

Supporting information

A DFT-based explanation of the effect of simple anionic ligands on the regioselectivity of the Heck arylation of acrolein acetals

Signe Teuber Henriksen, David Tanner, Sandro Cacchi, and Per-Ola Norrby

Geometries and energies at the B3LYP/LACVP* level, with numbering following the main text. All geometries were determined both in gas phase and with a continuum solvation model representing DMF.

1a

Gas phase:

 $E_{\text{scf}} = -933.83179730215$ a.u. $G(T)-E(0) = 0.220910$ a.u.Lowest frequency: 16.53 cm⁻¹

Pd	0.00000	0.00000	0.00000
C	0.00000	0.00000	4.79694
C	1.17165	0.00000	4.03761
C	1.11108	0.00861	2.64032
C	-0.13324	0.03099	1.99842
C	-1.30840	0.03130	2.75218
C	-1.23584	0.00964	4.15105
H	0.05125	-0.01276	5.88262
H	2.14223	-0.01538	4.52821
H	2.02926	-0.02537	2.06194
H	-2.27767	0.04562	2.26641
H	-2.15578	0.00350	4.73188
C	-1.52545	1.64816	-0.11161
C	-1.97251	0.59979	-0.88644
H	-0.89459	2.42196	-0.54230
H	-1.63473	0.52216	-1.91901
H	-1.96378	1.85509	0.85731
C	-3.15971	-0.30745	-0.60680
H	-2.83474	-1.35621	-0.56340
O	-4.05831	-0.28810	-1.70036
O	-3.76875	0.07002	0.59839
C	-4.73689	-0.86928	1.06226
H	-5.13597	-0.46892	1.99641
H	-5.54825	-0.99379	0.33679
H	-4.27275	-1.84704	1.25385
C	-4.66842	0.97305	-1.97124
H	-5.37451	0.79551	-2.78506
H	-5.20580	1.35663	-1.09657
H	-3.93398	1.72333	-2.29346
O	0.90514	-0.48461	-2.03762
C	1.84587	-1.04763	-1.40749
O	1.83086	-1.08574	-0.12130
C	3.01029	-1.67688	-2.13255
H	2.83347	-1.67982	-3.20992
H	3.92381	-1.11221	-1.91420
H	3.16363	-2.69928	-1.77278

Solution:

 $E_{\text{sol}} = -933.85194$ a.u.

Pd	-0.02105	-0.01658	-0.02081
C	0.05100	0.19566	4.75403
C	1.15877	0.55383	3.98042
C	1.07923	0.53948	2.58153
C	-0.12032	0.16697	1.96299
C	-1.23708	-0.17302	2.72726
C	-1.14264	-0.16803	4.12632
H	0.11903	0.20127	5.83939
H	2.09283	0.84105	4.45897
H	1.95490	0.79784	1.99357
H	-2.17123	-0.43706	2.24364
H	-2.01008	-0.44692	4.72087
C	-1.58300	1.63588	-0.03389
C	-1.97328	0.67832	-0.94208
H	-0.95307	2.46610	-0.34386
H	-1.60333	0.74518	-1.96509
H	-2.06584	1.71971	0.93316
C	-3.16353	-0.26022	-0.82794
H	-2.88089	-1.26708	-1.16203
O	-4.15880	0.13308	-1.76593
O	-3.64280	-0.29685	0.48434
C	-4.61285	-1.32786	0.71026
H	-4.89304	-1.26929	1.76370
H	-5.50235	-1.18131	0.08813
H	-4.18441	-2.31745	0.50020
C	-4.76248	1.41556	-1.53967
H	-5.57007	1.50110	-2.27147
H	-5.17874	1.48896	-0.52880
H	-4.05118	2.23626	-1.69843
O	0.89587	-0.82478	-1.99128
C	1.81772	-1.32577	-1.28233
O	1.80360	-1.15312	-0.00814
C	2.94039	-2.12469	-1.89740
H	2.80734	-2.20961	-2.97901
H	3.89930	-1.63848	-1.68231
H	2.96845	-3.12528	-1.45008

2a

Gas phase:

E_{scf} = -933.81475230992 a.u.

G(T)-E(0) = 0.222237 a.u.

Lowest frequency: -291.77 cm⁻¹

Solution:

E_{sol} = -933.83836 a.u.

Pd	0.00000	0.00000	0.00000
C	0.00000	0.00000	4.69715
C	1.22785	0.00000	4.03159
C	1.29403	0.33697	2.67815
C	0.11969	0.65029	1.97975
C	-1.10943	0.68280	2.65643
C	-1.16665	0.34292	4.00812
H	-0.04672	-0.25650	5.75214
H	2.13818	-0.26006	4.56590
H	2.25313	0.33876	2.16649
H	-2.01036	0.97193	2.12227
H	-2.12282	0.35234	4.52554
C	0.34287	2.22732	0.68438
C	0.09717	1.95450	-0.69368
H	1.36375	2.43753	0.98737
H	0.94772	1.95312	-1.37598
H	-0.41781	2.76822	1.23392
C	-1.20746	2.34210	-1.37344
H	-1.44679	1.61300	-2.15811
O	-1.10363	3.56480	-2.08688
O	-2.22412	2.37172	-0.40023
C	-3.53649	2.44588	-0.94740
H	-4.22768	2.46684	-0.10188
H	-3.66763	3.35041	-1.55247
H	-3.75101	1.56524	-1.56909
C	-0.81325	4.71713	-1.30537
H	-0.87012	5.56853	-1.98762
H	-1.54100	4.85289	-0.49605
H	0.19632	4.67831	-0.87246
O	-0.23454	-1.17815	-1.77647
C	-0.26218	-2.26781	-1.09886
O	-0.15590	-2.23764	0.16165
C	-0.41687	-3.57814	-1.83488
H	-1.30757	-3.54278	-2.47086
H	0.44688	-3.73389	-2.49068
H	-0.49514	-4.40740	-1.12915

Pd	0.06836	0.00329	-0.01879
C	-0.09450	0.07017	4.67272
C	1.16074	0.07618	4.05636
C	1.27751	0.38512	2.69719
C	0.12504	0.66446	1.94874
C	-1.13278	0.69118	2.57311
C	-1.23992	0.37866	3.92999
H	-0.17930	-0.16039	5.73208
H	2.05375	-0.15136	4.63410
H	2.25680	0.40404	2.22683
H	-2.01557	0.96033	1.99935
H	-2.21664	0.38794	4.40915
C	0.40007	2.25773	0.64821
C	0.10508	1.97013	-0.71406
H	1.43692	2.43469	0.91918
H	0.93606	1.96232	-1.42093
H	-0.33134	2.80587	1.23039
C	-1.21881	2.36128	-1.35740
H	-1.43837	1.68540	-2.19424
O	-1.14138	3.63668	-1.98687
O	-2.23719	2.29709	-0.39291
C	-3.55627	2.39216	-0.93714
H	-4.24942	2.25665	-0.10322
H	-3.73077	3.36890	-1.40336
H	-3.72773	1.60442	-1.68414
C	-0.89506	4.75313	-1.12788
H	-1.01155	5.64507	-1.74918
H	-1.61468	4.79277	-0.30328
H	0.12392	4.74009	-0.71910
O	-0.20795	-1.25087	-1.78725
C	-0.27717	-2.32301	-1.08937
O	-0.13327	-2.26741	0.17008
C	-0.54102	-3.63889	-1.78393
H	-1.52383	-3.60730	-2.26958
H	0.20841	-3.80336	-2.56630
H	-0.51649	-4.46746	-1.07216

3a

Gas phase:

 $E_{\text{scf}} = -933.85334845696$ a.u. $G(T)-E(0) = 0.225689$ a.u.Lowest frequency: 32.37 cm⁻¹

Solution:

 $E_{\text{sol}} = -933.87596$ a.u.

Pd	0.00000	0.00000	0.00000
H	0.00000	0.00000	3.51599
C	0.68278	0.00000	2.66142
C	0.51046	-1.29660	1.86329
C	-0.79605	-1.71726	1.50199
C	1.60707	-2.12288	1.51080
C	1.40278	-3.32408	0.84922
C	0.10264	-3.73459	0.50370
C	-0.98646	-2.94003	0.82604
H	-1.64931	-1.14225	1.85069
H	2.61220	-1.81039	1.78283
H	2.25232	-3.95175	0.59436
H	-0.04594	-4.67626	-0.01761
H	-1.99332	-3.25314	0.56463
C	0.37077	1.11957	1.66116
H	1.70750	0.07101	3.04231
H	1.24522	1.71279	1.37799
C	-0.80473	2.05192	1.93020
H	-1.10398	2.53887	0.99347
O	-1.87488	1.28959	2.44893
O	-0.48755	3.15682	2.76854
C	-3.11582	1.98509	2.46512
H	-3.06091	2.88872	3.08296
H	-3.41998	2.26846	1.44707
H	-3.85646	1.29940	2.88385
C	-0.04018	2.85093	4.08163
H	-0.73096	2.17468	4.60089
H	0.96477	2.40598	4.08421
H	0.00000	3.80165	4.61958
O	-0.07969	1.49101	-1.49354
C	-0.27712	0.65043	-2.45230
O	-0.34162	-0.58485	-2.21882
C	-0.42186	1.20145	-3.85291
H	-1.22609	1.94440	-3.87893
H	0.50280	1.71130	-4.14507
H	-0.63611	0.39658	-4.55877

Pd	-0.00731	-0.00844	0.00901
H	-0.05518	-0.03041	3.50783
C	0.65196	-0.01758	2.67343
C	0.50726	-1.30642	1.85661
C	-0.79097	-1.75908	1.49952
C	1.62497	-2.10780	1.50345
C	1.44601	-3.31943	0.85018
C	0.15229	-3.76192	0.51097
C	-0.95634	-2.98867	0.82824
H	-1.66014	-1.21028	1.85155
H	2.62300	-1.77355	1.77912
H	2.30821	-3.93411	0.60364
H	0.02390	-4.71631	0.00623
H	-1.95781	-3.33179	0.58163
C	0.35819	1.10487	1.67634
H	1.66449	0.05711	3.08424
H	1.24562	1.67376	1.38146
C	-0.79652	2.06480	1.94108
H	-1.07655	2.56829	1.00610
O	-1.89279	1.34600	2.45244
O	-0.43275	3.15736	2.78636
C	-3.11446	2.08652	2.45677
H	-3.04166	2.97800	3.09047
H	-3.38576	2.39521	1.43709
H	-3.88684	1.42135	2.85077
C	-0.03221	2.83342	4.12036
H	-0.76831	2.19266	4.61902
H	0.95091	2.34583	4.14860
H	0.03639	3.78189	4.66013
O	-0.13854	1.49313	-1.51992
C	-0.29794	0.66168	-2.48986
O	-0.32407	-0.58050	-2.26732
C	-0.44822	1.21300	-3.89106
H	-1.30605	1.89515	-3.93461
H	0.44483	1.78967	-4.16028
H	-0.58931	0.40269	-4.61059

4a

Gas phase:

 $E_{\text{scf}} = -933.83189121881$ a.u. $G(T)-E(0) = 0.223114$ a.u.Lowest frequency: -80.07 cm⁻¹

Pd	-0.78550	0.17458	-0.44595
H	-1.62277	-0.66670	1.77346
C	-0.57829	-0.51827	2.12014
C	0.19013	-1.80772	1.94663
C	0.03950	-2.55067	0.76843
C	1.10430	-2.25774	2.90603
C	1.85872	-3.41104	2.68365
C	1.71184	-4.13091	1.49675
C	0.79848	-3.69794	0.53436
H	-0.70851	-2.24734	0.02626
H	1.22987	-1.70072	3.83204
H	2.56493	-3.74658	3.43881
H	2.30175	-5.02714	1.32493
H	0.66823	-4.25520	-0.38927
C	0.03025	0.64572	1.33282
H	-0.69974	-0.25355	3.17850
H	1.11528	0.57401	1.20723
C	-0.36154	2.06725	1.72450
H	-0.29809	2.71516	0.84033
O	-1.68122	2.03152	2.21491
O	0.54059	2.69025	2.63096
C	-2.28176	3.31418	2.34772
H	-1.73180	3.94429	3.05652
H	-2.32805	3.82782	1.37672
H	-3.29683	3.14821	2.71612
C	0.70993	2.06524	3.89460
H	-0.25202	1.86401	4.38296
H	1.27894	1.12744	3.81832
H	1.28071	2.76674	4.50887
O	-0.40571	1.88107	-1.62964
C	-1.03518	1.40956	-2.65402
O	-1.56666	0.27046	-2.60836
C	-1.11116	2.27517	-3.89000
H	-1.64107	3.20497	-3.65598
H	-0.10220	2.54664	-4.21713
H	-1.63291	1.74601	-4.68958

Solution:

 $E_{\text{sol}} = -933.85559$ a.u.

Pd	-0.85308	0.08257	-0.43650
H	-1.63197	-0.68847	2.07387
C	-0.55703	-0.51596	2.25525
C	0.22203	-1.79109	2.01596
C	-0.03541	-2.56516	0.87491
C	1.27093	-2.17455	2.86245
C	2.05439	-3.29314	2.56599
C	1.79978	-4.04638	1.41565
C	0.75162	-3.68011	0.56692
H	-0.89019	-2.32231	0.23157
H	1.48384	-1.59039	3.75574
H	2.86727	-3.57342	3.23265
H	2.41270	-4.91402	1.18358
H	0.54147	-4.26569	-0.32487
C	-0.05837	0.61004	1.34497
H	-0.49906	-0.21378	3.30939
H	1.02161	0.54799	1.16706
C	-0.41085	2.05522	1.69278
H	-0.35178	2.66944	0.78552
O	-1.71125	2.09928	2.22549
O	0.54841	2.67891	2.54756
C	-2.23764	3.42421	2.33685
H	-1.63973	4.03800	3.01954
H	-2.27141	3.91256	1.35244
H	-3.25362	3.32793	2.72768
C	0.73828	2.12019	3.84861
H	-0.21583	1.92784	4.35191
H	1.33125	1.19697	3.81596
H	1.29518	2.86557	4.42370
O	-0.44845	1.86156	-1.54513
C	-0.94099	1.44508	-2.66065
O	-1.43461	0.28834	-2.74581
C	-0.89291	2.37968	-3.84731
H	-1.47365	3.28382	-3.63207
H	0.14182	2.68872	-4.03398
H	-1.29472	1.89165	-4.73834

5a

Gas phase:

 $E_{\text{scf}} = -933.84076389605$ a.u. $G(T)-E(0) = 0.222411$ a.u.Lowest frequency: 29.24 cm⁻¹

Pd	0.00000	0.00000	0.00000
H	0.00000	0.00000	1.86610
C	1.16608	0.00000	2.07204
C	1.42915	-1.25427	2.87563
C	1.13023	-2.52136	2.35849
C	2.00055	-1.15929	4.14962
C	2.28243	-2.31076	4.88817
C	1.99080	-3.56896	4.36210
C	1.41176	-3.67095	3.09475
H	0.66891	-2.60330	1.37560
H	2.22503	-0.18057	4.56790
H	2.72698	-2.22117	5.87595
H	2.20715	-4.46523	4.93734
H	1.17357	-4.64723	2.68086
C	1.86968	0.12521	0.75316
H	1.24921	0.91552	2.66265
H	2.44854	-0.74614	0.44194
C	2.57607	1.42055	0.37952
H	2.54862	1.54407	-0.71185
O	1.90526	2.48364	1.01210
O	3.96580	1.40698	0.66368
C	2.28581	3.76992	0.53666
H	3.35192	3.96027	0.70620
H	2.07167	3.86955	-0.53688
H	1.68944	4.49724	1.09178
C	4.32243	1.23298	2.03015
H	3.85141	1.98829	2.67198
H	4.05907	0.23303	2.40128
H	5.40771	1.35007	2.07803
O	0.04130	0.02796	-2.10520
C	-1.23813	-0.08445	-2.19600
O	-1.94199	-0.15633	-1.15147
C	-1.85285	-0.12527	-3.57432
H	-1.61695	0.80089	-4.10953
H	-1.41965	-0.95221	-4.14688
H	-2.93537	-0.24685	-3.50616

Solution:

 $E_{\text{sol}} = -933.86307$ a.u.

Pd	0.07849	-0.01381	-0.07383
H	0.03059	-0.06115	1.85257
C	1.17825	-0.02161	2.08792
C	1.47943	-1.23918	2.94578
C	1.37838	-2.54059	2.43506
C	1.91861	-1.06361	4.26482
C	2.26845	-2.16640	5.05105
C	2.17606	-3.45792	4.52920
C	1.72501	-3.64278	3.21810
H	1.02640	-2.69242	1.41629
H	1.99478	-0.06073	4.67958
H	2.61559	-2.01235	6.07024
H	2.45144	-4.31567	5.13867
H	1.64437	-4.64572	2.80510
C	1.90455	0.06913	0.77442
H	1.23765	0.91036	2.65574
H	2.44629	-0.83149	0.47491
C	2.70885	1.30766	0.40528
H	2.80737	1.35448	-0.68841
O	2.04889	2.44954	0.89014
O	4.06158	1.23325	0.84166
C	2.59782	3.68186	0.41330
H	3.62416	3.82682	0.76811
H	2.58885	3.71283	-0.68494
H	1.96039	4.47960	0.80254
C	4.27842	1.16874	2.25497
H	3.75080	1.97103	2.78267
H	3.97621	0.19964	2.67000
H	5.35428	1.29192	2.40440
O	0.35692	-0.18820	-2.17485
C	-0.86810	-0.47440	-2.43854
O	-1.73182	-0.46335	-1.51759
C	-1.22951	-0.84366	-3.85711
H	-0.85935	-0.08298	-4.55252
H	-0.74596	-1.79327	-4.11702
H	-2.31119	-0.94989	-3.96396

6a

Gas phase:

 $E_{\text{scf}} = -933.83006293228$ a.u. $G(T)-E(0) = 0.220907$ a.u.Lowest frequency: -539.06 cm $^{-1}$

Solution:

 $E_{\text{sol}} = -933.85300$ a.u.

Pd	0.00000	0.00000	0.00000
H	0.00000	0.00000	1.58232
C	1.69299	0.00000	1.55684
C	1.95293	-1.27441	2.28370
C	2.00122	-2.51980	1.63813
C	2.19961	-1.21846	3.66250
C	2.50472	-2.37593	4.37955
C	2.55945	-3.60706	3.72708
C	2.30379	-3.67447	2.35432
H	1.77969	-2.58742	0.57625
H	2.15633	-0.26038	4.17600
H	2.69601	-2.31364	5.44748
H	2.79172	-4.51098	4.28376
H	2.33347	-4.63216	1.84161
C	2.08215	0.22764	0.20959
H	1.64770	0.88560	2.18633
H	2.55164	-0.58701	-0.33956
C	2.52072	1.59627	-0.28968
H	2.18207	1.74210	-1.32383
O	1.97493	2.57694	0.55339
O	3.93279	1.68850	-0.39510
C	2.08027	3.90071	0.04081
H	3.12704	4.19002	-0.10859
H	1.54258	3.99436	-0.91313
H	1.61872	4.55859	0.78022
C	4.65387	1.55129	0.82523
H	4.32712	2.28389	1.57309
H	4.55751	0.54265	1.25002
H	5.70268	1.73132	0.57837
O	-0.46394	0.00048	-2.13394
C	-1.69907	-0.13579	-1.84865
O	-2.06703	-0.19405	-0.63036
C	-2.71893	-0.22537	-2.95789
H	-2.69378	0.69437	-3.55236
H	-2.46156	-1.05343	-3.62670
H	-3.72092	-0.37364	-2.55093

Pd	0.01785	0.06154	-0.00217
H	0.06155	0.07704	1.56344
C	1.79678	-0.01063	1.53088
C	1.99564	-1.30928	2.22938
C	2.13987	-2.53045	1.54748
C	2.08593	-1.30029	3.63096
C	2.32765	-2.48143	4.33600
C	2.47347	-3.68866	3.64862
C	2.37638	-3.70908	2.25186
H	2.05353	-2.56614	0.46439
H	1.97063	-0.36279	4.17146
H	2.40003	-2.45629	5.42083
H	2.65769	-4.61068	4.19510
H	2.48310	-4.64699	1.71172
C	2.12680	0.23433	0.17428
H	1.76353	0.85810	2.18580
H	2.54338	-0.58439	-0.41071
C	2.62245	1.59023	-0.30812
H	2.42275	1.69417	-1.38262
O	1.98477	2.61171	0.41123
O	4.04114	1.67135	-0.23330
C	2.20988	3.92077	-0.12234
H	3.27021	4.19445	-0.07876
H	1.86363	3.98172	-1.16375
H	1.62927	4.61352	0.49154
C	4.61341	1.58626	1.07516
H	4.17212	2.31938	1.75776
H	4.50626	0.58133	1.50279
H	5.67762	1.80428	0.95515
O	-0.60689	-0.01006	-2.14843
C	-1.81081	-0.17974	-1.77558
O	-2.08726	-0.18132	-0.52691
C	-2.90608	-0.38425	-2.79358
H	-2.96970	0.49383	-3.44731
H	-2.66480	-1.24993	-3.42162
H	-3.86975	-0.54494	-2.30478

7a

Gas phase:

$E_{\text{scf}} = -933.84008856092$ a.u.

$G(T)-E(0) = 0.221512$ a.u.

Lowest frequency: -38.60 cm $^{-1}$

Pd	0.00000	0.00000	0.00000
H	0.00000	0.00000	1.53572
C	2.22622	0.00000	0.21301
C	2.74339	-0.93537	-0.80305
C	2.63780	-0.70970	-2.18858
C	3.38653	-2.10462	-0.35956
C	3.91789	-3.01713	-1.26772
C	3.81013	-2.77910	-2.63885
C	3.16646	-1.62471	-3.09384
H	2.12005	0.16780	-2.56155
H	3.46825	-2.29258	0.70859
H	4.41339	-3.91387	-0.90559
H	4.22086	-3.49046	-3.35051
H	3.07159	-1.43866	-4.16018
C	1.74383	1.29039	-0.00249
H	2.44003	-0.26836	1.24368
H	1.72939	1.70497	-1.00894
C	1.70874	2.37094	1.06817
H	0.73247	2.87298	1.06743
O	1.96805	1.79499	2.31708
O	2.61111	3.41798	0.74914
C	1.64651	2.64121	3.41492
H	2.21807	3.57623	3.38043
H	0.57268	2.87651	3.42554
H	1.90191	2.08791	4.32104
C	3.98802	3.05059	0.71076
H	4.30862	2.59141	1.65286
H	4.20622	2.35837	-0.11382
H	4.54265	3.97789	0.55067
O	-0.69894	-0.12729	-2.16980
C	-1.79061	-0.56329	-1.70234
O	-1.95368	-0.68672	-0.43182
C	-2.92350	-0.94721	-2.62470
H	-3.21040	-0.08023	-3.22944
H	-2.58310	-1.72785	-3.31342
H	-3.78576	-1.30408	-2.05822

Solution:

$E_{\text{sol}} = -933.86107$ a.u.

Pd	0.00877	0.03182	-0.03974
H	-0.02692	0.36707	1.44832
C	2.23657	0.07963	0.16524
C	2.75301	-0.83697	-0.86623
C	2.80508	-0.50681	-2.23480
C	3.23486	-2.09478	-0.45386
C	3.75198	-2.99843	-1.38078
C	3.79549	-2.65925	-2.73679
C	3.32059	-1.41221	-3.15892
H	2.44959	0.45917	-2.58221
H	3.20078	-2.35745	0.60210
H	4.12188	-3.96492	-1.04723
H	4.19912	-3.36234	-3.46167
H	3.35635	-1.14273	-4.21173
C	1.74044	1.36862	-0.03891
H	2.43871	-0.21559	1.19228
H	1.71998	1.79096	-1.04286
C	1.72788	2.45427	1.03036
H	0.83184	3.07853	0.91664
O	1.77547	1.88699	2.30711
O	2.79550	3.36707	0.79722
C	1.49651	2.81466	3.36076
H	2.22991	3.62869	3.38035
H	0.48892	3.24077	3.25013
H	1.55005	2.25190	4.29564
C	4.11810	2.84003	0.95917
H	4.25435	2.39924	1.95168
H	4.35620	2.08920	0.19489
H	4.79731	3.68782	0.84371
O	-0.76642	-0.52398	-2.18513
C	-1.87355	-0.75626	-1.62976
O	-1.98972	-0.63934	-0.34756
C	-3.08191	-1.16732	-2.43531
H	-3.29129	-0.40342	-3.19270
H	-2.86636	-2.10271	-2.96196
H	-3.95824	-1.29984	-1.79907

8a

Gas phase:

E_{scf} = -1103.74766595511 a.u.

G(T)-E(0) = 0.260318 a.u.

Lowest frequency: 10.27 cm⁻¹

H	-0.20927	-0.23518	2.49608
C	0.85651	0.02174	2.44071
C	1.57379	-0.73356	3.55142
C	1.28263	-2.08540	3.78513
C	2.52340	-0.10733	4.36864
C	3.16500	-0.81097	5.38982
C	2.87078	-2.15783	5.60843
C	1.92560	-2.79388	4.80085
H	0.54013	-2.58550	3.16567
H	2.76689	0.93635	4.19056
H	3.89720	-0.30569	6.01579
H	3.37122	-2.70679	6.40245
H	1.68408	-3.84133	4.96576
C	1.34105	-0.30851	1.01822
H	0.94166	1.09813	2.61066
H	1.35628	-1.38876	0.84353
C	2.67747	0.30063	0.54230
H	2.53798	0.79758	-0.42773
O	3.11940	1.26063	1.48100
O	3.67774	-0.65795	0.23709
C	4.18659	2.06325	1.00559
H	5.07306	1.46388	0.76585
H	3.88960	2.62231	0.10407
H	4.43106	2.77089	1.80266
C	4.15557	-1.45275	1.31731
H	4.53113	-0.83648	2.14205
H	3.38403	-2.12572	1.71107
H	4.97473	-2.05075	0.90874
O	-0.93415	-1.65000	-0.61564
C	-1.86436	-1.23054	-1.40066
O	-1.98552	-0.00274	-1.66654
C	-2.81059	-2.26022	-1.97562
H	-2.24238	-3.08734	-2.41241
H	-3.42913	-2.67600	-1.17198
H	-3.45586	-1.80712	-2.73074
Pd	-0.14097	0.25139	-0.26574
C	-0.39195	3.16015	-0.57106
O	0.38277	2.33261	-0.07041
H	-1.28464	2.85557	-1.13368
H	-0.84711	5.14090	-0.87965
N	-0.20105	4.48361	-0.46801
H	0.59691	4.83405	0.04725

Solution:

E_{sol} = -1103.78266 a.u.

H	-0.20283	-0.13060	2.39852
C	0.87338	0.06461	2.46014
C	1.47319	-0.95495	3.41945
C	1.03005	-2.28679	3.38102
C	2.46693	-0.60693	4.34484
C	3.00411	-1.56452	5.21121
C	2.55666	-2.88775	5.16301
C	1.56653	-3.24674	4.24254
H	0.24952	-2.57024	2.67487
H	2.82660	0.41852	4.37723
H	3.77286	-1.27536	5.92580
H	2.97309	-3.63295	5.83785
H	1.20535	-4.27285	4.20033
C	1.46227	-0.02254	1.03977
H	1.00233	1.07627	2.85038
H	1.60824	-1.07010	0.75941
C	2.76186	0.75184	0.74227
H	2.62318	1.40858	-0.12427
O	3.12377	1.53814	1.85220
O	3.82279	-0.10449	0.31333
C	4.19668	2.43978	1.58746
H	5.13478	1.90818	1.38833
H	3.96609	3.08391	0.72653
H	4.31477	3.05953	2.47980
C	4.32125	-1.03254	1.27894
H	4.67697	-0.52313	2.18015
H	3.56588	-1.77254	1.56892
H	5.15778	-1.55049	0.80163
O	-0.87476	-1.52149	0.00644
C	-1.88815	-1.38467	-0.77562
O	-2.07272	-0.30625	-1.40435
C	-2.85193	-2.54320	-0.89862
H	-2.30469	-3.48202	-1.03376
H	-3.43605	-2.63014	0.02627
H	-3.53461	-2.38763	-1.73715
Pd	-0.04643	0.39339	-0.27210
C	-0.24326	3.19865	-1.22592
O	0.56999	2.41176	-0.68035
H	-1.26443	2.88758	-1.47340
H	-0.64087	5.04975	-1.98611
N	0.05121	4.45311	-1.54544
H	0.96812	4.84704	-1.35839

9a

Gas phase:

E_{scf} = -933.83386795701 a.u.

G(T)-E(0) = 0.220833 a.u.

Lowest frequency: 20.93 cm⁻¹

Pd	0.00000	0.00000	0.00000
H	0.00000	0.00000	1.78384
C	4.79184	0.00000	1.98124
C	4.32720	-0.09389	0.66088
C	5.14305	-0.71466	-0.29355
C	6.39408	-1.22594	0.05690
C	6.84747	-1.12497	1.37252
C	6.04159	-0.50985	2.33307
H	4.16554	0.47289	2.73237
H	4.79753	-0.79308	-1.32250
H	7.01478	-1.70026	-0.69938
H	7.82186	-1.52090	1.64769
H	6.38821	-0.42540	3.36033
C	2.95399	0.43891	0.27127
H	2.89428	0.51369	-0.82044
H	2.80298	1.44388	0.67595
H	2.01573	-1.53081	0.49557
C	1.19389	-0.29030	2.07236
C	1.83648	-0.48317	0.74504
O	1.65477	0.79376	2.77192
O	1.02586	-1.37785	2.92847
C	0.84502	1.21147	3.87485
H	1.30853	2.12239	4.25620
H	-0.17603	1.43347	3.53348
C	0.37335	-2.52311	2.39869
H	-0.55628	-2.24034	1.88117
H	1.01437	-3.07604	1.70188
H	0.81468	0.44737	4.65575
H	0.13761	-3.16030	3.25334
O	0.10326	0.02699	-2.11106
C	-1.13249	0.36340	-2.22811
O	-1.84699	0.52171	-1.19876
C	-1.69042	0.56139	-3.61734
H	-1.57562	-0.36167	-4.19557
H	-2.74447	0.84098	-3.57035
H	-1.12176	1.34238	-4.13350

Solution:

E_{sol} = -933.85450 a.u.

Pd	0.00846	0.08325	0.02079
H	-0.04075	0.07668	1.77354
C	4.83596	-0.01525	1.98575
C	4.31539	-0.08019	0.68413
C	5.07782	-0.70064	-0.31574
C	6.33485	-1.23860	-0.02708
C	6.84677	-1.16412	1.27099
C	6.09276	-0.55101	2.27637
H	4.25554	0.46172	2.77172
H	4.68903	-0.75474	-1.33119
H	6.91503	-1.71048	-0.81715
H	7.82682	-1.57819	1.49693
H	6.48603	-0.48564	3.28864
C	2.94217	0.49369	0.35468
H	2.86715	0.62606	-0.73063
H	2.81673	1.47856	0.81286
H	1.97315	-1.47711	0.52482
C	1.16571	-0.25872	2.12820
C	1.82021	-0.43366	0.80795
O	1.61376	0.80356	2.85690
O	0.92597	-1.34795	2.94914
C	0.80726	1.19392	3.98378
H	1.26209	2.10723	4.37055
H	-0.22124	1.40124	3.65777
C	0.34077	-2.51307	2.36650
H	-0.53672	-2.24139	1.76162
H	1.05622	-3.05739	1.74038
H	0.80446	0.41933	4.75418
H	0.03277	-3.14546	3.20132
O	0.14534	0.06787	-2.12606
C	-1.09094	0.36796	-2.28849
O	-1.82569	0.57731	-1.27684
C	-1.64314	0.45149	-3.69112
H	-1.54381	-0.52439	-4.18148
H	-2.69454	0.74662	-3.67762
H	-1.06395	1.17518	-4.27623

10a

Gas phase:

 $E_{\text{scf}} = -933.83332877218$ a.u. $G(T)-E(0) = 0.218803$ a.u.Lowest frequency: -489.91 cm $^{-1}$

Solution:

 $E_{\text{sol}} = -933.85412$ a.u.

Pd	0.00000	0.00000	0.00000
H	0.00000	0.00000	1.67174
C	4.96115	0.00000	1.70527
C	4.36034	-0.26311	0.46593
C	5.03967	-1.08108	-0.44679
C	6.28687	-1.62315	-0.13286
C	6.87594	-1.35319	1.10323
C	6.20907	-0.53876	2.02042
H	4.44365	0.62832	2.42466
H	4.59023	-1.28817	-1.41626
H	6.80046	-2.25165	-0.85630
H	7.84896	-1.77128	1.34871
H	6.66303	-0.31972	2.98397
C	2.98654	0.29547	0.12046
H	2.89354	0.38416	-0.96756
H	2.86487	1.29791	0.53994
H	1.97708	-1.65274	0.30093
C	1.33140	-0.46224	1.97161
C	1.86751	-0.61529	0.61925
O	1.82649	0.56474	2.70252
O	1.01908	-1.53339	2.76913
C	1.08567	0.93814	3.87128
H	1.57664	1.83253	4.25639
H	0.04821	1.17082	3.59643
C	0.38463	-2.65843	2.16950
H	-0.47327	-2.33535	1.56262
H	1.08010	-3.22705	1.54240
H	1.10230	0.14328	4.62042
H	0.04478	-3.28405	2.99643
O	-0.11427	0.07250	-2.14371
C	-1.32739	0.47833	-2.08681
O	-1.89029	0.64622	-0.96271
C	-2.06516	0.76196	-3.37334
H	-1.98229	-0.09755	-4.04610
H	-3.11518	0.98338	-3.17313
H	-1.60136	1.61762	-3.87693

Pd	-0.01719	-0.00512	0.02865
H	-0.01621	-0.02777	1.71728
C	4.94065	-0.13747	1.71574
C	4.32812	-0.27660	0.46040
C	5.00076	-0.99155	-0.54184
C	6.25914	-1.54969	-0.30097
C	6.86340	-1.40041	0.95067
C	6.19953	-0.69267	1.95816
H	4.43175	0.41375	2.50328
H	4.54161	-1.10273	-1.52323
H	6.76950	-2.09486	-1.09293
H	7.84555	-1.82891	1.13817
H	6.66512	-0.56787	2.93407
C	2.95216	0.31839	0.18467
H	2.83044	0.44318	-0.89700
H	2.86375	1.30858	0.63972
H	1.93726	-1.62908	0.38076
C	1.29527	-0.42647	2.05340
C	1.83564	-0.58869	0.69440
O	1.76784	0.62502	2.75981
O	1.01647	-1.49408	2.86382
C	1.04946	0.99169	3.95508
H	1.50039	1.92672	4.29036
H	-0.01083	1.15261	3.72001
C	0.45566	-2.67201	2.27697
H	-0.38142	-2.40491	1.61726
H	1.20537	-3.23002	1.70684
H	1.14945	0.22445	4.72626
H	0.09756	-3.27980	3.10941
O	-0.04594	0.09640	-2.13747
C	-1.27188	0.46462	-2.16880
O	-1.91223	0.61817	-1.08359
C	-1.93092	0.70892	-3.50504
H	-1.80937	-0.17317	-4.14355
H	-2.99313	0.93133	-3.38156
H	-1.43902	1.55002	-4.00780

11a

Gas phase:

E_{scf} = -933.84602799511 a.u.

G(T)-E(0) = 0.220747 a.u.

Lowest frequency: -22.06 cm⁻¹

Solution:

E_{sol} = -933.87225 a.u.

Pd	0.00000	0.00000	0.00000
H	0.00000	0.00000	1.55732
C	5.26529	0.00000	-0.72100
C	4.11807	-0.14840	-1.51323
C	4.23839	-0.79772	-2.74888
C	5.47054	-1.28989	-3.18227
C	6.60539	-1.13716	-2.38441
C	6.49890	-0.48877	-1.15237
H	5.18927	0.50741	0.23779
H	3.35870	-0.91032	-3.37970
H	5.54477	-1.78699	-4.14642
H	7.56690	-1.51542	-2.72229
H	7.37967	-0.35818	-0.52811
C	2.76445	0.35593	-1.03878
H	2.12794	0.56416	-1.90472
H	2.87813	1.29575	-0.49059
H	1.91452	-1.64320	-0.62558
C	2.30282	-0.71954	1.22534
C	2.04036	-0.66708	-0.15761
O	2.91436	0.29187	1.82052
O	2.07074	-1.74683	2.03340
C	2.76308	0.45022	3.24490
H	3.27199	1.38483	3.47912
H	1.69929	0.52082	3.49242
C	1.31626	-2.87011	1.55578
H	0.35119	-2.52032	1.17119
H	1.86833	-3.40222	0.77552
H	3.22297	-0.38198	3.78149
H	1.18006	-3.51440	2.42405
O	-0.58645	0.23798	-2.15100
C	-1.71165	0.65336	-1.73504
O	-1.95740	0.71414	-0.48016
C	-2.77250	1.08686	-2.72060
H	-2.99225	0.26379	-3.40889
H	-3.68462	1.39154	-2.20359
H	-2.39242	1.92124	-3.32026

Pd	-0.06327	-0.12589	-0.14875
H	-0.17860	-0.64599	1.30292
C	5.24996	0.41611	-0.83089
C	4.09367	-0.14294	-1.38998
C	4.23233	-1.16242	-2.34462
C	5.49520	-1.61449	-2.73018
C	6.64425	-1.04856	-2.16787
C	6.51711	-0.03088	-1.21889
H	5.16070	1.21559	-0.09774
H	3.34330	-1.59767	-2.79915
H	5.58254	-2.40247	-3.47521
H	7.62907	-1.39487	-2.47222
H	7.40444	0.42137	-0.78117
C	2.70919	0.32968	-0.97666
H	2.09957	0.48427	-1.87396
H	2.77386	1.29550	-0.46852
H	1.94987	-1.68877	-0.50555
C	2.29771	-0.69536	1.31521
C	1.97701	-0.68359	-0.08189
O	2.78008	0.38902	1.87063
O	2.17679	-1.71515	2.13046
C	2.93605	0.46458	3.31576
H	3.31956	1.46846	3.49941
H	1.96365	0.32961	3.79690
C	1.66016	-2.98778	1.66984
H	0.67033	-2.83990	1.22968
H	2.34799	-3.43212	0.94644
H	3.64327	-0.29219	3.66120
H	1.60041	-3.60580	2.56491
O	-0.53753	0.77266	-2.22468
C	-1.72393	0.95201	-1.81757
O	-2.06040	0.58461	-0.63564
C	-2.75761	1.59834	-2.71188
H	-2.91147	0.97790	-3.60293
H	-3.70897	1.72362	-2.18902
H	-2.39248	2.57546	-3.04897

1b

Gas phase:

 $E_{\text{scf}} = -1165.55998823976$ a.u. $G(T)-E(0) = 0.176015$ a.u.Lowest frequency: 23.96 cm⁻¹

Pd	0.34659	0.02907	-0.11129
C	-1.44866	-0.18151	4.29207
C	-0.36367	0.65279	4.01956
C	0.17891	0.71377	2.73030
C	-0.39330	-0.06369	1.72784
C	-1.45908	-0.92279	1.98069
C	-1.99124	-0.96925	3.27579
H	-1.86190	-0.22687	5.29608
H	0.07214	1.26075	4.80851
H	1.03095	1.35516	2.52944
H	-1.86071	-1.56393	1.20291
H	-2.82119	-1.63968	3.48543
C	0.03527	2.22625	-0.42743
C	-1.06589	1.59696	-0.96488
H	0.90874	2.44849	-1.03758
H	-1.05660	1.27819	-2.00726
H	-0.04102	2.72665	0.53170
C	-2.46439	1.62840	-0.36432
H	-2.81472	0.61139	-0.14364
O	-3.39998	2.09422	-1.32236
O	-2.43244	2.40358	0.79734
C	-3.60146	2.28121	1.60407
H	-3.45672	2.94354	2.45989
H	-4.49973	2.58226	1.05238
H	-3.71975	1.25028	1.96212
C	-3.22679	3.44600	-1.74164
H	-4.05684	3.65912	-2.41857
H	-3.25849	4.13836	-0.89305
H	-2.28059	3.59160	-2.28095
Cl	1.45004	-1.99011	0.14409

Solution:

 $E_{\text{sol}} = -1165.58863$ a.u.

Pd	0.41798	0.03992	-0.17167
C	-1.42810	-0.10877	4.24729
C	-0.28930	0.65646	3.98683
C	0.26369	0.69543	2.69843
C	-0.34550	-0.03546	1.67948
C	-1.46717	-0.82585	1.92494
C	-2.01033	-0.85255	3.21844
H	-1.85523	-0.12874	5.24752
H	0.17693	1.23428	4.78237
H	1.14730	1.29728	2.51442
H	-1.92546	-1.42255	1.14356
H	-2.88863	-1.46548	3.41208
C	0.05937	2.23520	-0.33320
C	-1.03810	1.61684	-0.89353
H	0.92552	2.49681	-0.93688
H	-1.01883	1.33983	-1.94723
H	-0.00991	2.68399	0.65194
C	-2.44056	1.60589	-0.29621
H	-2.76777	0.58041	-0.07917
O	-3.37483	2.04830	-1.27368
O	-2.44958	2.38528	0.86270
C	-3.64613	2.26662	1.63836
H	-3.50718	2.89596	2.52009
H	-4.52212	2.61395	1.07904
H	-3.80379	1.22859	1.95542
C	-3.21590	3.40481	-1.70368
H	-4.00829	3.58525	-2.43425
H	-3.32319	4.10488	-0.86814
H	-2.24300	3.56831	-2.18585
Cl	1.48924	-2.06857	0.20770

2b

Gas phase:

 $E_{\text{scf}} = -1165.54248298259$ a.u. $G(T)-E(0) = 0.178354$ a.u.Lowest frequency: -230.49 cm⁻¹

Pd	0.00000	0.00000	0.00000
C	0.00000	0.00000	4.67184
C	1.22662	0.00000	4.00437
C	1.29056	0.33224	2.64797
C	0.10638	0.62361	1.95916
C	-1.12239	0.67190	2.63242
C	-1.17115	0.33667	3.98675
H	-0.04219	-0.24877	5.72863
H	2.13944	-0.25112	4.53831
H	2.24759	0.34413	2.13320
H	-2.02266	0.96096	2.09764
H	-2.12460	0.34787	4.50864
C	0.33882	2.19109	0.53977
C	0.03786	1.90252	-0.82762
H	1.37171	2.39016	0.80863
H	0.85535	1.87341	-1.54641
H	-0.40553	2.72901	1.11426
C	-1.29779	2.27708	-1.45735
H	-1.54790	1.55294	-2.23963
O	-1.20839	3.50974	-2.15288
O	-2.27800	2.29181	-0.44993
C	-3.61037	2.34767	-0.95566
H	-4.27331	2.36608	-0.08797
H	-3.76979	3.24854	-1.55918
H	-3.83202	1.46124	-1.56486
C	-0.93000	4.66202	-1.36484
H	-1.02015	5.51692	-2.03880
H	-1.64520	4.77286	-0.54115
H	0.08911	4.64579	-0.95291
Cl	-0.24890	-1.27064	-1.95574

Solution:

 $E_{\text{sol}} = -1165.57170$ a.u.

Pd	-0.11034	-0.01080	0.09418
C	0.31471	-0.02024	4.71671
C	1.47283	-0.00686	3.93342
C	1.39914	0.32835	2.57798
C	0.14612	0.60132	2.01322
C	-1.01302	0.64346	2.79781
C	-0.92296	0.30477	4.15202
H	0.37990	-0.26718	5.77313
H	2.43746	-0.24189	4.37612
H	2.30078	0.36699	1.97347
H	-1.96822	0.92205	2.36155
H	-1.82043	0.30848	4.76526
C	0.27041	2.24023	0.56056
C	0.04723	1.90249	-0.79690
H	1.28810	2.43705	0.88204
H	0.91657	1.80553	-1.44678
H	-0.51493	2.74480	1.11197
C	-1.20214	2.30547	-1.57059
H	-1.35527	1.60899	-2.40327
O	-0.98936	3.55480	-2.21839
O	-2.31038	2.31151	-0.71605
C	-3.55793	2.44140	-1.40914
H	-4.34654	2.39319	-0.65240
H	-3.62010	3.39733	-1.94328
H	-3.68972	1.61862	-2.12866
C	-0.82196	4.69917	-1.37299
H	-0.85128	5.56896	-2.03392
H	-1.62972	4.77773	-0.63868
H	0.14380	4.68754	-0.85179
Cl	-0.48066	-1.26804	-1.94026

3b

Gas phase:

 $E_{\text{scf}} = -1165.58500748121$ a.u. $G(T)-E(0) = 0.182112$ a.u.Lowest frequency: 39.94 cm⁻¹

Solution:

 $E_{\text{sol}} = -1165.60663$ a.u.

Pd	0.00000	0.00000	0.00000
H	0.00000	0.00000	3.48603
Cl	1.70467	0.00000	-1.58222
C	0.00362	-0.67482	2.62591
C	-1.30190	-0.50238	1.83680
C	-1.74138	0.80371	1.49687
C	-2.11577	-1.60605	1.47897
C	-3.32157	-1.41102	0.82115
C	-3.74501	-0.11322	0.48369
C	-2.96365	0.98428	0.81812
H	-1.17599	1.66014	1.85230
H	-1.78908	-2.60972	1.73888
H	-3.93890	-2.26585	0.55935
H	-4.68805	0.02890	-0.03715
H	-3.29276	1.98989	0.57114
C	1.14080	-0.34534	1.65070
H	0.08339	-1.70435	2.99021
H	1.75276	-1.20120	1.36182
C	2.03897	0.85671	1.93968
H	2.54835	1.15781	1.01906
O	1.23946	1.90572	2.43654
O	3.11179	0.53693	2.81431
C	1.90057	3.16817	2.45227
H	2.79569	3.14205	3.08397
H	2.18782	3.47070	1.43592
H	1.18803	3.89061	2.85720
C	2.77940	0.13551	4.13707
H	2.08468	0.83786	4.61373
H	2.34763	-0.87468	4.16921
H	3.71871	0.12745	4.69570

Pd	-0.26544	0.82452	0.27707
H	-0.21839	0.32180	3.31130
Cl	1.43151	1.50903	-1.24996
C	-0.11963	-0.51862	2.61898
C	-1.40407	-0.70608	1.81284
C	-2.29760	0.37441	1.62179
C	-1.71290	-1.95580	1.22229
C	-2.87344	-2.11923	0.47846
C	-3.74508	-1.03319	0.27049
C	-3.45898	0.20318	0.83624
H	-2.16109	1.29915	2.17644
H	-1.04171	-2.79802	1.37885
H	-3.10988	-3.09129	0.05224
H	-4.64824	-1.17072	-0.31959
H	-4.14225	1.03898	0.70903
C	0.93128	-0.25091	1.55118
H	0.10223	-1.42381	3.20131
H	1.14146	-1.15457	0.97286
C	2.24756	0.45221	1.87574
H	2.88128	0.41067	0.98472
O	2.03435	1.77958	2.26183
O	2.99161	-0.29234	2.84255
C	3.19120	2.60711	2.08326
H	4.01783	2.27591	2.72340
H	3.51408	2.59106	1.03464
H	2.90101	3.62438	2.35803
C	2.63861	-0.14795	4.22173
H	2.37913	0.88567	4.46648
H	1.80628	-0.80270	4.50448
H	3.52233	-0.43958	4.79487

4b

Gas phase:

 $E_{\text{scf}} = -1165.56371317025$ a.u. $G(T)-E(0) = 0.178786$ a.u.Lowest frequency: -55.78 cm⁻¹

Solution:

 $E_{\text{sol}} = -1165.58864$ a.u.

Pd	0.47510	1.58960	-0.16122
H	-0.51389	1.80612	2.12085
Cl	2.14268	1.01837	-1.65027
C	-0.36363	0.70767	2.13955
C	-1.60044	0.01017	1.60635
C	-2.56170	0.72403	0.87972
C	-1.79719	-1.36264	1.80810
C	-2.92071	-2.00416	1.28787
C	-3.86850	-1.28343	0.55616
C	-3.68653	0.08394	0.35335
H	-2.44207	1.79795	0.73798
H	-1.06484	-1.93451	2.37446
H	-3.05696	-3.06973	1.45297
H	-4.74233	-1.78534	0.15014
H	-4.41860	0.65648	-0.20980
C	0.91803	0.37674	1.37898
H	-0.22021	0.50006	3.20995
H	0.96533	-0.64144	0.98797
C	2.25973	0.79337	1.98135
H	3.00413	0.84680	1.17989
O	2.08350	2.04844	2.59022
O	2.81250	-0.17508	2.86294
C	3.30507	2.71595	2.89727
H	3.91192	2.13541	3.60171
H	3.88887	2.89732	1.98467
H	3.03296	3.67210	3.34964
C	2.13312	-0.42472	4.08606
H	1.80808	0.50506	4.56780
H	1.26622	-1.08713	3.95044
H	2.85142	-0.93068	4.73674

Pd	0.11569	1.75752	0.19236
H	-0.41411	0.73741	2.94554
Cl	2.02503	1.86761	-1.25065
C	-0.19732	-0.11691	2.28837
C	-1.43704	-0.56355	1.54825
C	-2.15426	0.36660	0.77759
C	-1.80647	-1.91242	1.49087
C	-2.86238	-2.32737	0.67460
C	-3.55012	-1.39917	-0.11345
C	-3.19609	-0.04807	-0.06184
H	-1.98077	1.44749	0.91780
H	-1.26376	-2.64342	2.08652
H	-3.14110	-3.37869	0.64723
H	-4.36112	-1.72700	-0.75917
H	-3.73448	0.68029	-0.66329
C	0.90364	0.21977	1.28268
H	0.16180	-0.92836	2.93412
H	0.96756	-0.57510	0.53199
C	2.33351	0.48894	1.80513
H	3.03024	0.11839	1.04642
O	2.56653	1.84822	2.03452
O	2.63847	-0.31166	2.95103
C	3.96106	2.18087	1.99439
H	4.51324	1.66829	2.79129
H	4.39069	1.90799	1.02240
H	4.03728	3.26142	2.13490
C	2.29890	0.19923	4.24526
H	2.18424	1.28511	4.23085
H	1.37338	-0.25474	4.61808
H	3.11701	-0.06445	4.92279

5b

Gas phase:

 $E_{\text{scf}} = -1165.56980642062$ a.u. $G(T)-E(0) = 0.178757$ a.u.Lowest frequency: 31.10 cm⁻¹

Pd	0.00000	0.00000	0.00000
H	0.00000	0.00000	1.96129
Cl	0.21722	0.00000	-2.28707
C	1.14210	0.06689	2.14150
C	1.51791	-1.14147	2.97360
C	1.30740	-2.44349	2.50230
C	2.10322	-0.96175	4.23243
C	2.48413	-2.06340	5.00190
C	2.27809	-3.35640	4.52214
C	1.68621	-3.54356	3.27053
H	0.84142	-2.59505	1.52991
H	2.26152	0.04414	4.61488
H	2.93983	-1.90786	5.97629
H	2.57250	-4.21442	5.12054
H	1.51596	-4.54826	2.89313
C	1.82522	0.20540	0.79931
H	1.20744	1.00332	2.70146
H	2.43644	-0.64299	0.48803
C	2.47274	1.53303	0.40918
H	2.44059	1.63751	-0.68124
O	1.75199	2.56434	1.03396
O	3.85745	1.56981	0.70339
C	2.03404	3.86139	0.51420
H	3.09400	4.11453	0.63029
H	1.76209	3.92158	-0.54817
H	1.42345	4.56442	1.08464
C	4.22094	1.46159	2.07604
H	3.70385	2.20760	2.69202
H	4.02052	0.45953	2.47907
H	5.29687	1.64603	2.11838

Solution:

 $E_{\text{sol}} = -1165.59860$ a.u.

Pd	-0.36900	0.12386	0.20061
H	-0.09839	-0.08642	2.17693
Cl	-0.03209	0.26247	-2.14463
C	1.04827	0.01024	2.21226
C	1.58473	-1.20544	2.95901
C	1.65382	-2.47680	2.37304
C	2.01670	-1.04874	4.28314
C	2.53466	-2.13333	4.99704
C	2.62300	-3.39031	4.39273
C	2.18100	-3.55863	3.07779
H	1.31289	-2.61903	1.34957
H	1.94792	-0.07251	4.75853
H	2.86401	-1.99112	6.02474
H	3.03129	-4.23432	4.94303
H	2.24686	-4.53574	2.60002
C	1.56418	0.17952	0.80150
H	1.17061	0.92334	2.80202
H	2.02348	-0.71980	0.38904
C	2.41712	1.37641	0.37564
H	2.49038	1.37948	-0.71868
O	1.84574	2.57556	0.82918
O	3.77563	1.23553	0.78667
C	2.48096	3.73899	0.27992
H	3.52564	3.81644	0.60349
H	2.45524	3.71213	-0.81954
H	1.92112	4.60744	0.63741
C	4.05377	1.31669	2.18947
H	3.56867	2.18852	2.65060
H	3.75622	0.40504	2.71859
H	5.13824	1.43003	2.27400

6b

Gas phase:

 $E_{\text{scf}} = -1165.54993099088$ a.u. $G(T)-E(0) = 0.172595$ a.u.Lowest frequency: -746.04 cm $^{-1}$

Pd	0.00000	0.00000	0.00000
H	0.00000	0.00000	1.56937
Cl	1.95353	0.00000	-1.23278
C	-1.60416	0.14329	1.66916
C	-1.76084	1.47033	2.32849
C	-1.72225	2.68036	1.61867
C	-1.99851	1.50095	3.70985
C	-2.21901	2.71237	4.36593
C	-2.19254	3.90869	3.64982
C	-1.93940	3.88851	2.27509
H	-1.49754	2.67796	0.55504
H	-2.01905	0.57028	4.27263
H	-2.40738	2.71898	5.43601
H	-2.35788	4.85387	4.15973
H	-1.90202	4.81855	1.71471
C	-2.08747	-0.14505	0.36520
H	-1.57236	-0.70993	2.34563
H	-2.55727	0.65621	-0.20381
C	-2.57828	-1.52822	-0.03714
H	-2.27321	-1.74519	-1.07065
O	-2.03631	-2.46734	0.84741
O	-3.99284	-1.57110	-0.10248
C	-2.15121	-3.81710	0.40168
H	-3.20029	-4.10296	0.26499
H	-1.60992	-3.96078	-0.54331
H	-1.69649	-4.43852	1.17526
C	-4.67742	-1.35413	1.12964
H	-4.35400	-2.06313	1.90044
H	-4.53793	-0.33058	1.50355
H	-5.73675	-1.51009	0.91529

Solution:

 $E_{\text{sol}} = -1165.58012$ a.u.

Pd	-0.15601	0.09176	-0.25062
H	0.01151	0.06251	1.30750
Cl	2.12375	0.16036	-1.01558
C	-1.57575	0.10007	1.67525
C	-1.68526	1.40125	2.38691
C	-1.55199	2.64014	1.74276
C	-2.00345	1.37372	3.75464
C	-2.21122	2.56433	4.45508
C	-2.07160	3.79298	3.80519
C	-1.73420	3.82838	2.44714
H	-1.25972	2.66666	0.69558
H	-2.10479	0.42047	4.26828
H	-2.47460	2.53034	5.50931
H	-2.21452	4.72089	4.35448
H	-1.60097	4.78220	1.94260
C	-2.14845	-0.20312	0.41401
H	-1.40284	-0.75943	2.32270
H	-2.71048	0.56408	-0.11650
C	-2.54368	-1.63735	0.06125
H	-2.20959	-1.88134	-0.95828
O	-1.96794	-2.51166	0.99445
O	-3.95248	-1.76197	-0.03154
C	-2.07266	-3.89869	0.66081
H	-3.11807	-4.20940	0.56026
H	-1.53785	-4.11942	-0.27161
H	-1.60914	-4.45098	1.48130
C	-4.68432	-1.46878	1.16322
H	-4.36534	-2.10312	1.99682
H	-4.57988	-0.41519	1.44967
H	-5.73230	-1.67284	0.93143

7b

Gas phase:

$E_{\text{scf}} = -1165.57106058436$ a.u.

$G(T)-E(0) = 0.174220$ a.u.

Lowest frequency: 29.36 cm⁻¹

Pd	0.00000	0.00000	0.00000
H	0.00000	0.00000	1.51116
Cl	2.30400	0.00000	0.06561
C	-2.09125	0.71538	-0.25871
C	-2.05331	1.33522	-1.59722
C	-2.01698	0.58869	-2.79160
C	-2.04386	2.74022	-1.68522
C	-2.00016	3.37863	-2.92116
C	-1.96030	2.62541	-4.09671
C	-1.96841	1.23020	-4.02650
H	-2.03961	-0.49714	-2.76057
H	-2.06705	3.32814	-0.77081
H	-1.99431	4.46409	-2.96798
H	-1.92393	3.12220	-5.06235
H	-1.94185	0.63913	-4.93777
C	-2.11523	-0.64780	0.01562
H	-2.27866	1.39085	0.57199
H	-2.16592	-1.37153	-0.79595
C	-2.58297	-1.23410	1.33794
H	-1.93866	-2.07520	1.62578
O	-2.55823	-0.23403	2.31747
O	-3.85780	-1.83904	1.19524
C	-2.73047	-0.72458	3.64356
H	-3.69811	-1.22537	3.76244
H	-1.92804	-1.42793	3.90710
H	-2.68049	0.14295	4.30445
C	-4.92883	-0.96010	0.85874
H	-5.01278	-0.13386	1.57398
H	-4.81892	-0.54503	-0.15210
H	-5.83672	-1.56614	0.89620

Solution:

$E_{\text{sol}} = -1165.60074$ a.u.

Pd	0.03987	-0.31691	-0.06484
H	-0.03902	-0.00885	1.40814
Cl	2.41253	-0.19449	0.06516
C	-1.97653	0.68008	-0.26405
C	-1.96894	1.34849	-1.57447
C	-1.84514	0.66429	-2.80027
C	-2.12598	2.75052	-1.59171
C	-2.16907	3.44721	-2.79781
C	-2.03069	2.75888	-4.00769
C	-1.86386	1.36847	-4.00314
H	-1.74103	-0.41803	-2.81851
H	-2.23138	3.28991	-0.65189
H	-2.31078	4.52567	-2.79532
H	-2.05621	3.30319	-4.94824
H	-1.75468	0.83022	-4.94137
C	-2.10749	-0.68147	0.02127
H	-2.07036	1.35287	0.58470
H	-2.25976	-1.40635	-0.77761
C	-2.58957	-1.17484	1.38478
H	-1.97075	-2.01443	1.72685
O	-2.53499	-0.11640	2.29942
O	-3.88133	-1.75273	1.27624
C	-2.72387	-0.50111	3.66436
H	-3.68906	-0.99923	3.80677
H	-1.91718	-1.16703	3.99976
H	-2.70103	0.42017	4.25066
C	-4.92913	-0.87539	0.84707
H	-5.00888	0.00225	1.49666
H	-4.78795	-0.55002	-0.19124
H	-5.85198	-1.45706	0.91100

8b

Gas phase:

E_{scf} = -1335.47922955366 a.u.

G(T)-E(0) = 0.219131 a.u.

Lowest frequency: 19.15 cm⁻¹

H	0.08876	0.08945	2.99806
Cl	2.34492	-0.84881	0.84708
C	-0.37688	1.03120	2.68947
C	-0.13272	2.06094	3.78669
C	1.12395	2.14772	4.40377
C	-1.14992	2.92053	4.22019
C	-0.92003	3.84503	5.24120
C	0.33690	3.92881	5.84286
C	1.35865	3.07538	5.42005
H	1.92115	1.47788	4.08755
H	-2.12611	2.86834	3.74525
H	-1.72468	4.50014	5.56715
H	0.51736	4.64828	6.63747
H	2.33900	3.12639	5.88739
C	0.21679	1.39280	1.31777
H	-1.45204	0.84929	2.60170
H	1.28643	1.59196	1.39001
C	-0.44041	2.49123	0.45455
H	-0.52426	2.14572	-0.58456
O	-1.75045	2.75025	0.95060
O	0.32511	3.66537	0.30830
C	-2.48785	3.64930	0.12987
H	-2.00038	4.62720	0.06477
H	-2.60407	3.25117	-0.89025
H	-3.47279	3.76227	0.59076
C	0.65201	4.40894	1.48093
H	-0.24030	4.67837	2.05613
H	1.34048	3.86413	2.13599
H	1.14288	5.31786	1.12388
Pd	0.17913	-0.33067	0.20621
C	-2.91828	0.04099	-0.07193
O	-1.84025	-0.31519	-0.56506
H	-2.96861	0.77240	0.74329
H	-4.96959	-0.11509	-0.10713
N	-4.09879	-0.41283	-0.52174
H	-4.11929	-1.09366	-1.27106

Solution:

E_{sol} = -1335.52315 a.u.

H	0.12784	0.08769	3.06267
Cl	2.25250	-1.06524	0.97057
C	-0.34129	1.02025	2.73066
C	-0.09055	2.07893	3.80228
C	1.17209	2.20236	4.40348
C	-1.12072	2.92767	4.23050
C	-0.89831	3.87805	5.23055
C	0.36432	3.99759	5.81737
C	1.39944	3.15552	5.40042
H	1.98397	1.54398	4.09843
H	-2.10188	2.84626	3.77018
H	-1.71294	4.52382	5.55263
H	0.53897	4.73548	6.59767
H	2.38342	3.23538	5.85800
C	0.22455	1.34294	1.33944
H	-1.41755	0.84193	2.65506
H	1.30379	1.50669	1.37357
C	-0.42620	2.46387	0.49959
H	-0.50742	2.13664	-0.54499
O	-1.70872	2.73433	1.00049
O	0.38475	3.62819	0.36777
C	-2.47767	3.60341	0.16808
H	-2.04891	4.61144	0.13303
H	-2.54213	3.21053	-0.85665
H	-3.47835	3.64971	0.60430
C	0.62462	4.42406	1.53133
H	-0.30748	4.69066	2.03778
H	1.28421	3.92026	2.24537
H	1.11501	5.33478	1.17546
Pd	0.09504	-0.39547	0.23808
C	-2.94736	-0.12662	-0.00141
O	-1.84232	-0.08585	-0.59478
H	-3.02362	-0.05411	1.08747
H	-4.97694	-0.28770	-0.13207
N	-4.10080	-0.25750	-0.64108
H	-4.12879	-0.34513	-1.65310

9b

Gas phase:

 $E_{\text{scf}} = -1165.56245921866$ a.u. $G(T)-E(0) = 0.177167$ a.u.Lowest frequency: 20.55 cm⁻¹

Solution:

 $E_{\text{sol}} = -1165.58932$ a.u.

Pd	0.00000	0.00000	0.00000
H	0.00000	0.00000	1.93085
Cl	0.31641	0.00000	-2.27903
C	4.36598	1.90508	2.10903
C	3.97667	1.57894	0.80211
C	4.96067	1.19184	-0.11776
C	6.30421	1.13930	0.25468
C	6.68270	1.47083	1.55675
C	5.70971	1.85424	2.48168
H	3.61012	2.19442	2.83320
H	4.67107	0.93842	-1.13544
H	7.05491	0.84351	-0.47383
H	7.72926	1.43203	1.84824
H	5.99753	2.11479	3.49731
C	2.51205	1.60290	0.38091
H	2.44740	1.67183	-0.70841
H	1.99502	2.46797	0.80326
H	2.40187	-0.57589	0.56906
C	1.14822	0.22360	2.16724
C	1.82410	0.31660	0.81737
O	1.18520	1.41265	2.85789
O	1.54797	-0.82853	3.00338
C	0.35606	1.46929	4.02114
H	0.44663	2.48684	4.40410
H	-0.69263	1.27105	3.75551
C	1.20927	-2.14098	2.57930
H	0.12825	-2.22810	2.38912
H	1.75323	-2.44129	1.67546
H	0.68554	0.75170	4.77719
H	1.48665	-2.80533	3.40014

Pd	-0.24480	0.08368	0.09579
H	0.18332	-0.27480	2.03393
Cl	-0.06387	0.71637	-2.18522
C	4.34635	1.78077	2.04628
C	4.00750	1.33597	0.75689
C	5.02187	0.78241	-0.04156
C	6.33389	0.67740	0.43283
C	6.65667	1.12230	1.71787
C	5.65623	1.67692	2.52099
H	3.57863	2.21413	2.67919
H	4.79341	0.44921	-1.05247
H	7.10760	0.25591	-0.20588
H	7.67730	1.04390	2.08672
H	5.89646	2.03485	3.52041
C	2.57355	1.46907	0.22243
H	2.60018	1.52021	-0.86963
H	2.13048	2.39777	0.58854
H	2.13886	-0.66707	0.25205
C	1.27181	0.14573	2.07906
C	1.72604	0.26766	0.64070
O	1.22225	1.38453	2.68734
O	1.97903	-0.75387	2.90097
C	0.48458	1.43816	3.91359
H	0.50054	2.48275	4.23207
H	-0.55512	1.12276	3.74593
C	2.05801	-2.09752	2.43568
H	1.07503	-2.45655	2.09769
H	2.77921	-2.20745	1.61731
H	0.94329	0.80669	4.67951
H	2.38971	-2.69995	3.28327

10b

Gas phase:

E_{scf} = -1165.55666908888 a.u.

G(T)-E(0) = 0.174761 a.u.

Lowest frequency: -620.06 cm⁻¹

Pd	0.00000	0.00000	0.00000
H	0.00000	0.00000	1.65286
Cl	0.14638	0.00000	-2.33569
C	-4.79926	-1.65333	1.39772
C	-4.19290	-1.16952	0.23044
C	-4.99587	-0.54847	-0.73676
C	-6.37107	-0.41564	-0.54475
C	-6.96530	-0.90340	0.62077
C	-6.17573	-1.52388	1.59015
H	-4.18926	-2.13763	2.15538
H	-4.53947	-0.17867	-1.65291
H	-6.97920	0.06193	-1.30879
H	-8.03757	-0.80526	0.76960
H	-6.63254	-1.91234	2.49711
C	-2.69082	-1.28177	0.01015
H	-2.47740	-1.38462	-1.05721
H	-2.28807	-2.16419	0.51351
H	-2.38142	0.89828	0.08644
C	-1.59185	0.08687	1.91307
C	-1.98089	-0.02378	0.50768
O	-1.77928	-0.99071	2.68237
O	-1.63478	1.23777	2.61552
C	-1.13841	-1.00492	3.96822
H	-1.33320	-1.99640	4.37689
H	-0.05943	-0.85286	3.84018
C	-1.38274	2.47578	1.94563
H	-0.45506	2.40333	1.36277
H	-2.21315	2.74531	1.28594
H	-1.55137	-0.23368	4.62139
H	-1.28232	3.21989	2.73631

Solution:

E_{sol} = -1165.58623 a.u.

Pd	0.12204	-0.13589	0.12405
H	-0.23241	0.23891	1.69857
Cl	0.49600	-0.71671	-2.18543
C	-4.80627	-1.76171	1.13088
C	-4.22885	-0.96539	0.13009
C	-5.03994	-0.02998	-0.53356
C	-6.39146	0.10441	-0.20366
C	-6.95568	-0.69652	0.79421
C	-6.15855	-1.63269	1.45821
H	-4.19608	-2.49706	1.64988
H	-4.62157	0.58711	-1.32723
H	-7.00749	0.82976	-0.73175
H	-8.00864	-0.59552	1.04882
H	-6.58935	-2.26708	2.23045
C	-2.75064	-1.12107	-0.22595
H	-2.62839	-1.17329	-1.31242
H	-2.37561	-2.05754	0.19094
H	-2.14482	0.99173	-0.24839
C	-1.73114	0.24929	1.72801
C	-1.92921	0.06411	0.28158
O	-2.00176	-0.81373	2.50027
O	-1.93740	1.42673	2.36352
C	-1.49948	-0.79011	3.85151
H	-1.73445	-1.77024	4.26789
H	-0.41139	-0.64286	3.82957
C	-1.87535	2.64842	1.61089
H	-0.96048	2.67696	1.00860
H	-2.75228	2.75096	0.96483
H	-1.97672	-0.00084	4.43582
H	-1.86339	3.45156	2.34784

11b

Gas phase:

 $E_{\text{scf}} = -1165.57622320558$ a.u. $G(T)-E(0) = 0.174240$ a.u.Lowest frequency: 16.52 cm⁻¹

Pd	0.11151	-0.18973	0.21901
H	0.31816	1.26249	-0.16804
Cl	2.32181	-0.74967	-0.19361
C	-4.86383	-1.53363	1.16334
C	-4.25662	-0.95094	0.04290
C	-5.06089	-0.25486	-0.86895
C	-6.43644	-0.13915	-0.66634
C	-7.03026	-0.72193	0.45441
C	-6.23974	-1.42133	1.36756
H	-4.25325	-2.08118	1.87691
H	-4.60647	0.19281	-1.75105
H	-7.04537	0.40031	-1.38748
H	-8.10241	-0.63696	0.61155
H	-6.69565	-1.88583	2.23850
C	-2.75199	-1.03874	-0.16821
H	-2.53427	-1.09317	-1.23995
H	-2.36769	-1.95907	0.28327
H	-2.26102	1.11912	-0.07378
C	-1.74195	0.25599	1.78355
C	-2.01972	0.17600	0.40693
O	-1.79270	-0.85603	2.52134
O	-1.54527	1.35794	2.50716
C	-1.24415	-0.83466	3.85573
H	-1.34409	-1.85908	4.21331
H	-0.19104	-0.54248	3.82744
C	-1.54582	2.64132	1.86948
H	-0.74680	2.68978	1.12261
H	-2.51685	2.83927	1.40555
H	-1.80830	-0.15064	4.49313
H	-1.35923	3.35824	2.66870

Solution:

 $E_{\text{sol}} = -1165.60592$ a.u.

Pd	0.00039	-0.22615	0.01276
H	0.39084	1.15193	0.51655
Cl	2.07738	-0.73965	-1.09256
C	-4.87621	-1.62881	1.44818
C	-4.18855	-0.98392	0.41309
C	-4.91691	-0.23173	-0.51962
C	-6.30530	-0.12822	-0.42277
C	-6.98592	-0.77975	0.61075
C	-6.26698	-1.52987	1.54513
H	-4.32440	-2.22612	2.17082
H	-4.39424	0.26255	-1.33697
H	-6.85515	0.45189	-1.16070
H	-8.06829	-0.70886	0.68211
H	-6.78730	-2.04735	2.34797
C	-2.67791	-1.09428	0.28764
H	-2.42746	-1.22551	-0.77246
H	-2.32842	-1.98977	0.80761
H	-2.25605	1.07391	0.35743
C	-1.65395	0.25602	2.20303
C	-1.92394	0.13828	0.80391
O	-1.64698	-0.82413	2.94911
O	-1.40591	1.36367	2.85477
C	-1.23300	-0.73897	4.34254
H	-1.28305	-1.76490	4.70506
H	-0.21149	-0.35552	4.40096
C	-1.42322	2.66335	2.21264
H	-0.62780	2.71783	1.46391
H	-2.39854	2.84944	1.75812
H	-1.91313	-0.09149	4.89926
H	-1.23432	3.37185	3.01827