1-spar-Cl
Gas phase Energy: -1284.39036949836 hartrees
Solvation Energy: -1284.40362732283 hartrees
Zero Point Energy: 265.123 kcal/mol
Coordinates:

Pd1	-0.2009386652	-0.0244805590	0.1400799797
C2	0.0632305815	0.0802383548	3.6733096288
C3	2.2609461878	0.0769314904	2.5807280176
C4	1.8898697941	-1.2262501504	1.8504225533
N5	0.4197523465	-1.4467027873	1.6792984001
C6	-0.3173483097	-1.2424424931	2.9742131377
C7	-1.8203966190	-1.4524728565	2.7617238380
C8	-2.1040632617	-2.8819844989	2.2802468262
C9	-1.2741128703	-3.2015674581	1.0300771353
C10	0.2028822617	-2.8574588365	1.2238093653
C11	1.5704058861	0.0704874194	3.9523119912
C12	-0.2955268343	1.3875888357	2.9450998308
N13	0.4672207882	1.6006059934	1.6895683187
C14	1.9474320055	1.3896410522	1.8210926863
C15	2.6972857967	2.5850255292	2.4561100586
C16	0.8378982474	4.1187623334	1.7791491734
C17	2.3560193620	3.9147556757	1.7742737792
C18	0.1560034451	2.9319354818	1.0911512901
H19	-0.4934044862	0.0870763667	4.6191445276
H20	3.3503223977	0.0444244788	2.7081340712
H21	2.3400684153	-1.2651892369	0.8549394124
H22	2.3026143575	-2.0627069548	2.4396867731
H23	0.0297411942	-2.0403632745	3.6572616610
H24	-2.3382460156	-1.2558346770	3.7083605173
H25	-2.1891472501	-0.7297803436	2.0242596389
H26	-1.8540631382	-3.5884274359	3.0842534611
H27	-3.1709904476	-3.0094443445	2.0686724419
H28	-1.3472414621	-4.2661583935	0.7783563514
H29	-1.6574265507	-2.6352430713	0.1759303626
H30	0.7554910892	-2.9865809813	0.2904398577
H31	0.6449127925	-3.5279742880	1.9806499322
H32	1.8605894102	0.9351947895	4.5561650878
H33	1.8552123262	-0.8247445197	4.5179889281
H34	-0.1259467467	2.2103393569	3.6573167306
H35	-1.3561663413	1.4108158617	2.6781930217
H36	2.3099979828	1.2898840838	0.7892903763
H37	3.7734598239	2.3820265341	2.3922271333
H38	2.4587198980	2.6653959948	3.5235293327
H39	0.5628868647	5.0322467201	1.2394652415

H40	0.4805585150	4.2448108805	2.8101201760
H41	2.7153563042	3.9009321914	0.7361389273
H42	2.8701605736	4.7409397251	2.2781207097
H43	-0.9320166034	3.0353991454	1.0815134126
H44	0.4615163845	2.8918968925	0.0428164850
H45	-0.5547578582	-1.1087351654	-0.8658382777
Cl46	-0.8138825555	1.3664852120	-1.6557827494

2-spar-Cl
Gas phase Energy: -1434.70946303218 hartrees
Solvation Energy: -1434.72291362442 hartrees
Zero Point Energy: 267.344 kcal/mol
Coordinates:

Pd1	-0.2011186950	-0.0258494637	0.1401858042
C2	0.0640049478	0.0812836641	3.6733775830
C3	2.2615351288	0.0778816021	2.5803306275
C4	1.8905157127	-1.2257103265	1.8503532023
N5	0.4203290704	-1.4469035022	1.6798180418
C6	-0.3169981021	-1.2415059337	2.9744458513
C7	-1.8200521350	-1.4501689505	2.7608052033
C8	-2.1046964512	-2.8793575265	2.2789923425
C9	-1.2737110665	-3.2003961808	1.0299317152
C10	0.2034146018	-2.8576292227	1.2247003829
C11	1.5712508369	0.0714175875	3.9520653399
C12	-0.2946378145	1.3886345433	2.9452279487
N13	0.4677091359	1.6011827986	1.6893538991
C14	1.9479262179	1.3907199730	1.8208425147
C15	2.6971685441	2.5863278309	2.4563371733
C16	0.8370145635	4.1196522858	1.7799773227
C17	2.3552192245	3.9163996171	1.7752413004
C18	0.1558555225	2.9326755944	1.0913812335
H19	-0.4924719747	0.0884129642	4.6193037207
H20	3.3509112077	0.0455087088	2.7076017700
H21	2.3402974376	-1.2649633092	0.8546669700
H22	2.3038364877	-2.0618343155	2.4396702745
H23	0.0290970124	-2.0394875176	3.6579258987
H24	-2.3385038852	-1.2529978538	3.7070176346
H25	-2.1875299073	-0.7270228738	2.0230941120
H26	-1.8563734358	-3.5859707044	3.0833373375
H27	-3.1715480439	-3.0056103196	2.0662055622
H28	-1.3474857652	-4.2651566321	0.7792683736
H29	-1.6563478190	-2.6347988898	0.1750253211
H30	0.7559548823	-2.9883784957	0.2917391120
H31	0.6444931555	-3.5281369424	1.9820735105
H32	1.8615250275	0.9361196190	4.5558967735
H33	1.8561157787	-0.8238300694	4.5176817004

H34	-0.1246457387	2.2114633586	3.6572813053
H35	-1.3554756397	1.4122562487	2.6788186390
H36	2.3107216069	1.2913480407	0.7890838499
H37	3.7734398384	2.3840003269	2.3923803342
H38	2.4586220335	2.6660826790	3.5238191726
H39	0.5615789726	5.0332876838	1.2407076905
H40	0.4794356284	4.2450311420	2.8109737555
H41	2.7146325546	3.9034617230	0.7371386286
H42	2.8688019372	4.7425822851	2.2796063750
H43	-0.9322394304	3.0357503961	1.0820722383
H44	0.4612303479	2.8933646982	0.0430062198
H45	-0.5593169458	-1.1082048693	-0.8633223406
O46	-0.4736324119	-3.2098580520	-2.7587726702
O47	0.6525704297	-3.5934347887	-2.5154600574
Cl48	-0.8147914820	1.3637102130	-1.6564674348

3A-spar-Cl
Gas phase Energy: -1434.72814931058 hartrees
Solvation Energy: -1434.73845436812 hartrees
Zero Point Energy: 274.908 kcal/mol
Coordinates:

Pd1	-.1220159457	-.0840678896	.0655475965
C2	.0824911057	.0490034871	3.6690111015
C3	2.3103965558	.0591838449	2.6415581488
C4	1.9860057548	-1.2708299398	1.9379359906
N5	.5336382508	-1.5237195045	1.7416660573
C6	-.2522232681	-1.2995724297	2.9942741401
C7	-1.7453787710	-1.5197758506	2.7247980918
C8	-2.0045564160	-2.9498578524	2.2342094565
C9	-1.1296134341	-3.2582150750	1.0137692716
C10	.3410070229	-2.9244737553	1.2725054401
C11	1.5801403422	.0762283691	3.9920742158
C12	-.2803277341	1.3303163585	2.8954993276
N13	.5120039331	1.5249935430	1.6549777101
C14	1.9916579670	1.3426865454	1.8356134266
C15	2.6947031795	2.5718121067	2.4614173073
C16	.8319998304	4.0514384034	1.6754221702
C17	2.3526956677	3.8762788332	1.7324933620
C18	.1967332522	2.8304022828	1.0016052236
H19	-.5020760254	.0729143493	4.5976368289
H20	3.3959402424	.0568613706	2.8013542016
H21	2.4609188234	-1.3198026841	.9530761440
H22	2.4150058592	-2.0821195064	2.5531989792
H23	.0649575599	-2.0740585490	3.7201828341
H24	-2.3024987457	-1.3203612625	3.6483281324
H25	-2.0896819989	-.8015852666	1.9696321212

H26	-1.7743649890	-3.6557912413	3.0445817302
H27	-3.0633340224	-3.0847843496	1.9882255862
H28	-1.2000032410	-4.3174043335	.7408558725
H29	-1.4776604464	-2.6825058236	.1504589123
H30	.9219130709	-3.0496288745	.3553486524
H31	.7535404339	-3.6098616926	2.0345886453
H32	1.8371603797	.9605718456	4.5827536908
H33	1.8637735425	-.7997099588	4.5876891344
H34	-.1427357084	2.1751688791	3.5888682487
H35	-1.3342661964	1.3292182172	2.6022731072
H36	2.3883331142	1.2241071842	.8185974991
H37	3.7761470838	2.3893958311	2.4407082415
H38	2.4174188815	2.6752182852	3.5172828936
H39	.5600418696	4.9430239242	1.0990219695
H40	.4334398673	4.1995516606	2.6880061931
H41	2.7516084486	3.8439730346	.7092165363
H42	2.8314508969	4.7253818636	2.2330720331
H43	-.8917018837	2.9126997794	.9493880990
H44	.5458848900	2.7643795552	-.0318921186
O45	-.0390716396	-1.6797103289	-1.5156428703
O46	-.2795965480	-1.2938784857	-2.7707037076
H47	-.5925744340	-.3293363014	-2.6626653095
Cl48	-1.0420392932	1.3594432569	-1.8084780647

4-spar-Cl
Gas phase Energy: -1434.75041929779 hartrees
Solvation Energy: -1434.76292810816 hartrees
Zero Point Energy: 273.699 kcal/mol
Coordinates:

Pd1	.0096826346	-.0637632119	.0449799171
C2	-.0525781224	.0539277457	3.5640457036
C3	2.2181937827	.0640177728	2.6326271515
C4	1.9210167066	-1.2640515594	1.9138371097
N5	.4709394798	-1.5001437325	1.6388318803
C6	-.3589081075	-1.2887128897	2.8731097424
C7	-1.8407405306	-1.5334510037	2.5718784523
C8	-2.0594928950	-2.9861322003	2.1337302867
C9	-1.1627379040	-3.3046068693	.9331783262
C10	.2973251949	-2.9173345583	1.1725980117
C11	1.4299911241	.0813426316	3.9508077257
C12	-.3892160240	1.3251627462	2.7694060433
N13	.4589165419	1.5266219093	1.5593540381
C14	1.9382056499	1.3523260867	1.8192314713
C15	2.6065870779	2.5737325734	2.4948303607
C16	.7673675126	4.0607321545	1.6950551317
C17	2.2859092381	3.8952963641	1.7905907271

C18	.1709937073	2.8669570168	.9463779411
H19	-.6769771489	.0781295880	4.4659787721
H20	3.2959098200	.0583671828	2.8375163843
H21	2.4474959861	-1.3279473277	.9574844252
H22	2.2947833469	-2.0793588927	2.5553459015
H23	-.0425346468	-2.0660871177	3.5928640695
H24	-2.4215090192	-1.3045442961	3.4737999019
H25	-2.1750536153	-.8514249993	1.7805152806
H26	-1.8273752420	-3.6534357211	2.9761660558
H27	-3.1104727003	-3.1545157752	1.8758837387
H28	-1.1875303190	-4.3768150944	.7053363363
H29	-1.5220284743	-2.7795693912	.0469772984
H30	.8591556813	-3.0269569747	.2445350120
H31	.7440878107	-3.5660479464	1.9443738520
H32	1.6619427163	.9637912926	4.5537132809
H33	1.6860494705	-.7952141684	4.5572247701
H34	-.2830141055	2.1788685316	3.4533801665
H35	-1.4272414178	1.3146462974	2.4261100795
H36	2.3833389111	1.2464123819	.8220296650
H37	3.6880187000	2.3918713485	2.5051346974
H38	2.2955930963	2.6516455050	3.5429652471
H39	.5039358016	4.9679158167	1.1395593806
H40	.3358242226	4.1730329674	2.6984509503
H41	2.7142522604	3.8927614901	.7792126295
H42	2.7454300965	4.7307369364	2.3300898777
H43	-.9137704487	2.9429033527	.8435077217
H44	.5701517481	2.8438234257	-.0678437123
O45	-.0765224187	-1.5306915132	-1.2728527795
O46	-1.3594742921	-1.5722156170	-1.9012351015
H47	-1.3150669661	-.7665563629	-2.4525441430
Cl48	-.4644133338	1.4034919541	-1.8186119973

TS1-spar-Cl
Gas phase Energy: -1434.68823732667 hartrees
Solvation Energy: -1434.70080756780 hartrees
Zero Point Energy: 259.270 kcal/mol
Number and Magnitude of negative Eigen values: 1 (-1589.24 cm^{-1})
Coordinates:

atom	x	y	z
Pd1	-.1663269412	-.1199830008	.0777426038
C2	.0603147995	.0522212190	3.6272194733
C3	2.2737119271	.0455785677	2.5671424853
C4	1.9199580171	-1.2695945117	1.8476326124
N5	.4551703816	-1.5014834953	1.6587024096
C6	-.3038374620	-1.2816123299	2.9390641344
C7	-1.8044748182	-1.5019486923	2.7116281242

C8	-2.0755395715	-2.9368307458	2.2367524072
C9	-1.2281009540	-3.2571558729	.9989573989
C10	.2479083785	-2.9153729081	1.2151932150
C11	1.5635029787	.0532891716	3.9287120537
C12	-.2958030326	1.3491250192	2.8779112904
N13	.4841410732	1.5464160178	1.6332233488
C14	1.9623702563	1.3482159922	1.7886413736
C15	2.6864959120	2.5618205887	2.4236702643
C16	.8268784849	4.0674244278	1.6697295331
C17	2.3475170170	3.8792175307	1.7139480730
C18	.1730536826	2.8568183377	.9924509470
H19	-.5093093233	.0683302745	4.5652348893
H20	3.3613631428	.0213605538	2.7103057172
H21	2.3869574596	-1.3195396300	.8596407528
H22	2.3319266312	-2.0964926037	2.4510904589
H23	.0364647468	-2.0686835818	3.6377183441
H24	-2.3330817241	-1.3009922549	3.6516242645
H25	-2.1735492093	-.7861535157	1.9664640310
H26	-1.8294770721	-3.6371908659	3.0475346656
H27	-3.1396316909	-3.0727631046	2.0154544113
H28	-1.2978060684	-4.3201157604	.7413737968
H29	-1.6044996268	-2.6956153839	.1378468317
H30	.8091203287	-3.0631304735	.2893217807
H31	.6765655161	-3.5804164758	1.9848357816
H32	1.8419324584	.9260998819	4.5270963922
H33	1.8437265733	-.8329883750	4.5110256063
H34	-.1396377231	2.1828262009	3.5813059395
H35	-1.3535773276	1.3660529375	2.5982563821
H36	2.3444452801	1.2430902619	.7644865802
H37	3.7661086609	2.3696276670	2.3868031378
H38	2.4242230412	2.6548127888	3.4845571672
H39	.5590925087	4.9646377758	1.0996938471
H40	.4369474278	4.2163768522	2.6858670707
H41	2.7396455612	3.8583023391	.6877295923
H42	2.8362648036	4.7182702615	2.2223092791
H43	-.9151893061	2.9499926717	.9524044114
H44	.5067309597	2.7942233548	-.0462442056
H45	-.2978868363	-1.2728040586	-1.1412324483
O46	-.3503944242	-2.0850552213	-2.1923493656
O47	.2765301140	-3.1649177211	-2.0173139012
Cl48	-.8733585344	1.2177831796	-1.7306586299

1-bipyr-Cl
Gas phase Energy: -1082.99831472470 hartrees
Solvation Energy: -1083.02922554232 hartrees
Zero Point Energy: 106.467 kcal/mol

Coordinates:

Pd1	.1025425149	1.3815374069	-2.0379855191
N2	.4208234633	1.9030842361	.0875547677
N3	-1.6666918681	2.3755137588	-1.5315747824
C4	1.5105216071	1.6199046935	.8085554162
C5	1.6262253184	1.9906228579	2.1482845101
C6	.5675092028	2.6763035172	2.7413983271
C7	-.5665126217	2.9693247721	1.9862820648
C8	-.6146606441	2.5665282985	.6460894741
C9	-1.7715329526	2.8256587270	-.2503826075
C10	-2.9237508170	3.4970584715	.1741097545
C11	-3.9720868922	3.7088869376	-.7159381729
C12	-3.8508916757	3.2436048008	-2.0237344898
C13	-2.6825976612	2.5828627527	-2.3891493966
H14	2.2909202785	1.0838231289	.2748281446
H15	2.5237934822	1.7458067250	2.7052759007
H16	.6194636914	2.9822953295	3.7816960817
H17	-1.3927487223	3.5021702309	2.4409374386
H18	-3.0034618953	3.8527360350	1.1937251779
H19	-4.8673821453	4.2289494538	-.3909400375
H20	-4.6398777614	3.3846279434	-2.7536751597
H21	-2.5333311553	2.2003078399	-3.3904824974
Cl22	2.1304366141	.2929203517	-2.4520730858
H23	-.2448674481	1.0857018393	-3.4948986842

2- bipyr-Cl
Gas phase Energy: -1233.31673859978 hartrees
Solvation Energy: -1233.34450898148 hartrees
Zero Point Energy: 109.071 kcal/mol
Coordinates:

Pd1	.4532763414	.1261927740	-.1663349621
N2	.2108933327	.1191078968	1.9131944023
N3	2.5351502695	.0158976657	.5721378423
C4	-.9831802128	.1729001895	2.5308812639
C5	-1.1121458182	.1694627714	3.9162533997
C6	.0424499100	.1075600552	4.6936009026
C7	1.2791457189	.0512692767	4.0584520328
C8	1.3475123787	.0578692887	2.6607848905
C9	2.6342076648	.0002195017	1.9190169747
C10	3.8859719687	-.0661781871	2.5429405932
C11	5.0342107706	-.1161793853	1.7548965053
C12	4.9126569908	-.0991608237	.3664856971
C13	3.6342727241	-.0320037938	-.1875398809
H14	-1.8466173593	.2190552077	1.8800033496
H15	-2.0983020417	.2146620721	4.3642892673
H16	-.0152746171	.1029816408	5.7773017720

H17	2.1854942960	.0027201585	4.6489326317
H18	3.9736205847	-.0790178509	3.6224917484
H19	6.0115669056	-.1678092464	2.2246076063
H20	5.7838361554	-.1367677703	-.2780240279
H21	3.4557143943	-.0145847660	-1.2595391835
H22	-1.0227870868	.2030517346	-.5395920901
O23	-3.8165083521	-.3919112124	-.5836305104
O24	-4.0858429314	.0053846379	.5318611906
Cl25	.8736460718	.1280135236	-2.4663301091

3A- bipyr-Cl
Gas phase Energy: -1233.33457321476 hartrees
Solvation Energy: -1233.36008187731 hartrees
Zero Point Energy: 111.121 kcal/mol
Coordinates:

Pd1	-0.0699106870	1.1320165194	-1.9036577560
N2	0.1735944821	1.8845970501	0.1997021228
N3	-1.7208255889	2.5848708207	-1.5819998627
C4	1.1385064268	1.4806312780	1.0368057758
C5	1.2473340542	1.9539716125	2.3427867280
C6	0.3089966597	2.8839897053	2.7872679259
C7	-0.6944766249	3.3044598243	1.9183086147
C8	-0.7424436601	2.7873989978	0.6170366737
C9	-1.7836053727	3.1846144295	-0.3735652305
C10	-2.7843121888	4.1243012501	-0.0967857427
C11	-3.7199855772	4.4344645640	-1.0813420572
C12	-3.6404899636	3.8043129442	-2.3219213754
C13	-2.6176459148	2.8807315784	-2.5310297544
H14	1.8379070273	0.7544831953	0.6333723520
H15	2.0448839471	1.5996698326	2.9864802505
H16	0.3542988640	3.2785318046	3.7975612079
H17	-1.4294634672	4.0246391637	2.2561629782
H18	-2.8388858321	4.6121395637	0.8687436345
H19	-4.5004246714	5.1610326336	-0.8780800100
H20	-4.3496112905	4.0182363161	-3.1137497618
H21	-2.4910237227	2.3516221507	-3.4713263006
H22	1.1203837409	-0.6023448804	-3.6408803963
O23	1.6451683295	-0.2375980450	-1.8956231821
O24	1.8609066496	-0.9208598090	-3.0216613161
Cl25	-0.4847255807	0.3944895908	-4.2813081459

4- bipyr-Cl
Gas phase Energy: -1233.36137111896 hartrees
Solvation Energy: -1233.39923630028 hartrees
Zero Point Energy: 112.709 kcal/mol
Coordinates:

Pd1	0.0077203179	1.2677662484	-1.9578868403
N2	0.2233265962	1.8289861424	0.0268913324
N3	-1.6646850030	2.5430629911	-1.6948888822
C4	1.2175519159	1.3794611890	0.8037307280
C5	1.3236747601	1.7627310439	2.1386695304
C6	0.3664576462	2.6306571908	2.6632027808
C7	-0.6648898810	3.0907119546	1.8458785851
C8	-0.7199440592	2.6727323473	0.5132783613
C9	-1.7683244709	3.0814718500	-0.4523894098
C10	-2.8127146788	3.9568815480	-0.1427161075
C11	-3.7526099878	4.2714261232	-1.1224742335
C12	-3.6318286002	3.7060526925	-2.3903158961
C13	-2.5668363375	2.8415139498	-2.6395970446
H14	1.9074246375	0.7054423305	0.3009344602
H15	2.1382353864	1.3842885218	2.7458570972
H16	0.4178589964	2.9477542433	3.6999002260
H17	-1.4149187618	3.7629157993	2.2447751752
H18	-2.8941283037	4.3896578208	0.8471036242
H19	-4.5677102811	4.9508557594	-0.8942590417
H20	-4.3429895890	3.9261288712	-3.1785106640
H21	-2.4030030530	2.3638325597	-3.6009472779
H22	1.2401991411	-1.1504770395	-3.1225632427
O23	1.6630680669	0.2096832512	-1.9010052765
O24	1.3539864669	-1.1633155511	-2.1547357834
Cl25	-0.3845572112	0.7164657390	-4.2445088309

5- bipyr-Cl
Gas phase Energy: -1233.74330865486 hartrees
Solvation Energy: -1233.83633811619 hartrees
Zero Point Energy: 120.65 kcal/mol
Coordinates:

Pd1	-0.2026223862	1.0760880285	-1.8065225185
N2	0.1755723656	1.7479353558	0.1228695825
N3	-1.6241194784	2.5148819721	-1.6599013496
C4	1.1465803546	1.3109218913	0.9390269893
C5	1.3266778824	1.8226125352	2.2197033563
C6	0.4657733510	2.8266705442	2.6600428531
C7	-0.5357507012	3.2882831670	1.8085205618
C8	-0.6658631331	2.7354774652	0.5329154965
C9	-1.6726723967	3.1568371542	-0.4571539495
C10	-2.6274731000	4.1472832918	-0.2317200199
C11	-3.5297154524	4.4793139882	-1.2420886311
C12	-3.4590953884	3.8130777789	-2.4617837323
C13	-2.4893288302	2.8289041483	-2.6397074607
H14	1.7980515976	0.5367000486	0.5514606207
H15	2.1234664445	1.4394360319	2.8463789610

H16	0.5733555854	3.2502920860	3.6528430353
H17	-1.2052813313	4.0733587945	2.1366412192
H18	-2.6702716913	4.6574296654	0.7223180232
H19	-4.2753474420	5.2489000729	-1.0730814847
H20	-4.1389874305	4.0386466033	-3.2751062119
H21	-2.3855693418	2.2744360720	-3.5638631877
H22	1.6089358644	-0.2519438291	-3.7955352744
O23	1.2028751899	-0.5167705806	-1.9912427261
O24	2.1982508008	-0.2003201224	-3.0106572583
Cl25	-0.7117538009	0.4687061463	-4.0067961297
H26	1.7802882916	-0.8146632764	-1.2694401331

6- bipyr-Cl
Gas phase Energy: -1542.63146883203 hartrees
Solvation Energy: -1542.67053091060 hartrees
Zero Point Energy: 102.65 kcal/mol
Coordinates:

Pd1	.1145686479	1.3344091711	-2.0104746276
N2	.4180003959	1.8781050971	-.0136323006
N3	-1.6723157734	2.3371882219	-1.5882183001
C4	1.5203836982	1.5962922765	.6966300426
C5	1.6498056262	1.9798472949	2.0299562199
C6	.6035907051	2.6730951586	2.6345044277
C7	-.5377702136	2.9644434187	1.8911491072
C8	-.6120639150	2.5558143394	.5568355064
C9	-1.7726340112	2.8158315590	-.3205913199
C10	-2.9161378738	3.5083467262	.0863534933
C11	-3.9560515791	3.7061115404	-.8189327515
C12	-3.8331803193	3.2084090212	-2.1141881093
C13	-2.6701693941	2.5255960012	-2.4647273556
H14	2.2872530542	1.0518875384	.1529965275
H15	2.5556800245	1.7334053723	2.5722958529
H16	.6708060982	2.9851715666	3.6718141914
H17	-1.3595950481	3.5023654463	2.3472958902
H18	-2.9958751591	3.8912153381	1.0962351163
H19	-4.8482255668	4.2430728212	-.5129064530
H20	-4.6184263864	3.3410761781	-2.8499221364
H21	-2.4964170848	2.1070709444	-3.4519167328
Cl22	2.1805700577	.2704192452	-2.2249018156
Cl23	-.4690924594	.8426947812	-4.2143196257

TS1- bipyr-Cl
Gas phase Energy: -1233.29530813908 hartrees
Solvation Energy: -1233.32297355022 hartrees
Zero Point Energy: 106.873 kcal/mol
Number and Magnitude of negative Eigen values: 1 (-1621.30 cm^{-1})

Coordinates:

Pd1	.3106450294	.0733792027	-.1276718595
N2	.1399376547	.0788349054	1.9780922645
N3	2.4312735518	.0464698348	.5720624131
C4	-1.0375380090	.1028240286	2.6261449813
C5	-1.1263660406	.1167501278	4.0158430074
C6	.0509669168	.1060302219	4.7598559624
C7	1.2711061524	.0798702968	4.0905187158
C8	1.2987069663	.0651070918	2.6918367086
C9	2.5654253695	.0344485031	1.9145403759
C10	3.8353552341	-.0066088682	2.5032915018
C11	4.9620466240	-.0336497243	1.6837618649
C12	4.8026316571	-.0197159826	.2989678615
C13	3.5084972586	.0200729446	-.2193595328
H14	-1.9247340127	.1092600770	1.9993427963
H15	-2.1002897008	.1360312195	4.4916284880
H16	.0245052627	.1178642099	5.8448073756
H17	2.1947477584	.0726094122	4.6556634788
H18	3.9529840565	-.0199015218	3.5800322427
H19	5.9525909706	-.0660218467	2.1263575253
H20	5.6563821800	-.0403124093	-.3693071664
H21	3.3019867199	.0310961551	-1.2860742554
H22	-1.3309483829	.0726577306	-.5035954209
O23	-2.6208400163	.0660870263	-.7654113977
O24	-3.3218271930	.0646471593	.2839965298
Cl25	.6118801288	.0625400911	-2.4485223903

1-bipyr-CH_3
Gas phase Energy: -662.66064953707 hartrees
Solvation Energy: -662.68127561673 hartrees
Zero Point Energy: 127.637 kcal/mol
Coordinates:

Pd1	0.0078274022	1.1692799951	-2.0318428305
N2	0.1935151876	1.8094243986	0.0669334619
N3	-1.6803451465	2.6214889787	-1.6816794022
C4	1.1619625157	1.3772272846	0.8872278371
C5	1.2872095903	1.8103386917	2.2047440604
C6	0.3652465843	2.7358434524	2.6883622278
C7	-0.6419245014	3.1874558374	1.8419117911
C8	-0.7095982401	2.7054604606	0.5279317693
C9	-1.7597187058	3.1373047063	-0.4336682230
C10	-2.7854620770	4.0256903512	-0.0842017788
C11	-3.7353454272	4.3852037717	-1.0347248584
C12	-3.6429498444	3.8493137221	-2.3170413636
C13	-2.5971922825	2.9705273200	-2.5915171765
H14	1.8508092898	0.6602716324	0.4550099576

H15	2.0890904812	1.4295322056	2.8282254688
H16	0.4269023469	3.1031121665	3.7084328531
H17	-1.3628930604	3.9099832771	2.2050879382
H18	-2.8495442447	4.4322692475	0.9179372825
H19	-4.5349030021	5.0724005748	-0.7741335644
H20	-4.3613906849	4.1008330931	-3.0899353455
H21	-2.4784064461	2.5224054960	-3.5729654831
H22	1.1857044263	0.1750739100	-2.1767983420
C23	-0.2232694758	0.6374914211	-3.9914954545
H24	-1.0542041956	1.2259002166	-4.4085078081
H25	0.6768938439	0.8436909155	-4.5775698265
H26	-0.4636843735	-0.4258544602	-4.0868176282

2- bipyr- CH_3
Gas phase Energy: -812.97899435790 hartrees
Solvation Energy: -812.99708165398 hartrees
Zero Point Energy: 130.185 kcal/mol
Coordinates:

Pd1	0.4629886526	0.0695558773	-0.2323059003
N2	0.2473751394	0.0780947809	1.9614500917
N3	2.5607880844	0.0318094604	0.5907707939
C4	-0.9400689218	0.1133351125	2.5852472914
C5	-1.0632143713	0.1520680499	3.9721624666
C6	0.0992645451	0.1561119482	4.7410077527
C7	1.3331593458	0.1188082381	4.0984279428
C8	1.3829744854	0.0778347891	2.6987689811
C9	2.6623181459	0.0331003481	1.9399060926
C10	3.9152623554	-0.0087778923	2.5673145325
C11	5.0703978428	-0.0501439570	1.7915257829
C12	4.9526716509	-0.0503774935	0.4027844063
C13	3.6742984120	-0.0093696554	-0.1502463194
H14	-1.8084980960	0.1106312886	1.9364768343
H15	-2.0464268937	0.1796375646	4.4289363836
H16	0.0496675733	0.1884731308	5.8249072619
H17	2.2433460143	0.1245100193	4.6853037264
H18	3.9953182127	-0.0122459544	3.6473984381
H19	6.0456960057	-0.0827332037	2.2673051743
H20	5.8246401820	-0.0825388947	-0.2413419925
H21	3.5229026500	-0.0090993523	-1.2250539087
H22	-1.0078286700	0.0873509347	-0.7140528524
O23	-3.8633326426	-0.0191779614	-0.6702457887
O24	-4.0985472643	0.0398561676	0.5199063323
C25	0.7496237387	0.0826345976	-2.2559999977
H26	1.8292432098	0.1796455819	-2.4463785887
H27	0.3959092032	-0.8493210328	-2.7069182717
H28	0.2361669586	0.9180410763	-2.7383545318

3A- bipyr- CH_3
Gas phase Energy: -812.96300567677 hartrees
Solvation Energy: -812.98048583728 hartrees
Zero Point Energy: 132.058 kcal/mol
Coordinates:

Pd1	0.0146635658	1.2358572495	-2.0287456931
N2	0.2844457765	2.0193830570	0.0949245589
N3	-1.9100956036	2.3342768280	-1.4832107582
C4	1.2735303403	1.6445961202	0.9196941637
C5	1.3096422021	2.0005894911	2.2642788175
C6	0.2556390418	2.7599118808	2.7794373337
C7	-0.7851609436	3.1293311434	1.9362645819
C8	-0.7448601636	2.7510950569	0.5852787639
C9	-1.8080513172	3.1129872039	-0.3736377366
C10	-2.6676611710	4.2033328420	-0.1691402762
C11	-3.6732726799	4.4657391191	-1.0905680506
C12	-3.7921281772	3.6384495854	-2.2135423164
C13	-2.8809336376	2.6027808284	-2.3736951426
H14	2.0526476568	1.0367459737	0.4693756991
H15	2.1390729362	1.6868324300	2.8888595102
H16	0.2372753163	3.0448126855	3.8272704940
H17	-1.6346485146	3.6805767548	2.3239652036
H18	-2.5351457741	4.8468846747	0.6938336993
H19	-4.3466290990	5.3049305200	-0.9443243785
H20	-4.5716211140	3.7960621115	-2.9515433116
H21	-2.9115946473	1.9510106209	-3.2412956952
H22	0.9715974238	-1.0000684787	-3.2727575447
O23	1.5018836914	-0.2126574532	-1.6873461271
O24	1.4867532945	-1.3185781865	-2.5025118175
C25	-0.3374035694	0.8164890696	-4.0773356926
H26	-0.6071313816	1.7532286930	-4.5792470404
H27	0.5469879537	0.4253047266	-4.6016270253
H28	-1.1668149915	0.1077057739	-4.1994722329

3B- bipyr- CH_3
Gas phase Energy: -812.96105504788 hartrees
Solvation Energy: -812.97593147028 hartrees
Zero Point Energy: 131.194 kcal/mol
Coordinates:

Pd1	0.3046046712	0.0333790177	-0.2055788594
N2	0.1650351295	0.0781221095	2.0140477325
N3	2.4789048834	0.0255896944	0.6198944537
C4	-1.0158498648	0.0989502955	2.6540350328
C5	-1.1177678269	0.1041201055	4.0439892866
C6	0.0546889124	0.0867122201	4.7959207511

C7	1.2798295754	0.0666184774	4.1352358315
C8	1.3114561429	0.0635404452	2.7345133724
C9	2.5877608280	0.0437187419	1.9648126989
C10	3.8478362915	0.0444100992	2.5809571753
C11	4.9952734246	0.0250367186	1.7926243514
C12	4.8664855019	0.0060134864	0.4048016447
C13	3.5816311399	0.0074991052	-0.1354126450
H14	-1.8968464718	0.1122623761	2.0168169360
H15	-2.0947418666	0.1207864737	4.5143641942
H16	0.0209455935	0.0885938818	5.8810070154
H17	2.1975848332	0.0519495414	4.7099930742
H18	3.9409095427	0.0609541260	3.6599236240
H19	5.9755858146	0.0252552493	2.2591394555
H20	5.7339307488	-0.0093717673	-0.2461372026
H21	3.4158423802	-0.0065824028	-1.2085849970
H22	-1.7823155330	0.1376389333	-0.7519267939
O23	-2.7882590512	0.1804953357	-0.9186255344
O24	-3.3738767597	0.1781420979	0.2673031404
C25	0.4731750610	-0.0249468318	-2.2482521175
H26	1.5237891990	-0.1360143539	-2.5468336092
H27	-0.0882772032	-0.8758771307	-2.6549348485
H28	0.0854459528	0.9000262139	-2.6937754986

4- bipyr- CH_3
Gas phase Energy: -813.01999829421 hartrees
Solvation Energy: -813.04975709439 hartrees
Zero Point Energy: 121.829 kcal/mol
Coordinates:

Pd1	0.0171310004	1.2820080227	-2.0483544308
N2	0.2385629532	1.8273674372	0.0393144142
N3	-1.6598664083	2.5395873605	-1.6966110550
C4	1.2529717520	1.4137821355	0.8031494326
C5	1.3690898720	1.8057363979	2.1360680248
C6	0.3947648978	2.6499223220	2.6678921782
C7	-0.6596228280	3.0776857586	1.8620657322
C8	-0.7133896829	2.6444778580	0.5320906644
C9	-1.7793900422	3.0270617272	-0.4320265191
C10	-2.8626289745	3.8396337400	-0.0821463569
C11	-3.8280061636	4.1532307063	-1.0336852836
C12	-3.6927582554	3.6471621739	-2.3244444336
C13	-2.5921745074	2.8449033971	-2.6109214744
H14	1.9594395994	0.7620156023	0.2919860797
H15	2.2025013846	1.4568766444	2.7367202483
H16	0.4525260470	2.9760486794	3.7021191309
H17	-1.4177708942	3.7363401581	2.2692582897
H18	-2.9540010150	4.2227261923	0.9269837967

H19	-4.6719650703	4.7822486665	-0.7678090828
H20	-4.4200592216	3.8643843728	-3.0990454267
H21	-2.4335882940	2.4240458452	-3.5974846658
H22	1.2585572323	-1.5403900899	-2.7458643545
O23	1.6749351010	0.1645745308	-2.0364704577
O24	1.2554413528	-1.2190795719	-1.8306570838
C25	-0.2538819472	0.8912503474	-4.0333092823
H26	-0.3491060194	1.8314513426	-4.5917462496
H27	0.6137863062	0.3431373973	-4.4087685624
H28	-1.1617504240	0.2890033621	-4.1692364508

TS1- bipyr- CH_3
Gas phase Energy: -812.95523481632 hartrees
Solvation Energy: -812.97057436522 hartrees
Zero Point Energy: 128.193 kcal/mol
Number and Magnitude of negative Eigen values: 1 (-1421.04 cm^{-1})
Coordinates:

Pd1	0.2979284085	0.0426540994	-0.1984660628
N2	0.1517016562	0.0775118305	2.0036202374
N3	2.4567069616	0.0170659903	0.5965135872
C4	-1.0259716054	0.1037501825	2.6466363598
C5	-1.1215249863	0.1177830478	4.0369045938
C6	0.0531383666	0.1034354592	4.7843114467
C7	1.2750916837	0.0769495124	4.1188396619
C8	1.3005045854	0.0651503942	2.7185732887
C9	2.5716885797	0.0396252342	1.9415589385
C10	3.8331944914	0.0402423624	2.5533662145
C11	4.9785876139	0.0167352893	1.7632396043
C12	4.8446575000	-0.0066014208	0.3768367882
C13	3.5585872533	-0.0051154041	-0.1592720886
H14	-1.9092598422	0.1147404797	2.0117895087
H15	-2.0964757084	0.1391923635	4.5118072528
H16	0.0238918517	0.1126746856	5.8698306437
H17	2.1950000039	0.0648293690	4.6902647504
H18	3.9282868787	0.0601321319	3.6322097586
H19	5.9605049934	0.0172404575	2.2270399440
H20	5.7099335132	-0.0250709838	-0.2772366710
H21	3.3928582396	-0.0219057698	-1.2324194692
H22	-1.3681530824	0.0823256899	-0.6167261348
O23	-2.6189100118	0.1141755620	-0.8380853582
O24	-3.2846217882	0.1523752623	0.2546887786
C25	0.4990222030	0.0100224042	-2.2318540591
H26	1.5624060877	-0.0614393356	-2.4975546347
H27	-0.0270965500	-0.8517827783	-2.6577012148
H28	0.0881703463	0.9275514431	-2.6686331805

1-bipyr-OAc
Gas phase Energy: -851.25413428759 hartrees
Solvation Energy: -851.28469041901 hartrees
Zero Point Energy: 137.899 kcal/mol
Coordinates:

Pd1	0.2184810518	1.5571955682	-2.0638091345
N2	0.4660191188	2.0645573851	0.1273216449
N3	-1.6176915993	2.3811503625	-1.5473698345
C4	1.5594294058	1.9211626675	0.8882183537
C5	1.5472260745	2.1710856235	2.2613042858
C6	0.3618356309	2.5927884426	2.8551841266
C7	-0.7679510670	2.7657446351	2.0595776725
C8	-0.6851063739	2.4968772141	0.6881750386
C9	-1.8283627461	2.6904171359	-0.2399782921
C10	-3.0686839834	3.1837726024	0.1820681789
C11	-4.0958537273	3.3633072124	-0.7369243316
C12	-3.8645305829	3.0478304032	-2.0738933212
C13	-2.6144080379	2.5597615309	-2.4353316554
H14	2.4568967092	1.6360518295	0.3478637437
H15	2.4548689084	2.0398649693	2.8406500283
H16	0.3127784291	2.7945948447	3.9212371894
H17	-1.6933708504	3.1055747900	2.5084532832
H18	-3.2307059255	3.4299936533	1.2239058391
H19	-5.0588087698	3.7451612159	-0.4122603828
H20	-4.6321643008	3.1726827744	-2.8294635642
H21	-2.3815467035	2.2954647631	-3.4581476342
H22	-0.1842966546	1.2937051988	-3.5122975673
O23	1.8929360408	0.5299948651	-2.6193204975
C24	3.0643656444	0.9194566006	-2.2154448700
O25	3.3089829759	1.8929104334	-1.4934831910
C26	4.1918982792	0.0224635408	-2.7259477300
H27	4.2249350673	0.0533086804	-3.8194332868
H28	5.1483712824	0.3561918450	-2.3202704861
H29	4.0063221394	-1.0170740724	-2.4381151271

2- bipyr- OAc
Gas phase Energy: -1001.57268434527 hartrees
Solvation Energy: -1001.60098501887 hartrees
Zero Point Energy: 140.467 kcal/mol
Coordinates:

Pd1	0.2468645813	-0.2228090472	-0.1805963892
N2	0.1890138386	0.0037697009	1.8866770496
N3	2.3956327774	0.2347802011	0.3632474355
C4	-0.9533950184	-0.0727835630	2.5965573761
C5	-0.9824545591	0.0176662694	3.9837358752
C6	0.2197952082	0.1942060567	4.6655139404

C7	1.4003796167	0.2777440058	3.9355104335
C8	1.3694293664	0.1804542492	2.5390647976
C9	2.5908459075	0.2792001402	1.7003313325
C10	3.8734559093	0.4315910730	2.2403983690
C11	4.9623760280	0.5506887166	1.3796721365
C12	4.7443019127	0.5303628674	0.0050711616
C13	3.4394098848	0.3741144817	-0.4660763519
H14	-1.8566561146	-0.2136317626	2.0181592465
H15	-1.9295864030	-0.0508433005	4.5067610462
H16	0.2409311258	0.2682735909	5.7480775963
H17	2.3414557623	0.4219495147	4.4505735462
H18	4.0304160263	0.4564271941	3.3116915004
H19	5.9637855114	0.6658390591	1.7831535261
H20	5.5620118864	0.6366551905	-0.6992891070
H21	3.1826637476	0.3934205321	-1.5209293244
H22	-1.2413549728	-0.5330477091	-0.2985817521
O23	-4.1162301160	-0.9390228361	-0.3691879925
O24	-4.2045824980	-0.6975811498	0.8172841796
O25	0.2172793849	-0.6832815346	-2.1696999655
C26	0.9077087440	0.0162743766	-3.0184130954
O27	1.6479969978	0.9714352121	-2.7574682292
C28	0.7246664411	-0.4633894583	-4.4573380804
H29	-0.3163080462	-0.3195730299	-4.7633863786
H30	1.3825335571	0.0943067916	-5.1257376484
H31	0.9363681176	-1.5343235663	-4.5282619083

3A- bipyr- OAc
Gas phase Energy: -1001.60016324321 hartrees
Solvation Energy: -1001.62225618539 hartrees
Zero Point Energy: 142.401 kcal/mol
Coordinates:

Pd1	-0.3318327111	1.0513152339	-1.8021026614
N2	0.1595966654	1.9013724140	0.1783552569
N3	-1.8976957676	2.6133687302	-1.4064502162
C4	1.2039915870	1.4942608946	0.9129322268
C5	1.5015397568	2.0379729659	2.1597036628
C6	0.6748006252	3.0449985026	2.6551353956
C7	-0.4100016767	3.4686189008	1.8931882971
C8	-0.6509943132	2.8773437556	0.6456743170
C9	-1.7887045473	3.2722977575	-0.2322399454
C10	-2.7062580760	4.2688015282	0.1194814661
C11	-3.7430142732	4.5803428568	-0.7572887263
C12	-3.8407896670	3.8918427041	-1.9629468050
C13	-2.8935103746	2.9087506950	-2.2544809439
H14	1.8098245089	0.7073366202	0.4734460629
H15	2.3573188292	1.6783434817	2.7207920888

H16	0.8700030533	3.4968672759	3.6230506858
H17	-1.0582139332	4.2503789846	2.2698011958
H18	-2.6205018094	4.7987925340	1.0605908270
H19	-4.4616248987	5.3518342211	-0.4963973940
H20	-4.6328893451	4.1041423688	-2.6731119454
H21	-2.9038449238	2.3276597199	-3.1768927007
H22	0.5215763803	-0.7663749715	-3.5396761926
O23	1.3673336230	-0.4369880117	-1.9053143295
O24	1.3704305195	-1.1513032502	-3.0287506219
O25	-0.6147966984	0.0528607253	-3.7452828610
C26	-1.5109217889	0.1901890506	-4.6876625521
O27	-2.4425510764	0.9908121836	-4.6508005776
C28	-1.3199362974	-0.7407585369	-5.8802502220
H29	-1.3532804263	-1.7845529089	-5.5505551729
H30	-2.1002658497	-0.5665680804	-6.6218796406
H31	-0.3375884200	-0.5726974743	-6.3341919963

4- bipyr- OAc
Gas phase Energy: -1001.62289065933 hartrees
Solvation Energy: -1001.65797808454 hartrees
Zero Point Energy: 144.436 kcal/mol
Coordinates:

Pd1	-0.2337726730	1.0572927797	-1.8570495861
N2	0.2544868362	1.8299828672	-0.0102163381
N3	-1.8237677033	2.4677347396	-1.5323894386
C4	1.3443359606	1.4305147835	0.6606270005
C5	1.6566252411	1.9524617640	1.9124918961
C6	0.8056556101	2.9040136395	2.4725093322
C7	-0.3286052252	3.3045497942	1.7706160685
C8	-0.5907824633	2.7482769481	0.5151105640
C9	-1.7599358658	3.0908799512	-0.3267909493
C10	-2.7454767586	3.9987482703	0.0665915609
C11	-3.8070452378	4.2692510681	-0.7941969785
C12	-3.8499075568	3.6357937434	-2.0318595837
C13	-2.8343077869	2.7410873447	-2.3717637884
H14	1.9351877338	0.6755187430	0.1468223310
H15	2.5471823269	1.6142187600	2.4305564323
H16	1.0188839941	3.3313053452	3.4475718300
H17	-0.9981303033	4.0421275755	2.1963906177
H18	-2.6888543233	4.4896644486	1.0308844527
H19	-4.5815280553	4.9710298017	-0.4995378363
H20	-4.6494053439	3.8282130465	-2.7389562540
H21	-2.7676150288	2.2501740727	-3.3406551490
H22	0.6040917946	-1.3307490049	-2.9678997154
O23	1.3764994191	-0.0743140039	-1.8285556028
O24	0.9881772243	-1.4293451234	-2.0721312584

O25	-0.5950860278	0.0459343045	-3.6330874993
C26	-1.1103210061	0.5236612653	-4.7297853567
O27	-1.6906600318	1.6054817780	-4.8494419409
C28	-0.9289078844	-0.4029131556	-5.9287775066
H29	-1.2555683844	-1.4173147735	-5.6815275582
H30	-1.4928697613	-0.0252625379	-6.7828138887
H31	0.1333384214	-0.4563803232	-6.1902514339

TS1- bipyr- OAc
Gas phase Energy: -1001.55369041006 hartrees
Solvation Energy: -1001.57936274656 hartrees
Zero Point Energy: 138.387 kcal/mol
Number and Magnitude of negative Eigen values: 1 (-1443.61 cm^{-1})
Coordinates:

Pd1	0.1299791197	-0.1528119173	-0.1643188609
N2	0.0867567523	0.0192088668	1.9268394607
N3	2.3044949712	0.2820625318	0.4232503235
C4	-1.0588279962	-0.0764018031	2.6259175196
C5	-1.0972118614	-0.0047391187	4.0145747937
C6	0.0979752424	0.1736737286	4.7062873651
C7	1.2828673824	0.2729810858	3.9853900298
C8	1.2612771432	0.1911358034	2.5883330781
C9	2.4895044734	0.2967894831	1.7599611491
C10	3.7708014760	0.4165995586	2.3106012183
C11	4.8669560559	0.5322876013	1.4586256332
C12	4.6577761703	0.5352741570	0.0829798171
C13	3.3533492280	0.4095424381	-0.3991767568
H14	-1.9652441905	-0.2226072206	2.0455900761
H15	-2.0475847656	-0.0889958194	4.5298040288
H16	0.1112531177	0.2359139226	5.7901008136
H17	2.2198486502	0.4179420041	4.5082718254
H18	3.9212785501	0.4158170724	3.3834368918
H19	5.8678494811	0.6226722783	1.8704897322
H20	5.4827749969	0.6339031428	-0.6145111992
H21	3.0990337753	0.4273335553	-1.4568381756
H22	-1.4891576018	-0.4694581842	-0.2962575849
O23	-2.7726106511	-0.7420319187	-0.5293550914
O24	-3.4611001116	-0.7113521142	0.5296215206
O25	-0.0388247089	-0.5505969201	-2.1525581855
C26	0.7515770760	-0.0651029718	-3.0645939595
O27	1.7226408908	0.6725998422	-2.8733524170
C28	0.3709736672	-0.5112275022	-4.4737407212
H29	-0.6609814476	-0.2218696332	-4.6935448718
H30	1.0464557430	-0.0635728363	-5.2042578186
H31	0.4216822173	-1.6025725071	-4.5432522173

1-bipyr-I
Gas phase Energy: -634.19958772809 hartrees
Solvation Energy: -634.22456836302 hartrees
Zero Point Energy: 106.044 kcal/mol
Coordinates:

Pd1	-0.0339527609	1.1821714174	-1.8592243263
N2	0.1743510240	1.8392485222	0.1464455259
N3	-1.7278128512	2.6134099809	-1.5981674728
C4	1.1451356395	1.4173907203	0.9750208400
C5	1.2598402141	1.8634345931	2.2876001413
C6	0.3291098658	2.7855873273	2.7610279399
C7	-0.6771374559	3.2249309811	1.9072200035
C8	-0.7400163890	2.7387604961	0.5957260468
C9	-1.7891299491	3.1675432250	-0.3670279058
C10	-2.7925141409	4.0893241088	-0.0419902776
C11	-3.7362962917	4.4349291290	-1.0057415741
C12	-3.6601622982	3.8557540209	-2.2703252720
C13	-2.6346479238	2.9458390969	-2.5236938707
H14	1.8407810046	0.7014821259	0.5554870620
H15	2.0619356932	1.4917343605	2.9156000567
H16	0.3831012101	3.1588985661	3.7789241734
H17	-1.4074944474	3.9413787669	2.2620584541
H18	-2.8443153077	4.5354039504	0.9437168899
H19	-4.5197950850	5.1483039679	-0.7677548414
H20	-4.3759700223	4.0987146005	-3.0481360758
H21	-2.5165505523	2.4570034777	-3.4871460805
H22	1.1573463789	0.2348074445	-1.9041039361
I25	-0.3241128424	0.3838962797	-4.3651508298

2- bipyr- I
Gas phase Energy: -784.51806729102 hartrees
Solvation Energy: -784.54025846983 hartrees
Zero Point Energy: 108.657 kcal/mol
Coordinates:

Pd1	0.4428524336	0.0381702997	-0.0808743135
N2	0.2051048392	0.0566296067	2.0300703371
N3	2.5384260452	0.0048343439	0.6827122941
C4	-0.9879913720	0.0822949694	2.6494890837
C5	-1.1154012546	0.0933028927	4.0351728515
C6	0.0423764574	0.0771474623	4.8100452103
C7	1.2787528343	0.0506727546	4.1725339819
C8	1.3427961774	0.0406332797	2.7740250453
C9	2.6306678874	0.0122254158	2.0311974412
C10	3.8797828362	-0.0062327784	2.6646786086
C11	5.0364744070	-0.0324910100	1.8890098361
C12	4.9248522932	-0.0397873402	0.5001890660

C13	3.6494645972	-0.0203730956	-0.0626234393
H14	-1.8551806367	0.0940699396	2.0014481748
H15	-2.1013381095	0.1140202660	4.4855937298
H16	-0.0123690368	0.0849343283	5.8939573646
H17	2.1863962933	0.0378557757	4.7627519116
H18	3.9585456932	-0.0003744957	3.7447785409
H19	6.0107391578	-0.0470031445	2.3676109383
H20	5.8004862253	-0.0600065157	-0.1390709396
H21	3.4882666631	-0.0247096603	-1.1372982490
H22	-1.0281227831	0.0624772494	-0.4695476946
O23	-3.8709416101	0.0781666198	-0.4901953898
O24	-4.1081164456	0.1173667140	0.7001748702
I25	0.7700208908	0.0142531168	-2.7067363270

3A- bipyr- I
Gas phase Energy: -784.52881051369 hartrees
Solvation Energy: -784.55219217822 hartrees
Zero Point Energy: 110.928 kcal/mol
Coordinates:

Pd1	-0.0701479427	1.1946965055	-1.8086480662
N2	0.1785760303	1.9419038740	0.3010633120
N3	-1.7355487976	2.6671003611	-1.4604366792
C4	1.1497045524	1.5256864232	1.1228973264
C5	1.2736378175	1.9866857355	2.4315604930
C6	0.3444676285	2.9165495102	2.8934800737
C7	-0.6654968212	3.3489445694	2.0387274237
C8	-0.7289584152	2.8432168157	0.7334477524
C9	-1.7782596918	3.2531105172	-0.2434570099
C10	-2.7683374352	4.1950347279	0.0619328933
C11	-3.7184554896	4.5261248635	-0.9003487536
C12	-3.6624269067	3.9119247729	-2.1488339556
C13	-2.6488952624	2.9849542579	-2.3866226968
H14	1.8404899446	0.7997453619	0.7035968713
H15	2.0760570106	1.6229374483	3.0643723173
H16	0.4017224708	3.3021817376	3.9070333881
H17	-1.3932637619	4.0696767893	2.3913444513
H18	-2.8031694770	4.6695152493	1.0351713179
H19	-4.4905838883	5.2553627834	-0.6735853146
H20	-4.3829572458	4.1403322669	-2.9267665953
H21	-2.5468283972	2.4709760150	-3.3382440289
H22	1.3992847754	-0.7017433791	-3.3613965638
O23	1.6546460553	-0.1013954033	-1.6213856323
O24	2.0535201550	-0.8938255874	-2.6248417644
I25	-0.5341171564	0.3681747274	-4.4673731592

4- bipyr- I

Gas phase Energy: -784.55779703219 hartrees
Solvation Energy: -784.59105466409 hartrees
Zero Point Energy: 112.309 kcal/mol
Coordinates:

Pd1	0.0279129344	1.2832021177	-1.8708866363
N2	0.2292475596	1.8300096688	0.1461891749
N3	-1.6633886955	2.5580066922	-1.5838813944
C4	1.2312643036	1.3944583512	0.9180304621
C5	1.3295909205	1.7632251337	2.2574740945
C6	0.3528433790	2.6015572045	2.7922799932
C7	-0.6863753817	3.0488458008	1.9788167018
C8	-0.7286965097	2.6467910730	0.6401851467
C9	-1.7786708439	3.0561612982	-0.3244931522
C10	-2.8369819254	3.9036399986	0.0147432370
C11	-3.7824793311	4.2408774475	-0.9499435864
C12	-3.6500248384	3.7245435724	-2.2359687408
C13	-2.5736063515	2.8844331779	-2.5125937589
H14	1.9388027862	0.7437227703	0.4090188219
H15	2.1533472093	1.3972892292	2.8605669201
H16	0.3959279823	2.9067429412	3.8333892797
H17	-1.4503124725	3.7001417719	2.3862460787
H18	-2.9240102130	4.2972137067	1.0203538875
H19	-4.6086267324	4.8981049746	-0.6964102633
H20	-4.3618319504	3.9613832620	-3.0190039520
H21	-2.4135924658	2.4487485071	-3.4938685850
H22	1.1937755816	-1.3487181098	-2.7218495677
O23	1.6642140565	0.1983807135	-1.7684187833
O24	1.2722911021	-1.1780292610	-1.7650210524
I25	-0.2773952425	0.6699415056	-4.4954604500

TS1- bipyr- I
Gas phase Energy: -784.49488553333 hartrees
Solvation Energy: -784.51757539452 hartrees
Zero Point Energy: 106.488 kcal/mol
Number and Magnitude of negative Eigen values: 1 (-1621.62 cm^{-1})
Coordinates:

Pd1	0.3410854364	0.0424610864	-0.0428536013
N2	0.1703112447	0.0628444697	2.0862809298
N3	2.4650903067	0.0113784707	0.6742156327
C4	-1.0041267442	0.0881322958	2.7365770178
C5	-1.0915746583	0.0982345025	4.1262198570
C6	0.0862831355	0.0813870353	4.8681471350
C7	1.3040880023	0.0553998344	4.1958241813
C8	1.3276474407	0.0465097846	2.7966516421
C9	2.5932941726	0.0192588811	2.0179492175
C10	3.8594668097	0.0022698709	2.6165521709

C11	4.9941738818	-0.0232416895	1.8101083959
C12	4.8439206121	-0.0312245547	0.4253239041
C13	3.5537136430	-0.0131141677	-0.1022938982
H14	-1.8936516219	0.1005467160	2.1127845629
H15	-2.0648605156	0.1187641450	4.6039366621
H16	0.0622374336	0.0882865723	5.9535747192
H17	2.2283880078	0.0420168830	4.7600474414
H18	3.9672166860	0.0087764478	3.6944131773
H19	5.9815717111	-0.0366347965	2.2618393949
H20	5.7019487487	-0.0509571548	-0.2378256574
H21	3.3647946640	-0.0179842758	-1.1719904700
H22	-1.3112221082	0.0667899634	-0.4027017397
O23	-2.5908938778	0.0824209925	-0.6144510230
O24	-3.2682782280	0.1113842018	0.4517886151
I25	0.5626800339	0.0148827888	-2.6887203983

1-bipyr-CN
Gas phase Energy: -715.61340084282 hartrees
Solvation Energy: -715.64821575091 hartrees
Zero Point Energy: 110.745 kcal/mol
Coordinates:

Pd1	0.0084687031	1.1603447042	-2.0293832210
N2	0.2295090101	1.7895243370	0.0015746675
N3	-1.6584565262	2.5709350055	-1.7425285956
C4	1.1996126447	1.3608324562	0.8237880951
C5	1.3148515026	1.7936476589	2.1413756952
C6	0.3827758422	2.7099866810	2.6220305958
C7	-0.6255496939	3.1574335530	1.7732236371
C8	-0.6863200680	2.6823014070	0.4580898848
C9	-1.7344551483	3.1132274948	-0.5072549067
C10	-2.7497621835	4.0212023035	-0.1863605330
C11	-3.6873801813	4.3641494015	-1.1579392284
C12	-3.5940228157	3.7964552066	-2.4264930483
C13	-2.5577826143	2.8982427455	-2.6786589587
H14	1.8957515025	0.6496961075	0.3955855425
H15	2.1173980272	1.4170444023	2.7658091589
H16	0.4372891604	3.0734613278	3.6435223643
H17	-1.3561522266	3.8701434200	2.1349774417
H18	-2.8158868680	4.4577480852	0.8029168849
H19	-4.4804259870	5.0673526241	-0.9219524087
H20	-4.3052412550	4.0388432191	-3.2085515304
H21	-2.4241499896	2.4170168303	-3.6432886090
H22	1.1907147781	0.1860840346	-2.1607825251
C25	-0.3074690247	0.6718873326	-3.8887203645
N26	-0.6304315074	0.4852995546	-4.9974890288

2- bipyr- CN
Gas phase Energy: -865.93197230595 hartrees
Solvation Energy: -865.96514388287 hartrees
Zero Point Energy: 113.365 kcal/mol
Coordinates:

Pd1	0.4551423948	0.0547166565	-0.2041147974
N2	0.2151303895	0.0743144347	1.9223331259
N3	2.5234314823	0.0235549034	0.5469417913
C4	-0.9719103986	0.1008185940	2.5492610630
C5	-1.0879772428	0.1160352707	3.9365827665
C6	0.0772741669	0.1033046107	4.6997429828
C7	1.3098398419	0.0753284057	4.0530364788
C8	1.3594912528	0.0607980946	2.6546495513
C9	2.6383848982	0.0303393404	1.8933915392
C10	3.8990839400	0.0090999154	2.5012344811
C11	5.0397178238	-0.0186942910	1.7006996143
C12	4.9022658678	-0.0247374710	0.3140704217
C13	3.6167800958	-0.0030186829	-0.2256870526
H14	-1.8430863286	0.1095152211	1.9054522486
H15	-2.0694794453	0.1374501807	4.3963358090
H16	0.0314386070	0.1148801922	5.7840001062
H17	2.2226732877	0.0653596238	4.6353542988
H18	3.9992179366	0.0135521121	3.5796849972
H19	6.0233493569	-0.0354836005	2.1595133181
H20	5.7657374098	-0.0460230672	-0.3413804823
H21	3.4316970286	-0.0065897822	-1.2960328586
H22	-1.0104886795	0.0759827092	-0.6635352525
O23	-3.8214516264	0.0946653421	-0.8510275114
O24	-4.0575158967	0.0981976612	0.3400086275
C25	0.8136817118	0.0351725672	-2.1197109511
N26	1.1906790108	0.0212160985	-3.2272520499

3A- bipyr- CN
Gas phase Energy: -865.93241744829 hartrees
Solvation Energy: -865.95887961342 hartrees
Zero Point Energy: 115.161 kcal/mol
Coordinates:

Pd1	-0.1581612929	1.1804868955	-2.0006511347
N2	0.1056215605	1.9086967988	0.0705924543
N3	-1.8446771316	2.6830971754	-1.6102639394
C4	1.0931714349	1.4670035498	0.8620426129
C5	1.2572371652	1.9031588406	2.1745440511
C6	0.3530185872	2.8351670146	2.6789846345
C7	-0.6738526011	3.2951383187	1.8592828712
C8	-0.7779842014	2.8152485705	0.5475420727
C9	-1.8468033007	3.2601115383	-0.3919957303

C10	-2.8093462139	4.2207679634	-0.0562653911
C11	-3.7735082490	4.5756443951	-0.9964277005
C12	-3.7585980895	3.9683607393	-2.2503542572
C13	-2.7685226211	3.0231208048	-2.5138177698
H14	1.7662946629	0.7413371462	0.4151142972
H15	2.0723189060	1.5180278113	2.7776036127
H16	0.4425715802	3.2006988650	3.6975375067
H17	-1.3844673415	4.0170634589	2.2427615052
H18	-2.8119926800	4.6915495263	0.9196121931
H19	-4.5254180698	5.3190499750	-0.7493567932
H20	-4.4920367006	4.2171917352	-3.0097566018
H21	-2.6979786171	2.5142534516	-3.4706055170
H22	1.3641630694	-0.7514490752	-3.6745702651
O23	1.7583337582	-0.2666973941	-1.9103352639
O24	2.0678013313	-0.9871028287	-2.9783029046
C25	-0.2891812904	0.4325832770	-3.8875918686
N26	0.0359207439	-0.2299588492	-4.8022753501

4- bipyr- CN
Gas phase Energy: -865.96937589850 hartrees
Solvation Energy: -866.01287008899 hartrees
Zero Point Energy: 116.918 kcal/mol
Coordinates:

Pd1	0.0143671643	1.2553662916	-2.0194089288
N2	0.2358647989	1.8079301596	-0.0006756724
N3	-1.6473253883	2.5284267491	-1.7337758390
C4	1.2303149274	1.3627108044	0.7736249933
C5	1.3385339704	1.7462969470	2.1090318706
C6	0.3764626171	2.6081075864	2.6334714785
C7	-0.6601844836	3.0627880280	1.8185206949
C8	-0.7101130832	2.6439925609	0.4857548986
C9	-1.7598003343	3.0486690467	-0.4839758515
C10	-2.8172666365	3.9042203444	-0.1656157448
C11	-3.7601433755	4.2204054255	-1.1410245911
C12	-3.6283221639	3.6775133549	-2.4167146590
C13	-2.5521137934	2.8321463278	-2.6758533144
H14	1.9226220295	0.6908340072	0.2697067559
H15	2.1565324479	1.3739612009	2.7156848941
H16	0.4279097367	2.9255466074	3.6704174201
H17	-1.4131404634	3.7300334523	2.2202786304
H18	-2.9068663343	4.3192846686	0.8312088961
H19	-4.5862952254	4.8832684504	-0.9032890186
H20	-4.3402967958	3.8985630962	-3.2040424151
H21	-2.3869767723	2.3754137375	-3.6462489369
H22	1.2981719849	-1.3277392953	-3.0826390635
O23	1.6528613339	0.1430528981	-1.9607449038

O24	1.2846430882	-1.2405042546	-2.1141789961
C25	-0.3049176130	0.8489799130	-3.9278275779
N26	-0.5798596222	0.6459944764	-5.0462863880

TS1- bipyr- CN
Gas phase Energy: -865.90675257034 hartrees
Solvation Energy: -865.93943846715 hartrees
Zero Point Energy: 111.320 kcal/mol
Number and Magnitude of negative Eigen values: 1 (-1561.08 cm^{-1})
Coordinates:

Pd1	0.3078741688	0.0516909067	-0.1791834281
N2	0.1290484609	0.0705264470	1.9558056849
N3	2.4125604750	0.0238774166	0.5359311858
C4	-1.0455549219	0.0938038183	2.6037356211
C5	-1.1320890496	0.1106601584	3.9939157118
C6	0.0474040565	0.1041473012	4.7334492145
C7	1.2666238619	0.0799078993	4.0617868107
C8	1.2873089350	0.0621167972	2.6635180114
C9	2.5510792547	0.0331334844	1.8778232932
C10	3.8231791440	0.0145806176	2.4616686025
C11	4.9480889296	-0.0130363171	1.6401615135
C12	4.7840043225	-0.0217401922	0.2567923510
C13	3.4883154486	-0.0025676698	-0.2576964724
H14	-1.9330401390	0.0990499768	1.9758095714
H15	-2.1044136824	0.1289924274	4.4736030680
H16	0.0234391671	0.1177923505	5.8188173956
H17	2.1923034063	0.0757512019	4.6240924244
H18	3.9434951169	0.0206607780	3.5383481816
H19	5.9406334901	-0.0278154531	2.0802197430
H20	5.6352050889	-0.0431434617	-0.4150085652
H21	3.2836348887	-0.0081620536	-1.3245349215
H22	-1.3449518906	0.0759945262	-0.6431753887
O23	-2.5959504675	0.0982558740	-0.8643182525
O24	-3.2727464610	0.1055695866	0.2084065945
C25	0.6077181162	0.0334980828	-2.1177521171
N26	0.9438873857	0.0206873880	-3.2385365978

1-bipyr-CF_3
Gas phase Energy: -960.38780971527 hartrees
Solvation Energy: -960.40794598692 hartrees
Zero Point Energy: 114.009 kcal/mol
Coordinates:

Pd1	-0.0071116694	1.1917137833	-2.0404505618
N2	0.1728947509	1.8222750830	0.0254944984
N3	-1.7130187408	2.6443543444	-1.7095814895
C4	1.1494093111	1.3803610211	0.8308987177

C5	1.2829063682	1.7998384976	2.1516567944
C6	0.3611684445	2.7182820143	2.6489547691
C7	-0.6539787335	3.1788334146	1.8154792863
C8	-0.7305209126	2.7118651771	0.4970391975
C9	-1.7859034742	3.1505813073	-0.4568761572
C10	-2.8084315396	4.0356509837	-0.0932953179
C11	-3.7639803008	4.4024075981	-1.0371219078
C12	-3.6781887356	3.8766014236	-2.3229156494
C13	-2.6348723563	2.9990785315	-2.6149974911
H14	1.8352072162	0.6694145842	0.3848846563
H15	2.0898020970	1.4134625527	2.7643796591
H16	0.4291715979	3.0743031102	3.6723108049
H17	-1.3733326809	3.8954049012	2.1917740439
H18	-2.8667643194	4.4343110109	0.9117694641
H19	-4.5620374782	5.0875288356	-0.7669309862
H20	-4.4005914882	4.1338240614	-3.0901505180
H21	-2.5135145824	2.5545543721	-3.5949224716
H22	1.1869763504	0.2122762359	-2.0906904011
C23	-0.1586066878	0.6101462573	-3.9495016492
F24	-1.1863735335	1.2883803383	-4.6029760334
F25	0.9373702402	0.8512959030	-4.7178839293
F26	-0.4646661228	-0.7048881410	-4.1217958707

2- bipyr- CF_3
Gas phase Energy: -1110.70635125832 hartrees
Solvation Energy: -1110.72420037567 hartrees
Zero Point Energy: 116.641 kcal/mol
Coordinates:

Pd1	0.4624901300	0.0444583831	-0.2371471873
N2	0.2512074536	0.0714626411	1.9317564542
N3	2.5770926869	0.0176070209	0.5766060967
C4	-0.9427106879	0.1016940530	2.5433133827
C5	-1.0772112681	0.1244474178	3.9294342210
C6	0.0787638034	0.1162026907	4.7068743452
C7	1.3186282712	0.0854055001	4.0752311220
C8	1.3819252163	0.0628577671	2.6759889782
C9	2.6674926614	0.0282156736	1.9268621077
C10	3.9136127847	0.0065171901	2.5662057212
C11	5.0760406640	-0.0268014757	1.8000487878
C12	4.9699859573	-0.0379013181	0.4119607042
C13	3.6974563794	-0.0147061055	-0.1578019568
H14	-1.8052931770	0.1078428706	1.8878031251
H15	-2.0640371983	0.1481846702	4.3778588722
H16	0.0202580499	0.1335500207	5.7906277729
H17	2.2231612716	0.0795799821	4.6704369955
H18	3.9841519732	0.0142600820	3.6468513969

H19	6.0472117271	-0.0441695498	2.2850725657
H20	5.8476484956	-0.0641104788	-0.2242387165
H21	3.5442442729	-0.0212883792	-1.2297633788
H22	-1.0322185773	0.0630498676	-0.6167971026
O23	-3.8930140625	0.0894583302	-0.6688404462
O24	-4.0662241824	0.0741915597	0.5328304234
C25	0.6404201330	0.0218194332	-2.2353516663
F26	1.9804084618	0.0244528353	-2.6260774958
F27	0.1200024897	-1.0781352863	-2.8452903343
F28	0.1061511314	1.0980699931	-2.8751394666

3A- bipyr- CF_3
Gas phase Energy: -1110.69909006223 hartrees
Solvation Energy: -1110.71455999571 hartrees
Zero Point Energy: 118.870 kcal/mol
Coordinates:

Pd1	-0.0411522195	1.1924140265	-2.0114712259
N2	0.2023805130	1.9462554207	0.0869182974
N3	-1.9400778623	2.4502015165	-1.5102319075
C4	1.1749689152	1.5183042968	0.9046506790
C5	1.2358046307	1.8668723611	2.2513214764
C6	0.2305792359	2.6808451120	2.7709279253
C7	-0.7886149818	3.1152528867	1.9294023649
C8	-0.7758797991	2.7396708129	0.5797996046
C9	-1.8315877118	3.1703893765	-0.3736446682
C10	-2.6752593909	4.2607543661	-0.1229934994
C11	-3.6655523721	4.5799450630	-1.0476924544
C12	-3.7842710446	3.8124714886	-2.2061065273
C13	-2.8890057003	2.7633615219	-2.4019651526
H14	1.9176069516	0.8689852471	0.4514612783
H15	2.0473317535	1.5006948809	2.8707597335
H16	0.2314774269	2.9642728921	3.8191219055
H17	-1.5982612178	3.7192280198	2.3220190555
H18	-2.5494723460	4.8628731533	0.7697041969
H19	-4.3283584521	5.4212827843	-0.8689208318
H20	-4.5466537535	4.0223721040	-2.9488810648
H21	-2.9103650045	2.1446238290	-3.2930955717
H22	1.2264273938	-1.1439499465	-3.2121172444
O23	1.6204746142	-0.2904858930	-1.6176745073
O24	1.8040407581	-1.3448526819	-2.4277198401
C25	-0.3803728763	0.6717669682	-3.9844113087
F26	-1.7112510050	0.5294323992	-4.3174681803
F27	0.1227303851	1.5195397421	-4.9251608609
F28	0.1633222473	-0.5961291658	-4.3676801913

4- bipyr- CF_3

Gas phase Energy: -1110.74885907135 hartrees
Solvation Energy: -1110.77660983106 hartrees
Zero Point Energy: 120.520 kcal/mol
Coordinates:

Pd1	-0.0134291234	1.2420055902	-2.0415592339
N2	0.2006065128	1.8136967879	0.0030328413
N3	-1.6990875540	2.5588026906	-1.7186304254
C4	1.2049430827	1.3656994054	0.7617316036
C5	1.3252467241	1.7362855543	2.0994935709
C6	0.3670408605	2.5914982531	2.6405890923
C7	-0.6748687725	3.0542478594	1.8380934529
C8	-0.7350041881	2.6454922441	0.5019027192
C9	-1.7855205547	3.0687136827	-0.4611991309
C10	-2.8155500309	3.9481456739	-0.1161691994
C11	-3.7634181373	4.3094670746	-1.0691635737
C12	-3.6618439963	3.7823470316	-2.3527814675
C13	-2.6145296442	2.9087038345	-2.6349484334
H14	1.8966427584	0.7063382326	0.2403446943
H15	2.1496783851	1.3601404482	2.6953109663
H16	0.4267282930	2.8993191514	3.6800836299
H17	-1.4221676215	3.7195962065	2.2534737410
H18	-2.8776353963	4.3501699521	0.8875558536
H19	-4.5658422986	4.9928071511	-0.8086687181
H20	-4.3756231580	4.0350678013	-3.1291348456
H21	-2.4880478434	2.4610253327	-3.6120031674
H22	1.1441251284	-1.4541683481	-2.7590976653
O23	1.6609222076	0.1639361577	-1.9555149059
O24	1.2933699253	-1.2300092341	-1.8253239046
C25	-0.1864327054	0.7593589641	-3.9855824728
F26	-1.4805919074	0.8568980127	-4.4725040053
F27	0.5552118143	1.5584708909	-4.7978742513
F28	0.1839283733	-0.5272023035	-4.2935507448

TS1- bipyr- CF_3
Gas phase Energy: -1110.68137390433 hartrees
Solvation Energy: -1110.69842074766 hartrees
Zero Point Energy: 114.709 kcal/mol
Number and Magnitude of negative Eigen values: 1 (-1488.76 cm^{-1})
Coordinates:

Pd1	0.3211957922	0.0489704050	-0.1974051210
N2	0.1773785604	0.0682412152	1.9742825725
N3	2.4868695816	0.0008363082	0.5706227697
C4	-1.0034265033	0.0990793296	2.6104309655
C5	-1.1038221879	0.1208714815	3.9997434292
C6	0.0690963508	0.1104048223	4.7491816016
C7	1.2940063440	0.0772479487	4.0888200159

C8	1.3262617002	0.0557032280	2.6896308830
C9	2.5995000642	0.0167977896	1.9155782233
C10	3.8587063888	-0.0046806953	2.5293088700
C11	5.0043715925	-0.0454196901	1.7388873961
C12	4.8714869569	-0.0638737222	0.3531563195
C13	3.5873820062	-0.0376962892	-0.1889512518
H14	-1.8855080032	0.1059683747	1.9741689340
H15	-2.0803680254	0.1456249157	4.4705744991
H16	0.0363773485	0.1274895842	5.8343024436
H17	2.2116817660	0.0681019578	4.6632837952
H18	3.9531215334	0.0101509998	3.6082749099
H19	5.9856876362	-0.0622836319	2.2036592250
H20	5.7369582295	-0.0956431226	-0.3000324209
H21	3.4129353932	-0.0412591386	-1.2588809563
H22	-1.3624029327	0.0910494375	-0.5780162620
O23	-2.5924776653	0.1761745673	-0.8274488196
O24	-3.2850767471	0.1464463084	0.2441553443
C25	0.4970408971	0.0165592153	-2.1868240771
F26	1.7563615467	0.4292106080	-2.5953104480
F27	0.3471418259	-1.2336704659	-2.7192369305
F28	-0.3696043567	0.8230877672	-2.8639631796