Electronic Supplementary Material (ESI) for Dalton Transactions.

Electronic Supporting Information

Monomeric Alkoxide and Alkylcarbonate Complexes of Nickel and Palladium Complexes Stabilized with a^{iPr}PCP Pincer Ligand: A Model for the Catalytic Carboxylation of Alcohols to Alkyl Carbonates

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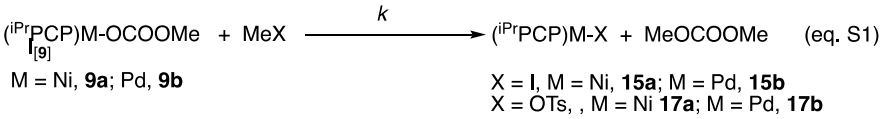
Kinetic data for the reactions of Methylcarbonate Complexes (**9a/b**) Complexes with Alkylating Agents

Table S1 collects the data corresponding to the reactions of **9a** and **9b** with MeI and MeOTs (Ec. S1). The consumption of the Ni or Pd complex is represented as the molar fraction ($f_{[9]}$), calculated from the intensities of the $^{31}P\{^1H\}$ signals of the starting ($I_{[9]}$) and product ($I_{[15]}$ or $I_{[17]}$) complexes, as shown in eq. S2. In the calculation of first-order rate constants, the molar fraction can be used directly, but for half-order rate constants, $f_{[9]}$ are to be converted into absolute concentrations multiplying by the initial concentration of the starting complex (C_0 = 0.041 M) (Eq. S3). The expressions used for the first and half-order kinetics are shown in Eqs S4 and S5.



$$f_{[9]} = \frac{I_{[9]}}{I_{[9]} + I_{[15]}} \quad or \quad \frac{I_{[9]}}{I_{[9]} + I_{[17]}} \qquad \text{(eq. S2)}$$

$$\text{at any } t,\ [\mathbf{9}] = C_0 \cdot f_{[9]} = 0.041 \cdot f_{[9]} \qquad \text{(eq. S3)}$$

$$\textit{first order kinetics}: \ ln \frac{f_{[9]\ \text{at t}=0}}{f_{[9]\ \text{at t}}} = k \cdot t \qquad \text{(eq. S4)}$$

$$\textit{half-order kinetics}: \ \sqrt{[\mathbf{9}]\ \text{at t=0}} - \sqrt{[\mathbf{9}]\ \text{at t}} = 1/2\ k \cdot t \qquad \text{(eq. S5)}$$

Table S1. Kinetic data.

MeX = Iodomethane									
M = Ni						M = Pd			
[MeI]/Ni=	10	[MeI]/Ni=	15	[MeI]/Ni=	20	[MeI]/Pd =	10	[MeI]/Pd =	20
t(s)	$f_{[9a]}$	t(s)	$f_{[9a]}$	t(s)	$f_{[9a]}$	t(s)	$f_{[9b]}$	t(s)	$f_{[9b]}$
0	0,848	0	0,958	0	0,966	0	0,663	0	1,000
1800	0,784	1800	0,681	900	0,563	1500	0,571	600	0,441
3600	0,734	3600	0,425	1800	0,367	3000	0,510	1200	0,206
5400	0,689	5400	0,206	2700	0,231	4500	0,435	2640	0,057
7200	0,649	7200	0,065	3600	0,130	6000	0,383		
9000	0,606			4500	0,057	7500	0,329		
10800	0,565			5400	0,020	9000	0,275		
12600	0,522					10500	0,248		
14400	0,471					12000	0,200		
16200	0,429					13500	0,180		
18000	0,379					15000	0,138		
19800	0,342					16500	0,115		
21600	0,301					18000	0,099		
23400	0,265					19500	0,074		
25200	0,225					21000	0,057		
27000	0,187					22500	0,048		
28800	0,160					24000	0,038		
30600	0,130					25500	0,029		
32400	0,099								
34200	0,074								
36000	0,057								
37800	0,038								
39600	0,020								
41400	0,010								
MeX = Methyl tosylate									
[MeI]/Ni=	10			[MeI]/Ni=	20	[MeI]/Pd =	10	[MeI]/Pd =	20
t(sec)	$f_{[9a]}$	t(sec)	$f_{[9a]}$	t(sec)	$f_{[9a]}$	t(sec)	$f_{[9b]}$	t(sec)	$f_{[9b]}$
0	0,968			0	0,934	0	0,958	0	0,722
1800	0,899			1800	0,805	19800	0,670	1800	0,512
70200	0,524			3600	0,722	88200	0,359	3600	0,408
97200	0,462			5400	0,668	99000	0,329	5400	0,333
154800	0,338			7200	0,615	172800	0,194	7200	0,270
172800	0,329			9000	0,574	189000	0,180	9000	0,225
241200	0,248			10800	0,541	255600	0,115	10800	0,187
262800	0,225			12600	0,507	270000	0,099	12600	0,167
414000	0,083			14400	0,479			14400	0,130
432000	0,074			16200	0,457			16200	0,107
507600	0,057			18000	0,435			18000	0,091
525600	0,048			19800	0,415			19800	0,074
590400	0,038			21600	0,398			21600	0,065
612000	0,029			23400	0,379			23400	0,057
763200	0,010			25200	0,363			25200	0,038
				27000	0,346			27000	0,029
				28800	0,333				
				30600	0,315				
				32400	0,306				
				34200	0,291				
				36000	0,281				
				37800	0,270				
				39600	0,259				
				41400	0,248				

Table S2. DFT (PBE functional, CPCM = benzene) SCF Energies and Free Energies (Kcal·mol^{-1})

Molecule		**6-31G***			**6-311++G(3df, 2p)**	**Corrected**	
	E (SCF)	G^{o}	ZPE	TC^{a}	E' (SCF)	E = E' + ZPE	G^{o} =E' + TC
[Ni]-OCOOH	-2031020,72	-2030732,38	330,77	288,34	-2030732,38	-2031093,29	-2031135,72
[Ni]-OCOOMe	-2055647,64	-2055344,13	347,79	303,51	-2055344,13	-2055706,28	-2055750,56
[Ni]-OCOOEt	-2080284,53	-2079964,89	365,22	319,64	-2079964,89	-2080332,93	-2080378,51
[Ni]-OCOOCH2CH2OMe	-2152061,32	-2151722,77	386,01	338,55	-2151722,77	-2152115,85	-2152163,31

[Pd]-OCOOH	-1164325,92	-1164039,97	329,91	285,95	-1164039,97	-1165014,93	-1165058,89
[Pd]-OCOOMe	-1188952,68	-1188651,07	347,09	301,61	-1188651,07	-1189627,82	-1189673,30
[Pd]-OCOOEt	-1213589,54	-1213271,46	365,22	318,08	-1213271,46	-1214253,67	-1214300,81
[Pd]-OCOOCH2CH2OMe	-1285366,40	-1285030,70	384,95	335,7	-1285030,70	-1286037,55	-1286086,80
			Data taken from ref 18e				
[Ni]-OH	-1912784,89	-1912503,41	320,81	281,48	-1912503,41	-1912824,94	-1912864,27
[Ni]-OMe	-1937407,29	-1937109,14	338,44	298,15	-1937109,14	-1937434,29	-1937474,58
[Ni]-OEt	-1962044,96	-1961730,25	356,27	314,71	-1961730,25	-1962060,73	-1962102,29
[Ni]-OCH2CH2OMe	-2033822,65	-2033491,89	375,92	330,76	-2033491,89	-2033845,29	-2033890,45
[Pd]-OH	-1046086,22	-1045805,36	320,58	280,86	-1045805,36	-1046743,93	-1046783,65
[Pd]-OMe	-1070711,70	-1070413,49	338,57	298,21	-1070413,49	-1071355,31	-1071395,67
[Pd]-OEt	-1095349,42	-1095035,19	356,11	314,23	-1095035,19	-1095982,15	-1096024,03
[Pd]-OCH2CH2OMe	-1167126,71	-1166796,67	375,67	330,04	-1166796,67	-1167766,65	-1167812,28

(a) Thermal correction (TC = G^o (6-31G*) – E (6-31G*))

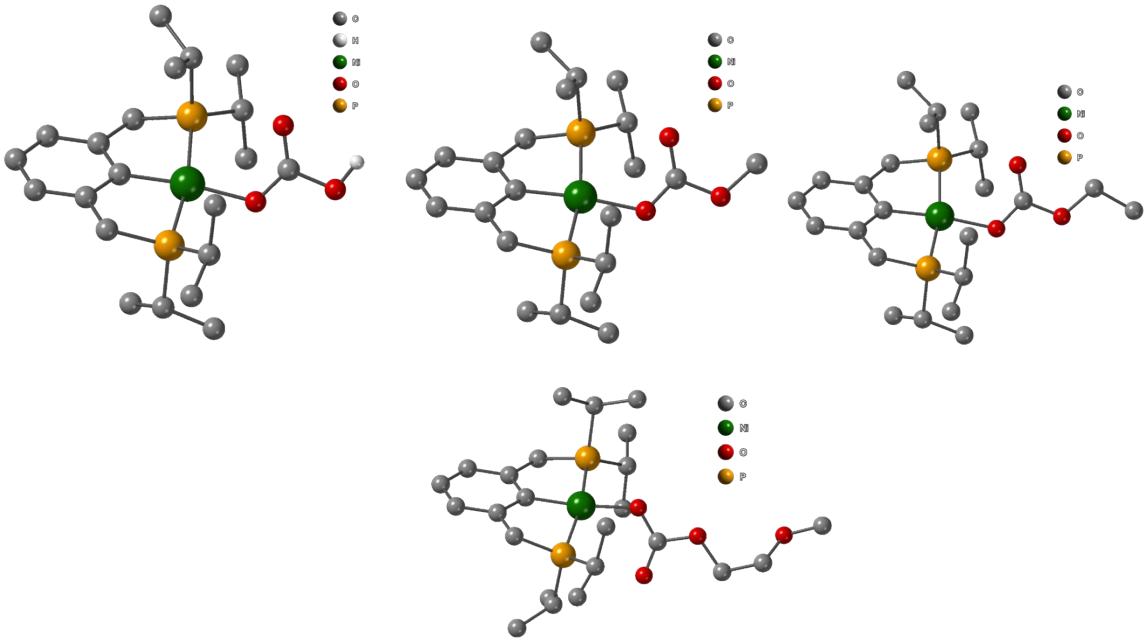


Figure S1. Molecular drawings for optimized geometries of nickel bicarbonate and alkylcarbonate complexes**.** Hydrogen atoms (except those of bicarbonate) have been omitted for simplicity. From left to right: [Ni]-OCOOH, [Ni]-OCOOMe, [Ni]-OCOOEt; below [Ni]-OCOOH.

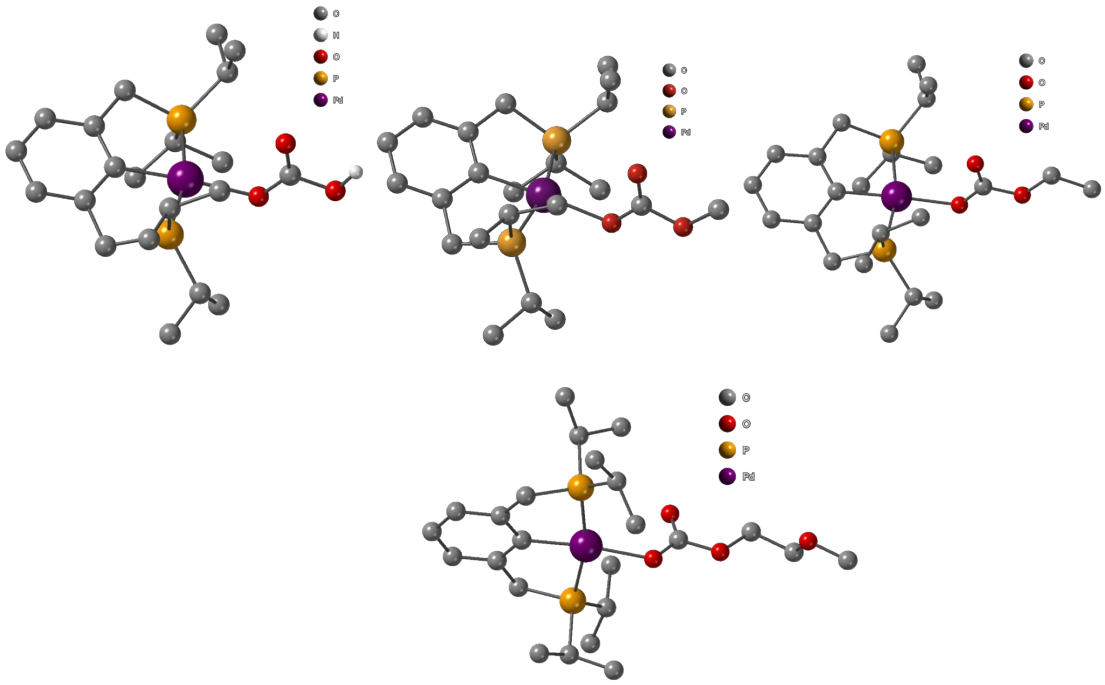


Figure S2. Molecular drawings for optimized geometries of palladium bicarbonate and alkylcarbonate complexes**.** Hydrogen atoms (except those of bicarbonate) have been omitted for simplicity. From left to right: [Pd]-OCOOH, [Pd]-OCOOMe, [Pd]-OCOOEt; below [Pd]-OCOOH.

Table S3. Molecular coordinates for bicarbonate and alkylcarbonate complexes.

[Ni]-OCOOH

63

H -0.601798 -3.592753 3.689475
H 0.019111 -3.231864 2.053359
H 3.572601 -2.962708 -1.720739
O 2.878334 -3.076483 -1.036240
C -1.112470 1.774190 1.612953
C -0.075173 1.410025 2.654764
C 2.271006 -0.467449 2.704833
C 3.148934 0.500127 1.893573
C 2.474253 -0.309103 4.217575
C -0.498600 -1.466022 3.244851
C 0.033236 -2.901956 3.106245
C -1.988022 -1.379907 2.874236
C 2.199902 -1.871992 -1.037529
H -2.025175 3.322042 2.824636
H 2.531409 -1.498544 2.399177
H -0.366052 -1.125402 4.291007
H -0.463108 1.462628 3.688629
H 0.803062 2.082289 2.604859
H 2.922822 1.554375 2.133845
H 3.006290 0.358059 0.808658
H 4.215095 0.328037 2.125882
H 3.539755 -0.451478 4.475192
H 1.890607 -1.043984 4.797099
H 2.183612 0.701383 4.556562
H 1.066767 -3.002515 3.477755
H -2.143103 -1.707887 1.831487
H -2.382857 -0.354328 2.959363
H -2.578819 -2.037531 3.537025
Ni 0.121932 -0.323678 0.044115
O 1.243879 -1.869414 -0.163923
P 0.486298 -0.287599 2.170291
C -0.413147 -1.414920 -3.215279
C -0.996560 -1.105213 -4.603364
C -1.157962 -2.578358 -2.537212
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H -1.026071 -2.030780 -5.207068
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H -1.078102 -3.490146 -3.156072
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C -0.172786 2.299695 -3.826446
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H -3.756792 2.715530 -1.094436
H -2.457756 1.264189 -2.743435
H -2.765533 -0.228132 -1.826593
H 1.380099 0.816493 -3.472007
H 2.035975 2.976378 -2.368295
H 2.050920 1.589307 -1.233077
H 0.707959 2.770522 -1.185613
H -0.871419 2.936992 -3.255556
H -0.757779 1.742061 -4.575589
H 0.515343 2.972734 -4.369643
H -0.392744 -0.367765 -5.157063
H -2.030296 -0.722696 -4.532438
O 2.543126 -0.967212 -1.825965
P -0.363716 0.040518 -2.041673

[Ni]-OCOOMe

66

H -0.817681 -3.425265 3.834697
H -0.222146 -3.089844 2.184073
O 2.702903 -2.930075 -0.942021
C -1.309158 1.898810 1.698067
C -0.256527 1.556725 2.730861
C 2.078806 -0.328666 2.814289
C 2.963832 0.625834 1.995207
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C -0.696912 -1.305277 3.363751
C -0.184642 -2.748798 3.232829
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H 1.979836 0.862866 4.651259
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H -2.571821 -0.173294 3.094516
H -2.779912 -1.852603 3.678193
Ni -0.066560 -0.206717 0.143163
O 1.081428 -1.730764 -0.066088
P 0.296298 -0.150455 2.271017
C -0.573991 -1.237401 -3.178223
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P -0.553007 0.170063 -1.942932
C 3.764119 -3.026847 -1.903954
H 4.519148 -2.237738 -1.747661
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H 4.214224 -4.018444 -1.746467

[Ni]-OCOOEt

69

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H -2.261320 -2.874464 -0.394814
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C -2.073720 0.856271 2.758328
C -4.404576 0.079009 2.070300
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C -3.310230 -2.532707 -0.370170
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H 1.091868 1.889785 1.710958
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H 2.864883 3.284477 -1.384888
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H 3.966387 3.527726 -0.007096
H 4.953241 0.156245 -0.856302
H 4.345830 -0.379073 -2.448654
O 1.685485 -0.609015 2.135425
P 1.868361 0.386606 -0.747064
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H 0.661962 -4.373875 4.560197

[Ni]-OCOOCH$_2$CH$_2$OMe

73

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H 0.641550 -2.293339 2.507769
O -2.223749 0.783230 2.353116
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C 0.815424 -2.849828 -2.137214
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C -1.726284 -4.475867 -0.490388
C 1.201607 -3.461106 0.738744
C 0.648077 -3.343218 2.168218
C 2.686708 -3.069724 0.676422
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P 0.217444 -2.390976 -0.444128
C 1.009223 2.986089 0.750023
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C 3.726647 0.187362 -3.105818
C 2.780495 0.416893 -2.092424
C 2.759990 1.719834 -1.323284
C 0.005537 2.682799 -2.077392
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H -1.343587 2.150891 -3.700111
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H 2.595336 4.360338 0.099975
O -1.937432 1.534210 0.208188
P 1.005803 1.837806 -0.725045
C -3.347415 1.678987 2.438014
H -4.177779 1.304809 1.811185
H -3.065533 2.679489 2.065988
C -3.779379 1.765531 3.887228
H -4.524931 2.586977 3.986037
H -2.906961 2.028572 4.525319
O -4.343555 0.524530 4.289595
C -4.747590 0.554073 5.648939
H -5.509733 1.341198 5.835965
H -3.890102 0.735750 6.331629
H -5.185366 -0.430313 5.878412

[Pd]OCOOH

63

C -3.262896 -3.619680 0.628232
C -1.908148 -2.965798 -1.416396
H -3.565789 -4.554937 0.123579
H -0.904776 -2.730341 -1.807230
H -2.285371 -3.875714 -1.918074
C -0.387559 2.564451 0.976547
C 0.883372 2.988675 0.267680
C 3.102623 1.742626 -1.312997
C 3.816277 1.236725 -0.048334
C 3.633633 3.109694 -1.773482
C 0.511072 2.412083 -2.653331
C 0.880672 1.489773 -3.828269
C -1.010971 2.572709 -2.517598
C 2.196940 -2.102143 -1.252356
H -0.745498 4.533425 1.812086
H 3.267644 0.997921 -2.114923
H 0.963033 3.410297 -2.814554
H 0.818757 4.018994 -0.127046
H 1.745106 2.964687 0.961701
H 3.665446 1.920189 0.806472
H 3.465901 0.227356 0.225329
H 4.903946 1.186811 -0.237665
H 4.729439 3.055966 -1.904794
H 3.196685 3.430170 -2.734190
H 3.428106 3.894023 -1.023133
H 1.967556 1.471579 -4.017751
H 0.554319 0.452592 -3.635517
H -1.485928 1.595247 -2.325206
H -1.291311 3.248884 -1.692097
H -1.426947 2.983440 -3.455221
O 1.095041 -1.538046 -1.613269
P 1.242785 1.736011 -1.064257
Pd 0.164870 -0.151084 -0.234154
H 0.384835 1.842989 -4.750225
H 3.478063 -3.355377 -1.836613
O 2.650067 -2.993983 -2.220037
C -0.846404 1.221454 0.867161
C -1.109594 3.501427 1.741010
C -2.280349 3.127001 2.412321
C -2.752192 1.812369 2.302713
C -2.057491 0.866148 1.526168
C -2.619058 -0.528951 1.344143
C -0.454815 -2.132234 2.605003
C 0.858312 -2.910366 2.416478
C -1.407740 -2.861890 3.563929
C -1.881039 -3.186322 0.107408
H -2.828798 3.860327 3.013115
H -3.677900 1.518555 2.811923
H -3.205540 -0.875134 2.212636
H -3.289932 -0.566147 0.463772
H -0.215429 -1.137878 3.031738
H 1.547881 -2.405346 1.718537
H 1.362492 -3.025238 3.392825
H -0.926441 -2.957340 4.554226
H -2.363909 -2.330912 3.709850
H -1.627909 -3.883072 3.208556
H -1.142285 -3.980301 0.331464
H -3.279278 -3.800504 1.714205
O 2.863795 -1.955197 -0.205453
P -1.189230 -1.650582 0.943757
H 0.666231 -3.927801 2.028358
H -2.585125 -2.133383 -1.684977
H -4.029246 -2.858899 0.396231

[Pd]-OCOOMe

66

C 3.357540 -3.534371 0.791213
C 2.819716 -2.171498 -1.287391
H 4.315408 -3.867288 0.351471
H 2.616331 -1.164110 -1.686517
H 3.736201 -2.568349 -1.761143
C -2.746815 -0.533345 1.069355
C -3.153387 0.731209 0.339055
C -1.875099 2.917758 -1.251119
C -1.362844 3.633424 0.009894
C -3.236547 3.462463 -1.713221
C -2.579162 0.325640 -2.575782
C -1.658641 0.682236 -3.756003
C -2.747969 -1.194757 -2.429964
C 1.931576 1.957248 -1.216348
H -4.719154 -0.842615 1.915877
H -1.128844 3.071088 -2.053775
H -3.575324 0.782546 -2.735812
H -4.182602 0.672443 -0.059451
H -3.123503 1.602556 1.020782
H -2.046795 3.491569 0.865731
H -0.356016 3.277406 0.284381
H -1.305480 4.719822 -0.184627
H -3.168854 4.556366 -1.853477
H -3.565558 3.021914 -2.669401
H -4.021558 3.273439 -0.959165
H -1.635212 1.767697 -3.952961
H -0.622763 0.351238 -3.564210
H -1.772127 -1.673391 -2.237873
H -3.422511 -1.466126 -1.600047
H -3.164442 -1.614516 -3.363381
O 1.372797 0.843120 -1.557393
P -1.892903 1.059068 -0.992034
Pd -0.023773 -0.046653 -0.158241
H -2.017727 0.182252 -4.673417
O 2.795754 2.388744 -2.219078
C -1.411338 -1.015470 0.964826
C -3.693491 -1.225066 1.849695
C -3.336689 -2.388429 2.542914
C -2.029835 -2.882406 2.439957
C -1.074575 -2.218153 1.647774
C 0.310448 -2.807179 1.476721
C 1.947455 -0.639808 2.684098

C 2.746868 0.655670 2.463904
C 2.664020 -1.577986 3.667353
C 2.992259 -2.145972 0.241727
H -4.077162 -2.913544 3.155678
H -1.748939 -3.802465 2.966462
H 0.647330 -3.376840 2.359962
H 0.332306 -3.502849 0.615517
H 0.957041 -0.375433 3.104819
H 2.248258 1.340611 1.757150
H 2.878838 1.176024 3.429546
H 2.779565 -1.065204 4.639612
H 2.112928 -2.516079 3.851796
H 3.677238 -1.833411 3.312304
H 3.801149 -1.431667 0.490159
H 3.464975 -3.545158 1.886975
O 1.791224 2.628754 -0.174524
P 1.456482 -1.405717 1.039787
H 3.757851 0.438638 2.071169
H 1.981310 -2.829946 -1.581323
H 2.592730 -4.281860 0.516383
C 3.463814 3.624619 -1.932892
H 4.085651 3.837085 -2.815989
H 4.100362 3.540631 -1.034998
H 2.742217 4.444385 -1.772490

[Pd]-OCOOEt

69

C 3.152282 0.948663 3.714937
C 2.617671 -1.132099 2.353582
H 4.111231 0.512146 4.049032
H 2.415354 -1.532016 1.346301
H 3.534030 -1.605079 2.751651
C -2.949500 1.225839 0.711694
C -3.356901 0.495389 -0.552538
C -2.077840 -1.087526 -2.743435
C -1.569095 0.176619 -3.456093
C -3.438354 -1.551334 -3.288935
C -2.779171 -2.419579 -0.154100
C -1.856701 -3.597610 -0.512922
C -2.948356 -2.276861 1.366544
C 1.723261 -1.067693 -1.781641
H -4.922128 2.071457 1.021687
H -1.329486 -1.887772 -2.899325
H -3.775021 -2.580312 -0.611432
H -4.385230 0.094874 -0.491896
H -3.330308 1.177814 -1.423405
H -2.255792 1.030062 -3.313097
H -0.563246 0.452683 -3.098707
H -1.510283 -0.015537 -4.542835
H -3.370483 -1.688690 -4.383198
H -3.765438 -2.509315 -2.850846
H -4.224835 -0.799283 -3.098031
H -1.832366 -3.791781 -1.598896
H -0.821292 -3.404940 -0.180955
H -1.972894 -2.083587 1.845500
H -3.624590 -1.448742 1.639285
H -3.363019 -3.211806 1.784699
O 1.170715 -1.401504 -0.661497
P -2.094929 -0.833354 -0.883980
Pd -0.226230 -0.001916 0.224694
H -2.214655 -4.516827 -0.015412
O 2.585654 -2.071442 -2.210090
C -1.613539 1.122218 1.192867
C -3.896216 2.005974 1.403595
C -3.539173 2.700042 2.566374
C -2.231825 2.598424 3.059268
C -1.276469 1.806580 2.394706
C 0.108953 1.637307 2.983404
C 1.749830 2.835252 0.812716
C 2.550650 2.607925 -0.480745
C 2.467735 3.820296 1.748015
C 2.789419 0.397034 2.326821
H -4.279731 3.312506 3.091729
H -1.950601 3.125716 3.978788
H 0.446146 2.522609 3.549736
H 0.130606 0.779109 3.682774
H 0.760735 3.257230 0.545543
H 2.050840 1.900626 -1.164272
H 2.686860 3.571385 -1.004069
H 2.586651 4.790198 1.231543
H 1.915756 4.010068 2.684551
H 3.479638 3.463580 2.006383
H 3.599088 0.645183 1.613316
H 3.256292 2.044777 3.724758
O 1.576179 -0.029322 -2.457660
P 1.254696 1.194594 1.583548
H 3.559912 2.212426 -0.260543
H 1.778781 -1.425936 3.011442
H 2.387798 0.672249 4.462147
C 3.247199 -1.812539 -3.464839
H 3.816358 -0.867463 -3.397530
H 2.492203 -1.682777 -4.262184
C 4.160074 -2.995656 -3.748381
H 4.913349 -3.109800 -2.950698
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H 3.581480 -3.932646 -3.813880

[Pd]-OCOOCH$_2$CH$_2$OMe

73

C 2.799671 1.249376 3.911882
C 2.318493 -0.840474 2.542162
H 3.770151 0.840880 4.248137
H 2.125696 -1.241483 1.533449
H 3.244403 -1.295410 2.938914
C -3.292782 1.431620 0.887492
C -3.680886 0.703646 -0.384379
C -2.369633 -0.866173 -2.565531
C -1.856331 0.398843 -3.273629
C -3.724468 -1.330458 -3.124900
C -3.079516 -2.205778 0.017754
C -2.146685 -3.376600 -0.337966
C -3.255718 -2.066393 1.537987
C 1.430394 -0.781546 -1.580311
H -5.277872 2.250529 1.189807
H -1.619757 -1.666132 -2.715169
H -4.072184 -2.373525 -0.443995
H -4.706862 0.295194 -0.338413
H -3.648173 1.390025 -1.251999
H -2.545186 1.251265 -3.135136
H -0.853922 0.678468 -2.909197
H -1.789515 0.207579 -4.360080
H -3.644352 -1.471409 -4.217881
H -4.057830 -2.286727 -2.687682
H -4.512188 -0.576874 -2.945433
H -2.114616 -3.568980 -1.424037
H -1.114666 -3.177500 0.000620
H -2.283179 -1.867622 2.020571
H -3.937986 -1.242915 1.809540
H -3.665760 -3.004690 1.953105
O 0.859550 -1.143113 -0.479698
P -2.404673 -0.613033 -0.706386
Pd -0.552546 0.238727 0.411911
H -2.501068 -4.299068 0.156060
O 2.290915 -1.781277 -2.026899

C	-1.959019	1.341595	1.377238
C	-4.253617	2.195629	1.577768
C	-3.912332	2.887137	2.746851
C	-2.606840	2.799315	3.247300
C	-1.637401	2.023346	2.584343
C	-0.252239	1.869799	3.177751
C	1.365403	3.116416	1.018944
C	2.192220	2.920145	-0.262857
C	2.038094	4.119301	1.968712
C	2.456505	0.691966	2.521325
H	-4.663820	3.487022	3.271191
H	-2.337809	3.325239	4.171227
H	0.069712	2.755159	3.752535
H	-0.219523	1.004984	3.868548
H	0.368562	3.509933	0.737386
H	1.724372	2.200740	-0.956180
H	2.305495	3.889789	-0.780270
H	2.130184	5.095413	1.458588
H	1.468808	4.284701	2.899374
H	3.058382	3.795993	2.237493
H	3.262747	0.960979	1.811633
H	2.870919	2.348046	3.924007
O	1.302096	0.275522	-2.230562
P	0.905710	1.458577	1.777282
H	3.209892	2.555679	-0.029422
H	1.485275	-1.154376	3.197771
H	2.041271	0.949408	4.656205
C	3.000609	-1.467620	-3.236106
H	3.704202	-0.632884	-3.061002
H	2.294410	-1.152874	-4.025497
C	3.751917	-2.706235	-3.680450
H	4.156081	-2.531020	-4.703334
H	3.052165	-3.568927	-3.742353
O	4.805265	-2.976665	-2.764622
C	5.520981	-4.146208	-3.125427
H	6.317019	-4.283446	-2.376450
H	5.984232	-4.054461	-4.131939
H	4.869153	-5.046088	-3.127672