SUPPORTING INFORMATION FOR:

Unprecedented Hydrogen Transfer from Water to Alkenes and Alkynes Mediated by Ti^{III} and Late Transition Metals

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General Details.

For all reactions solvents and reagents were thoroughly deoxygenated prior to use. Compounds **4-12** were purchased from commercial sources. Products **13-21** were isolated as pure samples by flash chromatography and **14-21** showed NMR data matching those reported: **14**,¹ **15**,¹ **16**,¹ **17**,² **18**,¹ **19**,³ **20**,⁴ **21**.⁵ Despite of **13** is a well-known ester;⁶ we could not find its NMR data in the bibliography. Deuterium incorporation was determined using ¹H NMR and MS techniques.

General procedure for the H₂O/Cp₂TiCl₂-based hydrogenation of alkenes and alkynes.

Deoxygenated THF (25 mL) was added to a mixture of Cp₂TiCl₂ (1.25 mmol), Mn dust (4 mmol) and a hydrogenation catalyst (Pd/C, Pd/alumina, Pd(dba)₂, Rh/alumina, Wilkinson, or Lindlar catalysts) (0.05 mmol) under an Ar atmosphere and the suspension was stirred at rt until it turned lime green (after about 15 min). Subsequently, a deoxygenated solution of H₂O (5 mmol) and the corresponding alkene

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¹ Sigma-Aldrich database.

² Profit, J. A.; Ong, H. H. *J. Org. Chem.* **1979**, *44*, 3972-3974.

³ Johnson, C. R.; Elliot, R. C. *J. Am. Chem. Soc.* **1982**, *104*, 7041-7044.

⁴ Jankowski, P.; Marczak, S.; Masnyk, M.; Wicha, J. *J. Organometallic Chem.* **1991**, *403*, 49-62.

⁵ (a) Gibson, J. S.; Herbert, J. M. *J. Label Comp. Radiopharm.* **2003**, *46*, 531-537. (b) Concellón, J. M.; Huerta, M. *J. Org. Chem.* **2005**, *70*, 4714-4719.

⁶ Corset, J.; Froment, F.; Deschamps, E.; Loupy, A.; Nee, G.; Le Ny, G.; Tchoubar, B. *Tetrahedron* **1978**, *34*, 2645-2654.

(**4-9**) or alkyne (**10-12**) (0.5 mmol) in THF (5 mL) was added and the mixture was stirred at rt for 24 h. The reaction mixture was then diluted with EtOAc, filtered, washed with brine, dried (anhyd Na₂SO₄) and the solvent removed. The residue was submitted to flash chromatography (hexane/EtOAc mixtures) to give the corresponding hydrogenation product (**13-18**, **4**, **19**, or **20** respectively). The yields obtained appear in Table 1 (cf. main text).

NMR data for product 13. ¹H NMR (300 MHz, CDCl₃) δ 3.72 (s, 6H), 3.37 (t, *J* = 7.6 Hz, 1H), 1.88 (q, *J* = 7.6 Hz, 2H), 1.34 (hex, *J* = 7.6 Hz, 2H), 0.92 (t, *J* = 7.6 Hz, 3H); ¹³C NMR (75 MHz, CDCl₃, DEPT) δ 170.2 (C), 52.6 (CH₃), 51.7 (CH), 31.3 (CH₂), 20.8 (CH₂), 13.9 (CH₃).

Synthesis of double-deuterated derivative 21.

Deoxygenated THF (25 mL) was added to a mixture of Cp₂TiCl₂ (352 mg, 1.4 mmol), Mn dust (250 mg, 4.5 mmol) and Wilkinson catalyst (53 mg, 0.06 mmol) under an Ar atmosphere and the suspension was stirred at room temperature until it turned lime green (after about 15 min). Subsequently, a solution of ethyl cinnamate (**17**) (100 mg, 0.6 mmol) and D₂O (114 mg, 5.7 mmol) in THF (10 mL) was added and the mixture was stirred for 60 h. The reaction was then diluted with EtOAc, washed with brine, dried (anhyd Na₂SO₄) and the solvent removed. The residue was submitted to flash chromatography (hexane: EtOAc, 9:1) to give 74 mg of **21** (72% yield, 75% deuterium incorporation).

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Computational methods

Calculations were performed with the GAUSSIAN 03 series of programs.⁷ The geometries of all complexes were optimized at the DFT level using the B3LYP hybrid functional,⁸ using the standard 6-31G(d) basis set for C, H, O, Cl and P. The standard LANL2DZ basis set, which includes a relativistic pseudopotential, was used for Pd and Ti. Unrestricted B3LYP was used for the radical species. Transition states were graphically located. Harmonic frequencies were calculated at the same level of theory to characterize the stationary points and to determine the zero-point energies (ZPE).

(kcal mol ⁻¹)	$\Delta(E+ZPE)^\ddagger$	$\Delta E^\ddagger$	$\Delta G^\ddagger$	ΔE
R = H	17.3	19.8	31.4	+ 15.7
R = D	18.4	19.8	32.6	-

Cp₂Ti (H₂O) Cl (1)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	22	0	0.009211	-0.005296	0.082282
2	17	0	-0.072211	2.379758	-0.745033
3	8	0	0.080776	1.293809	1.948538
4	1	0	-0.746863	1.280449	2.454117
5	1	0	0.059753	2.133089	1.425021

⁷ Gaussian 03, Revision B.03,

Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, Jr., J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; Pople, J. A. Gaussian, Inc., Pittsburgh PA, 2003.

⁸ Becke, A. D. *Phys. Rev. A* **1988**, 38, 3098-3100. (b) Lee, C.; Yang, W.; Parr, R. G. *Phys. Rev. B* **1988**, 37, 785-789.

6	6	0	-2.347142	0.157914	0.446013
7	6	0	-1.902091	-1.033704	1.086519
8	6	0	-1.448881	-1.914798	0.077997
9	6	0	-1.619783	-1.273383	-1.182980
10	6	0	-2.187657	-0.002823	-0.953063
11	1	0	-2.740468	1.044358	0.927405
12	1	0	-1.905394	-1.237159	2.150716
13	1	0	-1.040806	-2.903908	0.236356
14	1	0	-1.358082	-1.685647	-2.148812
15	1	0	-2.388827	0.751486	-1.700003
16	6	0	2.197978	-0.487001	1.008878
17	6	0	2.342428	0.395442	-0.089873
18	6	0	1.932994	-0.290260	-1.267602
19	6	0	1.520717	-1.587599	-0.885058
20	6	0	1.671138	-1.705286	0.527379
21	1	0	2.383652	-0.240960	2.045795
22	1	0	2.670999	1.423814	-0.044103
23	1	0	1.911519	0.124781	-2.266293
24	1	0	1.145168	-2.356310	-1.547487
25	1	0	1.429862	-2.574849	1.125067

Zero-point correction= 0.195675
(Hartree/Particle)
Thermal correction to Energy= 0.209428
Thermal correction to Enthalpy= 0.210372
Thermal correction to Gibbs Free Energy= 0.154235
Sum of electronic and zero-point Energies= -981.694360
Sum of electronic and thermal Energies= -981.680606
Sum of electronic and thermal Enthalpies= -981.679662
Sum of electronic and thermal Free Energies= -981.735800

Cp₂Ti (D₂O) Cl

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	22	0	0.095978	-0.208982	-0.021961
2	17	0	-0.110758	-2.721793	-0.171568
3	8	0	0.181364	-0.700132	-2.241688
4	1	0	-0.626570	-0.452982	-2.718002
5	1	0	0.107986	-1.673373	-2.079494
6	6	0	-2.250598	-0.101243	-0.461397
7	6	0	-1.735431	1.220289	-0.589478
8	6	0	-1.283187	1.626022	0.687087
9	6	0	-1.524451	0.561835	1.603577
10	6	0	-2.134547	-0.494420	0.895221
11	1	0	-2.662011	-0.715900	-1.252075
12	1	0	-1.692747	1.814018	-1.494779
13	1	0	-0.830216	2.578653	0.926273
14	1	0	-1.280819	0.560810	2.658048
15	1	0	-2.392333	-1.465263	1.293197
16	6	0	2.333883	0.477780	-0.655553
17	6	0	2.403575	-0.763044	0.024377
18	6	0	1.980553	-0.558378	1.367496
19	6	0	1.634700	0.805941	1.503239
20	6	0	1.839773	1.445468	0.246135
21	1	0	2.546184	0.636621	-1.704314
22	1	0	2.691852	-1.711510	-0.405596
23	1	0	1.906923	-1.321174	2.130897
24	1	0	1.267153	1.281956	2.402688

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25          1          0          1.655127    2.488279    0.022453
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Zero-point correction=                      0.189115
(Hartree/Particle)
Thermal correction to Energy=              0.203247
Thermal correction to Enthalpy=            0.204191
Thermal correction to Gibbs Free Energy=    0.147259
Sum of electronic and zero-point Energies=  -981.700919
Sum of electronic and thermal Energies=     -981.686787
Sum of electronic and thermal Enthalpies=   -981.685843
Sum of electronic and thermal Free Energies= -981.742775

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Pd(acrol)₂ (acrol = CH₂CHO)

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Center      Atomic      Atomic      Coordinates (Angstroms)
Number      Number      Type          X           Y           Z
-----
  1          46          0          0.689800    -0.191824    0.169194
  2           6          0          0.962335    -2.365466    0.417461
  3           6          0         -0.168585    -2.190600   -0.361601
  4           6          0         -1.524092    -2.155925    0.237212
  5           8          0         -2.552830    -2.087874   -0.406797
  6           6          0          0.006738     1.763427    0.952716
  7           6          0          0.947673     2.015420   -0.031904
  8           6          0          0.555401     2.295864   -1.432423
  9           8          0          1.337876     2.615072   -2.306580
 10          1          0          0.877713    -2.538364    1.489445
 11          1          0          1.921189    -2.613813   -0.031012
 12          1          0         -0.130420    -2.258147   -1.447263
 13          1          0         -1.541716    -2.215391    1.348825
 14          1          0          0.271870     1.791840    2.006074
 15          1          0         -1.057837     1.802349    0.727866
 16          1          0          1.989623     2.212284    0.217658
 17          1          0         -0.534735     2.206147   -1.637872
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Zero-point correction=                      0.125915
(Hartree/Particle)
Thermal correction to Energy=              0.137242
Thermal correction to Enthalpy=            0.138186
Thermal correction to Gibbs Free Energy=    0.085822
Sum of electronic and zero-point Energies=  -510.491443
Sum of electronic and thermal Energies=     -510.480116
Sum of electronic and thermal Enthalpies=   -510.479171
Sum of electronic and thermal Free Energies= -510.531536

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TS

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Center      Atomic      Atomic      Coordinates (Angstroms)
Number      Number      Type          X           Y           Z
-----
  1          22          0          2.225413    -0.272586    0.044425
  2          17          0          1.268570     0.092664    2.197353
  3           8          0          0.690080     0.283657   -0.935528
  4           1          0          0.565572     1.256319   -1.040893
  5           1          0         -0.801250    -0.005393   -0.652934
  6          46          0         -2.393158     0.250638   -0.198265
  7           6          0         -2.686035    -1.689342   -1.130128
  8           6          0         -3.987951    -1.289628   -0.796948
  9           6          0         -4.625313    -1.657512    0.471109

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10	8	0	-5.786461	-1.405519	0.760462
11	6	0	-2.917328	2.082710	1.085968
12	6	0	-1.607726	2.148623	0.609571
13	6	0	-1.299006	2.852398	-0.639713
14	8	0	-0.181368	2.927716	-1.155585
15	1	0	-2.168011	-2.411316	-0.500265
16	1	0	-2.351832	-1.643209	-2.162707
17	1	0	-4.629246	-0.805566	-1.530936
18	1	0	-3.971920	-2.222396	1.174637
19	1	0	-3.130368	1.737788	2.092217
20	1	0	-3.731290	2.573812	0.556639
21	1	0	-0.767495	1.853643	1.235796
22	1	0	-2.157493	3.357233	-1.126760
23	6	0	2.842449	2.064199	-0.048460
24	6	0	3.214153	1.470634	-1.282785
25	6	0	4.213494	0.506205	-1.021011
26	6	0	4.473964	0.513737	0.382023
27	6	0	3.640686	1.490291	0.970232
28	1	0	2.054772	2.792378	0.087635
29	1	0	2.771854	1.680844	-2.247527
30	1	0	4.706213	-0.115025	-1.756123
31	1	0	5.193120	-0.103303	0.903560
32	1	0	3.569806	1.707866	2.025331
33	6	0	1.361352	-2.299603	-1.009037
34	6	0	1.215037	-2.443880	0.383946
35	6	0	2.517378	-2.485052	0.963513
36	6	0	3.458956	-2.346125	-0.074842
37	6	0	2.742966	-2.188580	-1.298625
38	1	0	0.559252	-2.167242	-1.720144
39	1	0	0.283457	-2.460834	0.931050
40	1	0	2.735063	-2.562260	2.019655
41	1	0	4.534376	-2.339519	0.036902
42	1	0	3.175422	-2.052853	-2.280992

-293.1735 cm⁻¹

Zero-point correction=	0.317636
(Hartree/Particle)	
Thermal correction to Energy=	0.342927
Thermal correction to Enthalpy=	0.343872
Thermal correction to Gibbs Free Energy=	0.258594
Sum of electronic and zero-point Energies=	-1492.158227
Sum of electronic and thermal Energies=	-1492.132935
Sum of electronic and thermal Enthalpies=	-1492.131991
Sum of electronic and thermal Free Energies=	-1492.217268

TS containing D₂O

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	22	0	2.225413	-0.272586	0.044425
2	17	0	1.268570	0.092664	2.197353
3	8	0	0.690080	0.283657	-0.935528
4	1	0	0.565572	1.256319	-1.040893
5	1	0	-0.801250	-0.005393	-0.652934
6	46	0	-2.393158	0.250638	-0.198265
7	6	0	-2.686035	-1.689342	-1.130128
8	6	0	-3.987951	-1.289628	-0.796948

9	6	0	-4.625313	-1.657512	0.471109
10	8	0	-5.786461	-1.405519	0.760462
11	6	0	-2.917328	2.082710	1.085968
12	6	0	-1.607726	2.148623	0.609571
13	6	0	-1.299006	2.852398	-0.639713
14	8	0	-0.181368	2.927716	-1.155585
15	1	0	-2.168011	-2.411316	-0.500265
16	1	0	-2.351832	-1.643209	-2.162707
17	1	0	-4.629246	-0.805566	-1.530936
18	1	0	-3.971920	-2.222396	1.174637
19	1	0	-3.130368	1.737788	2.092217
20	1	0	-3.731290	2.573812	0.556639
21	1	0	-0.767495	1.853643	1.235796
22	1	0	-2.157493	3.357233	-1.126760
23	6	0	2.842449	2.064199	-0.048460
24	6	0	3.214153	1.470634	-1.282785
25	6	0	4.213494	0.506205	-1.021011
26	6	0	4.473964	0.513737	0.382023
27	6	0	3.640686	1.490291	0.970232
28	1	0	2.054772	2.792378	0.087635
29	1	0	2.771854	1.680844	-2.247527
30	1	0	4.706213	-0.115025	-1.756123
31	1	0	5.193120	-0.103303	0.903560
32	1	0	3.569806	1.707866	2.025331
33	6	0	1.361352	-2.299603	-1.009037
34	6	0	1.215037	-2.443880	0.383946
35	6	0	2.517378	-2.485052	0.963513
36	6	0	3.458956	-2.346125	-0.074842
37	6	0	2.742966	-2.188580	-1.298625
38	1	0	0.559252	-2.167242	-1.720144
39	1	0	0.283457	-2.460834	0.931050
40	1	0	2.735063	-2.562260	2.019655
41	1	0	4.534376	-2.339519	0.036902
42	1	0	3.175422	-2.052853	-2.280992

-265.3815 cm⁻¹

Zero-point correction=	0.312786
(Hartree/Particle)	
Thermal correction to Energy=	0.338510
Thermal correction to Enthalpy=	0.339454
Thermal correction to Gibbs Free Energy=	0.253493
Sum of electronic and zero-point Energies=	-1492.163077
Sum of electronic and thermal Energies=	-1492.137353
Sum of electronic and thermal Enthalpies=	-1492.136409
Sum of electronic and thermal Free Energies=	-1492.222369

H-Pd(acrol)₂ (acrol = CH₂CHO)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	46	0	0.322169	-0.134273	0.113024
2	6	0	0.409690	-2.334484	0.105088
3	6	0	-0.927354	-2.076424	-0.190974
4	6	0	-1.961299	-1.993567	0.852176
5	8	0	-3.150627	-1.839426	0.624278
6	6	0	-0.588236	1.940508	0.528752
7	6	0	0.731622	2.089337	0.144534
8	6	0	1.089011	2.396644	-1.265803
9	8	0	2.193282	2.747948	-1.624307
10	1	0	1.886584	-0.342637	0.386775

11	1	0	0.703395	-2.603083	1.117779
12	1	0	1.102341	-2.624872	-0.678732
13	1	0	-1.280235	-2.045521	-1.220027
14	1	0	-1.585534	-2.108432	1.893360
15	1	0	-0.881697	1.948323	1.573642
16	1	0	-1.392678	2.003873	-0.202698
17	1	0	1.518570	2.244253	0.877787
18	1	0	0.247610	2.304397	-1.989397

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Zero-point correction=                0.131546
(Hartree/Particle)
Thermal correction to Energy=         0.143676
Thermal correction to Enthalpy=       0.144620
Thermal correction to Gibbs Free Energy= 0.090334
Sum of electronic and zero-point Energies= -511.031969
Sum of electronic and thermal Energies= -511.019839
Sum of electronic and thermal Enthalpies= -511.018895
Sum of electronic and thermal Free Energies= -511.073181

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D-Pd(acrol)₂ (acrol = CH₂CHO)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	46	0	-0.040628	-0.303534	-0.201288
2	6	0	1.667968	-1.685525	-0.064026
3	6	0	2.120322	-0.563337	0.627446
4	6	0	2.878011	0.512455	-0.030288
5	8	0	3.349074	1.473559	0.556755
6	6	0	-1.100036	1.726679	-0.448579
7	6	0	-2.035785	0.711233	-0.520782
8	6	0	-2.825165	0.309970	0.673629
9	8	0	-3.798624	-0.412547	0.631512
10	1	0	-0.663763	-1.577387	-0.945743
11	1	0	1.972606	-1.851816	-1.095285
12	1	0	1.327040	-2.564717	0.473794
13	1	0	2.033953	-0.496852	1.710288
14	1	0	3.021994	0.380797	-1.125903
15	1	0	-0.688652	2.186596	-1.341444
16	1	0	-0.891126	2.226593	0.496201
17	1	0	-2.408766	0.355428	-1.477464
18	1	0	-2.469910	0.746991	1.634251

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Zero-point correction=                0.129897
(Hartree/Particle)
Thermal correction to Energy=         0.142246
Thermal correction to Enthalpy=       0.143190
Thermal correction to Gibbs Free Energy= 0.088327
Sum of electronic and zero-point Energies= -511.033618
Sum of electronic and thermal Energies= -511.021269
Sum of electronic and thermal Enthalpies= -511.020325
Sum of electronic and thermal Free Energies= -511.075188

```

Cp₂Ti (OH) Cl

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z

1	22	0	0.003990	0.055320	0.228722
2	8	0	0.088047	0.252776	2.074418
3	17	0	-0.012283	2.374195	-0.298695
4	1	0	-0.739305	0.535521	2.493259
5	6	0	-2.417853	0.163613	0.472569
6	6	0	-2.016734	-1.149945	0.819545
7	6	0	-1.463396	-1.755942	-0.331255
8	6	0	-1.557096	-0.822176	-1.406511
9	6	0	-2.157121	0.351345	-0.908810
10	1	0	-2.835965	0.908678	1.137225
11	1	0	-2.058393	-1.595086	1.804830
12	1	0	-1.064199	-2.759184	-0.389758
13	1	0	-1.230942	-0.982834	-2.424922
14	1	0	-2.323926	1.262659	-1.462847
15	6	0	2.252210	-0.662966	0.884605
16	6	0	2.398393	0.443258	0.028704
17	6	0	1.911244	0.073573	-1.260380
18	6	0	1.458319	-1.258120	-1.186621
19	6	0	1.626699	-1.705111	0.157235
20	1	0	2.451027	-0.668309	1.946119
21	1	0	2.752427	1.424374	0.309852
22	1	0	1.863058	0.720320	-2.125643
23	1	0	1.035503	-1.833180	-1.998641
24	1	0	1.359377	-2.678689	0.546643

```

Zero-point correction=                0.184905
(Hartree/Particle)
Thermal correction to Energy=          0.197771
Thermal correction to Enthalpy=        0.198716
Thermal correction to Gibbs Free Energy= 0.145377
Sum of electronic and zero-point Energies= -981.115351
Sum of electronic and thermal Energies=   -981.102484
Sum of electronic and thermal Enthalpies=  -981.101540
Sum of electronic and thermal Free Energies= -981.154879

```

Cp₂Ti (OD) C1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	22	0	-0.177806	-0.199892	-0.044947
2	8	0	-1.450969	-0.619209	1.241809
3	17	0	-1.441554	-0.912584	-1.929241
4	1	0	-1.548253	-1.565763	1.427255
5	6	0	0.616326	-2.489972	0.202671
6	6	0	1.139291	-1.742115	1.286137
7	6	0	2.009708	-0.760867	0.759664
8	6	0	2.052929	-0.927822	-0.657086
9	6	0	1.204218	-2.001363	-0.991848
10	1	0	-0.115330	-3.285653	0.259880
11	1	0	0.872329	-1.849789	2.329104
12	1	0	2.563598	-0.030867	1.333760
13	1	0	2.634856	-0.340431	-1.354027
14	1	0	0.981967	-2.346897	-1.990081
15	6	0	-1.019783	1.940849	0.796936
16	6	0	-1.325963	1.879848	-0.574200
17	6	0	-0.098886	1.866167	-1.302106

18	6	0	0.957250	1.909214	-0.371231
19	6	0	0.389414	1.909904	0.937076
20	1	0	-1.733668	1.878134	1.604894
21	1	0	-2.313102	1.789160	-1.003486
22	1	0	-0.003955	1.793479	-2.376791
23	1	0	2.012785	1.916426	-0.605107
24	1	0	0.934357	1.921823	1.871863

```

Zero-point correction=                                0.181798
(Hartree/Particle)
Thermal correction to Energy=                          0.194902
Thermal correction to Enthalpy=                       0.195846
Thermal correction to Gibbs Free Energy=              0.142047
Sum of electronic and zero-point Energies=            -981.118458
Sum of electronic and thermal Energies=               -981.105354
Sum of electronic and thermal Enthalpies=             -981.104410
Sum of electronic and thermal Free Energies=          -981.158209

```

Association complex between **Cp₂Ti(OH)Cl** and **H-Pd(acrol)₂**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	22	0	-3.130942	0.116607	-0.657084
2	17	0	-1.352818	1.327391	-1.773899
3	8	0	-2.044658	-0.725001	0.552932
4	1	0	-1.738531	-0.266068	1.364845
5	1	0	1.913680	-1.585173	2.148780
6	46	0	2.386692	-0.786877	0.837505
7	6	0	3.596636	-2.579766	0.476635
8	6	0	4.420772	-1.549860	0.023254
9	6	0	4.390113	-1.069515	-1.366682
10	8	0	5.145203	-0.218030	-1.810737
11	6	0	2.186133	1.502248	0.933893
12	6	0	0.943999	0.928012	1.140699
13	6	0	0.415769	0.745866	2.506900
14	8	0	-0.746471	0.460773	2.767900
15	1	0	2.982395	-3.139098	-0.229154
16	1	0	3.802480	-3.076527	1.418184
17	1	0	5.210058	-1.144479	0.652381
18	1	0	3.631957	-1.559515	-2.018079
19	1	0	2.478316	1.856422	-0.050723
20	1	0	2.819352	1.802137	1.766360
21	1	0	0.235833	0.831770	0.317316
22	1	0	1.138152	0.921905	3.327969
23	6	0	-3.286834	1.894228	0.995399
24	6	0	-4.227429	0.895103	1.348148
25	6	0	-5.197383	0.826302	0.320722
26	6	0	-4.865836	1.804846	-0.662077
27	6	0	-3.696733	2.468027	-0.233215
28	1	0	-2.394628	2.146702	1.550584
29	1	0	-4.179330	0.254644	2.218713
30	1	0	-6.050367	0.162164	0.296489
31	1	0	-5.410459	2.008162	-1.574017
32	1	0	-3.165102	3.230216	-0.782488
33	6	0	-3.168067	-2.241975	-1.328563
34	6	0	-2.538643	-1.522286	-2.358235

35	6	0	-3.502921	-0.642317	-2.939372
36	6	0	-4.717115	-0.816680	-2.252366
37	6	0	-4.500595	-1.773873	-1.215276
38	1	0	-2.681672	-2.923966	-0.646790
39	1	0	-1.494088	-1.575374	-2.629043
40	1	0	-3.312963	0.061423	-3.737850
41	1	0	-5.642374	-0.293380	-2.450117
42	1	0	-5.235134	-2.120114	-0.500039

A flat potential energy surface around this geometry accounts for the high displacements observed. No actual minimum has been found. The energy data below give an idea of the reaction energy. Nevertheless, coordination of an additional ligand to Pd complex would render an exothermic process.

```
SCF Done:  E(UB+HF-LYP) = -1492.48240826      A.U. after  11 cycles
              Convg  =    0.6082D-08              -V/T =   2.0881
              S**2   =    0.7615
```

Item	Value	Threshold	Converged?
Maximum Force	0.000346	0.000450	YES
RMS Force	0.000052	0.000300	YES
Maximum Displacement	0.012637	0.001800	NO
RMS Displacement	0.002174	0.001200	NO

Predicted change in Energy=-1.016169D-06