

Supporting Information for “A Computational Model Relating Structure and Reactivity in Enantioselective Oxidations of Secondary Alcohols by (-)-Sparteine-Pd(II) Complexes”

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Included are energies, coordinates and imaginary frequencies for numbered structures, representative structures from Table 1, and peripheral species (necessary for calculating relative energies.)

No. (Structure Number)

GPE: (Gas phase energy in Hartrees)

SE: (Solvation energy in Hartrees, using gas-phase geometry)

or

SPE: (Solution phase energy in Hartrees, optimized in solvent)

freqs: (Imaginary frequencies in cm⁻¹)

(Coordinates in Angstroms)

No. 1

GPE: -1744.01967

SE: -.01661

Pd1	.1194434933	-.5651117570	-2.1409019737
C2	1.1837736473	-.7041065141	1.2249289507
C3	-.1730534138	1.2783568264	.7085712885
C4	.8293521845	1.6849254735	-.3838318983
N5	1.6034407915	.5384264249	-.9490653809
C6	2.2007303506	-.3192533087	.1365248722
C7	2.9637240400	-1.5004980870	-.4745817368
C8	4.1350423656	-.9950163353	-1.3263332204
C9	3.6256429957	-.0006362088	-2.3753037045
C10	2.7400292221	1.0883772078	-1.7673309496
C11	.6022999475	.5767081479	1.8346825150
C12	.0374263440	-1.6202265191	.7796952366
N13	-.9021617220	-.9804575203	-.1860663523
C14	-1.3623019684	.4007438797	.2446020502
C15	-2.4611575494	.3874894723	1.3367272900
C16	-3.0879137772	-1.9477042103	.7308428500
C17	-3.6306915469	-.5446763445	1.0105176453
C18	-2.0799996389	-1.8867104735	-.4196438502
H19	1.7492648709	-1.2594084150	1.9838668602
H20	-.6101801056	2.2141634445	1.0783216684
H21	.3344932103	2.1832436496	-1.2221639778
H22	1.5374337958	2.4019151010	.0629308406
H23	2.9440884893	.3188938270	.6471359796
H24	3.3222062727	-2.1411559002	.3406363408
H25	2.2849488571	-2.1012404133	-1.0926371582
H26	4.8729890781	-.5122155301	-.6697510214
H27	4.6443107671	-1.8336112124	-1.8132459642
H28	4.4622264398	.4942388090	-2.8823482639
H29	3.0516386178	-.5218090806	-3.1457017996
H30	2.3081819920	1.7044342859	-2.5557586829
H31	3.3329192472	1.7293834936	-1.0944663197
H32	-.0379767539	.3474384185	2.6913561308
H33	1.4049977515	1.2265998642	2.2024715963
H34	-.5080360024	-1.9316265355	1.6810561440
H35	.4140122315	-2.5270028341	.2992267243
H36	-1.8008873630	.8393110571	-.6598321808
H37	-2.0373443816	.0902828369	2.3029109705
H38	-2.8087091474	1.4207981596	1.4559629114

H39	-2.6479213118	-2.3718988172	1.6431466741
H40	-3.8909733293	-2.6291850898	.4276756437
H41	-4.3480482364	-.5508254603	1.8388278022
H42	-4.1669511444	-.1786942087	.1245556191
H43	-1.6783051375	-2.8700880375	-.6702023736
H44	-2.5837567455	-1.5283232944	-1.3168189005
C145	-1.2997175204	-1.9284384463	-3.4352481802
C146	.8007301006	.3845306439	-4.1900190343

No. 2

GPE: -2130.03622

SE: -0.01373

Pd1	-0.1530030556	0.4613806572	-2.0250937358
C2	1.8159670290	-0.9721470927	0.6258015963
C3	-0.2936378445	-0.0744003581	1.4828396609
C4	0.0803805821	1.3089917834	0.9228353747
N5	1.0492835171	1.2792471914	-0.2264907536
C6	2.2358141254	0.4320849565	0.1470372574
C7	3.3457794993	0.4708099543	-0.9059831406
C8	3.8677464051	1.9053653238	-1.0515338498
C9	2.7069311318	2.8414901073	-1.4025200481
C10	1.5084394590	2.6967546487	-0.4583093151
C11	0.9891029380	-0.8044194933	1.9063678004
C12	1.0356904458	-1.8503952600	-0.3687175602
N13	-0.3462372547	-1.3614736032	-0.6860160575
C14	-1.1384629625	-0.9661109135	0.5460052215
C15	-1.7232592584	-2.1722185974	1.3222744811
C16	-1.5789110623	-3.6006446225	-0.7083019901
C17	-2.4951079452	-3.1439964278	0.4276058775
C18	-1.0875392805	-2.3843379437	-1.4976400381
H19	2.7467084929	-1.5117193392	0.8428971094
H20	-0.9242441346	0.1273392751	2.3576756913
H21	-0.8065912438	1.8472500552	0.5848494594
H22	0.5551061918	1.8767452137	1.7382612866
H23	2.6635544463	0.9174072473	1.0436587924
H24	4.1465116363	-0.2051687929	-0.5818098177
H25	2.9811875333	0.1008544560	-1.8720473430
H26	4.3397354855	2.2099778415	-0.1062962370
H27	4.6416498619	1.9592024957	-1.8248224967
H28	3.0253871309	3.8899489253	-1.3583663168
H29	2.3830164218	2.6522886343	-2.4259825483
H30	0.6484511417	3.2536736264	-0.8359982643
H31	1.7759149088	3.1033472464	0.5300198596
H32	0.7788775625	-1.7717822139	2.3707388171
H33	1.5437501462	-0.2116637279	2.6432097014
H34	0.9593976740	-2.8517702453	0.0749625100
H35	1.5638202709	-1.9559964357	-1.3191400500
H36	-1.9720783992	-0.3767738454	0.1540124719
H37	-2.3762948836	-1.7567591174	2.0990779317
H38	-0.9364242044	-2.7303316029	1.8431957467
H39	-2.1095508907	-4.2502931342	-1.4139145276
H40	-0.7441555128	-4.1921808940	-0.3085815958
H41	-2.8543650794	-3.9960135436	1.0159546715
H42	-3.3778076187	-2.6451834627	0.0066549989
H43	-0.4406487388	-2.6659398109	-2.3290884514
H44	-1.9398477698	-1.8664667869	-1.9365162314
C145	0.2233178571	2.2528699789	-3.5232264916
C46	-2.6932087891	0.7161372776	-4.7664034406
C47	-1.4320285076	-0.1507816931	-4.7658079758
C48	-1.6092855287	-1.4462031884	-5.5594706977
C49	-2.6384769201	-2.3464148678	-5.2407209650

H50	-3.3156613374	-2.1141112959	-4.4240874929
C51	-2.8023732328	-3.5267426008	-5.9658236284
H52	-3.6076632850	-4.2109304264	-5.7105291447
C53	-1.9379414886	-3.8270445206	-7.0236514671
H54	-2.0685319285	-4.7437030918	-7.5926460734
C55	-0.9083809057	-2.9399048227	-7.3466320462
H56	-0.2340370741	-3.1635841832	-8.1691673393
C57	-0.7428499828	-1.7615349614	-6.6135425739
H58	0.0596634688	-1.0726458824	-6.8668760930
O59	-1.0612478736	-0.6062513432	-3.4720357821
H60	-2.5290075978	1.6228501643	-4.1828363857
H61	-2.9584192193	0.9905218868	-5.7942404270
H62	-3.5363523132	0.1802952822	-4.3206463882
H63	-0.6103515406	0.4108903798	-5.2251230427
C164	-2.3662299996	1.5186726694	-1.2886797445
H65	1.1354953985	-0.0880295219	-2.5971489817

No. 6

GPE: -2130.11851

SE: -0.01708

freqs: -80.27

Pd1	-.0067074015	-.0165780968	.0122559034
C2	.0376486853	-.0176230521	3.5316149106
C3	2.2685131530	.0108922596	2.5050162232
C4	1.9321091993	-1.2913275457	1.7535998940
N5	.4620358661	-1.5293498178	1.5544947141
C6	-.2950435591	-1.3504188929	2.8409394348
C7	-1.7900870154	-1.6233518057	2.6446129675
C8	-2.0078232787	-3.0816513825	2.2234023257
C9	-1.1869841682	-3.3813543275	.9652091674
C10	.2766651346	-2.9545184997	1.0987638698
C11	1.5366212969	.0015654603	3.8554758232
C12	-.3409323742	1.2440726136	2.7427611210
N13	.4694341658	1.4596587205	1.5075454639
C14	1.9640116004	1.3166993859	1.7356793882
C15	2.6001383835	2.5424437039	2.4335110621
C16	.7244649750	3.9984886436	1.6595198608
C17	2.2470171635	3.8616714662	1.7394003710
C18	.1326761582	2.8015890250	.9070491362
H19	-.5504089563	.0046419616	4.4579147992
H20	3.3543751040	-.0079251062	2.6615668665
H21	2.4003791794	-1.3170319066	.7663437198
H22	2.3353664296	-2.1291709362	2.3441180942
H23	.0843714522	-2.1345780219	3.5206150654
H24	-2.3066832885	-1.4090564829	3.5883112223
H25	-2.2000077390	-.9480640243	1.8833826366
H26	-1.7042562350	-3.7422465252	3.0479744938
H27	-3.0697599234	-3.2743143468	2.0382939064
H28	-1.1952780567	-4.4548866136	.7412403855
H29	-1.6224751879	-2.8730836809	.1029022782
H30	.7920746971	-3.0636761713	.1447554830
H31	.7806525500	-3.5870077470	1.8479187508
H32	1.7981460469	.8702122554	4.4654926651
H33	1.8116366288	-.8870536144	4.4357285346
H34	-.2153638228	2.1065775858	3.4097988657
H35	-1.3906956032	1.2234986275	2.4365609797
H36	2.3838134515	1.2570806221	.7264322094
H37	3.6853774109	2.3843901257	2.4313589779
H38	2.2973612492	2.6047911580	3.4854555027
H39	.2987827163	4.1026441068	2.6666856827

H40	.4392195636	4.9014203188	1.1079844671
H41	2.6670030888	3.8724935938	.7262324838
H42	2.6895039590	4.7026706996	2.2846533453
H43	-.9552423622	2.8539695992	.8361561517
H44	.5382724673	2.7916010312	-.1045705443
O45	-1.2069886223	1.5563233745	-1.4460385079
C146	-.3792207612	-1.5698555778	-1.7143093179
C47	-2.2398233925	1.1972200509	-2.3896817247
C48	-2.2213946292	2.1895248295	-3.5580072821
C49	-3.5673242613	1.1769873845	-1.6592475313
C50	-3.9699741602	2.2566587858	-.8607211542
H51	-3.3088476470	3.1115994193	-.7493195299
C52	-5.2061872802	2.2406461188	-.2137416626
H53	-5.5071027028	3.0865965790	.3991822250
C54	-6.0613672448	1.1447115341	-.3587043925
H55	-7.0257729325	1.1343138971	.1426347543
C56	-5.6707455063	.0669867590	-1.1541423760
H57	-6.3284742444	-.7896724754	-1.2736154254
C58	-4.4301719159	.0836097276	-1.7966479802
H59	-4.1247395888	-.7608644603	-2.4096132745
H60	-1.2495645810	2.1629704019	-4.0616056381
H61	-2.9926039595	1.9282013161	-4.2898035696
H62	-2.4061574860	3.2106284028	-3.2101259553
H63	-2.0304813532	.1923855694	-2.7696200107

No. 7

GPE: -2130.12730

SE: -0.01844

Pd1	0.0145417371	0.1039351140	-0.1793277251
C2	-0.3263322389	0.3399094081	3.3066507662
C3	1.9684510306	-0.0997293977	2.5427093570
C4	1.4830922448	-1.3590678149	1.8052034766
N5	0.0267600205	-1.3255383074	1.4305521081
C6	-0.8344001140	-0.9268142004	2.6024757174
C7	-2.3137284604	-0.8991546197	2.2008547361
C8	-2.7795227497	-2.3025643538	1.7931646367
C9	-1.8713395059	-2.8499363546	0.6872599806
C10	-0.3864601200	-2.7228165775	1.0306557115
C11	1.1043892072	0.0906554981	3.7981171617
C12	-0.3662412679	1.6188138530	2.4641508091
N13	0.5847527189	1.6139547608	1.3165795602
C14	1.9964405004	1.1972801128	1.7023027208
C15	2.7967808406	2.3040101808	2.4317157004
C16	1.3086801515	4.0613262007	1.4772719340
C17	2.7649329249	3.6454094749	1.6946864438
C18	0.5849913288	2.9760676143	0.6730629269
H19	-0.9962999972	0.5038231946	4.1603432341
H20	3.0082287411	-0.3040559689	2.8263041975
H21	2.0485046435	-1.5314375281	0.8857258119
H22	1.6421804808	-2.2220975657	2.4690305979
H23	-0.7158776880	-1.7389893878	3.3399532224
H24	-2.8964750364	-0.5285333223	3.0529675317
H25	-2.4643019701	-0.1982617056	1.3703354380
H26	-2.7491200904	-2.9594390327	2.6737352939
H27	-3.8198428312	-2.2782445302	1.4528061133
H28	-2.0765060782	-3.9117091629	0.5057521989
H29	-2.0611315937	-2.3263442252	-0.2519399340
H30	0.2291601294	-3.0191755603	0.1827772618
H31	-0.1440846497	-3.3696675400	1.8883246149

H32	1.4583938133	0.9227551513	4.4120652214
H33	1.1407848940	-0.8059505539	4.4284957157
H34	-0.1329033758	2.4623072985	3.1261576935
H35	-1.3652962341	1.7976068235	2.0557245229
H36	2.4990715743	1.0197792984	0.7435598304
H37	3.8272788687	1.9395336123	2.5182600036
H38	2.4303355492	2.4508404595	3.4550888304
H39	0.8171206975	4.2664083334	2.4378742986
H40	1.2482778795	4.9876938612	0.8946603356
H41	3.2615396247	3.5430991866	0.7230606162
H42	3.3086543267	4.4020302073	2.2713501561
H43	-0.4596590868	3.2321843387	0.4793221739
H44	1.0947578066	2.8795087376	-0.2815397908
C145	-0.1998270639	-1.5270568332	-1.8731493199
C46	0.0281867121	2.5866854025	-3.8944601019
C47	-0.5612038534	1.4993183327	-2.9908592777
C48	-2.0319042119	1.6983162527	-2.6936321691
C49	-2.4723062075	2.8050184134	-1.9541325562
H50	-1.7459629654	3.5216174694	-1.5808757122
C51	-3.8305317369	2.9990777609	-1.7048595580
H52	-4.1581801270	3.8661571219	-1.1368238820
C53	-4.7708344876	2.0892575998	-2.1963732682
H54	-5.8296781953	2.2433269600	-2.0079217700
C55	-4.3418431335	0.9865502883	-2.9356183285
H56	-5.0654452832	0.2743895406	-3.3228154737
C57	-2.9804720298	0.7912778941	-3.1784954273
H58	-2.6474776265	-0.0765150543	-3.7413907577
O59	0.1681109175	1.5237054958	-1.7313595417
H60	1.0957426494	2.4115015386	-4.0536285683
H61	-0.4808964186	2.5693168132	-4.8632518771
H62	-0.0992478919	3.5811097467	-3.4563987062
H63	-0.4159381981	0.5211901920	-3.4540927281
C164	3.0376916926	1.6600430081	-1.7055462403
H65	1.1922415529	1.5432925584	-1.8898683165

No. 8

GPE: -1669.28921

SE: -.01169

Pd1	0.0192465080	-0.0110054020	-0.0694406102
C2	-0.2305717639	0.0802519049	3.4627787263
C3	2.0810029522	0.0418421777	2.6297459471
C4	1.7915940926	-1.2794202375	1.8946866087
N5	0.3509269414	-1.4807940782	1.5500369567
C6	-0.5420296898	-1.2422207570	2.7374850493
C7	-2.0116355141	-1.4204338226	2.3367583302
C8	-2.2666530865	-2.8613807057	1.8743306765
C9	-1.2889645632	-3.2299007012	0.7519860324
C10	0.1615360434	-2.9057017544	1.1133579098
C11	1.2354895006	0.0691544225	3.9127795075
C12	-0.5039630214	1.3647676372	2.6695029486
N13	0.3937214062	1.5514825826	1.4932654140
C14	1.8613736941	1.3392340243	1.8094469754
C15	2.5309473722	2.5431242180	2.5155724677
C16	0.7675705822	4.0749469586	1.6426801596
C17	2.2769562956	3.8687405974	1.7917953743
C18	0.1497551447	2.8997618350	0.8806816056
H19	-0.8929811814	0.1080551602	4.3374885137
H20	3.1486444630	0.0170532295	2.8820457871
H21	2.3584063955	-1.3521299050	0.9619670563
H22	2.1181748288	-2.1031186569	2.5512077142
H23	-0.3028990498	-2.0380791112	3.4668203971

H24	-2.6419428183	-1.1701447396	3.1992802505
H25	-2.2641633584	-0.7212449913	1.5299634699
H26	-2.1371281358	-3.5411402451	2.7289291827
H27	-3.3008738067	-2.9761826637	1.5313909148
H28	-1.3465809175	-4.2998488418	0.5185910886
H29	-1.5414899071	-2.6901263915	-0.1646054453
H30	0.8081123192	-3.0729438129	0.2516749117
H31	0.4985933079	-3.5477552065	1.9446651316
H32	1.4613845685	0.9425631043	4.5318846080
H33	1.4450946732	-0.8176293447	4.5227609315
H34	-0.3944772456	2.2120086013	3.3618712973
H35	-1.5282542158	1.3877965344	2.2892142815
H36	2.3423478627	1.2281611097	0.8301285425
H37	3.6054509580	2.3306776670	2.5748730891
H38	2.1745865452	2.6332573670	3.5485673384
H39	0.5479664812	4.9888437378	1.0780497082
H40	0.3091103478	4.2039329292	2.6328001288
H41	2.7402248728	4.6955481859	2.3422865819
H42	2.7413954240	3.8451237294	0.7964535185
H43	-0.9327931931	3.0041742428	0.7833612971
H44	0.5347030823	2.8589847950	-0.1391735912
C145	0.2028046232	-1.5978526334	-1.8453679219
O46	-0.1670712366	1.4311199848	-1.4328813419
C47	-1.2192017073	1.3583302195	-2.3681451736
C48	-0.9127744458	2.3891716436	-3.4672725481
C49	-2.5846050584	1.5852045621	-1.7151503823
C50	-2.9392165249	2.8311742356	-1.1725910549
H51	-2.2433825410	3.6629136929	-1.2499963086
C52	-4.1734156995	3.0191453515	-0.5473722633
H53	-4.4331511669	3.9951439348	-0.1436657312
C54	-5.0811558369	1.9576931760	-0.4493623886
H55	-6.0439865405	2.1035411053	0.0335092122
C56	-4.7428214866	0.7135806566	-0.9865592820
H57	-5.4428490407	-0.1162559979	-0.9231007070
C58	-3.5045465474	0.5330017095	-1.6126697798
H59	-3.2412093768	-0.4375748635	-2.0274023187
H60	0.0466239548	2.1452447997	-3.9322201549
H61	-1.6937127172	2.3813370978	-4.2355235993
H62	-0.8447436334	3.4011936813	-3.0538333167
H63	-1.2376255458	0.3680977636	-2.8421517976

No. 9

GPE: -1669.25353

SE: -0.01745

freqs: -598.08

Pd1	-0.0122865885	0.0161979040	0.0016788393
C2	0.0038858019	-0.0069473735	3.4514489672
C3	2.2975126118	-0.0108932143	2.5702879643
C4	1.9952130277	-1.2950193857	1.7805349116
N5	0.5402089343	-1.4802335629	1.4669150920
C6	-0.3039939457	-1.3254409890	2.7012385381
C7	-1.7856201969	-1.5623535246	2.3842879593
C8	-2.0009627012	-2.9705386166	1.8097376653
C9	-1.0931890409	-3.2040186609	0.5942971776
C10	0.3646795416	-2.8545339933	0.8961481807
C11	1.4799736575	-0.0176764589	3.8706965258
C12	-0.2767390439	1.3078417035	2.6957462307
N13	0.5908941058	1.4932776022	1.4987546728
C14	2.0648565087	1.2957010537	1.7748883795
C15	2.7176680124	2.5092035917	2.4745516735

C16	0.9410822938	4.0179604846	1.5559156003
C17	2.4494866146	3.8260127576	1.7362514679
C18	0.3452744749	2.8105207778	0.8254271731
H19	-0.6431949812	-0.0018711381	4.3383177040
H20	3.3704223186	-0.0466871602	2.7964968375
H21	2.5270589334	-1.2969884103	0.8239109265
H22	2.3233710762	-2.1547649260	2.3872214284
H23	0.0092668423	-2.1311492364	3.3898276953
H24	-2.3623411570	-1.4338970331	3.3088269203
H25	-2.1393866909	-0.8100019597	1.6681969691
H26	-1.7762579326	-3.7139109424	2.5871720424
H27	-3.0507325502	-3.1119408137	1.5320502236
H28	-1.1318632197	-4.2543516402	0.2813351408
H29	-1.4498209620	-2.6066222580	-0.2510608558
H30	0.9851237871	-2.9035725460	-0.0018581175
H31	0.7667315366	-3.5725082540	1.6294538595
H32	1.7101568054	0.8453682540	4.5031698912
H33	1.7072028344	-0.9140584624	4.4601866504
H34	-0.1279658078	2.1319515066	3.4084707901
H35	-1.3149388031	1.3622638229	2.3541187534
H36	2.5192702114	1.1776707784	0.7830772242
H37	3.7956869761	2.3148511549	2.5274336432
H38	2.3686529892	2.6052108131	3.5106772434
H39	0.4591200013	4.1697700946	2.5311333922
H40	0.7252947166	4.9124783034	0.9601538370
H41	2.9324823315	3.8001437585	0.7509031772
H42	2.8889611397	4.6653215634	2.2869038803
H43	-0.7351054546	2.9080191642	0.6880407274
H44	-0.5338384183	-0.9356826683	-1.2141570624
C145	2.6268629955	-0.2259499614	-1.3977952011
O46	-0.8861730229	1.2253020003	-1.4560525508
C47	-1.1683726461	0.1519792014	-2.1359825030
C48	-2.6057551897	-0.3309586730	-2.1145836792
C49	-3.5809199500	0.4696791793	-1.5021661373
H50	-3.2693162304	1.4036593633	-1.0462545472
C51	-4.9188273901	0.0786569680	-1.5007873298
H52	-5.6663958154	0.7159982382	-1.0363192608
C53	-5.3009718458	-1.1233420047	-2.1022922861
H54	-6.3438900532	-1.4275813773	-2.1021790526
C55	-4.3358908855	-1.9283445946	-2.7104286203
H56	-4.6247158894	-2.8631591189	-3.1826183252
C57	-2.9976684229	-1.5333690392	-2.7215330636
H58	-2.2591178520	-2.1682615631	-3.2017254407
C59	-0.3316274111	-0.1150663067	-3.3778802806
H60	0.7236912439	0.0429595047	-3.1414707285
H61	-0.4683034502	-1.1229119615	-3.7748054104
H62	-0.6557006672	0.6009644970	-4.1436215324
H63	0.7892875194	2.7346555446	-0.1709801635

No. 10

GPE: -1669.27609

SE: -0.01620

Pd1	0.1442749079000	0.0129587376000	-0.0288216657000
C2	-0.2684249188000	-0.0339030731000	3.4352581696000
C3	2.1192583783000	-0.0825994613000	2.8796122731000
C4	1.8921895476000	-1.3290143349000	2.0069984953000
N5	0.4825963643000	-1.5005068858000	1.5133228855000
C6	-0.5052710156000	-1.3344159364000	2.6319502587000
C7	-1.9335974722000	-1.5445189159000	2.1214319578000
C8	-2.0977739795000	-2.9602198499000	1.5459173794000
C9	-1.0381345082000	-3.2345431527000	0.4700995131000

C10	0.3696340432000	-2.8856877789000	0.9502823860000
C11	1.1326133411000	-0.1038506758000	4.0541549075000
C12	-0.4097841363000	1.3057983901000	2.6839424407000
N13	0.6301822822000	1.5114958140000	1.6434301836000
C14	2.0355932422000	1.2578622581000	2.1220452770000
C15	2.6149488130000	2.4138586230000	2.9669420949000
C16	1.0452064823000	4.0174628973000	1.8559278163000
C17	2.5034360363000	3.7630791428000	2.2482898662000
C18	0.5250271390000	2.8537329282000	1.0039109616000
H19	-1.0292946783000	-0.0281911212000	4.2254668934000
H20	3.1490301157000	-0.1673595816000	3.2473253035000
H21	2.5405308250000	-1.3094409165000	1.1316981601000
H22	2.1354230136000	-2.2115590548000	2.6176332190000
H23	-0.2988435618000	-2.1522300502000	3.3468584446000
H24	-2.6300774738000	-1.3858970870000	2.9535594632000
H25	-2.1562625911000	-0.7980261544000	1.3495695872000
H26	-1.9971097549000	-3.6913481856000	2.3600038906000
H27	-3.1022276491000	-3.0903409261000	1.1288814709000
H28	-1.0461336624000	-4.2920595871000	0.1797599050000
H29	-1.2621331708000	-2.6483898403000	-0.4262096291000
H30	1.0940367963000	-2.9561925718000	0.1363095643000
H31	0.6722144444000	-3.5907051104000	1.7420222941000
H32	1.2985477419000	0.7329773860000	4.7400606787000
H33	1.2484966843000	-1.0246106605000	4.6381491810000
H34	-0.3759526252000	2.1048811565000	3.4413727796000
H35	-1.3809020341000	1.3758842343000	2.1847456703000
H36	2.6297256264000	1.1657582923000	1.2076896939000
H37	3.6645133583000	2.1794122920000	3.1759399972000
H38	2.1121485669000	2.4870232807000	3.9396598382000
H39	0.9495552197000	4.9422116699000	1.2749168209000
H40	0.4297625212000	4.1476265045000	2.7560450181000
H41	2.8850236004000	4.5692752130000	2.8861347662000
H42	3.1244696976000	3.7460921846000	1.3438146912000
H43	-0.5191662382000	3.0003528825000	0.7171300317000
H44	1.1108341405000	2.8000635166000	0.0813961470000
C145	2.9409603675000	-0.0359236002000	-1.0868777775000
O46	-0.6467935433000	1.4711568889000	-1.4715877905000
C47	-0.4434297445000	1.6162426307000	-2.6912930400000
C48	-1.1266168122000	2.7409426740000	-3.3883559223000
C49	-0.9581814980000	2.9588820051000	-4.7710314427000
H50	-0.3212251027000	2.3008669872000	-5.3628930484000
C51	-1.6048185598000	4.0237241421000	-5.3961910716000
H52	-1.4627333962000	4.1837574498000	-6.4640985419000
C53	-2.4278344310000	4.8820832753000	-4.6490341359000
H54	-2.9279297177000	5.7146235891000	-5.1354375284000
C55	-2.6089534663000	4.6678884249000	-3.2742521143000
H56	-3.2519179063000	5.3321922235000	-2.6931885832000
C57	-1.9660906950000	3.6045493374000	-2.6493112716000
H58	-2.0982183653000	3.4231554769000	-1.5857584930000
C59	0.4697656311000	0.6852991475000	-3.4359800774000
H60	1.1812989127000	0.2757722119000	-2.7136727040000
H61	-0.1187776935000	-0.1401909404000	-3.8724645333000
H62	1.0078620589000	1.1851651984000	-4.2438316432000
H63	-0.1925091103000	-1.0472837991000	-1.0688816473000

No. 11

GPE: -1284.39037

SE: -0.01326

Pd1	.0260880224	-.0399352927	-.0352194150
C2	.1097722297	.0585537852	3.5113250268

C3	2.3604752114	-.0245684569	2.5335298208
C4	1.9805077968	-1.3141816860	1.7827442835
N5	.5135880031	-1.4799526417	1.5342662556
C6	-.2811824239	-1.2499320555	2.7905157515
C7	-1.7785731248	-1.4046224938	2.5013988543
C8	-2.0897537868	-2.8228679141	2.0012696113
C9	-1.2081012997	-3.1721697769	.7943403788
C10	.2690271122	-2.8830229240	1.0660715129
C11	1.5997610550	-.0052660278	3.8677958253
C12	-.1643936130	1.3770139822	2.7659804491
N13	.6693065216	1.5602815848	1.5510276704
C14	2.1328948295	1.2987502631	1.7610938932
C15	2.8865498943	2.4682854582	2.4395217434
C16	1.1206957918	4.0657999240	1.6611998616
C17	2.6294311835	3.8094020556	1.7416555044
C18	.4361038107	2.9014321281	.9372570655
H19	-.4943605445	.0858148484	4.4274027701
H20	3.4400987823	-.0958486362	2.7172384601
H21	2.4810405534	-1.3701811795	.8122012418
H22	2.3296715077	-2.1655331169	2.3919395879
H23	.0017117136	-2.0606098426	3.4881927112
H24	-2.3357106547	-1.1907905252	3.4219235899
H25	-2.0836674943	-.6676185713	1.7489235330
H26	-1.9077272493	-3.5388864070	2.8152502050
H27	-3.1485198183	-2.9103829125	1.7343383073
H28	-1.3077190364	-4.2331039638	.5354691046
H29	-1.5249972277	-2.5901564554	-.0766513224
H30	.8655453919	-3.0333958410	.1631541974
H31	.6453439935	-3.5682899750	1.8450983315
H32	1.8897959779	.8488986722	4.4868846209
H33	1.8220560082	-.9101266270	4.4465602219
H34	-.0022964191	2.1949567395	3.4857361916
H35	-1.2085259741	1.4370814195	2.4447120839
H36	2.5470149446	1.1880058668	.7500879271
H37	3.9573333654	2.2287549989	2.4359826561
H38	2.5908797393	2.5572828778	3.4919758591
H39	.7110629200	4.2065150915	2.6708204139
H40	.9083902475	4.9873546858	1.1067049633
H41	3.1418318756	4.6178523729	2.2758878637
H42	3.0467168763	3.7834086563	.7254823265
H43	-.6459358810	3.0420630510	.8708797911
H44	.7949950118	2.8492706027	-.0937394735
H63	-.3076202872	-1.1134508874	-1.0595845482
C164	-.4457439572	1.3620004892	-1.8673467597

No. 12

GPE: -2130.10381

SE: -.01298

Pd1	.0000000000	.0000000000	.0000000000
C2	.0000000000	.0000000000	3.8792974665
C3	2.3848742006	.0000000000	3.3789749941
C4	2.3403744501	-1.4961798809	3.0362223902
N5	1.0250179648	-1.9390119385	2.5442240549
C6	-.1027697304	-1.4767089210	3.4156128156
C7	-1.4458964248	-1.8449889625	2.7736963890
C8	-1.5532002527	-3.3615496819	2.5616849660
C9	-.3341576022	-3.8798130575	1.7866782965
C10	.9710678018	-3.4147513064	2.4401667790
C11	1.3736859249	.2357444312	4.5072016200
C12	-.2582594788	1.1393981833	2.8802946227
N13	.7470521010	1.2598484404	1.7743007638

C14	2.1970086438	1.0390841782	2.2229614254
C15	2.9297202317	2.3240215285	2.7126199979
C16	1.1791639817	3.8012840086	1.7807840583
C17	2.6845724142	3.5969675042	1.9079647063
C18	.5846301312	2.5894248001	1.0677430899
H19	-.7849145211	.1093612294	4.6393858238
H20	3.4013299077	.1773776747	3.7511436120
H21	3.0943003432	-1.7386308460	2.2787514434
H22	2.6227725335	-2.0483584832	3.9530045139
H23	-.0252061848	-2.0538507744	4.3607262882
H24	-2.2567878517	-1.4919005476	3.4226111858
H25	-1.5527706648	-1.3266520841	1.8148011500
H26	-1.6061936451	-3.8647946695	3.5381027871
H27	-2.4764394162	-3.6057764056	2.0255091339
H28	-.3396275304	-4.9751559845	1.7373547039
H29	-.3745616225	-3.5066840645	.7566096890
H30	1.8353326966	-3.7492010851	1.8542359045
H31	1.0745668201	-3.8670659123	3.4452200317
H32	1.4404315105	1.2475103500	4.9212857087
H33	1.5635805487	-.4628041982	5.3309736426
H34	-.2563666484	2.0686089306	3.4698239462
H35	-1.2381371350	1.0584806215	2.4085957970
H36	2.7069370437	.6769267389	1.3279007859
H37	3.9990047576	2.0795574185	2.722289583
H38	2.6523029783	2.5240438930	3.7536742166
H39	.7246680905	3.9437612002	2.7671364757
H40	.9359551559	4.6918647612	1.1913628400
H41	3.1235772799	3.5140003726	.9062909380
H42	3.1722852679	4.4417932470	2.3994925449
H43	-.4821548111	2.7103640768	.8766722544
H44	1.0774295101	2.4919238367	.0921262286
C145	-.6725448118	-1.2055590591	-1.8883984806
O46	1.8872702211	-1.0189773711	.0101823886
C47	2.5269148856	-1.6725986408	-1.1378227873
C48	3.9950297263	-1.2853753532	-1.1392812285
C49	4.9068428018	-1.8384241144	-.2266978483
H50	4.5729025412	-2.5811632696	.4931919215
C51	6.2478953462	-1.4535360353	-.2362469273
H52	6.9411001763	-1.8920118177	.4767364867
C53	6.7002800334	-.5116500426	-1.1652938738
H54	7.7453584682	-.2150179256	-1.1757172791
C55	5.8033505813	.0416472742	-2.0817762655
H56	6.1470656510	.7707696669	-2.8100251726
C57	4.4597557475	-.3426396688	-2.0651977873
H58	3.7630410382	.0889807018	-2.7802322354
C59	2.2658741608	-3.1734127670	-1.1382922496
H60	1.1904336935	-3.3616890893	-1.1692046994
H61	2.7206567665	-3.6206934856	-2.0273160472
H62	2.7006430633	-3.6670756225	-.2623031244
H63	2.0343698325	-1.2354286962	-2.0079308858
C164	-2.1343409016	.9816055047	.0464579814
H65	1.6186341193	-1.6191830952	.7475522378

No. 13

GPE: -2130.10314

SE: -0.01711

Pd1	0.2280000000000	-0.3360000000000	-0.0070000000000
C2	-0.0440000000000	0.1430000000000	3.9520000000000
C3	2.2800000000000	-0.2900000000000	3.3160000000000
C4	1.9160000000000	-1.7100000000000	2.8490000000000

N5	0.440000000000	-1.915000000000	2.581000000000
C6	-0.481000000000	-1.302000000000	3.624000000000
C7	-1.941000000000	-1.478000000000	3.198000000000
C8	-2.282000000000	-2.955000000000	2.947000000000
C9	-1.329000000000	-3.554000000000	1.906000000000
C10	0.131000000000	-3.371000000000	2.317000000000
C11	1.386000000000	0.098000000000	4.501000000000
C12	-0.139000000000	1.213000000000	2.835000000000
N13	0.867000000000	1.096000000000	1.727000000000
C14	2.267000000000	0.810000000000	2.220000000000
C15	3.030000000000	2.056000000000	2.732000000000
C16	1.521000000000	3.570000000000	1.453000000000
C17	2.983000000000	3.238000000000	1.760000000000
C18	0.832000000000	2.336000000000	0.864000000000
H19	-0.739000000000	0.475000000000	4.734000000000
H20	3.325000000000	-0.367000000000	3.641000000000
H21	2.409000000000	-1.945000000000	1.903000000000
H22	2.186000000000	-2.433000000000	3.626000000000
H23	-0.302000000000	-1.900000000000	4.530000000000
H24	-2.566000000000	-1.065000000000	3.997000000000
H25	-2.140000000000	-0.894000000000	2.293000000000
H26	-2.213000000000	-3.521000000000	3.887000000000
H27	-3.316000000000	-3.039000000000	2.599000000000
H28	-1.508000000000	-4.627000000000	1.776000000000
H29	-1.483000000000	-3.083000000000	0.928000000000
H30	0.813000000000	-3.686000000000	1.524000000000
H31	0.372000000000	-3.914000000000	3.238000000000
H32	1.673000000000	1.067000000000	4.917000000000
H33	1.472000000000	-0.635000000000	5.313000000000
H34	-0.008000000000	2.182000000000	3.336000000000
H35	-1.122000000000	1.212000000000	2.362000000000
H36	2.785000000000	0.416000000000	1.341000000000
H37	4.067000000000	1.746000000000	2.906000000000
H38	2.638000000000	2.392000000000	3.700000000000
H39	1.441000000000	4.379000000000	0.718000000000
H40	1.012000000000	3.921000000000	2.361000000000
H41	3.505000000000	2.975000000000	0.830000000000
H42	3.505000000000	4.100000000000	2.190000000000
H43	-0.217000000000	2.516000000000	0.622000000000
H44	1.344000000000	2.077000000000	-0.068000000000
C145	-0.404000000000	-1.949000000000	-1.586000000000
O46	2.146000000000	-0.971000000000	-0.037000000000
C47	2.819000000000	-1.110000000000	-1.277000000000
C48	3.968000000000	-0.107000000000	-1.320000000000
C49	5.046000000000	-0.209000000000	-0.430000000000
H50	5.081000000000	-1.040000000000	0.268000000000
C51	6.069000000000	0.740000000000	-0.430000000000
H52	6.898000000000	0.640000000000	0.263000000000
C53	6.034000000000	1.813000000000	-1.326000000000
H54	6.831000000000	2.550000000000	-1.329000000000
C55	4.969000000000	1.925000000000	-2.218000000000
H56	4.934000000000	2.753000000000	-2.921000000000
C57	3.946000000000	0.971000000000	-2.212000000000
H58	3.120000000000	1.063000000000	-2.910000000000
C59	3.278000000000	-2.559000000000	-1.462000000000
H60	2.400000000000	-3.206000000000	-1.481000000000
H61	3.830000000000	-2.684000000000	-2.400000000000
H62	3.928000000000	-2.871000000000	-0.639000000000
H63	2.140000000000	-0.872000000000	-2.105000000000
C164	-2.018000000000	0.496000000000	0.103000000000
H65	0.239000000000	-1.420000000000	1.669000000000

No. 14
GPE: -1669.25418
SE: -0.00870
freqs: -438.97

Pd1	0.0000000000	0.0000000000	0.0000000000
C2	0.0000000000	0.0000000000	3.8541339576
C3	2.3107752386	0.0000000000	3.0301384624
C4	1.9813809180	-1.2103731282	2.1372497672
N5	0.5370788923	-1.3605746042	1.7687165982
C6	-0.3214977364	-1.2488314751	2.9989818655
C7	-1.8038169463	-1.4405131641	2.6577193912
C8	-2.0417590824	-2.8060522005	1.9921397905
C9	-1.0998824789	-3.0019335215	0.7959037354
C10	0.3541862831	-2.7250830201	1.1797389171
C11	1.4626039940	-0.0827513921	4.3067100452
C12	-0.2304531668	1.3813706574	3.2120043949
N13	0.7071416427	1.6758406196	2.1210148866
C14	2.1374281456	1.3786067929	2.3536471304
C15	2.8863735649	2.4930893426	3.1286392876
C16	1.1667251903	4.1530714822	2.3308604309
C17	2.6671177385	3.8733312149	2.4907962037
C18	0.5084009665	3.0110574698	1.5388191779
H19	-0.6652988549	-0.0585080781	4.7258889408
H20	3.3756318608	-0.1006427131	3.2786129274
H21	2.5514186900	-1.1833576803	1.2074502446
H22	2.2799512375	-2.1158188194	2.6931968053
H23	-0.0335191300	-2.1064417645	3.6380213914
H24	-2.3795835496	-1.3709445259	3.5894454735
H25	-2.1472398635	-0.6393030872	1.9988869405
H26	-1.8660834931	-3.6045397573	2.7269427315
H27	-3.0866385069	-2.8972795285	1.6744642971
H28	-1.1663039121	-4.0276232774	0.4136189732
H29	-1.3908229163	-2.3375085943	-0.0269107183
H30	1.0112707553	-2.7951638731	0.3102464596
H31	0.6874023269	-3.4691674711	1.9241734107
H32	1.6996771990	0.7271553089	5.0045718360
H33	1.6558401495	-1.0254595302	4.8338982210
H34	-0.1779750790	2.1216808026	4.0328776404
H35	-1.2394232893	1.4478897105	2.7903296614
H36	2.5920074135	1.3231292076	1.3534357781
H37	3.9566505287	2.2500344380	3.1501453454
H38	2.5519016042	2.5270124241	4.1736402471
H39	0.9998884851	5.1035966548	1.8089174375
H40	0.6984485609	4.2507678885	3.3195565371
H41	3.1500420399	4.6523389892	3.0922307116
H42	3.1452757257	3.8983370311	1.5011429174
H43	-0.5694675307	3.1709853830	1.4358492135
H44	-0.4512567915	0.8344947296	-1.2998693651
C145	1.9540434014	-0.5902822882	-1.2152372113
C46	-1.8833633352	1.0942727621	-0.9732151719
C47	-1.8499178292	2.5687597925	-1.3953109611
C48	-2.5854082207	0.1538227994	-1.9351768678
C49	-3.5757640459	-0.7037754523	-1.4389740510
H50	-3.7929717459	-0.6901196614	-0.3761572832
C51	-4.2741751643	-1.5462340024	-2.3042411882
H52	-5.0488382441	-2.1992322361	-1.9117971052
C53	-3.9812418455	-1.5500913451	-3.6690103150
H54	-4.5220805990	-2.2098009431	-4.3413550960
C55	-2.9890431076	-0.7025354722	-4.1676776527
H56	-2.7496711822	-0.7073157751	-5.2270726343
C57	-2.2989484422	0.1489593095	-3.3072677687

H58	-1.5161685922	0.7898900856	-3.7038534937
O59	-1.9677528082	0.8420955885	0.3000896283
H60	-2.8750089288	2.9506747818	-1.3206801036
H61	-1.2074182551	3.1391270112	-0.7256405713
H62	-1.5140410645	2.7010405050	-2.4256226995
H63	0.9382723553	2.9987113918	0.5270168002

No. 15

GPE: -2130.08720

SE: -0.01954

freqs: -415.67

Pd1	2.2303120977	-0.6312011747	1.4488054185
C2	-0.5292385901	3.8575376953	-1.4907607866
C3	0.1486869186	1.5062196771	-1.8693167281
C4	1.6118023500	1.8682108184	-1.5868564131
N5	1.7195658640	3.0446567688	-0.6426490331
C6	0.9246216359	4.2504076812	-1.1331910821
C7	1.0520889371	5.3870055825	-0.1125736078
C8	2.5182430003	5.7744978798	0.1274462156
C9	3.3197412740	4.5487092766	0.5826644784
C10	3.1717061226	3.3810847861	-0.3886527674
C11	-0.5301915503	2.7201594445	-2.5253186624
C12	-1.3675122253	3.4024279989	-0.2820295288
N13	-0.7553098523	2.2203426326	0.3328263876
C14	-0.5966563016	1.0622302302	-0.5864723932
C15	-1.9223581522	0.3238871823	-0.8631107302
C16	-2.7346181495	1.0947415563	1.4118534496
C17	-2.5762446414	-0.1051347335	0.4628744247
C18	-1.3859122139	1.8066651673	1.6055526849
H19	-0.9893426859	4.7583008732	-1.9173062042
H20	0.1712986453	0.6564150620	-2.5616105236
H21	2.1760868148	1.0488281195	-1.1348973398
H22	2.1180473311	2.1671270833	-2.5124504307
H23	1.4300968077	4.5503669655	-2.0623342155
H24	0.4757630593	6.2414595259	-0.4859477563
H25	0.5950990515	5.0803173972	0.8354776011
H26	2.9457470304	6.1831096930	-0.7993551352
H27	2.5780591558	6.5671425295	0.8804796286
H28	4.3868298982	4.7831700463	0.6642442322
H29	2.9890427028	4.2158107789	1.5725952008
H30	3.6274618145	2.4726938345	0.0084097058
H31	3.6035617612	3.6140656401	-1.3693588674
H32	-1.5586314069	2.4872953165	-2.8194964292
H33	0.0074774784	3.0130862742	-3.4368912431
H34	-2.4040487964	3.2452385041	-0.6306043362
H35	-1.4156436222	4.1861101365	0.4819063635
H36	0.0538343220	0.3566435853	-0.0503940443
H37	-1.7158223269	-0.5525863816	-1.4904852805
H38	-2.6132798837	0.9629933061	-1.4302016981
H39	-3.1046469762	0.7605185647	2.3880239379
H40	-3.4841100240	1.7929387154	1.0115472704
H41	-3.5470552606	-0.5772529813	0.2703971408
H42	-1.9393846490	-0.8557797453	0.9482316000
H43	-1.4933330750	2.6997488095	2.2316007418
H44	2.3354538695	-2.0826836754	0.8529685302
C145	2.1901458432	1.6298628257	2.3817191213
O46	3.6918238072	-0.3140750178	-0.1000030928
C47	3.4399856356	-1.5458282259	-0.3737856085
C48	2.5757703070	-1.8416565216	-1.5873314502
C49	3.0233637948	-1.3383767050	-2.8204426801
H50	3.9340481547	-0.7472073676	-2.8570097526

C51	2.3060071344	-1.5933172303	-3.9913086275
H52	2.6639035014	-1.2005786418	-4.9395691363
C53	1.1320627203	-2.3492298829	-3.9422470843
H54	0.5700240735	-2.5433439838	-4.8514129674
C55	0.6850639938	-2.8543061155	-2.7175849172
H56	-0.2289041724	-3.4387878038	-2.6695809164
C57	1.4051992566	-2.6080346485	-1.5459265847
H58	1.0418105981	-2.9824447706	-0.5925364822
C59	4.4809352404	-2.5979151011	-0.0133560422
H60	4.9416231697	-2.3590228747	0.9462546141
H61	4.0530574293	-3.6024170810	0.0149373222
H62	5.2509861582	-2.5782375821	-0.7957628700
H63	-0.6812898724	1.1411291756	2.1139290226
C164	0.5236762602	-1.5472754801	2.7843071946
H65	1.2727996425	2.7254382209	0.2497287554

No. 16

GPE: -1280.57956

SE: -.01492

Pd1	-.0581790005	-.0106141541	-.0576621529
C2	.0524199275	-.0306049386	3.4058059930
C3	2.2874503959	.0283738587	2.3781590942
C4	1.9786082080	-1.2707295783	1.6161772699
N5	.5144466033	-1.4953044478	1.3945040488
C6	-.2767234280	-1.3422042021	2.6683214471
C7	-1.7702470330	-1.5705151373	2.4042277221
C8	-2.0109447517	-2.9950263514	1.8878026594
C9	-1.1477792313	-3.2539442679	.6472600211
C10	.3209202831	-2.8975672593	.8856354934
C11	1.5522335503	-.0068277239	3.7276756472
C12	-.3321778393	1.2631865164	2.6728110164
N13	.4578055131	1.4918117194	1.4247065741
C14	1.9554331242	1.3341470081	1.6157427284
C15	2.6239678314	2.5490549450	2.3013239716
C16	.7429231865	4.0277584753	1.5897113360
C17	2.2659078366	3.8827882270	1.6389687667
C18	.1290321655	2.8409269536	.8428757090
H19	-.5325883158	-.0484460490	4.3341033934
H20	3.3727694812	.0334975600	2.5383683097
H21	2.4489734092	-1.2906198050	.6292430575
H22	2.3733232751	-2.1115210643	2.2092013575
H23	.0686711120	-2.1521095392	3.3356432524
H24	-2.3152338071	-1.4004995731	3.3411523447
H25	-2.1378222940	-.8405675222	1.6725869540
H26	-1.7600550193	-3.7141735521	2.6810916068
H27	-3.0702527613	-3.1399917658	1.6502286572
H28	-1.1922935889	-4.3109767780	.3576451649
H29	-1.5163262923	-2.6710930961	-.2000772724
H30	.9074784561	-2.9906731866	-.0277125503
H31	.7536569354	-3.5715098669	1.6431071921
H32	1.8045891075	.8546220895	4.3533375148
H33	1.8386702363	-.9034285245	4.2899883527
H34	-.1788383185	2.1000251393	3.3675777622
H35	-1.3838680344	1.2655059946	2.3767157779
H36	2.3574778971	1.2621090475	.5980241346
H37	3.7072614914	2.3802856654	2.2752233294
H38	2.3429465301	2.5957475232	3.3598909842
H39	.4495444354	4.9402884484	1.0579194905
H40	.3391324074	4.1184858814	2.6067001391
H41	2.6679226239	3.9113817536	.6169786515

H42	2.7275434604	4.7117759684	2.1872459902
H43	-.9596407996	2.8993973404	.7952694896
H44	.4949394154	2.8328146225	-.1850518550
O45	-.6559232221	1.3424653832	-1.4901958182
C46	-1.9139370866	1.6779555590	-1.4262432430
C47	-2.4245437024	2.3765124776	-2.6786442399
O48	-2.6605799912	1.4656677893	-.4605361295
H49	-2.7964645623	1.6115211031	-3.3693582175
H50	-1.6263695264	2.9239849787	-3.1845596331
H51	-3.2523628315	3.0424806242	-2.4274553366
O52	-.3241909967	-1.3412821055	-1.6077893072
C53	.7739955279	-1.6463891688	-2.2403033074
C54	.5374433220	-2.2937635117	-3.5968134520
O55	1.9214604258	-1.4435871418	-1.8170408100
H56	.4317100102	-1.4968128824	-4.3412914696
H57	-.3843105264	-2.8796088404	-3.6034838760
H58	1.3926076205	-2.9132388683	-3.8732089993

No. 17

GPE: -1437.56842

SE: -.01024

Pd1	-.0388412342	-.1512023069	.0353638928
C2	.3483347762	-.2432614752	3.5290518570
C3	2.4498471512	.1242649177	2.3064675830
C4	2.2404417015	-1.1962717092	1.5462334240
N5	.8027404437	-1.5989842879	1.4458383575
C6	.1132845550	-1.5698629114	2.7795601937
C7	-1.3633415357	-1.9565535067	2.6215594356
C8	-1.4950192001	-3.3762682976	2.0532675722
C9	-.7025865143	-3.4950227774	.7453090395
C10	.7348440653	-2.9967997810	.9072387207
C11	1.8558346021	-.0309847548	3.7154144305
C12	-.2550521603	1.0107021058	2.8808458811
N13	.3692582901	1.3787684907	1.5750240371
C14	1.8891646697	1.3940874948	1.6143789744
C15	2.4849488848	2.6692796789	2.2566250092
C16	.3785752965	3.9249937103	1.8098863022
C17	1.9020971788	3.9574372149	1.6687684232
C18	-.1884393072	2.6917592568	1.1023720638
H19	-.1410689515	-.3546009953	4.5055436953
H20	3.5361025617	.2668582679	2.3677930356
H21	2.6212825252	-1.1456362869	.5223558277
H22	2.7896079159	-1.9852189453	2.0870227370
H23	.5955382852	-2.3504262089	3.3968404403
H24	-1.8501320172	-1.8839044486	3.6023287313
H25	-1.8632955797	-1.2453152330	1.9522789178
H26	-1.1120559111	-4.0965919162	2.7904962890
H27	-2.5495377466	-3.6233592320	1.8862910469
H28	-.6659640978	-4.5379841851	.4076487085
H29	-1.1847291139	-2.9166261843	-.0478202592
H30	1.2662694296	-3.0010758573	-.0437270489
H31	1.2828795748	-3.6473264849	1.6098202682
H32	2.0502923268	.8450584503	4.3421681070
H33	2.3071690209	-.8929381046	4.2211807007
H34	-.1425819853	1.8402261445	3.5935044705
H35	-1.3245634633	.8877736311	2.6922959086
H36	2.1917470532	1.3839839164	.5609351514
H37	3.5709119368	2.6302365179	2.1075139222
H38	2.3194651630	2.6704717032	3.3407649508
H39	-.0795074739	4.8093390025	1.3509301339
H40	.1015125744	3.9474297249	2.8729369053

H41	2.1679164376	4.0356236420	.6056894944
H42	2.3306956390	4.8315362492	2.1723782729
H43	-1.2731773661	2.6236513834	1.2122072299
H44	-.0022005761	2.7468128938	.0291184441
C45	-1.8976625394	1.9193313826	-3.1721505317
C46	-1.8512536686	.9334815628	-1.9908795845
C47	-3.1426994130	.9677243477	-1.1707580936
C48	-3.9393372940	-.1767681856	-1.0400560927
H49	-3.6361308937	-1.0904425952	-1.5472423988
C50	-5.1077517851	-.1588380098	-.2700656689
H51	-5.7127933384	-1.0581842668	-.1834749760
C52	-5.4979132973	1.0122927135	.3828333478
H53	-6.4059828054	1.0310584104	.9797736752
C54	-4.7124472591	2.1641952231	.2584132978
H55	-5.0138847269	3.0831859093	.7556238108
C56	-3.5480532088	2.1386303746	-.5100066400
H57	-2.9443608935	3.0369903761	-.6078646087
O58	-.7253955078	1.2564771373	-1.2116191809
H59	-1.9728378870	2.9525640102	-2.8166455645
H60	-.9786300317	1.8275699713	-3.7585942209
H61	-2.7565899473	1.7147007456	-3.8213723940
H62	-1.7507844642	-.0790055761	-2.4083572491
O63	-.1560816881	-1.4650935265	-1.5645346049
C64	.9618569156	-1.6599291361	-2.2031997851
C65	.7952560906	-2.3090994340	-3.5716451724
O66	2.0907049736	-1.3710494808	-1.7796583639
H67	1.0866738028	-1.5814685893	-4.3363212546
H68	-.2339169468	-2.6249225956	-3.7505336551
H69	1.4730333085	-3.1630063802	-3.6601365658

No. 18

GPE: -1437.52449

SE: -0.01285

freqs: -549.83

Pd1	0.0000000000	0.0000000000	0.0000000000
C2	0.0000000000	0.0000000000	3.4703496102
C3	2.2783882377	0.0000000000	2.5470168804
C4	1.9676391692	-1.2907774373	1.7695040530
N5	0.5091978701	-1.4813996371	1.4792491430
C6	-0.3230853376	-1.3120368208	2.7186736002
C7	-1.8094230100	-1.5263590393	2.4074922229
C8	-2.0516024263	-2.9313080277	1.8362111076
C9	-1.1433465056	-3.1873354514	0.6257123268
C10	0.3202903064	-2.8668564515	0.9262392984
C11	1.4835271595	-0.0101160289	3.8611456493
C12	-0.2989917319	1.3128399422	2.7222143628
N13	0.5460769724	1.5008378474	1.5107736358
C14	2.0266364659	1.3086991347	1.7591787379
C15	2.6848435998	2.5236248882	2.4511546588
C16	0.8846990022	4.0270353914	1.5699443696
C17	2.3971729482	3.8385605819	1.7170104259
C18	0.2778439873	2.8183164668	0.8493903001
H19	-0.6296398034	0.0012308200	4.3699962683
H20	3.3550495215	-0.0296453330	2.7566618494
H21	2.4816034786	-1.3105619551	0.8085309304
H22	2.3083655177	-2.1444260570	2.3774895333
H23	-0.0175349476	-2.1230277282	3.4041716971
H24	-2.3826089498	-1.3834230683	3.3325624954
H25	-2.1495185313	-0.7692935719	1.6897505539
H26	-1.8435312168	-3.6756617956	2.6175148137

H27	-3.1043301212	-3.0521048820	1.5583732873
H28	-1.2033111727	-4.2375227586	0.3159151659
H29	-1.4828073773	-2.5873105177	-0.2257274268
H30	0.9431807069	-2.9224028998	0.0288817691
H31	0.7036620174	-3.5744353632	1.6801363860
H32	1.7244151769	0.8515767494	4.4917862171
H33	1.7220604078	-0.9073591136	4.4449883539
H34	-0.1445677378	2.1390326225	3.4313399571
H35	-1.3430160116	1.3596997802	2.3971180504
H36	2.4658699612	1.1944286069	0.7622734334
H37	3.7647666660	2.3357959790	2.4872679857
H38	2.3511040402	2.6172056404	3.4923126252
H39	0.4244107731	4.1738328823	2.5561582820
H40	0.6532185701	4.9229875536	0.9822244999
H41	2.8580233070	3.8109730849	0.7208138038
H42	2.8470885927	4.6804141103	2.2553708638
H43	-0.8067197657	2.9113716369	0.7416457088
H44	-0.3422397713	-0.9955180847	-1.2202781478
O45	2.6803026679	0.0593657163	-1.1072720669
O46	-0.7286191092	1.1932539466	-1.5470534388
C47	-0.8717606012	0.1157907794	-2.2563906323
C48	-2.2744468905	-0.4156664405	-2.4521804939
C49	-3.3596779236	0.3406516157	-1.9870829863
H50	-3.1566314934	1.2776918257	-1.4792481115
C51	-4.6654725888	-0.1004995165	-2.1914606146
H52	-5.4993697545	0.4997759163	-1.8377216242
C53	-4.9043460088	-1.3063538646	-2.8560166757
H54	-5.9227727713	-1.6498715082	-3.0150095380
C55	-3.8284677240	-2.0659445495	-3.3197023446
H56	-4.0065921770	-3.0043685655	-3.8372021683
C57	-2.5204280928	-1.6222667976	-3.1232692251
H58	-1.6912868524	-2.2226250300	-3.4849576026
C59	0.1471211707	-0.1355188115	-3.3555347701
H60	1.1044940657	0.2805414497	-3.0444693467
H61	0.2779718233	-1.1938875725	-3.5834819178
H62	-0.2119183385	0.3791851970	-4.2561533409
H63	0.6941186961	2.7530066475	-0.1593226869
C64	2.8730464864	-1.0587480245	-1.6823020296
O65	2.1334952429	-2.0778465613	-1.5722601004
C66	4.0849106690	-1.1595642829	-2.6190933622
H67	4.8915202579	-0.4984565852	-2.2912677165
H68	4.4396944509	-2.1907515329	-2.6922741218
H69	3.7832340507	-0.8386507197	-3.6242336828

No. 19

GPE: -1437.54533

SE: -0.01273

Pd1	0.0000000000	0.0000000000	0.0000000000
C2	0.0000000000	0.0000000000	3.4711709345
C3	2.2917876155	0.0000000000	2.5846601857
C4	1.9796703298	-1.2523838783	1.7480261992
N5	0.5094265844	-1.4617115009	1.4652037959
C6	-0.3214764811	-1.3054600284	2.7098774347
C7	-1.8035969021	-1.5384642879	2.3957083543
C8	-2.0227803717	-2.9643969406	1.8659374130
C9	-1.1091815106	-3.2435409396	0.6629582000
C10	0.3456036795	-2.8613975815	0.9414223079
C11	1.4772432403	-0.0399208773	3.8868864582
C12	-0.2753305556	1.3280478505	2.7375975838
N13	0.6106115504	1.5492559983	1.5631942973
C14	2.0775173254	1.3392024416	1.8466798438

C15	2.7245528529	2.5169607083	2.6107626585
C16	0.9638112226	4.0666776755	1.7259837110
C17	2.4710032912	3.8629264420	1.9197083481
C18	0.3826803018	2.8860689649	0.9390557222
H19	-0.6447896555	-0.0047317626	4.3602199882
H20	3.3644425087	-0.0620279870	2.8072792653
H21	2.5010126143	-1.2173823391	0.7808246371
H22	2.3288561036	-2.1297118344	2.3153306416
H23	-0.0042119472	-2.1186887578	3.3876760062
H24	-2.3859407270	-1.3759349080	3.3115123043
H25	-2.1404863966	-0.8056406690	1.6522453670
H26	-1.8063266951	-3.6807474230	2.6710117831
H27	-3.0721561707	-3.1124303869	1.5864221324
H28	-1.1350995075	-4.3073092663	0.3969606612
H29	-1.4649888006	-2.6824429185	-0.2068629262
H30	0.9599473659	-2.9378374851	0.0419518894
H31	0.7641330306	-3.5413910166	1.7008354875
H32	1.7187918129	0.8004522697	4.5453796976
H33	1.6929233667	-0.9578981035	4.4477091328
H34	-0.1583829549	2.1355583255	3.4762855363
H35	-1.3078038542	1.3719321752	2.3744735255
H36	2.5410532852	1.2828933546	0.8541892779
H37	3.8011920451	2.3184449629	2.6761382432
H38	2.3542099357	2.5728086157	3.6427639436
H39	0.4668609933	4.1776108869	2.6996866851
H40	0.7602023605	4.9868383952	1.1646213516
H41	2.9642954602	3.8673246071	0.9391762311
H42	2.9048575705	4.6808562209	2.5073426408
H43	-0.6958118947	2.9944625856	0.7839936614
H44	-0.4572895800	-1.0939040968	-0.9700136961
O45	2.9113184318	1.2763239466	-1.3095786068
O46	-0.4900573275	1.4281331803	-1.4995684861
C47	-0.1020172513	1.4591027065	-2.6855409264
C48	-0.3452174660	2.7101920444	-3.4546005308
C49	-0.9400027900	3.8074328474	-2.8030503936
H50	-1.2346360375	3.7005187242	-1.7659526773
C51	-1.1294862411	5.0116034124	-3.4752553959
H52	-1.5799505569	5.8550873208	-2.9609783044
C53	-0.7332820969	5.1389624710	-4.8119098837
H54	-0.8734402711	6.0802790811	-5.3316476628
C55	-0.1466114866	4.0554586757	-5.4706427651
H56	0.1663057391	4.1511133228	-6.5054454452
C57	0.0472914571	2.8484410591	-4.7987150141
H58	0.5180598288	2.0234400279	-5.3209187325
C59	0.6482930315	0.3184884250	-3.2854443671
H60	0.3560369891	-0.6079584236	-2.7837847445
H61	0.5387460710	0.2291723455	-4.3660383438
H62	1.7002088768	0.4915424258	-3.0173879410
H63	0.8587943753	2.8507976981	-0.0441001659
C64	3.7100745548	0.2864472380	-1.3634448654
O65	3.4500249977	-0.8916446394	-0.9932935304
C66	5.1005906757	0.5485250754	-1.9670447471
H67	5.4309785138	1.5678831666	-1.7596493793
H68	5.8320448316	-0.1722606483	-1.5968744258
H69	5.0444627273	0.4375563086	-3.0579814479

No. 20

GPE: -1437.53028

SE: -0.00698

fregs: -503.09 -16.50

Pd1	0.0030268331	0.0471022443	0.0074813868
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C2	-0.0095635392	-0.0348793401	3.8648495541
C3	2.3025568450	-0.0025612437	3.0479454799
C4	2.0775973483	-1.3820352810	2.4045424906
N5	0.6675849383	-1.7018847689	2.1394881777
C6	-0.2297504603	-1.4493806447	3.2814350944
C7	-1.6874464684	-1.7343407645	2.8882704613
C8	-1.8540903031	-3.1716320837	2.3766369490
C9	-0.8653422408	-3.4418069741	1.2359581009
C10	0.5599686497	-3.0868373598	1.6618354096
C11	1.4477880058	0.0798868719	4.3212611475
C12	-0.3442818369	1.1657482253	2.9535538579
N13	0.5791450884	1.3697035287	1.7960759008
C14	2.0406370871	1.2204218079	2.1307802038
C15	2.6781713222	2.4876246522	2.7600140266
C16	0.8480096524	3.9203343916	1.8482116016
C17	2.3640456456	3.7801523119	2.0005079724
C18	0.2941850986	2.6854616532	1.1301569831
H19	-0.6818279917	0.0507141157	4.7292171228
H20	3.3681504804	0.0420544355	3.3091768143
H21	2.6096436220	-1.4484039098	1.4504750865
H22	2.5230208706	-2.1339706951	3.0884011980
H23	0.0252616355	-2.1496807749	4.1088256287
H24	-2.3265031930	-1.5642570128	3.7647035651
H25	-2.0001368494	-1.0323671193	2.1084244503
H26	-1.6674055613	-3.8788826478	3.1977183759
H27	-2.8838091699	-3.3415024609	2.0424951125
H28	-0.8997003797	-4.4954195962	0.9327318596
H29	-1.1415190867	-2.8402193842	0.3619941919
H30	1.2539455977	-3.2009770170	0.8226108063
H31	0.8919196172	-3.7918394970	2.4526091540
H32	1.6168330116	1.0094428595	4.8744894661
H33	1.7047302069	-0.7430524162	4.9993656065
H34	-0.3364978390	2.0601924131	3.5954068065
H35	-1.3481280830	1.0779017643	2.5320946646
H36	2.5358693201	1.0467769905	1.1674655981
H37	3.7619970837	2.3216992916	2.8027440783
H38	2.3444262606	2.6076565205	3.7972207261
H39	0.5873085412	4.8057336663	1.2565832811
H40	0.3800053357	4.0529018120	2.8322206689
H41	2.7933588263	4.6403089072	2.5268312025
H42	2.8279302744	3.7543668871	1.0044496677
H43	-0.7876343488	2.7384462032	0.9903747888
H44	-0.3934155302	-0.6498395669	-1.3690193215
O45	-1.9741016694	0.6492958634	0.2426254782
C46	1.0917357266	-0.8476464579	-1.8551958690
C47	0.8644811309	-2.3009793271	-2.2725875419
C48	1.1526384343	0.1632111912	-2.9794342552
C49	2.2399194966	1.0449242698	-3.0316975845
H50	2.9855239858	0.9995254793	-2.2447308701
C51	2.3622391244	1.9496149106	-4.0858199170
H52	3.2161536465	2.6204103683	-4.1246536033
C53	1.3933524674	1.9905984052	-5.0907600579
H54	1.4874129232	2.6969315419	-5.9107746132
C55	0.3014843370	1.1211846506	-5.0361702215
H56	-0.4625752659	1.1570183170	-5.8073253052
C57	0.1813490198	0.2076855248	-3.9896982251
H58	-0.6891683930	-0.4388542618	-3.9364243852
O59	1.8261952070	-0.6343471243	-0.7993062342
H60	1.7580896129	-2.6338481318	-2.8152073677
H61	0.7286064380	-2.9296068879	-1.3924061113
H62	0.0030705519	-2.4119701879	-2.9337906704
H63	0.7452186018	2.6417712251	0.1322817734

C64	-2.7910752772	0.3508404740	-0.7286645778
O65	-2.5042747520	-0.3167016952	-1.7325346057
C66	-4.1907613840	0.9316797444	-0.5629374855
H67	-4.9060131251	0.3647187002	-1.1602430322
H68	-4.1841011419	1.9670860287	-0.9224242439
H69	-4.4940305876	0.9472122186	0.4866490477

No. 21

GPE: -1208.85688

SE: -0.03653

freqs: -381.03

Pd1	.0056801017	-.0003447376	-.0038464877
C2	-.0051411036	-.0006722668	3.4418177207
C3	2.2784289508	-.0006866181	2.5231612203
C4	1.9618501724	-1.2931157173	1.7510007129
N5	.5013066281	-1.4822484874	1.4524269292
C6	-.3384203899	-1.3137284461	2.6993015378
C7	-1.8231280215	-1.5184922111	2.3734828000
C8	-2.0744737637	-2.9185443628	1.7943147423
C9	-1.1661786041	-3.1723362804	.5836132108
C10	.2973551574	-2.8709297533	.9067962708
C11	1.4783881331	-.0138922390	3.8351790315
C12	-.3076054891	1.3051393232	2.6858103528
N13	.5430147405	1.4921594401	1.4680421239
C14	2.0240075306	1.3094763903	1.7390206045
C15	2.6648784169	2.5298939800	2.4358129579
C16	.8633219884	4.0234064852	1.5316847424
C17	2.3758087200	3.8419701070	1.6961212724
C18	.2655768492	2.8168479294	.8042761714
H19	-.6331465109	.0074503076	4.3408226879
H20	3.3538839039	-.0319397137	2.7347830355
H21	2.4963822227	-1.3314915279	.7969481203
H22	2.3020124701	-2.1457043493	2.3571986527
H23	-.0338519964	-2.1277974127	3.3784952381
H24	-2.4001522604	-1.3750488240	3.2942177054
H25	-2.1598440120	-.7544581904	1.6604681629
H26	-1.8751312589	-3.6708716046	2.5688966833
H27	-3.1253489756	-3.0294535687	1.5095855945
H28	-1.2341013646	-4.2165436892	.2587409174
H29	-1.4926776916	-2.5561474124	-.2628585383
H30	.9308691095	-2.9695620663	.0210616444
H31	.6651605051	-3.5796623200	1.6639491232
H32	1.7231320959	.8446156453	4.4663797133
H33	1.7168451840	-.9118841594	4.4160215475
H34	-.1503560922	2.1406027967	3.3795318027
H35	-1.3489881235	1.3495819386	2.3561725868
H36	2.4814078617	1.2235454485	.7449464398
H37	3.7441923696	2.3470463291	2.4925146838
H38	2.3095178409	2.6153457434	3.4688042622
H39	.3891097547	4.1714385834	2.5099873285
H40	.6357633274	4.9158733380	.9383744115
H41	2.8518316468	3.8234643440	.7062132963
H42	2.8131688939	4.6839325161	2.2418383745
H43	-.8191233991	2.8967694033	.6964343152
H44	-.3867179169	-.9312345998	-1.3485298482
O46	-.4631243012	1.1810300602	-1.6032782833
C47	-.6425837472	.0857273282	-2.3226491476
C48	-2.0590027146	-.2721881323	-2.7073068001
C49	-3.0985663411	.6095510399	-2.3768296475
H50	-2.8609971253	1.5250239290	-1.8458977373

C51	-4.4094228573	.3189117859	-2.7542569241
H52	-5.2072885199	1.0139729277	-2.5105445167
C53	-4.6960455704	-.8589878824	-3.4510066739
H54	-5.7173440767	-1.0841068928	-3.7433729406
C55	-3.6651897721	-1.7454338111	-3.7755150425
H56	-3.8829485640	-2.6613867315	-4.3165424932
C57	-2.3514374929	-1.4533108806	-3.4092136056
H58	-1.5615284750	-2.1522241885	-3.6683416578
C59	.4560126752	-.2339095424	-3.3355020918
H60	1.4326983470	.0038634002	-2.9109779126
H61	.4444481458	-1.2752722074	-3.6619602612
H62	.2881107777	.3979996237	-4.2145421350
H63	.6814947841	2.7559843298	-.2043768167

No. (Table 1, Entry 1-R1)

SPE: -1669.26540

freqs: -617.47 -16.61

Pd1	.0011709063	-.0053307189	.0002844449
C2	-.0001272803	-.0000548384	3.4424060461
C3	2.2933970222	.0100733284	2.5569283987
C4	1.9980547962	-1.2810814733	1.7775490413
N5	.5418639687	-1.4837075249	1.4698294912
C6	-.3065222028	-1.3218832356	2.7020762986
C7	-1.7848360649	-1.5555853278	2.3717774424
C8	-2.0012872752	-2.9687752479	1.8113763059
C9	-1.0823934813	-3.2192782247	.6082128329
C10	.3732380136	-2.8679466101	.9156148851
C11	1.4767972385	.0006626495	3.8581432477
C12	-.2927480947	1.3049147057	2.6796630383
N13	.5771463322	1.4965622632	1.4801206470
C14	2.0521561517	1.3138662465	1.7603832966
C15	2.6841637050	2.5359370832	2.4629358866
C16	.8853391872	4.0246230768	1.5480293331
C17	2.3965697457	3.8505703298	1.7276081153
C18	.3063718509	2.8124186528	.8138112516
H19	-.6445060380	.0087023936	4.3307550440
H20	3.3662395288	-.0176386951	2.7821741923
H21	2.5261670656	-1.3022001782	.8192762770
H22	2.3315902197	-2.1309762997	2.3932203103
H23	.0031472285	-2.1246234351	3.3944311716
H24	-2.3738730887	-1.4105410264	3.2853678334
H25	-2.1239700467	-.8102432079	1.6412208234
H26	-1.7877878528	-3.7037800940	2.5995913919
H27	-3.0490729829	-3.1076719396	1.5239758360
H28	-1.1207570812	-4.2711855856	.3020158502
H29	-1.4300863936	-2.6279168694	-.2454572721
H30	.9997072482	-2.9262556256	.0225331837
H31	.7709306232	-3.5729510665	1.6626654032
H32	1.7009217160	.8656157136	4.4901158493
H33	1.7120371072	-.8942566773	4.4460698634
H34	-.1570578914	2.1364713788	3.3852367458
H35	-1.3285983990	1.3431791975	2.3309125858
H36	2.5168047166	1.2042226730	.7728212594
H37	3.7639416831	2.3580436073	2.5246326076
H38	2.3232767159	2.6208065074	3.4950981453
H39	.4007039546	4.1628308336	2.5234949857
H40	.6571528263	4.9190856378	.9566940398
H41	2.8789044503	3.8359870768	.7412218876
H42	2.8249623762	4.6945543388	2.2798004292
H43	-.7759099998	2.8930397166	.6839147627
H44	-.5298914297	-.9918672324	-1.1677521878

C145	2.6218945829	-.7013122911	-1.5120665999
O46	-.7844365138	1.2038697450	-1.5167684827
C47	-1.1900521617	.1262563719	-2.1172727538
C48	-2.6475291683	-.2489490502	-1.9656038325
C49	-3.5108303655	.6504038787	-1.3217059021
H50	-3.1020134136	1.5828490900	-.9468097303
C51	-4.8657654500	.3555994961	-1.1832322266
H52	-5.5255470126	1.0673953632	-.6935873332
C53	-5.3765342271	-.8489507380	-1.6776241641
H54	-6.4325193677	-1.0804122478	-1.5689201070
C55	-4.5233635360	-1.7511511317	-2.3184090804
H56	-4.9126558251	-2.6889164228	-2.7062879971
C57	-3.1685239144	-1.4515362922	-2.4672494578
H58	-2.5192657977	-2.1648626241	-2.9662954419
C59	-.4548898104	-.2751662670	-3.3831139619
H60	.6224872950	-.2275075639	-3.2088062430
H61	-.7239413650	-1.2727549557	-3.7328751917
H62	-.7399003002	.4460177229	-4.1598736916
H63	.7437066296	2.7536296710	-.1861915506

No. (Table 1, Entry 1-R2)

SPE: -1669.26264

freqs: -860.41

Pd1	-.0053777716	-.0026411143	-.0041576524
C2	.0091814078	-.0003559276	3.4573772287
C3	2.2858384828	-.0016568783	2.5302478557
C4	1.9635939022	-1.3044447908	1.7777114493
N5	.5070679067	-1.5087863510	1.5109006417
C6	-.3102430117	-1.3402566723	2.7616165681
C7	-1.7967328367	-1.5733257274	2.4742617817
C8	-2.0281244831	-2.9796645648	1.9076915538
C9	-1.1601139158	-3.1938092512	.6631143576
C10	.3087151447	-2.8806067088	.9457643389
C11	1.4930826675	.0042251335	3.8466436711
C12	-.3162132237	1.2808753286	2.6662843102
N13	.5486549709	1.4778720296	1.4527177674
C14	2.0257897489	1.2995235143	1.7330359575
C15	2.6681507617	2.5177493324	2.4362431221
C16	.8555027088	4.0133739374	1.5800105369
C17	2.3706275556	3.8403608752	1.7225199423
C18	.2653284558	2.8211536658	.8238918973
H19	-.6171417109	.0312787256	4.3571078087
H20	3.3636325412	-.0286236320	2.7349781699
H21	2.4807212394	-1.3420714234	.8136231851
H22	2.3322163355	-2.1470565683	2.3854233501
H23	.0250836298	-2.1304354431	3.4585121965
H24	-2.3425137655	-1.4454359362	3.4168492405
H25	-2.1778500726	-.8170202220	1.7765015090
H26	-1.7761426411	-3.7321179916	2.6692387434
H27	-3.0853008466	-3.1182793076	1.6591537387
H28	-1.2230531001	-4.2311776107	.3129338465
H29	-1.5106656413	-2.5562141447	-.1528050285
H30	.9009519058	-2.9455508830	.0290537016
H31	.7190227697	-3.6054554228	1.6685034040
H32	1.7366184888	.8738349885	4.4638497202
H33	1.7409960151	-.8847158431	4.4386862403
H34	-.1804351107	2.1299525239	3.3487058104
H35	-1.3485283536	1.2979571817	2.3036086575
H36	2.4940316723	1.2094248031	.7447792431
H37	3.7485333262	2.3354081609	2.4828157967
H38	2.3209330217	2.5912402249	3.4725024246

H39	.3919672487	4.1302308064	2.5672803269
H40	.6118018154	4.9199822675	1.0141177065
H41	2.8330680958	3.8379937115	.7253595391
H42	2.8158327278	4.6741724528	2.2764781551
H43	-.8195224510	2.8809526300	.7017116967
H44	-.2572738491	1.0153507391	-1.2206030487
C145	-2.9676413244	1.2521779822	.2768601843
O46	-.3336680742	-1.1826992092	-1.7040507343
C47	-.3024213163	-.1003359769	-2.4185956818
C48	.9873831713	.2301340299	-3.1340270467
C49	2.0070687477	-.7330836812	-3.1612066969
H50	1.8420848571	-1.6778112105	-2.6547054037
C51	3.1996058875	-.4838475370	-3.8384680153
H52	3.9761215534	-1.2435873343	-3.8619294826
C53	3.3943404768	.7371904846	-4.4906737548
H54	4.3244128492	.9330902197	-5.0176253979
C55	2.3851910107	1.7032912949	-4.4656702380
H56	2.5294538047	2.6546994732	-4.9701198578
C57	1.1865714554	1.4502283905	-3.7975061005
H58	.4146413317	2.2134797070	-3.7843968704
C59	-1.6158182688	.3797039439	-3.0058221426
H60	-2.3849551318	.3989743473	-2.2300982910
H61	-1.5380069994	1.3672850068	-3.4621298205
H62	-1.8934134133	-.3358993526	-3.7905529645
H63	.7126028362	2.7934869042	-.1739385808

No. (Table 1, Entry 1-S1)

SPE: -1669.26090

freqs: -373.91

Pd1	0.0161802159	-0.0037423668	0.0026524258
C2	-0.0172629549	0.0042418836	3.4746845882
C3	2.2649187427	0.0083656484	2.5604516990
C4	1.9373465471	-1.2817623906	1.7858088771
N5	0.4756116520	-1.4818532834	1.5026412544
C6	-0.3335046300	-1.3315097218	2.7678389339
C7	-1.8190550438	-1.5907534411	2.5058336240
C8	-2.0433411263	-2.9891747283	1.9149015259
C9	-1.1796509507	-3.1819645957	0.6625153838
C10	0.2855953550	-2.8649794992	0.9519769170
C11	1.4648197682	0.0052465565	3.8723526323
C12	-0.3340066876	1.2900112414	2.6873198513
N13	0.5459503425	1.4883568446	1.4911224968
C14	2.0149240650	1.3177537046	1.7766476965
C15	2.6422268653	2.5416586946	2.4802663945
C16	0.8394236866	4.0150401243	1.5458338632
C17	2.3515159429	3.8477247678	1.7311065680
C18	0.2577574834	2.7997261636	0.8175989995
H19	-0.6489956949	0.0293838398	4.3705691021
H20	3.3413361533	-0.0323658049	2.7699305153
H21	2.4632987810	-1.3125622048	0.8270027893
H22	2.2886822235	-2.1347235967	2.3875501748
H23	0.0313815665	-2.1239782044	3.4460932269
H24	-2.3442128848	-1.4962487045	3.4642104167
H25	-2.2313589787	-0.8294031443	1.8327513361
H26	-1.7843952388	-3.7575082794	2.6578048195
H27	-3.1009857511	-3.1270925444	1.6681610588
H28	-1.2407117891	-4.2132377793	0.2947036027
H29	-1.5426361544	-2.5276706935	-0.1379928175
H30	0.8999326644	-2.9464204985	0.0509113225
H31	0.6794949327	-3.5779267134	1.6941359124
H32	1.7055539067	0.8734511869	4.4925995621

H33	1.7091372665	-0.8857588336	4.4627329713
H34	-0.2124911013	2.1366194495	3.3766388128
H35	-1.3619798842	1.2995066849	2.3127004225
H36	2.4901570576	1.2334960228	0.7906155833
H37	3.7224609073	2.3672299921	2.5541269921
H38	2.2693637706	2.6301856906	3.5067013930
H39	0.3541509571	4.1610530797	2.5191312697
H40	0.6128506020	4.9054821620	0.9482758685
H41	2.8386555163	3.8255280621	0.7461663924
H42	2.7784610891	4.6966783967	2.2765889736
H43	-0.8264441022	2.8567472891	0.6937956957
H44	-0.2900410695	-1.0037291231	-1.2565738568
C145	-2.9268254692	0.9542594180	0.2678174867
O46	0.0583406564	1.0898811805	-1.7978045120
C47	-0.1740502694	-0.0318223195	-2.4160910191
C48	0.9890539228	-0.6936434271	-3.1329047191
C49	2.2176726942	-0.0210836960	-3.1911005476
H50	2.2999339186	0.9488592787	-2.7125086872
C51	3.3015161623	-0.5840680148	-3.8643569164
H52	4.2454531719	-0.0476350002	-3.9119670488
C53	3.1735797589	-1.8308884421	-4.4829704404
H54	4.0181245861	-2.2704173166	-5.0066557141
C55	1.9522327918	-2.5074903748	-4.4288678343
H56	1.8437985625	-3.4762946233	-4.9085724082
C57	0.8648867981	-1.9409734230	-3.7620115686
H58	-0.0773673153	-2.4796595669	-3.7299542866
C59	-1.5728708467	-0.2139935092	-2.9875401537
H60	-1.6222382046	0.3726002658	-3.9133950295
H61	-1.8028763549	-1.2528464705	-3.2330884626
H62	-2.3003764484	0.1733431975	-2.2701013443
H63	0.6949635870	2.7410533289	-0.1829239992

No. (Table 1, Entry 1-S2)

SPE: -1669.26217

freqs: -518.07

Pd1	-0.0026714816	0.0028008721	0.0002942342
C2	0.0027809274	-0.0009449420	3.4591719542
C3	2.2838933425	-0.0047093128	2.5505311671
C4	1.9746674950	-1.2926185466	1.7681879133
N5	0.5130495883	-1.5103720131	1.5089038008
C6	-0.3101366630	-1.3355468680	2.7524773879
C7	-1.7953562364	-1.5725247475	2.4587964046
C8	-2.0206161196	-2.9980651526	1.9411162490
C9	-1.1395219765	-3.2541434514	0.7129071670
C10	0.3261757050	-2.8957118645	0.9694221216
C11	1.4827469629	-0.0105393682	3.8609891677
C12	-0.3042803092	1.2863273070	2.6685028248
N13	0.5628530725	1.4742906458	1.4600115653
C14	2.0424542480	1.3044356710	1.7666702651
C15	2.6437235884	2.5183377292	2.5095073695
C16	0.8675404170	4.0146843394	1.5813286700
C17	2.3749213446	3.8417010680	1.7862212544
C18	0.3124088179	2.8139025155	0.8120824218
H19	-0.6338832261	0.0309373234	4.3525397868
H20	3.3589991436	-0.0387261537	2.7628851009
H21	2.4817594938	-1.2804312546	0.7987750040
H22	2.3512600366	-2.1464484933	2.3536010695
H23	0.0100413460	-2.1256081656	3.4557306505
H24	-2.3639805245	-1.3988833426	3.3803169715
H25	-2.1471781045	-0.8460283005	1.7150475928
H26	-1.7745527438	-3.7125946421	2.7390968128

H27	-3.0765095316	-3.1540100471	1.6927714364
H28	-1.1815060642	-4.3088302221	0.4169746615
H29	-1.5016618110	-2.6673421117	-0.1335276149
H30	0.9073169732	-2.9666369493	0.0469772648
H31	0.7615701320	-3.5981350178	1.6989398657
H32	1.7249132610	0.8497670642	4.4911645291
H33	1.7114993931	-0.9086703220	4.4467728652
H34	-0.1686653177	2.1322687224	3.3546247863
H35	-1.3429746703	1.3094136122	2.3275665023
H36	2.5225298587	1.2349956440	0.7821085252
H37	3.7218760988	2.3390801644	2.5926490361
H38	2.2610435021	2.5918617509	3.5345555136
H39	0.3608110936	4.1403764487	2.5468594429
H40	0.6473343914	4.9144480465	0.9948557669
H41	2.8749755989	3.8355042593	0.8096466019
H42	2.7916099909	4.6789519246	2.3570660506
H43	-0.7665768863	2.8945974334	0.6527542710
H44	-0.4353044019	1.0446209123	-1.1507076052
C145	2.8966957481	0.4786299983	-1.4615391830
O46	-0.7581063977	-1.1177340269	-1.6071159720
C47	-1.0457115079	-0.0077617006	-2.2150767680
C48	-2.4855566267	0.4530539520	-2.2008283358
C49	-3.4746288635	-0.4263398144	-1.7367274817
H50	-3.1775097563	-1.4088212957	-1.3872242710
C51	-4.8172645521	-0.0497190268	-1.7435077470
H52	-5.5746827119	-0.7458877181	-1.3932658900
C53	-5.1890252681	1.2159475758	-2.2048816750
C55	-4.2091572806	2.0996249658	-2.6658439838
C57	-2.8671555253	1.7191978109	-2.6702495305
H58	-2.1176533027	2.4189672679	-3.0274174143
C59	-0.1631643324	0.3870180743	-3.3829158608
H60	-0.4086983517	-0.2983524090	-4.2048018076
H61	-0.3469675805	1.4056014628	-3.7287810420
H62	0.8891411514	0.2730665064	-3.1079006330
H63	0.7994653149	2.7656878191	-0.1645658185
H64	-4.4899869729	3.0857017047	-3.0255228659
H65	-6.2348487283	1.5109111215	-2.2087083351

No. (Table 1, Entry 2-R1)

SPE: -1783.79113

freqs: -669.12

Pd1	0.0017067175	0.0005582510	0.0006796641
C2	0.0034695380	0.0030516310	3.4486405320
C3	2.2939195677	0.0056957232	2.5548430343
C4	1.9894974728	-1.2822918998	1.7728047179
N5	0.5307655198	-1.4760850285	1.4683536579
C6	-0.3129214620	-1.3134626208	2.7039801182
C7	-1.7942837596	-1.5342842205	2.3781056916
C8	-2.0226714713	-2.9426091655	1.8109164646
C9	-1.1085158829	-3.1929358513	0.6037433318
C10	0.3516492760	-2.8578000193	0.9093184789
C11	1.4817728991	-0.0043411118	3.8592600735
C12	-0.2864204512	1.3103951757	2.6900955027
N13	0.5798744704	1.5020822238	1.4873946206
C14	2.0544822555	1.3152231143	1.7667301210
C15	2.6901141034	2.5324306108	2.4753130074
C16	0.8917634233	4.0294202835	1.5728143042
C17	2.4029984607	3.8524757602	1.7497454604
C18	0.3098298175	2.8230203429	0.8307298922
H19	-0.6376700907	0.0125005750	4.3391784276
H20	3.3674418366	-0.0269659336	2.7762055321

H21	2.5158387832	-1.3158751365	0.8126762117
H22	2.3175047505	-2.1338769374	2.3891828514
H23	-0.0067748215	-2.1210922563	3.3919614360
H24	-2.3785974943	-1.3891689840	3.2947245983
H25	-2.1313160587	-0.7826282932	1.6529771745
H26	-1.8110570317	-3.6826608179	2.5949096249
H27	-3.0728275564	-3.0733450058	1.5276454431
H28	-1.1581477374	-4.2419605174	0.2899582887
H29	-1.4521607275	-2.5921706915	-0.2454938029
H30	0.9796772415	-2.9176908141	0.0167718924
H31	0.7417998626	-3.5670398498	1.6564237240
H32	1.7119174687	0.8566741543	4.4944186675
H33	1.7150689463	-0.9026670062	4.4423565697
H34	-0.1450835098	2.1402452861	3.3963761872
H35	-1.3231996422	1.3534252373	2.3449395237
H36	2.5185691889	1.2138140349	0.7781345402
H37	3.7695475043	2.3523778954	2.5349243422
H38	2.3304784025	2.6103379422	3.5082722538
H39	0.4086570914	4.1618236903	2.5497155725
H40	0.6641559496	4.9282698911	0.9882752394
H41	2.8847735447	3.8453820305	0.7629664509
H42	2.8326714067	4.6915968806	2.3080596204
H43	-0.7727176275	2.9062530534	0.7049642734
H44	-0.5470864511	-0.9656673215	-1.1903567136
C145	2.6298094168	-1.0892763898	-1.5614866573
O46	-0.7191623158	1.2107155371	-1.5262990027
C47	-1.1325964617	0.1416676385	-2.1517087768
C48	-2.6044562676	-0.1773478875	-2.0805635225
C49	-3.4632581940	0.6920860238	-1.3826921304
H50	-3.0369195268	1.5664769584	-0.9029614156
C51	-4.8282459826	0.4577620288	-1.3243054254
H52	-5.4946198595	1.1360405430	-0.7996825807
C53	-5.3786614481	-0.6679630528	-1.9630302105
O54	-6.7276605469	-0.8115703746	-1.8542427771
C55	-4.5384152517	-1.5485805475	-2.6563567070
H56	-4.9373358916	-2.4227891900	-3.1570359240
C57	-3.1663022398	-1.2948507781	-2.7105468269
H58	-2.5371442367	-1.9928338023	-3.2535863674
C59	-0.3514831564	-0.2685381686	-3.3879170084
H60	0.7179744872	-0.2682540012	-3.1660266860
H61	-0.6373833449	-1.2520888946	-3.7631532137
H62	-0.5750127039	0.4721472181	-4.1659791563
H63	0.7432653760	2.7719066678	-0.1714353371
C64	-7.3490502440	-1.9177764083	-2.5051735931
H65	-6.9752974958	-2.8732054297	-2.1179678541
H66	-7.1950799792	-1.8807191789	-3.5902965521
H67	-8.4151778269	-1.8351667509	-2.2891179545

No. (Table 1, Entry 3-R1)

SPE: -1768.49584

freqs: -744.85

Pd1	0.0097299484	0.0049795202	-0.0034771088
C2	-0.0106492944	0.0053781365	3.4407291499
C3	2.2841373090	0.0303592238	2.5569233195
C4	1.9950946288	-1.2606523743	1.7738278957
N5	0.5383242226	-1.4686356453	1.4637228062
C6	-0.3114656227	-1.3146088840	2.6960494468
C7	-1.7891026134	-1.5531866753	2.3659771656
C8	-1.9990658099	-2.9653984281	1.8012247266
C9	-1.0791813017	-3.2073013134	0.5969974026
C10	0.3760344899	-2.8526833120	0.9038467197

C11	1.4658444411	0.0115602976	3.8575217396
C12	-0.3095157710	1.3095139039	2.6803512926
N13	0.5625551417	1.5115158707	1.4833319332
C14	2.0374462925	1.3389566313	1.7696316966
C15	2.6564261383	2.5614835212	2.4833766277
C16	0.8463900074	4.0415553029	1.5743557067
C17	2.3583725590	3.8799414979	1.7588051725
C18	0.2819070973	2.8305519927	0.8268841286
H19	-0.6558052487	0.0099034369	4.3285039506
H20	3.3566036604	0.0066702843	2.7840316128
H21	2.5240251078	-1.2931619555	0.8150802620
H22	2.3274916922	-2.1085950936	2.3927546326
H23	0.0018209414	-2.1189073224	3.3846372957
H24	-2.3779045389	-1.4135936320	3.2805776096
H25	-2.1326486876	-0.8065035483	1.6387056329
H26	-1.7809384443	-3.7013526694	2.5872258544
H27	-3.0467526437	-3.1094277023	1.5155102720
H28	-1.1142744371	-4.2577083017	0.2859927699
H29	-1.4286305495	-2.6133226540	-0.2546027034
H30	1.0047131602	-2.9052723309	0.0113041659
H31	0.7746255049	-3.5569830467	1.6509095695
H32	1.6849712917	0.8742335189	4.4941415375
H33	1.7049189439	-0.8848585882	4.4413308420
H34	-0.1822217879	2.1406171053	3.3874877789
H35	-1.3444753689	1.3411593301	2.3284298915
H36	2.5074330196	1.2432713184	0.7833142963
H37	3.7374249429	2.3933760333	2.5475359495
H38	2.2910383813	2.6336913106	3.5146604161
H39	0.3562319026	4.1668173946	2.5486522836
H40	0.6124375119	4.9390117493	0.9900199398
H41	2.8449325546	3.8802637814	0.7743919739
H42	2.7760353843	4.7225216509	2.3209224762
H43	-0.8008527325	2.9024768072	0.6956339896
H44	-0.5236037890	-0.9792305039	-1.1752354708
C145	2.6658270955	-0.9964841047	-1.5587770356
O46	-0.6913244745	1.2164681458	-1.5473594898
C47	-1.1294209567	0.1506506541	-2.1491004645
C48	-2.6068773250	-0.1474109942	-2.0327950397
C49	-3.4331514870	0.7882237355	-1.3901694783
H50	-2.9816744909	1.6879944477	-0.9875811037
C51	-4.8061532092	0.5826594414	-1.2845600490
H52	-5.4562942093	1.3058307778	-0.8022980418
C53	-5.3459794866	-0.5811260497	-1.8247383775
F54	-6.6759587193	-0.7903743519	-1.7263767711
C55	-4.5606836901	-1.5331355824	-2.4659505186
H56	-5.0215609121	-2.4263084596	-2.8748807529
C57	-3.1885368208	-1.3057997533	-2.5711522431
H58	-2.5750512920	-2.0482205195	-3.0713259653
C59	-0.3841250334	-0.2977517490	-3.3917793675
H60	0.6905319728	-0.3018596484	-3.1937636422
H61	-0.6918190890	-1.2854683345	-3.7378040322
H62	-0.6168177313	0.4277473447	-4.1819603653
H63	0.7217579044	2.7860584901	-0.1727332959

No. (Table 1, Entry 9-R1)

SPE: -1669.27679

freqs: -569.96 -47.82

Pd1	0.0272229769	-0.0099072328	-0.0237746165
C2	-0.0825060456	0.0024830351	3.4160148432
C3	2.2371310959	0.0564590757	2.6004682694
C4	1.9908552939	-1.2404643453	1.8140217105

N5	0.5484372915	-1.4712539118	1.4600713589
C6	-0.3415530448	-1.3242460240	2.6675582869
C7	-1.8038313775	-1.5877795251	2.2914976365
C8	-1.9754551875	-3.0066379859	1.7299464863
C9	-1.0145766756	-3.2444431664	0.5573937175
C10	0.4228046269	-2.8630555202	0.9101155427
C11	1.3811196985	0.0300578666	3.8758957608
C12	-0.3772987389	1.3010065991	2.6438664675
N13	0.5243320259	1.5069125588	1.4686591860
C14	1.9935709993	1.3552968891	1.7969018595
C15	2.5767099940	2.5895402259	2.5200705054
C16	0.7806620213	4.0417476723	1.5445652639
C17	2.2882461026	3.8975994560	1.7737686695
C18	0.2484626179	2.8180445482	0.7940311703
H19	-0.7527216322	-0.0011115081	4.2846828407
H20	3.3028538195	0.0497359717	2.8584854615
H21	2.5495107475	-1.2545642603	0.8739096754
H22	2.3211649668	-2.0835416362	2.4401463909
H23	-0.0360619742	-2.1214884127	3.3672059688
H24	-2.4232994291	-1.4520101873	3.1858468818
H25	-2.1353716819	-0.8507944376	1.548836107
H26	-1.7726865480	-3.7344007009	2.5274682950
H27	-3.0106945910	-3.1670347431	1.4100793146
H28	-1.0215915251	-4.2983205900	0.2559257813
H29	-1.3458530917	-2.6644914366	-0.3107821135
H30	1.0786138841	-2.9179883197	0.0386412198
H31	0.8097745285	-3.5546179815	1.6743893057
H32	1.5703488341	0.8986463961	4.5138543123
H33	1.6156740897	-0.8605479250	4.4705569386
H34	-0.2757989337	2.1357169363	3.3506505090
H35	-1.4035374497	1.3218459996	2.2664617416
H36	2.4923129766	1.2585516272	0.8248440603
H37	3.6568288857	2.4322839639	2.6193336961
H38	2.1789673997	2.6671431248	3.5389074671
H39	0.2617163614	4.1718671429	2.5030725468
H40	0.5545533413	4.9299581721	0.9432100534
H41	2.8034365614	3.8927251921	0.8038232000
H42	2.6812892536	4.7501486612	2.3387501480
H43	-0.8306873575	2.8787812858	0.6318751672
H44	-0.4405697107	-1.0181023343	-1.2007953909
C145	2.8395068945	-0.5828313953	-1.4783229894
O46	-0.7217590427	1.1770008772	-1.5781909579
C47	-1.0959634809	0.0896428378	-2.1829665952
C48	-2.5505608951	-0.3074494867	-2.0736095158
C49	-3.4423603050	0.5686535343	-1.4362605402
H50	-3.0579119724	1.4995670637	-1.0335363864
C51	-4.7965955201	0.2542414627	-1.3399110173
H52	-5.4781902698	0.9478416119	-0.8546795696
C53	-5.2780046054	-0.9462664502	-1.8718227060
H54	-6.3336561403	-1.1923776051	-1.7968620875
C55	-4.3964878641	-1.8253499075	-2.5061666045
H56	-4.7631915756	-2.7591166630	-2.9235065468
C57	-3.0417219395	-1.5069225013	-2.6118062707
H58	-2.3717246386	-2.2028942936	-3.1071298785
C59	-0.3192095924	-0.3083803081	-3.4258151010
H60	0.7512487953	-0.2154100172	-3.2311508533
H61	-0.5438102068	-1.3209962970	-3.7640756007
H62	-0.6136047216	0.3872741695	-4.2223897762
H63	0.7187864186	2.7695709334	-0.1914821373

No. (Table 1, Entry 11-R3)

GPE: -1437.53000

SE: -0.00641
freqs: -431.49

Pd1	-0.0410762307	-0.0000346039	0.0107967700
C2	0.0188246853	0.0360157850	3.9150267152
C3	2.3184472940	-0.0298437547	3.0604497189
C4	1.9359952602	-1.2150733410	2.1513196642
N5	0.4797212144	-1.3446034464	1.8325547857
C6	-0.3528350793	-1.2059863573	3.0730483918
C7	-1.8437390052	-1.3455184238	2.7435523893
C8	-2.1315924524	-2.7135652009	2.1050102703
C9	-1.2109464519	-2.9555842150	0.9008628975
C10	0.2568626842	-2.7043272010	1.2539968831
C11	1.4839741035	-0.0966991305	4.3469269822
C12	-0.1795181355	1.4189683085	3.2638561935
N13	0.7614470708	1.6874487084	2.1695530724
C14	2.1812188386	1.3620116660	2.4056688658
C15	2.9476552752	2.4562130100	3.1943804924
C16	1.2680675760	4.1535903448	2.3772223269
C17	2.7607457796	3.8440567131	2.5606241487
C18	0.5946559549	3.0227008872	1.5806217229
H19	-0.6350708071	0.0051731233	4.7967023241
H20	3.3822547978	-0.1700503533	3.2948145745
H21	2.4675010192	-1.1693812302	1.1988233001
H22	2.2521362580	-2.1355956158	2.6727449689
H23	-0.0907515827	-2.0695799660	3.7164844821
H24	-2.4149731954	-1.2356145977	3.6741969258
H25	-2.1556008533	-0.5441601957	2.0676090364
H26	-1.9711072252	-3.5037101453	2.8523775989
H27	-3.1820102103	-2.7799371281	1.8000199295
H28	-1.3084600740	-3.9868868786	0.5405492925
H29	-1.5008237554	-2.2991756413	0.0712634648
H30	0.8921106105	-2.7891037432	0.3692009283
H31	0.5933475966	-3.4564664478	1.9896894296
H32	1.7583201685	0.6988831613	5.0472798550
H33	1.6521673161	-1.0492316964	4.8651211598
H34	-0.1110146219	2.1636585207	4.0799904286
H35	-1.1871526935	1.5044094615	2.8428080129
H36	2.6416957783	1.3101307272	1.4070364057
H37	4.0130540862	2.1927472615	3.2265178922
H38	2.6024544888	2.4912949130	4.2354260144
H39	1.1305395134	5.1054130456	1.8494073914
H40	0.7885091767	4.2672567634	3.3588042986
H41	3.2482178321	4.6112812075	3.1732482474
H42	3.2554416856	3.8661474732	1.5789009318
H43	-0.4777788390	3.2021705454	1.4594982890
H44	-0.3411632981	0.7365836890	-1.3635243982
O45	1.6831473209	-0.7255930539	-0.8914997589
C46	-1.8162006844	1.1495906898	-0.9895945993
C47	-1.6264407341	2.5820649278	-1.4938195628
C48	-2.5966851748	0.2254933254	-1.8999473553
C49	-3.6495340010	-0.5236379258	-1.3568741212
H50	-3.8540554626	-0.4408859084	-0.2945426488
C51	-4.4251280156	-1.3437572379	-2.1758568386
H52	-5.2482648357	-1.9097552581	-1.7480197198
C53	-4.1475218735	-1.4351922551	-3.5412417655
H54	-4.7497062021	-2.0767172148	-4.1783883742
C55	-3.0921070739	-0.6992719694	-4.0849873093
H56	-2.8637719822	-0.7749667224	-5.1443605943
C57	-2.3226193535	0.1318909584	-3.2725175252
H58	-1.4837236700	0.6738064701	-3.6981314837
O59	-1.9124478328	0.9685918264	0.2958715460

H60	-2.6129060004	3.0619814368	-1.5020675153
H61	-0.9673934417	3.1328104401	-0.8236700024
H62	-1.2222014593	2.6140132218	-2.5068980605
H63	1.0358151344	2.9973036816	0.5740260357
C64	1.8867607727	-0.3717364328	-2.1289353795
O65	1.1525712555	0.3704885051	-2.7979257475
C66	3.1524776062	-0.9690156299	-2.7330529953
H67	3.3131893755	-0.5811824574	-3.7389185973
H68	3.0596576352	-2.0591533789	-2.7714715154
H69	4.0155660520	-0.7392412323	-2.1013651174

No. (sparteineH-Cl)

GPE: -1157.60820

SE: -0.01421

C1	1.1554329869	-.4019431610	1.2854766203
C2	-.2332990710	1.3794663515	.2950724929
C3	.9014724373	1.6696090883	-.7000061042
N4	1.7649061323	.5179995324	-.9266245427
C5	2.3036925275	-.0912430507	.2908158507
C6	3.1429511012	-1.3329555238	-.0573232771
C7	4.2583567273	-.9978021936	-1.0551579125
C8	3.6409003937	-.3713100889	-2.3093820828
C9	2.7807793682	.8362227062	-1.9381446361
C10	.3930908716	.8888946572	1.6093291281
C11	.1400877380	-1.4649013900	.8305553853
N12	-.7539302244	-1.0336388116	-.2963080935
C13	-1.2998659300	.3854939554	-.2262520098
C14	-2.6024982630	.4757983167	.5878013555
C15	-3.0615438141	-1.9621545222	.2773217439
C16	-3.6551086887	-.5551606865	.1670022333
C17	-1.8221415683	-2.0668272714	-.5975923224
H18	1.6197416634	-.8047998621	2.1948644305
H19	-.7651785430	2.3244242217	.4627037517
H20	.4836010971	1.9659271870	-1.6693684647
H21	1.4708507647	2.5425546038	-.3135154237
H22	2.9754815194	.6207454412	.8240457806
H23	3.5554270934	-1.7532557962	.8691537545
H24	2.4976686401	-2.0925077830	-.5132857307
H25	4.9696101390	-.2967916748	-.5938233762
H26	4.8227371875	-1.9026522081	-1.3093278209
H27	4.4203394352	-.0507713564	-3.0114004918
H28	3.0054308296	-1.1018421687	-2.8208149659
H29	2.2530681331	1.1967345238	-2.8270037649
H30	3.4329686242	1.6611997985	-1.5794633732
H31	-.3613528127	.7160224668	2.3856075935
H32	1.0827074206	1.6489838118	1.9934080942
H33	-.4963628891	-1.7337695972	1.6804101606
H34	.6335467531	-2.3740576790	.4793527695
H35	-1.5219394053	.6155539425	-1.2755010415
H36	-2.9890449761	1.4934886351	.4617117566
H37	-2.3892718512	.3537297920	1.6570772029
H38	-3.7737661233	-2.7214904787	-.0649684459
H39	-2.8320096004	-2.1955132309	1.3256132534
H40	-3.9631351051	-.3710343562	-.8711586788
H41	-4.5505384240	-.4564026547	.7896280641
H42	-1.3317735944	-3.0403783749	-.5289433940
H43	-2.0651696589	-1.9150966873	-1.6522534004
H44	-.1857672140	-1.0793864559	-1.2433160673
C145	.1152945900	-1.4706707487	-3.0256292235

No. (sparteine-HOAc)

GPE: -925.89913
SE: -0.00457

C1	-.0170421832	-.1760546585	-.0685836840
C2	.0606087335	-.0219419269	2.3816115752
C3	1.5965465425	.0093231498	2.3175793301
N4	2.1231807314	.4867601393	1.0354607327
C5	1.5290407707	-.1689074075	-.1404476358
C6	2.0675237658	.4709448401	-1.4294800981
C7	3.5985496906	.4085021811	-1.4876671170
C8	4.1903319901	1.0465854403	-.2255998239
C9	3.5868554145	.4134407246	1.0304308236
C10	-.4490201592	-.8861857393	1.2194258445
C11	-.7159313318	1.1974036777	-.1263668102
N12	-.4491536590	2.0500765497	1.0509310906
C13	-.6111593080	1.3721982971	2.3727605801
C14	-2.0845901783	1.2743069066	2.8369581432
C15	-2.6793373678	3.2323988858	1.3835533279
C16	-2.8034167298	2.6286337648	2.7873283496
C17	-1.1972384283	3.3293647816	.9991402045
H18	-.3659859411	-.7397956111	-.9441293796
H19	-.2027562363	-.4882944751	3.3398215207
H20	1.9913218786	.6644139812	3.1031790052
H21	1.9600978618	-1.0173020715	2.5366769310
H22	1.8286158416	-1.2420522224	-.1619450491
H23	1.6246035128	-.0425621146	-2.2925616070
H24	1.7524444954	1.5199376480	-1.4738647663
H25	3.9190230379	-.6412234267	-1.5538272111
H26	3.9697734745	.9108999535	-2.3887838783
H27	5.2807239598	.9295419126	-.2024746810
H28	3.9697094215	2.1201798044	-.2207825311
H29	3.9511787625	.9302071906	1.9260403973
H30	3.9268730300	-.6416404050	1.1092090856
H31	-1.5368012992	-1.0127820140	1.2501831500
H32	-.0068929386	-1.8889410563	1.2728969757
H33	-1.7950665513	1.0041585629	-.2541447990
H34	-.3960889331	1.7599877057	-1.0107166332
H35	-.0784427519	2.0152110672	3.0855506576
H36	-2.0974313577	.8718929423	3.8576438113
H37	-2.6358417220	.5589140489	2.2134010359
H38	-3.1253491705	4.2337413686	1.3440684027
H39	-3.2271644668	2.6143242277	.6597714578
H40	-2.3465480239	3.3133209835	3.5157039216
H41	-3.8551626386	2.5138833631	3.0752136987
H42	-1.0730408040	3.7452285806	-.0067911863
H43	-.7040048828	4.0170279718	1.6974027446
H44	1.1506889229	2.8495772578	.9530868188
O45	1.7221637728	3.8160662339	3.0505864762
C46	2.1975964218	4.1333173596	1.9687581101
C47	3.2575001952	5.1979158787	1.7960224502
O48	1.8420523556	3.5782301377	.8109815242
H49	4.1684311083	4.7477225677	1.3888789321
H50	3.4750992506	5.6640628094	2.7565862413
H51	2.9206643358	5.9521069499	1.0787612103

No. ((R)-1-phenylethanol)

GPE: -386.10065
SE: -0.00472

No. (Cl-)

GPE: -460.27146
SE: -0.07588