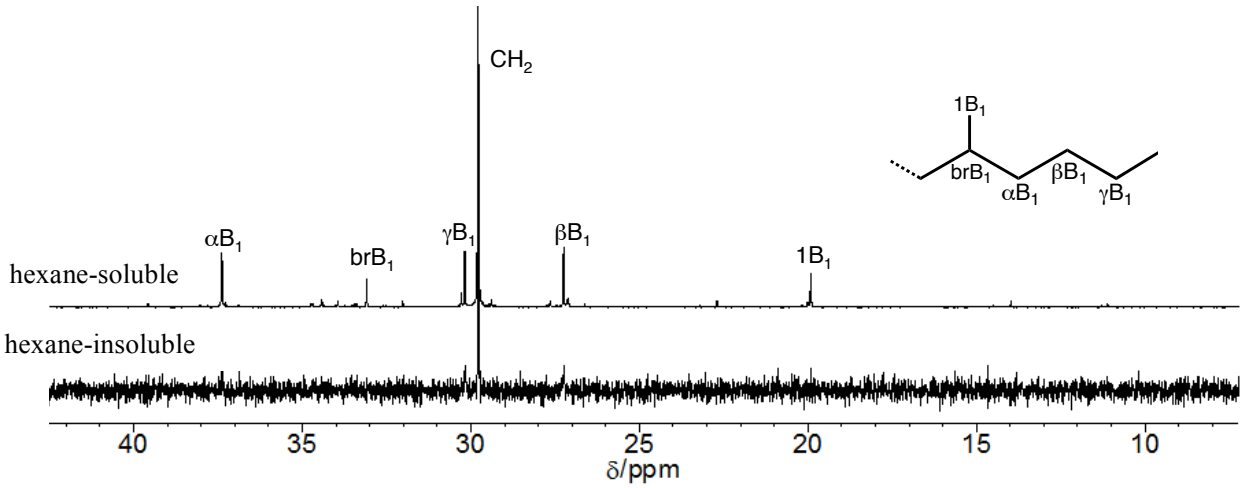

Figure S-5. $^{13}C\{^{1}H\}$ NMR spectra of hexane-soluble and -insoluble fractions of polyethylene obtained by $[Ni_2Me_2(PMe_3)_2(\mathbf{1})]/Ni(cod)_2$.

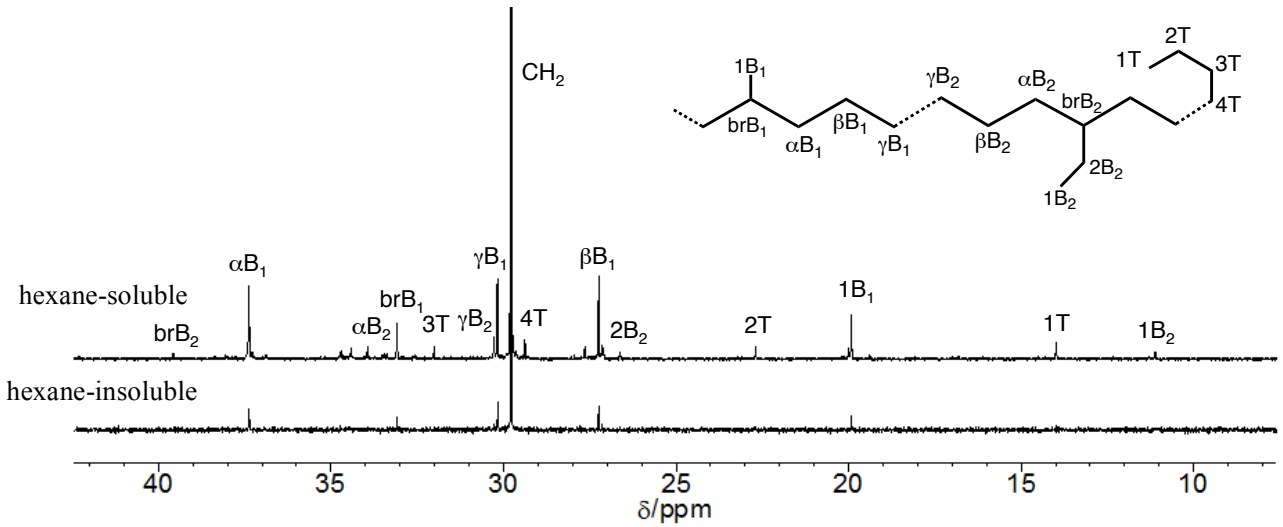

Figure S-6. $^{13}C\{^{1}H\}$ NMR spectra of hexane-soluble and -insoluble fractions of polyethylene obtained by $[Ni_2Me_2(PMe_3)_2(\mathbf{2})]/Ni(cod)_2$.

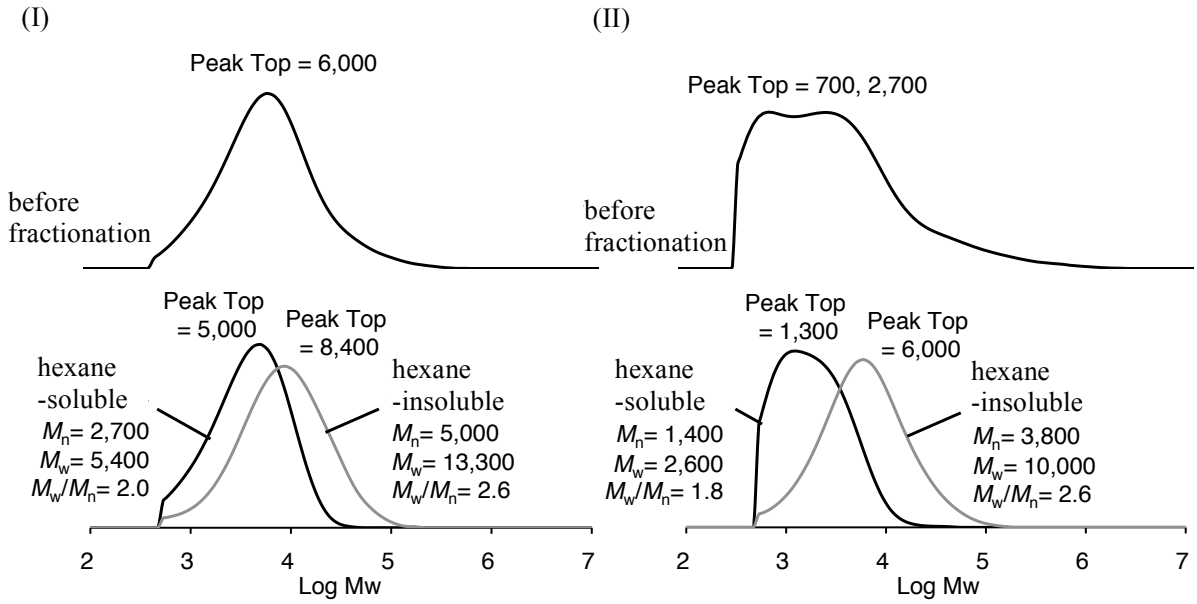

Figure S-7. GPC profiles of polyethylene obtained by (I) $[Ni_2Me_2(PMe_3)_2(\mathbf{1})]/Ni(cod)_2$ and by (I) $[Ni_2Me_2(PMe_3)_2(\mathbf{2})]/Ni(cod)_2$.

Table S-1. Crystallographic data details of refinement of the ligand of $[Ni_2Me_2(PMe_3)_2$(**2**)].

	$[Ni_2Me_2(PMe_3)_2$(**2**)]
fomula	$C_{60}H_{72}N_2Ni_2O_4P_2\cdot(C_6H_{14})$
formula wt	1150.76
cryst size/ mm	0.27×0.15×0.12
cryst syst	monoclinic
cryst color	red
space group	$P2_1/n$ (*No*. 14)
a/Å	15.456(3)
b/Å	15.227(3)
c/Å	26.465(5)
β/ deg	94.403(3)
V/ Å^3	6210(2)
Z	4
D_{calcd}/ g cm^{-3}	1.231
F(000)	2456
μ/mm^{-1}	7.049
no. of reflns measd	50274
no. of unique reflns	13968
R_{int}	0.0927
no. of obsed reflns ($I > 2\sigma(I)$)	13968
no. of variables	705
R ($I > 2\sigma(I)$)	0.0859
R, R_w (all data)	0.1346, 0.2636
GOF on F^2	1.034

Table S-2. Atomic coordinates and B_{iso}/B_{eq}

atom	x	y	z	B_{eq}
Ni1	0.36700(4)	0.89852(4)	0.12058(2)	2.69(2)
Ni2	0.67127(4)	0.82904(4)	0.10398(2)	2.65(2)
P1	0.43044(9)	1.02328(8)	0.12209(5)	3.04(3)
P2	0.76086(9)	0.93542(9)	0.12209(5)	3.37(3)
O1	0.3845(3)	0.8955(2)	0.19207(11)	2.90(6)
O2	0.6768(2)	0.8128(2)	0.17533(11)	2.69(6)
O3	0.5575(2)	0.8916(2)	0.29451(13)	3.21(7)
O4	0.4380(2)	0.7193(2)	0.05085(11)	2.56(6)
N1	0.3247(3)	0.7785(3)	0.11616(13)	2.59(7)
N2	0.6048(3)	0.7228(3)	0.09107(13)	2.50(7)
C1	0.3432(4)	0.9196(4)	0.0484(2)	3.68(11)
C2	0.6644(4)	0.8629(4)	0.0340(2)	3.61(10)
C3	0.3213(3)	0.7268(3)	0.1553(2)	2.68(8)
C4	0.3709(3)	0.8325(3)	0.2236(2)	2.44(8)
C5	0.3413(3)	0.7480(3)	0.2071(2)	2.47(8)
C6	0.3306(4)	0.6814(4)	0.2434(2)	3.04(9)
C7	0.3472(4)	0.6959(4)	0.2943(2)	3.05(9)
C8	0.3760(3)	0.7801(4)	0.3100(2)	2.97(9)
C9	0.3871(3)	0.8474(3)	0.2768(2)	2.62(8)
C10	0.5737(3)	0.6747(3)	0.1260(2)	2.45(8)
C11	0.6378(3)	0.7548(3)	0.2016(2)	2.52(8)
C12	0.5854(3)	0.6863(3)	0.1793(2)	2.36(8)
C13	0.5448(3)	0.6264(3)	0.2108(2)	2.73(8)
C14	0.5553(4)	0.6312(4)	0.2626(2)	3.06(9)
C15	0.6066(3)	0.6999(3)	0.2850(2)	2.89(9)
C16	0.6472(3)	0.7605(3)	0.2558(2)	2.50(8)
C17	0.2938(3)	0.7405(3)	0.0685(2)	2.60(8)
C18	0.2055(3)	0.7342(4)	0.0555(2)	3.04(9)
C19	0.1728(4)	0.7052(4)	0.0078(2)	3.18(9)
C20	0.2324(3)	0.6793(4)	-0.0252(2)	2.95(9)

C21	0.3223(3)	0.6820(3)	-0.0139(2)	2.64(8)
C22	0.3509(3)	0.7130(3)	0.0337(2)	2.65(8)
C23	0.5850(3)	0.6896(3)	0.0406(2)	2.46(8)
C24	0.6500(4)	0.6596(4)	0.0119(2)	3.05(9)
C25	0.6319(4)	0.6278(4)	-0.0366(2)	3.28(9)
C26	0.5468(4)	0.6282(4)	-0.0567(2)	3.00(9)
C27	0.4779(3)	0.6575(3)	-0.0289(2)	2.57(8)
C28	0.4987(3)	0.6888(3)	0.0197(2)	2.57(8)
C29	0.3855(3)	0.6532(3)	-0.0520(2)	2.75(9)
C30	0.3640(4)	0.5596(4)	-0.0693(2)	3.49(10)
C31	0.3743(4)	0.7169(4)	-0.0982(2)	3.48(10)
C32	0.0754(4)	0.6993(4)	-0.0072(3)	4.07(12)
C33	0.0461(6)	0.6109(8)	0.0012(9)	21.4(10)
C34	0.0537(5)	0.734(2)	-0.0548(5)	22.2(10)
C35	0.0228(6)	0.7461(13)	0.0301(5)	16.9(7)
C36	0.7041(4)	0.5935(4)	-0.0692(2)	3.78(11)
C37	0.7132(8)	0.6500(7)	-0.1106(5)	14.2(6)
C38	0.6778(7)	0.5051(7)	-0.0921(5)	11.2(4)
C39	0.7821(6)	0.5720(13)	-0.0385(4)	18.6(8)
C40	0.4144(3)	0.9375(4)	0.2949(2)	2.74(8)
C41	0.3540(4)	1.0021(4)	0.3027(2)	3.55(10)
C42	0.3810(4)	1.0847(4)	0.3202(3)	4.16(12)
C43	0.4675(4)	1.1033(4)	0.3286(2)	3.34(10)
C44	0.5311(3)	1.0406(4)	0.3203(2)	2.87(9)
C45	0.5020(3)	0.9586(3)	0.3043(2)	2.60(8)
C46	0.6453(3)	0.9074(4)	0.2958(2)	2.66(8)
C47	0.6931(3)	0.8384(3)	0.2784(2)	2.73(8)
C48	0.7823(3)	0.8500(4)	0.2783(2)	3.01(9)
C49	0.8217(4)	0.9282(4)	0.2938(2)	3.18(9)
C50	0.7717(4)	0.9956(4)	0.3102(2)	3.19(9)
C51	0.6815(4)	0.9876(4)	0.3120(2)	2.90(9)
C52	0.6277(4)	1.0636(4)	0.3281(2)	3.30(10)
C53	0.6454(4)	1.1450(4)	0.2946(3)	4.72(13)

C54	0.6522(4)	1.0853(5)	0.3842(3)	5.0(2)
C55	0.3643(4)	1.1213(4)	0.1108(2)	3.96(11)
C56	0.5116(4)	1.0345(4)	0.0769(2)	3.82(11)
C57	0.4906(4)	1.0496(4)	0.1823(2)	4.10(12)
C58	0.7989(5)	1.0080(5)	0.0746(3)	5.4(2)
C59	0.8611(4)	0.8898(4)	0.1508(2)	4.09(11)
C60	0.7276(4)	1.0113(4)	0.1698(2)	4.10(11)
C61	0.1071(9)	1.0358(8)	0.0769(6)	12.1(4)
C62	0.1042(11)	0.9626(11)	0.1108(6)	14.5(6)
C63	0.1322(9)	0.9493(6)	0.1685(7)	13.6(5)
C64	0.1092(6)	0.8591(7)	0.1909(4)	9.5(4)
C65	0.103(2)	0.8771(12)	0.2440(6)	24.0(13)
C66	0.0804(12)	0.7933(12)	0.2616(6)	17.5(8)

$B_{eq} = 8/3\ p^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}(aa^*bb^*)\cos g + 2U_{13}(aa^*cc^*)\cos b + 2U_{23}(bb^*cc^*)\cos a)$

Table S-3. Atomic coordinates and B_{iso} involving hydrogen atoms

atom	x	y	z	B_{iso}
H1	0.3487	0.9825	0.0415	4.42
H2	0.2841	0.9002	0.0378	4.42
H3	0.3848	0.8868	0.0296	4.42
H4	0.6081	0.8450	0.0176	4.33
H5	0.7110	0.8341	0.0170	4.33
H6	0.6705	0.9267	0.0314	4.33
H7	0.3034	0.6682	0.1482	3.22
H8	0.3114	0.6249	0.2321	3.65
H9	0.3394	0.6507	0.3182	3.66
H10	0.3883	0.7906	0.3452	3.56
H11	0.5391	0.6261	0.1145	2.94
H12	0.5091	0.5814	0.1956	3.27
H13	0.5288	0.5892	0.2831	3.68
H14	0.6132	0.7046	0.3209	3.47
H15	0.1661	0.7500	0.0798	3.65
H16	0.2113	0.6583	-0.0577	3.54
H17	0.7085	0.6609	0.0259	3.66
H18	0.5341	0.6079	-0.0904	3.60
H19	0.3718	0.5197	-0.0402	4.19
H20	0.4027	0.5420	-0.0951	4.19
H21	0.3037	0.5569	-0.0836	4.19
H22	0.3158	0.7106	-0.1148	4.17
H23	0.4173	0.7027	-0.1223	4.17
H24	0.3830	0.7775	-0.0864	4.17
H25	0.0342	0.5813	-0.0315	25.62
H26	-0.0070	0.6127	0.0192	25.62
H27	0.0912	0.5787	0.0216	25.62
H28	-0.0074	0.7518	-0.0574	26.68
H29	0.0628	0.6893	-0.0806	26.68
H30	0.0904	0.7850	-0.0603	26.68

H31	-0.0389	0.7428	0.0186	20.31
H32	0.0408	0.8078	0.0326	20.31
H33	0.0323	0.7182	0.0634	20.31
H34	0.7272	0.6154	-0.1401	17.01
H35	0.7599	0.6921	-0.1020	17.01
H36	0.6587	0.6817	-0.1186	17.01
H37	0.7278	0.4783	-0.1068	13.49
H38	0.6307	0.5134	-0.1186	13.49
H39	0.6581	0.4666	-0.0656	13.49
H40	0.8112	0.6262	-0.0266	22.28
H41	0.8210	0.5382	-0.0587	22.28
H42	0.7674	0.5370	-0.0093	22.28
H43	0.2939	0.9901	0.2961	4.26
H44	0.3391	1.1283	0.3263	4.99
H45	0.4848	1.1601	0.3403	4.01
H46	0.8169	0.8033	0.2672	3.61
H47	0.8827	0.9351	0.2932	3.81
H48	0.7990	1.0492	0.3206	3.83
H49	0.6055	1.1925	0.3020	5.67
H50	0.6364	1.1288	0.2587	5.67
H51	0.7054	1.1647	0.3021	5.67
H52	0.7139	1.1007	0.3887	6.04
H53	0.6411	1.0340	0.4051	6.04
H54	0.6172	1.1350	0.3945	6.04
H55	0.3311	1.1165	0.0779	4.75
H56	0.4020	1.1731	0.1109	4.75
H57	0.3243	1.1271	0.1376	4.75
H58	0.5388	1.0925	0.0806	4.58
H59	0.4841	1.0281	0.0425	4.58
H60	0.5558	0.9888	0.0832	4.58
H61	0.5234	1.1041	0.1787	4.92
H62	0.5309	1.0016	0.1919	4.92
H63	0.4499	1.0572	0.2086	4.92

H64	0.8425	1.0482	0.0905	6.53
H65	0.7500	1.0420	0.0591	6.53
H66	0.8249	0.9733	0.0485	6.53
H67	0.8997	0.9376	0.1630	4.91
H68	0.8894	0.8552	0.1255	4.91
H69	0.8485	0.8520	0.1793	4.91
H70	0.6830	1.0509	0.1546	4.92
H71	0.7779	1.0456	0.1833	4.92
H72	0.7040	0.9782	0.1974	4.92
H73	0.1668	1.0578	0.0773	14.49
H74	0.0690	1.0826	0.0877	14.49
H75	0.0876	1.0171	0.0424	14.49
H76	0.1355	0.9156	0.0939	17.38
H77	0.0424	0.9447	0.1077	17.38
H78	0.1958	0.9576	0.1737	16.30
H79	0.1047	0.9958	0.1879	16.30
H80	0.0533	0.8370	0.1750	11.44
H81	0.1552	0.8153	0.1859	11.44
H82	0.1595	0.8973	0.2605	28.75
H83	0.0579	0.9213	0.2494	28.75
H84	0.1303	0.7536	0.2608	21.04
H85	0.0318	0.7699	0.2397	21.04
H86	0.0634	0.7981	0.2964	21.04

Table S-4. Anisotropic displacement parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ni1	0.0432(4)	0.0300(4)	0.0295(4)	-0.0017(3)	0.0058(3)	0.0018(3)
Ni2	0.0362(4)	0.0337(4)	0.0303(4)	-0.0036(3)	-0.0007(3)	0.0036(3)
P1	0.0503(8)	0.0317(7)	0.0341(7)	-0.0044(6)	0.0054(6)	0.0022(5)
P2	0.0460(8)	0.0418(8)	0.0395(7)	-0.0127(6)	-0.0007(6)	0.0071(6)
O1	0.050(2)	0.034(2)	0.028(2)	-0.001(2)	0.007(2)	0.0035(13)
O2	0.036(2)	0.036(2)	0.030(2)	-0.006(2)	-0.001(2)	0.005(2)
O3	0.029(2)	0.033(2)	0.059(3)	0.002(2)	-0.002(2)	-0.004(2)
O4	0.030(2)	0.040(2)	0.027(2)	-0.001(2)	0.0018(13)	-0.0055(13)
N1	0.039(3)	0.031(2)	0.030(2)	-0.003(2)	0.008(2)	-0.001(2)
N2	0.033(2)	0.033(2)	0.029(2)	0.001(2)	-0.000(2)	-0.001(2)
C1	0.074(4)	0.037(3)	0.030(3)	-0.002(3)	0.006(3)	0.005(2)
C2	0.057(4)	0.043(3)	0.036(3)	-0.006(3)	-0.002(3)	0.008(3)
C3	0.028(3)	0.031(3)	0.042(3)	-0.003(2)	0.004(2)	-0.000(2)
C4	0.031(3)	0.029(3)	0.033(3)	-0.004(2)	0.006(2)	0.001(2)

C5	0.029(3)	0.033(3)	0.032(3)	-0.003(2)	0.002(2)
	0.004(2)				
C6	0.042(3)	0.034(3)	0.040(3)	-0.009(2)	0.006(3)
	0.005(2)				
C7	0.044(3)	0.037(3)	0.035(3)	-0.010(3)	0.007(3)
	0.007(2)				
C8	0.036(3)	0.044(3)	0.034(3)	-0.002(3)	0.004(2)
	0.002(2)				
C9	0.027(3)	0.042(3)	0.033(3)	0.002(2)	0.012(2)
	0.000(2)				
C10	0.032(3)	0.029(3)	0.032(3)	0.004(2)	-0.002(2)
	0.003(2)				
C11	0.034(3)	0.032(3)	0.029(3)	0.003(2)	0.001(2)
	0.000(2)				
C12	0.024(2)	0.030(3)	0.035(3)	0.001(2)	0.000(2)
	0.003(2)				
C13	0.037(3)	0.029(3)	0.038(3)	0.002(2)	0.004(2)
	0.001(2)				
C14	0.046(3)	0.034(3)	0.037(3)	0.001(3)	0.010(3)
	0.009(2)				
C15	0.040(3)	0.037(3)	0.033(3)	0.007(2)	0.006(2)
	0.002(2)				
C16	0.028(3)	0.038(3)	0.029(3)	0.005(2)	-0.000(2)
	-0.001(2)				
C17	0.030(3)	0.035(3)	0.035(3)	-0.001(2)	0.003(2)
	0.001(2)				
C18	0.033(3)	0.045(3)	0.037(3)	0.001(3)	0.001(2)
	0.002(3)				
C19	0.035(3)	0.046(3)	0.039(3)	-0.005(3)	-0.001(2)
	0.003(3)				
C20	0.035(3)	0.043(3)	0.033(3)	-0.007(2)	-0.005(2)
	-0.001(2)				

C21	0.031(3)	0.037(3)	0.032(3)	-0.002(2)	-0.002(2)
	-0.001(2)				
C22	0.032(3)	0.034(3)	0.033(3)	-0.001(2)	-0.005(2)
	-0.000(2)				
C23	0.035(3)	0.028(3)	0.031(3)	0.002(2)	0.006(2)
	0.002(2)				
C24	0.037(3)	0.044(3)	0.035(3)	0.004(3)	0.003(2)
	0.005(2)				
C25	0.043(3)	0.046(3)	0.037(3)	0.003(3)	0.013(3)
	0.004(3)				
C26	0.040(3)	0.043(3)	0.032(3)	0.004(3)	0.005(2)
	-0.001(2)				
C27	0.039(3)	0.035(3)	0.022(3)	-0.002(2)	-0.002(2)
	0.000(2)				
C28	0.036(3)	0.032(3)	0.030(3)	0.003(2)	0.005(2)
	0.000(2)				
C29	0.043(3)	0.033(3)	0.029(3)	-0.005(2)	-0.002(2)
	-0.004(2)				
C30	0.050(4)	0.042(3)	0.041(3)	-0.005(3)	0.003(3)
	-0.009(3)				
C31	0.045(3)	0.052(4)	0.034(3)	-0.006(3)	-0.004(3)
	0.005(3)				
C32	0.027(3)	0.063(4)	0.062(4)	0.001(3)	-0.007(3)
	-0.003(3)				
C33	0.039(5)	0.099(9)	0.66(4)	-0.030(6)	-0.076(12)
	0.05(2)				
C34	0.023(4)	0.68(4)	0.135(10)	0.002(10)	-0.015(5)
	0.20(2)				
C35	0.034(5)	0.41(3)	0.191(13)	0.027(9)	-0.029(6)
	-0.14(2)				
C36	0.050(4)	0.058(4)	0.038(3)	0.013(3)	0.014(3)
	0.001(3)				

C37	0.215(13)	0.115(9)	0.236(13)	0.083(9)	0.199(12)
	0.097(9)				
C38	0.123(8)	0.110(8)	0.209(11)	-0.045(6)	0.108(8)
	-0.106(8)				
C39	0.065(6)	0.54(3)	0.096(8)	0.119(12)	-0.019(6)
	-0.116(12)				
C40	0.037(3)	0.039(3)	0.029(3)	0.000(2)	0.006(2)
	0.000(2)				
C41	0.032(3)	0.053(4)	0.050(3)	0.004(3)	0.004(3)
	-0.008(3)				
C42	0.043(3)	0.043(3)	0.074(4)	0.003(3)	0.013(3)
	-0.019(3)				
C43	0.042(3)	0.036(3)	0.049(3)	0.003(3)	0.007(3)
	-0.008(3)				
C44	0.036(3)	0.040(3)	0.032(3)	-0.002(2)	-0.002(2)
	-0.002(2)				
C45	0.033(3)	0.036(3)	0.030(3)	0.004(2)	0.003(2)
	-0.005(2)				
C46	0.028(3)	0.043(3)	0.029(3)	0.000(2)	-0.002(2)
	0.002(2)				
C47	0.040(3)	0.038(3)	0.025(3)	0.002(2)	0.001(2)
	0.006(2)				
C48	0.033(3)	0.053(3)	0.027(3)	0.001(3)	-0.004(2)
	-0.000(2)				
C49	0.036(3)	0.051(3)	0.033(3)	-0.000(3)	-0.004(2)
	-0.005(3)				
C50	0.036(3)	0.046(3)	0.038(3)	-0.004(3)	-0.009(3)
	-0.000(3)				
C51	0.036(3)	0.041(3)	0.032(3)	-0.001(2)	-0.001(2)
	0.002(2)				
C52	0.038(3)	0.039(3)	0.048(3)	-0.001(3)	-0.003(3)
	-0.009(3)				

C53	0.041(3)	0.044(4)	0.093(5)	-0.004(3)	-0.003(3)
	0.007(3)				
C54	0.053(4)	0.080(5)	0.056(4)	0.012(4)	-0.017(3)
	-0.033(4)				
C55	0.065(4)	0.038(3)	0.047(3)	-0.001(3)	0.002(3)
	-0.000(3)				
C56	0.052(4)	0.048(4)	0.044(3)	-0.008(3)	0.003(3)
	0.004(3)				
C57	0.072(4)	0.045(3)	0.038(3)	-0.018(3)	-0.002(3)
	0.002(3)				
C58	0.069(5)	0.072(5)	0.064(4)	-0.029(4)	-0.006(4)
	0.024(4)				
C59	0.045(4)	0.054(4)	0.056(4)	-0.009(3)	0.001(3)
	0.006(3)				
C60	0.059(4)	0.046(4)	0.049(4)	-0.009(3)	-0.007(3)
	0.000(3)				
C61	0.128(10)	0.104(9)	0.23(2)	-0.004(8)	0.030(10)
	-0.040(10)				
C62	0.21(2)	0.21(2)	0.135(11)	-0.11(2)	0.066(11)
	0.004(11)				
C63	0.168(12)	0.046(6)	0.30(2)	0.006(7)	0.031(12)
	-0.066(9)				
C64	0.080(6)	0.147(10)	0.130(9)	0.038(7)	-0.030(6)
	-0.060(8)				
C65	0.45(4)	0.15(2)	0.28(3)	0.03(2)	-0.20(3)
	-0.10(2)				
C66	0.26(2)	0.20(2)	0.20(2)	0.06(2)	-0.05(2)
	-0.12(2)				

The general temperature factor expression: $\exp(-2p^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl))$

Table S-5. Bond lengths (Å)

atom	atom	distance	atom	atom	distance
Ni1	P1	2.1368(15)	Ni1	O1	1.891(3)
Ni1	N1	1.942(4)	Ni1	C1	1.944(5)
Ni2	P2	2.1608(16)	Ni2	O2	1.900(3)
Ni2	N2	1.933(4)	Ni2	C2	1.918(5)
P1	C55	1.821(6)	P1	C56	1.805(6)
P1	C57	1.826(6)	P2	C58	1.805(7)
P2	C59	1.811(6)	P2	C60	1.815(6)
O1	C4	1.300(6)	O2	C11	1.302(6)
O3	C45	1.371(6)	O3	C46	1.377(6)
O4	C22	1.389(6)	O4	C28	1.377(6)
N1	C3	1.304(6)	N1	C17	1.435(6)
N2	C10	1.300(6)	N2	C23	1.440(6)
C3	C5	1.420(6)	C4	C5	1.424(7)
C4	C9	1.429(7)	C5	C6	1.415(7)

C6	C7	1.369(7)	C7	C8
	1.409(7)			
C8	C9	1.369(7)	C9	C40
	1.502(7)			
C10	C12	1.419(6)	C11	C12
	1.421(6)			
C11	C16	1.433(6)	C12	C13
	1.415(7)			
C13	C14	1.371(7)	C14	C15
	1.415(7)			
C15	C16	1.385(7)	C16	C47
	1.485(7)			
C17	C18	1.385(7)	C17	C22
	1.389(7)			
C18	C19	1.395(7)	C19	C20
	1.376(7)			
C19	C32	1.529(7)	C20	C21
	1.399(7)			
C21	C22	1.385(7)	C21	C29
	1.522(7)			
C23	C24	1.383(7)	C23	C28
	1.404(7)			
C24	C25	1.380(7)	C25	C26
	1.380(7)			
C25	C36	1.552(8)	C26	C27
	1.413(7)			
C27	C28	1.385(6)	C27	C29
	1.512(7)			
C29	C30	1.527(7)	C29	C31
	1.559(7)			
C32	C33	1.443(14)	C32	C34
	1.384(15)			

C32	C35	1.505(15)	C36	C37
	1.410(13)			
C36	C38	1.518(12)	C36	C39
	1.438(12)			
C40	C41	1.382(8)	C40	C45
	1.394(7)			
C41	C42	1.393(8)	C42	C43
	1.368(8)			
C43	C44	1.400(7)	C44	C45
	1.383(7)			
C44	C52	1.531(7)	C46	C47
	1.383(7)			
C46	C51	1.397(7)	C47	C48
	1.389(7)			
C48	C49	1.385(8)	C49	C50
	1.376(8)			
C50	C51	1.403(7)	C51	C52
	1.505(8)			
C52	C53	1.560(8)	C52	C54
	1.540(8)			
C61	C62	1.43(2)	C62	C63
	1.57(3)			
C63	C64	1.548(16)	C64	C65
	1.443(18)			
C65	C66	1.41(3)		

Table S-6. Bond lengths involving hydrogens (Å)

atom	atom	distance	atom	atom	distance
C1	H1	0.980	C1	H2	0.980
C1	H3	0.980	C2	H4	0.980
C2	H5	0.980	C2	H6	0.980
C3	H7	0.950	C6	H8	0.950
C7	H9	0.950	C8	H10	0.950
C10	H11	0.950	C13	H12	0.950
C14	H13	0.950	C15	H14	0.950
C18	H15	0.950	C20	H16	0.950
C24	H17	0.950	C26	H18	0.950
C30	H19	0.980	C30	H20	0.980
C30	H21	0.980	C31	H22	0.980
C31	H23	0.980	C31	H24	0.980
C33	H25	0.980	C33	H26	0.980
C33	H27	0.980	C34	H28	0.980

C34	H29	0.980	C34	H30
	0.980			
C35	H31	0.980	C35	H32
	0.980			
C35	H33	0.980	C37	H34
	0.980			
C37	H35	0.980	C37	H36
	0.980			
C38	H37	0.980	C38	H38
	0.980			
C38	H39	0.980	C39	H40
	0.980			
C39	H41	0.980	C39	H42
	0.980			
C41	H43	0.950	C42	H44
	0.950			
C43	H45	0.950	C48	H46
	0.950			
C49	H47	0.950	C50	H48
	0.950			
C53	H49	0.980	C53	H50
	0.980			
C53	H51	0.980	C54	H52
	0.980			
C54	H53	0.980	C54	H54
	0.980			
C55	H55	0.980	C55	H56
	0.980			
C55	H57	0.980	C56	H58
	0.980			
C56	H59	0.980	C56	H60
	0.980			

C57	H61	0.980	C57	H62
	0.980			
C57	H63	0.980	C58	H64
	0.980			
C58	H65	0.980	C58	H66
	0.980			
C59	H67	0.980	C59	H68
	0.980			
C59	H69	0.980	C60	H70
	0.980			
C60	H71	0.980	C60	H72
	0.980			
C61	H73	0.980	C61	H74
	0.980			
C61	H75	0.980	C62	H76
	0.990			
C62	H77	0.990	C63	H78
	0.990			
C63	H79	0.990	C64	H80
	0.990			
C64	H81	0.990	C65	H82
	0.990			
C65	H83	0.990	C66	H84
	0.980			
C66	H85	0.980	C66	H86
	0.980			

Table S-7. Bond angles (^{O})

atom	atom	atom	angle	atom	atom	atom	angle
P1	Ni1	O1	88.44(11)	P1	Ni1	N1	171.85(13)
P1	Ni1	C1	85.61(17)	O1	Ni1	N1	93.38(14)
O1	Ni1	C1	171.41(19)	N1	Ni1	C1	93.37(19)
P2	Ni2	O2	84.12(10)	P2	Ni2	N2	171.72(12)
P2	Ni2	C2	90.02(17)	O2	Ni2	N2	92.86(14)
O2	Ni2	C2	171.86(19)	N2	Ni2	C2	93.7(2)
Ni1	P1	C55	118.4(2)	Ni1	P1	C56	114.36(19)
Ni1	P1	C57	114.43(19)	C55	P1	C56	102.9(3)
C55	P1	C57	101.8(3)	C56	P1	C57	102.9(3)
Ni2	P2	C58	122.8(3)	Ni2	P2	C59	108.6(2)
Ni2	P2	C60	114.9(2)	C58	P2	C59	102.3(3)
C58	P2	C60	102.7(3)	C59	P2	C60	103.4(3)
Ni1	O1	C4	130.0(3)	Ni2	O2	C11	129.2(3)
C45	O3	C46	119.8(4)	C22	O4	C28	117.9(4)
Ni1	N1	C3	123.6(3)	Ni1	N1	C17	121.3(3)

C3	N1	C17	115.0(4)	Ni2	N2	C10
	124.5(3)					
Ni2	N2	C23	122.0(3)	C10	N2	C23
	113.5(4)					
N1	C3	C5	127.7(5)	O1	C4	C5
	122.2(4)					
O1	C4	C9	119.5(4)	C5	C4	C9
	118.3(4)					
C3	C5	C4	122.9(4)	C3	C5	C6
	117.8(4)					
C4	C5	C6	119.4(4)	C5	C6	C7
	121.9(5)					
C6	C7	C8	118.0(5)	C7	C8	C9
	122.9(5)					
C4	C9	C8	119.5(5)	C4	C9	C40
	118.8(4)					
C8	C9	C40	121.7(4)	N2	C10	C12
	127.6(4)					
O2	C11	C12	123.3(4)	O2	C11	C16
	118.5(4)					
C12	C11	C16	118.1(4)	C10	C12	C11
	122.0(4)					
C10	C12	C13	118.5(4)	C11	C12	C13
	119.5(4)					
C12	C13	C14	122.1(5)	C13	C14	C15
	118.5(5)					
C14	C15	C16	121.5(5)	C11	C16	C15
	120.2(4)					
C11	C16	C47	117.4(4)	C15	C16	C47
	122.1(4)					
N1	C17	C18	120.1(5)	N1	C17	C22
	121.2(4)					

C18	C17	C22	118.6(5)	C17	C18	C19
	121.9(5)					
C18	C19	C20	116.9(5)	C18	C19	C32
	122.3(5)					
C20	C19	C32	120.8(5)	C19	C20	C21
	123.9(5)					
C20	C21	C22	116.6(5)	C20	C21	C29
	121.7(4)					
C22	C21	C29	121.6(4)	O4	C22	C17
	114.3(4)					
O4	C22	C21	123.6(5)	C17	C22	C21
	122.1(5)					
N2	C23	C24	120.9(4)	N2	C23	C28
	119.8(4)					
C24	C23	C28	119.3(4)	C23	C24	C25
	121.5(5)					
C24	C25	C26	118.4(5)	C24	C25	C36
	122.1(5)					
C26	C25	C36	119.5(5)	C25	C26	C27
	122.4(5)					
C26	C27	C28	117.5(5)	C26	C27	C29
	120.1(4)					
C28	C27	C29	122.4(5)	O4	C28	C23
	115.6(4)					
O4	C28	C27	123.4(4)	C23	C28	C27
	120.9(5)					
C21	C29	C27	110.7(4)	C21	C29	C30
	109.4(4)					
C21	C29	C31	107.6(4)	C27	C29	C30
	109.8(4)					
C27	C29	C31	109.6(4)	C30	C29	C31
	109.8(4)					

C19	C32	C33	109.2(6)	C19	C32	C34
	112.3(6)					
C19	C32	C35	111.8(6)	C33	C32	C34
	116.0(12)					
C33	C32	C35	98.6(11)	C34	C32	C35
	108.2(10)					
C25	C36	C37	110.1(7)	C25	C36	C38
	109.8(6)					
C25	C36	C39	111.8(6)	C37	C36	C38
	105.7(8)					
C37	C36	C39	116.6(9)	C38	C36	C39
	102.2(9)					
C9	C40	C41	121.4(5)	C9	C40	C45
	120.8(5)					
C41	C40	C45	117.8(5)	C40	C41	C42
	120.3(5)					
C41	C42	C43	120.3(5)	C42	C43	C44
	121.5(5)					
C43	C44	C45	116.6(5)	C43	C44	C52
	120.8(5)					
C45	C44	C52	122.6(5)	O3	C45	C40
	114.1(4)					
O3	C45	C44	122.4(5)	C40	C45	C44
	123.5(5)					
O3	C46	C47	114.2(4)	O3	C46	C51
	122.1(5)					
C47	C46	C51	123.7(5)	C16	C47	C46
	119.4(5)					
C16	C47	C48	123.0(5)	C46	C47	C48
	117.3(5)					
C47	C48	C49	121.5(5)	C48	C49	C50
	119.3(5)					

C49	C50	C51	122.0(5)	C46	C51	C50
	116.1(5)					
C46	C51	C52	122.8(5)	C50	C51	C52
	121.0(5)					
C44	C52	C51	110.0(4)	C44	C52	C53
	108.5(4)					
C44	C52	C54	110.1(5)	C51	C52	C53
	109.0(5)					
C51	C52	C54	109.7(5)	C53	C52	C54
	109.6(5)					
C61	C62	C63	133.6(13)	C62	C63	C64
	115.6(11)					
C63	C64	C65	103.7(12)	C64	C65	C66
	100.7(13)					

Table S-8. Bond angles involving hydrogens (^{O})

atom	atom	atom	angle	atom	atom	atom	angle
Ni1	C1	H1	109.5	Ni1	C1	H2	109.5
Ni1	C1	H3	109.5	H1	C1	H2	109.5
H1	C1	H3	109.5	H2	C1	H3	109.5
Ni2	C2	H4	109.5	Ni2	C2	H5	109.5
Ni2	C2	H6	109.5	H4	C2	H5	109.5
H4	C2	H6	109.5	H5	C2	H6	109.5
N1	C3	H7	116.2	C5	C3	H7	116.2
C5	C6	H8	119.0	C7	C6	H8	119.0
C6	C7	H9	121.0	C8	C7	H9	121.0
C7	C8	H10	118.5	C9	C8	H10	118.5
N2	C10	H11	116.2	C12	C10	H11	116.2
C12	C13	H12	118.9	C14	C13	H12	118.9
C13	C14	H13	120.7	C15	C14	H13	120.7
C14	C15	H14	119.3	C16	C15	H14	119.3
C17	C18	H15	119.0	C19	C18	H15	119.0

C19	C20	H16	118.1	C21	C20	H16
	118.1					
C23	C24	H17	119.3	C25	C24	H17
	119.3					
C25	C26	H18	118.8	C27	C26	H18
	118.8					
C29	C30	H19	109.5	C29	C30	H20
	109.5					
C29	C30	H21	109.5	H19	C30	H20
	109.5					
H19	C30	H21	109.5	H20	C30	H21
	109.5					
C29	C31	H22	109.5	C29	C31	H23
	109.5					
C29	C31	H24	109.5	H22	C31	H23
	109.5					
H22	C31	H24	109.5	H23	C31	H24
	109.5					
C32	C33	H25	109.5	C32	C33	H26
	109.5					
C32	C33	H27	109.5	H25	C33	H26
	109.5					
H25	C33	H27	109.5	H26	C33	H27
	109.5					
C32	C34	H28	109.5	C32	C34	H29
	109.5					
C32	C34	H30	109.5	H28	C34	H29
	109.5					
H28	C34	H30	109.5	H29	C34	H30
	109.5					
C32	C35	H31	109.5	C32	C35	H32
	109.5					

C32	C35	H33	109.5	H31	C35	H32
	109.5					
H31	C35	H33	109.5	H32	C35	H33
	109.5					
C36	C37	H34	109.5	C36	C37	H35
	109.5					
C36	C37	H36	109.5	H34	C37	H35
	109.5					
H34	C37	H36	109.5	H35	C37	H36
	109.5					
C36	C38	H37	109.5	C36	C38	H38
	109.5					
C36	C38	H39	109.5	H37	C38	H38
	109.5					
H37	C38	H39	109.5	H38	C38	H39
	109.5					
C36	C39	H40	109.5	C36	C39	H41
	109.5					
C36	C39	H42	109.5	H40	C39	H41
	109.5					
H40	C39	H42	109.5	H41	C39	H42
	109.5					
C40	C41	H43	119.9	C42	C41	H43
	119.9					
C41	C42	H44	119.8	C43	C42	H44
	119.8					
C42	C43	H45	119.3	C44	C43	H45
	119.3					
C47	C48	H46	119.2	C49	C48	H46
	119.2					
C48	C49	H47	120.4	C50	C49	H47
	120.3					

C49	C50	H48	119.0	C51	C50	H48
	119.0					
C52	C53	H49	109.5	C52	C53	H50
	109.5					
C52	C53	H51	109.5	H49	C53	H50
	109.5					
H49	C53	H51	109.5	H50	C53	H51
	109.5					
C52	C54	H52	109.5	C52	C54	H53
	109.5					
C52	C54	H54	109.5	H52	C54	H53
	109.5					
H52	C54	H54	109.5	H53	C54	H54
	109.5					
P1	C55	H55	109.5	P1	C55	H56
	109.5					
P1	C55	H57	109.5	H55	C55	H56
	109.5					
H55	C55	H57	109.5	H56	C55	H57
	109.5					
P1	C56	H58	109.5	P1	C56	H59
	109.5					
P1	C56	H60	109.5	H58	C56	H59
	109.5					
H58	C56	H60	109.5	H59	C56	H60
	109.5					
P1	C57	H61	109.5	P1	C57	H62
	109.5					
P1	C57	H63	109.5	H61	C57	H62
	109.5					
H61	C57	H63	109.5	H62	C57	H63
	109.5					

P2	C58	H64	109.5	P2	C58	H65
	109.5					
P2	C58	H66	109.5	H64	C58	H65
	109.5					
H64	C58	H66	109.5	H65	C58	H66
	109.5					
P2	C59	H67	109.5	P2	C59	H68
	109.5					
P2	C59	H69	109.5	H67	C59	H68
	109.5					
H67	C59	H69	109.5	H68	C59	H69
	109.5					
P2	C60	H70	109.5	P2	C60	H71
	109.5					
P2	C60	H72	109.5	H70	C60	H71
	109.5					
H70	C60	H72	109.5	H71	C60	H72
	109.5					
C62	C61	H73	109.5	C62	C61	H74
	109.5					
C62	C61	H75	109.5	H73	C61	H74
	109.5					
H73	C61	H75	109.5	H74	C61	H75
	109.5					
C61	C62	H76	103.8	C61	C62	H77
	103.8					
C63	C62	H76	103.8	C63	C62	H77
	103.8					
H76	C62	H77	105.4	C62	C63	H78
	108.4					
C62	C63	H79	108.4	C64	C63	H78
	108.4					

C64	C63	H79	108.4	H78	C63	H79
	107.4					
C63	C64	H80	111.0	C63	C64	H81
	111.0					
C65	C64	H80	111.0	C65	C64	H81
	111.0					
H80	C64	H81	109.0	C64	C65	H82
	111.6					
C64	C65	H83	111.6	C66	C65	H82
	111.6					
C66	C65	H83	111.6	H82	C65	H83
	109.4					
C65	C66	H84	109.5	C65	C66	H85
	109.5					
C65	C66	H86	109.5	H84	C66	H85
	109.5					
H84	C66	H86	109.5	H85	C66	H86
	109.5					