Nickel Pincer Complexes with Frequent Aliphatic Alkoxo Ligands [(^{iPr}PCP)Ni-OR] (R = Et, *n*Bu, *i*Pr, 2-hydroxyethyl). An Assessment of the Hydrolytic Stability of Nickel and Palladium Alkoxides.

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Electronic Supporting Information (ESI)

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1. Estimation of the aggregation degree of 5 using DOSY.

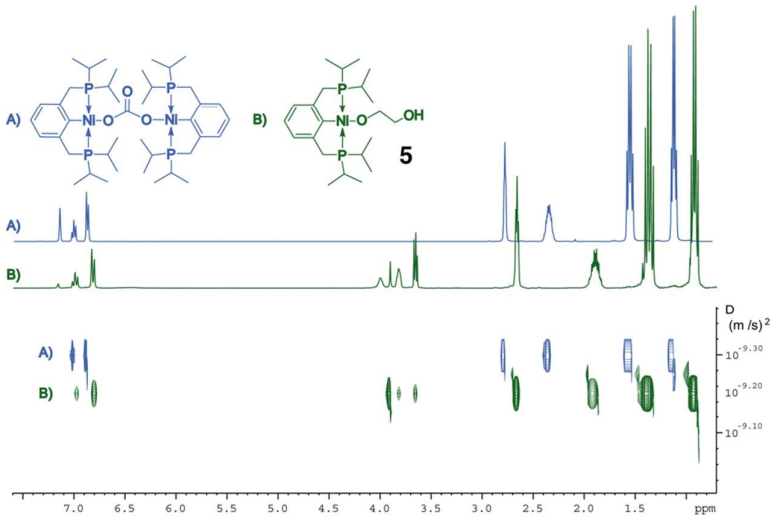


Figure S1: DOSY spectra of **5** and [{(^{iPr}PCP)Ni}$_2$-μ-κ^2-*O,O'*-CO_3]

The diffusion coefficients measured for **5** and the reference binuclear complexes are $10^{-9.1}$ and $10^{-9.2}$ m^2/s, indicating that **5** is significantly smaller, and therefore it is likely a monomeric compound. This conclusion can be refined as follows: The size of two given molecules A and B can be compared on the basis of the diffusion coefficients measured in the DOSY.[1] From the Stokes-Einstein equation (1), it is deduced that the ratio of the hydrodynamic radii r_A and r_B, is the inverse of the diffussion coefficients D_A and D_B (2). Assuming that the shape of molecules **A** and **B** can be approximated to spheres, their radii are proportional to the cubic root of their mass. Therefore, the relationship (3) holds, which relates the diffusion coefficients to the molecular weights, M_A and M_B. Feeding the diffusion coefficients of the binuclear compound and **5** as $D_A = 10^{-9.1}$ and $D_B = 10^{-9.2}$ m^2/s, respectively, and the molecular weight of the reference compound (850.3) as M_A, gives M_B = 435.3, which is a very good estimate of the correct molecular weight of monomeric **5**, 456.2.

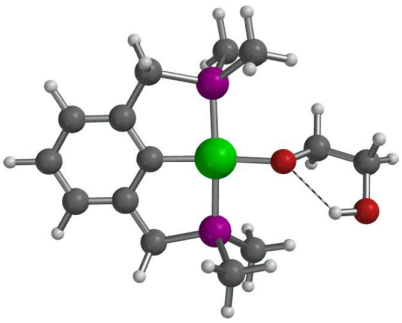
$$D = \frac{kT}{6\pi\eta r} \quad (1)$$

$$\frac{D_A}{D_B} = \frac{r_B}{r_A} \quad (2)$$

$$\frac{D_A}{D_B} = \left(\frac{M_B}{M_A}\right)^{1/3} \quad (3)$$

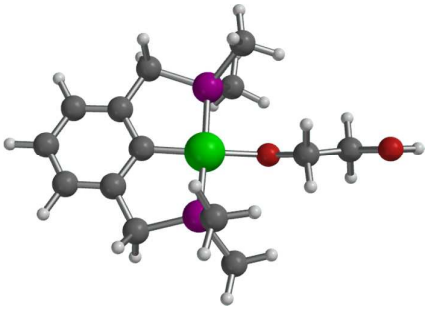
1): a) Cabrita, E. J.; Beger, S. *Magn. Reson. Chem.* **2002**, *40*, S122 - S127; b) Thureau, P.; Ancian, B.; Viel, S.; Thevand, A. *Chem. Commun.*, **2006**, 200 - 202; c) Díez, J.; Gimeno, I.; Merino, E.; Rubio, F. Suárez, F. J. *Inorg. Chem.*, **2011**, *50*, 4868 - 4881.

2. Computational model of intramolecular hydrogen bonding in glycoxide complex 5 in solution



E (SCF) = -1812190.95 -1812002.75

ΔGº (298 K) = -1812002.75 -1812002.75



E (SCF) = -1812184.09 95 Kcal·mol^{-1}

ΔGº (298 K) = -1811997.63 Kcal·mol^{-1}

Figure S2. Drawings of the optimized geometries of the hypothetical complex [(^{Me}PCP)NiOCH2CH2OH] (model for complex **5**) in solution (PBE-D3/6-31*/CPCM, solvent = benzene), showing SCF electronic and free energies. Left, H-Bonded; Right, Non-bonded.

3. IR spectral calculations

Table S1. SCF (PBE) and Free energies(Kcal·mol^{-1}) corresponding to the molecules of complexes **1a, 1b, 2, 4 and 5**, and alcohols MeOH, EtOH and iPrOH, used for vibrational spectra calculations (PBE/6-31+G*).

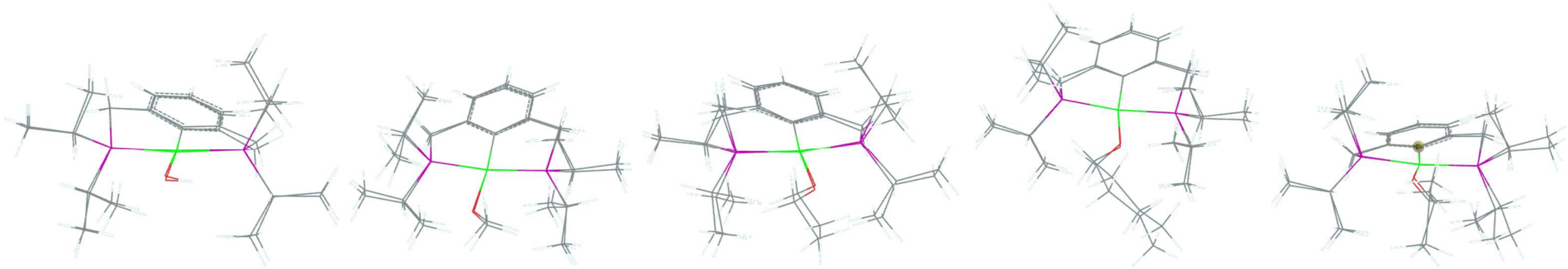
Compound	SCF E	ΔGº (298 K)
[(^{iPr}PCP)Ni-OMe]	-1937426.72	-1937131.98
[(^{iPr}PCP)Pd-OMe]	-1071753.53	-1071456.26
[(^{iPr}PCP)Ni-OEt]	-1962064.69	-1961753.16
[(^{iPr}PCP)Ni-OnBu]	-2011332.79	-2010988.67
[(^{iPr}PCP)Ni-OiPr]	-1986701.66	-1986373.21
MeOH	-72528.0259	-72510.9833
EtOH	-97165.9356	-97133.0572
nBuOH	-146434.463	-146370.261
iPrOH	-121803.887	-121755.210

4. Calculation of the energy balances in hydroxide / alcohol exchanges (Eq. 1 in main text).

Table S2. Comparison of key bond distances and angles of nickel and palladium alkoxides in PBE/6-31G* optimized geometries and experimental x-ray diffraction data

	Without CPCM solvent correction							With CPCM solvent correction						Experimental (X ray)						
	6a Ni-OH	**1a** Ni-OMe	**2** Ni-OEt	**3** Ni-OnBu	**4** Ni-OiPr	**6b** Pd-OH	**1b** Pd-OMe	**6a** Ni-OH	**1a** Ni-OMe	**2** Ni-OEt	**3** Ni-OiPr	**6b** Pd-OH	**1b** Pd-OMe	**6a** Ni-OH	**1a** Ni-OMe	**2** Ni-OEt	**3** Ni-OiPr	**4** Ni-OnBu	**6b** Pd-OH	**1b** PdOMe
Distances (Å)																				
M-O	1.857	1.875	1.865	1.866	1.873	2.074	2.093	1.864	1.880	1.870	1.876	2.086	2.104	1.865	1.850	1.897	1.852	1.887	2.105	2.081
O-C		1.396	1.399	1.401	1.404		1.395		1.398	1.401	1.405		1.394		1.295	1.273	1.335	1.280		1.296
M-C	1.887	1.894	1.894	1.890	1.895	2.050	2.059	1.886	1.893	1.893	1.895	2.045	2.055	1.918	1.918	1.926	1.920	1.919	1.993	2.020
M-P1	2.139	2.163	2.169	2.157	2.173	2.311	2.322	2.147	2.173	2.176	2.180	2.313	2.306	2.157	2.191	2.182	2.164	2.176	2.274	2.283
M-P2	2.147	2.142	2.144	2.154	2.149	2.305	2.302	2.153	2.146	2.150	2.156	2.308	2.324	2.157	2.154	2.157	2.173	2.156	2.256	2.266
M-P ave	2.143	2.153	2.157	2.156	2.161	2.308	2.312	2.150	2.160	2.163	2.168	2.311	2.315	2.157	2.173	2.170	2.169	2.166	2.265	2.275
Angles and Torsion Angles (º)																				
C-M-O	175.06	167.81	167.90	170.17	168.71	175.24	170.76	176.05	167.95	168.03	169.17	176.54	171.65	175.47	169.75	170.56	171.11	171.50	174.25	170.15
P-M-P	169.77	171.18	167.92	169.43	169.31	166.22	166.78	170.10	171.33	167.63	169.33	166.08	166.62	169.38	170.25	169.78	168.87	168.61	164.97	166.49
M-O-C/H	112.48	128.68	128.45	131.15	130.07	105.32	120.89	111.39	125.34	128.03	129.71	104.10	120.51	109.94	125.85	129.64	142.10	132.98	99.46	125.82
P-M-O-R	1.48	40.23	-27.62	-15.80	-36.33	3.49	28.79	-0.02	43.92	-28.82	-36.70	-0.77	29.73	12.75	46.63	-32.28	-17.95	17.68	5.54	23.52
PMP^*m.m'*-C_6H_3	17.31	-11.17	15.77	-17.18	-14.66	14.12	-9.91	16.52	-10.45	15.39	-14.61	14.03	-9.77	14.68	-8.58	10.23	-13.86	-13.52	-5.82	10.08

Figure S3. Overlaid experimental (X-ray) and opitimzed (PBE/6-31G*, vacuum) structures of nickel hydroxide and alkoxide complexes.



6a, [(^{iPr}PCP)Ni-OH] **1a**, [(^{iPr}PCP)Ni-OMe] **2**, [(^{iPr}PCP)Ni-OEt] **3**, [(^{iPr}PCP)Ni-OnBu] **4**, [(^{iPr}PCP)Ni-OnBu]

Table S3. Computed SCF, Zero-Point, Thermal Corrections and Free Energies (Kcal·mol^{-1}).

	PBE/6-31G*/CPCM (Benzene)					PBE/6-31G*/CPCM//PBE/6-311++G(3df,2p)/CPCM		
Molecule	SCF Energy	ZPE	ΔGº (298 K)	T.C.[(a)]		SCF Energy	E+ZPE[(b)]	ΔGº (298 K)[(c)]
[(^{iPr}PCP)Ni-OH]	-1912784.89	320.81	-1912503.41	281.48		-1913145.75	-1912824.94	-1912864.27
[(^{iPr}PCP)Ni-OMe]	-1937407.29	338.44	-1937109.15	298.15		-1937772.73	-1937434.29	-1937474.59
[(^{iPr}PCP)Ni-OEt]	-1962044.96	356.27	-1961730.25	314.71		-1962417.00	-1962060.73	-1962102.29
[(^{iPr}PCP)Ni-OiPr]	-1986681.21	373.21	-1986350.42	330.79		-1987060.46	-1986687.25	-1986729.67
[(^{iPr}PCP)Ni-OC_3H_7O]	-2033822.65	375.92	-2033491.89	330.76		-2034221.21	-2033845.29	-2033890.45
[(^{iPr}PCP)Pd-OH]	-1046086.22	320.58	-1045805.36	280.86		-1047064.51	-1046743.93	-1046783.65
[(^{iPr}PCP)Pd-OMe]	-1070711.70	338.57	-1070413.49	298.21		-1071693.88	-1071355.31	-1071395.67
[(^{iPr}PCP)Pd-OEt]	-1095349.42	356.11	-1095035.19	314.23		-1096338.26	-1095982.15	-1096024.03
[(^{iPr}PCP)Pd-OiPr]	-1119985.71	372.84	-1119656.13	329.59		-1120981.91	-1120609.07	-1120652.33
[(^{iPr}PCP)Pd-OC_3H_7O]	-1167126.71	375.67	-1166796.67	330.04		-1168142.32	-1167766.65	-1167812.28
H_2O	-47896.58	12.92	-47894.77	1.81		-47929.54	-47916.62	-47927.73
MeOH	-72523.14	31.40	-72506.01	17.13		-72557.79	-72526.39	-72540.67
EtOH	-97160.19	48.93	-97127.26	32.93		-97202.29	-97153.36	-97169.36
iPrOH	-121797.77	66.20	-121748.85	48.92		-121847.00	-121780.80	-121798.08
$(C_3H_7O)OH$	-168939.98	69.63	-168889.26	50.71		-169008.02	-168938.39	-168957.31
[(^{iPr}PCP)Ni•]	-1865219.95	309.26	-1864947.03	272.92		-1865566.82	-1865257.56	-1865293.90
[(^{iPr}PCP)Pd•]	-998536.34	308.85	-998264.56	271.78		-999489.99	-999181.14	-999218.20
HO(•)	-47465.10	4.91	-47470.43	-5.33		-47490.60	-47470.43	-47495.93
MeO(•)	-72107.90	21.06	-72100.51	7.39		-72137.14	-72100.51	-72129.75
EtO(•)	-96746.03	38.71	-96722.65	23.38		-96782.51	-96722.65	-96759.13
iPrO(•)	-121382.42	57.16	-121342.26	40.15		-121426.10	-121342.26	-121385.95
$(C_3H_7O)O(•)$	-168522.81	59.39	-168482.25	40.57		-168585.99	-168482.25	-168545.43
H(•)						-313.63	-313.63	
[(^{iPr}PCP)Ni]$^+$	-1865132.20	313.12	-1864856.95	275.26		-1865454.18	-1865141.06	-1865178.93
[(^{iPr}PCP)Pd]$^+$	-998453.76	312.73	-998179.50	274.26		-999384.59	-999071.86	-999110.32
OH^-	-47511.33	4.88	-47516.67	-5.35		-47550.05	-47545.17	-47555.40
MeO^-	-72161.48	21.21	-72154.23	7.25		-72177.19	-72155.98	-72169.94
EtO($^-$	-96800.47	39.21	-96776.92	23.55		-96829.31	-96790.10	-96805.76
$iPrO^-$	-121438.23	57.57	-121398.72	39.51		-121475.73	-121419.16	-121436.22
$(C_3H_7O)O^-$	--168580.1	59.46	-168539.41	40.69		-168639.76	-168580.30	-168599.07

(a) Thermal Correction (T. C.) = ΔGº (298 K, 6-31G*/CPCM) – E(SCF, 6-31G*/CPCM).

(b) ZPE from 6-31G* calculation

(c) ΔGº (298 K, 6-31G*) = E(SCF, 6-311++G(3df, 2p)/CPCM) + Thermal Correction (T. C.).

Table S4. Mulliken Electrostatic Charges at the metal center and oxygen atom in hydroxides and alkoxides.

	[(^{iPr}PCP)Ni-OR]		[(^{iPr}PCP)Pd-OR]	
OR	q(Ni)	q(O)	q(Pd)	q(O)
OH	+0.493	-0.747	+0.290	-0.723
OMe	+0.415	-0.412	+0.427	-0.561
OEt	+0.412	-0.361	+0.403	-0.525
OiPr	+0.358	-0.207	+0.424	-0.378
O(C_3H_7O)	+0.434	-0.291	+0.354	-0.476

5. XYZ coordinates

5.1 Intramolecular hydrogen bond in glycoxide complex (PBE-D3/6-31+G**/CPCM)

H-bonded [(^{Me}PCP)Ni-OCH$_2$CH$_2$OH]

43

C	1.776871	0.422300	0.010599
C	4.530629	1.138310	0.090811
C	2.795001	-0.568395	0.172049
C	2.190392	1.783810	-0.127007
C	3.550420	2.131118	-0.069621
C	4.152836	-0.208765	0.201985
H	3.851180	3.181316	-0.160613
H	4.919859	-0.982344	0.326664
H	5.588795	1.414574	0.128796
C	2.374841	-2.022925	0.356884
H	2.983043	-2.724278	-0.243207
H	2.477286	-2.332053	1.414902
C	1.119325	2.839754	-0.371764
H	1.084994	3.119368	-1.442137
H	1.294582	3.768830	0.199459
Ni	-0.021724	-0.044948	0.071358
P	0.564067	-2.084461	-0.063567
P	-0.497445	2.016586	0.043919
O	-1.865119	-0.456432	0.437101
C	-2.790434	-0.942922	-0.501310
H	-2.571168	-1.984241	-0.854081
H	-2.845397	-0.309848	-1.419105
C	-0.292255	-3.261311	1.070095
H	-0.258171	-2.882336	2.101906
C	0.377169	-2.929926	-1.696849
H	0.836537	-2.321602	-2.489325
C	-1.124905	2.712108	1.631872
H	-2.085942	2.220297	1.856362
C	-1.789297	2.563376	-1.154257
H	-2.747390	2.108383	-0.847966
H	-0.423642	2.480648	2.446365
H	-1.283477	3.801700	1.571280
H	-1.897925	3.660575	-1.169970
H	-1.547030	2.201947	-2.165055
H	-1.353581	-3.291508	0.771813
H	0.131407	-4.278492	1.026346
H	-0.700539	-3.020330	-1.912068
H	0.828086	-3.936526	-1.689267
C	-4.179138	-0.945265	0.160662
H	-4.230678	-1.757271	0.918448
H	-4.974544	-1.111815	-0.587042
O	-4.414400	0.324286	0.777766

H	-3.533122	0.508707	1.176771

[(^{Me}PCP)Ni-OCH_2CH_2OH]

43

C	1.838563	0.217332	0.033731
C	4.677718	0.447214	0.049871
C	2.479044	1.492272	-0.061615
C	2.675386	-0.939804	0.153975
C	4.074640	-0.816910	0.148165
C	3.880197	1.598792	-0.046284
H	4.700750	-1.713979	0.225077
H	4.354823	2.583840	-0.125157
H	5.768714	0.533168	0.047885
C	1.602961	2.730066	-0.223862
H	1.893597	3.549116	0.459124
H	1.670348	3.130139	-1.253270
C	2.024809	-2.315960	0.304997
H	2.157312	-2.706835	1.331889
H	2.463060	-3.065431	-0.378890
Ni	-0.002494	0.053500	-0.100654
P	-0.152168	2.159389	0.035334
P	0.210133	-2.049984	-0.010655
O	-1.824978	-0.301144	-0.569728
C	-2.964696	-0.074065	0.206621
H	-3.207182	1.010479	0.352285
H	-2.906037	-0.506908	1.234606
C	-1.243674	2.994784	-1.195278
H	-0.994996	2.646497	-2.208781
C	-0.776479	2.823661	1.640597
H	-0.243088	2.335613	2.469532
C	-0.333274	-2.970005	-1.512678
H	-1.369331	-2.636221	-1.697911
C	-0.764292	-2.910855	1.302744
H	-1.831987	-2.797413	1.049069
H	0.280087	-2.698063	-2.383590
H	-0.308796	-4.062725	-1.366089
H	-0.519414	-3.984973	1.358356
H	-0.595207	-2.443810	2.284177
H	-2.278939	2.678003	-0.985625
H	-1.182113	4.094785	-1.149272
H	-1.844332	2.557135	1.717898
H	-0.668266	3.918535	1.717378
C	-4.180829	-0.710983	-0.479481
H	-3.999534	-1.800193	-0.595855
H	-4.298026	-0.272334	-1.490804
O	-5.334552	-0.458640	0.342797
H	-6.118627	-0.806168	-0.116147

5.2 Alkoxide complexes and alcohols for IR calculations (See main text, Table 2; PBE/6-31+G*, LACVP* for M = Pd).

[(^{iPr}PCP)Ni-OMe]

63

C	-1.284209	-0.571741	-0.992478
C	-2.411349	-1.235115	-0.410542
C	-3.527587	-1.620659	-1.172791
C	-3.566592	-1.378332	-2.553426
C	-2.473414	-0.749281	-3.164209
C	-1.355914	-0.354156	-2.406487
C	-2.374739	-1.540530	1.071585
C	-0.197285	0.337560	-3.100696
C	-0.357513	-1.410451	3.238610
C	0.385661	-2.657220	2.728902
C	-1.411297	-1.761609	4.300284
C	-1.983605	0.998670	2.502122
C	-1.036598	1.931525	3.277746
C	-2.708284	1.756846	1.377678
C	2.434826	-0.782795	-2.347339
C	1.860410	-2.204530	-2.219451
C	3.722219	-0.626888	-1.521574
C	1.929420	2.148474	-1.999782
C	0.915573	3.240158	-1.617315
C	2.553890	2.394789	-3.382079
C	2.324782	0.667191	1.988261
H	-4.373869	-2.118135	-0.681152
H	-4.437964	-1.678420	-3.146230
H	-2.489110	-0.556297	-4.244903
H	0.394484	-0.736027	3.689224
H	-2.738036	0.577616	3.196562
H	2.653195	-0.580206	-3.416127
H	2.713087	2.137377	-1.219851
H	1.136671	-2.395637	1.963284
H	-0.305822	-3.394503	2.282910
H	0.906444	-3.159449	3.564810
H	-0.943273	-2.330009	5.125830
H	-1.878657	-0.863657	4.740641
H	-2.216402	-2.393781	3.882817
H	-0.221340	2.293769	2.625809
H	-0.579838	1.439004	4.153976
H	-1.596963	2.810024	3.647973
H	-1.985361	2.125271	0.628275
H	-3.439366	1.126814	0.843916
H	-3.246674	2.625236	1.800634
H	2.587060	-2.941180	-2.609705
H	0.912623	-2.333665	-2.769918
H	1.659038	-2.444824	-1.160319

H	3.507460	-0.698025	-0.441338
H	4.222353	0.340932	-1.697924
H	4.436754	-1.427926	-1.787108
H	0.069240	3.284585	-2.326982
H	1.408617	4.230100	-1.630583
H	0.520523	3.065767	-0.602714
H	3.366180	1.683467	-3.611881
H	2.983573	3.413017	-3.425656
H	1.800626	2.320433	-4.188036
H	3.206912	1.339939	2.081963
H	1.755479	0.758260	2.946877
H	2.720158	-0.376461	1.952514
H	-2.095278	-2.597872	1.243985
H	-3.352206	-1.381916	1.565536
H	0.137262	-0.210811	-4.002401
H	-0.483266	1.353083	-3.437998
Ni	0.167946	0.070516	0.055410
O	1.586630	1.029063	0.857978
P	-1.044764	-0.453558	1.773866
P	1.137475	0.466179	-1.820984

[(^{iPr}PCP)Pd-OMe]

63

C	-1.288667	-0.582788	-1.012337
C	-2.401915	-1.240292	-0.412405
C	-3.495346	-1.667156	-1.189886
C	-3.504575	-1.469973	-2.577776
C	-2.415166	-0.835276	-3.189931
C	-1.319717	-0.387686	-2.425775
C	-2.398665	-1.509692	1.080979
C	-0.183275	0.342907	-3.123922
C	-0.477803	-1.408772	3.359746
C	0.274742	-2.659614	2.872935
C	-1.562705	-1.753390	4.392104
C	-2.081125	1.006297	2.608729
C	-1.150062	1.971089	3.365504
C	-2.862796	1.744065	1.509495
C	2.522065	-0.769876	-2.543215
C	1.957093	-2.194651	-2.399885
C	3.843506	-0.609767	-1.771996
C	2.031835	2.164953	-2.173162
C	1.100184	3.244202	-1.596054
C	2.456711	2.458493	-3.620646
C	2.434000	0.621806	2.244490
H	-4.345578	-2.164439	-0.705044
H	-4.356633	-1.807469	-3.178375
H	-2.419915	-0.675273	-4.275952
H	0.264091	-0.734080	3.825973
H	-2.806714	0.563059	3.319640

H	2.690757	-0.562250	-3.619866
H	2.921295	2.118140	-1.516237
H	1.037455	-2.406369	2.116297
H	-0.410486	-3.402207	2.426324
H	0.781569	-3.150612	3.723674
H	-1.121616	-2.338726	5.220526
H	-2.024697	-0.853962	4.834094
H	-2.368440	-2.367784	3.949701
H	-0.364700	2.365896	2.696078
H	-0.653269	1.493834	4.227948
H	-1.733755	2.827469	3.751076
H	-2.177222	2.162388	0.753349
H	-3.578909	1.089021	0.985597
H	-3.431049	2.578876	1.959746
H	2.668896	-2.922672	-2.831219
H	0.987649	-2.322770	-2.912025
H	1.805457	-2.449423	-1.336436
H	3.665582	-0.621338	-0.682317
H	4.358130	0.335464	-2.015796
H	4.527778	-1.439604	-2.028203
H	0.144889	3.307175	-2.149075
H	1.587298	4.234681	-1.662675
H	0.881771	3.031047	-0.535976
H	3.186943	1.724721	-4.004357
H	2.927070	3.457395	-3.683267
H	1.586792	2.460687	-4.302752
H	3.412849	1.114247	2.451632
H	1.739436	0.951808	3.059656
H	2.597243	-0.475147	2.386110
H	-2.120838	-2.563372	1.277284
H	-3.395091	-1.355571	1.537152
H	0.111596	-0.154095	-4.067812
H	-0.499731	1.368944	-3.398138
Pd	0.291525	0.098204	0.107006
O	2.003535	0.966994	0.962927
P	-1.104799	-0.427951	1.881723
P	1.255518	0.480184	-1.944979

[(^{iPr}PCP)Ni-OEt]

66

C	-0.689050	0.358313	-1.727838
C	-2.013469	0.838567	-1.981953
C	-2.464305	1.116465	-3.284822
C	-1.623558	0.917076	-4.389123
C	-0.330228	0.416245	-4.180717
C	0.124927	0.131990	-2.881440
C	1.499690	-0.461136	-2.671847
C	-2.944174	1.035112	-0.800384
C	-2.896783	-1.528041	0.696307

C	-2.328282	-2.311035	1.892278
C	-2.685478	-2.293595	-0.620961
C	-2.596357	1.053707	2.174002
C	-4.117078	1.128402	2.383650
C	-1.929647	2.440267	2.213261
C	3.032925	-1.548441	-0.374943
C	2.186509	-2.826848	-0.239203
C	4.241351	-1.761788	-1.301272
C	3.013024	1.398015	-0.970729
C	3.545561	1.766348	0.422463
C	2.227956	2.570658	-1.584362
C	1.407080	-0.397645	2.583881
C	1.311001	-0.049174	4.074799
H	-3.485173	1.490809	-3.436609
H	-1.975505	1.140629	-5.402424
H	0.331497	0.237904	-5.038379
H	-3.983858	-1.368195	0.843777
H	-2.136823	0.452593	2.980086
H	3.399615	-1.279067	0.633356
H	3.861746	1.148037	-1.639003
H	-2.766838	-3.325641	1.923983
H	-2.542007	-1.824232	2.859226
H	-1.231620	-2.413046	1.805406
H	-1.607877	-2.435856	-0.817425
H	-3.108706	-1.763027	-1.490422
H	-3.166264	-3.287097	-0.556150
H	-4.340238	1.639189	3.339048
H	-4.594729	0.132787	2.424124
H	-4.607695	1.708125	1.580217
H	-2.285886	3.095174	1.396111
H	-0.834742	2.330666	2.140697
H	-2.172116	2.945241	3.167076
H	1.784968	-3.155082	-1.214803
H	1.332213	-2.677075	0.444290
H	2.804818	-3.652860	0.158185
H	4.855898	-2.605500	-0.934864
H	4.896613	-0.874816	-1.350315
H	3.925075	-2.008593	-2.330819
H	4.145616	2.693251	0.363096
H	4.191157	0.980404	0.851006
H	2.707925	1.942396	1.120654
H	1.354578	2.826865	-0.958780
H	1.853756	2.348143	-2.597745
H	2.879891	3.461648	-1.648319
H	2.449848	-0.174608	2.240491
H	1.280079	-1.501955	2.471124
H	1.453319	1.035795	4.224989
H	2.081538	-0.587873	4.658839
H	0.317248	-0.321815	4.473479
H	2.257560	-0.054934	-3.368498
H	1.475036	-1.557558	-2.828192

H	-3.965524	0.655444	-0.995669
H	-3.044080	2.106044	-0.535836
Ni	-0.026861	0.140219	0.041466
O	0.448986	0.320377	1.859148
P	-2.100443	0.168116	0.604335
P	1.916391	-0.124484	-0.891001

[(^{iPr}PCP)Ni-OnBu]

72

C	-1.043664	0.489017	2.038768
C	-1.733904	-0.450401	2.865872
C	-2.351429	-0.070874	4.069920
C	-2.308734	1.262649	4.502182
C	-1.637244	2.212738	3.718297
C	-1.014082	1.837753	2.514890
C	-1.795235	-1.885979	2.394725
C	-0.293937	2.872228	1.673329
C	1.022075	-2.705864	2.144807
C	1.428903	-1.716694	3.251938
C	2.225055	-3.027201	1.243214
C	-0.950733	-3.448221	0.019941
C	-1.342960	-4.731872	0.769111
C	-2.074952	-2.965167	-0.915877
C	-1.631880	2.823547	-0.974964
C	-2.961176	2.392242	-0.332273
C	-1.560321	2.387553	-2.449228
C	1.360790	2.706727	-0.841635
C	2.587143	2.198516	-0.065955
C	1.412228	4.224234	-1.072297
C	0.965920	-1.333455	-2.008633
C	2.082366	-0.839433	-2.948336
C	1.583293	0.010521	-4.122490
C	2.712850	0.508280	-5.034460
H	-2.875972	-0.825129	4.671037
H	-2.794879	1.558689	5.438438
H	-1.596211	3.259851	4.045217
H	0.668679	-3.641377	2.623645
H	-0.065707	-3.660846	-0.608204
H	-1.545271	3.927799	-0.905070
H	1.334511	2.174801	-1.811129
H	2.253246	-2.151707	3.847000
H	0.600063	-1.475396	3.937779
H	1.781570	-0.766063	2.815279
H	2.579153	-2.114639	0.731094
H	1.996999	-3.786326	0.474423
H	3.059613	-3.414224	1.856819
H	-2.215402	-4.566189	1.425614
H	-0.520763	-5.129043	1.389182
H	-1.620361	-5.521503	0.045931

H	-2.324066	-3.759297	-1.643556
H	-1.771789	-2.060573	-1.469869
H	-2.999681	-2.728826	-0.358262
H	-3.805538	2.853545	-0.877514
H	-3.036140	2.684768	0.728512
H	-3.075848	1.294879	-0.381824
H	-1.475681	1.289127	-2.527653
H	-0.692581	2.826402	-2.972286
H	-2.472298	2.715774	-2.981390
H	3.509506	2.396625	-0.642668
H	2.517478	1.111718	0.114907
H	2.696965	2.705005	0.910456
H	1.381873	4.783653	-0.118918
H	0.581935	4.583769	-1.703822
H	2.355453	4.495898	-1.582365
H	0.265573	-1.964738	-2.615091
H	1.438578	-2.020302	-1.270744
H	2.818719	-0.258640	-2.355204
H	2.623277	-1.727141	-3.340995
H	1.015487	0.871760	-3.724306
H	0.858653	-0.583086	-4.716228
H	3.439034	1.122927	-4.469889
H	2.325092	1.127014	-5.864129
H	3.272837	-0.334704	-5.480598
H	-2.749230	-2.095094	1.872146
H	-1.715847	-2.614979	3.223652
H	0.734469	3.046576	2.046549
H	-0.806006	3.853497	1.676739
Ni	-0.284559	-0.024989	0.374308
O	0.277474	-0.271780	-1.403663
P	-0.197574	2.100765	-0.010611
P	-0.425206	-2.039098	1.146417

[(^{iPr}PCP)Ni-OiPr]

69

C	1.767529	0.799284	-0.621649
C	2.984058	0.403600	0.015308
C	4.235465	0.903394	-0.385532
C	4.326567	1.842955	-1.422383
C	3.150296	2.295796	-2.036103
C	1.897071	1.791767	-1.644252
C	2.883460	-0.534218	1.194384
C	0.636296	2.319762	-2.295285
C	1.711321	-3.056009	0.329872
C	0.608194	-4.114542	0.474959
C	2.122927	-2.873818	-1.141320
C	0.718955	-1.702618	2.825517
C	1.795576	-2.408461	3.666212
C	0.257406	-0.381471	3.465697

C	-1.177204	3.187841	-0.101049
C	-2.459205	2.887539	0.697687
C	0.006536	3.488169	0.834002
C	-2.216011	1.477237	-2.327691
C	-1.917299	0.381741	-3.364665
C	-2.693008	2.768737	-3.013047
C	-2.285579	-1.525968	0.696246
C	-2.631788	-2.174468	-0.655982
C	-3.552765	-1.337648	1.548832
H	5.145381	0.562605	0.125425
H	5.301962	2.230068	-1.737710
H	3.205727	3.051875	-2.830030
H	2.598618	-3.384258	0.908479
H	-0.164761	-2.364579	2.753549
H	-1.340230	4.061534	-0.764079
H	-3.000976	1.102420	-1.644013
H	0.945217	-5.064665	0.020344
H	0.354194	-4.322541	1.529213
H	-0.316123	-3.805837	-0.042564
H	1.271073	-2.504462	-1.739672
H	2.946660	-2.150323	-1.261854
H	2.448989	-3.842411	-1.564097
H	1.408575	-2.608908	4.682892
H	2.105292	-3.376277	3.234364
H	2.698107	-1.781000	3.777778
H	1.085660	0.348392	3.541674
H	-0.554280	0.076881	2.875315
H	-0.111235	-0.567602	4.491864
H	-2.617565	3.673856	1.458779
H	-3.355267	2.862699	0.052390
H	-2.383218	1.905604	1.197900
H	0.208450	2.621036	1.487495
H	0.936588	3.709809	0.283968
H	-0.232356	4.359157	1.472405
H	-1.176145	0.717359	-4.113212
H	-1.538428	-0.541047	-2.895859
H	-2.841392	0.127276	-3.916146
H	-3.540602	2.542761	-3.687024
H	-3.036027	3.535373	-2.297888
H	-1.891759	3.213107	-3.632316
H	-1.623007	-2.249081	1.239634
H	-1.718684	-2.282986	-1.269891
H	-3.089752	-3.174638	-0.529618
H	-3.341465	-1.535405	-1.213443
H	-4.256447	-0.658077	1.033616
H	-4.065989	-2.300087	1.732090
H	-3.297072	-0.887539	2.524154
H	3.726260	-1.248093	1.260436
H	2.880585	0.040817	2.141865
H	0.650190	3.420390	-2.411100
H	0.493068	1.893778	-3.306705

Ni	0.082332	0.081280	-0.089770
O	-1.662323	-0.279089	0.539431
P	1.234101	-1.381322	1.046398
P	-0.740723	1.733552	-1.204225

MeOH

6

C	-0.123381	0.000000	0.342586
H	0.385161	0.902579	0.737956
H	0.385161	-0.902578	0.737956
H	-1.163023	-0.000000	0.704732
O	-0.197731	-0.000000	-1.085762
H	0.713812	-0.000000	-1.437468

EtOH

9

C	-0.378522	-0.000001	0.951479
H	-1.023523	-0.893884	1.002988
H	-1.023526	0.893880	1.002988
H	0.290290	0.000001	1.829960
C	0.432708	0.000001	-0.334730
H	1.086259	-0.897171	-0.374657
H	1.086256	0.897174	-0.374657
O	-0.491884	-0.000000	-1.435685
H	0.021941	-0.000001	-2.267687

nBuOH

15

C	-0.385571	0.000000	2.190645
H	-1.037398	0.891103	2.244327
H	0.256419	0.000000	3.089202
H	-1.037398	-0.891103	2.244327
C	0.449291	0.000000	0.903561
H	1.115705	0.885605	0.898365
H	1.115705	-0.885605	0.898365
C	-0.412863	0.000000	-0.366833
H	-1.075031	0.887418	-0.375699
H	-1.075031	-0.887418	-0.375699
C	0.413024	0.000000	-1.648190
H	1.068230	0.897466	-1.676825
H	1.068230	-0.897466	-1.676825
O	-0.494874	0.000000	-2.762367
H	0.031562	0.000000	-3.586354

iPrOH

15

C	0.032236	0.301543	-0.342945
H	0.026043	0.350083	-1.454547
C	1.359283	-0.295361	0.115350
H	2.201956	0.331703	-0.221160
H	1.491232	-1.310916	-0.296298
H	1.390877	-0.355080	1.217769
C	-1.173977	-0.518319	0.126110
H	-1.141012	-1.542278	-0.287945
H	-2.125332	-0.059739	-0.203099
H	-1.187159	-0.585725	1.228506
O	-0.008157	1.643868	0.186913
H	-0.865990	2.040223	-0.068653

5.3 Hydroxde / Alcohol Exchange (PBE/6-31G*/CPCM)

[(^{iPr}PCP)Ni-OH]

60

C	0.229949	1.023179	-1.049540
C	1.273602	0.874366	-2.017899
C	1.496690	1.824240	-3.028901
C	0.681583	2.960852	-3.129809
C	-0.358394	3.139283	-2.205850
C	-0.576970	2.197743	-1.185509
C	-1.696808	2.397211	-0.183846
C	2.139398	-0.364128	-1.925723
C	3.349964	-0.269023	0.771716
C	3.435245	-0.897678	2.170599
C	3.236207	1.261677	0.851633
C	2.183081	-2.821982	-0.243514
C	0.976717	-3.490647	-0.924198
C	3.519297	-3.215197	-0.891004
C	-3.403170	-0.016316	-0.456762
C	-3.007542	-0.197310	-1.930374
C	-3.855649	-1.351468	0.159442
C	-2.638597	0.937322	2.259267
C	-1.543287	1.545510	3.150266
C	-3.942386	1.748143	2.316516
H	2.312232	1.668417	-3.746081
H	0.853194	3.698354	-3.921402
H	-1.007240	4.021454	-2.272971
H	4.262226	-0.529932	0.199149

H	2.196573	-3.151652	0.814954
H	-4.228911	0.719291	-0.395540
H	-2.823116	-0.093560	2.614066
H	3.645840	-1.979615	2.130451
H	4.247304	-0.420218	2.747790
H	2.494162	-0.752803	2.731480
H	3.184752	1.730106	-0.144842
H	2.322893	1.553163	1.399346
H	4.110421	1.674551	1.387181
H	0.876211	-3.172295	-1.977567
H	1.092688	-4.589416	-0.915828
H	0.045871	-3.223657	-0.396070
H	3.569488	-2.875937	-1.940386
H	4.384371	-2.789450	-0.354976
H	3.633608	-4.314438	-0.890869
H	-3.876996	-0.565057	-2.505285
H	-2.195656	-0.939496	-2.023875
H	-2.658288	0.739536	-2.394601
H	-2.999832	-2.041166	0.267669
H	-4.607387	-1.830843	-0.493227
H	-4.311790	-1.221773	1.155547
H	-0.624748	0.937033	3.110186
H	-1.890585	1.586470	4.198604
H	-1.293439	2.577829	2.845841
H	-3.797670	2.759438	1.896131
H	-4.765426	1.264733	1.763022
H	-4.269706	1.867299	3.365681
H	-2.602159	2.849341	-0.630095
H	-1.381447	3.062078	0.644035
H	3.199691	-0.177529	-2.178933
H	1.780400	-1.155498	-2.612260
Ni	-0.064514	-0.254811	0.306119
O	-0.481010	-1.508620	1.620551
P	-1.979801	0.704914	0.525444
P	1.898449	-0.969296	-0.187717
H	0.250418	-2.142724	1.752766

[(^{iPr}PCP)Ni-OMe]

63

C	-1.269524	-0.533860	-0.982006
C	-2.389169	-1.215712	-0.404999
C	-3.497862	-1.619011	-1.168339
C	-3.536237	-1.385043	-2.549575
C	-2.449109	-0.746455	-3.159678
C	-1.341592	-0.330873	-2.399603
C	-2.353183	-1.521779	1.075729
C	-0.187474	0.366499	-3.092602
C	-0.348303	-1.409672	3.234200
C	0.397847	-2.641358	2.695565

C	-1.405687	-1.788934	4.281442
C	-1.991173	1.000388	2.536698
C	-1.048769	1.946188	3.300041
C	-2.756429	1.741777	1.429215
C	2.425645	-0.791105	-2.339179
C	1.834292	-2.205452	-2.222493
C	3.715515	-0.658745	-1.515152
C	1.957447	2.146540	-2.028658
C	0.953967	3.250619	-1.657702
C	2.565469	2.356169	-3.423458
C	2.265213	0.688157	2.012452
H	-4.336433	-2.126707	-0.675278
H	-4.401151	-1.700379	-3.143444
H	-2.459641	-0.561766	-4.241259
H	0.397708	-0.742426	3.703068
H	-2.721992	0.560846	3.242929
H	2.645542	-0.583014	-3.405387
H	2.753674	2.145506	-1.262702
H	1.161113	-2.358026	1.950388
H	-0.291329	-3.357606	2.214059
H	0.902633	-3.173751	3.521573
H	-0.937200	-2.369906	5.096943
H	-1.880774	-0.902370	4.735253
H	-2.202945	-2.417414	3.845713
H	-0.247709	2.319216	2.637357
H	-0.572834	1.453224	4.165028
H	-1.614995	2.815746	3.680118
H	-2.060118	2.120690	0.660335
H	-3.486758	1.091590	0.919784
H	-3.300836	2.600902	1.861210
H	2.547434	-2.946937	-2.626071
H	0.880934	-2.312765	-2.767075
H	1.639987	-2.454549	-1.164452
H	3.504824	-0.761408	-0.436691
H	4.215864	0.312302	-1.669195
H	4.426202	-1.454380	-1.803552
H	0.092978	3.271065	-2.349563
H	1.445104	4.239242	-1.712054
H	0.578836	3.104494	-0.631350
H	3.373729	1.637111	-3.639669
H	2.992442	3.372808	-3.500394
H	1.800672	2.255895	-4.214688
H	3.107013	1.393591	2.198623
H	1.636975	0.702938	2.936141
H	2.720776	-0.329611	1.957132
H	-2.062524	-2.574937	1.252142
H	-3.331125	-1.372533	1.569424
H	0.143342	-0.169070	-4.002091
H	-0.463335	1.389800	-3.412597
Ni	0.169876	0.115006	0.061444
O	1.581185	1.069780	0.854924

P	-1.034695	-0.427928	1.786226
P	1.146668	0.477393	-1.814200

[(^{iPr}PCP)Ni-OEt]

66

C	-0.667279	0.372477	-1.691232
C	-1.979739	0.878736	-1.962786
C	-2.431552	1.120340	-3.271564
C	-1.600314	0.867845	-4.371368
C	-0.317078	0.349731	-4.149038
C	0.134563	0.096470	-2.842549
C	1.496773	-0.516222	-2.619349
C	-2.898152	1.132255	-0.784656
C	-2.958057	-1.478684	0.633920
C	-2.445329	-2.307042	1.823918
C	-2.746196	-2.222834	-0.693962
C	-2.602830	1.039839	2.191861
C	-4.116311	1.021462	2.454501
C	-2.022707	2.464235	2.219950
C	3.060467	-1.545904	-0.341722
C	2.229956	-2.834327	-0.211587
C	4.262417	-1.736602	-1.279245
C	3.010261	1.392163	-0.979814
C	3.568457	1.793871	0.392325
C	2.207987	2.542923	-1.609822
C	1.449943	-0.407995	2.567672
C	1.412348	-0.037655	4.055287
H	-3.445709	1.508523	-3.429288
H	-1.952462	1.062677	-5.390211
H	0.340248	0.129315	-4.999502
H	-4.040710	-1.284139	0.762186
H	-2.080467	0.457928	2.972943
H	3.431159	-1.276245	0.664050
H	3.847985	1.130659	-1.655571
H	-2.913776	-3.307708	1.816522
H	-2.673609	-1.835478	2.794637
H	-1.350509	-2.439107	1.762846
H	-1.670084	-2.393434	-0.874235
H	-3.139203	-1.659561	-1.556426
H	-3.256788	-3.202128	-0.657448
H	-4.338841	1.542216	3.403721
H	-4.513755	-0.004663	2.535767
H	-4.674085	1.539363	1.653492
H	-2.460729	3.104467	1.433029
H	-0.929161	2.436051	2.087399
H	-2.246106	2.939358	3.192459
H	1.825507	-3.155609	-1.187559
H	1.378258	-2.701983	0.477783
H	2.860436	-3.656269	0.172730

H	4.888554	-2.576800	-0.926549
H	4.904674	-0.840906	-1.323885
H	3.937475	-1.975643	-2.307076
H	4.169715	2.716390	0.299314
H	4.215453	1.013419	0.827415
H	2.745872	1.992574	1.101544
H	1.329060	2.790085	-0.988504
H	1.837021	2.294054	-2.617566
H	2.843190	3.443896	-1.687712
H	2.440556	-0.097577	2.156470
H	1.422670	-1.521512	2.485746
H	1.471297	1.058126	4.179229
H	2.254642	-0.497197	4.604493
H	0.468231	-0.381110	4.514389
H	2.260651	-0.149430	-3.329731
H	1.455318	-1.616763	-2.734101
H	-3.944614	0.837604	-0.985129
H	-2.914394	2.202163	-0.500168
Ni	-0.026613	0.131539	0.073730
O	0.380632	0.201250	1.897957
P	-2.109577	0.192120	0.601950
P	1.924960	-0.135593	-0.851878

[(^{iPr}PCP)Ni-OiPr]

69

C	1.751231	0.810838	-0.592013
C	2.964728	0.422888	0.057039
C	4.220005	0.916075	-0.336923
C	4.322393	1.841381	-1.384892
C	3.152954	2.284142	-2.017001
C	1.896517	1.784468	-1.631894
C	2.847794	-0.505636	1.239596
C	0.642726	2.297422	-2.306153
C	1.739535	-3.029297	0.279867
C	0.646521	-4.100041	0.396622
C	2.147061	-2.801995	-1.184812
C	0.695969	-1.767364	2.799600
C	1.801935	-2.412234	3.649628
C	0.143788	-0.476929	3.427047
C	-1.137798	3.232657	-0.124456
C	-2.423149	2.990277	0.684418
C	0.052278	3.535790	0.799301
C	-2.217635	1.494195	-2.307316
C	-1.943772	0.350288	-3.295664
C	-2.657094	2.775584	-3.032787
C	-2.281011	-1.559082	0.701897
C	-2.698225	-2.305518	-0.578521
C	-3.505382	-1.317613	1.601920
H	5.122560	0.578945	0.187962

H	5.300650	2.225197	-1.694263
H	3.214187	3.027076	-2.822010
H	2.628377	-3.357234	0.853969
H	-0.139826	-2.485246	2.708453
H	-1.285734	4.087744	-0.812847
H	-3.011794	1.163753	-1.612616
H	0.986014	-5.031924	-0.090574
H	0.401721	-4.341207	1.445216
H	-0.281135	-3.777218	-0.105982
H	1.286065	-2.431447	-1.769895
H	2.955590	-2.058743	-1.282112
H	2.490498	-3.751398	-1.634788
H	1.414967	-2.638966	4.660016
H	2.171037	-3.356883	3.214246
H	2.664098	-1.734074	3.771878
H	0.932546	0.291395	3.529614
H	-0.658353	-0.062416	2.793438
H	-0.256833	-0.680045	4.436787
H	-2.577008	3.821435	1.396352
H	-3.317345	2.930718	0.040372
H	-2.353134	2.046596	1.251753
H	0.235531	2.682810	1.475820
H	0.983801	3.718818	0.239190
H	-0.165670	4.428804	1.412940
H	-1.144530	0.609632	-4.013346
H	-1.651030	-0.573298	-2.770105
H	-2.854720	0.137426	-3.883990
H	-3.507885	2.552306	-3.702407
H	-2.980098	3.569918	-2.339208
H	-1.841520	3.180060	-3.659300
H	-1.587285	-2.238451	1.256490
H	-1.821807	-2.483495	-1.227450
H	-3.162305	-3.283781	-0.351217
H	-3.426872	-1.702130	-1.151009
H	-4.227120	-0.660543	1.083008
H	-4.017211	-2.262977	1.858588
H	-3.203251	-0.818857	2.539041
H	3.700276	-1.201693	1.344581
H	2.789012	0.075889	2.180900
H	0.656831	3.392561	-2.458617
H	0.493427	1.836748	-3.301071
Ni	0.075022	0.073774	-0.102892
O	-1.682978	-0.318379	0.423019
P	1.224279	-1.386914	1.036693
P	-0.732414	1.745416	-1.199131

[(^{iPr}PCP)Ni-OCH_2CH_2OMe]

70

C	-0.674792	-1.950128	-0.946286

C	0.269748	-2.799717	-1.603744
C	-0.105084	-4.014745	-2.201931
C	-1.443956	-4.429240	-2.194458
C	-2.406280	-3.609762	-1.589004
C	-2.034515	-2.398629	-0.980240
C	1.705404	-2.334879	-1.675276
C	-3.088845	-1.519153	-0.341871
C	2.668089	-1.948896	1.076711
C	1.739509	-3.078345	1.552951
C	2.985511	-0.976655	2.224192
C	3.198981	0.122751	-1.031814
C	4.493427	-0.589394	-1.452491
C	2.598910	0.944113	-2.186077
C	-2.738129	1.146564	-1.647190
C	-2.243586	0.470492	-2.935555
C	-2.185335	2.574500	-1.512306
C	-3.052021	0.954921	1.320975
C	-2.690454	0.176951	2.597284
C	-4.567616	1.155237	1.170028
C	1.106390	2.027727	1.074015
C	0.840276	3.116216	2.120929
O	1.906937	4.060132	2.080404
C	1.727071	5.097583	3.028222
H	0.658953	-4.635570	-2.686422
H	-1.735531	-5.375381	-2.663273
H	-3.460838	-3.912411	-1.586508
H	3.608322	-2.398716	0.701579
H	3.426763	0.815351	-0.201010
H	-3.844240	1.185741	-1.667742
H	-2.547955	1.936889	1.379196
H	2.223622	-3.630355	2.378948
H	1.502042	-3.797458	0.752149
H	0.784091	-2.670252	1.926719
H	2.069226	-0.449223	2.543500
H	3.735503	-0.219174	1.938617
H	3.381703	-1.534489	3.092017
H	4.309021	-1.315323	-2.263352
H	4.968132	-1.125516	-0.614226
H	5.222791	0.149894	-1.831249
H	3.346291	1.662740	-2.568003
H	1.710822	1.511460	-1.859322
H	2.295918	0.300128	-3.031376
H	-2.511188	1.089597	-3.811189
H	-2.682237	-0.531305	-3.075959
H	-1.146227	0.349345	-2.911635
H	-1.087143	2.565570	-1.393552
H	-2.613814	3.109722	-0.648080
H	-2.424997	3.156300	-2.420680
H	-3.111881	0.690516	3.480592
H	-1.595989	0.119391	2.712132
H	-3.102702	-0.848283	2.585506

H	-5.093259	0.189831	1.057362
H	-4.827901	1.786675	0.303414
H	-4.972368	1.648299	2.072956
H	1.205318	2.535589	0.085360
H	2.108072	1.586449	1.298670
H	-0.134166	3.610893	1.907259
H	0.760331	2.653782	3.130288
H	0.797954	5.677735	2.837316
H	2.593284	5.773859	2.942639
H	1.677378	4.705532	4.067056
H	1.914921	-1.860203	-2.653700
H	2.434124	-3.157945	-1.559047
H	-3.350777	-1.871610	0.674345
H	-4.030253	-1.489721	-0.922105
Ni	-0.164588	-0.367504	-0.048267
O	0.069113	1.093041	1.114141
P	-2.256208	0.123260	-0.152084
P	1.880931	-1.034796	-0.360446

[(^{iPr}PCP)Pd-OH]

60

C	0.243163	1.055911	-1.083381
C	1.335387	0.921833	-1.989629
C	1.568661	1.889666	-2.984627
C	0.716526	2.994715	-3.117534
C	-0.373641	3.136282	-2.247782
C	-0.610716	2.186863	-1.235086
C	-1.779107	2.374519	-0.281514
C	2.235280	-0.296475	-1.896122
C	3.462503	-0.334621	0.815336
C	3.545410	-1.015895	2.190735
C	3.307957	1.188806	0.959318
C	2.376696	-2.874174	-0.350806
C	1.132640	-3.565323	-0.936774
C	3.661114	-3.203907	-1.125942
C	-3.556258	-0.021318	-0.408452
C	-3.148297	-0.288595	-1.866874
C	-4.018966	-1.315603	0.282954
C	-2.781286	1.088611	2.258710
C	-1.662048	1.663229	3.143806
C	-4.043732	1.964434	2.276662
H	2.419308	1.770868	-3.667088
H	0.899622	3.741141	-3.898010
H	-1.046361	3.996796	-2.350201
H	4.389406	-0.547718	0.245846
H	2.491116	-3.222637	0.694444
H	-4.376192	0.723642	-0.397510
H	-3.027930	0.082747	2.648776
H	3.809526	-2.083875	2.114558

H	4.320505	-0.524146	2.805374
H	2.584223	-0.937525	2.730560
H	3.281918	1.704576	-0.015080
H	2.372902	1.436801	1.492346
H	4.157420	1.594003	1.538777
H	0.932620	-3.231412	-1.971363
H	1.283753	-4.659745	-0.962357
H	0.242201	-3.338557	-0.323816
H	3.583581	-2.888337	-2.181226
H	4.550435	-2.719131	-0.688521
H	3.836961	-4.294880	-1.119364
H	-4.013862	-0.688666	-2.425501
H	-2.333559	-1.032588	-1.912623
H	-2.799683	0.621457	-2.383852
H	-3.166174	-2.000674	0.438632
H	-4.768289	-1.830062	-0.345340
H	-4.482491	-1.123205	1.265473
H	-0.782413	0.997283	3.152925
H	-2.027510	1.775267	4.180580
H	-1.337697	2.661951	2.799333
H	-3.841295	2.970105	1.866699
H	-4.873690	1.520681	1.700611
H	-4.393368	2.097003	3.316885
H	-2.671414	2.783822	-0.790836
H	-1.516353	3.092066	0.521154
H	3.290603	-0.066441	-2.133990
H	1.911088	-1.072757	-2.617235
Pd	-0.100268	-0.355136	0.355852
O	-0.561094	-1.818553	1.768558
P	-2.126903	0.733886	0.539874
P	2.041083	-1.034646	-0.192685
H	0.236989	-2.382365	1.796343

[(^{iPr}PCP)Pd-OMe]

63

C	-1.285877	-0.568948	-1.013173
C	-2.401009	-1.221043	-0.410613
C	-3.491219	-1.656281	-1.187722
C	-3.494804	-1.475963	-2.576856
C	-2.403570	-0.849436	-3.191881
C	-1.312188	-0.391509	-2.428649
C	-2.406057	-1.481909	1.082838
C	-0.175343	0.328390	-3.134102
C	-0.476389	-1.425416	3.346353
C	0.258507	-2.675988	2.835076
C	-1.564846	-1.771040	4.373462
C	-2.065941	1.010771	2.633958
C	-1.137482	1.942497	3.432170
C	-2.814459	1.788899	1.539951

C	2.536065	-0.755383	-2.520291
C	1.979913	-2.179450	-2.348921
C	3.847551	-0.564096	-1.739801
C	2.016095	2.181958	-2.226246
C	1.070662	3.263226	-1.677829
C	2.431570	2.438841	-3.682271
C	2.402689	0.568871	2.273266
H	-4.341796	-2.147373	-0.698649
H	-4.343959	-1.821121	-3.176632
H	-2.400899	-0.703616	-4.279265
H	0.272682	-0.765229	3.820194
H	-2.809180	0.557212	3.318040
H	2.709785	-0.567844	-3.598646
H	2.913685	2.164951	-1.580308
H	1.024239	-2.415971	2.083497
H	-0.437767	-3.397488	2.372187
H	0.756593	-3.191376	3.675558
H	-1.128161	-2.366039	5.196370
H	-2.019774	-0.870672	4.819640
H	-2.373156	-2.374680	3.922747
H	-0.329278	2.331087	2.786831
H	-0.671963	1.437886	4.295747
H	-1.713022	2.803603	3.817472
H	-2.101148	2.283115	0.858862
H	-3.469096	1.142359	0.932212
H	-3.440122	2.570710	2.007120
H	2.700248	-2.912753	-2.754463
H	1.017124	-2.323009	-2.869050
H	1.819231	-2.407056	-1.280656
H	3.649627	-0.524865	-0.654072
H	4.362516	0.369467	-2.022675
H	4.533862	-1.404570	-1.947124
H	0.118758	3.296657	-2.238052
H	1.543873	4.257832	-1.765862
H	0.843671	3.071159	-0.615321
H	3.167418	1.700426	-4.043518
H	2.889379	3.440486	-3.774492
H	1.558176	2.409785	-4.357468
H	3.394319	1.021101	2.516184
H	1.713618	0.892576	3.095603
H	2.533159	-0.535008	2.391953
H	-2.144190	-2.537501	1.288696
H	-3.400455	-1.311401	1.535343
H	0.128156	-0.186148	-4.064619
H	-0.491088	1.347816	-3.431174
Pd	0.294012	0.117766	0.107328
O	2.001753	0.964255	0.997996
P	-1.101433	-0.418167	1.887255
P	1.256737	0.494649	-1.953505

[(^{iPr}PCP)Pd-OEt]

66

C	-0.699436	0.282734	-1.770278
C	-2.026695	0.738608	-2.023761
C	-2.486856	0.918557	-3.342244
C	-1.643984	0.669128	-4.433514
C	-0.334173	0.227383	-4.205704
C	0.135906	0.025661	-2.893688
C	1.539445	-0.498885	-2.671901
C	-2.948877	1.053155	-0.859914
C	-3.230912	-1.420249	0.795150
C	-2.929242	-2.102240	2.140398
C	-2.875507	-2.334820	-0.388731
C	-2.729662	1.228136	2.139734
C	-4.233170	1.515031	2.254065
C	-1.872933	2.503920	2.140205
C	3.332764	-1.422214	-0.480252
C	2.682873	-2.815789	-0.415086
C	4.549736	-1.405802	-1.418180
C	2.991605	1.493983	-1.039330
C	3.582833	1.898289	0.319400
C	2.093587	2.605767	-1.604730
C	1.525735	-0.681018	2.729405
C	1.430426	-0.786100	4.259120
H	-3.514347	1.262750	-3.514129
H	-2.007214	0.817015	-5.456266
H	0.330672	0.027537	-5.055230
H	-4.307930	-1.166522	0.742498
H	-2.399339	0.605716	2.992381
H	3.658031	-1.152956	0.542294
H	3.813856	1.307239	-1.758102
H	-3.407906	-3.097828	2.170968
H	-3.310583	-1.521600	2.997685
H	-1.841923	-2.234740	2.278680
H	-1.793075	-2.553952	-0.386682
H	-3.119503	-1.876679	-1.361985
H	-3.430517	-3.286771	-0.306560
H	-4.438857	2.101499	3.167812
H	-4.830025	0.589221	2.310071
H	-4.594455	2.103882	1.392093
H	-2.105082	3.155233	1.277197
H	-0.802779	2.238737	2.105975
H	-2.066375	3.088788	3.057970
H	2.350801	-3.156362	-1.412033
H	1.809362	-2.826760	0.259150
H	3.417205	-3.552319	-0.042704
H	5.250406	-2.213101	-1.137190
H	5.104127	-0.453615	-1.372077
H	4.249339	-1.577521	-2.466990
H	4.149863	2.841003	0.214452

H	4.268647	1.137033	0.728153
H	2.779215	2.066934	1.057973
H	1.244054	2.805831	-0.928312
H	1.677671	2.346710	-2.592337
H	2.678951	3.537367	-1.710251
H	2.390325	-0.008388	2.491146
H	1.816487	-1.688043	2.336644
H	1.189537	0.200132	4.694803
H	2.380704	-1.140043	4.701145
H	0.628032	-1.488957	4.546492
H	2.265732	-0.090666	-3.399174
H	1.559887	-1.599796	-2.789258
H	-4.001216	0.787504	-1.069922
H	-2.935974	2.138023	-0.635211
Pd	-0.034798	-0.009223	0.152313
O	0.314547	-0.220983	2.207269
P	-2.279234	0.191036	0.649921
P	2.040221	-0.125597	-0.910833

[(^{iPr}PCP)Pd-OiPr]

69

C	1.798586	0.809032	-0.644401
C	2.998731	0.370081	-0.015651
C	4.253209	0.836597	-0.450702
C	4.341375	1.773713	-1.489405
C	3.169413	2.263953	-2.079744
C	1.906518	1.795645	-1.667126
C	2.906006	-0.551733	1.182934
C	0.651724	2.359643	-2.308360
C	1.781573	-3.136599	0.391511
C	0.681291	-4.198414	0.536205
C	2.196332	-2.959124	-1.078392
C	0.831125	-1.821336	2.912833
C	1.994076	-2.372386	3.753188
C	0.201013	-0.558061	3.522945
C	-1.172590	3.371442	-0.166623
C	-2.473638	3.144673	0.623677
C	0.009871	3.639121	0.778387
C	-2.275987	1.692323	-2.387696
C	-2.050270	0.532371	-3.370687
C	-2.643865	2.992908	-3.121161
C	-2.435113	-1.646757	0.760244
C	-2.629423	-2.303838	-0.620175
C	-3.760621	-1.645306	1.546044
H	5.166627	0.473552	0.036550
H	5.319769	2.133184	-1.826146
H	3.234575	3.019701	-2.872266
H	2.669038	-3.454184	0.974448
H	0.042737	-2.593935	2.845620

H	-1.290980	4.237326	-0.847035
H	-3.097141	1.407079	-1.703189
H	1.020310	-5.145194	0.078244
H	0.431031	-4.408176	1.589966
H	-0.243740	-3.887900	0.020645
H	1.343177	-2.602393	-1.681626
H	3.017834	-2.233090	-1.198213
H	2.529962	-3.928088	-1.492378
H	1.638952	-2.612727	4.771838
H	2.427248	-3.292760	3.325030
H	2.804991	-1.629954	3.854681
H	0.925609	0.276183	3.558809
H	-0.667646	-0.235032	2.923092
H	-0.125538	-0.760124	4.559448
H	-2.611523	3.962532	1.353921
H	-3.362147	3.127490	-0.030753
H	-2.435551	2.185578	1.169913
H	0.146792	2.789566	1.470248
H	0.959354	3.785987	0.237085
H	-0.190153	4.547078	1.375929
H	-1.238221	0.756064	-4.085715
H	-1.800466	-0.403429	-2.845009
H	-2.968567	0.361397	-3.960771
H	-3.492823	2.805727	-3.803549
H	-2.942662	3.800043	-2.431832
H	-1.800313	3.359059	-3.733533
H	-1.719296	-2.300430	1.328397
H	-1.678606	-2.264798	-1.183211
H	-2.955690	-3.358558	-0.540817
H	-3.390754	-1.749273	-1.200691
H	-4.517966	-1.047456	1.006044
H	-4.157727	-2.668364	1.681901
H	-3.614551	-1.190827	2.541438
H	3.767357	-1.239802	1.268249
H	2.886746	0.050556	2.113148
H	0.708312	3.456130	-2.441719
H	0.490004	1.930821	-3.316119
Pd	-0.020921	0.080909	-0.040675
O	-1.967487	-0.331942	0.664634
P	1.283381	-1.473979	1.122525
P	-0.802673	1.878505	-1.244399

[(^{iPr}PCP)Pd-OCH$_2$CH$_2$OMe]

70

C	-0.695509	-1.991873	-1.058401
C	0.275467	-2.830363	-1.676585
C	-0.108488	-4.012185	-2.338617
C	-1.457811	-4.380085	-2.415344
C	-2.430048	-3.566183	-1.818502

C	-2.063025	-2.389274	-1.138871
C	1.736959	-2.429986	-1.651551
C	-3.134566	-1.552217	-0.463327
C	2.715567	-2.031677	1.138693
C	1.726186	-3.084633	1.664450
C	3.079362	-1.021187	2.241230
C	3.349304	-0.015705	-0.990482
C	4.636350	-0.759093	-1.376066
C	2.792561	0.822689	-2.153899
C	-2.930737	1.208928	-1.621707
C	-2.371475	0.599764	-2.918009
C	-2.435681	2.651941	-1.425603
C	-3.325456	0.851743	1.330703
C	-2.743389	0.237666	2.614836
C	-4.852805	0.713870	1.241676
C	1.150988	2.277550	1.062426
C	1.005453	3.380077	2.120891
O	2.112361	4.276068	2.034819
C	2.008631	5.322479	2.983129
H	0.658067	-4.644278	-2.803893
H	-1.751052	-5.297272	-2.937408
H	-3.488159	-3.850342	-1.874059
H	3.631557	-2.546507	0.787654
H	3.563041	0.670255	-0.148283
H	-4.037320	1.205240	-1.668496
H	-3.054826	1.923971	1.319135
H	2.181077	-3.626833	2.513059
H	1.447076	-3.825324	0.896483
H	0.799936	-2.601233	2.020970
H	2.199490	-0.410383	2.512677
H	3.888572	-0.336041	1.936360
H	3.417682	-1.558898	3.145388
H	4.456031	-1.473856	-2.198003
H	5.069726	-1.313823	-0.527525
H	5.397367	-0.038109	-1.726211
H	3.543554	1.562918	-2.483120
H	1.876421	1.359433	-1.853508
H	2.543885	0.191352	-3.026111
H	-2.632487	1.242797	-3.777945
H	-2.768741	-0.410356	-3.110686
H	-1.271612	0.517987	-2.857320
H	-1.345409	2.675996	-1.250742
H	-2.925404	3.152000	-0.573531
H	-2.653386	3.245064	-2.332042
H	-3.236096	0.680768	3.499530
H	-1.659727	0.434849	2.670419
H	-2.908838	-0.854351	2.655584
H	-5.161070	-0.346837	1.246575
H	-5.269191	1.185290	0.334940
H	-5.323985	1.197906	2.116287
H	1.223513	2.781196	0.065189

H	2.144318	1.787120	1.229447
H	0.047443	3.924171	1.959912
H	0.954790	2.915101	3.131184
H	1.096945	5.938523	2.822212
H	2.897480	5.963829	2.865185
H	1.978885	4.936228	4.025168
H	2.027501	-1.973086	-2.618419
H	2.407913	-3.296446	-1.503518
H	-3.376672	-1.971324	0.533583
H	-4.080641	-1.533398	-1.035614
Pd	-0.166755	-0.289966	-0.049182
O	0.066566	1.410847	1.175448
P	-2.433780	0.146935	-0.156151
P	1.986114	-1.129430	-0.336512

H2O

3

H	0.000000	0.761519	0.204154
O	0.000000	0.000000	-0.408307
H	0.000000	-0.761519	0.204154

MeOH

6

C	-0.124340	0.000000	0.332273
H	0.386517	0.898933	0.736088
H	0.386517	-0.898933	0.736089
H	-1.160175	-0.000000	0.708467
O	-0.204332	-0.000000	-1.091408
H	0.715813	-0.000000	-1.421510

EtOH

9

C	-0.378374	-0.000001	0.949927
H	-1.023202	-0.893625	1.003878
H	-1.023206	0.893622	1.003878
H	0.292899	0.000001	1.825236
C	0.425751	0.000001	-0.341795
H	1.086260	-0.893587	-0.375036
H	1.086258	0.893590	-0.375036
O	-0.499505	-0.000000	-1.435219
H	0.033119	-0.000000	-2.255833

iPrOH

12

C	0.032908	0.306937	-0.341663

H	0.025863	0.347106	-1.454172
C	1.359028	-0.294268	0.115823
H	2.203611	0.332541	-0.215906
H	1.490354	-1.307787	-0.298821
H	1.386887	-0.359496	1.217839
C	-1.171609	-0.515705	0.126797
H	-1.145552	-1.536784	-0.292764
H	-2.120018	-0.046735	-0.193690
H	-1.178034	-0.589108	1.228539
O	-0.011599	1.642727	0.191993
H	-0.871840	2.020572	-0.083975

$HOCH_2CH_2OMe$

13

C	0.213674	0.592935	0.176230
H	0.140153	0.539041	1.283997
H	-0.129911	1.600659	-0.145545
C	1.648650	0.333204	-0.262462
H	2.321562	1.081345	0.190164
H	1.713563	0.437726	-1.367333
O	2.092351	-0.951395	0.168917
H	1.372585	-1.560036	-0.105885
O	-0.580313	-0.432834	-0.420959
C	-1.925278	-0.407448	0.035628
H	-1.988313	-0.546501	1.135172
H	-2.452743	-1.235336	-0.463910
H	-2.425979	0.548638	-0.224014

[(^{iPr}PCP)Ni]

58

C	0.217974	0.990875	-1.035037
C	1.308279	0.871238	-1.945663
C	1.542645	1.841722	-2.935320
C	0.683913	2.946462	-3.056939
C	-0.408717	3.082366	-2.185400
C	-0.636130	2.121645	-1.183702
C	-1.791406	2.257086	-0.206541
C	2.191218	-0.357465	-1.818284
C	3.343985	-0.402256	0.878765
C	3.443403	-1.076768	2.254579
C	3.231051	1.125252	1.012657
C	2.211317	-2.906897	-0.282093
C	1.055960	-3.544847	-1.069430
C	3.580750	-3.257252	-0.880837
C	-3.453578	-0.170122	-0.313931
C	-3.063237	-0.419889	-1.779232
C	-3.926146	-1.465711	0.362120

C	-2.679822	0.989890	2.323279
C	-1.547561	1.578317	3.180588
C	-3.924740	1.889185	2.324744
H	2.392377	1.732372	-3.621407
H	0.864749	3.699503	-3.832275
H	-1.080879	3.944821	-2.281146
H	4.254326	-0.638556	0.292556
H	2.163111	-3.292139	0.755116
H	-4.270449	0.577354	-0.284945
H	-2.949336	0.006393	2.754113
H	3.639721	-2.159760	2.178497
H	4.268061	-0.627072	2.836875
H	2.509967	-0.940722	2.830794
H	3.201395	1.630649	0.033135
H	2.308733	1.405005	1.553232
H	4.096094	1.518169	1.578048
H	1.038282	-3.197902	-2.117774
H	1.160861	-4.644706	-1.085408
H	0.080957	-3.293505	-0.614314
H	3.693936	-2.835811	-1.895081
H	4.414154	-2.881880	-0.262871
H	3.694904	-4.353886	-0.963126
H	-3.929407	-0.820973	-2.336750
H	-2.241502	-1.155461	-1.842483
H	-2.721694	0.497716	-2.286663
H	-3.096416	-2.192723	0.436165
H	-4.733271	-1.933066	-0.231153
H	-4.317191	-1.292802	1.379494
H	-0.676924	0.898783	3.211694
H	-1.896127	1.744598	4.215987
H	-1.201893	2.551262	2.786723
H	-3.708800	2.874206	1.874414
H	-4.768759	1.440148	1.773330
H	-4.263611	2.068027	3.362158
H	-2.722764	2.606079	-0.692148
H	-1.557742	2.992769	0.588005
H	3.261541	-0.140401	-1.996985
H	1.898916	-1.125267	-2.560449
Ni	-0.064357	-0.270717	0.307962
P	-2.004418	0.579561	0.615378
P	1.884294	-1.062894	-0.103021

[(^{iPr}PCP)Pd]

58

C	0.212629	0.958511	-1.037101
C	1.338423	0.838644	-1.889117
C	1.577116	1.817063	-2.874823
C	0.693795	2.896551	-3.029486
C	-0.429989	3.012163	-2.197346

C	-0.673204	2.052417	-1.193380
C	-1.856032	2.204153	-0.249239
C	2.253154	-0.366307	-1.755552
C	3.460452	-0.492293	0.930512
C	3.587058	-1.202976	2.286472
C	3.299643	1.025920	1.113009
C	2.496808	-2.985261	-0.399181
C	1.336094	-3.694943	-1.114809
C	3.825810	-3.163273	-1.150641
C	-3.654231	-0.143276	-0.247104
C	-3.277187	-0.439164	-1.707623
C	-4.159444	-1.409417	0.460933
C	-2.880563	1.163958	2.329978
C	-1.736573	1.689436	3.212001
C	-4.031719	2.176835	2.227689
H	2.451392	1.730416	-3.532539
H	0.881858	3.650296	-3.802231
H	-1.115966	3.859852	-2.322005
H	4.376177	-0.681148	0.335681
H	2.596301	-3.427311	0.610763
H	-4.452375	0.624895	-0.237192
H	-3.265376	0.234028	2.791399
H	3.810083	-2.278134	2.179938
H	4.404514	-0.747982	2.874675
H	2.653213	-1.105126	2.869083
H	3.256948	1.562048	0.150139
H	2.371860	1.260587	1.664796
H	4.154726	1.425313	1.689013
H	1.187711	-3.295696	-2.134507
H	1.546279	-4.775732	-1.209105
H	0.389184	-3.567637	-0.561163
H	3.767555	-2.743918	-2.170650
H	4.671547	-2.681050	-0.630942
H	4.063926	-4.238532	-1.248929
H	-4.160559	-0.820284	-2.251939
H	-2.483865	-1.205664	-1.760822
H	-2.910759	0.456711	-2.236736
H	-3.350887	-2.159538	0.534254
H	-4.992099	-1.859151	-0.110161
H	-4.526917	-1.204274	1.481120
H	-0.932988	0.939570	3.315000
H	-2.115158	1.938315	4.219933
H	-1.289454	2.607424	2.789149
H	-3.699716	3.117830	1.754344
H	-4.886239	1.785959	1.649946
H	-4.402060	2.428769	3.238669
H	-2.761942	2.559632	-0.775973
H	-1.631565	2.964872	0.525050
H	3.313785	-0.110311	-1.938967
H	1.983585	-1.131040	-2.510812
Pd	-0.125216	-0.459341	0.450133

P	-2.184390	0.591209	0.669756
P	2.024848	-1.184601	-0.073360

OH·

2

O	0.000000	0.000000	0.495777
H	0.000000	0.000000	-0.495777

MeO·

5

C	-0.040844	-0.000003	0.023440
H	0.545243	0.870546	0.416789
H	0.545225	-0.870565	0.416787
H	-1.056207	0.000007	0.478524
O	0.006556	-0.000001	-1.335539

EtO·

8

C	-0.427010	0.000000	0.675230
H	-1.072783	-0.893377	0.716602
H	-1.072783	0.893377	0.716602
H	0.226058	-0.000000	1.565172
C	0.399202	-0.000000	-0.612493
H	1.118798	-0.864633	-0.638509
H	1.118797	0.864633	-0.638509
O	-0.290279	0.000000	-1.784094

iPrO·

11

C	-0.013840	0.525752	-0.350369
H	-0.082976	0.532449	-1.466964
C	1.298430	-0.128511	0.109960
H	2.157248	0.488975	-0.202304
H	1.413741	-1.133173	-0.333603
H	1.315952	-0.218725	1.209577
C	-1.256853	-0.308226	0.134438
H	-1.160592	-1.321978	-0.287845
H	-2.191516	0.155018	-0.214815
H	-1.258413	-0.362198	1.234333
O	-0.221183	1.770617	0.167592

$MeOCH_2CH_2O$·

12

C	0.326898	0.396044	0.222855
H	0.276940	0.275978	1.327008
H	-0.007927	1.429691	-0.022842
C	1.765398	0.180876	-0.246265
H	2.393143	1.086912	-0.037030
H	1.786537	0.131546	-1.368321
O	2.386095	-0.926684	0.241206
O	-0.484325	-0.569611	-0.431614
C	-1.836917	-0.506168	-0.001234
H	-1.927637	-0.700652	1.087947
H	-2.388220	-1.282321	-0.554764
H	-2.289985	0.484388	-0.216946

[(^{iPr}PCP)Ni]+

58

C	0.222047	0.982180	-1.014953
C	1.258986	0.786535	-1.966654
C	1.469545	1.744979	-2.972828
C	0.657361	2.883584	-3.054635
C	-0.372612	3.077024	-2.124814
C	-0.595829	2.140387	-1.100629
C	-1.700993	2.327908	-0.084880
C	2.119012	-0.453144	-1.866614
C	3.373679	-0.311408	0.853013
C	3.281115	-0.745185	2.325190
C	3.413111	1.218391	0.709079
C	2.141278	-2.885406	-0.116336
C	0.906317	-3.525905	-0.775004
C	3.452344	-3.337924	-0.778517
C	-3.412691	-0.113311	-0.425887
C	-3.088053	-0.072132	-1.926841
C	-3.699230	-1.545370	0.058801
C	-2.643304	0.799267	2.333509
C	-1.510611	1.322231	3.233787
C	-3.907507	1.668668	2.429911
H	2.280471	1.590667	-3.693484
H	0.826428	3.620919	-3.845544
H	-1.018159	3.960186	-2.188170
H	4.293735	-0.734481	0.405494
H	2.155973	-3.179712	0.951033
H	-4.299919	0.520599	-0.235339
H	-2.889199	-0.232903	2.649273
H	3.320792	-1.840395	2.445203
H	4.126304	-0.316187	2.890596
H	2.348261	-0.378430	2.791508
H	3.529789	1.538908	-0.338852
H	2.491469	1.682423	1.102300

H	4.267888	1.616632	1.283107
H	0.805451	-3.225277	-1.832993
H	0.996155	-4.625588	-0.748605
H	-0.027868	-3.248903	-0.253715
H	3.490142	-3.036722	-1.839646
H	4.340561	-2.927295	-0.271033
H	3.525019	-4.439202	-0.741227
H	-3.927822	-0.512610	-2.492166
H	-2.177532	-0.651482	-2.160458
H	-2.935789	0.955532	-2.295880
H	-2.812454	-2.193504	-0.067834
H	-4.517813	-1.981805	-0.539112
H	-4.004459	-1.583030	1.118248
H	-0.607509	0.688083	3.172647
H	-1.845194	1.334119	4.285456
H	-1.220761	2.353448	2.967126
H	-3.717246	2.691217	2.059977
H	-4.753907	1.247602	1.861874
H	-4.220212	1.748274	3.486025
H	-2.598050	2.808838	-0.513225
H	-1.365512	2.958934	0.759478
H	3.168048	-0.269688	-2.158868
H	1.736091	-1.259624	-2.519810
Ni	-0.047688	-0.242077	0.307087
P	-2.025026	0.626858	0.577581
P	1.945575	-1.025694	-0.112748

[(^{iPr}PCP)Pd]+

58

C	0.222361	0.978156	-1.045783
C	1.305087	0.799175	-1.940337
C	1.509326	1.769158	-2.942020
C	0.654961	2.870962	-3.061803
C	-0.415206	3.028335	-2.173706
C	-0.645590	2.092530	-1.145409
C	-1.783919	2.294164	-0.169057
C	2.217971	-0.402691	-1.845462
C	3.504931	-0.391605	0.848123
C	3.600335	-1.037418	2.239413
C	3.381519	1.138199	0.941855
C	2.368434	-2.959853	-0.256288
C	1.208064	-3.627860	-1.014253
C	3.737428	-3.307472	-0.863823
C	-3.614004	-0.065055	-0.352533
C	-3.225250	-0.290415	-1.822381
C	-4.113305	-1.366304	0.298570
C	-2.818346	0.993769	2.348359
C	-1.685268	1.529805	3.240416
C	-4.054609	1.908701	2.366167

H	2.350601	1.645818	-3.632883
H	0.823725	3.610197	-3.850834
H	-1.088711	3.887447	-2.266286
H	4.415845	-0.639464	0.268210
H	2.339179	-3.310849	0.793792
H	-4.413333	0.699798	-0.305779
H	-3.107103	-0.005884	2.725659
H	3.788642	-2.122612	2.190374
H	4.434437	-0.578759	2.798074
H	2.676957	-0.871711	2.823392
H	3.347217	1.622211	-0.047979
H	2.472679	1.432140	1.496380
H	4.255685	1.539301	1.484298
H	1.180677	-3.320808	-2.074278
H	1.334935	-4.724058	-0.991161
H	0.228780	-3.387431	-0.563782
H	3.832382	-2.919048	-1.892784
H	4.575006	-2.911580	-0.266343
H	3.850799	-4.404733	-0.911340
H	-4.108332	-0.652057	-2.377883
H	-2.433674	-1.055449	-1.910901
H	-2.870193	0.628619	-2.317008
H	-3.302350	-2.114486	0.364405
H	-4.917565	-1.800201	-0.320380
H	-4.521665	-1.208704	1.310731
H	-0.816476	0.848238	3.259296
H	-2.052898	1.641039	4.275260
H	-1.333621	2.522280	2.908111
H	-3.824007	2.910326	1.963290
H	-4.899108	1.490528	1.793200
H	-4.393638	2.042239	3.408695
H	-2.663879	2.752300	-0.654338
H	-1.473958	2.976286	0.645768
H	3.261277	-0.148784	-2.104168
H	1.894288	-1.186482	-2.555899
Pd	-0.091732	-0.382149	0.398380
P	-2.187534	0.656359	0.617530
P	2.081750	-1.114157	-0.130866

HO(-)

2

O	0.000000	0.000000	0.494505
H	0.000000	0.000000	-0.494505

MeO(-)

5

C	-0.001200	-0.000003	-0.062320

H	0.525930	0.895693	0.472089
H	0.525911	-0.895712	0.472087
H	-1.025381	0.000007	0.500215
O	-0.025288	-0.000001	-1.382071

EtO(-)

8

C	-0.404723	0.000000	0.656258
H	-1.064151	-0.890365	0.696653
H	-1.064151	0.890365	0.696653
H	0.243435	-0.000000	1.561781
C	0.392118	0.000000	-0.694650
H	1.130841	-0.895459	-0.567638
H	1.130841	0.895459	-0.567638
O	-0.364209	0.000000	-1.781417

iPrO(-)

8

C	-0.050752	0.597914	-0.312287
H	-0.047806	0.491996	-1.475494
C	1.281633	-0.123558	0.106359
H	2.141839	0.493581	-0.216767
H	1.410823	-1.146922	-0.312267
H	1.324159	-0.189388	1.213299
C	-1.243767	-0.331509	0.117020
H	-1.212760	-1.355782	-0.316694
H	-2.196331	0.144528	-0.185165
H	-1.258645	-0.419258	1.223167
O	-0.148395	1.838399	0.158829

$MeOCH_2CH_2O(-)$

12

C	0.354106	0.349734	0.183354
H	0.279946	0.261538	1.293590
H	-0.005215	1.372201	-0.106472
C	1.836302	0.123222	-0.239859
H	2.305834	1.145705	0.091558
H	1.794765	0.277310	-1.392692
O	2.405428	-0.981778	0.202452
O	-0.501763	-0.636458	-0.419654
C	-1.833217	-0.500203	0.010815
H	-1.937099	-0.621951	1.114316
H	-2.433470	-1.284314	-0.486681
H	-2.265617	0.494994	-0.250728