

Pd_trPPh3_Cl_olefin_mal_min.out

E_solv = -2169.56937544701 a.u.

C	-0.05378	0.05827	-0.07435
C	0.20118	-0.16113	1.49402
H	0.80227	-0.36409	-0.60971
C	-0.09765	1.54072	-0.31278
O	-1.07027	2.25814	-0.11811
H	0.85797	1.99389	-0.63325
C	-1.30342	-0.68844	-0.45292
O	-2.44092	-0.27424	-0.27570
H	-1.14935	-1.69150	-0.88580
Na	-3.29075	1.79264	0.46046
Pd	0.64897	-1.88013	3.97552
Cl	2.10542	0.15317	4.72199
C	0.56585	-1.58110	1.83930
C	-0.36573	-2.57674	2.20440
H	1.00458	0.52018	1.79110
H	-0.15024	-3.62807	2.02314
H	-0.70939	0.16271	2.00687
H	-1.42756	-2.33899	2.27711
H	1.52519	-1.89976	1.42780
P	0.39843	-3.18957	5.94133
C	4.45562	-5.43474	6.50807
C	3.92823	-5.18844	5.23703
C	2.70910	-4.52344	5.10284
C	1.98712	-4.10419	6.23355
C	2.52539	-4.35923	7.50415
C	3.75177	-5.01745	7.63960
H	5.41325	-5.93985	6.61436
H	4.47385	-5.50137	4.34911
H	2.31483	-4.30308	4.11293
H	1.99319	-4.03728	8.39477
H	4.15852	-5.19865	8.63237
C	-2.87261	-6.51748	5.76077
C	-1.63078	-6.81966	6.32426
C	-0.63167	-5.84417	6.38871
C	-0.85681	-4.55415	5.88324
C	-2.10356	-4.26831	5.30324
C	-3.10741	-5.23695	5.25089
H	-3.65035	-7.27660	5.71328
H	-1.43739	-7.81572	6.71742
H	0.32748	-6.09164	6.83526
H	-2.27831	-3.28141	4.88143
H	-4.06983	-4.99541	4.80432
C	-0.30973	-1.19448	10.11002
C	0.47348	-0.57941	9.12934
C	0.65748	-1.19120	7.88730
C	0.06942	-2.43817	7.61154
C	-0.71845	-3.04644	8.60222
C	-0.90762	-2.42805	9.84172
H	-0.45619	-0.71358	11.07511
H	0.93702	0.38430	9.32929
H	1.25164	-0.69857	7.11969
H	-1.18653	-4.00795	8.41240
H	-1.52194	-2.91287	10.59796

Pd_trPPh3_Cl_olefin_mal_18min.out

E_solv = -2169.56421298489 a.u.

C	0.00880	0.25548	0.02004
C	-0.11154	0.07286	1.80671
H	1.07327	0.38259	-0.18028
C	-0.75150	1.49334	-0.25870
O	-1.97636	1.57740	-0.33642
H	-0.14262	2.41141	-0.33943
C	-0.51693	-1.01488	-0.52982
O	-1.70846	-1.29688	-0.63583
H	0.24186	-1.76211	-0.82208
Na	-3.64373	-0.03383	-0.29375
Pd	0.36304	-1.25317	4.42812
Cl	-0.18745	1.05972	5.47079
C	0.91219	-0.83164	2.36330
C	0.73507	-2.22146	2.55564
H	-0.00881	1.09753	2.16458
H	1.59985	-2.88069	2.60381
H	-1.14063	-0.26531	1.92972
H	-0.18555	-2.70777	2.23022
H	1.92653	-0.43296	2.36067
P	0.37590	-2.77292	6.25332
C	4.43712	-2.15099	8.46970
C	4.28881	-1.82607	7.11900
C	3.06300	-2.03018	6.48302
C	1.96879	-2.56802	7.18051
C	2.12950	-2.88955	8.53781
C	3.35464	-2.68150	9.17693
H	5.38770	-1.98264	8.97119
H	5.12274	-1.40302	6.56267
H	2.93560	-1.75373	5.43823
H	1.29527	-3.29460	9.10418
H	3.46142	-2.92838	10.23106
C	0.21897	-7.27370	5.01749
C	1.27583	-6.82724	5.81246
C	1.34600	-5.48646	6.20505
C	0.36370	-4.57047	5.80024
C	-0.68540	-5.02848	4.98326
C	-0.76466	-6.36829	4.60428
H	0.16268	-8.31786	4.71753
H	2.04817	-7.52271	6.13533
H	2.16863	-5.15884	6.83409
H	-1.44476	-4.32821	4.64075
H	-1.59072	-6.70561	3.98128
C	-2.76666	-2.50142	9.69935
C	-2.34793	-1.36312	9.00546
C	-1.41786	-1.47106	7.96866
C	-0.88514	-2.72313	7.61671
C	-1.31408	-3.86189	8.31850
C	-2.24893	-3.75148	9.35154
H	-3.49508	-2.41488	10.50292
H	-2.75244	-0.38783	9.26729
H	-1.10849	-0.58415	7.41889
H	-0.92034	-4.84080	8.05987
H	-2.57126	-4.64357	9.88479

Pd_trPPh3_Cl_olefin_mal_19min.out

E_solv = -2169.56116378232 a.u.

C	-0.05403	0.13360	0.00534
C	-0.08209	-0.00003	1.90043
H	1.00794	0.23225	-0.21623
C	-0.80235	1.36834	-0.24581
O	-2.03209	1.47796	-0.27368
H	-0.18209	2.27570	-0.36508
C	-0.61738	-1.15182	-0.42428
O	-1.81803	-1.42624	-0.49573
H	0.12388	-1.93711	-0.65539
Na	-3.70965	-0.10816	-0.20956
Pd	0.39712	-1.25604	4.50229
Cl	-0.19596	1.01169	5.57054
C	0.96089	-0.87782	2.41731
C	0.79363	-2.26297	2.66800
H	0.03978	1.04766	2.17057
H	1.66555	-2.91173	2.72309
H	-1.10906	-0.33306	2.03934
H	-0.12305	-2.76697	2.35876
H	1.96984	-0.46714	2.40445
P	0.41373	-2.79889	6.31082
C	4.43352	-2.21031	8.61421
C	4.30684	-1.84852	7.27035
C	3.09511	-2.04425	6.60431
C	1.99216	-2.60955	7.26497
C	2.13023	-2.96840	8.61587
C	3.34141	-2.76954	9.28423
H	5.37257	-2.04815	9.13861
H	5.14676	-1.40247	6.74184
H	2.98833	-1.73832	5.56563
H	1.28872	-3.39491	9.15506
H	3.42916	-3.04597	10.33267
C	0.21327	-7.28054	5.01027
C	1.28060	-6.85223	5.80169
C	1.36511	-5.51746	6.21308
C	0.38610	-4.58911	5.83033
C	-0.67437	-5.02797	5.01773
C	-0.76697	-6.36149	4.61994
H	0.14584	-8.31960	4.69650
H	2.05042	-7.55750	6.10820
H	2.19535	-5.20516	6.83979
H	-1.43372	-4.31834	4.69593
H	-1.60210	-6.68309	4.00106
C	-2.79266	-2.52161	9.69677
C	-2.33502	-1.37957	9.03457
C	-1.38533	-1.48708	8.01587
C	-0.87188	-2.74321	7.65009
C	-1.34011	-3.88601	8.31955
C	-2.29402	-3.77516	9.33513
H	-3.53612	-2.43515	10.48645
H	-2.72414	-0.40089	9.30663
H	-1.04790	-0.59616	7.49036
H	-0.96132	-4.86799	8.05151
H	-2.64606	-4.67029	9.84377

Pd_trPPh3_Cl_olefin_mal_20min_intopt.out

E_solv = -2169.55958544004 a.u.

C	0.00104	-0.00354	-0.00557
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C	0.01886	-0.00162	1.99434
H	1.06930	0.00101	-0.21445
C	-0.66269	1.25609	-0.29387
O	-1.88656	1.44812	-0.31178
H	0.01691	2.11156	-0.45931
C	-0.65441	-1.27302	-0.28201
O	-1.87722	-1.47671	-0.28816
H	0.02792	-2.12810	-0.44037
Na	-3.65051	-0.00569	-0.14846
Pd	0.38393	-1.11771	4.62845
Cl	-0.07334	1.10489	5.81756
C	1.04081	-0.85533	2.52831
C	0.83202	-2.21607	2.87944
H	0.17405	1.06521	2.12740
H	1.69213	-2.87386	2.99167
H	-1.01741	-0.30018	2.11332
H	-0.07895	-2.72514	2.56289
H	2.05797	-0.46431	2.51206
P	0.39027	-2.70716	6.40531
C	4.43968	-2.13970	8.64885
C	4.29946	-1.77723	7.30822
C	3.07729	-1.97052	6.65948
C	1.98150	-2.52585	7.33600
C	2.13263	-2.88242	8.68385
C	3.35317	-2.69003	9.33492
H	5.38767	-1.98630	9.16114
H	5.13723	-1.34565	6.76549
H	2.95982	-1.67007	5.62036
H	1.29276	-3.30011	9.23295
H	3.45401	-2.96124	10.38299
C	0.22869	-7.13236	4.93325
C	1.32005	-6.71083	5.69261
C	1.38937	-5.39291	6.15666
C	0.37047	-4.47897	5.86102
C	-0.71774	-4.90864	5.08006
C	-0.79314	-6.22534	4.62873
H	0.17271	-8.15885	4.57696
H	2.12078	-7.40741	5.93373
H	2.24013	-5.08285	6.75707
H	-1.50917	-4.20646	4.82162
H	-1.64789	-6.54537	4.03619
C	-2.77890	-2.56358	9.82477
C	-2.36720	-1.39644	9.17510
C	-1.43061	-1.45881	8.14184
C	-0.89008	-2.69305	7.74908
C	-1.30893	-3.86420	8.40268
C	-2.24796	-3.79716	9.43612
H	-3.51246	-2.51387	10.62688
H	-2.78486	-0.43628	9.46919
H	-1.12368	-0.54997	7.62736
H	-0.89983	-4.82793	8.11593
H	-2.56427	-4.71076	9.93632

Pd_trPPh3_Cl_olefin_mal_21min.out

E_solv = -2169.55932318904 a.u.

C	0.04286	0.04741	0.06939
C	0.06564	-0.09488	2.16444

H	1.11474	-0.03830	-0.09098
C	-0.48724	1.37597	-0.10788
O	-1.68795	1.70341	-0.14035
H	0.27538	2.17514	-0.17708
C	-0.72066	-1.13265	-0.24720
O	-1.96022	-1.21873	-0.31831
H	-0.12377	-2.05168	-0.39685
Na	-3.57384	0.41207	-0.21472
Pd	0.32872	-1.20497	4.70121
Cl	-0.24896	1.01903	5.79454
C	1.05435	-1.01374	2.61063
C	0.77720	-2.35877	2.98408
H	0.27092	0.96088	2.30731
H	1.60292	-3.05597	3.10923
H	-0.98416	-0.36205	2.23937
H	-0.15924	-2.82432	2.67254
H	2.08612	-0.66637	2.61595
P	0.38518	-2.75842	6.49667
C	4.42909	-2.02690	8.69967
C	4.26650	-1.68386	7.35601
C	3.04785	-1.92259	6.71838
C	1.97637	-2.51254	7.40871
C	2.15131	-2.85349	8.75906
C	3.36961	-2.61130	9.39849
H	5.37369	-1.83149	9.20230
H	5.08238	-1.21956	6.80670
H	2.91233	-1.63253	5.67926
H	1.33454	-3.29884	9.31987
H	3.48830	-2.87338	10.44687
C	0.29027	-7.23007	5.16700
C	1.38190	-6.76227	5.90081
C	1.43341	-5.42815	6.31959
C	0.39478	-4.54186	6.00162
C	-0.69289	-5.01923	5.24840
C	-0.74996	-6.35234	4.84254
H	0.24939	-8.26869	4.84700
H	2.19717	-7.43577	6.15616
H	2.28483	-5.08462	6.89986
H	-1.50236	-4.34373	4.98015
H	-1.60462	-6.70593	4.26959
C	-2.75657	-2.55906	9.93633
C	-2.37060	-1.40813	9.24447
C	-1.44289	-1.48862	8.20384
C	-0.88244	-2.72637	7.84675
C	-1.27916	-3.87985	8.54383
C	-2.21001	-3.79512	9.58212
H	-3.48152	-2.49327	10.74461
H	-2.79681	-0.44387	9.51184
H	-1.15474	-0.59127	7.66098
H	-0.86190	-4.84730	8.28061
H	-2.50623	-4.69653	10.11429

Pd_trPPh3_Cl_olefin_mal_22min.out

E_solv = -2169.56104691802 a.u.

C	0.00846	-0.10163	0.08698
C	0.12305	-0.12487	2.28387
H	1.07977	-0.14366	-0.09004

C	-0.59446	1.18200	-0.10126
O	-1.81377	1.45431	-0.08530
H	0.12004	2.01598	-0.24113
C	-0.69865	-1.33221	-0.09516
O	-1.93604	-1.49909	-0.07466
H	-0.05854	-2.22465	-0.23351
Na	-3.60921	0.05997	0.01355
Pd	0.32860	-1.12679	4.80447
Cl	-0.30017	1.03441	5.94014
C	1.13942	-0.99519	2.72157
C	0.88587	-2.32853	3.16293
H	0.30790	0.94284	2.31323
H	1.72782	-2.99499	3.33718
H	-0.91899	-0.42136	2.33794
H	-0.02468	-2.83585	2.84124
H	2.15979	-0.61671	2.73027
P	0.38074	-2.69947	6.57524
C	4.45157	-2.13389	8.77737
C	4.30205	-1.77849	7.43427
C	3.07291	-1.95772	6.79664
C	1.97759	-2.50414	7.48641
C	2.13816	-2.85821	8.83569
C	3.36678	-2.67205	9.47531
H	5.40475	-1.98383	9.27913
H	5.13730	-1.35001	6.88478
H	2.95165	-1.65636	5.75875
H	1.30345	-3.27114	9.39510
H	3.47400	-2.94361	10.52300
C	0.23369	-7.11577	5.09680
C	1.34049	-6.68109	5.82725
C	1.40723	-5.36301	6.29031
C	0.36808	-4.46230	6.01958
C	-0.73630	-4.90595	5.27065
C	-0.80761	-6.22329	4.82035
H	0.18140	-8.14251	4.74186
H	2.15524	-7.36822	6.04483
H	2.27013	-5.04342	6.86692
H	-1.54795	-4.21814	5.04303
H	-1.67385	-6.55306	4.25082
C	-2.80815	-2.59900	9.97510
C	-2.41403	-1.42617	9.32651
C	-1.46859	-1.47103	8.29899
C	-0.90074	-2.69616	7.91104
C	-1.30387	-3.87218	8.56729
C	-2.25122	-3.82188	9.59269
H	-3.54787	-2.56077	10.77189
H	-2.84793	-0.47190	9.61629
H	-1.17650	-0.55654	7.78856
H	-0.88205	-4.83078	8.28023
H	-2.55381	-4.73982	10.09199

Pd_trPPH3_Cl_olefin_mal_23min_intopt.out

E_solv = -2169.56390961251 a.u.

C	-0.01343	-0.09965	-0.02432
C	-0.02094	0.00134	2.27345
H	1.07041	-0.12663	-0.07975
C	-0.62060	1.15782	-0.29627

O	-1.84391	1.40839	-0.40442
H	0.08689	2.00474	-0.39154
C	-0.67838	-1.34982	-0.14201
O	-1.91441	-1.55439	-0.19338
H	-0.01209	-2.23451	-0.15185
Na	-3.59412	-0.02920	-0.42504
Pd	0.08952	-0.71550	4.76397
Cl	-1.06792	1.31427	5.64588
C	1.08542	-0.69824	2.76443
C	0.97115	-2.00152	3.33389
H	0.02062	1.07922	2.19233
H	1.87353	-2.52120	3.64490
H	-1.00705	-0.44452	2.24002
H	0.15796	-2.65769	3.01941
H	2.04313	-0.18160	2.80042
P	0.34949	-1.99219	6.74435
C	3.61006	0.09256	9.33605
C	3.56648	0.27093	7.95103
C	2.57767	-0.36210	7.19612
C	1.62651	-1.19157	7.81165
C	1.67781	-1.36576	9.20396
C	2.66327	-0.72544	9.95946
H	4.37125	0.59543	9.92789
H	4.29229	0.91359	7.45798
H	2.52856	-0.20191	6.12153
H	0.94485	-1.99256	9.70435
H	2.68753	-0.86179	11.03810
C	1.86395	-6.29696	5.82108
C	2.67051	-5.43739	6.56783
C	2.23007	-4.14632	6.87754
C	0.97867	-3.69921	6.43419
C	0.17727	-4.56864	5.67202
C	0.61253	-5.85910	5.37509
H	2.20715	-7.30139	5.58406
H	3.64541	-5.76940	6.91713
H	2.86565	-3.49214	7.46676
H	-0.79292	-4.23559	5.30901
H	-0.02263	-6.52205	4.79160
C	-3.26192	-2.64556	9.61711
C	-3.14861	-1.47316	8.86553
C	-2.06794	-1.29208	7.99890
C	-1.08211	-2.28540	7.87744
C	-1.20362	-3.46221	8.63675
C	-2.28670	-3.63915	9.50103
H	-4.10732	-2.78569	10.28748
H	-3.90717	-0.69791	8.94851
H	-1.98886	-0.38229	7.40897
H	-0.45582	-4.24566	8.55540
H	-2.36767	-4.55565	10.08181

Pd_trPPh3_Cl_olefin_mal_24min_intopt.out

E_solv = -2169.56728209338 a.u.

C	0.01928	0.01677	-0.01642
C	-0.00947	-0.00609	2.38330
H	1.10467	0.05078	-0.02700
C	-0.64901	1.25086	-0.20955
O	-1.88468	1.44754	-0.32152

H	0.01200	2.13977	-0.24139
C	-0.57649	-1.25886	-0.16660
O	-1.80184	-1.52999	-0.24316
H	0.13490	-2.10848	-0.18539
Na	-3.54342	-0.07899	-0.43149
Pd	0.00144	-0.79657	4.76430
Cl	-1.13614	1.17389	5.76237
C	1.08708	-0.74742	2.81988
C	0.93134	-2.06616	3.34408
H	0.05532	1.07104	2.30656
H	1.81186	-2.60905	3.67712
H	-0.99217	-0.44622	2.26454
H	0.12063	-2.69706	2.97687
H	2.05134	-0.24934	2.90273
P	0.15848	-2.09310	6.74189
C	2.77070	0.25957	9.78696
C	2.88544	0.48861	8.41391
C	2.09084	-0.22916	7.51913
C	1.17994	-1.19059	7.98383
C	1.07152	-1.41462	9.36539
C	1.86296	-0.69158	10.26001
H	3.37980	0.82692	10.48696
H	3.58176	1.23532	8.03889
H	2.15971	-0.03250	6.45216
H	0.36321	-2.14405	9.74807
H	1.76568	-0.86713	11.32883
C	2.22905	-6.19745	6.01814
C	2.84163	-5.26357	6.85445
C	2.22893	-4.03129	7.10458
C	0.99793	-3.71870	6.51237
C	0.39320	-4.66184	5.66182
C	0.99987	-5.89376	5.42278
H	2.70599	-7.15610	5.82780
H	3.79777	-5.49163	7.32017
H	2.71350	-3.31759	7.76415
H	-0.55805	-4.43372	5.18533
H	0.51505	-6.61534	4.76893
C	-3.74745	-3.15519	9.04878
C	-3.64563	-1.96346	8.32668
C	-2.47463	-1.66098	7.62734
C	-1.38648	-2.54967	7.64724
C	-1.49683	-3.74642	8.37541
C	-2.67047	-4.04540	9.07153
H	-4.66194	-3.39026	9.58907
H	-4.48127	-1.26759	8.30275
H	-2.39890	-0.73247	7.06742
H	-0.67041	-4.45034	8.39943
H	-2.74166	-4.97553	9.63079

Pd_trPPh3_Cl_olefin_mal_25min.out

E_solv = -2169.57137812064 a.u.

C	-0.45586	-0.33280	0.23146
C	0.36281	-0.95242	2.51090
H	0.03746	-1.22049	-0.15275
C	0.25028	0.88596	0.11238
O	-0.14044	2.04139	0.42152
H	1.27959	0.79010	-0.28846

C	-1.83085	-0.44735	0.53702
O	-2.61260	0.45877	0.92709
H	-2.25014	-1.46807	0.43298
Na	-2.19051	2.68454	1.12453
Pd	0.56866	-1.85508	4.76719
Cl	2.11119	-0.09652	5.59604
C	0.28997	-2.34060	2.61534
C	-0.68848	-2.95987	3.44577
H	1.26868	-0.47433	2.16392
H	-0.68968	-4.04158	3.54724
H	-0.45104	-0.30888	2.81998
H	-1.66157	-2.48514	3.57706
H	1.10728	-2.93822	2.21569
P	0.37885	-3.16093	6.75323
C	4.51878	-5.17720	7.41258
C	4.09391	-4.80803	6.13407
C	2.84898	-4.20150	5.96164
C	2.00765	-3.96709	7.06148
C	2.44222	-4.34253	8.34220
C	3.69191	-4.94218	8.51432
H	5.49412	-5.63808	7.55097
H	4.73549	-4.97858	5.27235
H	2.53127	-3.89034	4.96898
H	1.81323	-4.16128	9.20909
H	4.02176	-5.22175	9.51214
C	-2.75109	-6.58119	6.33066
C	-1.40835	-6.90772	6.52464
C	-0.45046	-5.89862	6.67060
C	-0.82822	-4.55000	6.61542
C	-2.18210	-4.23069	6.40838
C	-3.13680	-5.23766	6.27474
H	-3.49463	-7.36730	6.22148
H	-1.10066	-7.95009	6.56820
H	0.58918	-6.16847	6.83015
H	-2.49362	-3.18973	6.35359
H	-4.18118	-4.97412	6.12325
C	-0.66721	-1.17107	10.83327
C	0.04087	-0.46635	9.85649
C	0.33651	-1.06589	8.63008
C	-0.07217	-2.38408	8.36908
C	-0.78582	-3.08594	9.35538
C	-1.07935	-2.48179	10.57993
H	-0.89842	-0.70104	11.78669
H	0.36179	0.55534	10.04677
H	0.88581	-0.51326	7.87212
H	-1.11383	-4.10479	9.17243
H	-1.63084	-3.03742	11.33508