1
Gas phase Energy: -1121.52944957348 hartrees
Solvation Energy: -1121.53821566197 hartrees
Zero Point Energy: 107.368 kcal/mol
Free Energy: -23.933 kcal/mol
final geometry:

angstroms

atom	x	y	z
Pd1	-0.0087289642	-0.1853027357	-0.1742667191
C2	0.0816154994	0.2840516883	1.8935569690
P3	2.2407155306	-0.4904926026	0.1442819713
C4	1.3217423677	0.5022929080	2.5354093663
C5	2.6026768181	0.4423895517	1.7192300953
C6	-1.0966135487	0.3890009094	2.6671923511
H7	3.2928843435	-0.1200415430	-0.7239547417
C8	1.3778219659	0.8049569474	3.9019135361
H9	2.9161108504	1.4492206880	1.4119373491
C10	0.2020791261	0.9146759610	4.6442258074
H11	3.4407015433	0.0026175264	2.2704512812
C12	-1.0331397654	0.7122594286	4.0286392646
H13	2.6618570054	-1.8094475140	0.4256107171
C14	-2.4415887774	0.1109484314	2.0155404679
P15	-2.2298526353	0.2678567938	0.1681243801
H16	-1.9460734483	0.7983213906	4.6145046976
H17	-2.7566127960	-0.9250219140	2.1995529515
H18	0.2484059210	1.1577830518	5.7023540156
H19	-3.2408436742	0.7585954848	2.3913440669
H20	2.3378299341	0.9648056604	4.3886966955
H21	-2.6516940470	1.5869503150	-0.1115060859
H22	-3.3428448704	-0.4210762865	-0.3654309455
H23	-0.0774624436	-0.5430265691	-1.7553052049

2
Gas phase Energy: -1271.84775687578 hartrees
Solvation Energy: -1271.85559109325 hartrees
Zero Point Energy: 109.963 kcal/mol
Free Energy: -28.176 kcal/mol
final geometry:

angstroms

atom	x	y	z
Pd1	-0.0367924548	0.3409028405	-0.4072654335
C2	0.1617034450	0.2652864542	1.7037249300
P3	2.2414230789	0.1367493769	-0.2801317935
C4	1.4196703329	0.4466901489	2.3209235298

C5	2.6430183816	0.6976342093	1.4535717103
C6	-0.9669639208	0.0723324187	2.5323119061
H7	3.2207448003	0.7668181186	-1.0815967679
C8	1.5410342396	0.4334017919	3.7162457563
H9	2.8574266849	1.7724746470	1.3830471365
C10	0.4120062669	0.2572309666	4.5159508392
H11	3.5477054095	0.2163199666	1.8401049345
C12	-0.8402433326	0.0800794456	3.9269866630
H13	2.7481891487	-1.1812602098	-0.3363739940
C14	-2.3219311049	-0.1775510882	1.8908923593
P15	-2.2608375291	0.4816063759	0.1457238759
H16	-1.7162351745	-0.0584739438	4.5574819058
H17	-2.5155566205	-1.2551255875	1.8009707700
H18	0.5075128754	0.2592992856	5.5983978524
H19	-3.1525557601	0.2497806141	2.4624462067
H20	2.5143026767	0.5720388589	4.1827570791
H21	-2.8233661212	1.7729854181	0.2512664618
H22	-3.3413691825	-0.1610523901	-0.5011098958
H23	-0.1868418133	0.4321856333	-2.0201054250
O24	-1.4576092186	-2.4052919003	-2.5143047377
O25	-1.2793502547	-2.6564686489	-1.3401893580

3
Gas phase Energy: -1271.83997495622 hartrees
Solvation Energy: -1271.84533806202 hartrees
Zero Point Energy: 112.004 kcal/mol
Free Energy: -27.855 kcal/mol
final geometry:

angstroms

atom	x	y	z
Pd1	-0.3440219136	0.0412034236	-0.2877561468
C2	-0.0550775272	0.3315008846	1.7740964092
P3	1.9625808810	-0.3301854645	-0.2766534560
C4	1.2477358703	0.4840111621	2.2830335607
C5	2.4317316355	0.4930066496	1.3326083240
C6	-1.1613670871	0.3580147403	2.6404137824
H7	3.0025716077	0.0963479234	-1.1323577959
C8	1.4350311780	0.6565684728	3.6617885092
H9	2.7063702477	1.5235092497	1.0720452772
C10	0.3351322112	0.6967638484	4.5190030264
H11	3.3200577028	0.0331991436	1.7753422703
C12	-0.9580139126	0.5536661382	4.0134221467
H13	2.3651085174	-1.6701331182	-0.0906976423
C14	-2.5596172220	0.1348026654	2.0927171798
P15	-2.5728704276	0.4631892952	0.2499327384
H16	-1.8084653487	0.5849992144	4.6913823597

H17	-2.8499940140	-0.9169100716	2.2092120674
H18	0.4863693955	0.8399512371	5.5854770455
H19	-3.3123393736	0.7301787972	2.6170605314
H20	2.4389400763	0.7668910586	4.0667002619
H21	-2.9790906071	1.8160901424	0.1616018142
H22	-3.8028117288	-0.1290969652	-0.1367758544
H23	0.2499905713	-0.8509975119	-2.3941817549
O24	0.5720717531	-1.3656916601	-3.1991278458
O25	1.8008692885	-1.7152456871	-2.8673331251

4
Gas phase Energy: -1271.89067143898 hartrees
Solvation Energy: -1271.90437808260 hartrees
Zero Point Energy: 113.520 kcal/mol
Free Energy: -26.508 kcal/mol
final geometry:

angstroms

atom	x	y	z
Pd1	0.0804138907	-0.2677198075	-0.1159738522
C2	0.1022089376	0.3044661018	1.8833197643
P3	2.3511390101	-0.5517655513	0.3006564964
C4	1.3145823424	0.6044483116	2.5479808419
C5	2.6258574049	0.5294303135	1.7864298026
C6	-1.1059235964	0.4352366761	2.6120705025
H7	3.4207405881	-0.2433336964	-0.5708855810
C8	1.3159540483	1.0047961366	3.8897950048
H9	2.9059230434	1.5176399330	1.3977620553
C10	0.1165651854	1.1373098199	4.5869269617
H11	3.4579043983	0.1804999366	2.4061295442
C12	-1.0897079680	0.8586010610	3.9464687536
H13	2.7847886602	-1.8292538527	0.7203565628
C14	-2.4307926202	0.0821292467	1.9556120310
P15	-2.1744627035	0.1286370873	0.1173409088
H16	-2.0260068473	0.9638507022	4.4905425270
H17	-2.7172436017	-0.9499515819	2.1981875368
H18	0.1213913164	1.4573423228	5.6251006640
H19	-3.2504172057	0.7274089213	2.2871952660
H20	2.2576542265	1.2230794858	4.3891768783
H21	-2.6769697788	1.3806013914	-0.2963693651
H22	-3.1586369164	-0.7122107318	-0.4361127710
O23	0.0188479646	-0.8294140605	-2.0776288075
O24	-1.2350117791	-0.3362198110	-2.6692280588
H25	-0.8890853543	0.3853879066	-3.2150371320

4 triplet
Gas phase Energy: -1271.83959920689 hartrees

Solvation Energy: - -1271.84800761887hartrees
Zero Point Energy: 112.110 kcal/mol
Free Energy: -28.191 kcal/mol
final geometry:

angstroms

atom	x	y	z
Pd1	0.1589929141	0.2957941677	-0.3193576694
C2	0.0813288234	0.1518260463	1.7975730825
P3	2.5208277552	-0.0182709554	0.0783387143
C4	1.2563982756	0.1897337430	2.5651281702
C5	2.6022724169	0.4183747515	1.8962826002
C6	-1.1695642622	0.0062728974	2.4240730356
H7	3.7678025114	0.5047029220	-0.3630285383
C8	1.1752089277	0.0597532294	3.9588948982
H9	2.8670263151	1.4839585480	1.9325088400
C10	-0.0655132915	-0.0854317196	4.5802231840
H11	3.4090832704	-0.1245414098	2.3988312765
C12	-1.2352680291	-0.1052907795	3.8189615398
H13	2.8932966987	-1.3829783853	0.0818364400
C14	-2.4302703886	-0.0592626754	1.5793172024
P15	-2.1791215778	0.9096950252	-0.0004348438
H16	-2.1991336248	-0.2137260809	4.3120042736
H17	-2.6142607955	-1.0875272566	1.2413733343
H18	-0.1219044208	-0.1795604511	5.6612807993
H19	-3.3171104280	0.2704296855	2.1285861748
H20	2.0811421588	0.0804054390	4.5617404443
H21	-2.5218643129	2.2200339694	0.4171835057
H22	-3.3724397527	0.6114366479	-0.7063481248
O23	-0.1681702101	-1.5963440589	-1.3518239351
O24	-1.4382317126	-2.1123744430	-1.0479614917
H25	-1.2239699459	-2.8251890894	-0.4216670995

6
Gas phase Energy: -1121.56311965546 hartrees
Solvation Energy: -1121.56567261868 hartrees
Zero Point Energy: 109.906 kcal/mol
Free Energy: -24.413 kcal/mol
final geometry:

angstroms

atom	x	y	z
Pd1	0.0095947420	0.0746530894	-0.8315119145
C2	0.0218225441	-0.7473622342	2.0875880931
P3	2.2438281621	-0.0528168767	-0.1452900316
C4	1.3001627292	-0.3118804747	2.4474509286
C5	2.4550750456	-0.7883423720	1.6025699924
C6	-1.1331040691	-0.0897043891	2.5199906195

H7	2.8662580539	1.2043039982	0.0784804830
C8	1.4130782571	0.7027186432	3.4050134673
H9	3.4269864098	-0.5029197921	2.0137885990
C10	0.2627068167	1.2845172585	3.9454453871
H11	2.4422910997	-1.8766375210	1.4777401196
C12	-1.0038137883	0.9235625617	3.4769252989
H13	3.3811236883	-0.6467033566	-0.7668487969
C14	-2.4029507305	-0.3447196424	1.7472254544
P15	-2.1657145534	0.3507768745	-0.0135774413
H16	-1.8857761161	1.4490143952	3.8358901429
H17	-2.5942769924	-1.4166774390	1.6270440647
H18	0.3561659157	2.0619353208	4.6988564565
H19	-3.2813666916	0.1090480591	2.2137573342
H20	2.3951637437	1.0578004426	3.7087174890
H21	-2.5356247692	1.6985254028	0.2405464341
H22	-3.4264884091	-0.0235449648	-0.5638282827
H23	-0.0724750007	-1.5387958207	1.3488590717

7
Gas phase Energy: -1121.50336393231 hartrees
Solvation Energy: - -1121.50813301884 hartrees
Zero Point Energy: 105.984 kcal/mol
Free Energy: -26.435 kcal/mol
final geometry:

	angstroms		
atom	x	y	z
Pd1	0.0959054625	-0.1150612037	-0.0519551191
C2	0.3026963406	0.3088343585	1.8769101289
P3	2.5200747116	-0.2942808160	0.2649039846
C4	1.4297411514	0.4906529501	2.6683156527
C5	2.7848176012	0.4222304492	1.9936064436
C6	-1.0000138628	0.3802018203	2.3283405086
H7	3.6843208167	0.1766190284	-0.4029358272
C8	1.1858352608	0.7489902385	4.0287095105
H9	3.2175675647	1.4225475964	1.8633362409
C10	-0.1294462536	0.8195623336	4.5100614164
H11	3.5177894768	-0.1714622265	2.5497064637
C12	-1.2481048334	0.6414947467	3.6748426849
H13	2.9752459922	-1.6240347504	0.4463223514
C14	-1.7731874254	0.1196687527	1.0503281309
P15	-0.7152926648	-0.5698263438	-2.2666538806
H16	-2.2540890287	0.7070889135	4.0840701345
H17	-2.3570796644	-0.8036632621	1.0294489042
H18	-0.2856590520	1.0213577894	5.5671347353
H19	-2.3527565663	0.9652737427	0.6725988968
H20	2.0134930469	0.8996330325	4.7197001721

H21	0.0672585634	-0.8122829801	-3.4255995618
H22	-1.5860436390	-1.6738404576	-2.4347043920
H23	-1.5667916458	0.3961372259	-2.8556304452

8
Gas phase Energy: -1121.49829128369 hartrees
Solvation Energy: -1121.50588015165 hartrees
Zero Point Energy: 106.678 kcal/mol
Free Energy: -25.238 kcal/mol
final geometry:

angstroms

atom	x	y	z
Pd1	-0.1379062012	-0.0838928165	-0.0295424778
C2	0.0071092402	0.6082191475	1.8696050815
P3	2.1126434429	-0.9751311735	0.3605671783
C4	1.3278696110	0.7252172819	2.3614408439
C5	2.5273285598	0.4691852428	1.4708903370
C6	-1.0883357997	0.8273804594	2.7286245272
H7	3.2330203409	-1.0488486965	-0.5047757960
C8	1.5484022540	1.0633431870	3.7021523436
H9	2.7115408070	1.3188514235	0.8023310017
C10	0.4747219319	1.2928097119	4.5526604115
H11	3.4321833867	0.3016982305	2.0600065429
C12	-0.8217384810	1.1702587523	4.0666620398
H13	2.4295747503	-2.0950216529	1.1664548295
C14	-2.5406216201	0.6964880787	2.3353180235
P15	-3.2522475083	-1.0558685008	2.2392602518
H16	-1.6617155826	1.3425294585	4.7352323973
H17	-3.1689193777	1.2410292583	3.0476433684
H18	0.6471336332	1.5597747626	5.5913730903
H19	-2.7123921037	1.1281241983	1.3446156493
H20	2.5675205377	1.1470971055	4.0718570505
H21	-2.2353761826	-1.6217197387	1.4182865293
H22	-2.6825380821	-1.5547407440	3.4476298134
H23	-1.3996219105	0.8182748994	-0.1278706000

TS1
Gas phase Energy: -1271.82464798774 hartrees
Solvation Energy: -1271.83186884053 hartrees
Zero Point Energy: 108.228 kcal/mol
Free Energy: -28.277 kcal/mol
Number and Magnitude of negative Eigen values: 1 (-1360.28cm^{-1})
final geometry:

angstroms

atom	x	y	z
Pd1	-0.2439779381	-0.0270403072	-0.2459198711

C2	-0.0217983735	0.3817702541	1.8208882816
P3	2.0346508641	-0.3314155075	-0.1393644855
C4	1.2653358310	0.5577596141	2.3678568292
C5	2.4868069758	0.5147025419	1.4626920195
C6	-1.1511752125	0.4573332464	2.6591462994
H7	3.0026333209	0.1340279873	-1.0545831113
C8	1.4111286361	0.8064931311	3.7387172628
H9	2.7974188852	1.5317558439	1.1885586465
C10	0.2867492249	0.8983937524	4.5596440941
H11	3.3487174538	0.0398499863	1.9429263532
C12	-0.9903079772	0.7284974295	4.0241906999
H13	2.5078853833	-1.6517787014	0.0186271144
C14	-2.5351192651	0.1989248905	2.0857862526
P15	-2.4661566684	0.4022008472	0.2298448237
H16	-1.8606744170	0.7982074227	4.6734379124
H17	-2.8360003943	-0.8421205938	2.2635375953
H18	0.4063828269	1.1006773736	5.6203533215
H19	-3.3053320308	0.8343319820	2.5348443194
H20	2.4030909000	0.9362559396	4.1667665742
H21	-2.9154729098	1.7262694378	0.0241437788
H22	-3.6277614525	-0.2725668970	-0.2143352212
H23	-0.2211005299	-0.4642148383	-1.9339072723
O24	0.1402094928	-0.9403099538	-3.1673587010
O25	1.3450113185	-1.3320733713	-3.1633118370

MECP
Gas phase Energy: -1271.83757028133 hartrees
Solvation Energy: -1271.85558113356 hartrees
Zero Point Energy: 111.989 kcal/mol
Free Energy: 21.04 kcal/mol

final geometry:

C1	0.07776652	0.12842125	4.08922455
C2	0.48880929	1.27479863	3.40704006
C3	0.51377015	1.28716716	2.00544951
C4	0.09796671	0.15198968	1.27050594
C5	-0.30898623	-1.00341036	1.97976825
C6	-0.30849944	-1.00988204	3.38203535
Pd7	0.11107739	0.17305723	-0.80553304
C8	-0.78536402	-2.23515076	1.22713823
P9	-0.03877984	-2.27450188	-0.48481157
C10	1.04821167	2.51503753	1.28972334
P11	0.17944308	2.80032987	-0.34588683
H12	0.65368899	4.12691991	-0.60384244
H13	-0.72396100	-3.38790526	-1.04738641
H14	1.19776193	-2.93147299	-0.26515927

H15	-1.11607308	3.18850839	0.07358385
H16	0.06283876	0.12138442	5.17573296
H17	0.80646428	2.15034503	3.97204236
H18	-0.61848873	-1.90066891	3.92634326
H19	-0.59403001	-3.16008086	1.78304858
H20	-1.86986453	-2.17907427	1.05564144
H21	1.00064337	3.41263056	1.91640363
H22	2.10291654	2.36411470	1.02202131
O23	0.26251154	0.35910000	-2.96506240
O24	0.47277440	1.61320281	-3.43059006
H25	0.40418274	2.17840880	-2.61639499

Isolated (PCP)Pd radical
Gas phase Energy: -1120.92598478847 hartrees
Solvation Energy: -1120.92978548690 hartrees
Zero Point Energy: 102.097 kcal/mol
Free Energy: -24.513 kcal/mol
final geometry:

angstroms

atom	x	y	z
Pd1	-0.3461324479	0.0353521914	-0.2965142317
C2	-0.0533936597	0.3218059284	1.7718543284
P3	1.9775848036	-0.3459871902	-0.2678341939
C4	1.2458429530	0.4916930040	2.2824674479
C5	2.4316349331	0.5158462197	1.3323730919
C6	-1.1568690548	0.3437122701	2.6433620300
H7	3.0790878736	0.0189092506	-1.0886051384
C8	1.4341761755	0.6719086519	3.6595497000
H9	2.6772432045	1.5490876770	1.0523782444
C10	0.3358443529	0.7045042295	4.5197234863
H11	3.3327644632	0.0838002531	1.7794525027
C12	-0.9557443239	0.5466714850	4.0154236912
H13	2.3891933764	-1.6759558877	-0.0099963549
C14	-2.5550365845	0.1103972985	2.0952494678
P15	-2.5870791872	0.4970396651	0.2623921330
H16	-1.8064642632	0.5742823825	4.6937800266
H17	-2.8272756893	-0.9503696668	2.1784798221
H18	0.4868159125	0.8530223349	5.5855781899
H19	-3.3161340736	0.6789687651	2.6392823777
H20	2.4380671042	0.7948776536	4.0617591293
H21	-2.9634849538	1.8620283323	0.2583639418
H22	-3.8555371324	-0.0320853752	-0.0999064925

O_2
Gas phase Energy: -150.31662268192 hartrees

Solvation Energy: -150.31662292754 hartrees
Zero Point Energy: 2.374 kcal/mol
Free Energy: -12.537 kcal/mol
final geometry:

angstroms

atom	x	y	z
O1	0.0000000000	0.0000000000	-0.0071239380
O2	0.0000000000	0.0000000000	1.2071239380

HO_2 radical
Gas phase Energy: -150.90084968382 hartrees
Solvation Energy: -150.90616540387 hartrees
Zero Point Energy: 8.864 kcal/mol
Free Energy: -13.923 kcal/mol
final geometry:

angstroms

atom	x	y	z
H1	0.0903646611	0.0000000000	0.0494563780
O2	-0.0850528388	0.0000000000	1.0129913814
O3	1.1185895282	0.0000000000	1.5838924172