PNacAu (1)

81

1 PNacAu Singlet E(DFT)=-2509.0321081 ZPVE=0.6523657

Au	-0.0438378	-0.5413403	-0.4538730
P	1.1022562	0.8220599	-1.9856580
P	-1.5666001	-1.7135514	0.8958605
N	0.6483406	-0.6791873	2.3464964
N	2.4770011	0.6395935	0.4488466
C	0.2804682	-1.8796971	2.8693862
C	2.4395019	1.5717227	1.3710435
C	0.9061309	0.4142824	3.0314314
C	-2.6742341	-0.4823657	1.6725216
C	3.3810530	0.5793449	-0.5758206
C	0.1465583	1.6582433	-4.5317078
H	0.0293079	2.6591315	-4.1121348
C	1.6277900	1.5113383	2.5252462
H	1.6620507	2.3910053	3.1708743
C	0.7735099	-0.6588366	-4.2977205
H	1.1478372	-1.4823038	-3.6820995
C	-0.7746932	-2.5990296	2.2459398
C	0.6481750	0.6214980	-3.7425439
C	1.4719374	4.9057651	-1.8199032
H	2.0938239	5.6713466	-2.2909983
C	-2.6891141	-2.9048021	0.0929713
C	3.7457048	0.4556453	-3.0003041
H	3.3393264	0.4711822	-4.0149345
C	1.6328588	3.5699735	-2.1727540
H	2.3924314	3.2888170	-2.9072734
C	-2.9638804	-0.5134373	3.0377199
H	-2.5280532	-1.2942726	3.6653741

C	0.8424346	2.5813558	-1.5750552
C	0.5311746	5.2635692	-0.8541766
H	0.4135999	6.3122247	-0.5682836
C	-0.0702186	0.1508239	-6.4073317
H	-0.3503079	-0.0320323	-7.4480452
C	-2.2359651	-3.6012153	-1.0312703
H	-1.2402870	-3.3890347	-1.4312364
C	-0.0931415	2.9462469	-0.6045808
H	-0.6856966	2.1773998	-0.1020680
C	-0.2123738	1.4212601	-5.8583346
H	-0.6061057	2.2405610	-6.4655251
C	0.4250653	-0.8910701	-5.6228663
H	0.5334466	-1.8933305	-6.0454184
C	-1.1363493	-3.8791557	2.6727081
H	-1.9466393	-4.4101784	2.1666572
C	-3.0477575	-4.5507547	-1.6451502
H	-2.6845470	-5.0903256	-2.5235445
C	2.8901150	0.5932395	-1.9056404
C	-0.2466230	4.2830069	-0.2446575
H	-0.9714021	4.5535111	0.5271434
C	5.1122513	0.2989340	-2.8005930
H	5.7850816	0.1906301	-3.6544191
C	0.5641903	-3.7813711	4.3675553
H	1.0980220	-4.2464720	5.2017629
C	4.7699768	0.4080445	-0.4008094
H	5.1663796	0.3618514	0.6158265
C	3.2852393	2.8244801	1.2110137
H	4.3465079	2.6169256	1.4273977
H	2.9504970	3.6212681	1.8911949
H	3.2308743	3.1983982	0.1757048

C -3.9715348 -3.1615637 0.5879061

H -4.3391656 -2.6156243 1.4603118

C 5.6125844 0.2749024 -1.4943548

H 6.6859944 0.1426834 -1.3292606

C -0.4736301 -4.4773986 3.7367969

H -0.7553748 -5.4785550 4.0705993

C -4.7851655 -4.1070287 -0.0307886

H -5.7874930 -4.2996804 0.3604992

C -3.7956625 0.4530638 3.6003509

H -4.0110269 0.4245054 4.6716507

C -4.3236955 -4.8040979 -1.1457347

H -4.9643483 -5.5450170 -1.6313034

C -4.3454059 1.4535521 2.8032954

H -4.9947344 2.2128785 3.2470353

C -3.2280658 0.5267565 0.8764360

H -2.9989926 0.5615396 -0.1927081

C 0.9392327 -2.5156198 3.9473390

H 1.7731071 -1.9992114 4.4269540

C -4.0627426 1.4873451 1.4381362

H -4.4898513 2.2715624 0.8076022

C 0.3926212 0.5722099 4.4557258

H -0.4555428 -0.0979842 4.6594545

H 0.0710229 1.6112820 4.6292641

H 1.1847772 0.3485829 5.1908482

81

1 PNacAu Triplet E(DFT)=-2508.9433759 ZPVE=0.6493884

Au -0.1266753 -0.5741607 -0.5614554

P 1.0755752 0.7828337 -2.0528644

P -1.5970325 -1.7020532 0.8741268

N 0.5329445 -0.6700068 2.4336434

N	2.3853496	0.7657072	0.4514061
C	0.2333003	-1.9085249	2.8751542
C	2.4538859	1.6325647	1.4849785
C	1.0122536	0.3167008	3.2262970
C	-2.6518165	-0.4457773	1.6829109
C	3.3120254	0.7099070	-0.5411173
C	0.2731270	1.5561915	-4.6686416
H	0.1536464	2.5713167	-4.2853482
C	1.7831905	1.3886739	2.7028343
H	1.9843916	2.1627237	3.4532332
C	0.8376270	-0.7649821	-4.3318386
H	1.1606541	-1.5762076	-3.6724097
C	-0.7929845	-2.6294196	2.1878866
C	0.7069725	0.5337590	-3.8226486
C	1.3719202	4.8728040	-1.9141177
H	2.0180947	5.6416054	-2.3455301
C	-2.7778989	-2.8519522	0.0935579
C	3.7595660	0.4778601	-2.9460450
H	3.3843757	0.4164822	-3.9708652
C	1.5806947	3.5351396	-2.2330619
H	2.4014652	3.2559409	-2.8991998
C	-2.8309592	-0.4122933	3.0662812
H	-2.3396478	-1.1583319	3.6948962
C	0.7609928	2.5424981	-1.6837955
C	0.3525264	5.2288358	-1.0311992
H	0.1970630	6.2792839	-0.7712390
C	0.1318376	-0.0030487	-6.5087429
H	-0.0925346	-0.2117552	-7.5580456
C	-2.4166065	-3.4973502	-1.0922086
H	-1.4508215	-3.2742002	-1.5545356

C	-0.2542905	2.9056432	-0.7962212
H	-0.8744348	2.1340419	-0.3323251
C	-0.0147794	1.2860466	-6.0060915
H	-0.3562066	2.0939032	-6.6585344
C	0.5602516	-1.0302368	-5.6676192
H	0.6721917	-2.0464600	-6.0543049
C	-1.1309172	-3.9336263	2.5423659
H	-1.9246098	-4.4550870	2.0019088
C	-3.2818397	-4.4112005	-1.6880438
H	-2.9902575	-4.9110139	-2.6152844
C	2.8625426	0.6099511	-1.8864550
C	-0.4566237	4.2443902	-0.4703522
H	-1.2451758	4.5143625	0.2364889
C	5.1283682	0.4276970	-2.7035466
H	5.8317076	0.3178181	-3.5319792
C	0.5566928	-3.8954965	4.2588334
H	1.1004906	-4.4005473	5.0628710
C	4.7105113	0.6637354	-0.3241448
H	5.0809761	0.7028541	0.7018822
C	3.2024982	2.9408424	1.3313792
H	4.2993081	2.8196705	1.2777079
H	2.9877090	3.6202923	2.1711547
H	2.8978676	3.4520420	0.3997226
C	-4.0230098	-3.1236240	0.6703480
H	-4.3182115	-2.6173181	1.5928725
C	5.5893817	0.5195948	-1.3851382
H	6.6638515	0.4723020	-1.1843042
C	-0.4608379	-4.5786017	3.5783169
H	-0.7210967	-5.6039713	3.8497400
C	-4.8897145	-4.0330126	0.0710407

H -5.8619787 -4.2377435 0.5267112

C -3.6243666 0.5760521 3.6456197

H -3.7521936 0.5992935 4.7309333

C -4.5193215 -4.6793354 -1.1071683

H -5.2017927 -5.3921588 -1.5775954

C -4.2457866 1.5332249 2.8478738

H -4.8649584 2.3095511 3.3050931

C -3.2768593 0.5193040 0.8853587

H -3.1364253 0.5020167 -0.1996496

C 0.8956856 -2.5954784 3.9312428

H 1.7127305 -2.0963552 4.4519347

C -4.0736641 1.5016252 1.4644068

H -4.5587415 2.2503810 0.8326094

C 0.7011047 0.3665137 4.7088949

H -0.2363304 -0.1707119 4.9312347

H 0.5726472 1.4125689 5.0378535

H 1.4814050 -0.0745036 5.3600628

PNacAg (2)

81

2 PNacAg Singlet E(DFT)=-2520.2702651 ZPVE=0.6523166

Ag -0.6828390 -0.4823248 -0.0500829

P -0.2076315 -0.5356187 -2.4694716

P -1.0235373 1.1903822 1.7595524

N -0.4886962 -1.5846068 2.1376814

N 0.6006094 -2.5269981 -0.5146896

C -1.4491594 -1.1628481 3.0459427

C -1.8670428 0.1896169 3.0201966

C -2.4455165 0.1772235 -3.9411906

H -2.9944052 -0.2149490 -3.0797478

C -1.0465282 0.1727795 -3.9279513

C	1.7056205	-2.4693294	1.6331733
H	2.6668759	-2.6795033	2.1040091
C	-0.0016290	-2.2933654	-2.8430905
C	0.7137007	-1.9738514	2.5086423
C	1.6341486	-2.7907704	0.2663141
C	0.4036914	-3.1022374	-1.7484141
C	-2.0902550	-2.0348000	3.9413120
H	-1.7987161	-3.0874520	3.9437415
C	-0.2725939	-2.8621828	-4.0909726
H	-0.5856241	-2.2198124	-4.9178757
C	-2.8725657	0.6410234	3.8777967
H	-3.1839698	1.6882201	3.8437623
C	-3.0855149	-1.5740509	4.7933176
H	-3.5677188	-2.2720949	5.4836729
C	0.6094927	1.5520155	2.5012332
C	0.5007437	-4.4919401	-1.9722688
H	0.7656058	-5.1382542	-1.1334803
C	1.4782848	0.1815871	-2.5247003
C	-1.9207978	2.7814293	1.7311019
C	-1.3568520	3.9960054	2.1297415
H	-0.3389169	4.0230207	2.5235253
C	-2.4415896	1.1905248	-6.1299578
H	-2.9857797	1.5897612	-6.9899799
C	-3.2240117	2.7763108	1.2149253
H	-3.6709353	1.8344353	0.8819115
C	-0.3526920	0.6912126	-5.0257517
H	0.7399386	0.6985353	-5.0251478
C	-3.3867091	5.1623522	1.5305233
H	-3.9580851	6.0911214	1.4536839
C	-3.1401331	0.6765701	-5.0389382

H	-4.2332192	0.6718159	-5.0393597
C	-2.0870645	5.1795775	2.0275685
H	-1.6329665	6.1227827	2.3428249
C	2.5993181	-0.5625676	-2.8976955
H	2.4752137	-1.5970461	-3.2260927
C	-1.0483572	1.1994731	-6.1201441
H	-0.4967632	1.6038740	-6.9729911
C	-3.4810005	-0.2348048	4.7706537
H	-4.2656905	0.1224596	5.4419220
C	-3.9552777	3.9550006	1.1244823
H	-4.9732338	3.9334855	0.7266361
C	1.1198679	-1.8567403	3.9673304
H	0.8436125	-0.8678256	4.3672564
H	2.2035622	-1.9941185	4.0900731
H	0.6068415	-2.6115089	4.5856658
C	-0.1490189	-4.2314980	-4.2899555
H	-0.3608127	-4.6680136	-5.2687952
C	1.6494429	1.5056447	-2.1007999
H	0.7794658	2.0934264	-1.7919118
C	2.8839957	-3.4484402	-0.3017404
H	2.8883563	-4.5350588	-0.1117493
H	3.7801380	-3.0294019	0.1814570
H	2.9666295	-3.2991431	-1.3881761
C	0.2364145	-5.0406177	-3.2176248
H	0.3212425	-6.1226060	-3.3548676
C	1.7582743	1.3901949	1.7230236
H	1.6725184	1.0718690	0.6805859
C	2.9173830	2.0761235	-2.0576571
H	3.0367820	3.1103247	-1.7241322
C	3.0200434	1.6077784	2.2720927

H 3.9088471 1.4671468 1.6519003

C 4.0330204 1.3238849 -2.4253201

H 5.0314014 1.7672519 -2.3824331

C 0.7413376 1.9242912 3.8442811

H -0.1502579 2.0261698 4.4690188

C 3.8709569 0.0060188 -2.8447722

H 4.7418804 -0.5888911 -3.1323377

C 3.1422897 1.9879578 3.6055267

H 4.1319037 2.1533362 4.0399440

C 2.0006613 2.1465366 4.3919385

H 2.0939956 2.4347198 5.4423256

81

2 PNacAg Triplet E(DFT)=-2520.1833300 ZPVE=0.6498092

Ag -0.9446591 -1.0080173 0.0105895

P -0.5865100 -0.6607657 -2.3838312

P -0.7619421 1.0222282 1.5862384

N -0.9336638 -1.7779004 2.1517062

N 0.8263721 -2.4511387 -0.4930755

C -1.8101656 -1.0754459 2.9845291

C -1.8460415 0.3376581 2.8835039

C -2.8226397 -0.7710859 -4.0181483

H -3.2186963 -1.4250919 -3.2354769

C -1.5431767 -0.2225318 -3.8761978

C 1.2941122 -2.7551036 1.8910428

H 2.1041610 -3.1262547 2.5269676

C 0.3074713 -2.1815208 -2.8316837

C 0.2048310 -2.3171790 2.6693999

C 1.6609384 -2.8412878 0.5169731

C 0.8940163 -2.9372078 -1.7610952

C -2.6872584 -1.7070113 3.8757959

H	-2.6826004	-2.7973015	3.9340506
C	0.3697867	-2.6474883	-4.1420555
H	-0.0723564	-2.0527264	-4.9447797
C	-2.7263686	1.0751873	3.6771714
H	-2.7474753	2.1646245	3.5909485
C	-3.5601537	-0.9595325	4.6583677
H	-4.2388306	-1.4718782	5.3459823
C	0.9167743	0.9930773	2.3086699
C	1.4640586	-4.1938855	-2.1022339
H	1.8447626	-4.8307096	-1.3057673
C	0.6938495	0.6471109	-2.2642518
C	-1.1990160	2.7908443	1.4618412
C	-0.3281794	3.8235424	1.8206082
H	0.6387799	3.5881332	2.2699474
C	-3.0935174	0.3569402	-6.1330365
H	-3.6991288	0.5848918	-7.0141981
C	-2.4284660	3.1156062	0.8713309
H	-3.1101706	2.3154074	0.5661537
C	-1.0512555	0.6267788	-4.8724023
H	-0.0558003	1.0655262	-4.7710772
C	-1.9133591	5.4674703	1.0287397
H	-2.1908072	6.5112415	0.8597992
C	-3.5908589	-0.4899308	-5.1437186
H	-4.5873116	-0.9276853	-5.2454411
C	-0.6844765	5.1538911	1.6029853
H	0.0063957	5.9517210	1.8886182
C	2.0517362	0.3875937	-2.4601520
H	2.3722301	-0.6045476	-2.7863159
C	-1.8253320	0.9164358	-5.9938120
H	-1.4322984	1.5828836	-6.7661900

C	-3.5805008	0.4324961	4.5687042
H	-4.2667679	1.0161342	5.1871859
C	-2.7878225	4.4430295	0.6654581
H	-3.7524248	4.6803663	0.2091098
C	0.3783449	-2.3607278	4.1721277
H	0.2419909	-1.3613492	4.6218295
H	1.3845366	-2.7133885	4.4427609
H	-0.3529908	-3.0279906	4.6623915
C	0.9715190	-3.8676170	-4.4483125
H	1.0087555	-4.2185359	-5.4820999
C	0.2983360	1.9199957	-1.8309661
H	-0.7590347	2.1297613	-1.6467379
C	3.0900385	-3.2632715	0.2395486
H	3.2659206	-4.3570797	0.2371096
H	3.7631925	-2.8376665	1.0046770
H	3.4261133	-2.8851815	-0.7398754
C	1.4992819	-4.6417424	-3.4112829
H	1.9394884	-5.6189276	-3.6300964
C	1.9922374	0.7170587	1.4586083
H	1.8155753	0.5411712	0.3950397
C	1.2414816	2.9159815	-1.6050481
H	0.9157750	3.8987267	-1.2547593
C	3.2868507	0.6413053	1.9648078
H	4.1172527	0.4181462	1.2900981
C	2.5969985	2.6475673	-1.7977982
H	3.3419678	3.4239901	-1.6052165
C	1.1536510	1.1864247	3.6734045
H	0.3155020	1.3873767	4.3461318
C	2.9984851	1.3851816	-2.2262937
H	4.0596185	1.1690673	-2.3765766

C 3.5158382 0.8325152 3.3254023

H 4.5310290 0.7627432 3.7255176

C 2.4479613 1.1069191 4.1794660

H 2.6240390 1.2519549 5.2486646

PNacAuCu (3)

83

3 PNacAuCuI Singlet E(DFT)=-4447.2902640 ZPVE=0.6560765

Au 13.9465975 0.6008259 15.4521887

I 16.7210152 -0.5654832 13.9553992

Cu 14.5062413 -0.0152135 12.8958512

P 13.0108632 -1.5174125 15.8929568

P 14.4066598 2.8965223 15.1963546

C 17.8873172 3.1796759 17.2889526

H 18.8184004 2.6094491 17.3374844

C 15.5057460 4.6233854 17.1585185

H 14.5746986 5.1926195 17.1126452

C 12.0073214 3.4887148 16.4885631

H 12.1733347 2.5394698 17.0053322

N 12.8560820 -1.1367987 12.9190867

N 13.6038651 1.7067538 12.4816415

C 10.8820690 4.2535730 16.7808093

H 10.1667311 3.9023854 17.5289909

C 14.9884755 3.4206792 13.5524682

C 13.2604183 -2.8144078 14.6366313

C 11.4252664 0.6851718 12.2526048

H 10.3901491 0.9183570 12.0048024

C 13.5528880 -4.7705896 12.6705650

H 13.6758722 -5.5306188 11.8941904

C 13.2422950 -3.4666103 12.3095412

H 13.1378043 -3.1879123 11.2586815

C	15.6809629	3.4945828	16.3552211
C	12.9321852	3.9240437	15.5334564
C	14.4699476	2.7994503	12.3940962
C	12.7127466	5.1369810	14.8737432
H	13.4260908	5.4854708	14.1234276
C	17.7112126	4.3083298	18.0893357
H	18.5059775	4.6269490	18.7691208
C	11.6723464	-0.6668110	12.5718667
C	13.0837989	-2.4675421	13.2792836
C	10.4882106	-1.6085579	12.5285537
H	10.6214697	-2.3619400	11.7346414
H	9.5512195	-1.0660211	12.3408283
H	10.3912431	-2.1575883	13.4785488
C	10.6660942	5.4587181	16.1146783
H	9.7782797	6.0563948	16.3373169
C	11.5829212	5.8990638	15.1628868
H	11.4176966	6.8431097	14.6373776
C	16.8763444	2.7675883	16.4279029
H	17.0149491	1.8771233	15.8052016
C	13.7228420	-5.1097390	14.0125355
H	13.9787810	-6.1324555	14.2987656
C	16.3651186	4.8792393	12.1844368
H	17.1068341	5.6774685	12.1075947
C	15.9343647	4.4462175	13.4315027
H	16.3447791	4.9085953	14.3318940
C	15.8540833	4.2705448	11.0377373
H	16.1945801	4.5906087	10.0491883
C	11.7123632	3.1239371	11.8502300
H	11.9336605	3.8653128	12.6347048
H	10.6219301	3.0573489	11.7314009

H	12.1425338	3.5106623	10.9122421
C	12.3112364	1.7798693	12.2088269
C	13.5800413	-4.1294543	14.9874463
H	13.7282776	-4.3892376	16.0378108
C	16.5204254	5.0267863	18.0249745
H	16.3766861	5.9099037	18.6529911
C	14.9271048	3.2443898	11.1433856
H	14.5505766	2.7404335	10.2505196
C	11.1935408	-1.4401916	16.0583744
C	13.6729352	-2.2226956	17.4369468
C	12.8854351	-2.5383615	18.5451253
H	11.8032561	-2.3981515	18.5101676
C	10.5353620	-0.2147451	15.9371045
H	11.1158449	0.6954737	15.7700023
C	10.4399698	-2.6099406	16.2191977
H	10.9422979	-3.5790539	16.2787750
C	9.1441891	-0.1545007	15.9895542
H	8.6413628	0.8097903	15.8810599
C	15.0639979	-2.3872574	17.5051420
H	15.6888585	-2.1198525	16.6459675
C	13.4799900	-3.0288596	19.7073425
H	12.8567821	-3.2725563	20.5717408
C	15.6496798	-2.8839392	18.6634915
H	16.7340967	-3.0128159	18.7066464
C	9.0522611	-2.5478966	16.2815443
H	8.4723210	-3.4656238	16.4083370
C	8.4022102	-1.3185112	16.1661617
H	7.3106151	-1.2724575	16.2041340
C	14.8588870	-3.2064592	19.7668588
H	15.3223403	-3.5925072	20.6786212

83

3 PNacAuCuI Triplet E(DFT)=-4447.2063707 ZPVE=0.6535198

Au 13.9209648 0.6670778 15.8142956

I 16.5880657 -0.4008657 13.6279634

Cu 14.1835062 0.1700601 13.1403946

P 13.0379095 -1.5074684 16.0188518

P 14.4804941 2.9151139 15.3756172

C 18.0484817 3.2363792 17.3088899

H 18.9546875 2.6302708 17.3853883

C 15.7333824 4.7781158 17.1043301

H 14.8291737 5.3860071 17.0264585

C 12.1049339 3.6492602 16.6370773

H 12.2406909 2.7287627 17.2122010

N 12.6668241 -0.9963402 13.1840706

N 13.2255188 1.8235423 12.9241182

C 10.9993512 4.4604257 16.8748591

H 10.2723251 4.1767079 17.6400222

C 15.0003191 3.2778868 13.6705779

C 13.4375268 -2.7006940 14.7030325

C 11.2294766 0.6533473 12.1238478

H 10.2419940 0.8049991 11.6815474

C 13.7654388 -4.5035703 12.6099130

H 13.8999952 -5.2083310 11.7846767

C 13.2663499 -3.2351182 12.3503101

H 13.0333405 -2.9282205 11.3288650

C 15.8227886 3.5628701 16.4228767

C 13.0400397 3.9984841 15.6579312

C 14.2147155 2.7389872 12.6157597

C 12.8521867 5.1673491 14.9149146

H 13.5690851 5.4386114 14.1366677

C	17.9559700	4.4504905	17.9896491
H	18.7907898	4.7982040	18.6038938
C	11.5081494	-0.6609660	12.5042747
C	13.0966442	-2.2994848	13.3866762
C	10.4519477	-1.7209160	12.3480710
H	10.7487035	-2.5344758	11.6614877
H	9.5200618	-1.2813675	11.9616424
H	10.2279420	-2.1982820	13.3194904
C	10.8167440	5.6244292	16.1307480
H	9.9443407	6.2580021	16.3110005
C	11.7438428	5.9762208	15.1520112
H	11.6005445	6.8847979	14.5616803
C	16.9850984	2.7885252	16.5332148
H	17.0585664	1.8353657	15.9992282
C	14.1215742	-4.8765763	13.9069815
H	14.5261410	-5.8716067	14.1059968
C	16.3702591	4.4864291	12.0837439
H	17.2118986	5.1513179	11.8773318
C	16.0731332	4.1246844	13.3951079
H	16.6797733	4.5184783	14.2131890
C	15.5834325	3.9930683	11.0403157
H	15.8144412	4.2684292	10.0074938
C	11.3881978	3.1538345	11.9486173
H	11.3460130	3.7865260	12.8562961
H	10.3627735	3.0353236	11.5663219
H	11.9607384	3.7280125	11.1975826
C	11.9930788	1.8128077	12.2683465
C	13.9572577	-3.9705382	14.9507774
H	14.2237868	-4.2651356	15.9677406
C	16.7987622	5.2177559	17.8885509

H 16.7216777 6.1683634 18.4226237

C 14.5269228 3.1333686 11.2972158

H 13.9407846 2.7099845 10.4790138

C 11.2176287 -1.4813231 16.0101167

C 13.5986444 -2.2871993 17.5692343

C 12.7390671 -2.6905890 18.5921735

H 11.6589528 -2.5821682 18.4782311

C 10.5377404 -0.2802487 15.7987194

H 11.0997103 0.6477271 15.6668748

C 10.4935125 -2.6752378 16.1133101

H 11.0201584 -3.6256340 16.2337864

C 9.1482832 -0.2690547 15.7084080

H 8.6279006 0.6739256 15.5244432

C 14.9843354 -2.4109507 17.7460167

H 15.6665452 -2.0771979 16.9571752

C 13.2569230 -3.2265633 19.7710387

H 12.5756879 -3.5376355 20.5672810

C 15.4958087 -2.9546407 18.9182199

H 16.5771966 -3.0521297 19.0429888

C 9.1050731 -2.6598828 16.0370742

H 8.5458033 -3.5953179 16.1191927

C 8.4310637 -1.4555307 15.8340079

H 7.3404273 -1.4463744 15.7597364

C 14.6317161 -3.3645273 19.9340953

H 15.0345239 -3.7869675 20.8583322

PNacAuZn (4)

84

4 PNacAuZnCl2 Singlet E(DFT)=-5208.6509165 ZPVE=0.6584522

Au 3.7112247 14.4980744 18.8486778

Zn 1.4038993 12.5278315 20.0058754

Cl	3.2578032	11.5845558	19.0423404
Cl	-0.2149234	11.2967817	20.8740578
P	2.7176689	14.6771447	16.7235203
P	4.8920472	14.6322227	20.8787568
N	0.6325215	13.9232026	18.7333355
N	1.9432174	14.0048982	21.3105050
C	3.9084818	14.2249276	15.4213159
C	1.2453251	15.1235706	21.4221422
C	1.2811876	13.5995522	16.4111018
C	0.0851595	15.0435391	19.1711790
C	4.1735256	13.6992914	22.2664878
C	0.3715501	15.6046944	20.4298444
H	-0.1443479	16.5351494	20.6626584
C	-0.7126312	12.5238733	17.2672194
H	-1.3553704	12.3035641	18.1222411
C	2.1117946	16.3575970	16.3522183
C	1.0678619	12.9840297	15.1729271
H	1.7809181	13.1366023	14.3594419
C	6.5784537	13.9590436	20.7154286
C	2.7788681	13.5247074	22.3313313
C	0.3723545	13.3858216	17.4632942
C	-0.9172216	11.9244434	16.0309999
H	-1.7672789	11.2512246	15.8927034
C	-0.8903136	15.7798236	18.2838050
H	-0.4509289	15.9790315	17.2939202
H	-1.1957176	16.7357745	18.7311265
H	-1.7893223	15.1628407	18.1194665
C	2.3558663	17.3960769	17.2537844
H	2.9269256	17.1953545	18.1638141
C	-0.0336266	12.1591649	14.9772341

H	-0.1895245	11.6794411	14.0080334
C	4.4775845	12.9461991	15.5113808
H	4.1816826	12.2728560	16.3231514
C	1.4002884	15.9578674	22.6722643
H	1.0960999	15.3805422	23.5604046
H	0.7937773	16.8725742	22.6212294
H	2.4544193	16.2438084	22.8187610
C	9.1026713	12.8128638	20.4031093
H	10.0919014	12.3638930	20.2804899
C	4.3029487	15.0886560	14.3992098
H	3.8752865	16.0910685	14.3292760
C	7.7209605	14.6741741	21.0778700
H	7.6324410	15.6840767	21.4846089
C	4.9918143	13.1255980	23.2485016
H	6.0760063	13.2460481	23.1871331
C	2.2373032	12.7435815	23.3613322
H	1.1637607	12.5445680	23.3424177
C	8.9815190	14.0996806	20.9195126
H	9.8734095	14.6642859	21.2034909
C	5.1763891	16.6489290	22.8386761
H	5.0880386	15.8523806	23.5809998
C	5.1030004	16.3449343	21.4759815
C	6.7013548	12.6661026	20.1880168
H	5.8060015	12.1061016	19.8969087
C	4.4397842	12.3870129	24.2868085
H	5.0884296	11.9419558	25.0450077
C	7.9612748	12.0976930	20.0392536
H	8.0520100	11.0879332	19.6310471
C	1.0952272	18.9160348	15.8674885
H	0.6928528	19.9149979	15.6798847

C 0.8439006 17.8826975 14.9643371

H 0.2446963 18.0693757 14.0695759

C 5.4166034 12.5376815 14.5719676

H 5.8536635 11.5386364 14.6448117

C 1.3440269 16.6083357 15.2081048

H 1.1214564 15.7966253 14.5107425

C 5.2057221 17.3774557 20.5376747

H 5.1390408 17.1440067 19.4712967

C 5.8049513 13.4008246 13.5464350

H 6.5470121 13.0781075 12.8114110

C 3.0588328 12.1902640 24.3335407

H 2.6190039 11.5807530 25.1272775

C 5.2511024 14.6746463 13.4638015

H 5.5569494 15.3561159 12.6657240

C 5.3505991 17.9667567 23.2548134

H 5.4008545 18.1952937 24.3224244

C 1.8487033 18.6711496 17.0118207

H 2.0372230 19.4740142 17.7289275

C 5.4573107 18.9893139 22.3147260

H 5.5914511 20.0231490 22.6435464

C 5.3878368 18.6925854 20.9547443

H 5.4683450 19.4914139 20.2130820

84

4 PNacAuZnCl2 Triplet E(DFT)=-5208.5536873 ZPVE=0.6551558

Au 3.7484540 14.4828742 18.8304851

Zn 1.4327252 12.5444695 20.0238552

Cl 3.2551834 11.5662690 19.0486250

Cl -0.1799224 11.3948601 20.9971022

P 2.7101810 14.6801843 16.7277109

P 4.9347724 14.5953293 20.8605348

N	0.6121686	13.8624835	18.7185783
N	1.9941430	14.0432731	21.2996908
C	3.9077314	14.2642152	15.4189206
C	1.1933725	15.1373174	21.4607049
C	1.2933255	13.5823741	16.4011574
C	0.0161652	15.0142422	19.1382744
C	4.2032871	13.6889747	22.2554507
C	0.3175716	15.5411502	20.4179805
H	-0.2377025	16.4550162	20.6504501
C	-0.6918082	12.4635837	17.2266279
H	-1.3408681	12.2289645	18.0729389
C	2.0898405	16.3594441	16.3819908
C	1.0949629	12.9829049	15.1521262
H	1.8089203	13.1602615	14.3445720
C	6.6140081	13.9057017	20.7026112
C	2.8029893	13.5739200	22.3388099
C	0.3823622	13.3345734	17.4439071
C	-0.8796297	11.8807708	15.9802286
H	-1.7200284	11.1991076	15.8251344
C	-0.9830637	15.7123718	18.2568086
H	-0.5585098	15.9658616	17.2690681
H	-1.3278869	16.6496843	18.7198193
H	-1.8724423	15.0831331	18.0663552
C	2.3777066	17.3984319	17.2701915
H	2.9828726	17.1958415	18.1579452
C	0.0077707	12.1445723	14.9364948
H	-0.1350258	11.6786885	13.9586086
C	4.5082832	12.9992930	15.4984476
H	4.2324623	12.3139133	16.3071790
C	1.2710448	15.9529547	22.7222966

H	0.9216934	15.3937810	23.6099990
H	0.6551754	16.8619230	22.6399264
H	2.3081603	16.2700944	22.9388174
C	9.1275468	12.7323898	20.4081463
H	10.1127260	12.2728138	20.2924032
C	4.2736632	15.1425059	14.3987439
H	3.8198207	16.1338793	14.3365432
C	7.7610966	14.6061480	21.0794316
H	7.6794621	15.6147005	21.4910894
C	5.0087712	13.1276938	23.2545602
H	6.0960308	13.2060107	23.1802991
C	2.2382674	12.8810076	23.4200112
H	1.1568859	12.7324744	23.4263064
C	9.0163528	14.0181661	20.9296864
H	9.9120044	14.5709329	21.2248728
C	5.1281938	16.6455165	22.7985777
H	4.9623090	15.8689092	23.5483194
C	5.1538873	16.3121272	21.4418051
C	6.7268177	12.6135551	20.1712111
H	5.8274018	12.0645698	19.8718178
C	4.4376221	12.4628719	24.3314142
H	5.0749574	12.0242214	25.1027694
C	7.9816024	12.0315056	20.0311675
H	8.0647880	11.0222818	19.6200308
C	1.0862663	18.9267067	15.9219989
H	0.6894466	19.9296635	15.7440684
C	0.7906486	17.8929200	15.0336575
H	0.1615381	18.0825208	14.1603326
C	5.4509729	12.6185886	14.5511384
H	5.9126306	11.6301000	14.6155756

C 1.2844962 16.6134857 15.2654241

H 1.0290500 15.8015553 14.5797102

C 5.3552152 17.3201067 20.4917841

H 5.3622785 17.0651245 19.4280161

C 5.8115001 13.4965470 13.5279580

H 6.5566513 13.1960252 12.7866945

C 3.0488181 12.3376118 24.4060463

H 2.5930443 11.7898573 25.2351200

C 5.2257818 14.7566446 13.4552914

H 5.5094360 15.4492578 12.6586302

C 5.3047540 17.9687827 23.1982805

H 5.2767581 18.2208878 24.2613822

C 1.8775778 18.6781035 17.0402309

H 2.1020601 19.4823697 17.7453487

C 5.5127145 18.9655743 22.2484522

H 5.6491647 20.0030790 22.5645492

C 5.5409854 18.6389364 20.8932198

H 5.7005280 19.4179307 20.1432482

PNacAuCd (5)

84

5 PNacAuCdI2 Singlet E(DFT)=-3272.3459289 ZPVE=0.6566880

Au 4.4700898 9.8562518 4.1820303

I 1.2505612 9.3372942 4.2766376

Cd 1.8442384 12.0434748 4.1679878

I 0.0435044 14.0570954 4.0307377

P 4.8054180 9.9324602 6.5126012

P 4.7969285 9.8149643 1.8505721

N 3.5807945 12.4511320 2.7348344

N 3.4412356 12.4465221 5.7413160

C 4.4714709 13.3921601 3.0112036

C	4.3454089	13.3955369	5.5657483
C	4.8093357	13.8267327	4.3072747
H	5.5578075	14.6169200	4.3437728
C	3.0405057	12.0024546	7.0122029
C	3.2471390	12.0925726	1.4180576
C	2.3764172	12.8921885	0.6633198
H	2.0063180	13.8196598	1.1058542
C	3.6721986	10.8619408	0.8775151
C	3.5332197	10.7779304	7.5049920
C	2.0664990	12.6863075	7.7490630
H	1.6535723	13.6111616	7.3395811
C	1.9581589	12.4941668	-0.5992669
H	1.2736209	13.1320048	-1.1644145
C	1.6112788	12.1779908	8.9597893
H	0.8468147	12.7236988	9.5188971
C	4.9422335	14.0719512	6.7792922
H	4.1806128	14.6990494	7.2723939
H	5.7945159	14.7084744	6.5048590
H	5.2797148	13.3309136	7.5198979
C	6.4802347	10.3789139	1.4125551
C	5.2064579	14.0570501	1.8675379
H	5.6587247	13.3027830	1.2051697
H	6.0000234	14.7222998	2.2344500
H	4.5087375	14.6504110	1.2545639
C	4.6522824	8.1549521	1.1094743
C	6.3400876	10.8215698	6.9474816
C	4.9359333	8.2607040	7.2271560
C	6.6727420	11.0554824	8.2879629
H	6.0269265	10.6778453	9.0851466
C	6.7387714	11.0761378	0.2288143

H	5.9201388	11.3114015	-0.4551880
C	3.0662236	10.2748943	8.7227443
H	3.4439985	9.3214861	9.0984455
C	2.3877713	11.2801355	-1.1352252
H	2.0490971	10.9591014	-2.1229767
C	9.0847943	11.1882635	0.7904139
H	10.1012704	11.5099325	0.5492021
C	3.2354327	10.4677101	-0.3932781
H	3.5570578	9.5066126	-0.8005698
C	2.1110451	10.9733646	9.4527987
H	1.7463146	10.5696554	10.4001855
C	7.5390017	10.0860983	2.2787674
H	7.3428115	9.5397801	3.2052335
C	7.1519727	11.3460658	5.9400911
H	6.8756930	11.2023286	4.8933887
C	8.2892770	12.0829716	6.2648354
H	8.9096833	12.4970106	5.4659932
C	7.8120401	11.7838566	8.6112304
H	8.0643790	11.9613136	9.6597205
C	8.6223666	12.2991376	7.5985143
H	9.5122737	12.8802760	7.8542062
C	8.0360210	11.4805101	-0.0785250
H	8.2267912	12.0306046	-1.0034851
C	4.3159357	5.6050056	0.0218282
H	4.1848151	4.6066300	-0.4037811
C	8.8352875	10.4858394	1.9682205
H	9.6538840	10.2517709	2.6536945
C	3.8285527	7.4145133	7.0734369
H	2.9278833	7.7792722	6.5696996
C	5.0269624	5.6343806	8.1784706

H 5.0625946 4.6076917 8.5521051

C 3.5126987 7.4019672 1.4194514

H 2.7526879 7.8113712 2.0918229

C 6.1336956 6.4661554 8.3183459

H 7.0422107 6.0954172 8.7999833

C 5.4539829 6.3474730 -0.2810678

H 6.2188568 5.9349632 -0.9440916

C 6.0907568 7.7769726 7.8447197

H 6.9665036 8.4191731 7.9558931

C 5.6234784 7.6210657 0.2592410

H 6.5188680 8.1968084 0.0155869

C 3.3456059 6.1348846 0.8719108

H 2.4516931 5.5556980 1.1164386

C 3.8741677 6.1112556 7.5540484

H 3.0043391 5.4607710 7.4330975

84

5 PNacAuCdI2 Triplet E(DFT)=-3272.2492061 ZPVE=0.6534610

Au 4.4402369 9.7837486 4.1807226

I 1.2339096 9.3045750 4.2884774

Cd 1.8814044 11.9967689 4.1461646

I 0.1158291 14.0222947 3.8842912

P 4.7928849 9.9297527 6.5061404

P 4.7587765 9.7522255 1.8467218

N 3.6445262 12.4112146 2.7313116

N 3.3800767 12.4486839 5.7812486

C 4.4790407 13.4556537 3.0131280

C 4.2912506 13.4505920 5.6366912

C 4.7298712 13.8629861 4.3534387

H 5.4485263 14.6861115 4.4074043

C 3.0047547 11.9777694 7.0455525

C	3.3103240	12.0894678	1.4133278
C	2.5309971	12.9564788	0.6291919
H	2.2200098	13.9105086	1.0588406
C	3.6619248	10.8303888	0.8807350
C	3.5187110	10.7523188	7.5143626
C	2.0467169	12.6510291	7.8137896
H	1.6247922	13.5801835	7.4244820
C	2.1113535	12.5809125	-0.6386117
H	1.4897165	13.2652994	-1.2218357
C	1.6196319	12.1255284	9.0268202
H	0.8651300	12.6608489	9.6090634
C	4.8522744	14.1371638	6.8539064
H	4.0768110	14.6998657	7.4059707
H	5.6462484	14.8466894	6.5756925
H	5.2858762	13.4141677	7.5669834
C	6.4514332	10.3080677	1.4346169
C	5.1950090	14.1757990	1.9000474
H	5.6892640	13.4642500	1.2145876
H	5.9720961	14.8441547	2.3022567
H	4.5191878	14.7930239	1.2795333
C	4.6005111	8.1038900	1.0858744
C	6.3200189	10.8468629	6.9038214
C	4.9678483	8.2639111	7.2258565
C	6.6602010	11.1257336	8.2330772
H	6.0171345	10.7783517	9.0461047
C	6.7193457	11.0889800	0.3073196
H	5.9038439	11.3900857	-0.3538006
C	3.0790029	10.2335040	8.7361912
H	3.4722401	9.2799403	9.0949394
C	2.4553260	11.3323259	-1.1595610

H	2.1137358	11.0328469	-2.1529838
C	9.0687483	11.1155196	0.8673734
H	10.0904612	11.4360535	0.6476418
C	3.2268523	10.4639344	-0.3982836
H	3.4954566	9.4842854	-0.7997475
C	2.1347462	10.9168005	9.4937060
H	1.7921566	10.4994678	10.4434025
C	7.5065790	9.9326019	2.2740364
H	7.3026167	9.3246291	3.1599125
C	7.1280985	11.3328207	5.8738078
H	6.8487314	11.1475213	4.8337362
C	8.2707062	12.0740217	6.1665483
H	8.8906221	12.4545031	5.3507464
C	7.8054083	11.8591166	8.5248603
H	8.0641030	12.0718853	9.5651623
C	8.6121013	12.3345562	7.4908325
H	9.5066988	12.9190645	7.7212922
C	8.0238028	11.4920975	0.0276243
H	8.2221951	12.1084763	-0.8528554
C	4.2426624	5.5753693	-0.0427949
H	4.1031528	4.5851559	-0.4845017
C	8.8089981	10.3302875	1.9900493
H	9.6246734	10.0305736	2.6531082
C	3.8877177	7.3847019	7.0631696
H	2.9829354	7.7206033	6.5467547
C	5.1232452	5.6475402	8.1950389
H	5.1841854	4.6245761	8.5755300
C	3.4671713	7.3452203	1.4041532
H	2.7202436	7.7426815	2.0980085
C	6.2031097	6.5123783	8.3440949

H 7.1155969 6.1713993 8.8399665

C 5.3744333 6.3240250 -0.3547723

H 6.1254617 5.9244842 -1.0411421

C 6.1280339 7.8186276 7.8617626

H 6.9825435 8.4874685 7.9806789

C 5.5545109 7.5871332 0.2058217

H 6.4439688 8.1691770 -0.0450246

C 3.2892791 6.0884716 0.8361218

H 2.4003002 5.5043524 1.0868097

C 3.9650438 6.0863670 7.5528581

H 3.1162948 5.4098458 7.4252601

PNacAuHg (6)

84

6 PNacAuHgCl2 Singlet E(DFT)=-3582.7344376 ZPVE=0.6567967

Au 3.4566680 8.4309196 14.7220908

Hg 2.4078257 10.8359021 12.3838579

Cl 3.4277676 8.6881982 11.6978285

P 5.6028119 9.3295384 15.0518844

P 1.4010409 7.2937397 14.8073354

Cl 1.6408911 12.9256401 11.4935484

N 0.8976105 10.1147961 14.1086004

N 3.5592270 11.4479435 14.4298035

C 5.9286484 10.9205909 14.2390628

C 6.9308771 8.2334183 14.4546999

C 5.1019774 13.0414002 13.4212092

H 4.2562326 13.7064203 13.2320239

C 4.8581393 11.8224652 14.0759656

C 2.1556387 5.2236160 13.1598092

H 2.4279357 6.0323351 12.4732901

C 5.9482151 9.5992125 16.8257486

C	-0.0439909	9.2634003	13.5229098
C	1.5979199	5.5263986	14.4104330
C	8.0226965	7.8633784	15.2419706
H	8.1096881	8.2281034	16.2679872
C	0.0929224	7.8705351	13.6813789
C	6.3757283	13.3655733	12.9767650
H	6.5402236	14.3179276	12.4656322
C	7.2072952	11.2555811	13.7755851
H	8.0279470	10.5438486	13.8929552
C	2.0347262	2.8681158	13.6749161
H	2.2048304	1.8272959	13.3871355
C	-1.8980768	8.8749958	12.0107946
H	-2.6686976	9.2733148	11.3454216
C	2.9241239	11.9601249	15.4688929
C	6.8239929	7.7556172	13.1416033
H	5.9644768	8.0374105	12.5240067
C	-0.7697866	6.9983689	13.0104139
H	-0.6505313	5.9187734	13.1275189
C	1.5918239	11.6680708	15.8207064
H	1.2304294	12.1740954	16.7150473
C	2.3650326	3.8991866	12.7945485
H	2.7963916	3.6702722	11.8168001
C	-1.0421017	9.7502145	12.6670048
H	-1.1101988	10.8289122	12.5060498
C	1.2747614	4.4936912	15.2913198
H	0.8531116	4.7191961	16.2730543
C	0.6542962	10.8240061	15.1961800
C	7.4376073	12.4766413	13.1561888
H	8.4376248	12.7273603	12.7948595
C	0.6298132	7.4023836	16.4583748

C	6.7158781	10.6777379	17.2738828
H	7.1194035	11.3951343	16.5557677
C	-1.7684785	7.4961343	12.1814894
H	-2.4355975	6.8086481	11.6562608
C	3.6712761	12.9094869	16.3833682
H	3.0756330	13.1643503	17.2709135
H	3.9235730	13.8418331	15.8527124
H	4.6210867	12.4591152	16.7147497
C	6.4460334	9.9388085	19.5571463
H	6.6373427	10.0747974	20.6247877
C	-0.5826298	7.6924436	18.9606503
H	-1.0594825	7.8101711	19.9372925
C	7.8117740	6.9246532	12.6249461
H	7.7252141	6.5572597	11.5992652
C	1.4945077	3.1668389	14.9219651
H	1.2402466	2.3627404	15.6174348
C	-0.6699535	6.9274222	16.6739145
H	-1.2236564	6.4609260	15.8549253
C	8.9027492	6.5565180	13.4126175
H	9.6749528	5.8988432	13.0047504
C	-0.7087496	10.7182997	15.8467517
H	-1.4817900	11.1453717	15.1866546
H	-0.7370978	11.2500552	16.8079059
H	-0.9785658	9.6644415	16.0202678
C	5.4304067	8.6930738	17.7581908
H	4.8216069	7.8527379	17.4128528
C	-1.2699161	7.0655810	17.9206956
H	-2.2848521	6.6925858	18.0798474
C	1.3097070	8.0328434	17.5029432
H	2.3103694	8.4365996	17.3299147

C 9.0057577 7.0240253 14.7197346

H 9.8576590 6.7356444 15.3410235

C 6.9609174 10.8467683 18.6351137

H 7.5573677 11.6967634 18.9762169

C 0.7046280 8.1776631 18.7497527

H 1.2424578 8.6826757 19.5560168

C 5.6827913 8.8586797 19.1163543

H 5.2743534 8.1440280 19.8355197

84

6 PNacAuHgCl2 Triplet E(DFT)=-3582.6385375 ZPVE=0.6539473

Au 3.4506357 8.4630519 14.7011596

Hg 2.4007174 10.9121958 12.3894466

Cl 3.3119766 8.5647967 11.7666191

P 5.6329589 9.2706505 14.9983726

P 1.3494536 7.4345025 14.8780593

Cl 3.0108348 12.7742634 11.0399244

N 0.7841809 10.2713208 13.7681938

N 3.5685341 11.3905676 14.5820443

C 5.9230448 10.9157767 14.2951285

C 6.9339598 8.2149216 14.2880115

C 5.0924188 13.1399296 13.8155341

H 4.2556448 13.8341830 13.7353860

C 4.8467262 11.8318202 14.2731590

C 2.1455218 5.2883656 13.3407197

H 2.4127521 6.0634174 12.6140343

C 6.0286281 9.4333992 16.7758704

C -0.0527693 9.2636865 13.2595879

C 1.5707143 5.6489706 14.5685331

C 8.0873131 7.8604510 14.9915426

H 8.2331273 8.2056386 16.0178334

C	0.0585727	7.9226759	13.6806153
C	6.3561355	13.5141925	13.3873793
H	6.5139784	14.5276195	13.0093141
C	7.1920345	11.3090508	13.8593746
H	8.0138515	10.5890945	13.8736693
C	2.0552972	2.9621222	13.9834722
H	2.2444795	1.9100361	13.7544146
C	-1.8135725	8.6168587	11.7182305
H	-2.5337798	8.8944532	10.9442656
C	2.7992429	12.0132967	15.5211297
C	6.7491669	7.7639923	12.9741446
H	5.8403462	8.0307916	12.4229772
C	-0.7854024	6.9565593	13.1198864
H	-0.6896256	5.9129263	13.4266378
C	1.4524063	11.6529165	15.6902464
H	0.9937894	12.1270246	16.5634376
C	2.3786870	3.9494054	13.0515089
H	2.8240280	3.6749500	12.0919154
C	-0.9809714	9.5857951	12.2623540
H	-1.0355912	10.6234379	11.9255723
C	1.2546738	4.6610813	15.5016484
H	0.8200625	4.9323598	16.4658688
C	0.5370707	10.7953107	15.0069602
C	7.4145258	12.6033434	13.4064115
H	8.4064860	12.8990403	13.0573523
C	0.5873179	7.5844249	16.5274757
C	6.7052329	10.5418995	17.2907610
H	7.0209141	11.3467113	16.6234859
C	-1.7250231	7.2966583	12.1540016
H	-2.3722459	6.5265014	11.7280348

C	3.4225853	12.9855530	16.4934723
H	2.7420475	13.1854085	17.3359484
H	3.6765557	13.9586320	16.0373748
H	4.3631699	12.5761698	16.9059845
C	6.5705399	9.6081439	19.5145088
H	6.7799100	9.6787215	20.5851267
C	-0.5593702	7.8761762	19.0590819
H	-1.0098295	7.9933416	20.0482691
C	7.7233644	6.9737629	12.3732069
H	7.5768876	6.6264776	11.3473431
C	1.4979236	3.3193853	15.2071031
H	1.2487385	2.5505391	15.9431350
C	-0.7175899	7.1386574	16.7672616
H	-1.2989028	6.6877689	15.9586969
C	8.8752914	6.6211282	13.0760255
H	9.6359418	5.9956655	12.6011301
C	-0.8408364	10.6230257	15.5975497
H	-1.6129734	11.0874410	14.9538588
H	-0.9017993	11.0894617	16.5923678
H	-1.1285017	9.5660661	15.7178800
C	5.6190633	8.4154268	17.6457997
H	5.0718517	7.5546150	17.2504527
C	-1.2863519	7.2802522	18.0290287
H	-2.3064920	6.9311038	18.2076860
C	1.3087181	8.1839383	17.5628831
H	2.3203485	8.5525772	17.3710459
C	9.0551872	7.0624360	14.3844489
H	9.9555492	6.7856561	14.9391408
C	6.9717748	10.6282947	18.6564702
H	7.4965114	11.5024108	19.0505008

C 0.7369809 8.3281449 18.8248647

H 1.3080681 8.8029842 19.6266427

C 5.8955732 8.4984599 19.0061935

H 5.5741132 7.6963649 19.6756211

PNacAgZn (7)

84

7 PNacAgZnCl2 Singlet E(DFT)=-5219.8868958 ZPVE=0.6579637

Ag -0.3423278 -0.7059149 0.2325867

Zn 2.4207327 -1.9952821 -0.0969673

P -1.1140555 -0.7843566 -2.0706089

Cl 0.5547771 -3.1924064 0.5613534

P -0.0408334 0.2846889 2.4272177

Cl 4.3891321 -2.9448985 -0.3675886

N 1.8929777 -0.8348824 -1.6980664

N 2.5323739 -0.3346598 1.0877056

C -1.8776751 1.8865835 -2.1135126

H -2.0550043 1.7356939 -1.0447995

C -1.4068678 0.8231252 -2.8906999

C -0.3272734 -2.4765995 -4.1948911

H -1.3905570 -2.5567111 -4.4332320

C 0.0830053 -1.6679420 -3.1275430

C 2.5746632 -0.6194281 2.4668832

C 1.4509746 -1.5828542 -2.8081659

C 0.2329084 2.0906987 2.4339186

C -2.6644929 -1.7210920 -2.3031500

C 1.4368047 -0.3915675 3.2636441

C 2.9919289 0.8042301 0.5922905

C 2.4091725 0.3790541 -1.8373575

C 2.9274080 1.1378894 -0.7732678

H 3.3335850 2.1121765 -1.0407255

C	1.4649768	-0.7294418	4.6201421
H	0.5807271	-0.5630399	5.2398411
C	-1.4050913	-0.0483131	3.5928828
C	1.9522456	-3.1333925	-4.5996902
H	2.6853252	-3.7219136	-5.1575211
C	3.7016051	-1.2247227	3.0313113
H	4.5425006	-1.4633311	2.3760243
C	0.6003318	-3.1952116	-4.9387467
H	0.2659789	-3.8239480	-5.7674842
C	2.4475485	1.0057062	-3.2111972
H	3.0772175	0.4064244	-3.8886526
H	2.8458809	2.0288648	-3.1722334
H	1.4390673	1.0380602	-3.6523894
C	2.3733750	-2.3423377	-3.5391087
H	3.4182585	-2.3276253	-3.2211563
C	2.6034680	-1.2975123	5.1818982
H	2.6139328	-1.5606396	6.2424220
C	-1.1775857	1.0253772	-4.2551375
H	-0.8035574	0.2041865	-4.8713829
C	-3.7419158	-1.2541373	-3.0581723
H	-3.6832080	-0.2843812	-3.5575864
C	3.7164409	-1.5538893	4.3815762
H	4.6027883	-2.0279168	4.8112343
C	-2.1277698	0.9436277	4.2578268
H	-1.8659540	1.9955629	4.1276528
C	3.6255602	1.8108078	1.5217295
H	2.9758350	2.0217081	2.3841766
H	3.8392770	2.7550383	1.0023731
H	4.5701199	1.4046017	1.9207932
C	-4.8983526	-2.0242270	-3.1771764

H	-5.7384613	-1.6512354	-3.7689050
C	0.1224694	2.7933056	1.2321461
H	-0.1471552	2.2592111	0.3175303
C	-2.1205897	3.1304888	-2.6893402
H	-2.4892828	3.9529309	-2.0708519
C	-2.7563074	-2.9637450	-1.6607898
H	-1.9172716	-3.3315763	-1.0606630
C	-1.7717391	-1.3922670	3.7565171
H	-1.2234929	-2.1752422	3.2220018
C	-3.5409365	-0.7389116	5.2621883
H	-4.3747907	-1.0081166	5.9157686
C	-2.8273611	-1.7341020	4.5931944
H	-3.1004404	-2.7849831	4.7178934
C	-4.9819759	-3.2626150	-2.5473803
H	-5.8889339	-3.8654121	-2.6431602
C	-3.9080815	-3.7315541	-1.7902117
H	-3.9695051	-4.7017471	-1.2907314
C	0.6285057	2.7727786	3.5913794
H	0.7501541	2.2270867	4.5309973
C	-1.8845109	3.3256003	-4.0488457
H	-2.0660973	4.3038675	-4.5015777
C	0.3901616	4.1601951	1.1859601
H	0.3100248	4.6952266	0.2362866
C	0.7699601	4.8336605	2.3431493
H	0.9845816	5.9050290	2.3083691
C	0.8888782	4.1380916	3.5473108
H	1.1977489	4.6626197	4.4551421
C	-3.1930165	0.5970115	5.0890616
H	-3.7532808	1.3814697	5.6045612
C	-1.4136247	2.2719974	-4.8299319

H -1.2260126 2.4214063 -5.8963414

84

7 PNacAgZnCl2 Triplet E(DFT)=-5219.7895513 ZPVE=0.6548072

Ag -0.4075945 -0.8693497 0.2827272

Zn 2.4295965 -2.0014272 -0.1215357

P -1.1677809 -0.8830677 -2.0286914

Cl 0.6199812 -3.2919665 0.5165337

P -0.0073974 0.2465048 2.4014698

Cl 4.4114516 -2.8568786 -0.5338696

N 1.8324036 -0.7861009 -1.6579424

N 2.5895901 -0.4506776 1.1738933

C -2.1046268 1.7286507 -1.9231382

H -2.3200784 1.4889118 -0.8776862

C -1.5316314 0.7564456 -2.7505634

C -0.2916560 -2.3923201 -4.2523183

H -1.3495463 -2.5281683 -4.4893408

C 0.0735524 -1.6394800 -3.1291384

C 2.5696685 -0.7433923 2.5461323

C 1.4357690 -1.4804805 -2.8133802

C 0.3376678 2.0342110 2.2713254

C -2.6705680 -1.8769769 -2.3223927

C 1.4189457 -0.4520572 3.3035822

C 3.0980146 0.7350382 0.7276275

C 2.3823663 0.4621437 -1.7654988

C 2.9596619 1.0974944 -0.6337417

H 3.3796664 2.0818321 -0.8610365

C 1.3918614 -0.7699840 4.6647744

H 0.4987545 -0.5539754 5.2555839

C -1.4050928 0.0724933 3.5645044

C 2.0247334 -2.8363854 -4.7308760

H	2.7912561	-3.3203455	-5.3418409
C	3.6526307	-1.3869878	3.1517228
H	4.5060012	-1.6586169	2.5261787
C	0.6754544	-2.9801277	-5.0575006
H	0.3768847	-3.5678105	-5.9288949
C	2.4069011	1.1683954	-3.0941851
H	3.0414466	0.6488985	-3.8358638
H	2.7936018	2.1933389	-2.9845921
H	1.3979980	1.2392821	-3.5380620
C	2.4030986	-2.0986520	-3.6179115
H	3.4490297	-2.0249052	-3.3132742
C	2.4869255	-1.3800962	5.2679818
H	2.4545315	-1.6263365	6.3320728
C	-1.2504165	1.0746079	-4.0823726
H	-0.7966047	0.3263381	-4.7363232
C	-3.7606352	-1.4233182	-3.0674603
H	-3.7415134	-0.4279776	-3.5172880
C	3.6107863	-1.6978438	4.5059291
H	4.4621776	-2.2027263	4.9698251
C	-2.0439580	1.1451727	4.1889406
H	-1.6953275	2.1659231	4.0208575
C	3.8211705	1.6544666	1.6716125
H	3.2153289	1.8960604	2.5617746
H	4.0769213	2.6036435	1.1762457
H	4.7603430	1.2015518	2.0410077
C	-4.8775667	-2.2399352	-3.2402178
H	-5.7279259	-1.8776941	-3.8239148
C	0.1869253	2.6596132	1.0313047
H	-0.1317980	2.0736030	0.1650772
C	-2.3973811	2.9959090	-2.4184236

H -2.8449777 3.7460013 -1.7612702

C -2.7097426 -3.1535989 -1.7447379

H -1.8600742 -3.5115857 -1.1537016

C -1.8832353 -1.2285152 3.7781023

H -1.4007607 -2.0744987 3.2773361

C -3.5939590 -0.3749171 5.2496117

H -4.4485321 -0.5487644 5.9086945

C -2.9644794 -1.4506577 4.6224145

H -3.3238585 -2.4697975 4.7856260

C -4.9087745 -3.5113906 -2.6745045

H -5.7847821 -4.1506286 -2.8126468

C -3.8220759 -3.9674010 -1.9278364

H -3.8425296 -4.9637792 -1.4791253

C 0.7927185 2.7806354 3.3641327

H 0.9439555 2.2939780 4.3316176

C -2.1097316 3.3070257 -3.7464935

H -2.3305327 4.3044257 -4.1356282

C 0.4689549 4.0157263 0.8860733

H 0.3516335 4.4905376 -0.0914539

C 0.9078100 4.7555695 1.9814755

H 1.1334757 5.8193487 1.8691293

C 1.0702357 4.1366558 3.2208302

H 1.4259250 4.7126308 4.0789546

C -3.1356464 0.9198420 5.0274922

H -3.6295427 1.7671815 5.5102469

C -1.5373016 2.3454270 -4.5762246

H -1.3081708 2.5860806 -5.6175236

PNacAgCd (8)

84

8 PNacAgCdI2 Singlet E(DFT)=-3283.5812901 ZPVE=0.6563733

I	6.3519593	12.7790548	6.7133021
I	7.9284129	8.2558780	7.6838760
Cd	5.9758868	10.0883742	7.4089293
Ag	3.4910851	12.1359540	6.9692632
P	2.7238714	11.5294677	4.7361025
P	2.9499920	12.6564797	9.2884204
N	4.4716910	10.1288350	9.1173817
N	4.1683031	9.3224116	6.2294855
C	1.0388420	10.8208340	4.6560538
C	0.0581612	11.3481957	5.5028042
H	0.3161113	12.1605036	6.1881513
C	3.3492029	8.4504629	6.8064661
C	2.7022855	14.4373789	9.6073399
C	4.2803115	12.1642531	10.4403906
C	4.7276214	12.9703315	11.4910769
H	4.2659284	13.9454788	11.6613710
C	5.2816750	8.3672472	4.2841972
H	5.7653842	7.6486708	4.9500091
C	3.7534638	15.2969267	9.2554999
H	4.6844358	14.8843579	8.8539574
C	3.6103453	9.1325619	9.2562757
C	4.8813715	10.9096256	10.2168840
C	5.7686404	12.5487658	12.3114461
H	6.1138808	13.1892724	13.1265507
C	4.3926180	9.2994415	4.8369294
C	3.8132691	10.2685786	3.9933531
C	2.4286724	17.2074175	9.9036607
H	2.3217952	18.2889221	10.0212915
C	5.5687923	8.3757166	2.9255694
H	6.2691841	7.6416343	2.5189182

C	3.1090230	8.3612416	8.1896838
H	2.4116400	7.5781781	8.4827280
C	3.1146540	8.7783617	10.6396459
H	3.9407423	8.3584819	11.2375833
H	2.3016368	8.0409813	10.5967638
H	2.7524909	9.6706532	11.1719904
C	1.5101165	14.9807278	10.0906722
H	0.6750652	14.3283854	10.3531306
C	0.6971215	9.7863605	3.7799791
H	1.4529351	9.3693337	3.1101103
C	4.9824609	9.3246390	2.0887206
H	5.2131411	9.3400179	1.0209098
C	2.7019694	12.8770086	3.5014397
C	-0.6011597	9.2814163	3.7608942
H	-0.8562661	8.4683438	3.0763670
C	5.9412960	10.5054757	11.0355234
H	6.4292992	9.5497945	10.8291277
C	3.6190266	16.6714213	9.4114925
H	4.4477003	17.3297879	9.1388491
C	1.3758139	16.3612316	10.2370871
H	0.4377289	16.7750597	10.6162316
C	4.1165803	10.2687740	2.6262355
H	3.6761755	11.0290900	1.9772865
C	1.6318512	13.1001460	2.6316170
H	0.7527770	12.4529371	2.6650659
C	6.3777300	11.3171578	12.0763037
H	7.2088345	10.9870535	12.7048504
C	1.4762982	11.8014578	9.9501192
C	1.1215899	11.8852349	11.3026741
H	1.7147934	12.5000499	11.9850379

C 2.6005406 7.4654892 5.9355228

H 2.0806064 7.9844525 5.1163711

H 1.8605513 6.8998010 6.5179517

H 3.3015965 6.7518496 5.4729308

C 2.7963436 14.9808107 1.6620492

H 2.8325647 15.8034328 0.9429893

C -1.2405527 10.8479385 5.4799585

H -1.9959256 11.2684496 6.1488522

C -1.5703996 9.8086352 4.6117317

H -2.5874648 9.4082711 4.5976164

C 3.8184241 13.7219395 3.4499823

H 4.6574933 13.5607288 4.1336824

C 0.0283864 11.1753250 11.7867039

H -0.2416166 11.2462332 12.8434790

C 1.6801353 14.1507338 1.7166062

H 0.8373434 14.3187112 1.0409789

C 3.8662742 14.7633308 2.5297834

H 4.7440935 15.4134665 2.4953010

C 0.7334081 10.9803519 9.1002113

H 1.0283553 10.8758027 8.0540041

C -0.7142117 10.3634278 10.9274159

H -1.5681335 9.7995099 11.3120653

C -0.3589641 10.2637718 9.5857443

H -0.9246187 9.6188280 8.9084353

84

8 PNacAgCdI2 Triplet E(DFT)=-3283.4846507 ZPVE=0.6531703

I 6.4331970 12.7994228 6.7379515

I 7.9161864 8.2016978 7.2433707

Cd 6.0076468 10.0872614 7.3660690

Ag 3.5913003 12.2128209 6.9422721

P	2.7846215	11.6425268	4.7154106
P	2.9839145	12.5291897	9.2829290
N	4.7352439	10.1100392	9.2121960
N	4.0860546	9.4013448	6.2780067
C	1.0563785	11.0427826	4.6724673
C	0.1146379	11.6850085	5.4841842
H	0.4263772	12.5204706	6.1181774
C	3.2747833	8.5068436	6.9221966
C	2.5839160	14.2863990	9.5926230
C	4.3271397	12.1596556	10.4663481
C	4.6859017	13.0294414	11.5007300
H	4.1162477	13.9478409	11.6580736
C	5.0066068	8.2262803	4.3514234
H	5.4196022	7.4808983	5.0337730
C	3.5422110	15.2330619	9.2009773
H	4.4917472	14.9012104	8.7687491
C	3.7878260	9.1481393	9.4196408
C	5.0744671	10.9815031	10.2605302
C	5.7760835	12.7496118	12.3180489
H	6.0466266	13.4400955	13.1203966
C	4.2646688	9.2904191	4.8875355
C	3.7729888	10.2821897	4.0139682
C	2.0797702	17.0235041	9.8930825
H	1.8824854	18.0921326	10.0114964
C	5.2561249	8.1498811	2.9886529
H	5.8511474	7.3204095	2.5978543
C	3.1906345	8.4527886	8.3396952
H	2.4682519	7.7061316	8.6813246
C	3.3975760	8.7784693	10.8264140
H	4.2507993	8.3419313	11.3790972

H	2.5803190	8.0414018	10.8281310
H	3.0566817	9.6501557	11.4099142
C	1.3680721	14.7256940	10.1200621
H	0.6046850	14.0038643	10.4163232
C	0.6485306	9.9711553	3.8729511
H	1.3742569	9.4612258	3.2353308
C	4.7716300	9.1333981	2.1257312
H	4.9758362	9.0798509	1.0538037
C	2.8486281	12.9484210	3.4407216
C	-0.6783891	9.5463663	3.8911854
H	-0.9854496	8.7033138	3.2669323
C	6.1840614	10.7232798	11.0708238
H	6.7716185	9.8224673	10.8794143
C	3.2940971	16.5913025	9.3588107
H	4.0514353	17.3182438	9.0547815
C	1.1186223	16.0901541	10.2679565
H	0.1626381	16.4223176	10.6811887
C	4.0365238	10.1927847	2.6416485
H	3.6632816	10.9700629	1.9709207
C	1.7950071	13.2090146	2.5610919
H	0.8768587	12.6198387	2.6147332
C	6.5296582	11.5992375	12.0936102
H	7.3998673	11.3822896	12.7184717
C	1.5381506	11.5791723	9.8661807
C	1.1720610	11.5416246	11.2162754
H	1.7605467	12.0908908	11.9564016
C	2.4289108	7.5446376	6.1267867
H	1.8595323	8.0663305	5.3382322
H	1.7033391	7.0328412	6.7775599
H	3.0272781	6.7655151	5.6198150

C 3.0781507 14.9767062 1.5308322

H 3.1673318 15.7699327 0.7839030

C -1.2120434 11.2650600 5.4973023

H -1.9364121 11.7745248 6.1379218

C -1.6093662 10.1902894 4.7031422

H -2.6490761 9.8529871 4.7180150

C 4.0171319 13.7175072 3.3635491

H 4.8435788 13.5268341 4.0550592

C 0.0688971 10.7970697 11.6231004

H -0.2098828 10.7713685 12.6796462

C 1.9108338 14.2221987 1.6108261

H 1.0810859 14.4202869 0.9272681

C 4.1317996 14.7213646 2.4080995

H 5.0494573 15.3123993 2.3532453

C 0.7955825 10.8482058 8.9358081

H 1.0952237 10.8452528 7.8851228

C -0.6725917 10.0772815 10.6862698

H -1.5357050 9.4891116 11.0091950

C -0.3077749 10.1021194 9.3420613

H -0.8771854 9.5343707 8.6016205

PNacCu (9)

81

9 PNacCu Singlet E(DFT)=-4013.7692983 ZPVE=0.6535853

Cu 2.3194282 1.2636571 3.0122256

P 2.2474574 -0.7579626 4.0769189

P 1.5652805 3.2788767 3.6822716

N 2.1918272 0.0294587 1.3815686

N 3.9519752 2.3361142 2.3654166

C 3.1112740 0.0611935 0.4377371

C 4.0819795 1.0826741 0.3068569

H	4.6664388	1.0254300	-0.6133608
C	4.4281184	2.1650198	1.1447276
C	5.4113530	3.1513307	0.5397335
H	6.4537088	2.8830257	0.7828574
H	5.2376094	4.1727051	0.9103168
H	5.3181374	3.1537266	-0.5559822
C	3.1897774	-1.0385431	-0.6045522
H	2.9096348	-2.0135066	-0.1775538
H	4.2104343	-1.1107733	-1.0069999
H	2.5098680	-0.8399252	-1.4505237
C	1.2390699	-0.9761946	1.5509291
C	1.1034930	-1.5108061	2.8568293
C	0.1503358	-2.4892379	3.1240868
H	0.0577518	-2.8935275	4.1355617
C	-0.6986547	-2.9432024	2.1153369
H	-1.4492835	-3.7072046	2.3320528
C	-0.5908205	-2.4017025	0.8367887
H	-1.2654389	-2.7361280	0.0435924
C	0.3634406	-1.4273874	0.5550906
H	0.4193067	-0.9905841	-0.4429026
C	3.7780410	-1.7336809	3.8411989
C	3.7999969	-3.1321581	3.8952028
H	2.8829346	-3.6829174	4.1224323
C	4.9796925	-3.8261246	3.6485242
H	4.9890354	-4.9184652	3.6936149
C	6.1462160	-3.1285003	3.3317568
H	7.0717111	-3.6752529	3.1313697
C	6.1276112	-1.7386571	3.2603416
H	7.0352829	-1.1891175	2.9977847
C	4.9470951	-1.0421126	3.5133653

H	4.9207932	0.0482102	3.4327219
C	1.5714132	-1.2464383	5.7013354
C	2.3034728	-1.9416709	6.6678234
H	3.3070902	-2.3043413	6.4362560
C	1.7629861	-2.1733929	7.9322860
H	2.3482284	-2.7189198	8.6773975
C	0.4869667	-1.7146964	8.2461746
H	0.0647787	-1.8992982	9.2375128
C	-0.2485037	-1.0132529	7.2903121
H	-1.2477542	-0.6396882	7.5291606
C	0.2926961	-0.7747671	6.0324709
H	-0.2813042	-0.2042620	5.2963832
C	4.2901652	3.3633926	3.2422500
C	3.2393149	3.9618845	3.9862335
C	3.5142444	4.9515051	4.9282703
H	2.6924530	5.3918506	5.4994354
C	4.8219804	5.3696552	5.1634423
H	5.0283996	6.1422805	5.9078916
C	5.8618048	4.7688639	4.4577178
H	6.8966032	5.0653070	4.6516193
C	5.6036188	3.7776678	3.5163842
H	6.4345266	3.2908185	3.0054985
C	0.8005711	4.4263135	2.4796726
C	-0.3343117	3.9800803	1.7924166
H	-0.7181009	2.9732159	1.9824401
C	-0.9676773	4.8008380	0.8647002
H	-1.8544870	4.4412791	0.3361392
C	-0.4618849	6.0727242	0.5997706
H	-0.9531360	6.7155452	-0.1356214
C	0.6767739	6.5181567	1.2667352

H 1.0821447 7.5114635 1.0560586

C 1.3053685 5.6998468 2.2033980

H 2.2002606 6.0529923 2.7209913

C 0.6787503 3.6110155 5.2470106

C 0.8730817 2.6928519 6.2863494

H 1.5273204 1.8311392 6.1280345

C 0.2327089 2.8620812 7.5089119

H 0.3928579 2.1330540 8.3076644

C -0.6210250 3.9476839 7.7034508

H -1.1312814 4.0796032 8.6613886

C -0.8277942 4.8598076 6.6713573

H -1.4997317 5.7098074 6.8177976

C -0.1808041 4.6941346 5.4474387

H -0.3501793 5.4126862 4.6418628

81

9 PNacCu Triplet E(DFT)=-4013.6979333 ZPVE=0.6517480

Cu 2.6312380 1.2571430 2.6690772

P 2.0769525 -0.6147629 3.8770447

P 1.9194111 3.1024814 3.8200092

N 2.4789832 -0.0120592 1.1827638

N 4.0019729 2.4958146 1.9972460

C 3.3680080 0.0800453 0.1265622

C 4.1982593 1.1900775 -0.0557072

H 4.7499600 1.1617555 -1.0007655

C 4.4713177 2.3353353 0.7038620

C 5.2097893 3.4564854 0.0066984

H 6.3031333 3.4584619 0.1758990

H 4.8359684 4.4417332 0.3327506

H 5.0571479 3.3866244 -1.0813514

C 3.5456209 -1.0830595 -0.8231457

H	3.4317782	-2.0453470	-0.2953624
H	4.5548472	-1.0601119	-1.2622462
H	2.8297393	-1.0960110	-1.6660592
C	1.4771719	-0.9444055	1.2810505
C	1.0783865	-1.3701490	2.5831155
C	0.0316231	-2.2678910	2.7808775
H	-0.2442370	-2.5568045	3.7993185
C	-0.6640751	-2.7879402	1.6949636
H	-1.4858200	-3.4915842	1.8440832
C	-0.2967159	-2.3757253	0.4092698
H	-0.8503767	-2.7526709	-0.4560618
C	0.7396793	-1.4799587	0.1963049
H	0.9582129	-1.1475027	-0.8164575
C	3.5442264	-1.6698299	4.1034851
C	3.4336851	-3.0510254	4.2984011
H	2.4461249	-3.5193598	4.3302010
C	4.5769761	-3.8302305	4.4374997
H	4.4855782	-4.9090035	4.5884412
C	5.8383040	-3.2368379	4.3723056
H	6.7362075	-3.8519477	4.4757832
C	5.9544579	-1.8655302	4.1632299
H	6.9408180	-1.3999374	4.0957059
C	4.8098353	-1.0827069	4.0265254
H	4.9018548	-0.0090578	3.8368371
C	1.1138506	-0.6970244	5.4151161
C	1.6090692	-1.2667593	6.5906671
H	2.5910923	-1.7443909	6.5954334
C	0.8521863	-1.2317775	7.7608718
H	1.2477226	-1.6853157	8.6735448
C	-0.3996017	-0.6246810	7.7679319

H	-0.9903982	-0.5955917	8.6871470
C	-0.8958326	-0.0450878	6.6003425
H	-1.8721786	0.4453356	6.6021520
C	-0.1432314	-0.0769623	5.4338244
H	-0.5343284	0.3870174	4.5240211
C	4.4184875	3.4747136	2.8615157
C	3.5180972	3.9215331	3.8769634
C	3.8869082	4.8722742	4.8288266
H	3.1652702	5.1690943	5.5956229
C	5.1588211	5.4306983	4.8158430
H	5.4502878	6.1756309	5.5591675
C	6.0640506	4.9942085	3.8410629
H	7.0825555	5.3943355	3.8337799
C	5.7174064	4.0462247	2.8927866
H	6.4718034	3.6994097	2.1904548
C	0.7816328	4.1149633	2.8225004
C	-0.2335243	3.4684529	2.1099833
H	-0.3118348	2.3773073	2.1432477
C	-1.1323880	4.2058636	1.3442114
H	-1.9205451	3.6930828	0.7871851
C	-1.0136361	5.5925154	1.2772255
H	-1.7139490	6.1720077	0.6698144
C	0.0054016	6.2404418	1.9739661
H	0.1061888	7.3271546	1.9126039
C	0.9021998	5.5051804	2.7439871
H	1.7096570	6.0105650	3.2798348
C	1.2583698	3.1263824	5.5135014
C	1.9840232	2.4574038	6.5083933
H	2.9312483	1.9719891	6.2569980
C	1.5076898	2.4063456	7.8115093

H	2.0805651	1.8786797	8.5776806
C	0.2944697	3.0136490	8.1361608
H	-0.0829143	2.9681833	9.1610763
C	-0.4361625	3.6712251	7.1516461
H	-1.3872661	4.1492328	7.4006937
C	0.0422771	3.7286016	5.8432060
H	-0.5350673	4.2499484	5.0765042