Supporting Information

for

CfbA Promotes Insertion of Cobalt into Ruffled Tetrapyrroles

*Ariel E. Schuelke-Sanchez, Alissa A. Stone, and Matthew D. Liptak**

Department of Chemistry, University of Vermont, Burlington, Vermont, 05405, United States

Contents

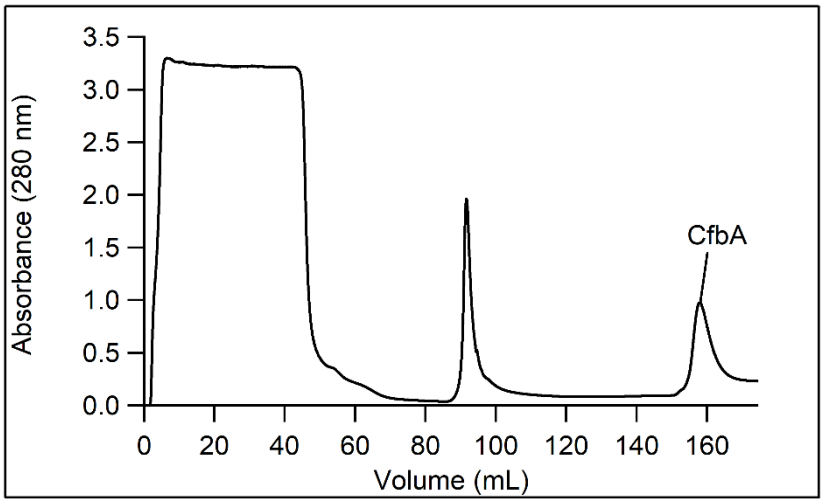

Figure S1. Purification of CfbA. The column was washed following a gradient of 50 mM HEPES pH 7.5, 500 mM NaCl, 5 mM imidazole, and 5% glycerol (*v/v*) to 50 mM HEPES pH 7.5, 500 mM NaCl, 500 mM imidazole, and 5% glycerol(*v/v*) at a flow rate of 5.0 mL/min. The protein eluted at 500 mM imidazole.

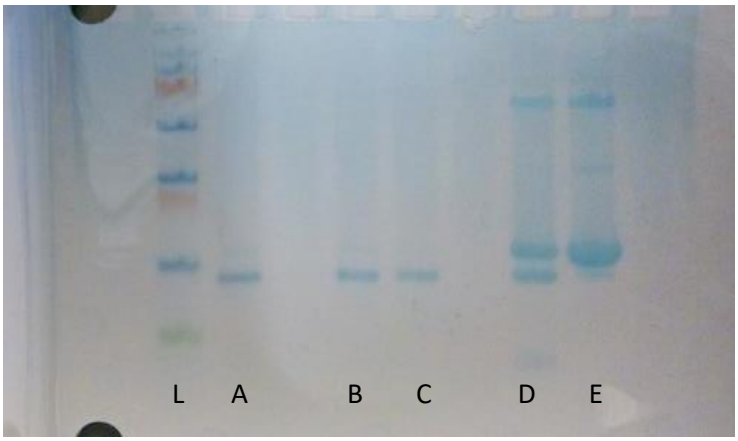

Figure S2. SDS-PAGE gel of CfbA. The lanes represent: PageRuler Plus prestained protein ladder (Pierce) (L), purified CfbA (A), 75 mM imidazole wash post-cleavage (B), post-cleavage flow-through (C), cleavage reaction (D), and uncleaved CfbA (E). CfbA was successfully purified and cleaved. All protein samples were in 10 mM HEPES pH 7.5, 500 mM NaCl.

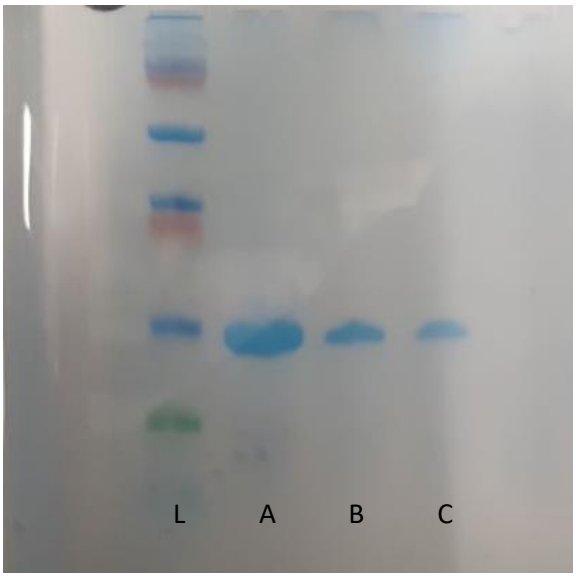

Figure S3. SDS-PAGE gel of CfbA. The lanes represent: PageRuler Plus prestained protein ladder (Pierce) (L), pure CfbA (A), 1/10 dilution of purified CfbA (B), 1/100 dilution of purified CfbA (C). CfbA is >99% pure according to SDS-PAGE gel. All protein samples were in 10 mM HEPES pH 7.5, 500 mM NaCl.

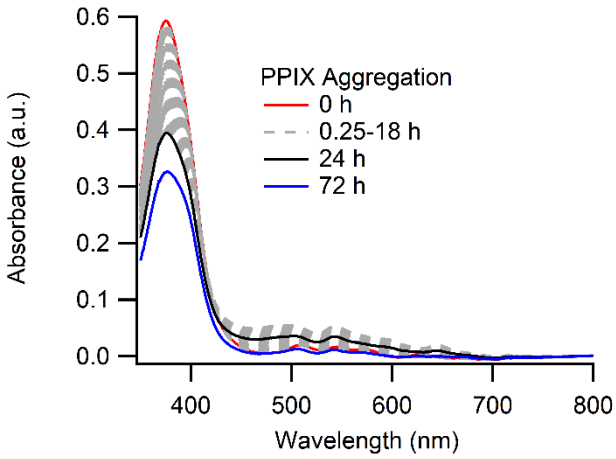

Figure S4. The decrease in intensity of PPIX throughout the assay is attributed to PPIX aggregation over time as seen in the absorption spectra in 50 mM Tris pH 8.0, 150 mM NaCl, 10% (*v/v*) methanol.

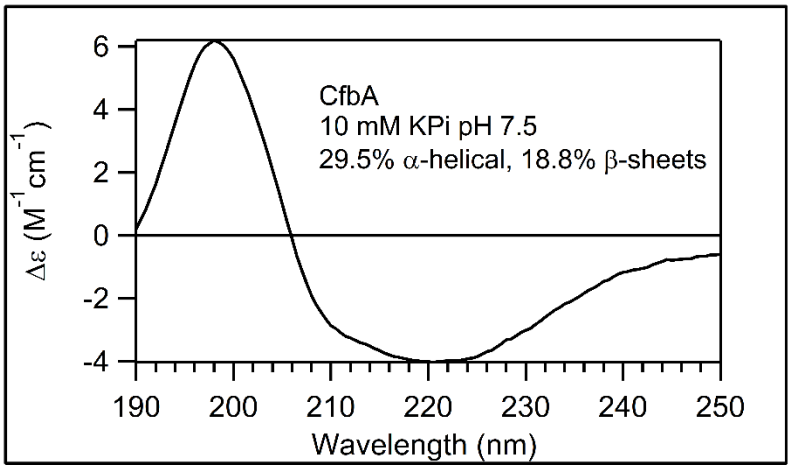

Figure S5. UV CD spectrum of CfbA collected in 10 mM KPi pH 7.5. The secondary structure is consistent with the monomeric crystal structure of *A. fulgidus* CbiX^{S} (PDB: 1TJN)[1] with 29.5% α-helical and 18.8% β-sheets calculated using the CD Multivariate SSE program (JASCO).

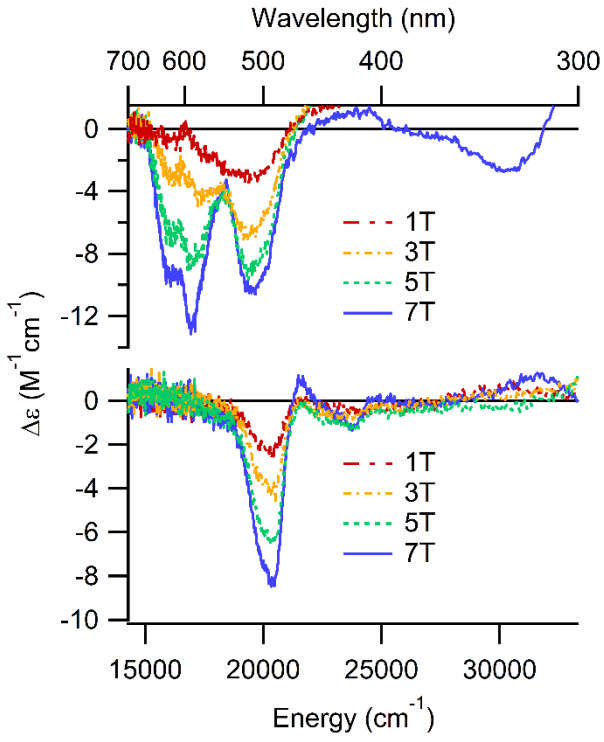

Figure S6. Cobalt (II) chloride (top) and cobalt-bound CfbA (bottom) MCD spectra at 5 K and 7 T (solid blue), 5 T (dotted green), 3 T (dashed yellow), and 1 T (dashed red) in 50 mM KPi pH 8.0, 50 mM NaCl, 60% (v/v) glycerol. The enzyme-free spectrum is consistent with a five-coordinate species, and the CfbA–Co(II) MCD spectrum indicates formation of an octahedral complex.

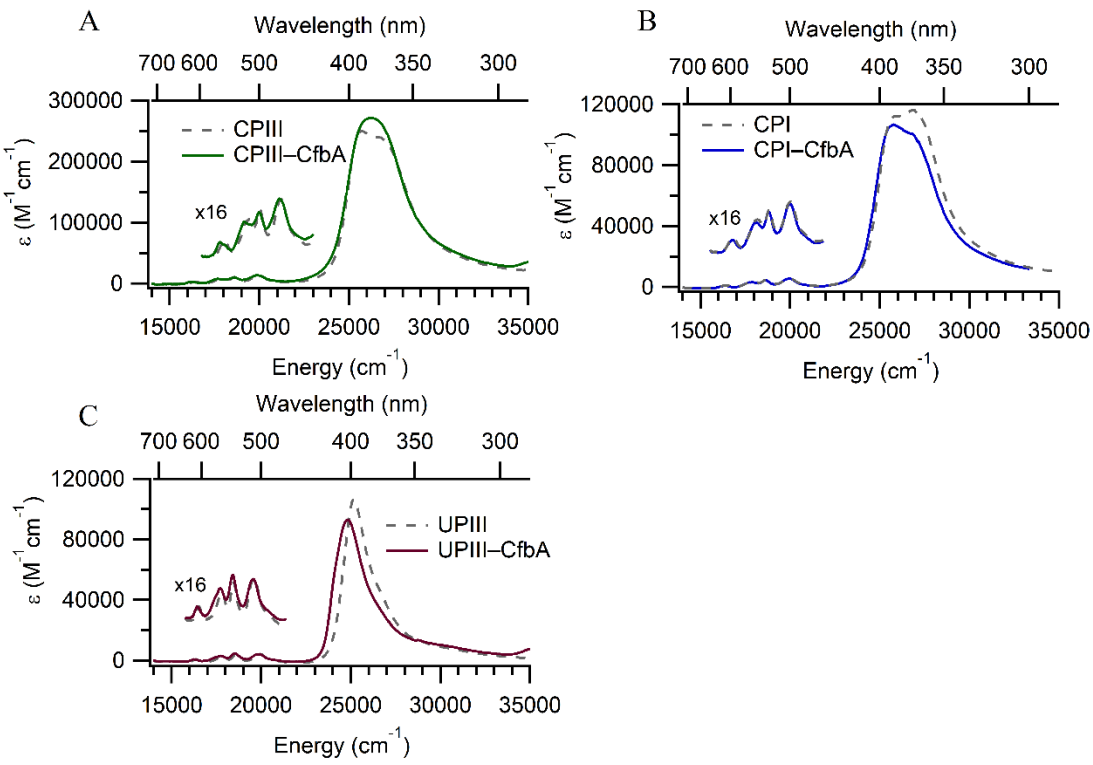

Figure S7. Binding to CfbA by the porphyrins CPIII (A), CPI (B) and UPIII (C) in 50 mM Tris pH 8.0, 150 mM NaCl. Upon addition of porphyrin to CfbA, the Soret bands red shift in energy, except for CPIII which exhibits a slight blue shift.

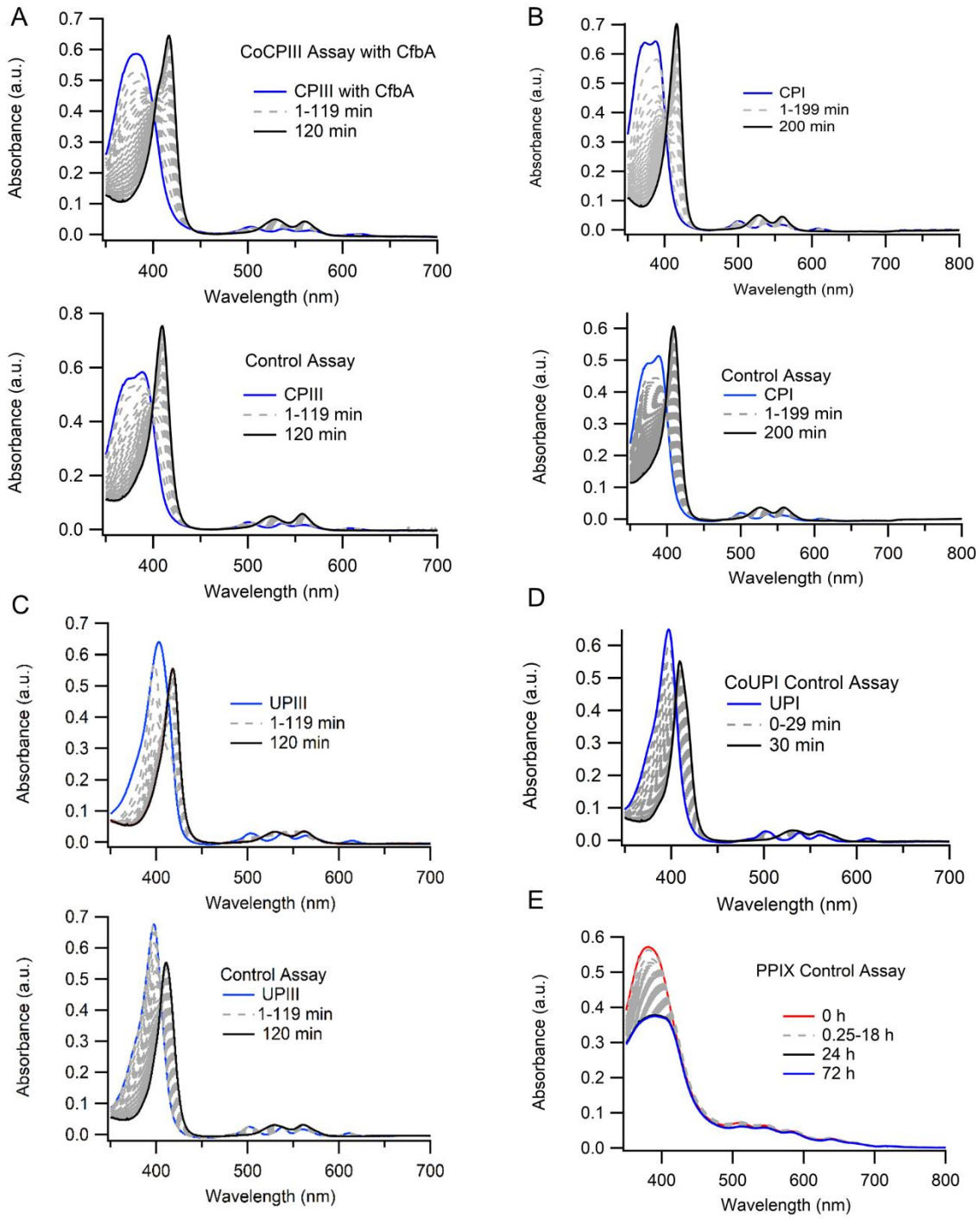

Figure S8. Activity and control assays with CPIII (A), CPI (B), and UPIII (C) in 50 mM Tris pH 8.0, 150 mM NaCl; in addition to the control assays for UPI (D) and PPIX (E). The PPIX assay was in 50 mM Tris pH 8.0, 150 mM NaCl, 10% (*v/v*) methanol.

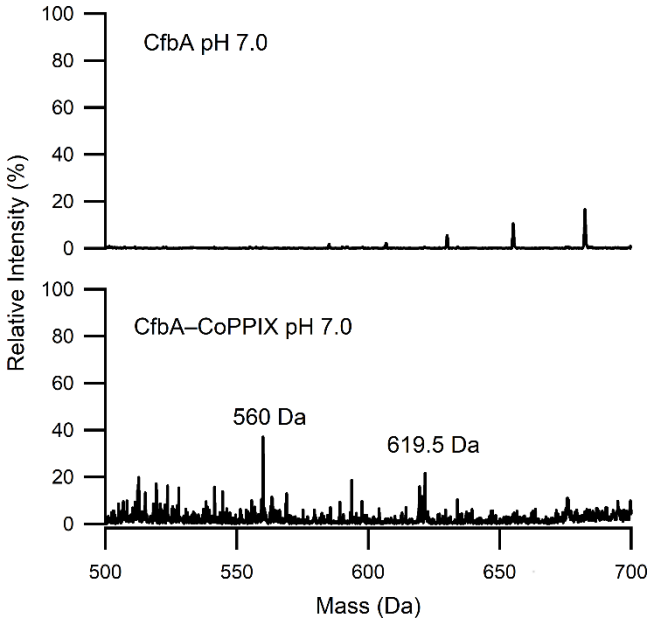

Figure S9. ESI-MS data for CfbA (top) and a reaction mixture containing CfbA, $CoCl_2$, and PPIX (bottom) in 50 mM Tris pH 7.0, 150 mM NaCl. The peak at 560 Da is consistent with the expected mas for PPIX (562.6 Da) and the peak at 619.5 Da is consistent with the expected mass for CoPPIX (619.58 Da). The relative intensities were normalized using a protein derived peak at 861.5 Da. These data indicate that Co is inserted into PPIX in the presence of CfbA yielding CoPPIX.

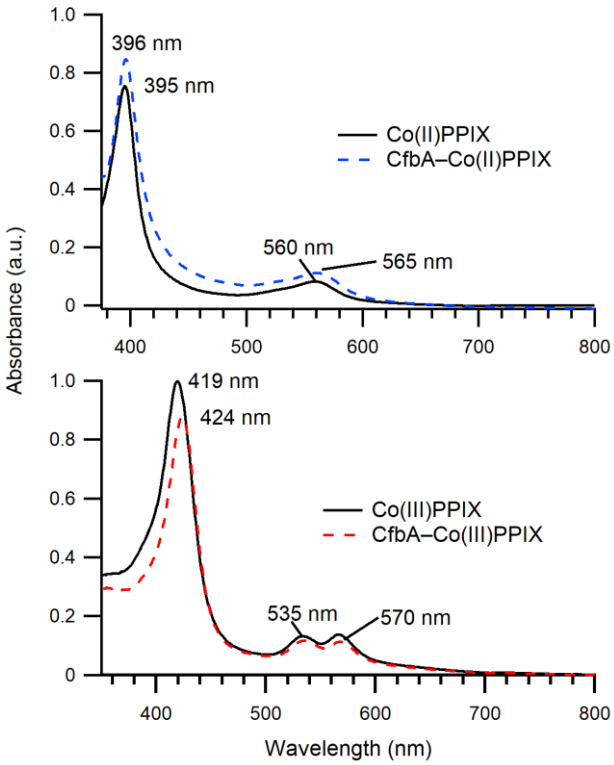

Figure S10. UV/Vis Abs spectra of anaerobic Co(II)PPIX (top, black) and Co(II)PPIX bound CfbA (top, blue dashed) in 50 mM Tris pH 8.0, 150 mM NaCl, 10% (*v/v*) methanol and 2 mM sodium dithionite. Abs spectra of Co(III)PPIX (bottom, black) and Co(III)PPIX bound CfbA (bottom, red dashed) in 50 mM Tris pH 8.0, 150 mM NaCl, 10% (*v/v*) methanol.

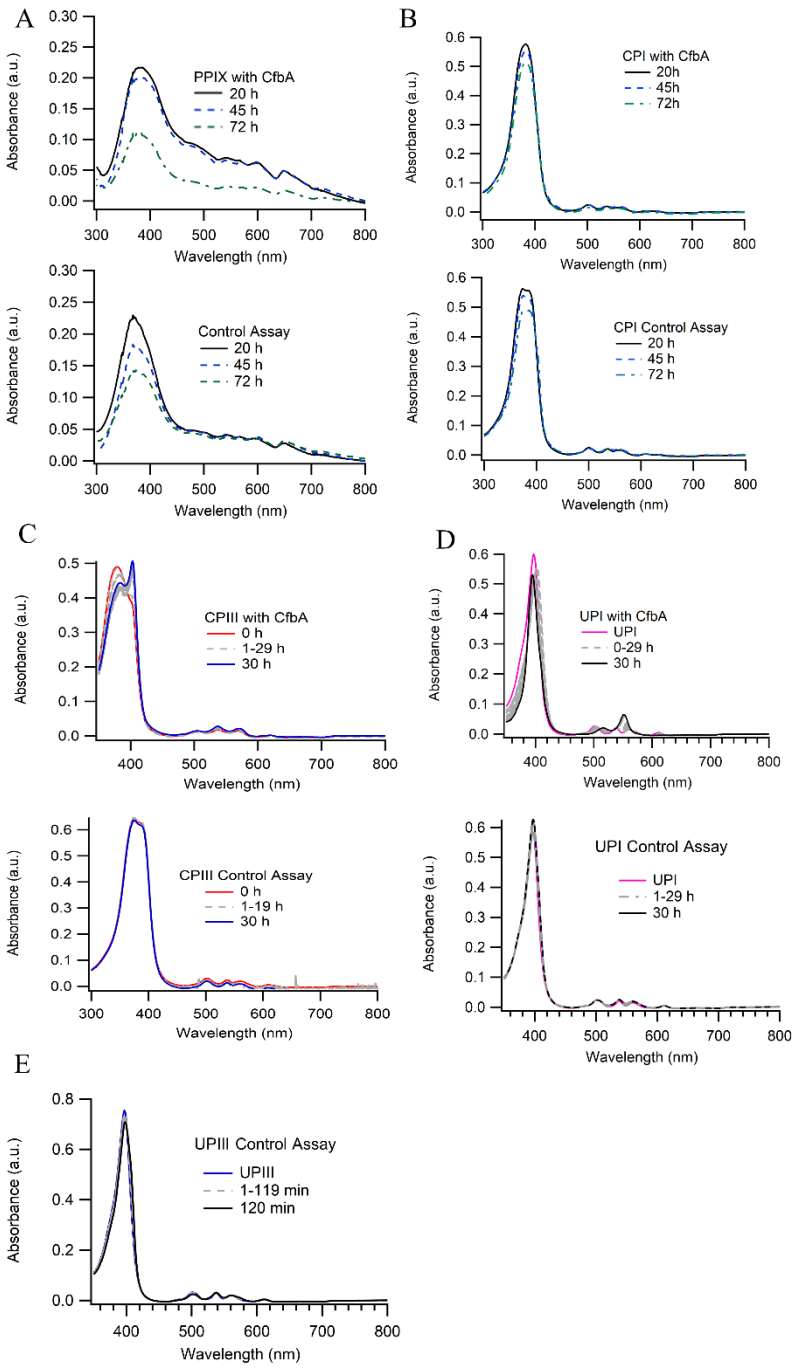

Figure S11. Nickel activity and control assays with PPIX (A), CPI (B), and CPIII (C) and UPI (D)in 50 mM Tris pH 8.0, 150 mM NaCl; in addition to the control assays for UPIII (E). The PPIX assay was in 50 mM Tris pH 8.0, 150 mM NaCl, 10% (*v/v*) methanol.

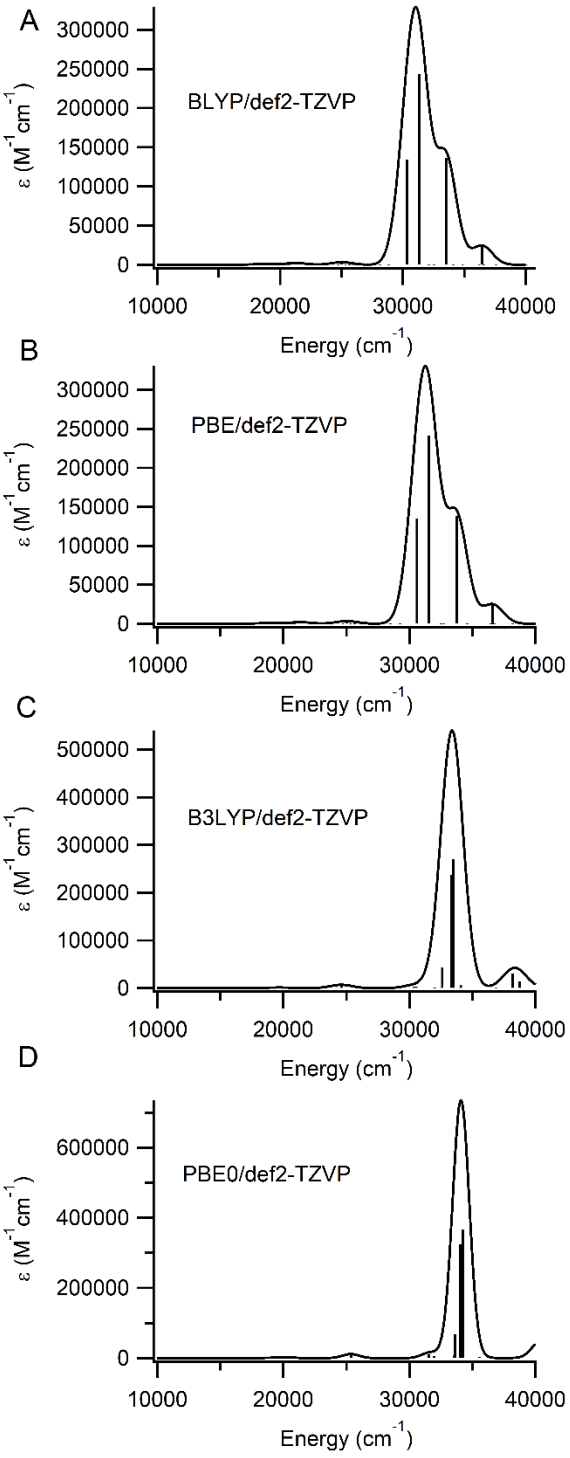

Figure S12. The predicted absorption spectra for neutral octamethylporphyrin using various functionals; BLYP (A), PBE (B), B3LYP (C), PBE0 (D) in order to identify an appropriate functional and basis set for the octamethyl porphyrin. The Q:Soret ratios of PBE, B3LYP, and PBE0 were 1:29, 1:40, 1:72, and 1:72, respectively. The BLYP-predicted ratio most closely agrees with the experimental ratio of 1:24.

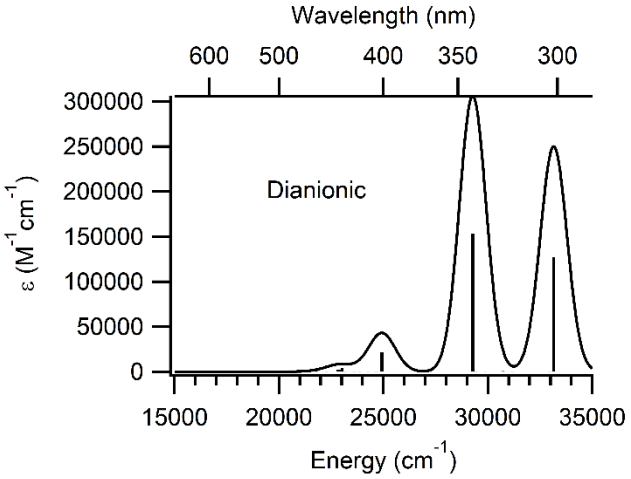

Figure S13. The BLYP-TDDFT predicted absorption spectrum of deprotonated octamethyl porphyrin. The Soret significantly red-shifted by 1,800 cm^{-1} and the Q-band region significantly changed. These spectral changes were not observed experimentally.

Table S1. cfbA (cbiX^S) gene sequence including N-terminal His$_6$-tag, linker, and TEV cleavage site. The polypeptide begins at S-1, after the S219V TEV cleavage.

M-32	G-31	H-30	H-29	H-28	H-27	H-26	H-25	D-24	Y-23	D-22	I-21
ATG	GGT	CAT	CAT	CAT	CAT	CAT	CAC	GAT	TAC	GAT	ATC
P-20	T-19	T-18	E-17	N-16	L-15	Y-14	F-16	Q-12	G-11	A-10	H-9
CCA	ACG	ACC	GAA	AAC	CTG	TAT	TTT	CAG	GGC	GCC	CAT
M-8	G-7	I-6	Q-5	R-4	S-3	T-2	S-1	T0	M1	R2	R3
ATG	GGA	ATT	CAA	AGG	CCT	ACG	TCG	ACC	ATG	CGT	CGC
G4	L5	V6	I7	V8	G9	H10	G11	S12	Q13	L14	N15
GGT	CTG	GTG	ATT	GTA	GGT	CAT	GGC	AGC	CAG	CTC	AAC
H16	Y17	R18	E19	V20	M21	E22	L23	H24	R25	K26	R27
CAC	TAC	CGT	GAG	GTT	ATG	GAA	CTC	CAC	CGG	AAA	CGT
I28	E29	E30	S31	G32	A33	F34	D35	E36	V37	K38	I39
ATT	GAA	GAA	TCA	GGC	GCC	TTT	GAT	GAA	GTC	AAA	ATT
A40	F41	A42	A43	R44	K45	R46	R47	P48	M49	P50	D51
GCC	TTT	GCG	GCG	CGC	AAA	CGC	CGG	CCG	ATG	CCA	GAC
E52	A53	I54	R55	E56	M57	N58	C59	D60	I61	I62	Y63
GAG	GCA	ATT	CGT	GAA	ATG	AAC	TGT	GAT	ATC	ATC	TAT
V64	V65	P66	L67	F68	I69	S70	Y71	G72	L73	H74	V75
GTC	GTG	CCA	TTA	TTC	ATC	TCG	TAT	GGT	CTT	CAT	GTT
T76	E77	D78	L79	P80	D81	L82	L83	G84	F85	P86	R87
ACC	GAG	GAC	CTG	CCT	GAT	CTT	CTG	GGC	TTT	CCG	CGC
G88	R89	G90	I91	K92	E93	G94	E95	F96	E97	G98	K99
GGT	CGC	GGG	ATC	AAA	GAG	GGC	GAG	TTC	GAA	GGC	AAA
K100	V101	V102	I103	C104	E105	P106	I107	G108	E109	D110	Y111
AAA	GTG	GTT	ATT	TGC	GAA	CCA	ATT	GGC	GAA	GAT	TAC
F112	V113	T114	Y115	A116	I117	L118	N119	S120	V121	F122	R123
TTT	GTG	ACT	TAT	GCA	ATT	CTG	AAC	TCG	GTA	TTC	CGC
I124	G125	R126	D127	G128	K129	G130	E131	E132			
ATT	GGT	CGC	GAT	GGC	AAA	GGT	GAG	GAA			

Table S2. The changes in Soret band intensity observed in the CfbA –tetrapyrrole UV/Vis Abs spectra.

ε ($M^{-1}cm^{-1}$)	Porphyrins	CfbA–porphyrin	Δ ε
UPI	$1.06x10^5$	$9.94x10^4$	-13100
UPIII	$1.06x10^5$	$9.29x10^4$	-13600
CPI	$1.16x10^5$	$1.06x10^5$	-10000
CPIII	$2.49x10^5$	$2.71x10^5$	+22000
PPIX	$1.72x10^5$	$2.14x10^5$	+42000

Table S3. Changes in Q-band transition energies observed for the tetrapyrroles upon the addition of CfbA.

Q-band (cm^{-1})	Porphyrins	CfbA–porphyrin	Δλ
UPI	16400, 17900, 18600, 19900	16300, 17800, 18500, 19900	-100, -100, -100, 0
UPIII	16300, 17900, 18600, 19900	16300, 17700, 18600, 19900	0, -200, 0, 0
CPI	16400, 17900, 18600, 20000	16400, 17800, 18600, 19900	0, -100, 0, -100
CPIII	16400, 18000, 18700 20000	16200, 17600, 18600, 19900	-200, -400, -100, -100
PPIX	15600, 17000,18600, 20700	15700, 17200, 18500, 19700	+100, +200, -100, -1000

References

1. Yin, J.; Xu, L. X.; Cherney, M. M.; Raux-Deery, E.; Bindley, A. A.; Savchenko, A.; Walker, J. R.; Cuff, M. E.; Warren, M. J.; James, M. N. G., Crystal structure of the vitamin B-12 biosynthetic cobaltochelatase, CbiX(S), from Archaeoglobus fulgidus. *J. Struct. Funct. Genomics* **2006**, *7*, 37-50

Geometry Optimized Coordinates: BLYP Protonated Model

C	-2.77863739330679	-1.35388648284353	0.08181194204246
C	-3.45469175696123	-2.66391637518981	0.09395113994764
C	-2.45537669937813	-3.60706053595191	0.10518052572536
C	-1.18650441152172	-2.85659312299248	0.09985020790616
N	-1.41188566841554	-1.50074973634926	0.08568893183253
C	-3.45829984447995	-0.12200083251168	0.06865003151742
C	0.08240010537495	-3.46444895308064	0.10917953679683
C	1.33561327370023	-2.84208644037830	0.10556352047388
C	2.64221192883155	-3.47175281787135	0.11833710747998
C	3.59773365266892	-2.46241343200429	0.10585335551374
C	2.89719766140810	-1.19268222587981	0.08486703976715
N	1.54672284082158	-1.47817526256034	0.08776812855187
C	3.44844067428806	0.09321559846750	0.06430063635009
C	2.76879620922741	1.32516077600814	0.04607831966678
C	3.44489445466784	2.63507328256750	0.02508625671086
C	2.44561724374676	3.57820249162596	0.01218454635071
C	1.17669253976437	2.82787433054748	0.02582586142463
N	1.40213022386468	1.47202170415145	0.04596967860795
C	-0.09211622723283	3.43577570233424	0.02020596162659
C	-1.34551971110096	2.81360950025809	0.03345739339524
C	-2.65193621801481	3.44330778069000	0.03291095858593
C	-3.60760848698251	2.43400404597903	0.04683119613623
C	-2.90733058800075	1.16424152153378	0.05597297091923
N	-1.55673683818044	1.44964511351491	0.04907725893609
C	-2.87410799169634	4.93057634745041	0.03454367604986
C	-5.10475887433428	2.57441262695395	0.06730935017729
C	-4.94453469027078	-2.87047976310209	0.09164644082926
C	-2.57622006370913	-5.10641698625929	0.12142451957832
C	2.86252952528782	-4.95893744297705	0.15334935587513

C	5.09520362236811	-2.60020397290911	0.12185394900841
C	4.93475438088887	2.84143681420870	0.02177484907994
C	2.56658300240951	5.07744167407514	-0.01018569793994
H	-4.54531258213237	-0.16630738100819	0.06870378789550
H	0.10090720170699	-4.55210363715762	0.12028608376598
H	0.80804867097390	-0.77713528757074	0.07059600291345
H	4.53546559201893	0.13717524421174	0.06180927588297
H	-0.11049726686234	4.52342647702705	0.00435289177990
H	-0.81839541187211	0.74806133815709	0.05086871311965
H	-2.26952762521960	5.42898881912054	-0.73515303538581
H	-2.59656378169539	5.37646365228425	1.00129669341901
H	-3.92478574866278	5.17674108907920	-0.15254331208373
H	-5.41135660992739	3.60676459874085	-0.13263633161605
H	-5.52089873247051	2.28885694666770	1.04494666745363
H	-5.57992872267845	1.93071889681227	-0.68518874610632
H	-5.42155432439119	-2.39015634147361	0.95852809644094
H	-5.20131586211876	-3.93565355523833	0.12063069861784
H	-5.41190400010118	-2.44086784754029	-0.80684131529841
H	-3.62540016675460	-5.42320548526033	0.10713689113613
H	-2.11016425692301	-5.54088509809599	1.01821147706193
H	-2.07959551013925	-5.56247343533533	-0.74751961412304
H	2.28906866016659	-5.46947361083131	-0.63247526771336
H	2.54497348253876	-5.38903931858273	1.11477479551697
H	3.91940457379576	-5.20897115232091	0.01253151985898
H	5.40095435596766	-3.64567860892434	0.00825264647914
H	5.52235336362650	-2.22998081417156	1.06555097477385
H	5.56074725309303	-2.02387169326256	-0.68948583380803
H	5.40989435267107	2.35088796095822	-0.84035508318199
H	5.40393523033264	2.42232164176432	0.92430848809953
H	5.19164698726194	3.90616993448146	-0.01987118542018

H	3.61574474652162	5.39361937532680	-0.03557348258627
H	2.10350157584034	5.53479749723272	0.87670689863601
H	2.06712749070068	5.51123509840430	-0.88888338645186

Geometry Optimized Coordinates: PBE Protonated Model

C	-2.75893068757527	-1.34539849853580	0.08203398582219
C	-3.43653216908122	-2.64646339786750	0.09411495501545
C	-2.43947871292660	-3.58927934104616	0.10568133205163
C	-1.17821055461159	-2.84064481603864	0.10038999400577
N	-1.39663420281272	-1.48843856023393	0.08588441404595
C	-3.44223971058541	-0.11994669731429	0.06953568289173
C	0.08392355580503	-3.45415595653982	0.11044894186166
C	1.33319691343222	-2.83273212984520	0.10494943681175
C	2.63426764121548	-3.46197461102466	0.12004813547879
C	3.58628814120578	-2.45348785118237	0.10577751376566
C	2.88323506274196	-1.19113400065145	0.08170714364972
N	1.53970448841629	-1.47524154366263	0.08408756690847
C	3.43235180035743	0.09141533399815	0.06091743544867
C	2.74848906689102	1.31666398997208	0.04437945648970
C	3.42611157038461	2.61733465865853	0.02287361951112
C	2.42948571649476	3.56056551455008	0.01199939615090
C	1.16801187970152	2.81223626748331	0.02726031654257
N	1.38616436373241	1.45986477954318	0.04656415595564
C	-0.09391633387566	3.42607358540348	0.02212945950819
C	-1.34342488397175	2.80494546796494	0.03470112761322
C	-2.64422547515435	3.43398420638286	0.03347469580874
C	-3.59612365120502	2.42503463525078	0.04701196049580
C	-2.89286060428816	1.16280142480812	0.05637060810448
N	-1.54938498538654	1.44709393331905	0.05015857590692
C	-2.86525372296428	4.91184822922726	0.03550380580190

C	-5.08374717958257	2.56044173109542	0.06751281839708
C	-4.91730030925085	-2.84827650377033	0.08551717874861
C	-2.55990214981916	-5.07885115473033	0.11522746330706
C	2.85403736920996	-4.93953085110343	0.16025552576832
C	5.07416716789784	-2.58708064648747	0.12714470755671
C	4.90708790922045	2.81764242172365	0.01701392661975
C	2.55014195829789	5.04998994503568	-0.00749784424723
H	-4.53299744498181	-0.16822264776681	0.07042091325858
H	0.09899659542477	-4.54575530376645	0.12527642313108
H	0.79731730845772	-0.77507551031846	0.06403124040925
H	4.52300787428685	0.14019540375773	0.05756966577961
H	-0.10866037705753	4.51773460687650	0.00680903667095
H	-0.80503429652481	0.74874383634494	0.05485515905308
H	-2.24843514215425	5.41428828057373	-0.72450899549086
H	-2.60047759730310	5.35667924571992	1.00853535514992
H	-3.91543028071934	5.15845033716696	-0.16522690309191
H	-5.39254340834981	3.59392389941579	-0.13315961341018
H	-5.50008781573486	2.27478408756042	1.04707750023843
H	-5.55935990558064	1.91284462379986	-0.68407036175377
H	-5.40564275663043	-2.31221005987539	0.91490188795259
H	-5.17859161128266	-3.91094302251155	0.17502576420273
H	-5.37363313261814	-2.47219003337851	-0.84493038392418
H	-3.60915896907570	-5.39433904450773	0.18178373209051
H	-2.02034163413184	-5.52515775051039	0.96587843750211
H	-2.13588416137958	-5.52734765615408	-0.79814566542010
H	2.25318174197895	-5.45883884228299	-0.60133140027570
H	2.56789426308653	-5.36193228693455	1.13708407060917
H	3.90787582436232	-5.19111894117623	-0.01274342298648
H	5.38345363264296	-3.62822249802097	-0.02723901864928
H	5.49423079741252	-2.25565246061938	1.09058636035404

H	5.54596828102095	-1.97335231902785	-0.65492932914438
H	5.38213134072533	2.31545937544286	-0.84117651039196
H	5.37731957746593	2.40368052803701	0.92401238692067
H	5.16838536397134	3.88278484089589	-0.03440419212600
H	3.60055711333038	5.36517163939693	-0.05431567955257
H	2.10595678500044	5.50624832003871	0.89221985161373
H	2.02933157344401	5.48869001844152	-0.87377884251597

Geometry Optimized Coordinates: PBE0 Protonated Model

C	-2.73940568708588	-1.32583987231343	0.13098738320255
C	-3.41414448906222	-2.61775419366290	0.08083669758795
C	-2.42556031044488	-3.54970526236265	0.03869344471403
C	-1.17353848073781	-2.81120530561642	0.08020763311334
N	-1.38995503703289	-1.47117178791298	0.12719501435062
C	-3.41629530242921	-0.10555816023688	0.16375051506040
C	0.07209421022034	-3.43802972927751	0.08449131689497
C	1.31367497678125	-2.82383126356361	0.12793685777739
C	2.61040272023769	-3.43693004327907	0.14362788616807
C	3.54123713138141	-2.42598424957470	0.17650340118251
C	2.83349398540433	-1.18221410455356	0.16564443976854
N	1.50449400835983	-1.47535248363727	0.15144761844461
C	3.38596967669120	0.08765487923455	0.13226875811654
C	2.70796731045840	1.30194214288432	0.07732511526814
C	3.39059285156575	2.58802592165479	0.01209964105869
C	2.40918762043022	3.52695108093381	-0.00740754685612
C	1.15221656763716	2.79035547077680	0.03056428978633
N	1.36009417531308	1.45129974042146	0.08125302300943
C	-0.09332236371862	3.41287458549847	0.01375809212966
C	-1.32997268466343	2.79026677996499	0.05174597429715
C	-2.61911577646523	3.41677546600830	0.06191282516246

C	-3.56128934996893	2.41866886643213	0.13425177522788
C	-2.86224862355041	1.16405739485055	0.14519755485156
N	-1.53080981540191	1.44605755862158	0.10164137389906
C	-2.82897072680218	4.88838934238345	0.00426754835119
C	-5.04130286747237	2.55394294234752	0.18623688161434
C	-4.88366110858707	-2.85970050927271	0.05521713532502
C	-2.55912012213142	-5.02925081409035	-0.03767606296202
C	2.88729624857067	-4.89908211845058	0.12740262465938
C	5.02165301559645	-2.55436309630553	0.19770110844608
C	4.86555363217571	2.77595450790869	-0.03140555583446
C	2.53257159701120	5.00749321569018	-0.06145111845231
H	-4.49911000701661	-0.14418535910010	0.18895503242369
H	0.07376029823163	-4.52121700449726	0.04974397319502
H	0.75669324060900	-0.79554052377168	0.13482426152106
H	4.46906785100343	0.13034784064611	0.13411472457546
H	-0.10512525272122	4.49571196230344	-0.02903573470861
H	-0.79136534854745	0.75713018512785	0.09571614166327
H	-2.12994399989833	5.35757551316214	-0.69118818430688
H	-2.66886863255420	5.35492342275684	0.98117296283184
H	-3.83927093813458	5.13232759726843	-0.32544737301706
H	-5.33535048515617	3.56355596229352	0.47404987120281
H	-5.47615263574439	1.86172524977928	0.91007220232540
H	-5.49765287845979	2.33101994788148	-0.78337078176220
H	-5.44671412042036	-2.00853781824581	0.44117114054672
H	-5.14813197930917	-3.72868977611220	0.66105626436545
H	-5.24074738589256	-3.05668238128477	-0.96092779311186
H	-3.56983800530763	-5.31871362828749	-0.33022119154248
H	-2.33766681768495	-5.50418043464746	0.92389508800124
H	-1.86800881270691	-5.45676575891917	-0.76784262276565
H	2.00547012393189	-5.47635307667615	-0.15242704589943

H	3.22029367592132	-5.25003203160692	1.10926594853619
H	3.68030523605488	-5.13767210877551	-0.58413293986079
H	5.32463819725327	-3.53817915195989	0.55915553177838
H	5.47650185684453	-1.80414278875734	0.84704285065294
H	5.44842058934249	-2.41627902572429	-0.80073657493685
H	5.33381221149051	2.07968733451471	-0.73133640459200
H	5.32490274517564	2.59938880284349	0.94644675450197
H	5.12680492008784	3.78669388460862	-0.34780697752294
H	3.54474138306382	5.33112590856320	0.18417416794448
H	1.85061351117175	5.49053941134469	0.64220208610120
H	2.28596328809210	5.39530117477080	-1.05552606550335

Geometry Optimized Coordinates: B3LYP Protonated Model

C	-2.75738017081285	-1.33447548023373	0.12802495001923
C	-3.43061772404491	-2.63435383138286	0.08153316056957
C	-2.43965854509652	-3.56761861694327	0.04007337013316
C	-1.18060449217087	-2.82777428658603	0.08025575837359
N	-1.40299871236194	-1.48317969986883	0.12438530429190
C	-3.43123281333855	-0.10853774684884	0.15759797481443
C	0.07272003118308	-3.44707065900221	0.08558454715656
C	1.31867445365524	-2.83272225648091	0.12544054383741
C	2.62034889539395	-3.44740419012557	0.14380335702582
C	3.55644939486387	-2.43649826263842	0.17336131020928
C	2.85246400780586	-1.18474146737773	0.15729003136078
N	1.51603226593980	-1.47776302105211	0.14394287126102
C	3.40428453443935	0.08975627823839	0.12199807628382
C	2.72918085948500	1.31023560861881	0.07097659774432
C	3.40895732891162	2.60531654272570	0.00741685611518
C	2.42424902035401	3.54482021231267	-0.00209364329487
C	1.16069435914348	2.80624258228377	0.03515592039174

N	1.37612095148322	1.46261838909598	0.07942730197160
C	-0.09244836674967	3.42222748743477	0.02161481101685
C	-1.33407031336126	2.80055457594331	0.05480587366383
C	-2.62953442088753	3.42648615497580	0.06161882446316
C	-3.57501260969723	2.42657928420461	0.12942244809884
C	-2.87785829882826	1.16545339467016	0.14066006987665
N	-1.53945431548843	1.44941789923776	0.10131649736811
C	-2.84666695666554	4.90545114001997	0.00711020507915
C	-5.06278286752675	2.56827386262522	0.17517985212891
C	-4.90823466699115	-2.87803338544906	0.05733069086106
C	-2.57658889606143	-5.05513970733147	-0.03358319024194
C	2.89642768123005	-4.91823149938787	0.13589390405052
C	5.04429070134460	-2.57436092411962	0.19714200794972
C	4.89101500602995	2.80112547609687	-0.04192084193268
C	2.55093545596307	5.03362245056742	-0.04722953096500
H	-4.51242146678492	-0.14673925316728	0.18004706374512
H	0.07848728063616	-4.52871259369328	0.05513710971062
H	0.77209965812146	-0.79445351857185	0.12449597262900
H	4.48573532265124	0.13148180492677	0.12201631087201
H	-0.10697938198591	4.50358069981942	-0.01651879483092
H	-0.80214350110413	0.75880342890323	0.09831681385697
H	-2.15571431843449	5.37996789349501	-0.69181672820911
H	-2.68432714490625	5.37177570225029	0.98342680461847
H	-3.85951117896328	5.14540041407836	-0.31486744585729
H	-5.35434480539196	3.58030586216453	0.45360340193815
H	-5.50371695693930	1.88430770576981	0.90234309335768
H	-5.51712616270257	2.34136776044196	-0.79408934251395
H	-5.46996136111295	-2.02947136564875	0.44867698161304
H	-5.17245545566267	-3.74930695813914	0.65888132927908
H	-5.26846628087944	-3.06798855524155	-0.95865118105849

H	-3.58951082221642	-5.34413538602914	-0.31570409374968
H	-2.34820505599476	-5.53014304167540	0.92598338807886
H	-1.89392328952412	-5.48496051160146	-0.76957069602802
H	2.01474480889993	-5.49589749173257	-0.14005716676051
H	3.22753766595461	-5.26529501106607	1.11930478226211
H	3.68771082459969	-5.16378838617214	-0.57436258602037
H	5.34145400825548	-3.55891009130269	0.55890199346154
H	5.50291241873087	-1.82801212559787	0.84730186778573
H	5.47482960830865	-2.44040497419668	-0.79987616350148
H	5.35891224026957	2.11827005612504	-0.75442440920249
H	5.35730921370652	2.61330809121526	0.93022228062767
H	5.14671554522666	3.81675693604487	-0.34407698246516
H	3.56655993897011	5.35338230856777	0.18540931702631
H	1.88167171832884	5.51344045751194	0.66995397393872
H	2.29225496380015	5.43041406929896	-1.03425784628534

Geometry Optmized Coordinates: BLYP Deprotonated Model

C	-2.80104422165809	-1.37058946483696	0.10432970082674
C	-3.47963781980575	-2.68585056930337	0.09268057944889
C	-2.47601239421489	-3.63462411105160	0.08595653218334
C	-1.20113727109828	-2.88311977147880	0.08923516789873
N	-1.44369415036390	-1.53726728582855	0.10467004878123
C	-3.45274484223004	-0.11115609151653	0.10378773691925
C	0.09280308843681	-3.46296376501342	0.07854701707578
C	1.35244013232533	-2.81261666835489	0.05754645390001
C	2.66734795612344	-3.48960190157938	0.10767963656490
C	3.61599829758496	-2.48596109239062	0.08985696120868
C	2.86491310755556	-1.21233550893165	0.02845594600953
N	1.51960224322266	-1.45657293300359	0.00196499210934
C	3.44327553334182	0.08212657847832	0.01698871625867

C	2.79182499152389	1.34160348512939	0.01414599005553
C	3.47044868035171	2.65685827611767	0.01717296394728
C	2.46667878015505	3.60565972946438	0.02376543308466
C	1.19176852028428	2.85404340571260	0.02823464077517
N	1.43451015613928	1.50824548285969	0.01920863803564
C	-0.10230609418870	3.43373409354199	0.04046639304626
C	-1.36200859600483	2.78353386786600	0.06521540598139
C	-2.67727958239740	3.46122178909532	0.03365037486956
C	-3.62593860562279	2.45761275744800	0.05176039173718
C	-2.87466854561956	1.18332065622236	0.09521878459250
N	-1.52912223928355	1.42708406847398	0.10844042346778
C	-2.89681566919400	4.95205780679445	-0.00725837382615
C	-5.12734743640136	2.59213781835843	0.03605279697897
C	-4.97124627136066	-2.90219186050755	0.08551126979306
C	-2.61040543469277	-5.13598378893286	0.06840855054001
C	2.88580603641538	-4.97908352316696	0.18531739914580
C	5.11673049539198	-2.61934481814093	0.14173173565440
C	4.96199568771033	2.87444089134919	0.01388976709694
C	2.60027871672103	5.10717473941776	0.03107428184923
H	-4.54348431883974	-0.14289910992290	0.09568273979460
H	0.12366946636821	-4.55365201452461	0.09569045343664
H	4.53403856018973	0.11335074525674	0.02618817834585
H	-0.13314775140866	4.52441280647808	0.02314267594076
H	-2.33736362527252	5.42535653424138	-0.82823147273421
H	-2.56298109115404	5.44234843586772	0.92122896701738
H	-3.95657359713323	5.20292145417093	-0.14378070650938
H	-5.44049731916913	3.63367440801176	-0.11170475245147
H	-5.58082888474757	2.24608786828053	0.97861504738080
H	-5.58311006583969	1.99376687233664	-0.76729002856397
H	-5.45929007910976	-2.42678164955729	0.95005936848481

H	-5.22865028573712	-3.96884685428709	0.11287370558263
H	-5.44360425412302	-2.47431423082104	-0.81267603729804
H	-3.66146273358218	-5.44909324337372	0.10942643520336
H	-2.09450743673372	-5.60324188927502	0.92143654627643
H	-2.17244155878592	-5.57715861504089	-0.84067794778620
H	2.36994936813012	-5.51142995160337	-0.62833994688965
H	2.50245371500688	-5.40232003881589	1.12738406430450
H	3.95086882115611	-5.23685215869599	0.12311450792379
H	5.43301563806017	-3.66880510558419	0.08483261384158
H	5.53512394168546	-2.20261919244270	1.07178509346009
H	5.60378083520824	-2.08315134125779	-0.68686596630772
H	5.44148137627163	2.41479039022891	-0.86427033533876
H	5.44310030529361	2.43100346422809	0.89968829217569
H	5.21660802725898	3.94197272973895	0.00414311422257
H	3.65162725496907	5.42097099638295	0.00585982724239
H	2.14593381658477	5.55543584291464	0.92846033208432
H	2.09945418030636	5.56717473577328	-0.83490800484911

Frequency Mode: Mode 6

* (null), Energy -1000.0000000

C	-2.778637	-1.353886	0.081812	0.003384	-0.000376	0.034392
C	-3.454692	-2.663916	0.093951	0.000998	0.002114	0.145598
C	-2.455377	-3.607061	0.105181	-0.000830	0.000790	0.179782
C	-1.186504	-2.856593	0.099850	0.000924	-0.002834	0.084166
N	-1.411886	-1.500750	0.085689	0.003574	-0.003176	0.013000
C	-3.458300	-0.122001	0.068650	0.004284	-0.001296	-0.056708
C	0.082400	-3.464449	0.109180	0.001220	-0.004536	0.038636
C	1.335613	-2.842086	0.105564	-0.000040	-0.002858	-0.018328
C	2.642212	-3.471753	0.118337	0.001956	-0.003712	-0.167128
C	3.597734	-2.462413	0.105853	0.000052	-0.002290	-0.160736

C	2.897198	-1.192682	0.084867	-0.003018	-0.000548	-0.008098
N	1.546723	-1.478175	0.087768	-0.002322	-0.001850	0.049926
C	3.448441	0.093216	0.064301	-0.003130	-0.000184	0.058118
C	2.768796	1.325161	0.046078	-0.002038	0.001296	0.096136
C	3.444894	2.635073	0.025086	-0.000028	0.001660	0.186902
C	2.445617	3.578202	0.012185	0.001360	0.002484	0.145800
C	1.176693	2.827874	0.025826	-0.000100	0.002902	0.034760
N	1.402130	1.472022	0.045970	-0.001670	0.001884	0.020478
C	-0.092116	3.435776	0.020206	0.000478	0.002862	-0.061976
C	-1.345520	2.813610	0.033457	-0.000096	0.001982	-0.128724
C	-2.651936	3.443308	0.032911	-0.000640	-0.000912	-0.164442
C	-3.607608	2.434004	0.046831	0.000832	-0.002954	-0.160298
C	-2.907331	1.164242	0.055973	0.002722	-0.000970	-0.124278
N	-1.556737	1.449645	0.049077	0.002248	0.001602	-0.113340
C	-2.874108	4.930576	0.034544	-0.010180	-0.002242	-0.180680
C	-5.104759	2.574413	0.067309	0.000922	0.000260	-0.168528
C	-4.944535	-2.870480	0.091646	0.000576	0.004574	0.229066
C	-2.576220	-5.106417	0.121425	-0.004082	0.002998	0.326346
C	2.862530	-4.958937	0.153349	-0.002914	-0.008576	-0.344392
C	5.095204	-2.600204	0.121854	0.002812	0.004320	-0.336754
C	4.934754	2.841437	0.021775	0.000164	0.002036	0.320796
C	2.566583	5.077442	-0.010186	0.005280	0.002922	0.213330
H	-4.545313	-0.166307	0.068704	0.004316	-0.001806	-0.055702
H	0.100907	-4.552104	0.120286	0.003112	-0.005200	0.024426
H	0.808049	-0.777135	0.070596	-0.005922	-0.000328	0.266488
H	4.535466	0.137175	0.061809	-0.003214	-0.000828	0.058270
H	-0.110497	4.523426	0.004353	0.002182	0.003010	-0.065962
H	-0.818395	0.748061	0.050869	0.004332	0.003764	-0.197066
H	-2.269528	5.428989	-0.735153	0.102026	0.010544	-0.083076
H	-2.596564	5.376464	1.001297	-0.162702	-0.010190	-0.132788

H	-3.924786	5.176741	-0.152543	0.015980	-0.008890	-0.336580
H	-5.411357	3.606765	-0.132636	0.001830	-0.023666	-0.293376
H	-5.520899	2.288857	1.044947	0.006434	0.123904	-0.129616
H	-5.579929	1.930719	-0.685189	-0.004876	-0.091816	-0.085022
H	-5.421554	-2.390156	0.958528	0.061518	-0.073956	0.306936
H	-5.201316	-3.935654	0.120631	0.001432	0.002396	0.153280
H	-5.411904	-2.440868	-0.806841	-0.062520	0.087040	0.301932
H	-3.625400	-5.423205	0.107137	0.000304	-0.000890	0.093400
H	-2.110164	-5.540885	1.018211	-0.237804	0.111558	0.501542
H	-2.079596	-5.562473	-0.747520	0.225824	-0.098320	0.512650
H	2.289069	-5.469474	-0.632475	0.106656	0.104564	-0.499322
H	2.544973	-5.389039	1.114775	-0.141618	-0.145434	-0.452058
H	3.919405	-5.208971	0.012532	0.015292	0.009582	-0.232614
H	5.400954	-3.645679	0.008253	-0.010312	-0.017938	-0.159868
H	5.522353	-2.229981	1.065551	0.133926	0.208046	-0.476864
H	5.560747	-2.023872	-0.689486	-0.112108	-0.167020	-0.525796
H	5.409894	2.350888	-0.840355	0.088052	-0.062072	0.405726
H	5.403935	2.422322	0.924308	-0.091380	0.069524	0.399776
H	5.191647	3.906170	-0.019871	0.004032	-0.000800	0.268954
H	3.615745	5.393619	-0.035573	0.006554	0.001360	0.244634
H	2.103502	5.534797	0.876707	-0.007234	-0.035460	0.226658
H	2.067127	5.511235	-0.888883	0.020078	0.043652	0.225036

* Frequency(6) 22.1800

C	-2.778252	-1.353929	0.085720	0.003384	-0.000376	0.034392
C	-3.454579	-2.663676	0.110497	0.000998	0.002114	0.145598
C	-2.455471	-3.606971	0.125612	-0.000830	0.000790	0.179782
C	-1.186399	-2.856915	0.109415	0.000924	-0.002834	0.084166
N	-1.411480	-1.501111	0.087166	0.003574	-0.003176	0.013000
C	-3.457813	-0.122148	0.062205	0.004284	-0.001296	-0.056708
C	0.082539	-3.464964	0.113571	0.001220	-0.004536	0.038636

C	1.335608	-2.842411	0.103481	-0.000040	-0.002858	-0.018328
C	2.642434	-3.472175	0.099344	0.001956	-0.003712	-0.167128
C	3.597740	-2.462673	0.087586	0.000052	-0.002290	-0.160736
C	2.896855	-1.192744	0.083947	-0.003018	-0.000548	-0.008098
N	1.546459	-1.478385	0.093442	-0.002322	-0.001850	0.049926
C	3.448085	0.093195	0.070906	-0.003130	-0.000184	0.058118
C	2.768564	1.325308	0.057003	-0.002038	0.001296	0.096136
C	3.444891	2.635262	0.046326	-0.000028	0.001660	0.186902
C	2.445772	3.578484	0.028754	0.001360	0.002484	0.145800
C	1.176682	2.828204	0.029776	-0.000100	0.002902	0.034760
N	1.401940	1.472236	0.048297	-0.001670	0.001884	0.020478
C	-0.092062	3.436101	0.013163	0.000478	0.002862	-0.061976
C	-1.345531	2.813835	0.018828	-0.000096	0.001982	-0.128724
C	-2.652009	3.443204	0.014223	-0.000640	-0.000912	-0.164442
C	-3.607513	2.433668	0.028614	0.000832	-0.002954	-0.160298
C	-2.907022	1.164132	0.041849	0.002722	-0.000970	-0.124278
N	-1.556482	1.449827	0.036196	0.002248	0.001602	-0.113340
C	-2.875265	4.930321	0.014011	-0.010180	-0.002242	-0.180680
C	-5.104654	2.574443	0.048157	0.000922	0.000260	-0.168528
C	-4.944470	-2.869960	0.117678	0.000576	0.004574	0.229066
C	-2.576684	-5.106076	0.158513	-0.004082	0.002998	0.326346
C	2.862199	-4.959912	0.114211	-0.002914	-0.008576	-0.344392
C	5.095524	-2.599713	0.083584	0.002812	0.004320	-0.336754
C	4.934773	2.841668	0.058232	0.000164	0.002036	0.320796
C	2.567183	5.077774	0.014058	0.005280	0.002922	0.213330
H	-4.544823	-0.166512	0.062374	0.004316	-0.001806	-0.055702
H	0.101261	-4.552695	0.123062	0.003112	-0.005200	0.024426
H	0.807376	-0.777172	0.100881	-0.005922	-0.000328	0.266488
H	4.535101	0.137081	0.068431	-0.003214	-0.000828	0.058270
H	-0.110249	4.523768	-0.003143	0.002182	0.003010	-0.065962

H	-0.817903	0.748489	0.028473	0.004332	0.003764	-0.197066
H	-2.257933	5.430187	-0.744594	0.102026	0.010544	-0.083076
H	-2.615054	5.375306	0.986206	-0.162702	-0.010190	-0.132788
H	-3.922970	5.175731	-0.190794	0.015980	-0.008890	-0.336580
H	-5.411149	3.604075	-0.165977	0.001830	-0.023666	-0.293376
H	-5.520168	2.302938	1.030217	0.006434	0.123904	-0.129616
H	-5.580483	1.920285	-0.694851	-0.004876	-0.091816	-0.085022
H	-5.414563	-2.398561	0.993410	0.061518	-0.073956	0.306936
H	-5.201153	-3.935382	0.138050	0.001432	0.002396	0.153280
H	-5.419009	-2.430976	-0.772528	-0.062520	0.087040	0.301932
H	-3.625365	-5.423306	0.117751	0.000304	-0.000890	0.093400
H	-2.137189	-5.528207	1.075209	-0.237804	0.111558	0.501542
H	-2.053932	-5.573647	-0.689260	0.225824	-0.098320	0.512650
H	2.301190	-5.457591	-0.689220	0.106656	0.104564	-0.499322
H	2.528879	-5.405567	1.063401	-0.141618	-0.145434	-0.452058
H	3.921143	-5.207882	-0.013903	0.015292	0.009582	-0.232614
H	5.399782	-3.647718	-0.009915	-0.010312	-0.017938	-0.159868
H	5.537573	-2.206338	1.011358	0.133926	0.208046	-0.476864
H	5.548007	-2.042853	-0.749240	-0.112108	-0.167020	-0.525796
H	5.419901	2.343834	-0.794246	0.088052	-0.062072	0.405726
H	5.393550	2.430223	0.969740	-0.091380	0.069524	0.399776
H	5.192105	3.906079	0.010694	0.004032	-0.000800	0.268954
H	3.616490	5.393774	-0.007772	0.006554	0.001360	0.244634
H	2.102680	5.530767	0.902466	-0.007234	-0.035460	0.226658
H	2.069409	5.516196	-0.863309	0.020078	0.043652	0.225036

* Frequency(6) 22.1800

C	-2.777910	-1.353967	0.089205	0.003384	-0.000376	0.034392
C	-3.454477	-2.663462	0.125251	0.000998	0.002114	0.145598
C	-2.455555	-3.606891	0.143830	-0.000830	0.000790	0.179782
C	-1.186305	-2.857202	0.117944	0.000924	-0.002834	0.084166

N	-1.411118	-1.501433	0.088484	0.003574	-0.003176	0.013000
C	-3.457379	-0.122280	0.056459	0.004284	-0.001296	-0.056708
C	0.082662	-3.465424	0.117486	0.001220	-0.004536	0.038636
C	1.335604	-2.842700	0.101624	-0.000040	-0.002858	-0.018328
C	2.642632	-3.472551	0.082409	0.001956	-0.003712	-0.167128
C	3.597745	-2.462905	0.071299	0.000052	-0.002290	-0.160736
C	2.896549	-1.192800	0.083126	-0.003018	-0.000548	-0.008098
N	1.546224	-1.478573	0.098501	-0.002322	-0.001850	0.049926
C	3.447768	0.093176	0.076795	-0.003130	-0.000184	0.058118
C	2.768358	1.325440	0.066745	-0.002038	0.001296	0.096136
C	3.444888	2.635430	0.065265	-0.000028	0.001660	0.186902
C	2.445909	3.578736	0.043528	0.001360	0.002484	0.145800
C	1.176672	2.828498	0.033299	-0.000100	0.002902	0.034760
N	1.401771	1.472427	0.050372	-0.001670	0.001884	0.020478
C	-0.092013	3.436391	0.006883	0.000478	0.002862	-0.061976
C	-1.345541	2.814036	0.005785	-0.000096	0.001982	-0.128724
C	-2.652074	3.443112	-0.002440	-0.000640	-0.000912	-0.164442
C	-3.607429	2.433369	0.012371	0.000832	-0.002954	-0.160298
C	-2.906746	1.164033	0.029256	0.002722	-0.000970	-0.124278
N	-1.556254	1.449989	0.024712	0.002248	0.001602	-0.113340
C	-2.876296	4.930094	-0.004298	-0.010180	-0.002242	-0.180680
C	-5.104561	2.574469	0.031080	0.000922	0.000260	-0.168528
C	-4.944411	-2.869497	0.140889	0.000576	0.004574	0.229066
C	-2.577098	-5.105773	0.191581	-0.004082	0.002998	0.326346
C	2.861904	-4.960781	0.079314	-0.002914	-0.008576	-0.344392
C	5.095809	-2.599275	0.049460	0.002812	0.004320	-0.336754
C	4.934789	2.841875	0.090738	0.000164	0.002036	0.320796
C	2.567718	5.078070	0.035674	0.005280	0.002922	0.213330
H	-4.544385	-0.166695	0.056729	0.004316	-0.001806	-0.055702
H	0.101576	-4.553222	0.125537	0.003112	-0.005200	0.024426

H	0.806776	-0.777206	0.127884	-0.005922	-0.000328	0.266488
H	4.534775	0.136997	0.074336	-0.003214	-0.000828	0.058270
H	-0.110028	4.524073	-0.009827	0.002182	0.003010	-0.065962
H	-0.817464	0.748870	0.008505	0.004332	0.003764	-0.197066
H	-2.247595	5.431256	-0.753012	0.102026	0.010544	-0.083076
H	-2.631541	5.374273	0.972751	-0.162702	-0.010190	-0.132788
H	-3.921351	5.174830	-0.224899	0.015980	-0.008890	-0.336580
H	-5.410964	3.601677	-0.195704	0.001830	-0.023666	-0.293376
H	-5.519516	2.315493	1.017083	0.006434	0.123904	-0.129616
H	-5.580977	1.910981	-0.703467	-0.004876	-0.091816	-0.085022
H	-5.408329	-2.406055	1.024511	0.061518	-0.073956	0.306936
H	-5.201008	-3.935139	0.153582	0.001432	0.002396	0.153280
H	-5.425344	-2.422157	-0.741933	-0.062520	0.087040	0.301932
H	-3.625335	-5.423396	0.127216	0.000304	-0.000890	0.093400
H	-2.161286	-5.516903	1.126030	-0.237804	0.111558	0.501542
H	-2.031050	-5.583609	-0.637313	0.225824	-0.098320	0.512650
H	2.311997	-5.446995	-0.739816	0.106656	0.104564	-0.499322
H	2.514529	-5.420304	1.017594	-0.141618	-0.145434	-0.452058
H	3.922692	-5.206911	-0.037474	0.015292	0.009582	-0.232614
H	5.398737	-3.649535	-0.026115	-0.010312	-0.017938	-0.159868
H	5.551144	-2.185256	0.963037	0.133926	0.208046	-0.476864
H	5.536647	-2.059777	-0.802519	-0.112108	-0.167020	-0.525796
H	5.428823	2.337544	-0.753134	0.088052	-0.062072	0.405726
H	5.384291	2.437268	1.010250	-0.091380	0.069524	0.399776
H	5.192514	3.905998	0.037947	0.004032	-0.000800	0.268954
H	3.617154	5.393911	0.017017	0.006554	0.001360	0.244634
H	2.101947	5.527174	0.925433	-0.007234	-0.035460	0.226658
H	2.071443	5.520619	-0.840506	0.020078	0.043652	0.225036
* Frequency(6)	22.1800					
C	-2.777645	-1.353996	0.091889	0.003384	-0.000376	0.034392

C	-3.454400	-2.663297	0.136612	0.000998	0.002114	0.145598
C	-2.455620	-3.606830	0.157859	-0.000830	0.000790	0.179782
C	-1.186233	-2.857423	0.124511	0.000924	-0.002834	0.084166
N	-1.410839	-1.501681	0.089498	0.003574	-0.003176	0.013000
C	-3.457045	-0.122381	0.052034	0.004284	-0.001296	-0.056708
C	0.082757	-3.465778	0.120501	0.001220	-0.004536	0.038636
C	1.335601	-2.842923	0.100194	-0.000040	-0.002858	-0.018328
C	2.642785	-3.472841	0.069367	0.001956	-0.003712	-0.167128
C	3.597749	-2.463084	0.058756	0.000052	-0.002290	-0.160736
C	2.896314	-1.192843	0.082494	-0.003018	-0.000548	-0.008098
N	1.546043	-1.478717	0.102397	-0.002322	-0.001850	0.049926
C	3.447524	0.093162	0.081330	-0.003130	-0.000184	0.058118
C	2.768199	1.325541	0.074247	-0.002038	0.001296	0.096136
C	3.444886	2.635559	0.079850	-0.000028	0.001660	0.186902
C	2.446015	3.578930	0.054906	0.001360	0.002484	0.145800
C	1.176664	2.828724	0.036011	-0.000100	0.002902	0.034760
N	1.401641	1.472574	0.051970	-0.001670	0.001884	0.020478
C	-0.091976	3.436615	0.002047	0.000478	0.002862	-0.061976
C	-1.345548	2.814191	-0.004260	-0.000096	0.001982	-0.128724
C	-2.652124	3.443041	-0.015272	-0.000640	-0.000912	-0.164442
C	-3.607364	2.433138	-0.000138	0.000832	-0.002954	-0.160298
C	-2.906533	1.163958	0.019559	0.002722	-0.000970	-0.124278
N	-1.556078	1.450114	0.015867	0.002248	0.001602	-0.113340
C	-2.877091	4.929919	-0.018397	-0.010180	-0.002242	-0.180680
C	-5.104489	2.574489	0.017929	0.000922	0.000260	-0.168528
C	-4.944366	-2.869140	0.158764	0.000576	0.004574	0.229066
C	-2.577416	-5.105539	0.217047	-0.004082	0.002998	0.326346
C	2.861676	-4.961450	0.052439	-0.002914	-0.008576	-0.344392
C	5.096028	-2.598938	0.023182	0.002812	0.004320	-0.336754
C	4.934802	2.842034	0.115771	0.000164	0.002036	0.320796

C	2.568130	5.078298	0.052321	0.005280	0.002922	0.213330
H	-4.544048	-0.166836	0.052383	0.004316	-0.001806	-0.055702
H	0.101819	-4.553628	0.127443	0.003112	-0.005200	0.024426
H	0.806314	-0.777231	0.148679	-0.005922	-0.000328	0.266488
H	4.534524	0.136932	0.078883	-0.003214	-0.000828	0.058270
H	-0.109858	4.524308	-0.014974	0.002182	0.003010	-0.065962
H	-0.817126	0.749164	-0.006873	0.004332	0.003764	-0.197066
H	-2.239634	5.432078	-0.759495	0.102026	0.010544	-0.083076
H	-2.644237	5.373478	0.962389	-0.162702	-0.010190	-0.132788
H	-3.920104	5.174136	-0.251164	0.015980	-0.008890	-0.336580
H	-5.410821	3.599831	-0.218598	0.001830	-0.023666	-0.293376
H	-5.519014	2.325162	1.006968	0.006434	0.123904	-0.129616
H	-5.581358	1.903816	-0.710101	-0.004876	-0.091816	-0.085022
H	-5.403529	-2.411826	1.048463	0.061518	-0.073956	0.306936
H	-5.200896	-3.934952	0.165543	0.001432	0.002396	0.153280
H	-5.430223	-2.415365	-0.718372	-0.062520	0.087040	0.301932
H	-3.625311	-5.423466	0.134504	0.000304	-0.000890	0.093400
H	-2.179843	-5.508198	1.165167	-0.237804	0.111558	0.501542
H	-2.013428	-5.591282	-0.597309	0.225824	-0.098320	0.512650
H	2.320320	-5.438836	-0.778780	0.106656	0.104564	-0.499322
H	2.503478	-5.431652	0.982318	-0.141618	-0.145434	-0.452058
H	3.923886	-5.206163	-0.055626	0.015292	0.009582	-0.232614
H	5.397932	-3.650935	-0.038590	-0.010312	-0.017938	-0.159868
H	5.561594	-2.169022	0.925826	0.133926	0.208046	-0.476864
H	5.527898	-2.072810	-0.843549	-0.112108	-0.167020	-0.525796
H	5.435694	2.332700	-0.721474	0.088052	-0.062072	0.405726
H	5.377160	2.442693	1.041446	-0.091380	0.069524	0.399776
H	5.192828	3.905936	0.058935	0.004032	-0.000800	0.268954
H	3.617665	5.394017	0.036107	0.006554	0.001360	0.244634
H	2.101382	5.524407	0.943120	-0.007234	-0.035460	0.226658

H	2.073010	5.524025	-0.822946	0.020078	0.043652	0.225036
* Frequency(6)	22.1800					
C	-2.777489	-1.354014	0.093481	0.003384	-0.000376	0.034392
C	-3.454353	-2.663199	0.143351	0.000998	0.002114	0.145598
C	-2.455659	-3.606793	0.166179	-0.000830	0.000790	0.179782
C	-1.186190	-2.857555	0.128407	0.000924	-0.002834	0.084166
N	-1.410673	-1.501828	0.090100	0.003574	-0.003176	0.013000
C	-3.456846	-0.122441	0.049410	0.004284	-0.001296	-0.056708
C	0.082814	-3.465988	0.122289	0.001220	-0.004536	0.038636
C	1.335599	-2.843056	0.099345	-0.000040	-0.002858	-0.018328
C	2.642876	-3.473012	0.061632	0.001956	-0.003712	-0.167128
C	3.597752	-2.463190	0.051317	0.000052	-0.002290	-0.160736
C	2.896174	-1.192868	0.082119	-0.003018	-0.000548	-0.008098
N	1.545935	-1.478803	0.104707	-0.002322	-0.001850	0.049926
C	3.447379	0.093154	0.084020	-0.003130	-0.000184	0.058118
C	2.768105	1.325601	0.078696	-0.002038	0.001296	0.096136
C	3.444884	2.635636	0.088500	-0.000028	0.001660	0.186902
C	2.446078	3.579045	0.061653	0.001360	0.002484	0.145800
C	1.176659	2.828859	0.037620	-0.000100	0.002902	0.034760
N	1.401563	1.472661	0.052918	-0.001670	0.001884	0.020478
C	-0.091954	3.436747	-0.000822	0.000478	0.002862	-0.061976
C	-1.345553	2.814282	-0.010218	-0.000096	0.001982	-0.128724
C	-2.652153	3.442999	-0.022883	-0.000640	-0.000912	-0.164442
C	-3.607326	2.433002	-0.007557	0.000832	-0.002954	-0.160298
C	-2.906407	1.163913	0.013807	0.002722	-0.000970	-0.124278
N	-1.555974	1.450189	0.010622	0.002248	0.001602	-0.113340
C	-2.877562	4.929815	-0.026759	-0.010180	-0.002242	-0.180680
C	-5.104446	2.574501	0.010129	0.000922	0.000260	-0.168528
C	-4.944340	-2.868928	0.169366	0.000576	0.004574	0.229066
C	-2.577605	-5.105400	0.232151	-0.004082	0.002998	0.326346

C	2.861541	-4.961847	0.036500	-0.002914	-0.008576	-0.344392
C	5.096158	-2.598738	0.007597	0.002812	0.004320	-0.336754
C	4.934810	2.842128	0.130618	0.000164	0.002036	0.320796
C	2.568374	5.078433	0.062195	0.005280	0.002922	0.213330
H	-4.543849	-0.166920	0.049805	0.004316	-0.001806	-0.055702
H	0.101963	-4.553868	0.128573	0.003112	-0.005200	0.024426
H	0.806040	-0.777246	0.161013	-0.005922	-0.000328	0.266488
H	4.534376	0.136894	0.081579	-0.003214	-0.000828	0.058270
H	-0.109757	4.524447	-0.018027	0.002182	0.003010	-0.065962
H	-0.816925	0.749338	-0.015994	0.004332	0.003764	-0.197066
H	-2.234912	5.432566	-0.763340	0.102026	0.010544	-0.083076
H	-2.651767	5.373007	0.956243	-0.162702	-0.010190	-0.132788
H	-3.919364	5.173725	-0.266741	0.015980	-0.008890	-0.336580
H	-5.410736	3.598735	-0.232176	0.001830	-0.023666	-0.293376
H	-5.518716	2.330896	1.000970	0.006434	0.123904	-0.129616
H	-5.581583	1.899567	-0.714036	-0.004876	-0.091816	-0.085022
H	-5.400682	-2.415249	1.062668	0.061518	-0.073956	0.306936
H	-5.200830	-3.934841	0.172637	0.001432	0.002396	0.153280
H	-5.433116	-2.411336	-0.704398	-0.062520	0.087040	0.301932
H	-3.625297	-5.423507	0.138827	0.000304	-0.000890	0.093400
H	-2.190849	-5.503034	1.188379	-0.237804	0.111558	0.501542
H	-2.002976	-5.595832	-0.573583	0.225824	-0.098320	0.512650
H	2.325256	-5.433996	-0.801890	0.106656	0.104564	-0.499322
H	2.496923	-5.438383	0.961396	-0.141618	-0.145434	-0.452058
H	3.924593	-5.205720	-0.066392	0.015292	0.009582	-0.232614
H	5.397455	-3.651765	-0.045989	-0.010312	-0.017938	-0.159868
H	5.567793	-2.159393	0.903756	0.133926	0.208046	-0.476864
H	5.522710	-2.080540	-0.867883	-0.112108	-0.167020	-0.525796
H	5.439769	2.329828	-0.702696	0.088052	-0.062072	0.405726
H	5.372931	2.445911	1.059948	-0.091380	0.069524	0.399776

H	5.193015	3.905899	0.071382	0.004032	-0.000800	0.268954
H	3.617969	5.394080	0.047429	0.006554	0.001360	0.244634
H	2.101048	5.522766	0.953610	-0.007234	-0.035460	0.226658
H	2.073939	5.526046	-0.812531	0.020078	0.043652	0.225036
* Frequency(6)	22.1800					
C	-2.777457	-1.354017	0.093808	0.003384	-0.000376	0.034392
C	-3.454344	-2.663179	0.144736	0.000998	0.002114	0.145598
C	-2.455667	-3.606785	0.167890	-0.000830	0.000790	0.179782
C	-1.186182	-2.857582	0.129207	0.000924	-0.002834	0.084166
N	-1.410639	-1.501858	0.090223	0.003574	-0.003176	0.013000
C	-3.456806	-0.122453	0.048870	0.004284	-0.001296	-0.056708
C	0.082826	-3.466031	0.122656	0.001220	-0.004536	0.038636
C	1.335599	-2.843083	0.099171	-0.000040	-0.002858	-0.018328
C	2.642894	-3.473048	0.060042	0.001956	-0.003712	-0.167128
C	3.597752	-2.463212	0.049788	0.000052	-0.002290	-0.160736
C	2.896145	-1.192873	0.082042	-0.003018	-0.000548	-0.008098
N	1.545913	-1.478820	0.105182	-0.002322	-0.001850	0.049926
C	3.447349	0.093152	0.084573	-0.003130	-0.000184	0.058118
C	2.768085	1.325613	0.079611	-0.002038	0.001296	0.096136
C	3.444884	2.635652	0.090278	-0.000028	0.001660	0.186902
C	2.446091	3.579068	0.063041	0.001360	0.002484	0.145800
C	1.176658	2.828886	0.037950	-0.000100	0.002902	0.034760
N	1.401547	1.472679	0.053113	-0.001670	0.001884	0.020478
C	-0.091949	3.436774	-0.001412	0.000478	0.002862	-0.061976
C	-1.345553	2.814301	-0.011443	-0.000096	0.001982	-0.128724
C	-2.652159	3.442990	-0.024447	-0.000640	-0.000912	-0.164442
C	-3.607318	2.432974	-0.009082	0.000832	-0.002954	-0.160298
C	-2.906382	1.163904	0.012624	0.002722	-0.000970	-0.124278
N	-1.555953	1.450204	0.009543	0.002248	0.001602	-0.113340
C	-2.877659	4.929794	-0.028478	-0.010180	-0.002242	-0.180680

C	-5.104437	2.574504	0.008526	0.000922	0.000260	-0.168528
C	-4.944334	-2.868885	0.171545	0.000576	0.004574	0.229066
C	-2.577644	-5.105371	0.235256	-0.004082	0.002998	0.326346
C	2.861514	-4.961928	0.033223	-0.002914	-0.008576	-0.344392
C	5.096185	-2.598697	0.004393	0.002812	0.004320	-0.336754
C	4.934811	2.842147	0.133670	0.000164	0.002036	0.320796
C	2.568425	5.078461	0.064224	0.005280	0.002922	0.213330
H	-4.543808	-0.166937	0.049275	0.004316	-0.001806	-0.055702
H	0.101992	-4.553918	0.128806	0.003112	-0.005200	0.024426
H	0.805983	-0.777249	0.163548	-0.005922	-0.000328	0.266488
H	4.534345	0.136886	0.082134	-0.003214	-0.000828	0.058270
H	-0.109736	4.524476	-0.018655	0.002182	0.003010	-0.065962
H	-0.816884	0.749374	-0.017869	0.004332	0.003764	-0.197066
H	-2.233941	5.432667	-0.764130	0.102026	0.010544	-0.083076
H	-2.653315	5.372910	0.954980	-0.162702	-0.010190	-0.132788
H	-3.919212	5.173640	-0.269944	0.015980	-0.008890	-0.336580
H	-5.410719	3.598510	-0.234967	0.001830	-0.023666	-0.293376
H	-5.518655	2.332075	0.999736	0.006434	0.123904	-0.129616
H	-5.581630	1.898693	-0.714845	-0.004876	-0.091816	-0.085022
H	-5.400096	-2.415952	1.065589	0.061518	-0.073956	0.306936
H	-5.200817	-3.934818	0.174096	0.001432	0.002396	0.153280
H	-5.433711	-2.410508	-0.701526	-0.062520	0.087040	0.301932
H	-3.625294	-5.423515	0.139715	0.000304	-0.000890	0.093400
H	-2.193111	-5.501973	1.193151	-0.237804	0.111558	0.501542
H	-2.000828	-5.596767	-0.568705	0.225824	-0.098320	0.512650
H	2.326271	-5.433002	-0.806641	0.106656	0.104564	-0.499322
H	2.495576	-5.439767	0.957095	-0.141618	-0.145434	-0.452058
H	3.924739	-5.205629	-0.068605	0.015292	0.009582	-0.232614
H	5.397357	-3.651936	-0.047510	-0.010312	-0.017938	-0.159868
H	5.569067	-2.157414	0.899219	0.133926	0.208046	-0.476864

H	5.521643	-2.082129	-0.872886	-0.112108	-0.167020	-0.525796
H	5.440607	2.329237	-0.698836	0.088052	-0.062072	0.405726
H	5.372061	2.446572	1.063752	-0.091380	0.069524	0.399776
H	5.193053	3.905891	0.073941	0.004032	-0.000800	0.268954
H	3.618031	5.394093	0.049756	0.006554	0.001360	0.244634
H	2.100979	5.522428	0.955766	-0.007234	-0.035460	0.226658
H	2.074130	5.526461	-0.810389	0.020078	0.043652	0.225036
* Frequency(6)	22.1800					
C	-2.777552	-1.354007	0.092835	0.003384	-0.000376	0.034392
C	-3.454372	-2.663238	0.140618	0.000998	0.002114	0.145598
C	-2.455643	-3.606808	0.162805	-0.000830	0.000790	0.179782
C	-1.186208	-2.857501	0.126827	0.000924	-0.002834	0.084166
N	-1.410740	-1.501768	0.089856	0.003574	-0.003176	0.013000
C	-3.456927	-0.122416	0.050474	0.004284	-0.001296	-0.056708
C	0.082791	-3.465903	0.121564	0.001220	-0.004536	0.038636
C	1.335600	-2.843002	0.099689	-0.000040	-0.002858	-0.018328
C	2.642839	-3.472943	0.064769	0.001956	-0.003712	-0.167128
C	3.597751	-2.463147	0.054334	0.000052	-0.002290	-0.160736
C	2.896231	-1.192858	0.082271	-0.003018	-0.000548	-0.008098
N	1.545979	-1.478768	0.103770	-0.002322	-0.001850	0.049926
C	3.447438	0.093157	0.082929	-0.003130	-0.000184	0.058118
C	2.768143	1.325576	0.076892	-0.002038	0.001296	0.096136
C	3.444885	2.635605	0.084992	-0.000028	0.001660	0.186902
C	2.446053	3.578998	0.058917	0.001360	0.002484	0.145800
C	1.176661	2.828804	0.036967	-0.000100	0.002902	0.034760
N	1.401595	1.472626	0.052534	-0.001670	0.001884	0.020478
C	-0.091963	3.436693	0.000341	0.000478	0.002862	-0.061976
C	-1.345551	2.814245	-0.007802	-0.000096	0.001982	-0.128724
C	-2.652141	3.443016	-0.019796	-0.000640	-0.000912	-0.164442
C	-3.607341	2.433057	-0.004548	0.000832	-0.002954	-0.160298

C	-2.906459	1.163931	0.016139	0.002722	-0.000970	-0.124278
N	-1.556016	1.450158	0.012749	0.002248	0.001602	-0.113340
C	-2.877371	4.929857	-0.023368	-0.010180	-0.002242	-0.180680
C	-5.104463	2.574496	0.013292	0.000922	0.000260	-0.168528
C	-4.944350	-2.869014	0.165066	0.000576	0.004574	0.229066
C	-2.577528	-5.105456	0.226026	-0.004082	0.002998	0.326346
C	2.861596	-4.961686	0.042964	-0.002914	-0.008576	-0.344392
C	5.096105	-2.598819	0.013917	0.002812	0.004320	-0.336754
C	4.934807	2.842090	0.124597	0.000164	0.002036	0.320796
C	2.568275	5.078379	0.058191	0.005280	0.002922	0.213330
H	-4.543930	-0.166886	0.050850	0.004316	-0.001806	-0.055702
H	0.101904	-4.553771	0.128115	0.003112	-0.005200	0.024426
H	0.806151	-0.777240	0.156011	-0.005922	-0.000328	0.266488
H	4.534436	0.136910	0.080486	-0.003214	-0.000828	0.058270
H	-0.109798	4.524391	-0.016789	0.002182	0.003010	-0.065962
H	-0.817007	0.749267	-0.012295	0.004332	0.003764	-0.197066
H	-2.236827	5.432369	-0.761781	0.102026	0.010544	-0.083076
H	-2.648713	5.373198	0.958736	-0.162702	-0.010190	-0.132788
H	-3.919664	5.173892	-0.260424	0.015980	-0.008890	-0.336580
H	-5.410770	3.599180	-0.226669	0.001830	-0.023666	-0.293376
H	-5.518837	2.328571	1.003402	0.006434	0.123904	-0.129616
H	-5.581492	1.901290	-0.712440	-0.004876	-0.091816	-0.085022
H	-5.401836	-2.413860	1.056907	0.061518	-0.073956	0.306936
H	-5.200857	-3.934886	0.169760	0.001432	0.002396	0.153280
H	-5.431943	-2.412970	-0.710066	-0.062520	0.087040	0.301932
H	-3.625303	-5.423490	0.137074	0.000304	-0.000890	0.093400
H	-2.186385	-5.505128	1.178966	-0.237804	0.111558	0.501542
H	-2.007215	-5.593987	-0.583205	0.225824	-0.098320	0.512650
H	2.323254	-5.435959	-0.792518	0.106656	0.104564	-0.499322
H	2.499582	-5.435654	0.969881	-0.141618	-0.145434	-0.452058

H	3.924306	-5.205900	-0.062026	0.015292	0.009582	-0.232614
H	5.397649	-3.651428	-0.042988	-0.010312	-0.017938	-0.159868
H	5.565279	-2.163298	0.912706	0.133926	0.208046	-0.476864
H	5.524814	-2.077405	-0.858014	-0.112108	-0.167020	-0.525796
H	5.438116	2.330993	-0.710311	0.088052	-0.062072	0.405726
H	5.374646	2.444606	1.052444	-0.091380	0.069524	0.399776
H	5.192939	3.905914	0.066334	0.004032	-0.000800	0.268954
H	3.617846	5.394055	0.042837	0.006554	0.001360	0.244634
H	2.101183	5.523431	0.949356	-0.007234	-0.035460	0.226658
H	2.073562	5.525226	-0.816754	0.020078	0.043652	0.225036

* Frequency(6) 22.1800

C	-2.777766	-1.353983	0.090668	0.003384	-0.000376	0.034392
C	-3.454435	-2.663372	0.131443	0.000998	0.002114	0.145598
C	-2.455591	-3.606858	0.151475	-0.000830	0.000790	0.179782
C	-1.186266	-2.857323	0.121523	0.000924	-0.002834	0.084166
N	-1.410966	-1.501568	0.089037	0.003574	-0.003176	0.013000
C	-3.457197	-0.122335	0.054047	0.004284	-0.001296	-0.056708
C	0.082714	-3.465617	0.119129	0.001220	-0.004536	0.038636
C	1.335603	-2.842822	0.100844	-0.000040	-0.002858	-0.018328
C	2.642716	-3.472709	0.075301	0.001956	-0.003712	-0.167128
C	3.597747	-2.463003	0.064463	0.000052	-0.002290	-0.160736
C	2.896421	-1.192823	0.082782	-0.003018	-0.000548	-0.008098
N	1.546125	-1.478651	0.100624	-0.002322	-0.001850	0.049926
C	3.447635	0.093169	0.079267	-0.003130	-0.000184	0.058118
C	2.768271	1.325495	0.070833	-0.002038	0.001296	0.096136
C	3.444887	2.635500	0.073214	-0.000028	0.001660	0.186902
C	2.445967	3.578842	0.049729	0.001360	0.002484	0.145800
C	1.176667	2.828621	0.034777	-0.000100	0.002902	0.034760
N	1.401700	1.472507	0.051243	-0.001670	0.001884	0.020478
C	-0.091993	3.436513	0.004247	0.000478	0.002862	-0.061976

C	-1.345545	2.814120	0.000310	-0.000096	0.001982	-0.128724
C	-2.652101	3.443073	-0.009433	-0.000640	-0.000912	-0.164442
C	-3.607394	2.433243	0.005554	0.000832	-0.002954	-0.160298
C	-2.906630	1.163992	0.023971	0.002722	-0.000970	-0.124278
N	-1.556158	1.450058	0.019892	0.002248	0.001602	-0.113340
C	-2.876729	4.929999	-0.011982	-0.010180	-0.002242	-0.180680
C	-5.104522	2.574480	0.023912	0.000922	0.000260	-0.168528
C	-4.944387	-2.869302	0.150631	0.000576	0.004574	0.229066
C	-2.577271	-5.105645	0.205460	-0.004082	0.002998	0.326346
C	2.861780	-4.961145	0.064667	-0.002914	-0.008576	-0.344392
C	5.095928	-2.599092	0.035139	0.002812	0.004320	-0.336754
C	4.934796	2.841961	0.104381	0.000164	0.002036	0.320796
C	2.567943	5.078194	0.044747	0.005280	0.002922	0.213330
H	-4.544202	-0.166772	0.054361	0.004316	-0.001806	-0.055702
H	0.101708	-4.553443	0.126576	0.003112	-0.005200	0.024426
H	0.806524	-0.777219	0.139218	-0.005922	-0.000328	0.266488
H	4.534638	0.136962	0.076814	-0.003214	-0.000828	0.058270
H	-0.109935	4.524201	-0.012632	0.002182	0.003010	-0.065962
H	-0.817279	0.749030	0.000124	0.004332	0.003764	-0.197066
H	-2.243256	5.431704	-0.756545	0.102026	0.010544	-0.083076
H	-2.638460	5.373840	0.967104	-0.162702	-0.010190	-0.132788
H	-3.920671	5.174452	-0.239213	0.015980	-0.008890	-0.336580
H	-5.410886	3.600671	-0.208181	0.001830	-0.023666	-0.293376
H	-5.519242	2.320763	1.011570	0.006434	0.123904	-0.129616
H	-5.581185	1.907076	-0.707082	-0.004876	-0.091816	-0.085022
H	-5.405713	-2.409200	1.037565	0.061518	-0.073956	0.306936
H	-5.200947	-3.935037	0.160101	0.001432	0.002396	0.153280
H	-5.428003	-2.418455	-0.729092	-0.062520	0.087040	0.301932
H	-3.625322	-5.423434	0.131188	0.000304	-0.000890	0.093400
H	-2.171399	-5.512158	1.147360	-0.237804	0.111558	0.501542

H	-2.021446	-5.587791	-0.615511	0.225824	-0.098320	0.512650
H	2.316533	-5.442548	-0.761052	0.106656	0.104564	-0.499322
H	2.508506	-5.426489	0.998369	-0.141618	-0.145434	-0.452058
H	3.923343	-5.206504	-0.047367	0.015292	0.009582	-0.232614
H	5.398299	-3.650298	-0.032914	-0.010312	-0.017938	-0.159868
H	5.556839	-2.176408	0.942757	0.133926	0.208046	-0.476864
H	5.531879	-2.066880	-0.824880	-0.112108	-0.167020	-0.525796
H	5.432568	2.334904	-0.735879	0.088052	-0.062072	0.405726
H	5.380404	2.440225	1.027252	-0.091380	0.069524	0.399776
H	5.192685	3.905964	0.049386	0.004032	-0.000800	0.268954
H	3.617433	5.393969	0.027421	0.006554	0.001360	0.244634
H	2.101639	5.525666	0.935072	-0.007234	-0.035460	0.226658
H	2.072297	5.522476	-0.830935	0.020078	0.043652	0.225036
* Frequency(6)	22.1800					
C	-2.778073	-1.353949	0.087541	0.003384	-0.000376	0.034392
C	-3.454526	-2.663564	0.118205	0.000998	0.002114	0.145598
C	-2.455515	-3.606929	0.135129	-0.000830	0.000790	0.179782
C	-1.186350	-2.857065	0.113871	0.000924	-0.002834	0.084166
N	-1.411291	-1.501279	0.087855	0.003574	-0.003176	0.013000
C	-3.457586	-0.122217	0.059203	0.004284	-0.001296	-0.056708
C	0.082603	-3.465205	0.115616	0.001220	-0.004536	0.038636
C	1.335606	-2.842562	0.102511	-0.000040	-0.002858	-0.018328
C	2.642538	-3.472371	0.090497	0.001956	-0.003712	-0.167128
C	3.597743	-2.462794	0.079077	0.000052	-0.002290	-0.160736
C	2.896695	-1.192773	0.083518	-0.003018	-0.000548	-0.008098
N	1.546336	-1.478483	0.096085	-0.002322	-0.001850	0.049926
C	3.447920	0.093185	0.073982	-0.003130	-0.000184	0.058118
C	2.768457	1.325377	0.062092	-0.002038	0.001296	0.096136
C	3.444889	2.635350	0.056220	-0.000028	0.001660	0.186902
C	2.445844	3.578616	0.036473	0.001360	0.002484	0.145800

C	1.176676	2.828357	0.031616	-0.000100	0.002902	0.034760
N	1.401852	1.472336	0.049381	-0.001670	0.001884	0.020478
C	-0.092036	3.436253	0.009882	0.000478	0.002862	-0.061976
C	-1.345536	2.813940	0.012014	-0.000096	0.001982	-0.128724
C	-2.652043	3.443156	0.005518	-0.000640	-0.000912	-0.164442
C	-3.607469	2.433512	0.020128	0.000832	-0.002954	-0.160298
C	-2.906878	1.164080	0.035271	0.002722	-0.000970	-0.124278
N	-1.556363	1.449912	0.030197	0.002248	0.001602	-0.113340
C	-2.875804	4.930203	0.004446	-0.010180	-0.002242	-0.180680
C	-5.104605	2.574456	0.039235	0.000922	0.000260	-0.168528
C	-4.944439	-2.869718	0.129804	0.000576	0.004574	0.229066
C	-2.576900	-5.105918	0.175788	-0.004082	0.002998	0.326346
C	2.862045	-4.960366	0.095980	-0.002914	-0.008576	-0.344392
C	5.095672	-2.599484	0.065757	0.002812	0.004320	-0.336754
C	4.934781	2.841776	0.075214	0.000164	0.002036	0.320796
C	2.567463	5.077929	0.025351	0.005280	0.002922	0.213330
H	-4.544594	-0.166608	0.059425	0.004316	-0.001806	-0.055702
H	0.101425	-4.552970	0.124355	0.003112	-0.005200	0.024426
H	0.807063	-0.777190	0.114988	-0.005922	-0.000328	0.266488
H	4.534931	0.137037	0.071516	-0.003214	-0.000828	0.058270
H	-0.110134	4.523927	-0.006635	0.002182	0.003010	-0.065962
H	-0.817673	0.748688	0.018041	0.004332	0.003764	-0.197066
H	-2.252532	5.430745	-0.748992	0.102026	0.010544	-0.083076
H	-2.623667	5.374767	0.979177	-0.162702	-0.010190	-0.132788
H	-3.922124	5.175260	-0.208611	0.015980	-0.008890	-0.336580
H	-5.411052	3.602823	-0.181507	0.001830	-0.023666	-0.293376
H	-5.519827	2.309497	1.023355	0.006434	0.123904	-0.129616
H	-5.580741	1.915424	-0.699352	-0.004876	-0.091816	-0.085022
H	-5.411306	-2.402476	1.009658	0.061518	-0.073956	0.306936
H	-5.201077	-3.935255	0.146165	0.001432	0.002396	0.153280

H	-5.422319	-2.426369	-0.756545	-0.062520	0.087040	0.301932
H	-3.625349	-5.423353	0.122696	0.000304	-0.000890	0.093400
H	-2.149778	-5.522301	1.101759	-0.237804	0.111558	0.501542
H	-2.041978	-5.578851	-0.662122	0.225824	-0.098320	0.512650
H	2.306836	-5.452056	-0.715653	0.106656	0.104564	-0.499322
H	2.521382	-5.413266	1.039470	-0.141618	-0.145434	-0.452058
H	3.921952	-5.207375	-0.026217	0.015292	0.009582	-0.232614
H	5.399236	-3.648667	-0.018378	-0.010312	-0.017938	-0.159868
H	5.544663	-2.195324	0.986114	0.133926	0.208046	-0.476864
H	5.542072	-2.051694	-0.777074	-0.112108	-0.167020	-0.525796
H	5.424562	2.340548	-0.772769	0.088052	-0.062072	0.405726
H	5.388713	2.433903	0.990903	-0.091380	0.069524	0.399776
H	5.192319	3.906037	0.024932	0.004032	-0.000800	0.268954
H	3.616837	5.393846	0.005179	0.006554	0.001360	0.244634
H	2.102297	5.528890	0.914464	-0.007234	-0.035460	0.226658
H	2.070472	5.518507	-0.851396	0.020078	0.043652	0.225036
* Frequency(6)	22.1800					
C	-2.778442	-1.353908	0.083793	0.003384	-0.000376	0.034392
C	-3.454635	-2.663794	0.102339	0.000998	0.002114	0.145598
C	-2.455425	-3.607015	0.115538	-0.000830	0.000790	0.179782
C	-1.186451	-2.856756	0.104699	0.000924	-0.002834	0.084166
N	-1.411680	-1.500933	0.086438	0.003574	-0.003176	0.013000
C	-3.458053	-0.122076	0.065383	0.004284	-0.001296	-0.056708
C	0.082470	-3.464710	0.111406	0.001220	-0.004536	0.038636
C	1.335611	-2.842251	0.104508	-0.000040	-0.002858	-0.018328
C	2.642325	-3.471967	0.108709	0.001956	-0.003712	-0.167128
C	3.597737	-2.462545	0.096593	0.000052	-0.002290	-0.160736
C	2.897024	-1.192714	0.084400	-0.003018	-0.000548	-0.008098
N	1.546589	-1.478282	0.090644	-0.002322	-0.001850	0.049926
C	3.448261	0.093205	0.067649	-0.003130	-0.000184	0.058118

C	2.768679	1.325236	0.051616	-0.002038	0.001296	0.096136
C	3.444892	2.635169	0.035853	-0.000028	0.001660	0.186902
C	2.445695	3.578345	0.020584	0.001360	0.002484	0.145800
C	1.176687	2.828041	0.027828	-0.000100	0.002902	0.034760
N	1.402034	1.472131	0.047150	-0.001670	0.001884	0.020478
C	-0.092088	3.435941	0.016636	0.000478	0.002862	-0.061976
C	-1.345526	2.813724	0.026041	-0.000096	0.001982	-0.128724
C	-2.651973	3.443255	0.023438	-0.000640	-0.000912	-0.164442
C	-3.607560	2.433834	0.037597	0.000832	-0.002954	-0.160298
C	-2.907174	1.164186	0.048814	0.002722	-0.000970	-0.124278
N	-1.556607	1.449737	0.042548	0.002248	0.001602	-0.113340
C	-2.874694	4.930447	0.024135	-0.010180	-0.002242	-0.180680
C	-5.104706	2.574428	0.057600	0.000922	0.000260	-0.168528
C	-4.944502	-2.870217	0.104842	0.000576	0.004574	0.229066
C	-2.576455	-5.106244	0.140225	-0.004082	0.002998	0.326346
C	2.862362	-4.959431	0.133509	-0.002914	-0.008576	-0.344392
C	5.095366	-2.599955	0.102454	0.002812	0.004320	-0.336754
C	4.934763	2.841554	0.040255	0.000164	0.002036	0.320796
C	2.566887	5.077610	0.002104	0.005280	0.002922	0.213330
H	-4.545064	-0.166411	0.065495	0.004316	-0.001806	-0.055702
H	0.101086	-4.552404	0.121693	0.003112	-0.005200	0.024426
H	0.807708	-0.777154	0.085948	-0.005922	-0.000328	0.266488
H	4.535281	0.137127	0.065166	-0.003214	-0.000828	0.058270
H	-0.110371	4.523599	0.000553	0.002182	0.003010	-0.065962
H	-0.818145	0.748278	0.039516	0.004332	0.003764	-0.197066
H	-2.263650	5.429596	-0.739939	0.102026	0.010544	-0.083076
H	-2.605937	5.375877	0.993647	-0.162702	-0.010190	-0.132788
H	-3.923865	5.176229	-0.171933	0.015980	-0.008890	-0.336580
H	-5.411252	3.605402	-0.149537	0.001830	-0.023666	-0.293376
H	-5.520528	2.295995	1.037480	0.006434	0.123904	-0.129616

H	-5.580210	1.925430	-0.690087	-0.004876	-0.091816	-0.085022
H	-5.418010	-2.394416	0.976210	0.061518	-0.073956	0.306936
H	-5.201234	-3.935516	0.129461	0.001432	0.002396	0.153280
H	-5.415506	-2.435854	-0.789447	-0.062520	0.087040	0.301932
H	-3.625382	-5.423256	0.112518	0.000304	-0.000890	0.093400
H	-2.123863	-5.534458	1.047104	-0.237804	0.111558	0.501542
H	-2.066587	-5.568137	-0.717987	0.225824	-0.098320	0.512650
H	2.295213	-5.463450	-0.661240	0.106656	0.104564	-0.499322
H	2.536815	-5.397417	1.088733	-0.141618	-0.145434	-0.452058
H	3.920286	-5.208419	-0.000868	0.015292	0.009582	-0.232614
H	5.400360	-3.646712	-0.000957	-0.010312	-0.017938	-0.159868
H	5.530068	-2.217996	1.038080	0.133926	0.208046	-0.476864
H	5.554289	-2.033494	-0.719776	-0.112108	-0.167020	-0.525796
H	5.414967	2.347312	-0.816982	0.088052	-0.062072	0.405726
H	5.398671	2.426327	0.947338	-0.091380	0.069524	0.399776
H	5.191879	3.906124	-0.004377	0.004032	-0.000800	0.268954
H	3.616123	5.393697	-0.021480	0.006554	0.001360	0.244634
H	2.103085	5.532754	0.889764	-0.007234	-0.035460	0.226658
H	2.068284	5.513750	-0.875919	0.020078	0.043652	0.225036
* Frequency(6)	22.1800					
C	-2.778832	-1.353864	0.079831	0.003384	-0.000376	0.034392
C	-3.454749	-2.664038	0.085563	0.000998	0.002114	0.145598
C	-2.455329	-3.607107	0.094824	-0.000830	0.000790	0.179782
C	-1.186557	-2.856430	0.095001	0.000924	-0.002834	0.084166
N	-1.412092	-1.500567	0.084940	0.003574	-0.003176	0.013000
C	-3.458547	-0.121926	0.071917	0.004284	-0.001296	-0.056708
C	0.082330	-3.464188	0.106954	0.001220	-0.004536	0.038636
C	1.335615	-2.841921	0.106620	-0.000040	-0.002858	-0.018328
C	2.642099	-3.471539	0.127965	0.001956	-0.003712	-0.167128
C	3.597731	-2.462281	0.115113	0.000052	-0.002290	-0.160736

C	2.897372	-1.192650	0.085334	-0.003018	-0.000548	-0.008098
N	1.546857	-1.478068	0.084892	-0.002322	-0.001850	0.049926
C	3.448621	0.093227	0.060953	-0.003130	-0.000184	0.058118
C	2.768913	1.325086	0.040540	-0.002038	0.001296	0.096136
C	3.444896	2.634977	0.014319	-0.000028	0.001660	0.186902
C	2.445539	3.578059	0.003786	0.001360	0.002484	0.145800
C	1.176699	2.827707	0.023824	-0.000100	0.002902	0.034760
N	1.402226	1.471913	0.044790	-0.001670	0.001884	0.020478
C	-0.092144	3.435611	0.023776	0.000478	0.002862	-0.061976
C	-1.345514	2.813496	0.040873	-0.000096	0.001982	-0.128724
C	-2.651899	3.443361	0.042384	-0.000640	-0.000912	-0.164442
C	-3.607656	2.434174	0.056065	0.000832	-0.002954	-0.160298
C	-2.907488	1.164298	0.063132	0.002722	-0.000970	-0.124278
N	-1.556867	1.449553	0.055606	0.002248	0.001602	-0.113340
C	-2.873522	4.930705	0.044953	-0.010180	-0.002242	-0.180680
C	-5.104812	2.574398	0.077018	0.000922	0.000260	-0.168528
C	-4.944568	-2.870743	0.078450	0.000576	0.004574	0.229066
C	-2.575985	-5.106590	0.102625	-0.004082	0.002998	0.326346
C	2.862698	-4.958443	0.173189	-0.002914	-0.008576	-0.344392
C	5.095042	-2.600453	0.141254	0.002812	0.004320	-0.336754
C	4.934745	2.841320	0.003295	0.000164	0.002036	0.320796
C	2.566279	5.077274	-0.022476	0.005280	0.002922	0.213330
H	-4.545562	-0.166203	0.071913	0.004316	-0.001806	-0.055702
H	0.100728	-4.551804	0.118879	0.003112	-0.005200	0.024426
H	0.808390	-0.777116	0.055244	-0.005922	-0.000328	0.266488
H	4.535651	0.137223	0.058452	-0.003214	-0.000828	0.058270
H	-0.110623	4.523253	0.008153	0.002182	0.003010	-0.065962
H	-0.818645	0.747844	0.062222	0.004332	0.003764	-0.197066
H	-2.275406	5.428382	-0.730367	0.102026	0.010544	-0.083076
H	-2.587191	5.377051	1.008947	-0.162702	-0.010190	-0.132788

H	-3.925707	5.177253	-0.133153	0.015980	-0.008890	-0.336580
H	-5.411462	3.608128	-0.115735	0.001830	-0.023666	-0.293376
H	-5.521270	2.281719	1.052414	0.006434	0.123904	-0.129616
H	-5.579648	1.936008	-0.680291	-0.004876	-0.091816	-0.085022
H	-5.425098	-2.385896	0.940846	0.061518	-0.073956	0.306936
H	-5.201398	-3.935792	0.111801	0.001432	0.002396	0.153280
H	-5.408302	-2.445882	-0.824235	-0.062520	0.087040	0.301932
H	-3.625418	-5.423154	0.101756	0.000304	-0.000890	0.093400
H	-2.096465	-5.547312	0.989318	-0.237804	0.111558	0.501542
H	-2.092605	-5.556809	-0.777053	0.225824	-0.098320	0.512650
H	2.282925	-5.475498	-0.603710	0.106656	0.104564	-0.499322
H	2.553131	-5.380661	1.140817	-0.141618	-0.145434	-0.452058
H	3.918524	-5.209523	0.025932	0.015292	0.009582	-0.232614
H	5.401548	-3.644646	0.017463	-0.010312	-0.017938	-0.159868
H	5.514638	-2.241966	1.093022	0.133926	0.208046	-0.476864
H	5.567205	-2.014250	-0.659196	-0.112108	-0.167020	-0.525796
H	5.404821	2.354464	-0.863728	0.088052	-0.062072	0.405726
H	5.409199	2.418317	0.901278	-0.091380	0.069524	0.399776
H	5.191415	3.906216	-0.035365	0.004032	-0.000800	0.268954
H	3.615367	5.393541	-0.049666	0.006554	0.001360	0.244634
H	2.103919	5.536840	0.863650	-0.007234	-0.035460	0.226658
H	2.065970	5.508720	-0.901847	0.020078	0.043652	0.225036

* Frequency(6) 22.1800

C	-2.779201	-1.353823	0.076083	0.003384	-0.000376	0.034392
C	-3.454858	-2.664268	0.069697	0.000998	0.002114	0.145598
C	-2.455239	-3.607193	0.075233	-0.000830	0.000790	0.179782
C	-1.186658	-2.856121	0.085829	0.000924	-0.002834	0.084166
N	-1.412481	-1.500221	0.083523	0.003574	-0.003176	0.013000
C	-3.459014	-0.121785	0.078097	0.004284	-0.001296	-0.056708
C	0.082197	-3.463693	0.102744	0.001220	-0.004536	0.038636

C	1.335620	-2.841610	0.108617	-0.000040	-0.002858	-0.018328
C	2.641886	-3.471135	0.146177	0.001956	-0.003712	-0.167128
C	3.597725	-2.462032	0.132629	0.000052	-0.002290	-0.160736
C	2.897701	-1.192591	0.086216	-0.003018	-0.000548	-0.008098
N	1.547110	-1.477867	0.079451	-0.002322	-0.001850	0.049926
C	3.448962	0.093247	0.054620	-0.003130	-0.000184	0.058118
C	2.769135	1.324945	0.030064	-0.002038	0.001296	0.096136
C	3.444899	2.634796	-0.006048	-0.000028	0.001660	0.186902
C	2.445390	3.577788	-0.012103	0.001360	0.002484	0.145800
C	1.176710	2.827391	0.020036	-0.000100	0.002902	0.034760
N	1.402408	1.471708	0.042559	-0.001670	0.001884	0.020478
C	-0.092196	3.435299	0.030530	0.000478	0.002862	-0.061976
C	-1.345504	2.813280	0.054900	-0.000096	0.001982	-0.128724
C	-2.651829	3.443460	0.060304	-0.000640	-0.000912	-0.164442
C	-3.607747	2.434496	0.073534	0.000832	-0.002954	-0.160298
C	-2.907784	1.164404	0.076675	0.002722	-0.000970	-0.124278
N	-1.557111	1.449378	0.067957	0.002248	0.001602	-0.113340
C	-2.872412	4.930949	0.064642	-0.010180	-0.002242	-0.180680
C	-5.104913	2.574370	0.095383	0.000922	0.000260	-0.168528
C	-4.944631	-2.871242	0.053488	0.000576	0.004574	0.229066
C	-2.575540	-5.106916	0.067062	-0.004082	0.002998	0.326346
C	2.863015	-4.957508	0.210718	-0.002914	-0.008576	-0.344392
C	5.094736	-2.600924	0.177951	0.002812	0.004320	-0.336754
C	4.934727	2.841098	-0.031664	0.000164	0.002036	0.320796
C	2.565703	5.076955	-0.045723	0.005280	0.002922	0.213330
H	-4.546032	-0.166006	0.077983	0.004316	-0.001806	-0.055702
H	0.100389	-4.551238	0.116217	0.003112	-0.005200	0.024426
H	0.809035	-0.777080	0.026204	-0.005922	-0.000328	0.266488
H	4.536001	0.137313	0.052102	-0.003214	-0.000828	0.058270
H	-0.110860	4.522925	0.015341	0.002182	0.003010	-0.065962

H	-0.819117	0.747434	0.083697	0.004332	0.003764	-0.197066
H	-2.286524	5.427233	-0.721314	0.102026	0.010544	-0.083076
H	-2.569461	5.378161	1.023417	-0.162702	-0.010190	-0.132788
H	-3.927448	5.178222	-0.096475	0.015980	-0.008890	-0.336580
H	-5.411662	3.610707	-0.083765	0.001830	-0.023666	-0.293376
H	-5.521971	2.268217	1.066539	0.006434	0.123904	-0.129616
H	-5.579117	1.946014	-0.671026	-0.004876	-0.091816	-0.085022
H	-5.431802	-2.377836	0.907398	0.061518	-0.073956	0.306936
H	-5.201555	-3.936053	0.095097	0.001432	0.002396	0.153280
H	-5.401489	-2.455367	-0.857137	-0.062520	0.087040	0.301932
H	-3.625451	-5.423057	0.091578	0.000304	-0.000890	0.093400
H	-2.070550	-5.559469	0.934663	-0.237804	0.111558	0.501542
H	-2.117214	-5.546095	-0.832918	0.225824	-0.098320	0.512650
H	2.271302	-5.486892	-0.549297	0.106656	0.104564	-0.499322
H	2.568564	-5.364812	1.190080	-0.141618	-0.145434	-0.452058
H	3.916858	-5.210567	0.051281	0.015292	0.009582	-0.232614
H	5.402672	-3.642691	0.034884	-0.010312	-0.017938	-0.159868
H	5.500043	-2.264638	1.144988	0.133926	0.208046	-0.476864
H	5.579422	-1.996050	-0.601898	-0.112108	-0.167020	-0.525796
H	5.395226	2.361228	-0.907941	0.088052	-0.062072	0.405726
H	5.419157	2.410741	0.857713	-0.091380	0.069524	0.399776
H	5.190975	3.906303	-0.064674	0.004032	-0.000800	0.268954
H	3.614653	5.393392	-0.076325	0.006554	0.001360	0.244634
H	2.104707	5.540704	0.838950	-0.007234	-0.035460	0.226658
H	2.063782	5.503963	-0.926370	0.020078	0.043652	0.225036
* Frequency(6)	22.1800					
C	-2.779508	-1.353789	0.072956	0.003384	-0.000376	0.034392
C	-3.454949	-2.664460	0.056459	0.000998	0.002114	0.145598
C	-2.455163	-3.607264	0.058887	-0.000830	0.000790	0.179782
C	-1.186742	-2.855863	0.078177	0.000924	-0.002834	0.084166

N	-1.412806	-1.499932	0.082341	0.003574	-0.003176	0.013000
C	-3.459403	-0.121667	0.083253	0.004284	-0.001296	-0.056708
C	0.082086	-3.463281	0.099231	0.001220	-0.004536	0.038636
C	1.335623	-2.841350	0.110284	-0.000040	-0.002858	-0.018328
C	2.641708	-3.470797	0.161373	0.001956	-0.003712	-0.167128
C	3.597721	-2.461823	0.147243	0.000052	-0.002290	-0.160736
C	2.897975	-1.192541	0.086952	-0.003018	-0.000548	-0.008098
N	1.547321	-1.477699	0.074912	-0.002322	-0.001850	0.049926
C	3.449247	0.093263	0.049335	-0.003130	-0.000184	0.058118
C	2.769321	1.324827	0.021323	-0.002038	0.001296	0.096136
C	3.444901	2.634646	-0.023042	-0.000028	0.001660	0.186902
C	2.445267	3.577562	-0.025359	0.001360	0.002484	0.145800
C	1.176719	2.827127	0.016875	-0.000100	0.002902	0.034760
N	1.402560	1.471537	0.040697	-0.001670	0.001884	0.020478
C	-0.092239	3.435039	0.036165	0.000478	0.002862	-0.061976
C	-1.345495	2.813100	0.066604	-0.000096	0.001982	-0.128724
C	-2.651771	3.443543	0.075255	-0.000640	-0.000912	-0.164442
C	-3.607822	2.434765	0.088108	0.000832	-0.002954	-0.160298
C	-2.908032	1.164492	0.087975	0.002722	-0.000970	-0.124278
N	-1.557316	1.449232	0.078262	0.002248	0.001602	-0.113340
C	-2.871487	4.931153	0.081070	-0.010180	-0.002242	-0.180680
C	-5.104996	2.574346	0.110706	0.000922	0.000260	-0.168528
C	-4.944683	-2.871658	0.032661	0.000576	0.004574	0.229066
C	-2.575169	-5.107189	0.037390	-0.004082	0.002998	0.326346
C	2.863280	-4.956729	0.242031	-0.002914	-0.008576	-0.344392
C	5.094480	-2.601316	0.208569	0.002812	0.004320	-0.336754
C	4.934712	2.840913	-0.060831	0.000164	0.002036	0.320796
C	2.565223	5.076690	-0.065119	0.005280	0.002922	0.213330
H	-4.546424	-0.165842	0.083047	0.004316	-0.001806	-0.055702
H	0.100106	-4.550765	0.113996	0.003112	-0.005200	0.024426

H	0.809574	-0.777051	0.001974	-0.005922	-0.000328	0.266488
H	4.536294	0.137388	0.046804	-0.003214	-0.000828	0.058270
H	-0.111059	4.522651	0.021338	0.002182	0.003010	-0.065962
H	-0.819511	0.747092	0.101614	0.004332	0.003764	-0.197066
H	-2.295800	5.426274	-0.713761	0.102026	0.010544	-0.083076
H	-2.554668	5.379088	1.035490	-0.162702	-0.010190	-0.132788
H	-3.928901	5.179030	-0.065873	0.015980	-0.008890	-0.336580
H	-5.411828	3.612859	-0.057091	0.001830	-0.023666	-0.293376
H	-5.522556	2.256951	1.078324	0.006434	0.123904	-0.129616
H	-5.578673	1.954362	-0.663296	-0.004876	-0.091816	-0.085022
H	-5.437395	-2.371112	0.879491	0.061518	-0.073956	0.306936
H	-5.201685	-3.936271	0.081161	0.001432	0.002396	0.153280
H	-5.395805	-2.463281	-0.884590	-0.062520	0.087040	0.301932
H	-3.625478	-5.422976	0.083086	0.000304	-0.000890	0.093400
H	-2.048929	-5.569612	0.889062	-0.237804	0.111558	0.501542
H	-2.137746	-5.537155	-0.879529	0.225824	-0.098320	0.512650
H	2.261605	-5.496400	-0.503898	0.106656	0.104564	-0.499322
H	2.581440	-5.351589	1.231181	-0.141618	-0.145434	-0.452058
H	3.915467	-5.211438	0.072431	0.015292	0.009582	-0.232614
H	5.403609	-3.641060	0.049420	-0.010312	-0.017938	-0.159868
H	5.487867	-2.283554	1.188345	0.133926	0.208046	-0.476864
H	5.589615	-1.980864	-0.554092	-0.112108	-0.167020	-0.525796
H	5.387220	2.366872	-0.944831	0.088052	-0.062072	0.405726
H	5.427466	2.404419	0.821364	-0.091380	0.069524	0.399776
H	5.190609	3.906376	-0.089128	0.004032	-0.000800	0.268954
H	3.614057	5.393269	-0.098567	0.006554	0.001360	0.244634
H	2.105365	5.543928	0.818342	-0.007234	-0.035460	0.226658
H	2.061957	5.499994	-0.946831	0.020078	0.043652	0.225036
* Frequency(6)	22.1800					
C	-2.779722	-1.353765	0.070789	0.003384	-0.000376	0.034392

C	-3.455012	-2.664594	0.047284	0.000998	0.002114	0.145598
C	-2.455111	-3.607314	0.047557	-0.000830	0.000790	0.179782
C	-1.186800	-2.855685	0.072873	0.000924	-0.002834	0.084166
N	-1.413032	-1.499732	0.081522	0.003574	-0.003176	0.013000
C	-3.459673	-0.121586	0.086826	0.004284	-0.001296	-0.056708
C	0.082009	-3.462995	0.096796	0.001220	-0.004536	0.038636
C	1.335626	-2.841170	0.111439	-0.000040	-0.002858	-0.018328
C	2.641585	-3.470563	0.171905	0.001956	-0.003712	-0.167128
C	3.597717	-2.461679	0.157372	0.000052	-0.002290	-0.160736
C	2.898165	-1.192506	0.087463	-0.003018	-0.000548	-0.008098
N	1.547467	-1.477582	0.071766	-0.002322	-0.001850	0.049926
C	3.449444	0.093275	0.045673	-0.003130	-0.000184	0.058118
C	2.769449	1.324746	0.015264	-0.002038	0.001296	0.096136
C	3.444903	2.634541	-0.034820	-0.000028	0.001660	0.186902
C	2.445181	3.577406	-0.034547	0.001360	0.002484	0.145800
C	1.176725	2.826944	0.014685	-0.000100	0.002902	0.034760
N	1.402665	1.471418	0.039406	-0.001670	0.001884	0.020478
C	-0.092269	3.434859	0.040071	0.000478	0.002862	-0.061976
C	-1.345489	2.812975	0.074716	-0.000096	0.001982	-0.128724
C	-2.651731	3.443600	0.085618	-0.000640	-0.000912	-0.164442
C	-3.607875	2.434951	0.098210	0.000832	-0.002954	-0.160298
C	-2.908203	1.164553	0.095807	0.002722	-0.000970	-0.124278
N	-1.557458	1.449132	0.085405	0.002248	0.001602	-0.113340
C	-2.870845	4.931295	0.092456	-0.010180	-0.002242	-0.180680
C	-5.105055	2.574330	0.121326	0.000922	0.000260	-0.168528
C	-4.944720	-2.871946	0.018226	0.000576	0.004574	0.229066
C	-2.574912	-5.107378	0.016824	-0.004082	0.002998	0.326346
C	2.863464	-4.956188	0.263734	-0.002914	-0.008576	-0.344392
C	5.094303	-2.601589	0.229791	0.002812	0.004320	-0.336754
C	4.934701	2.840784	-0.081047	0.000164	0.002036	0.320796

C	2.564891	5.076505	-0.078563	0.005280	0.002922	0.213330
H	-4.546696	-0.165728	0.086558	0.004316	-0.001806	-0.055702
H	0.099910	-4.550437	0.112457	0.003112	-0.005200	0.024426
H	0.809947	-0.777030	-0.014819	-0.005922	-0.000328	0.266488
H	4.536496	0.137440	0.043132	-0.003214	-0.000828	0.058270
H	-0.111196	4.522461	0.025495	0.002182	0.003010	-0.065962
H	-0.819783	0.746855	0.114033	0.004332	0.003764	-0.197066
H	-2.302229	5.425609	-0.708525	0.102026	0.010544	-0.083076
H	-2.544415	5.379730	1.043858	-0.162702	-0.010190	-0.132788
H	-3.929908	5.179590	-0.044662	0.015980	-0.008890	-0.336580
H	-5.411944	3.614350	-0.038603	0.001830	-0.023666	-0.293376
H	-5.522961	2.249143	1.086492	0.006434	0.123904	-0.129616
H	-5.578366	1.960148	-0.657938	-0.004876	-0.091816	-0.085022
H	-5.441272	-2.366452	0.860149	0.061518	-0.073956	0.306936
H	-5.201775	-3.936422	0.071502	0.001432	0.002396	0.153280
H	-5.391865	-2.468766	-0.903616	-0.062520	0.087040	0.301932
H	-3.625497	-5.422920	0.077200	0.000304	-0.000890	0.093400
H	-2.033943	-5.576642	0.857456	-0.237804	0.111558	0.501542
H	-2.151977	-5.530959	-0.911835	0.225824	-0.098320	0.512650
H	2.254884	-5.502989	-0.472432	0.106656	0.104564	-0.499322
H	2.590364	-5.342424	1.259669	-0.141618	-0.145434	-0.452058
H	3.914504	-5.212042	0.087090	0.015292	0.009582	-0.232614
H	5.404259	-3.639930	0.059494	-0.010312	-0.017938	-0.159868
H	5.479427	-2.296664	1.218396	0.133926	0.208046	-0.476864
H	5.596680	-1.970339	-0.520958	-0.112108	-0.167020	-0.525796
H	5.381672	2.370783	-0.970399	0.088052	-0.062072	0.405726
H	5.433224	2.400038	0.796172	-0.091380	0.069524	0.399776
H	5.190355	3.906426	-0.106076	0.004032	-0.000800	0.268954
H	3.613644	5.393183	-0.113983	0.006554	0.001360	0.244634
H	2.105821	5.546163	0.804058	-0.007234	-0.035460	0.226658

H	2.060692	5.497244	-0.961012	0.020078	0.043652	0.225036
* Frequency(6)	22.1800					
C	-2.779817	-1.353755	0.069816	0.003384	-0.000376	0.034392
C	-3.455040	-2.664653	0.043166	0.000998	0.002114	0.145598
C	-2.455087	-3.607337	0.042472	-0.000830	0.000790	0.179782
C	-1.186826	-2.855604	0.070493	0.000924	-0.002834	0.084166
N	-1.413133	-1.499642	0.081155	0.003574	-0.003176	0.013000
C	-3.459794	-0.121549	0.088430	0.004284	-0.001296	-0.056708
C	0.081974	-3.462867	0.095704	0.001220	-0.004536	0.038636
C	1.335627	-2.841089	0.111957	-0.000040	-0.002858	-0.018328
C	2.641530	-3.470458	0.176632	0.001956	-0.003712	-0.167128
C	3.597716	-2.461614	0.161918	0.000052	-0.002290	-0.160736
C	2.898251	-1.192491	0.087692	-0.003018	-0.000548	-0.008098
N	1.547533	-1.477530	0.070354	-0.002322	-0.001850	0.049926
C	3.449533	0.093280	0.044029	-0.003130	-0.000184	0.058118
C	2.769507	1.324709	0.012545	-0.002038	0.001296	0.096136
C	3.444904	2.634494	-0.040106	-0.000028	0.001660	0.186902
C	2.445143	3.577336	-0.038671	0.001360	0.002484	0.145800
C	1.176728	2.826862	0.013702	-0.000100	0.002902	0.034760
N	1.402713	1.471365	0.038827	-0.001670	0.001884	0.020478
C	-0.092283	3.434778	0.041824	0.000478	0.002862	-0.061976
C	-1.345487	2.812919	0.078357	-0.000096	0.001982	-0.128724
C	-2.651713	3.443626	0.090269	-0.000640	-0.000912	-0.164442
C	-3.607898	2.435034	0.102744	0.000832	-0.002954	-0.160298
C	-2.908280	1.164580	0.099322	0.002722	-0.000970	-0.124278
N	-1.557521	1.449086	0.088611	0.002248	0.001602	-0.113340
C	-2.870557	4.931358	0.097566	-0.010180	-0.002242	-0.180680
C	-5.105081	2.574322	0.126092	0.000922	0.000260	-0.168528
C	-4.944736	-2.872075	0.011747	0.000576	0.004574	0.229066
C	-2.574796	-5.107463	0.007594	-0.004082	0.002998	0.326346

C	2.863546	-4.955946	0.273475	-0.002914	-0.008576	-0.344392
C	5.094223	-2.601711	0.239315	0.002812	0.004320	-0.336754
C	4.934697	2.840727	-0.090120	0.000164	0.002036	0.320796
C	2.564741	5.076423	-0.084596	0.005280	0.002922	0.213330
H	-4.546818	-0.165677	0.088133	0.004316	-0.001806	-0.055702
H	0.099822	-4.550290	0.111766	0.003112	-0.005200	0.024426
H	0.810115	-0.777021	-0.022356	-0.005922	-0.000328	0.266488
H	4.536587	0.137464	0.041484	-0.003214	-0.000828	0.058270
H	-0.111258	4.522376	0.027361	0.002182	0.003010	-0.065962
H	-0.819906	0.746748	0.119607	0.004332	0.003764	-0.197066
H	-2.305115	5.425311	-0.706176	0.102026	0.010544	-0.083076
H	-2.539813	5.380018	1.047614	-0.162702	-0.010190	-0.132788
H	-3.930360	5.179842	-0.035142	0.015980	-0.008890	-0.336580
H	-5.411995	3.615020	-0.030305	0.001830	-0.023666	-0.293376
H	-5.523143	2.245639	1.090158	0.006434	0.123904	-0.129616
H	-5.578228	1.962745	-0.655533	-0.004876	-0.091816	-0.085022
H	-5.443012	-2.364360	0.851467	0.061518	-0.073956	0.306936
H	-5.201815	-3.936490	0.067166	0.001432	0.002396	0.153280
H	-5.390097	-2.471228	-0.912156	-0.062520	0.087040	0.301932
H	-3.625506	-5.422895	0.074559	0.000304	-0.000890	0.093400
H	-2.027217	-5.579797	0.843271	-0.237804	0.111558	0.501542
H	-2.158364	-5.528179	-0.926335	0.225824	-0.098320	0.512650
H	2.251867	-5.505946	-0.458309	0.106656	0.104564	-0.499322
H	2.594370	-5.338311	1.272455	-0.141618	-0.145434	-0.452058
H	3.914071	-5.212313	0.093669	0.015292	0.009582	-0.232614
H	5.404551	-3.639422	0.064016	-0.010312	-0.017938	-0.159868
H	5.475639	-2.302548	1.231883	0.133926	0.208046	-0.476864
H	5.599851	-1.965615	-0.506086	-0.112108	-0.167020	-0.525796
H	5.379181	2.372539	-0.981874	0.088052	-0.062072	0.405726
H	5.435809	2.398072	0.784864	-0.091380	0.069524	0.399776

H	5.190241	3.906449	-0.113683	0.004032	-0.000800	0.268954
H	3.613459	5.393145	-0.120902	0.006554	0.001360	0.244634
H	2.106025	5.547166	0.797648	-0.007234	-0.035460	0.226658
H	2.060124	5.496009	-0.967377	0.020078	0.043652	0.225036
* Frequency(6)	22.1800					
C	-2.779785	-1.353758	0.070143	0.003384	-0.000376	0.034392
C	-3.455031	-2.664633	0.044551	0.000998	0.002114	0.145598
C	-2.455095	-3.607329	0.044183	-0.000830	0.000790	0.179782
C	-1.186818	-2.855631	0.071293	0.000924	-0.002834	0.084166
N	-1.413099	-1.499672	0.081278	0.003574	-0.003176	0.013000
C	-3.459754	-0.121561	0.087890	0.004284	-0.001296	-0.056708
C	0.081986	-3.462910	0.096071	0.001220	-0.004536	0.038636
C	1.335627	-2.841116	0.111783	-0.000040	-0.002858	-0.018328
C	2.641548	-3.470494	0.175042	0.001956	-0.003712	-0.167128
C	3.597716	-2.461636	0.160389	0.000052	-0.002290	-0.160736
C	2.898222	-1.192496	0.087615	-0.003018	-0.000548	-0.008098
N	1.547511	-1.477547	0.070829	-0.002322	-0.001850	0.049926
C	3.449503	0.093278	0.044582	-0.003130	-0.000184	0.058118
C	2.769487	1.324721	0.013460	-0.002038	0.001296	0.096136
C	3.444904	2.634510	-0.038328	-0.000028	0.001660	0.186902
C	2.445156	3.577359	-0.037283	0.001360	0.002484	0.145800
C	1.176727	2.826889	0.014032	-0.000100	0.002902	0.034760
N	1.402697	1.471383	0.039022	-0.001670	0.001884	0.020478
C	-0.092278	3.434805	0.041234	0.000478	0.002862	-0.061976
C	-1.345487	2.812938	0.077132	-0.000096	0.001982	-0.128724
C	-2.651719	3.443617	0.088705	-0.000640	-0.000912	-0.164442
C	-3.607890	2.435006	0.101219	0.000832	-0.002954	-0.160298
C	-2.908255	1.164571	0.098139	0.002722	-0.000970	-0.124278
N	-1.557500	1.449101	0.087532	0.002248	0.001602	-0.113340
C	-2.870654	4.931337	0.095847	-0.010180	-0.002242	-0.180680

C	-5.105072	2.574325	0.124489	0.000922	0.000260	-0.168528
C	-4.944730	-2.872032	0.013926	0.000576	0.004574	0.229066
C	-2.574835	-5.107434	0.010699	-0.004082	0.002998	0.326346
C	2.863519	-4.956027	0.270198	-0.002914	-0.008576	-0.344392
C	5.094250	-2.601670	0.236111	0.002812	0.004320	-0.336754
C	4.934698	2.840746	-0.087068	0.000164	0.002036	0.320796
C	2.564792	5.076451	-0.082567	0.005280	0.002922	0.213330
H	-4.546777	-0.165694	0.087603	0.004316	-0.001806	-0.055702
H	0.099851	-4.550340	0.111999	0.003112	-0.005200	0.024426
H	0.810058	-0.777024	-0.019821	-0.005922	-0.000328	0.266488
H	4.536556	0.137456	0.042039	-0.003214	-0.000828	0.058270
H	-0.111237	4.522405	0.026733	0.002182	0.003010	-0.065962
H	-0.819865	0.746784	0.117732	0.004332	0.003764	-0.197066
H	-2.304144	5.425412	-0.706966	0.102026	0.010544	-0.083076
H	-2.541361	5.379921	1.046351	-0.162702	-0.010190	-0.132788
H	-3.930208	5.179757	-0.038345	0.015980	-0.008890	-0.336580
H	-5.411978	3.614795	-0.033096	0.001830	-0.023666	-0.293376
H	-5.523082	2.246818	1.088924	0.006434	0.123904	-0.129616
H	-5.578275	1.961871	-0.656342	-0.004876	-0.091816	-0.085022
H	-5.442426	-2.365063	0.854388	0.061518	-0.073956	0.306936
H	-5.201802	-3.936467	0.068625	0.001432	0.002396	0.153280
H	-5.390692	-2.470400	-0.909284	-0.062520	0.087040	0.301932
H	-3.625503	-5.422903	0.075447	0.000304	-0.000890	0.093400
H	-2.029479	-5.578736	0.848043	-0.237804	0.111558	0.501542
H	-2.156216	-5.529114	-0.921457	0.225824	-0.098320	0.512650
H	2.252882	-5.504952	-0.463060	0.106656	0.104564	-0.499322
H	2.593023	-5.339695	1.268154	-0.141618	-0.145434	-0.452058
H	3.914217	-5.212222	0.091456	0.015292	0.009582	-0.232614
H	5.404453	-3.639593	0.062495	-0.010312	-0.017938	-0.159868
H	5.476913	-2.300569	1.227346	0.133926	0.208046	-0.476864

H	5.598784	-1.967204	-0.511089	-0.112108	-0.167020	-0.525796
H	5.380019	2.371948	-0.978014	0.088052	-0.062072	0.405726
H	5.434939	2.398733	0.788668	-0.091380	0.069524	0.399776
H	5.190279	3.906441	-0.111124	0.004032	-0.000800	0.268954
H	3.613521	5.393158	-0.118575	0.006554	0.001360	0.244634
H	2.105956	5.546828	0.799804	-0.007234	-0.035460	0.226658
H	2.060315	5.496424	-0.965235	0.020078	0.043652	0.225036
* Frequency(6)	22.1800					
C	-2.779629	-1.353776	0.071735	0.003384	-0.000376	0.034392
C	-3.454984	-2.664535	0.051290	0.000998	0.002114	0.145598
C	-2.455134	-3.607292	0.052503	-0.000830	0.000790	0.179782
C	-1.186775	-2.855763	0.075189	0.000924	-0.002834	0.084166
N	-1.412933	-1.499819	0.081880	0.003574	-0.003176	0.013000
C	-3.459555	-0.121621	0.085266	0.004284	-0.001296	-0.056708
C	0.082043	-3.463120	0.097859	0.001220	-0.004536	0.038636
C	1.335625	-2.841249	0.110934	-0.000040	-0.002858	-0.018328
C	2.641639	-3.470665	0.167307	0.001956	-0.003712	-0.167128
C	3.597719	-2.461742	0.152950	0.000052	-0.002290	-0.160736
C	2.898082	-1.192521	0.087240	-0.003018	-0.000548	-0.008098
N	1.547403	-1.477633	0.073139	-0.002322	-0.001850	0.049926
C	3.449358	0.093270	0.047272	-0.003130	-0.000184	0.058118
C	2.769393	1.324781	0.017909	-0.002038	0.001296	0.096136
C	3.444902	2.634587	-0.029678	-0.000028	0.001660	0.186902
C	2.445219	3.577474	-0.030536	0.001360	0.002484	0.145800
C	1.176722	2.827024	0.015641	-0.000100	0.002902	0.034760
N	1.402619	1.471470	0.039970	-0.001670	0.001884	0.020478
C	-0.092256	3.434937	0.038365	0.000478	0.002862	-0.061976
C	-1.345492	2.813029	0.071174	-0.000096	0.001982	-0.128724
C	-2.651748	3.443575	0.081094	-0.000640	-0.000912	-0.164442
C	-3.607852	2.434870	0.093800	0.000832	-0.002954	-0.160298

C	-2.908129	1.164526	0.092387	0.002722	-0.000970	-0.124278
N	-1.557396	1.449176	0.082287	0.002248	0.001602	-0.113340
C	-2.871125	4.931233	0.087485	-0.010180	-0.002242	-0.180680
C	-5.105029	2.574337	0.116689	0.000922	0.000260	-0.168528
C	-4.944704	-2.871820	0.024528	0.000576	0.004574	0.229066
C	-2.575024	-5.107295	0.025803	-0.004082	0.002998	0.326346
C	2.863384	-4.956424	0.254259	-0.002914	-0.008576	-0.344392
C	5.094380	-2.601470	0.220526	0.002812	0.004320	-0.336754
C	4.934706	2.840840	-0.072221	0.000164	0.002036	0.320796
C	2.565036	5.076586	-0.072693	0.005280	0.002922	0.213330
H	-4.546578	-0.165778	0.085025	0.004316	-0.001806	-0.055702
H	0.099995	-4.550580	0.113129	0.003112	-0.005200	0.024426
H	0.809784	-0.777039	-0.007487	-0.005922	-0.000328	0.266488
H	4.536408	0.137418	0.044735	-0.003214	-0.000828	0.058270
H	-0.111136	4.522544	0.023680	0.002182	0.003010	-0.065962
H	-0.819664	0.746958	0.108611	0.004332	0.003764	-0.197066
H	-2.299422	5.425900	-0.710811	0.102026	0.010544	-0.083076
H	-2.548891	5.379450	1.040205	-0.162702	-0.010190	-0.132788
H	-3.929468	5.179346	-0.053922	0.015980	-0.008890	-0.336580
H	-5.411893	3.613699	-0.046674	0.001830	-0.023666	-0.293376
H	-5.522784	2.252552	1.082926	0.006434	0.123904	-0.129616
H	-5.578500	1.957622	-0.660277	-0.004876	-0.091816	-0.085022
H	-5.439579	-2.368486	0.868593	0.061518	-0.073956	0.306936
H	-5.201736	-3.936356	0.075719	0.001432	0.002396	0.153280
H	-5.393585	-2.466371	-0.895310	-0.062520	0.087040	0.301932
H	-3.625489	-5.422944	0.079770	0.000304	-0.000890	0.093400
H	-2.040485	-5.573572	0.871255	-0.237804	0.111558	0.501542
H	-2.145764	-5.533664	-0.897731	0.225824	-0.098320	0.512650
H	2.257818	-5.500112	-0.486170	0.106656	0.104564	-0.499322
H	2.586468	-5.346426	1.247232	-0.141618	-0.145434	-0.452058

H	3.914924	-5.211779	0.080690	0.015292	0.009582	-0.232614
H	5.403976	-3.640423	0.055096	-0.010312	-0.017938	-0.159868
H	5.483112	-2.290940	1.205276	0.133926	0.208046	-0.476864
H	5.593596	-1.974934	-0.535423	-0.112108	-0.167020	-0.525796
H	5.384094	2.369076	-0.959236	0.088052	-0.062072	0.405726
H	5.430710	2.401951	0.807170	-0.091380	0.069524	0.399776
H	5.190466	3.906404	-0.098677	0.004032	-0.000800	0.268954
H	3.613825	5.393221	-0.107253	0.006554	0.001360	0.244634
H	2.105622	5.545187	0.810294	-0.007234	-0.035460	0.226658
H	2.061244	5.498445	-0.954820	0.020078	0.043652	0.225036

* Frequency(6) 22.1800

C	-2.779364	-1.353805	0.074419	0.003384	-0.000376	0.034392
C	-3.454907	-2.664370	0.062651	0.000998	0.002114	0.145598
C	-2.455199	-3.607231	0.066532	-0.000830	0.000790	0.179782
C	-1.186703	-2.855984	0.081756	0.000924	-0.002834	0.084166
N	-1.412654	-1.500067	0.082894	0.003574	-0.003176	0.013000
C	-3.459221	-0.121722	0.080841	0.004284	-0.001296	-0.056708
C	0.082138	-3.463474	0.100874	0.001220	-0.004536	0.038636
C	1.335622	-2.841472	0.109504	-0.000040	-0.002858	-0.018328
C	2.641792	-3.470955	0.154265	0.001956	-0.003712	-0.167128
C	3.597723	-2.461921	0.140407	0.000052	-0.002290	-0.160736
C	2.897847	-1.192564	0.086608	-0.003018	-0.000548	-0.008098
N	1.547222	-1.477777	0.077035	-0.002322	-0.001850	0.049926
C	3.449114	0.093256	0.051807	-0.003130	-0.000184	0.058118
C	2.769234	1.324882	0.025411	-0.002038	0.001296	0.096136
C	3.444900	2.634716	-0.015093	-0.000028	0.001660	0.186902
C	2.445325	3.577668	-0.019158	0.001360	0.002484	0.145800
C	1.176714	2.827250	0.018353	-0.000100	0.002902	0.034760
N	1.402489	1.471617	0.041568	-0.001670	0.001884	0.020478
C	-0.092219	3.435161	0.033529	0.000478	0.002862	-0.061976

C	-1.345499	2.813184	0.061129	-0.000096	0.001982	-0.128724
C	-2.651798	3.443504	0.068262	-0.000640	-0.000912	-0.164442
C	-3.607787	2.434639	0.081291	0.000832	-0.002954	-0.160298
C	-2.907916	1.164451	0.082690	0.002722	-0.000970	-0.124278
N	-1.557220	1.449301	0.073442	0.002248	0.001602	-0.113340
C	-2.871920	4.931058	0.073386	-0.010180	-0.002242	-0.180680
C	-5.104957	2.574357	0.103538	0.000922	0.000260	-0.168528
C	-4.944659	-2.871463	0.042403	0.000576	0.004574	0.229066
C	-2.575342	-5.107061	0.051269	-0.004082	0.002998	0.326346
C	2.863156	-4.957093	0.227384	-0.002914	-0.008576	-0.344392
C	5.094599	-2.601133	0.194248	0.002812	0.004320	-0.336754
C	4.934719	2.840999	-0.047188	0.000164	0.002036	0.320796
C	2.565448	5.076814	-0.056046	0.005280	0.002922	0.213330
H	-4.546241	-0.165919	0.080679	0.004316	-0.001806	-0.055702
H	0.100238	-4.550986	0.115035	0.003112	-0.005200	0.024426
H	0.809322	-0.777064	0.013308	-0.005922	-0.000328	0.266488
H	4.536157	0.137353	0.049282	-0.003214	-0.000828	0.058270
H	-0.110966	4.522779	0.018533	0.002182	0.003010	-0.065962
H	-0.819326	0.747252	0.093233	0.004332	0.003764	-0.197066
H	-2.291461	5.426722	-0.717294	0.102026	0.010544	-0.083076
H	-2.561587	5.378655	1.029843	-0.162702	-0.010190	-0.132788
H	-3.928221	5.178652	-0.080187	0.015980	-0.008890	-0.336580
H	-5.411750	3.611853	-0.069568	0.001830	-0.023666	-0.293376
H	-5.522282	2.262221	1.072811	0.006434	0.123904	-0.129616
H	-5.578881	1.950457	-0.666911	-0.004876	-0.091816	-0.085022
H	-5.434779	-2.374257	0.892545	0.061518	-0.073956	0.306936
H	-5.201624	-3.936169	0.087680	0.001432	0.002396	0.153280
H	-5.398464	-2.459579	-0.871749	-0.062520	0.087040	0.301932
H	-3.625465	-5.423014	0.087058	0.000304	-0.000890	0.093400
H	-2.059042	-5.564867	0.910392	-0.237804	0.111558	0.501542

H	-2.128142	-5.541337	-0.857727	0.225824	-0.098320	0.512650
H	2.266141	-5.491953	-0.525134	0.106656	0.104564	-0.499322
H	2.575417	-5.357774	1.211956	-0.141618	-0.145434	-0.452058
H	3.916118	-5.211031	0.062538	0.015292	0.009582	-0.232614
H	5.403171	-3.641823	0.042621	-0.010312	-0.017938	-0.159868
H	5.493562	-2.274706	1.168065	0.133926	0.208046	-0.476864
H	5.584847	-1.987967	-0.576453	-0.112108	-0.167020	-0.525796
H	5.390965	2.364232	-0.927576	0.088052	-0.062072	0.405726
H	5.423579	2.407376	0.838366	-0.091380	0.069524	0.399776
H	5.190780	3.906342	-0.077689	0.004032	-0.000800	0.268954
H	3.614336	5.393327	-0.088163	0.006554	0.001360	0.244634
H	2.105057	5.542420	0.827981	-0.007234	-0.035460	0.226658
H	2.062811	5.501851	-0.937260	0.020078	0.043652	0.225036
* Frequency(6)	22.1800					
C	-2.779022	-1.353843	0.077904	0.003384	-0.000376	0.034392
C	-3.454805	-2.664156	0.077405	0.000998	0.002114	0.145598
C	-2.455283	-3.607151	0.084750	-0.000830	0.000790	0.179782
C	-1.186609	-2.856271	0.090285	0.000924	-0.002834	0.084166
N	-1.412292	-1.500389	0.084212	0.003574	-0.003176	0.013000
C	-3.458787	-0.121854	0.075095	0.004284	-0.001296	-0.056708
C	0.082261	-3.463934	0.104789	0.001220	-0.004536	0.038636
C	1.335618	-2.841761	0.107647	-0.000040	-0.002858	-0.018328
C	2.641990	-3.471331	0.137330	0.001956	-0.003712	-0.167128
C	3.597728	-2.462153	0.124120	0.000052	-0.002290	-0.160736
C	2.897541	-1.192620	0.085787	-0.003018	-0.000548	-0.008098
N	1.546987	-1.477965	0.082094	-0.002322	-0.001850	0.049926
C	3.448797	0.093237	0.057696	-0.003130	-0.000184	0.058118
C	2.769028	1.325014	0.035153	-0.002038	0.001296	0.096136
C	3.444897	2.634884	0.003846	-0.000028	0.001660	0.186902
C	2.445462	3.577920	-0.004384	0.001360	0.002484	0.145800

C	1.176704	2.827544	0.021876	-0.000100	0.002902	0.034760
N	1.402320	1.471808	0.043643	-0.001670	0.001884	0.020478
C	-0.092170	3.435451	0.027249	0.000478	0.002862	-0.061976
C	-1.345509	2.813385	0.048086	-0.000096	0.001982	-0.128724
C	-2.651863	3.443412	0.051599	-0.000640	-0.000912	-0.164442
C	-3.607703	2.434340	0.065048	0.000832	-0.002954	-0.160298
C	-2.907640	1.164352	0.070097	0.002722	-0.000970	-0.124278
N	-1.556992	1.449463	0.061958	0.002248	0.001602	-0.113340
C	-2.872951	4.930831	0.055077	-0.010180	-0.002242	-0.180680
C	-5.104864	2.574383	0.086461	0.000922	0.000260	-0.168528
C	-4.944600	-2.871000	0.065614	0.000576	0.004574	0.229066
C	-2.575756	-5.106758	0.084337	-0.004082	0.002998	0.326346
C	2.862861	-4.957962	0.192487	-0.002914	-0.008576	-0.344392
C	5.094884	-2.600695	0.160124	0.002812	0.004320	-0.336754
C	4.934735	2.841206	-0.014682	0.000164	0.002036	0.320796
C	2.565983	5.077110	-0.034430	0.005280	0.002922	0.213330
H	-4.545803	-0.166102	0.075034	0.004316	-0.001806	-0.055702
H	0.100553	-4.551513	0.117510	0.003112	-0.005200	0.024426
H	0.808722	-0.777098	0.040311	-0.005922	-0.000328	0.266488
H	4.535831	0.137269	0.055187	-0.003214	-0.000828	0.058270
H	-0.110745	4.523084	0.011849	0.002182	0.003010	-0.065962
H	-0.818887	0.747633	0.073265	0.004332	0.003764	-0.197066
H	-2.281123	5.427791	-0.725712	0.102026	0.010544	-0.083076
H	-2.578074	5.377622	1.016388	-0.162702	-0.010190	-0.132788
H	-3.926602	5.177751	-0.114292	0.015980	-0.008890	-0.336580
H	-5.411565	3.609455	-0.099295	0.001830	-0.023666	-0.293376
H	-5.521630	2.274776	1.059677	0.006434	0.123904	-0.129616
H	-5.579375	1.941153	-0.675527	-0.004876	-0.091816	-0.085022
H	-5.428545	-2.381751	0.923646	0.061518	-0.073956	0.306936
H	-5.201479	-3.935926	0.103212	0.001432	0.002396	0.153280

H	-5.404799	-2.450760	-0.841154	-0.062520	0.087040	0.301932
H	-3.625435	-5.423104	0.096523	0.000304	-0.000890	0.093400
H	-2.083139	-5.553563	0.961213	-0.237804	0.111558	0.501542
H	-2.105260	-5.551299	-0.805780	0.225824	-0.098320	0.512650
H	2.276948	-5.481357	-0.575730	0.106656	0.104564	-0.499322
H	2.561067	-5.372511	1.166149	-0.141618	-0.145434	-0.452058
H	3.917667	-5.210060	0.038967	0.015292	0.009582	-0.232614
H	5.402126	-3.643640	0.026421	-0.010312	-0.017938	-0.159868
H	5.507133	-2.253624	1.119744	0.133926	0.208046	-0.476864
H	5.573487	-2.004891	-0.629732	-0.112108	-0.167020	-0.525796
H	5.399887	2.357942	-0.886464	0.088052	-0.062072	0.405726
H	5.414320	2.414421	0.878876	-0.091380	0.069524	0.399776
H	5.191189	3.906261	-0.050436	0.004032	-0.000800	0.268954
H	3.615000	5.393464	-0.063374	0.006554	0.001360	0.244634
H	2.104324	5.538827	0.850948	-0.007234	-0.035460	0.226658
H	2.064845	5.506274	-0.914457	0.020078	0.043652	0.225036
* Frequency(6)	22.1800					
C	-2.778637	-1.353886	0.081812	0.003384	-0.000376	0.034392
C	-3.454692	-2.663916	0.093951	0.000998	0.002114	0.145598
C	-2.455377	-3.607061	0.105181	-0.000830	0.000790	0.179782
C	-1.186504	-2.856593	0.099850	0.000924	-0.002834	0.084166
N	-1.411886	-1.500750	0.085689	0.003574	-0.003176	0.013000
C	-3.458300	-0.122001	0.068650	0.004284	-0.001296	-0.056708
C	0.082400	-3.464449	0.109180	0.001220	-0.004536	0.038636
C	1.335613	-2.842086	0.105564	-0.000040	-0.002858	-0.018328
C	2.642212	-3.471753	0.118337	0.001956	-0.003712	-0.167128
C	3.597734	-2.462413	0.105853	0.000052	-0.002290	-0.160736
C	2.897198	-1.192682	0.084867	-0.003018	-0.000548	-0.008098
N	1.546723	-1.478175	0.087768	-0.002322	-0.001850	0.049926
C	3.448441	0.093216	0.064301	-0.003130	-0.000184	0.058118

C	2.768796	1.325161	0.046078	-0.002038	0.001296	0.096136
C	3.444894	2.635073	0.025086	-0.000028	0.001660	0.186902
C	2.445617	3.578202	0.012185	0.001360	0.002484	0.145800
C	1.176693	2.827874	0.025826	-0.000100	0.002902	0.034760
N	1.402130	1.472022	0.045970	-0.001670	0.001884	0.020478
C	-0.092116	3.435776	0.020206	0.000478	0.002862	-0.061976
C	-1.345520	2.813610	0.033457	-0.000096	0.001982	-0.128724
C	-2.651936	3.443308	0.032911	-0.000640	-0.000912	-0.164442
C	-3.607608	2.434004	0.046831	0.000832	-0.002954	-0.160298
C	-2.907331	1.164242	0.055973	0.002722	-0.000970	-0.124278
N	-1.556737	1.449645	0.049077	0.002248	0.001602	-0.113340
C	-2.874108	4.930576	0.034544	-0.010180	-0.002242	-0.180680
C	-5.104759	2.574413	0.067309	0.000922	0.000260	-0.168528
C	-4.944535	-2.870480	0.091646	0.000576	0.004574	0.229066
C	-2.576220	-5.106417	0.121425	-0.004082	0.002998	0.326346
C	2.862530	-4.958937	0.153349	-0.002914	-0.008576	-0.344392
C	5.095204	-2.600204	0.121854	0.002812	0.004320	-0.336754
C	4.934754	2.841437	0.021775	0.000164	0.002036	0.320796
C	2.566583	5.077442	-0.010186	0.005280	0.002922	0.213330
H	-4.545313	-0.166307	0.068704	0.004316	-0.001806	-0.055702
H	0.100907	-4.552104	0.120286	0.003112	-0.005200	0.024426
H	0.808049	-0.777135	0.070596	-0.005922	-0.000328	0.266488
H	4.535466	0.137175	0.061809	-0.003214	-0.000828	0.058270
H	-0.110497	4.523426	0.004353	0.002182	0.003010	-0.065962
H	-0.818395	0.748061	0.050869	0.004332	0.003764	-0.197066
H	-2.269528	5.428989	-0.735153	0.102026	0.010544	-0.083076
H	-2.596564	5.376464	1.001297	-0.162702	-0.010190	-0.132788
H	-3.924786	5.176741	-0.152543	0.015980	-0.008890	-0.336580
H	-5.411357	3.606765	-0.132636	0.001830	-0.023666	-0.293376
H	-5.520899	2.288857	1.044947	0.006434	0.123904	-0.129616

H	-5.579929	1.930719	-0.685189	-0.004876	-0.091816	-0.085022
H	-5.421554	-2.390156	0.958528	0.061518	-0.073956	0.306936
H	-5.201316	-3.935654	0.120631	0.001432	0.002396	0.153280
H	-5.411904	-2.440868	-0.806841	-0.062520	0.087040	0.301932
H	-3.625400	-5.423205	0.107137	0.000304	-0.000890	0.093400
H	-2.110164	-5.540885	1.018211	-0.237804	0.111558	0.501542
H	-2.079596	-5.562473	-0.747520	0.225824	-0.098320	0.512650
H	2.289069	-5.469474	-0.632475	0.106656	0.104564	-0.499322
H	2.544973	-5.389039	1.114775	-0.141618	-0.145434	-0.452058
H	3.919405	-5.208971	0.012532	0.015292	0.009582	-0.232614
H	5.400954	-3.645679	0.008253	-0.010312	-0.017938	-0.159868
H	5.522353	-2.229981	1.065551	0.133926	0.208046	-0.476864
H	5.560747	-2.023872	-0.689486	-0.112108	-0.167020	-0.525796
H	5.409894	2.350888	-0.840355	0.088052	-0.062072	0.405726
H	5.403935	2.422322	0.924308	-0.091380	0.069524	0.399776
H	5.191647	3.906170	-0.019871	0.004032	-0.000800	0.268954
H	3.615745	5.393619	-0.035573	0.006554	0.001360	0.244634
H	2.103502	5.534797	0.876707	-0.007234	-0.035460	0.226658
H	2.067127	5.511235	-0.888883	0.020078	0.043652	0.225036

Frequency Mode: Mode 8

* (null), Energy -1000.0000000

C	-2.778637	-1.353886	0.081812	0.005062	0.001168	0.075312
C	-3.454692	-2.663916	0.093951	0.003214	0.001552	0.061862
C	-2.455377	-3.607061	0.105181	0.002064	-0.001044	-0.070060
C	-1.186504	-2.856593	0.099850	0.003256	-0.003068	-0.103250
N	-1.411886	-1.500750	0.085689	0.005248	-0.002052	-0.019884

C	-3.458300	-0.122001	0.068650	0.004646	0.000838	0.140910
C	0.082400	-3.464449	0.109180	0.002252	-0.006558	-0.167564
C	1.335613	-2.842086	0.105564	0.002136	-0.006636	-0.108958
C	2.642212	-3.471753	0.118337	0.002926	-0.003708	-0.062634
C	3.597734	-2.462413	0.105853	0.000840	-0.000226	0.063852
C	2.897198	-1.192682	0.084867	-0.000692	-0.001326	0.067632
N	1.546723	-1.478175	0.087768	-0.000158	-0.005068	-0.031892
C	3.448441	0.093216	0.064301	-0.003722	0.000314	0.126156
C	2.768796	1.325161	0.046078	-0.004772	-0.001320	0.066432
C	3.444894	2.635073	0.025086	-0.002152	-0.002884	0.062430
C	2.445617	3.578202	0.012185	-0.000266	-0.003172	-0.061398
C	1.176693	2.827874	0.025826	-0.002284	-0.000688	-0.102286
N	1.402130	1.472022	0.045970	-0.004364	-0.000580	-0.027392
C	-0.092116	3.435776	0.020206	-0.000320	0.002532	-0.166856
C	-1.345520	2.813610	0.033457	-0.002108	0.004928	-0.106600
C	-2.651936	3.443308	0.032911	-0.001634	0.001844	-0.072200
C	-3.607608	2.434004	0.046831	0.000050	0.000772	0.064800
C	-2.907331	1.164242	0.055973	0.000248	0.002858	0.082430
N	-1.556737	1.449645	0.049077	-0.000092	0.004830	-0.016148
C	-2.874108	4.930576	0.034544	-0.027958	-0.001764	-0.143690
C	-5.104759	2.574413	0.067309	0.004540	0.026084	0.224150
C	-4.944535	-2.870480	0.091646	0.002714	0.004180	0.185102
C	-2.576220	-5.106417	0.121425	0.000980	-0.001848	-0.157322
C	2.862530	-4.958937	0.153349	0.012364	-0.003706	-0.119266
C	5.095204	-2.600204	0.121854	-0.001174	-0.002282	0.208708
C	4.934754	2.841437	0.021775	-0.001892	-0.003508	0.184218
C	2.566583	5.077442	-0.010186	0.004116	-0.005538	-0.135076
H	-4.545313	-0.166307	0.068704	0.005018	-0.001368	0.214112
H	0.100907	-4.552104	0.120286	0.001096	-0.007108	-0.232216
H	0.808049	-0.777135	0.070596	-0.001988	-0.007382	-0.053788

H	4.535466	0.137175	0.061809	-0.003938	0.003688	0.200488
H	-0.110497	4.523426	0.004353	0.002624	0.002188	-0.234542
H	-0.818395	0.748061	0.050869	0.002024	0.007056	-0.023424
H	-2.269528	5.428989	-0.735153	0.275680	0.019438	0.112602
H	-2.596564	5.376464	1.001297	-0.443442	-0.006222	-0.020860
H	-3.924786	5.176741	-0.152543	0.041558	-0.024438	-0.570014
H	-5.411357	3.606765	-0.132636	-0.016482	-0.092610	-0.366260
H	-5.520899	2.288857	1.044947	0.169118	0.652840	0.478754
H	-5.579929	1.930719	-0.685189	-0.133658	-0.438468	0.713310
H	-5.421554	-2.390156	0.958528	0.092940	-0.106422	0.296420
H	-5.201316	-3.935654	0.120631	0.004304	0.000894	0.076562
H	-5.411904	-2.440868	-0.806841	-0.090418	0.120358	0.289192
H	-3.625400	-5.423205	0.107137	0.001546	-0.001304	-0.206678
H	-2.110164	-5.540885	1.018211	-0.026238	-0.053996	-0.167742
H	-2.079596	-5.562473	-0.747520	0.028642	0.049472	-0.167688
H	2.289069	-5.469474	-0.632475	-0.107244	0.007532	-0.037562
H	2.544973	-5.389039	1.114775	0.164800	-0.020712	-0.075670
H	3.919405	-5.208971	0.012532	-0.007832	0.003226	-0.285190
H	5.400954	-3.645679	0.008253	0.014688	0.028796	-0.039860
H	5.522353	-2.229981	1.065551	-0.122422	-0.264990	0.367264
H	5.560747	-2.023872	-0.689486	0.101270	0.223882	0.429328
H	5.409894	2.350888	-0.840355	0.082618	-0.087618	0.278624
H	5.403935	2.422322	0.924308	-0.090600	0.084156	0.270994
H	5.191647	3.906170	-0.019871	0.002512	-0.007570	0.106556
H	3.615745	5.393619	-0.035573	0.006424	-0.009036	-0.082358
H	2.103502	5.534797	0.876707	-0.054472	0.045690	-0.191850
H	2.067127	5.511235	-0.888883	0.064014	-0.053870	-0.192896
* Frequency(8)	42.6000					
C	-2.778062	-1.353753	0.090371	0.005062	0.001168	0.075312
C	-3.454327	-2.663740	0.100981	0.003214	0.001552	0.061862

C	-2.455142	-3.607180	0.097219	0.002064	-0.001044	-0.070060
C	-1.186134	-2.856942	0.088116	0.003256	-0.003068	-0.103250
N	-1.411290	-1.500983	0.083429	0.005248	-0.002052	-0.019884
C	-3.457772	-0.121906	0.084664	0.004646	0.000838	0.140910
C	0.082656	-3.465194	0.090137	0.002252	-0.006558	-0.167564
C	1.335856	-2.842840	0.093181	0.002136	-0.006636	-0.108958
C	2.642545	-3.472174	0.111219	0.002926	-0.003708	-0.062634
C	3.597829	-2.462439	0.113109	0.000840	-0.000226	0.063852
C	2.897119	-1.192833	0.092553	-0.000692	-0.001326	0.067632
N	1.546705	-1.478751	0.084144	-0.000158	-0.005068	-0.031892
C	3.448018	0.093252	0.078638	-0.003722	0.000314	0.126156
C	2.768254	1.325011	0.053628	-0.004772	-0.001320	0.066432
C	3.444649	2.634745	0.032181	-0.002152	-0.002884	0.062430
C	2.445587	3.577842	0.005207	-0.000266	-0.003172	-0.061398
C	1.176433	2.827796	0.014202	-0.002284	-0.000688	-0.102286
N	1.401634	1.471956	0.042857	-0.004364	-0.000580	-0.027392
C	-0.092152	3.436064	0.001244	-0.000320	0.002532	-0.166856
C	-1.345760	2.814170	0.021342	-0.002108	0.004928	-0.106600
C	-2.652122	3.443518	0.024706	-0.001634	0.001844	-0.072200
C	-3.607602	2.434092	0.054195	0.000050	0.000772	0.064800
C	-2.907303	1.164567	0.065341	0.000248	0.002858	0.082430
N	-1.556747	1.450194	0.047242	-0.000092	0.004830	-0.016148
C	-2.877285	4.930376	0.018214	-0.027958	-0.001764	-0.143690
C	-5.104243	2.577377	0.092782	0.004540	0.026084	0.224150
C	-4.944227	-2.870005	0.112682	0.002714	0.004180	0.185102
C	-2.576109	-5.106627	0.103546	0.000980	-0.001848	-0.157322
C	2.863935	-4.959358	0.139795	0.012364	-0.003706	-0.119266
C	5.095071	-2.600463	0.145573	-0.001174	-0.002282	0.208708
C	4.934539	2.841038	0.042710	-0.001892	-0.003508	0.184218
C	2.567051	5.076813	-0.025537	0.004116	-0.005538	-0.135076

H	-4.544743	-0.166462	0.093037	0.005018	-0.001368	0.214112
H	0.101032	-4.552912	0.093896	0.001096	-0.007108	-0.232216
H	0.807823	-0.777974	0.064483	-0.001988	-0.007382	-0.053788
H	4.535018	0.137594	0.084593	-0.003938	0.003688	0.200488
H	-0.110199	4.523675	-0.022301	0.002624	0.002188	-0.234542
H	-0.818165	0.748863	0.048207	0.002024	0.007056	-0.023424
H	-2.238198	5.431198	-0.722356	0.275680	0.019438	0.112602
H	-2.646959	5.375757	0.998926	-0.443442	-0.006222	-0.020860
H	-3.920063	5.173964	-0.217322	0.041558	-0.024438	-0.570014
H	-5.413230	3.596240	-0.174260	-0.016482	-0.092610	-0.366260
H	-5.501680	2.363049	1.099355	0.169118	0.652840	0.478754
H	-5.595119	1.880889	-0.604125	-0.133658	-0.438468	0.713310
H	-5.410992	-2.402250	0.992215	0.092940	-0.106422	0.296420
H	-5.200827	-3.935552	0.129332	0.004304	0.000894	0.076562
H	-5.422180	-2.427190	-0.773976	-0.090418	0.120358	0.289192
H	-3.625224	-5.423353	0.083649	0.001546	-0.001304	-0.206678
H	-2.113146	-5.547021	0.999148	-0.026238	-0.053996	-0.167742
H	-2.076341	-5.556851	-0.766577	0.028642	0.049472	-0.167688
H	2.276881	-5.468618	-0.636744	-0.107244	0.007532	-0.037562
H	2.563702	-5.391393	1.106175	0.164800	-0.020712	-0.075670
H	3.918515	-5.208604	-0.019878	-0.007832	0.003226	-0.285190
H	5.402623	-3.642406	0.003723	0.014688	0.028796	-0.039860
H	5.508440	-2.260096	1.107289	-0.122422	-0.264990	0.367264
H	5.572256	-1.998429	-0.640695	0.101270	0.223882	0.429328
H	5.419283	2.340931	-0.808691	0.082618	-0.087618	0.278624
H	5.393639	2.431886	0.955105	-0.090600	0.084156	0.270994
H	5.191932	3.905310	-0.007761	0.002512	-0.007570	0.106556
H	3.616475	5.392592	-0.044933	0.006424	-0.009036	-0.082358
H	2.097312	5.539989	0.854904	-0.054472	0.045690	-0.191850
H	2.074402	5.505113	-0.910805	0.064014	-0.053870	-0.192896

* Frequency(8) 42.6000

C	-2.777549	-1.353635	0.098002	0.005062	0.001168	0.075312
C	-3.454001	-2.663582	0.107250	0.003214	0.001552	0.061862
C	-2.454933	-3.607285	0.090120	0.002064	-0.001044	-0.070060
C	-1.185804	-2.857253	0.077654	0.003256	-0.003068	-0.103250
N	-1.410758	-1.501191	0.081414	0.005248	-0.002052	-0.019884
C	-3.457301	-0.121821	0.098942	0.004646	0.000838	0.140910
C	0.082884	-3.465859	0.073158	0.002252	-0.006558	-0.167564
C	1.336072	-2.843513	0.082141	0.002136	-0.006636	-0.108958
C	2.642841	-3.472550	0.104872	0.002926	-0.003708	-0.062634
C	3.597915	-2.462462	0.119580	0.000840	-0.000226	0.063852
C	2.897049	-1.192967	0.099406	-0.000692	-0.001326	0.067632
N	1.546689	-1.479264	0.080912	-0.000158	-0.005068	-0.031892
C	3.447641	0.093284	0.091421	-0.003722	0.000314	0.126156
C	2.767770	1.324877	0.060359	-0.004772	-0.001320	0.066432
C	3.444431	2.634453	0.038507	-0.002152	-0.002884	0.062430
C	2.445560	3.577520	-0.001014	-0.000266	-0.003172	-0.061398
C	1.176202	2.827726	0.003837	-0.002284	-0.000688	-0.102286
N	1.401192	1.471897	0.040081	-0.004364	-0.000580	-0.027392
C	-0.092185	3.436320	-0.015664	-0.000320	0.002532	-0.166856
C	-1.345973	2.814669	0.010541	-0.002108	0.004928	-0.106600
C	-2.652287	3.443704	0.017390	-0.001634	0.001844	-0.072200
C	-3.607597	2.434170	0.060761	0.000050	0.000772	0.064800
C	-2.907278	1.164856	0.073693	0.000248	0.002858	0.082430
N	-1.556757	1.450683	0.045606	-0.000092	0.004830	-0.016148
C	-2.880118	4.930197	0.003654	-0.027958	-0.001764	-0.143690
C	-5.103783	2.580020	0.115496	0.004540	0.026084	0.224150
C	-4.943952	-2.869581	0.131438	0.002714	0.004180	0.185102
C	-2.576009	-5.106814	0.087605	0.000980	-0.001848	-0.157322
C	2.865188	-4.959734	0.127710	0.012364	-0.003706	-0.119266

C	5.094952	-2.600695	0.166721	-0.001174	-0.002282	0.208708
C	4.934347	2.840683	0.061377	-0.001892	-0.003508	0.184218
C	2.567468	5.076251	-0.039224	0.004116	-0.005538	-0.135076
H	-4.544234	-0.166601	0.114733	0.005018	-0.001368	0.214112
H	0.101143	-4.553632	0.070365	0.001096	-0.007108	-0.232216
H	0.807622	-0.778722	0.059033	-0.001988	-0.007382	-0.053788
H	4.534619	0.137968	0.104909	-0.003938	0.003688	0.200488
H	-0.109933	4.523896	-0.046068	0.002624	0.002188	-0.234542
H	-0.817960	0.749578	0.045833	0.002024	0.007056	-0.023424
H	-2.210264	5.433168	-0.710946	0.275680	0.019438	0.112602
H	-2.691893	5.375126	0.996813	-0.443442	-0.006222	-0.020860
H	-3.915852	5.171487	-0.275081	0.041558	-0.024438	-0.570014
H	-5.414900	3.586856	-0.211373	-0.016482	-0.092610	-0.366260
H	-5.484543	2.429201	1.147867	0.169118	0.652840	0.478754
H	-5.608662	1.836460	-0.531846	-0.133658	-0.438468	0.713310
H	-5.401574	-2.413034	1.022251	0.092940	-0.106422	0.296420
H	-5.200391	-3.935462	0.137090	0.004304	0.000894	0.076562
H	-5.431342	-2.414994	-0.744672	-0.090418	0.120358	0.289192
H	-3.625068	-5.423485	0.062707	0.001546	-0.001304	-0.206678
H	-2.115804	-5.552493	0.982151	-0.026238	-0.053996	-0.167742
H	-2.073439	-5.551838	-0.783569	0.028642	0.049472	-0.167688
H	2.266014	-5.467855	-0.640550	-0.107244	0.007532	-0.037562
H	2.580401	-5.393492	1.098508	0.164800	-0.020712	-0.075670
H	3.917721	-5.208277	-0.048777	-0.007832	0.003226	-0.285190
H	5.404112	-3.639489	-0.000316	0.014688	0.028796	-0.039860
H	5.496035	-2.286947	1.144503	-0.122422	-0.264990	0.367264
H	5.582517	-1.975743	-0.597191	0.101270	0.223882	0.429328
H	5.427655	2.332052	-0.780458	0.082618	-0.087618	0.278624
H	5.384458	2.440413	0.982565	-0.090600	0.084156	0.270994
H	5.192187	3.904543	0.003036	0.002512	-0.007570	0.106556

H	3.617126	5.391676	-0.053278	0.006424	-0.009036	-0.082358
H	2.091792	5.544619	0.835464	-0.054472	0.045690	-0.191850
H	2.080888	5.499654	-0.930351	0.064014	-0.053870	-0.192896
* Frequency(8)	42.6000					
C	-2.777154	-1.353544	0.103879	0.005062	0.001168	0.075312
C	-3.453750	-2.663461	0.112077	0.003214	0.001552	0.061862
C	-2.454772	-3.607367	0.084653	0.002064	-0.001044	-0.070060
C	-1.185550	-2.857492	0.069597	0.003256	-0.003068	-0.103250
N	-1.410348	-1.501351	0.079863	0.005248	-0.002052	-0.019884
C	-3.456939	-0.121755	0.109938	0.004646	0.000838	0.140910
C	0.083060	-3.466371	0.060082	0.002252	-0.006558	-0.167564
C	1.336239	-2.844030	0.073638	0.002136	-0.006636	-0.108958
C	2.643069	-3.472839	0.099985	0.002926	-0.003708	-0.062634
C	3.597980	-2.462479	0.124562	0.000840	-0.000226	0.063852
C	2.896995	-1.193071	0.104684	-0.000692	-0.001326	0.067632
N	1.546677	-1.479660	0.078423	-0.000158	-0.005068	-0.031892
C	3.447350	0.093308	0.101266	-0.003722	0.000314	0.126156
C	2.767398	1.324774	0.065543	-0.004772	-0.001320	0.066432
C	3.444263	2.634228	0.043379	-0.002152	-0.002884	0.062430
C	2.445539	3.577273	-0.005805	-0.000266	-0.003172	-0.061398
C	1.176024	2.827672	-0.004145	-0.002284	-0.000688	-0.102286
N	1.400851	1.471852	0.037944	-0.004364	-0.000580	-0.027392
C	-0.092210	3.436518	-0.028684	-0.000320	0.002532	-0.166856
C	-1.346138	2.815054	0.002222	-0.002108	0.004928	-0.106600
C	-2.652415	3.443848	0.011756	-0.001634	0.001844	-0.072200
C	-3.607593	2.434230	0.065818	0.000050	0.000772	0.064800
C	-2.907258	1.165079	0.080126	0.000248	0.002858	0.082430
N	-1.556764	1.451060	0.044346	-0.000092	0.004830	-0.016148
C	-2.882300	4.930059	-0.007558	-0.027958	-0.001764	-0.143690
C	-5.103429	2.582056	0.132987	0.004540	0.026084	0.224150

C	-4.943740	-2.869255	0.145882	0.002714	0.004180	0.185102
C	-2.575933	-5.106958	0.075328	0.000980	-0.001848	-0.157322
C	2.866153	-4.960023	0.118403	0.012364	-0.003706	-0.119266
C	5.094860	-2.600873	0.183007	-0.001174	-0.002282	0.208708
C	4.934200	2.840409	0.075752	-0.001892	-0.003508	0.184218
C	2.567789	5.075819	-0.049764	0.004116	-0.005538	-0.135076
H	-4.543843	-0.166708	0.131441	0.005018	-0.001368	0.214112
H	0.101228	-4.554187	0.052245	0.001096	-0.007108	-0.232216
H	0.807466	-0.779298	0.054836	-0.001988	-0.007382	-0.053788
H	4.534312	0.138256	0.120554	-0.003938	0.003688	0.200488
H	-0.109728	4.524067	-0.064370	0.002624	0.002188	-0.234542
H	-0.817802	0.750128	0.044006	0.002024	0.007056	-0.023424
H	-2.188751	5.434684	-0.702160	0.275680	0.019438	0.112602
H	-2.726496	5.374641	0.995185	-0.443442	-0.006222	-0.020860
H	-3.912609	5.169580	-0.319562	0.041558	-0.024438	-0.570014
H	-5.416186	3.579630	-0.239953	-0.016482	-0.092610	-0.366260
H	-5.471346	2.480145	1.185226	0.169118	0.652840	0.478754
H	-5.619092	1.802244	-0.476183	-0.133658	-0.438468	0.713310
H	-5.394322	-2.421339	1.045382	0.092940	-0.106422	0.296420
H	-5.200055	-3.935392	0.143064	0.004304	0.000894	0.076562
H	-5.438397	-2.405602	-0.722105	-0.090418	0.120358	0.289192
H	-3.624947	-5.423587	0.046579	0.001546	-0.001304	-0.206678
H	-2.117852	-5.556706	0.969061	-0.026238	-0.053996	-0.167742
H	-2.071204	-5.547977	-0.796654	0.028642	0.049472	-0.167688
H	2.257646	-5.467267	-0.643481	-0.107244	0.007532	-0.037562
H	2.593261	-5.395108	1.092603	0.164800	-0.020712	-0.075670
H	3.917110	-5.208026	-0.071031	-0.007832	0.003226	-0.285190
H	5.405258	-3.637242	-0.003426	0.014688	0.028796	-0.039860
H	5.486482	-2.307625	1.173162	-0.122422	-0.264990	0.367264
H	5.590420	-1.958273	-0.563689	0.101270	0.223882	0.429328

H	5.434102	2.325215	-0.758716	0.082618	-0.087618	0.278624
H	5.377388	2.446980	1.003711	-0.090600	0.084156	0.270994
H	5.192383	3.903952	0.011351	0.002512	-0.007570	0.106556
H	3.617627	5.390971	-0.059705	0.006424	-0.009036	-0.082358
H	2.087541	5.548185	0.820493	-0.054472	0.045690	-0.191850
H	2.085884	5.495451	-0.945403	0.064014	-0.053870	-0.192896

* Frequency(8) 42.6000

C	-2.776920	-1.353490	0.107365	0.005062	0.001168	0.075312
C	-3.453602	-2.663389	0.114940	0.003214	0.001552	0.061862
C	-2.454677	-3.607415	0.081410	0.002064	-0.001044	-0.070060
C	-1.185399	-2.857634	0.064818	0.003256	-0.003068	-0.103250
N	-1.410105	-1.501446	0.078943	0.005248	-0.002052	-0.019884
C	-3.456724	-0.121717	0.116459	0.004646	0.000838	0.140910
C	0.083164	-3.466674	0.052327	0.002252	-0.006558	-0.167564
C	1.336338	-2.844338	0.068596	0.002136	-0.006636	-0.108958
C	2.643205	-3.473011	0.097086	0.002926	-0.003708	-0.062634
C	3.598019	-2.462490	0.127517	0.000840	-0.000226	0.063852
C	2.896963	-1.193132	0.107814	-0.000692	-0.001326	0.067632
N	1.546669	-1.479895	0.076947	-0.000158	-0.005068	-0.031892
C	3.447178	0.093323	0.107104	-0.003722	0.000314	0.126156
C	2.767177	1.324713	0.068618	-0.004772	-0.001320	0.066432
C	3.444164	2.634094	0.046268	-0.002152	-0.002884	0.062430
C	2.445527	3.577126	-0.008647	-0.000266	-0.003172	-0.061398
C	1.175918	2.827641	-0.008879	-0.002284	-0.000688	-0.102286
N	1.400649	1.471825	0.036676	-0.004364	-0.000580	-0.027392
C	-0.092225	3.436635	-0.036407	-0.000320	0.002532	-0.166856
C	-1.346235	2.815282	-0.002711	-0.002108	0.004928	-0.106600
C	-2.652490	3.443934	0.008414	-0.001634	0.001844	-0.072200
C	-3.607591	2.434266	0.068817	0.000050	0.000772	0.064800
C	-2.907247	1.165212	0.083941	0.000248	0.002858	0.082430

N	-1.556768	1.451284	0.043598	-0.000092	0.004830	-0.016148
C	-2.883594	4.929977	-0.014209	-0.027958	-0.001764	-0.143690
C	-5.103219	2.583263	0.143361	0.004540	0.026084	0.224150
C	-4.943614	-2.869062	0.154449	0.002714	0.004180	0.185102
C	-2.575887	-5.107044	0.068047	0.000980	-0.001848	-0.157322
C	2.866725	-4.960194	0.112883	0.012364	-0.003706	-0.119266
C	5.094806	-2.600978	0.192667	-0.001174	-0.002282	0.208708
C	4.934112	2.840247	0.084278	-0.001892	-0.003508	0.184218
C	2.567980	5.075563	-0.056016	0.004116	-0.005538	-0.135076
H	-4.543610	-0.166771	0.141350	0.005018	-0.001368	0.214112
H	0.101279	-4.554516	0.041497	0.001096	-0.007108	-0.232216
H	0.807374	-0.779640	0.052346	-0.001988	-0.007382	-0.053788
H	4.534130	0.138426	0.129833	-0.003938	0.003688	0.200488
H	-0.109607	4.524168	-0.075225	0.002624	0.002188	-0.234542
H	-0.817708	0.750455	0.042921	0.002024	0.007056	-0.023424
H	-2.175993	5.435584	-0.696948	0.275680	0.019438	0.112602
H	-2.747019	5.374353	0.994219	-0.443442	-0.006222	-0.020860
H	-3.910686	5.168449	-0.345943	0.041558	-0.024438	-0.570014
H	-5.416949	3.575343	-0.256904	-0.016482	-0.092610	-0.366260
H	-5.463519	2.510359	1.207383	0.169118	0.652840	0.478754
H	-5.625278	1.781951	-0.443170	-0.133658	-0.438468	0.713310
H	-5.390020	-2.426264	1.059100	0.092940	-0.106422	0.296420
H	-5.199856	-3.935351	0.146608	0.004304	0.000894	0.076562
H	-5.442582	-2.400032	-0.708721	-0.090418	0.120358	0.289192
H	-3.624875	-5.423647	0.037013	0.001546	-0.001304	-0.206678
H	-2.119066	-5.559205	0.961298	-0.026238	-0.053996	-0.167742
H	-2.069878	-5.545688	-0.804415	0.028642	0.049472	-0.167688
H	2.252682	-5.466918	-0.645219	-0.107244	0.007532	-0.037562
H	2.600888	-5.396066	1.089101	0.164800	-0.020712	-0.075670
H	3.916748	-5.207876	-0.084230	-0.007832	0.003226	-0.285190

H	5.405937	-3.635909	-0.005271	0.014688	0.028796	-0.039860
H	5.480816	-2.319889	1.190160	-0.122422	-0.264990	0.367264
H	5.595107	-1.947911	-0.543819	0.101270	0.223882	0.429328
H	5.437925	2.321160	-0.745821	0.082618	-0.087618	0.278624
H	5.373195	2.450875	1.016254	-0.090600	0.084156	0.270994
H	5.192499	3.903602	0.016282	0.002512	-0.007570	0.106556
H	3.617925	5.390553	-0.063516	0.006424	-0.009036	-0.082358
H	2.085020	5.550299	0.811614	-0.054472	0.045690	-0.191850
H	2.088846	5.492957	-0.954331	0.064014	-0.053870	-0.192896
* Frequency(8)	42.6000					
C	-2.776871	-1.353479	0.108081	0.005062	0.001168	0.075312
C	-3.453571	-2.663375	0.115529	0.003214	0.001552	0.061862
C	-2.454657	-3.607425	0.080744	0.002064	-0.001044	-0.070060
C	-1.185368	-2.857663	0.063836	0.003256	-0.003068	-0.103250
N	-1.410055	-1.501466	0.078753	0.005248	-0.002052	-0.019884
C	-3.456679	-0.121709	0.117800	0.004646	0.000838	0.140910
C	0.083186	-3.466736	0.050733	0.002252	-0.006558	-0.167564
C	1.336358	-2.844401	0.067559	0.002136	-0.006636	-0.108958
C	2.643233	-3.473046	0.096490	0.002926	-0.003708	-0.062634
C	3.598027	-2.462492	0.128125	0.000840	-0.000226	0.063852
C	2.896957	-1.193145	0.108457	-0.000692	-0.001326	0.067632
N	1.546668	-1.479943	0.076644	-0.000158	-0.005068	-0.031892
C	3.447143	0.093326	0.108305	-0.003722	0.000314	0.126156
C	2.767132	1.324701	0.069250	-0.004772	-0.001320	0.066432
C	3.444143	2.634067	0.046862	-0.002152	-0.002884	0.062430
C	2.445524	3.577096	-0.009231	-0.000266	-0.003172	-0.061398
C	1.175896	2.827634	-0.009852	-0.002284	-0.000688	-0.102286
N	1.400608	1.471820	0.036416	-0.004364	-0.000580	-0.027392
C	-0.092228	3.436659	-0.037994	-0.000320	0.002532	-0.166856
C	-1.346255	2.815329	-0.003726	-0.002108	0.004928	-0.106600

C	-2.652506	3.443951	0.007727	-0.001634	0.001844	-0.072200
C	-3.607591	2.434273	0.069434	0.000050	0.000772	0.064800
C	-2.907244	1.165239	0.084725	0.000248	0.002858	0.082430
N	-1.556769	1.451330	0.043445	-0.000092	0.004830	-0.016148
C	-2.883860	4.929961	-0.015576	-0.027958	-0.001764	-0.143690
C	-5.103175	2.583511	0.145494	0.004540	0.026084	0.224150
C	-4.943588	-2.869022	0.156210	0.002714	0.004180	0.185102
C	-2.575878	-5.107062	0.066550	0.000980	-0.001848	-0.157322
C	2.866843	-4.960230	0.111748	0.012364	-0.003706	-0.119266
C	5.094795	-2.601000	0.194652	-0.001174	-0.002282	0.208708
C	4.934094	2.840213	0.086031	-0.001892	-0.003508	0.184218
C	2.568019	5.075510	-0.057301	0.004116	-0.005538	-0.135076
H	-4.543563	-0.166784	0.143387	0.005018	-0.001368	0.214112
H	0.101289	-4.554583	0.039288	0.001096	-0.007108	-0.232216
H	0.807356	-0.779710	0.051834	-0.001988	-0.007382	-0.053788
H	4.534092	0.138461	0.131740	-0.003938	0.003688	0.200488
H	-0.109582	4.524189	-0.077456	0.002624	0.002188	-0.234542
H	-0.817689	0.750522	0.042699	0.002024	0.007056	-0.023424
H	-2.173370	5.435769	-0.695877	0.275680	0.019438	0.112602
H	-2.751239	5.374294	0.994021	-0.443442	-0.006222	-0.020860
H	-3.910290	5.168217	-0.351366	0.041558	-0.024438	-0.570014
H	-5.417106	3.574462	-0.260389	-0.016482	-0.092610	-0.366260
H	-5.461910	2.516571	1.211939	0.169118	0.652840	0.478754
H	-5.626550	1.777779	-0.436383	-0.133658	-0.438468	0.713310
H	-5.389136	-2.427276	1.061921	0.092940	-0.106422	0.296420
H	-5.199815	-3.935342	0.147336	0.004304	0.000894	0.076562
H	-5.443442	-2.398887	-0.705970	-0.090418	0.120358	0.289192
H	-3.624861	-5.423660	0.035047	0.001546	-0.001304	-0.206678
H	-2.119316	-5.559719	0.959702	-0.026238	-0.053996	-0.167742
H	-2.069606	-5.545217	-0.806010	0.028642	0.049472	-0.167688

H	2.251662	-5.466847	-0.645577	-0.107244	0.007532	-0.037562
H	2.602456	-5.396263	1.088381	0.164800	-0.020712	-0.075670
H	3.916673	-5.207846	-0.086944	-0.007832	0.003226	-0.285190
H	5.406077	-3.635635	-0.005650	0.014688	0.028796	-0.039860
H	5.479652	-2.322411	1.193654	-0.122422	-0.264990	0.367264
H	5.596070	-1.945781	-0.539734	0.101270	0.223882	0.429328
H	5.438712	2.320326	-0.743170	0.082618	-0.087618	0.278624
H	5.372333	2.451676	1.018832	-0.090600	0.084156	0.270994
H	5.192523	3.903530	0.017296	0.002512	-0.007570	0.106556
H	3.617986	5.390467	-0.064300	0.006424	-0.009036	-0.082358
H	2.084502	5.550734	0.809789	-0.054472	0.045690	-0.191850
H	2.089455	5.492445	-0.956166	0.064014	-0.053870	-0.192896
* Frequency(8)	42.6000					
C	-2.777015	-1.353512	0.105951	0.005062	0.001168	0.075312
C	-3.453662	-2.663419	0.113779	0.003214	0.001552	0.061862
C	-2.454715	-3.607396	0.082725	0.002064	-0.001044	-0.070060
C	-1.185460	-2.857576	0.066756	0.003256	-0.003068	-0.103250
N	-1.410204	-1.501408	0.079316	0.005248	-0.002052	-0.019884
C	-3.456811	-0.121732	0.113815	0.004646	0.000838	0.140910
C	0.083122	-3.466551	0.055472	0.002252	-0.006558	-0.167564
C	1.336298	-2.844213	0.070641	0.002136	-0.006636	-0.108958
C	2.643150	-3.472941	0.098262	0.002926	-0.003708	-0.062634
C	3.598003	-2.462485	0.126319	0.000840	-0.000226	0.063852
C	2.896976	-1.193107	0.106544	-0.000692	-0.001326	0.067632
N	1.546672	-1.479799	0.077546	-0.000158	-0.005068	-0.031892
C	3.447248	0.093317	0.104737	-0.003722	0.000314	0.126156
C	2.767266	1.324738	0.067371	-0.004772	-0.001320	0.066432
C	3.444204	2.634149	0.045096	-0.002152	-0.002884	0.062430
C	2.445532	3.577185	-0.007494	-0.000266	-0.003172	-0.061398
C	1.175961	2.827653	-0.006959	-0.002284	-0.000688	-0.102286

N	1.400731	1.471836	0.037190	-0.004364	-0.000580	-0.027392
C	-0.092219	3.436588	-0.033275	-0.000320	0.002532	-0.166856
C	-1.346196	2.815190	-0.000711	-0.002108	0.004928	-0.106600
C	-2.652460	3.443899	0.009769	-0.001634	0.001844	-0.072200
C	-3.607592	2.434251	0.067601	0.000050	0.000772	0.064800
C	-2.907252	1.165158	0.082394	0.000248	0.002858	0.082430
N	-1.556766	1.451193	0.043901	-0.000092	0.004830	-0.016148
C	-2.883069	4.930011	-0.011512	-0.027958	-0.001764	-0.143690
C	-5.103304	2.582773	0.139154	0.004540	0.026084	0.224150
C	-4.943665	-2.869140	0.150975	0.002714	0.004180	0.185102
C	-2.575906	-5.107009	0.071000	0.000980	-0.001848	-0.157322
C	2.866493	-4.960125	0.115122	0.012364	-0.003706	-0.119266
C	5.094828	-2.600935	0.188749	-0.001174	-0.002282	0.208708
C	4.934148	2.840313	0.080821	-0.001892	-0.003508	0.184218
C	2.567902	5.075667	-0.053481	0.004116	-0.005538	-0.135076
H	-4.543705	-0.166745	0.137331	0.005018	-0.001368	0.214112
H	0.101258	-4.554382	0.045856	0.001096	-0.007108	-0.232216
H	0.807412	-0.779501	0.053356	-0.001988	-0.007382	-0.053788
H	4.534204	0.138357	0.126070	-0.003938	0.003688	0.200488
H	-0.109656	4.524127	-0.070823	0.002624	0.002188	-0.234542
H	-0.817746	0.750323	0.043361	0.002024	0.007056	-0.023424
H	-2.181167	5.435219	-0.699062	0.275680	0.019438	0.112602
H	-2.738696	5.374470	0.994611	-0.443442	-0.006222	-0.020860
H	-3.911466	5.168908	-0.335244	0.041558	-0.024438	-0.570014
H	-5.416640	3.577082	-0.250030	-0.016482	-0.092610	-0.366260
H	-5.466693	2.498106	1.198398	0.169118	0.652840	0.478754
H	-5.622769	1.790181	-0.456558	-0.133658	-0.438468	0.713310
H	-5.391765	-2.424266	1.053537	0.092940	-0.106422	0.296420
H	-5.199936	-3.935367	0.145171	0.004304	0.000894	0.076562
H	-5.440885	-2.402291	-0.714149	-0.090418	0.120358	0.289192

H	-3.624904	-5.423623	0.040892	0.001546	-0.001304	-0.206678
H	-2.118574	-5.558192	0.964446	-0.026238	-0.053996	-0.167742
H	-2.070416	-5.546616	-0.801267	0.028642	0.049472	-0.167688
H	2.254695	-5.467060	-0.644514	-0.107244	0.007532	-0.037562
H	2.597795	-5.395678	1.090521	0.164800	-0.020712	-0.075670
H	3.916895	-5.207937	-0.078877	-0.007832	0.003226	-0.285190
H	5.405662	-3.636449	-0.004523	0.014688	0.028796	-0.039860
H	5.483114	-2.314916	1.183267	-0.122422	-0.264990	0.367264
H	5.593206	-1.952113	-0.551878	0.101270	0.223882	0.429328
H	5.436375	2.322805	-0.751050	0.082618	-0.087618	0.278624
H	5.374896	2.449296	1.011167	-0.090600	0.084156	0.270994
H	5.192452	3.903744	0.014282	0.002512	-0.007570	0.106556
H	3.617804	5.390723	-0.061970	0.006424	-0.009036	-0.082358
H	2.086043	5.549442	0.815215	-0.054472	0.045690	-0.191850
H	2.087645	5.493969	-0.950710	0.064014	-0.053870	-0.192896

* Frequency(8) 42.6000

C	-2.777334	-1.353585	0.101205	0.005062	0.001168	0.075312
C	-3.453864	-2.663516	0.109881	0.003214	0.001552	0.061862
C	-2.454846	-3.607330	0.087140	0.002064	-0.001044	-0.070060
C	-1.185666	-2.857383	0.073263	0.003256	-0.003068	-0.103250
N	-1.410535	-1.501278	0.080569	0.005248	-0.002052	-0.019884
C	-3.457104	-0.121785	0.104935	0.004646	0.000838	0.140910
C	0.082980	-3.466138	0.066032	0.002252	-0.006558	-0.167564
C	1.336163	-2.843795	0.077507	0.002136	-0.006636	-0.108958
C	2.642965	-3.472708	0.102209	0.002926	-0.003708	-0.062634
C	3.597950	-2.462471	0.122295	0.000840	-0.000226	0.063852
C	2.897020	-1.193023	0.102282	-0.000692	-0.001326	0.067632
N	1.546682	-1.479480	0.079556	-0.000158	-0.005068	-0.031892

C	3.447483	0.093297	0.096787	-0.003722	0.000314	0.126156
C	2.767567	1.324821	0.063184	-0.004772	-0.001320	0.066432
C	3.444340	2.634330	0.041162	-0.002152	-0.002884	0.062430
C	2.445549	3.577385	-0.003625	-0.000266	-0.003172	-0.061398
C	1.176105	2.827697	-0.000513	-0.002284	-0.000688	-0.102286
N	1.401006	1.471873	0.038916	-0.004364	-0.000580	-0.027392
C	-0.092198	3.436428	-0.022760	-0.000320	0.002532	-0.166856
C	-1.346063	2.814879	0.006007	-0.002108	0.004928	-0.106600
C	-2.652357	3.443783	0.014319	-0.001634	0.001844	-0.072200
C	-3.607595	2.434203	0.063517	0.000050	0.000772	0.064800
C	-2.907267	1.164978	0.077199	0.000248	0.002858	0.082430
N	-1.556761	1.450889	0.044919	-0.000092	0.004830	-0.016148
C	-2.881307	4.930122	-0.002457	-0.027958	-0.001764	-0.143690
C	-5.103590	2.581130	0.125028	0.004540	0.026084	0.224150
C	-4.943836	-2.869404	0.139310	0.002714	0.004180	0.185102
C	-2.575968	-5.106893	0.080914	0.000980	-0.001848	-0.157322
C	2.865714	-4.959891	0.122638	0.012364	-0.003706	-0.119266
C	5.094902	-2.600792	0.175597	-0.001174	-0.002282	0.208708
C	4.934267	2.840534	0.069212	-0.001892	-0.003508	0.184218
C	2.567643	5.076016	-0.044969	0.004116	-0.005538	-0.135076
H	-4.544021	-0.166659	0.123839	0.005018	-0.001368	0.214112
H	0.101189	-4.553934	0.060490	0.001096	-0.007108	-0.232216
H	0.807537	-0.779036	0.056745	-0.001988	-0.007382	-0.053788
H	4.534452	0.138125	0.113435	-0.003938	0.003688	0.200488
H	-0.109821	4.523989	-0.056042	0.002624	0.002188	-0.234542
H	-0.817874	0.749878	0.044837	0.002024	0.007056	-0.023424
H	-2.198539	5.433994	-0.706158	0.275680	0.019438	0.112602
H	-2.710752	5.374862	0.995925	-0.443442	-0.006222	-0.020860
H	-3.914085	5.170448	-0.299324	0.041558	-0.024438	-0.570014
H	-5.415601	3.582918	-0.226949	-0.016482	-0.092610	-0.366260

H	-5.477351	2.456965	1.168228	0.169118	0.652840	0.478754
H	-5.614346	1.817812	-0.501509	-0.133658	-0.438468	0.713310
H	-5.397622	-2.417560	1.034857	0.092940	-0.106422	0.296420
H	-5.200208	-3.935424	0.140346	0.004304	0.000894	0.076562
H	-5.435187	-2.409875	-0.732373	-0.090418	0.120358	0.289192
H	-3.625002	-5.423541	0.053917	0.001546	-0.001304	-0.206678
H	-2.116920	-5.554789	0.975017	-0.026238	-0.053996	-0.167742
H	-2.072221	-5.549734	-0.790700	0.028642	0.049472	-0.167688
H	2.261453	-5.467534	-0.642147	-0.107244	0.007532	-0.037562
H	2.587410	-5.394372	1.095290	0.164800	-0.020712	-0.075670
H	3.917388	-5.208140	-0.060905	-0.007832	0.003226	-0.285190
H	5.404736	-3.638264	-0.002011	0.014688	0.028796	-0.039860
H	5.490829	-2.298217	1.160123	-0.122422	-0.264990	0.367264
H	5.586824	-1.966222	-0.578933	0.101270	0.223882	0.429328
H	5.431168	2.328326	-0.768608	0.082618	-0.087618	0.278624
H	5.380605	2.443992	0.994090	-0.090600	0.084156	0.270994
H	5.192294	3.904221	0.007568	0.002512	-0.007570	0.106556
H	3.617399	5.391292	-0.056780	0.006424	-0.009036	-0.082358
H	2.089475	5.546562	0.827305	-0.054472	0.045690	-0.191850
H	2.083611	5.497363	-0.938554	0.064014	-0.053870	-0.192896
* Frequency(8)	42.6000					
C	-2.777794	-1.353691	0.094358	0.005062	0.001168	0.075312
C	-3.454157	-2.663657	0.104256	0.003214	0.001552	0.061862
C	-2.455033	-3.607235	0.093510	0.002064	-0.001044	-0.070060
C	-1.185962	-2.857104	0.082650	0.003256	-0.003068	-0.103250
N	-1.411012	-1.501092	0.082377	0.005248	-0.002052	-0.019884
C	-3.457526	-0.121861	0.092123	0.004646	0.000838	0.140910
C	0.082775	-3.465541	0.081267	0.002252	-0.006558	-0.167564
C	1.335969	-2.843191	0.087414	0.002136	-0.006636	-0.108958
C	2.642699	-3.472371	0.107903	0.002926	-0.003708	-0.062634

C	3.597874	-2.462451	0.116490	0.000840	-0.000226	0.063852
C	2.897083	-1.192903	0.096133	-0.000692	-0.001326	0.067632
N	1.546697	-1.479019	0.082455	-0.000158	-0.005068	-0.031892
C	3.447821	0.093268	0.085316	-0.003722	0.000314	0.126156
C	2.768001	1.324941	0.057144	-0.004772	-0.001320	0.066432
C	3.444536	2.634593	0.035486	-0.002152	-0.002884	0.062430
C	2.445573	3.577674	0.001957	-0.000266	-0.003172	-0.061398
C	1.176313	2.827759	0.008787	-0.002284	-0.000688	-0.102286
N	1.401403	1.471925	0.041407	-0.004364	-0.000580	-0.027392
C	-0.092169	3.436198	-0.007589	-0.000320	0.002532	-0.166856
C	-1.345871	2.814431	0.015699	-0.002108	0.004928	-0.106600
C	-2.652208	3.443615	0.020884	-0.001634	0.001844	-0.072200
C	-3.607600	2.434133	0.057625	0.000050	0.000772	0.064800
C	-2.907290	1.164718	0.069704	0.000248	0.002858	0.082430
N	-1.556752	1.450450	0.046387	-0.000092	0.004830	-0.016148
C	-2.878765	4.930282	0.010608	-0.027958	-0.001764	-0.143690
C	-5.104003	2.578758	0.104648	0.004540	0.026084	0.224150
C	-4.944083	-2.869784	0.122481	0.002714	0.004180	0.185102
C	-2.576057	-5.106725	0.095218	0.000980	-0.001848	-0.157322
C	2.864590	-4.959554	0.133481	0.012364	-0.003706	-0.119266
C	5.095008	-2.600584	0.156621	-0.001174	-0.002282	0.208708
C	4.934439	2.840853	0.052462	-0.001892	-0.003508	0.184218
C	2.567269	5.076519	-0.032687	0.004116	-0.005538	-0.135076
H	-4.544477	-0.166535	0.104371	0.005018	-0.001368	0.214112
H	0.101090	-4.553288	0.081603	0.001096	-0.007108	-0.232216
H	0.807718	-0.778365	0.061636	-0.001988	-0.007382	-0.053788
H	4.534810	0.137789	0.095207	-0.003938	0.003688	0.200488
H	-0.110060	4.523790	-0.034717	0.002624	0.002188	-0.234542
H	-0.818058	0.749236	0.046967	0.002024	0.007056	-0.023424
H	-2.223605	5.432227	-0.716396	0.275680	0.019438	0.112602

H	-2.670433	5.375428	0.997822	-0.443442	-0.006222	-0.020860
H	-3.917863	5.172670	-0.247497	0.041558	-0.024438	-0.570014
H	-5.414103	3.591338	-0.193648	-0.016482	-0.092610	-0.366260
H	-5.492727	2.397608	1.124699	0.169118	0.652840	0.478754
H	-5.602194	1.857678	-0.566365	-0.133658	-0.438468	0.713310
H	-5.406072	-2.407884	1.007906	0.092940	-0.106422	0.296420
H	-5.200599	-3.935505	0.133385	0.004304	0.000894	0.076562
H	-5.426966	-2.420819	-0.758667	-0.090418	0.120358	0.289192
H	-3.625142	-5.423422	0.072708	0.001546	-0.001304	-0.206678
H	-2.114535	-5.549880	0.990268	-0.026238	-0.053996	-0.167742
H	-2.074825	-5.554232	-0.775454	0.028642	0.049472	-0.167688
H	2.271204	-5.468219	-0.638732	-0.107244	0.007532	-0.037562
H	2.572426	-5.392489	1.102170	0.164800	-0.020712	-0.075670
H	3.918100	-5.208434	-0.034975	-0.007832	0.003226	-0.285190
H	5.403401	-3.640882	0.001613	0.014688	0.028796	-0.039860
H	5.501960	-2.274123	1.126730	-0.122422	-0.264990	0.367264
H	5.577617	-1.986577	-0.617968	0.101270	0.223882	0.429328
H	5.423657	2.336292	-0.793941	0.082618	-0.087618	0.278624
H	5.388843	2.436341	0.969451	-0.090600	0.084156	0.270994
H	5.192065	3.904909	-0.002121	0.002512	-0.007570	0.106556
H	3.616815	5.392114	-0.049292	0.006424	-0.009036	-0.082358
H	2.094428	5.542408	0.844748	-0.054472	0.045690	-0.191850
H	2.077791	5.502261	-0.921016	0.064014	-0.053870	-0.192896
* Frequency(8)	42.6000					
C	-2.778345	-1.353819	0.086151	0.005062	0.001168	0.075312
C	-3.454507	-2.663827	0.097515	0.003214	0.001552	0.061862
C	-2.455258	-3.607121	0.101145	0.002064	-0.001044	-0.070060
C	-1.186316	-2.856770	0.093902	0.003256	-0.003068	-0.103250
N	-1.411584	-1.500868	0.084544	0.005248	-0.002052	-0.019884
C	-3.458032	-0.121953	0.076768	0.004646	0.000838	0.140910

C	0.082530	-3.464827	0.099527	0.002252	-0.006558	-0.167564
C	1.335736	-2.842468	0.099287	0.002136	-0.006636	-0.108958
C	2.642381	-3.471967	0.114729	0.002926	-0.003708	-0.062634
C	3.597782	-2.462426	0.109531	0.000840	-0.000226	0.063852
C	2.897158	-1.192758	0.088763	-0.000692	-0.001326	0.067632
N	1.546714	-1.478467	0.085931	-0.000158	-0.005068	-0.031892
C	3.448227	0.093234	0.071569	-0.003722	0.000314	0.126156
C	2.768521	1.325085	0.049905	-0.004772	-0.001320	0.066432
C	3.444770	2.634907	0.028682	-0.002152	-0.002884	0.062430
C	2.445602	3.578019	0.008648	-0.000266	-0.003172	-0.061398
C	1.176561	2.827834	0.019933	-0.002284	-0.000688	-0.102286
N	1.401879	1.471989	0.044392	-0.004364	-0.000580	-0.027392
C	-0.092134	3.435922	0.010594	-0.000320	0.002532	-0.166856
C	-1.345641	2.813894	0.027316	-0.002108	0.004928	-0.106600
C	-2.652030	3.443414	0.028752	-0.001634	0.001844	-0.072200
C	-3.607605	2.434048	0.050564	0.000050	0.000772	0.064800
C	-2.907317	1.164407	0.060722	0.000248	0.002858	0.082430
N	-1.556742	1.449923	0.048147	-0.000092	0.004830	-0.016148
C	-2.875719	4.930474	0.026266	-0.027958	-0.001764	-0.143690
C	-5.104497	2.575916	0.080222	0.004540	0.026084	0.224150
C	-4.944379	-2.870239	0.102309	0.002714	0.004180	0.185102
C	-2.576164	-5.106523	0.112362	0.000980	-0.001848	-0.157322
C	2.863242	-4.959150	0.146478	0.012364	-0.003706	-0.119266
C	5.095136	-2.600335	0.133877	-0.001174	-0.002282	0.208708
C	4.934645	2.841235	0.032387	-0.001892	-0.003508	0.184218
C	2.566820	5.077123	-0.017967	0.004116	-0.005538	-0.135076
H	-4.545024	-0.166386	0.081039	0.005018	-0.001368	0.214112
H	0.100970	-4.552513	0.106908	0.001096	-0.007108	-0.232216
H	0.807934	-0.777560	0.067497	-0.001988	-0.007382	-0.053788
H	4.535239	0.137387	0.073359	-0.003938	0.003688	0.200488

H	-0.110346	4.523552	-0.009159	0.002624	0.002188	-0.234542
H	-0.818278	0.748467	0.049520	0.002024	0.007056	-0.023424
H	-2.253647	5.430109	-0.728666	0.275680	0.019438	0.112602
H	-2.622110	5.376106	1.000095	-0.443442	-0.006222	-0.020860
H	-3.922392	5.175333	-0.185380	0.041558	-0.024438	-0.570014
H	-5.412306	3.601430	-0.153736	-0.016482	-0.092610	-0.366260
H	-5.511156	2.326466	1.072527	0.169118	0.652840	0.478754
H	-5.587629	1.905460	-0.644097	-0.133658	-0.438468	0.713310
H	-5.416200	-2.396287	0.975604	0.092940	-0.106422	0.296420
H	-5.201068	-3.935602	0.125042	0.004304	0.000894	0.076562
H	-5.417113	-2.433934	-0.790181	-0.090418	0.120358	0.289192
H	-3.625311	-5.423280	0.095231	0.001546	-0.001304	-0.206678
H	-2.111676	-5.543996	1.008548	-0.026238	-0.053996	-0.167742
H	-2.077946	-5.559623	-0.757180	0.028642	0.049472	-0.167688
H	2.282891	-5.469040	-0.634639	-0.107244	0.007532	-0.037562
H	2.554467	-5.390232	1.110416	0.164800	-0.020712	-0.075670
H	3.918954	-5.208785	-0.003897	-0.007832	0.003226	-0.285190
H	5.401800	-3.644020	0.005957	0.014688	0.028796	-0.039860
H	5.515301	-2.245247	1.086708	-0.122422	-0.264990	0.367264
H	5.566581	-2.010975	-0.664753	0.101270	0.223882	0.429328
H	5.414653	2.345840	-0.824304	0.082618	-0.087618	0.278624
H	5.398716	2.427170	0.939919	-0.090600	0.084156	0.270994
H	5.191792	3.905734	-0.013733	0.002512	-0.007570	0.106556
H	3.616115	5.393098	-0.040317	0.006424	-0.009036	-0.082358
H	2.100364	5.537429	0.865655	-0.054472	0.045690	-0.191850
H	2.070815	5.508132	-0.899995	0.064014	-0.053870	-0.192896

* Frequency(8) 42.6000

C	-2.778929	-1.353953	0.077473	0.005062	0.001168	0.075312
C	-3.454877	-2.664005	0.090387	0.003214	0.001552	0.061862
C	-2.455496	-3.607001	0.109217	0.002064	-0.001044	-0.070060

C	-1.186692	-2.856416	0.105798	0.003256	-0.003068	-0.103250
N	-1.412188	-1.500632	0.086834	0.005248	-0.002052	-0.019884
C	-3.458568	-0.122049	0.060532	0.004646	0.000838	0.140910
C	0.082270	-3.464071	0.118833	0.002252	-0.006558	-0.167564
C	1.335490	-2.841704	0.111841	0.002136	-0.006636	-0.108958
C	2.642043	-3.471539	0.121945	0.002926	-0.003708	-0.062634
C	3.597686	-2.462400	0.102175	0.000840	-0.000226	0.063852
C	2.897238	-1.192606	0.080971	-0.000692	-0.001326	0.067632
N	1.546732	-1.477883	0.089605	-0.000158	-0.005068	-0.031892
C	3.448655	0.093198	0.057033	-0.003722	0.000314	0.126156
C	2.769071	1.325237	0.042251	-0.004772	-0.001320	0.066432
C	3.445018	2.635239	0.021490	-0.002152	-0.002884	0.062430
C	2.445632	3.578385	0.015722	-0.000266	-0.003172	-0.061398
C	1.176825	2.827914	0.031719	-0.002284	-0.000688	-0.102286
N	1.402381	1.472055	0.047548	-0.004364	-0.000580	-0.027392
C	-0.092098	3.435630	0.029818	-0.000320	0.002532	-0.166856
C	-1.345399	2.813326	0.039598	-0.002108	0.004928	-0.106600
C	-2.651842	3.443202	0.037070	-0.001634	0.001844	-0.072200
C	-3.607611	2.433960	0.043098	0.000050	0.000772	0.064800
C	-2.907345	1.164077	0.051224	0.000248	0.002858	0.082430
N	-1.556732	1.449367	0.050007	-0.000092	0.004830	-0.016148
C	-2.872497	4.930678	0.042822	-0.027958	-0.001764	-0.143690
C	-5.105021	2.572910	0.054396	0.004540	0.026084	0.224150
C	-4.944691	-2.870721	0.080983	0.002714	0.004180	0.185102
C	-2.576276	-5.106311	0.130488	0.000980	-0.001848	-0.157322
C	2.861818	-4.958724	0.160220	0.012364	-0.003706	-0.119266
C	5.095272	-2.600073	0.109831	-0.001174	-0.002282	0.208708
C	4.934863	2.841639	0.011163	-0.001892	-0.003508	0.184218
C	2.566346	5.077761	-0.002405	0.004116	-0.005538	-0.135076
H	-4.545602	-0.166228	0.056369	0.005018	-0.001368	0.214112

H	0.100844	-4.551695	0.133664	0.001096	-0.007108	-0.232216
H	0.808164	-0.776710	0.073695	-0.001988	-0.007382	-0.053788
H	4.535693	0.136963	0.050259	-0.003938	0.003688	0.200488
H	-0.110648	4.523300	0.017865	0.002624	0.002188	-0.234542
H	-0.818512	0.747655	0.052218	0.002024	0.007056	-0.023424
H	-2.285409	5.427869	-0.741640	0.275680	0.019438	0.112602
H	-2.571018	5.376822	1.002499	-0.443442	-0.006222	-0.020860
H	-3.927180	5.178149	-0.119706	0.041558	-0.024438	-0.570014
H	-5.410408	3.612100	-0.111536	-0.016482	-0.092610	-0.366260
H	-5.530642	2.251248	1.017367	0.169118	0.652840	0.478754
H	-5.572229	1.955978	-0.726281	-0.133658	-0.438468	0.713310
H	-5.426908	-2.384025	0.941452	0.092940	-0.106422	0.296420
H	-5.201564	-3.935706	0.116220	0.004304	0.000894	0.076562
H	-5.406695	-2.447802	-0.823501	-0.090418	0.120358	0.289192
H	-3.625489	-5.423130	0.119043	0.001546	-0.001304	-0.206678
H	-2.108652	-5.537774	1.027874	-0.026238	-0.053996	-0.167742
H	-2.081246	-5.565323	-0.737860	0.028642	0.049472	-0.167688
H	2.295247	-5.469908	-0.630311	-0.107244	0.007532	-0.037562
H	2.535479	-5.387846	1.119134	0.164800	-0.020712	-0.075670
H	3.919856	-5.209157	0.028961	-0.007832	0.003226	-0.285190
H	5.400108	-3.647338	0.010549	0.014688	0.028796	-0.039860
H	5.529405	-2.214715	1.044394	-0.122422	-0.264990	0.367264
H	5.554913	-2.036769	-0.714219	0.101270	0.223882	0.429328
H	5.405135	2.355936	-0.856406	0.082618	-0.087618	0.278624
H	5.409154	2.417474	0.908697	-0.090600	0.084156	0.270994
H	5.191502	3.906606	-0.026009	0.002512	-0.007570	0.106556
H	3.615375	5.394140	-0.030829	0.006424	-0.009036	-0.082358
H	2.106640	5.532165	0.887759	-0.054472	0.045690	-0.191850
H	2.063439	5.514338	-0.877771	0.064014	-0.053870	-0.192896

* Frequency(8) 42.6000

C	-2.779480	-1.354081	0.069266	0.005062	0.001168	0.075312
C	-3.455227	-2.664175	0.083646	0.003214	0.001552	0.061862
C	-2.455721	-3.606887	0.116852	0.002064	-0.001044	-0.070060
C	-1.187046	-2.856082	0.117050	0.003256	-0.003068	-0.103250
N	-1.412760	-1.500408	0.089001	0.005248	-0.002052	-0.019884
C	-3.459074	-0.122141	0.045177	0.004646	0.000838	0.140910
C	0.082025	-3.463357	0.137093	0.002252	-0.006558	-0.167564
C	1.335257	-2.840981	0.123714	0.002136	-0.006636	-0.108958
C	2.641725	-3.471135	0.128771	0.002926	-0.003708	-0.062634
C	3.597594	-2.462375	0.095216	0.000840	-0.000226	0.063852
C	2.897313	-1.192461	0.073601	-0.000692	-0.001326	0.067632
N	1.546749	-1.477331	0.093081	-0.000158	-0.005068	-0.031892
C	3.449061	0.093164	0.043286	-0.003722	0.000314	0.126156
C	2.769591	1.325381	0.035012	-0.004772	-0.001320	0.066432
C	3.445252	2.635553	0.014686	-0.002152	-0.002884	0.062430
C	2.445661	3.578730	0.022413	-0.000266	-0.003172	-0.061398
C	1.177073	2.827989	0.042865	-0.002284	-0.000688	-0.102286
N	1.402857	1.472119	0.050533	-0.004364	-0.000580	-0.027392
C	-0.092063	3.435354	0.048001	-0.000320	0.002532	-0.166856
C	-1.345169	2.812789	0.051215	-0.002108	0.004928	-0.106600
C	-2.651664	3.443001	0.044938	-0.001634	0.001844	-0.072200
C	-3.607616	2.433875	0.036037	0.000050	0.000772	0.064800
C	-2.907372	1.163766	0.042242	0.000248	0.002858	0.082430
N	-1.556722	1.448840	0.051767	-0.000092	0.004830	-0.016148
C	-2.869451	4.930870	0.058480	-0.027958	-0.001764	-0.143690
C	-5.105515	2.570068	0.029970	0.004540	0.026084	0.224150
C	-4.944987	-2.871176	0.060811	0.002714	0.004180	0.185102
C	-2.576383	-5.106109	0.147632	0.000980	-0.001848	-0.157322
C	2.860470	-4.958320	0.173217	0.012364	-0.003706	-0.119266
C	5.095400	-2.599824	0.087087	-0.001174	-0.002282	0.208708

C	4.935069	2.842021	-0.008912	-0.001892	-0.003508	0.184218
C	2.565897	5.078365	0.012315	0.004116	-0.005538	-0.135076
H	-4.546149	-0.166079	0.033037	0.005018	-0.001368	0.214112
H	0.100724	-4.550920	0.158969	0.001096	-0.007108	-0.232216
H	0.808380	-0.775905	0.079556	-0.001988	-0.007382	-0.053788
H	4.536122	0.136561	0.028411	-0.003938	0.003688	0.200488
H	-0.110934	4.523062	0.043423	0.002624	0.002188	-0.234542
H	-0.818732	0.746886	0.054771	0.002024	0.007056	-0.023424
H	-2.315451	5.425751	-0.753910	0.275680	0.019438	0.112602
H	-2.522695	5.377500	1.004772	-0.443442	-0.006222	-0.020860
H	-3.931709	5.180812	-0.057589	0.041558	-0.024438	-0.570014
H	-5.408611	3.622192	-0.071624	-0.016482	-0.092610	-0.366260
H	-5.549071	2.180106	0.965195	0.169118	0.652840	0.478754
H	-5.557664	2.003760	-0.804013	-0.133658	-0.438468	0.713310
H	-5.437036	-2.372428	0.909150	0.092940	-0.106422	0.296420
H	-5.202033	-3.935803	0.107877	0.004304	0.000894	0.076562
H	-5.396842	-2.460917	-0.855015	-0.090418	0.120358	0.289192
H	-3.625658	-5.422988	0.141566	0.001546	-0.001304	-0.206678
H	-2.105793	-5.531890	1.046154	-0.026238	-0.053996	-0.167742
H	-2.084367	-5.570714	-0.719586	0.028642	0.049472	-0.167688
H	2.306934	-5.470729	-0.626218	-0.107244	0.007532	-0.037562
H	2.517520	-5.385589	1.127380	0.164800	-0.020712	-0.075670
H	3.920710	-5.209508	0.060039	-0.007832	0.003226	-0.285190
H	5.398507	-3.650476	0.014893	0.014688	0.028796	-0.039860
H	5.542746	-2.185839	1.004372	-0.122422	-0.264990	0.367264
H	5.543877	-2.061167	-0.761004	0.101270	0.223882	0.429328
H	5.396131	2.365484	-0.886769	0.082618	-0.087618	0.278624
H	5.419027	2.408303	0.879165	-0.090600	0.084156	0.270994
H	5.191229	3.907431	-0.037621	0.002512	-0.007570	0.106556
H	3.614675	5.395124	-0.021854	0.006424	-0.009036	-0.082358

H	2.112576	5.527186	0.908666	-0.054472	0.045690	-0.191850
H	2.056463	5.520209	-0.856750	0.064014	-0.053870	-0.192896
* Frequency(8)	42.6000					
C	-2.779940	-1.354187	0.062419	0.005062	0.001168	0.075312
C	-3.455520	-2.664316	0.078021	0.003214	0.001552	0.061862
C	-2.455908	-3.606792	0.123222	0.002064	-0.001044	-0.070060
C	-1.187342	-2.855803	0.126437	0.003256	-0.003068	-0.103250
N	-1.413237	-1.500222	0.090809	0.005248	-0.002052	-0.019884
C	-3.459496	-0.122217	0.032365	0.004646	0.000838	0.140910
C	0.081820	-3.462760	0.152328	0.002252	-0.006558	-0.167564
C	1.335063	-2.840377	0.133621	0.002136	-0.006636	-0.108958
C	2.641459	-3.470798	0.134465	0.002926	-0.003708	-0.062634
C	3.597518	-2.462355	0.089411	0.000840	-0.000226	0.063852
C	2.897376	-1.192341	0.067452	-0.000692	-0.001326	0.067632
N	1.546764	-1.476870	0.095980	-0.000158	-0.005068	-0.031892
C	3.449399	0.093135	0.031815	-0.003722	0.000314	0.126156
C	2.770025	1.325501	0.028972	-0.004772	-0.001320	0.066432
C	3.445448	2.635816	0.009010	-0.002152	-0.002884	0.062430
C	2.445685	3.579019	0.027995	-0.000266	-0.003172	-0.061398
C	1.177281	2.828051	0.052165	-0.002284	-0.000688	-0.102286
N	1.403254	1.472171	0.053024	-0.004364	-0.000580	-0.027392
C	-0.092034	3.435124	0.063172	-0.000320	0.002532	-0.166856
C	-1.344977	2.812341	0.060907	-0.002108	0.004928	-0.106600
C	-2.651515	3.442833	0.051503	-0.001634	0.001844	-0.072200
C	-3.607621	2.433805	0.030145	0.000050	0.000772	0.064800
C	-2.907395	1.163506	0.034747	0.000248	0.002858	0.082430
N	-1.556713	1.448401	0.053235	-0.000092	0.004830	-0.016148
C	-2.866909	4.931030	0.071545	-0.027958	-0.001764	-0.143690
C	-5.105928	2.567696	0.009590	0.004540	0.026084	0.224150
C	-4.945234	-2.871556	0.043982	0.002714	0.004180	0.185102

C	-2.576472	-5.105941	0.161936	0.000980	-0.001848	-0.157322
C	2.859346	-4.957983	0.184060	0.012364	-0.003706	-0.119266
C	5.095506	-2.599616	0.068111	-0.001174	-0.002282	0.208708
C	4.935241	2.842340	-0.025662	-0.001892	-0.003508	0.184218
C	2.565523	5.078868	0.024597	0.004116	-0.005538	-0.135076
H	-4.546605	-0.165955	0.013569	0.005018	-0.001368	0.214112
H	0.100625	-4.550274	0.180082	0.001096	-0.007108	-0.232216
H	0.808561	-0.775234	0.084447	-0.001988	-0.007382	-0.053788
H	4.536480	0.136225	0.010183	-0.003938	0.003688	0.200488
H	-0.111173	4.522863	0.064748	0.002624	0.002188	-0.234542
H	-0.818916	0.746244	0.056901	0.002024	0.007056	-0.023424
H	-2.340517	5.423984	-0.764148	0.275680	0.019438	0.112602
H	-2.482376	5.378066	1.006669	-0.443442	-0.006222	-0.020860
H	-3.935487	5.183034	-0.005762	0.041558	-0.024438	-0.570014
H	-5.407113	3.630612	-0.038323	-0.016482	-0.092610	-0.366260
H	-5.564447	2.120749	0.921666	0.169118	0.652840	0.478754
H	-5.545512	2.043626	-0.868869	-0.133658	-0.438468	0.713310
H	-5.445486	-2.362752	0.882199	0.092940	-0.106422	0.296420
H	-5.202424	-3.935884	0.100916	0.004304	0.000894	0.076562
H	-5.388621	-2.471861	-0.881309	-0.090418	0.120358	0.289192
H	-3.625798	-5.422869	0.160357	0.001546	-0.001304	-0.206678
H	-2.103408	-5.526981	1.061405	-0.026238	-0.053996	-0.167742
H	-2.086971	-5.575212	-0.704340	0.028642	0.049472	-0.167688
H	2.316685	-5.471414	-0.622803	-0.107244	0.007532	-0.037562
H	2.502536	-5.383706	1.134260	0.164800	-0.020712	-0.075670
H	3.921422	-5.209802	0.085969	-0.007832	0.003226	-0.285190
H	5.397172	-3.653094	0.018517	0.014688	0.028796	-0.039860
H	5.553877	-2.161745	0.970979	-0.122422	-0.264990	0.367264
H	5.534670	-2.081522	-0.800039	0.101270	0.223882	0.429328
H	5.388620	2.373450	-0.912102	0.082618	-0.087618	0.278624

H	5.427265	2.400652	0.854526	-0.090600	0.084156	0.270994
H	5.191000	3.908119	-0.047310	0.002512	-0.007570	0.106556
H	3.614091	5.395946	-0.014366	0.006424	-0.009036	-0.082358
H	2.117529	5.523032	0.926109	-0.054472	0.045690	-0.191850
H	2.050643	5.525107	-0.839212	0.064014	-0.053870	-0.192896
* Frequency(8)	42.6000					
C	-2.780259	-1.354260	0.057673	0.005062	0.001168	0.075312
C	-3.455722	-2.664413	0.074123	0.003214	0.001552	0.061862
C	-2.456039	-3.606726	0.127637	0.002064	-0.001044	-0.070060
C	-1.187548	-2.855610	0.132944	0.003256	-0.003068	-0.103250
N	-1.413568	-1.500092	0.092062	0.005248	-0.002052	-0.019884
C	-3.459789	-0.122270	0.023485	0.004646	0.000838	0.140910
C	0.081678	-3.462347	0.162888	0.002252	-0.006558	-0.167564
C	1.334928	-2.839959	0.140487	0.002136	-0.006636	-0.108958
C	2.641274	-3.470565	0.138412	0.002926	-0.003708	-0.062634
C	3.597465	-2.462341	0.085387	0.000840	-0.000226	0.063852
C	2.897420	-1.192257	0.063190	-0.000692	-0.001326	0.067632
N	1.546774	-1.476551	0.097990	-0.000158	-0.005068	-0.031892
C	3.449634	0.093115	0.023865	-0.003722	0.000314	0.126156
C	2.770326	1.325584	0.024785	-0.004772	-0.001320	0.066432
C	3.445584	2.635997	0.005076	-0.002152	-0.002884	0.062430
C	2.445702	3.579219	0.031864	-0.000266	-0.003172	-0.061398
C	1.177425	2.828095	0.058611	-0.002284	-0.000688	-0.102286
N	1.403529	1.472208	0.054750	-0.004364	-0.000580	-0.027392
C	-0.092013	3.434964	0.073687	-0.000320	0.002532	-0.166856
C	-1.344844	2.812030	0.067625	-0.002108	0.004928	-0.106600
C	-2.651412	3.442717	0.056053	-0.001634	0.001844	-0.072200
C	-3.607624	2.433757	0.026061	0.000050	0.000772	0.064800
C	-2.907410	1.163326	0.029552	0.000248	0.002858	0.082430
N	-1.556708	1.448097	0.054253	-0.000092	0.004830	-0.016148

C	-2.865147	4.931141	0.080600	-0.027958	-0.001764	-0.143690
C	-5.106214	2.566053	-0.004536	0.004540	0.026084	0.224150
C	-4.945405	-2.871820	0.032317	0.002714	0.004180	0.185102
C	-2.576534	-5.105825	0.171850	0.000980	-0.001848	-0.157322
C	2.858567	-4.957749	0.191576	0.012364	-0.003706	-0.119266
C	5.095580	-2.599473	0.054959	-0.001174	-0.002282	0.208708
C	4.935360	2.842561	-0.037271	-0.001892	-0.003508	0.184218
C	2.565264	5.079217	0.033109	0.004116	-0.005538	-0.135076
H	-4.546921	-0.165869	0.000077	0.005018	-0.001368	0.214112
H	0.100556	-4.549826	0.194716	0.001096	-0.007108	-0.232216
H	0.808686	-0.774769	0.087836	-0.001988	-0.007382	-0.053788
H	4.536728	0.135993	-0.002452	-0.003938	0.003688	0.200488
H	-0.111338	4.522725	0.079529	0.002624	0.002188	-0.234542
H	-0.819044	0.745799	0.058377	0.002024	0.007056	-0.023424
H	-2.357889	5.422759	-0.771244	0.275680	0.019438	0.112602
H	-2.454432	5.378458	1.007983	-0.443442	-0.006222	-0.020860
H	-3.938106	5.184574	0.030158	0.041558	-0.024438	-0.570014
H	-5.406074	3.636448	-0.015242	-0.016482	-0.092610	-0.366260
H	-5.575105	2.079608	0.891496	0.169118	0.652840	0.478754
H	-5.537089	2.071257	-0.913820	-0.133658	-0.438468	0.713310
H	-5.451343	-2.356046	0.863519	0.092940	-0.106422	0.296420
H	-5.202696	-3.935941	0.096091	0.004304	0.000894	0.076562
H	-5.382923	-2.479445	-0.899533	-0.090418	0.120358	0.289192
H	-3.625896	-5.422787	0.173382	0.001546	-0.001304	-0.206678
H	-2.101754	-5.523578	1.071976	-0.026238	-0.053996	-0.167742
H	-2.088776	-5.578330	-0.693773	0.028642	0.049472	-0.167688
H	2.323443	-5.471888	-0.620436	-0.107244	0.007532	-0.037562
H	2.492151	-5.382400	1.139029	0.164800	-0.020712	-0.075670
H	3.921915	-5.210005	0.103941	-0.007832	0.003226	-0.285190
H	5.396246	-3.654909	0.021029	0.014688	0.028796	-0.039860

H	5.561592	-2.145046	0.947835	-0.122422	-0.264990	0.367264
H	5.528288	-2.095631	-0.827094	0.101270	0.223882	0.429328
H	5.383413	2.378971	-0.929660	0.082618	-0.087618	0.278624
H	5.432974	2.395348	0.837449	-0.090600	0.084156	0.270994
H	5.190842	3.908596	-0.054024	0.002512	-0.007570	0.106556
H	3.613686	5.396515	-0.009176	0.006424	-0.009036	-0.082358
H	2.120961	5.520152	0.938199	-0.054472	0.045690	-0.191850
H	2.046609	5.528501	-0.827056	0.064014	-0.053870	-0.192896
* Frequency(8)	42.6000					
C	-2.780403	-1.354293	0.055543	0.005062	0.001168	0.075312
C	-3.455813	-2.664457	0.072373	0.003214	0.001552	0.061862
C	-2.456097	-3.606697	0.129618	0.002064	-0.001044	-0.070060
C	-1.187640	-2.855523	0.135864	0.003256	-0.003068	-0.103250
N	-1.413717	-1.500034	0.092625	0.005248	-0.002052	-0.019884
C	-3.459921	-0.122293	0.019500	0.004646	0.000838	0.140910
C	0.081614	-3.462162	0.167627	0.002252	-0.006558	-0.167564
C	1.334868	-2.839771	0.143569	0.002136	-0.006636	-0.108958
C	2.641191	-3.470460	0.140184	0.002926	-0.003708	-0.062634
C	3.597441	-2.462334	0.083581	0.000840	-0.000226	0.063852
C	2.897439	-1.192219	0.061277	-0.000692	-0.001326	0.067632
N	1.546778	-1.476407	0.098892	-0.000158	-0.005068	-0.031892
C	3.449739	0.093106	0.020297	-0.003722	0.000314	0.126156
C	2.770460	1.325621	0.022906	-0.004772	-0.001320	0.066432
C	3.445645	2.636079	0.003310	-0.002152	-0.002884	0.062430
C	2.445710	3.579308	0.033601	-0.000266	-0.003172	-0.061398
C	1.177490	2.828114	0.061504	-0.002284	-0.000688	-0.102286
N	1.403652	1.472224	0.055524	-0.004364	-0.000580	-0.027392
C	-0.092004	3.434893	0.078406	-0.000320	0.002532	-0.166856
C	-1.344785	2.811891	0.070640	-0.002108	0.004928	-0.106600
C	-2.651366	3.442665	0.058095	-0.001634	0.001844	-0.072200

C	-3.607625	2.433735	0.024228	0.000050	0.000772	0.064800
C	-2.907418	1.163245	0.027221	0.000248	0.002858	0.082430
N	-1.556705	1.447960	0.054709	-0.000092	0.004830	-0.016148
C	-2.864356	4.931191	0.084664	-0.027958	-0.001764	-0.143690
C	-5.106343	2.565315	-0.010876	0.004540	0.026084	0.224150
C	-4.945482	-2.871938	0.027082	0.002714	0.004180	0.185102
C	-2.576562	-5.105772	0.176300	0.000980	-0.001848	-0.157322
C	2.858217	-4.957644	0.194950	0.012364	-0.003706	-0.119266
C	5.095613	-2.599408	0.049056	-0.001174	-0.002282	0.208708
C	4.935414	2.842661	-0.042481	-0.001892	-0.003508	0.184218
C	2.565147	5.079374	0.036929	0.004116	-0.005538	-0.135076
H	-4.547063	-0.165830	-0.005979	0.005018	-0.001368	0.214112
H	0.100525	-4.549625	0.201284	0.001096	-0.007108	-0.232216
H	0.808742	-0.774560	0.089358	-0.001988	-0.007382	-0.053788
H	4.536840	0.135889	-0.008122	-0.003938	0.003688	0.200488
H	-0.111412	4.522663	0.086162	0.002624	0.002188	-0.234542
H	-0.819101	0.745600	0.059039	0.002024	0.007056	-0.023424
H	-2.365686	5.422209	-0.774429	0.275680	0.019438	0.112602
H	-2.441889	5.378634	1.008573	-0.443442	-0.006222	-0.020860
H	-3.939282	5.185265	0.046280	0.041558	-0.024438	-0.570014
H	-5.405608	3.639068	-0.004883	-0.016482	-0.092610	-0.366260
H	-5.579888	2.061143	0.877955	0.169118	0.652840	0.478754
H	-5.533308	2.083659	-0.933995	-0.133658	-0.438468	0.713310
H	-5.453972	-2.353036	0.855135	0.092940	-0.106422	0.296420
H	-5.202817	-3.935966	0.093926	0.004304	0.000894	0.076562
H	-5.380366	-2.482849	-0.907712	-0.090418	0.120358	0.289192
H	-3.625939	-5.422750	0.179227	0.001546	-0.001304	-0.206678
H	-2.101012	-5.522051	1.076720	-0.026238	-0.053996	-0.167742
H	-2.089586	-5.579729	-0.689030	0.028642	0.049472	-0.167688
H	2.326476	-5.472101	-0.619373	-0.107244	0.007532	-0.037562

H	2.487490	-5.381815	1.141169	0.164800	-0.020712	-0.075670
H	3.922137	-5.210096	0.112008	-0.007832	0.003226	-0.285190
H	5.395831	-3.655723	0.022156	0.014688	0.028796	-0.039860
H	5.565054	-2.137551	0.937448	-0.122422	-0.264990	0.367264
H	5.525424	-2.101963	-0.839238	0.101270	0.223882	0.429328
H	5.381076	2.381450	-0.937540	0.082618	-0.087618	0.278624
H	5.435537	2.392968	0.829784	-0.090600	0.084156	0.270994
H	5.190771	3.908810	-0.057038	0.002512	-0.007570	0.106556
H	3.613504	5.396771	-0.006846	0.006424	-0.009036	-0.082358
H	2.122502	5.518860	0.943625	-0.054472	0.045690	-0.191850
H	2.044799	5.530025	-0.821600	0.064014	-0.053870	-0.192896
* Frequency(8)	42.6000					
C	-2.780354	-1.354282	0.056259	0.005062	0.001168	0.075312
C	-3.455782	-2.664443	0.072962	0.003214	0.001552	0.061862
C	-2.456077	-3.606707	0.128952	0.002064	-0.001044	-0.070060
C	-1.187609	-2.855552	0.134882	0.003256	-0.003068	-0.103250
N	-1.413667	-1.500054	0.092435	0.005248	-0.002052	-0.019884
C	-3.459876	-0.122285	0.020841	0.004646	0.000838	0.140910
C	0.081636	-3.462224	0.166033	0.002252	-0.006558	-0.167564
C	1.334888	-2.839834	0.142532	0.002136	-0.006636	-0.108958
C	2.641219	-3.470495	0.139588	0.002926	-0.003708	-0.062634
C	3.597449	-2.462336	0.084189	0.000840	-0.000226	0.063852
C	2.897433	-1.192232	0.061920	-0.000692	-0.001326	0.067632
N	1.546777	-1.476455	0.098589	-0.000158	-0.005068	-0.031892
C	3.449704	0.093109	0.021498	-0.003722	0.000314	0.126156
C	2.770415	1.325609	0.023538	-0.004772	-0.001320	0.066432
C	3.445624	2.636052	0.003904	-0.002152	-0.002884	0.062430
C	2.445707	3.579278	0.033017	-0.000266	-0.003172	-0.061398
C	1.177468	2.828107	0.060531	-0.002284	-0.000688	-0.102286
N	1.403611	1.472219	0.055264	-0.004364	-0.000580	-0.027392

C	-0.092007	3.434917	0.076819	-0.000320	0.002532	-0.166856
C	-1.344805	2.811938	0.069625	-0.002108	0.004928	-0.106600
C	-2.651382	3.442682	0.057408	-0.001634	0.001844	-0.072200
C	-3.607625	2.433742	0.024845	0.000050	0.000772	0.064800
C	-2.907415	1.163272	0.028005	0.000248	0.002858	0.082430
N	-1.556706	1.448006	0.054556	-0.000092	0.004830	-0.016148
C	-2.864622	4.931175	0.083297	-0.027958	-0.001764	-0.143690
C	-5.106299	2.565563	-0.008743	0.004540	0.026084	0.224150
C	-4.945456	-2.871898	0.028843	0.002714	0.004180	0.185102
C	-2.576553	-5.105790	0.174803	0.000980	-0.001848	-0.157322
C	2.858335	-4.957680	0.193815	0.012364	-0.003706	-0.119266
C	5.095602	-2.599430	0.051041	-0.001174	-0.002282	0.208708
C	4.935396	2.842627	-0.040728	-0.001892	-0.003508	0.184218
C	2.565186	5.079321	0.035644	0.004116	-0.005538	-0.135076
H	-4.547016	-0.165843	-0.003942	0.005018	-0.001368	0.214112
H	0.100535	-4.549692	0.199075	0.001096	-0.007108	-0.232216
H	0.808724	-0.774630	0.088846	-0.001988	-0.007382	-0.053788
H	4.536802	0.135924	-0.006215	-0.003938	0.003688	0.200488
H	-0.111387	4.522684	0.083931	0.002624	0.002188	-0.234542
H	-0.819082	0.745667	0.058817	0.002024	0.007056	-0.023424
H	-2.363063	5.422394	-0.773358	0.275680	0.019438	0.112602
H	-2.446109	5.378575	1.008375	-0.443442	-0.006222	-0.020860
H	-3.938886	5.185033	0.040857	0.041558	-0.024438	-0.570014
H	-5.405765	3.638187	-0.008368	-0.016482	-0.092610	-0.366260
H	-5.578279	2.067355	0.882511	0.169118	0.652840	0.478754
H	-5.534580	2.079487	-0.927208	-0.133658	-0.438468	0.713310
H	-5.453088	-2.354048	0.857956	0.092940	-0.106422	0.296420
H	-5.202776	-3.935957	0.094654	0.004304	0.000894	0.076562
H	-5.381226	-2.481704	-0.904961	-0.090418	0.120358	0.289192
H	-3.625925	-5.422763	0.177261	0.001546	-0.001304	-0.206678

H	-2.101262	-5.522565	1.075124	-0.026238	-0.053996	-0.167742
H	-2.089314	-5.579258	-0.690625	0.028642	0.049472	-0.167688
H	2.325456	-5.472030	-0.619731	-0.107244	0.007532	-0.037562
H	2.489058	-5.382012	1.140449	0.164800	-0.020712	-0.075670
H	3.922062	-5.210066	0.109294	-0.007832	0.003226	-0.285190
H	5.395971	-3.655449	0.021777	0.014688	0.028796	-0.039860
H	5.563890	-2.140073	0.940942	-0.122422	-0.264990	0.367264
H	5.526387	-2.099833	-0.835153	0.101270	0.223882	0.429328
H	5.381863	2.380616	-0.934889	0.082618	-0.087618	0.278624
H	5.434675	2.393769	0.832362	-0.090600	0.084156	0.270994
H	5.190795	3.908738	-0.056024	0.002512	-0.007570	0.106556
H	3.613565	5.396685	-0.007630	0.006424	-0.009036	-0.082358
H	2.121984	5.519295	0.941800	-0.054472	0.045690	-0.191850
H	2.045408	5.529513	-0.823435	0.064014	-0.053870	-0.192896
* Frequency(8)	42.6000					
C	-2.780120	-1.354228	0.059745	0.005062	0.001168	0.075312
C	-3.455634	-2.664371	0.075825	0.003214	0.001552	0.061862
C	-2.455982	-3.606755	0.125709	0.002064	-0.001044	-0.070060
C	-1.187458	-2.855694	0.130103	0.003256	-0.003068	-0.103250
N	-1.413424	-1.500149	0.091515	0.005248	-0.002052	-0.019884
C	-3.459661	-0.122247	0.027362	0.004646	0.000838	0.140910
C	0.081740	-3.462527	0.158278	0.002252	-0.006558	-0.167564
C	1.334987	-2.840142	0.137490	0.002136	-0.006636	-0.108958
C	2.641355	-3.470667	0.136689	0.002926	-0.003708	-0.062634
C	3.597488	-2.462347	0.087144	0.000840	-0.000226	0.063852
C	2.897401	-1.192293	0.065050	-0.000692	-0.001326	0.067632
N	1.546769	-1.476690	0.097113	-0.000158	-0.005068	-0.031892
C	3.449532	0.093124	0.027336	-0.003722	0.000314	0.126156
C	2.770194	1.325548	0.026613	-0.004772	-0.001320	0.066432
C	3.445525	2.635918	0.006793	-0.002152	-0.002884	0.062430

C	2.445695	3.579131	0.030175	-0.000266	-0.003172	-0.061398
C	1.177362	2.828076	0.055797	-0.002284	-0.000688	-0.102286
N	1.403409	1.472192	0.053996	-0.004364	-0.000580	-0.027392
C	-0.092022	3.435034	0.069096	-0.000320	0.002532	-0.166856
C	-1.344902	2.812166	0.064692	-0.002108	0.004928	-0.106600
C	-2.651457	3.442768	0.054066	-0.001634	0.001844	-0.072200
C	-3.607623	2.433778	0.027844	0.000050	0.000772	0.064800
C	-2.907404	1.163405	0.031820	0.000248	0.002858	0.082430
N	-1.556710	1.448230	0.053808	-0.000092	0.004830	-0.016148
C	-2.865916	4.931093	0.076646	-0.027958	-0.001764	-0.143690
C	-5.106089	2.566770	0.001631	0.004540	0.026084	0.224150
C	-4.945330	-2.871705	0.037410	0.002714	0.004180	0.185102
C	-2.576507	-5.105876	0.167522	0.000980	-0.001848	-0.157322
C	2.858907	-4.957851	0.188295	0.012364	-0.003706	-0.119266
C	5.095548	-2.599535	0.060701	-0.001174	-0.002282	0.208708
C	4.935308	2.842465	-0.032202	-0.001892	-0.003508	0.184218
C	2.565377	5.079065	0.029392	0.004116	-0.005538	-0.135076
H	-4.546783	-0.165906	0.005967	0.005018	-0.001368	0.214112
H	0.100586	-4.550021	0.188327	0.001096	-0.007108	-0.232216
H	0.808632	-0.774972	0.086356	-0.001988	-0.007382	-0.053788
H	4.536620	0.136094	0.003064	-0.003938	0.003688	0.200488
H	-0.111266	4.522785	0.073076	0.002624	0.002188	-0.234542
H	-0.818988	0.745994	0.057732	0.002024	0.007056	-0.023424
H	-2.350305	5.423294	-0.768146	0.275680	0.019438	0.112602
H	-2.466632	5.378287	1.007409	-0.443442	-0.006222	-0.020860
H	-3.936963	5.183902	0.014476	0.041558	-0.024438	-0.570014
H	-5.406528	3.633900	-0.025319	-0.016482	-0.092610	-0.366260
H	-5.570452	2.097569	0.904668	0.169118	0.652840	0.478754
H	-5.540766	2.059194	-0.894195	-0.133658	-0.438468	0.713310
H	-5.448786	-2.358973	0.871674	0.092940	-0.106422	0.296420

H	-5.202577	-3.935916	0.098198	0.004304	0.000894	0.076562
H	-5.385411	-2.476134	-0.891577	-0.090418	0.120358	0.289192
H	-3.625853	-5.422823	0.167695	0.001546	-0.001304	-0.206678
H	-2.102476	-5.525064	1.067361	-0.026238	-0.053996	-0.167742
H	-2.087988	-5.576969	-0.698386	0.028642	0.049472	-0.167688
H	2.320492	-5.471681	-0.621469	-0.107244	0.007532	-0.037562
H	2.496685	-5.382970	1.136947	0.164800	-0.020712	-0.075670
H	3.921700	-5.209916	0.096095	-0.007832	0.003226	-0.285190
H	5.396650	-3.654116	0.019932	0.014688	0.028796	-0.039860
H	5.558224	-2.152337	0.957940	-0.122422	-0.264990	0.367264
H	5.531074	-2.089471	-0.815283	0.101270	0.223882	0.429328
H	5.385686	2.376561	-0.921994	0.082618	-0.087618	0.278624
H	5.430482	2.397664	0.844905	-0.090600	0.084156	0.270994
H	5.190911	3.908388	-0.051093	0.002512	-0.007570	0.106556
H	3.613863	5.396267	-0.011441	0.006424	-0.009036	-0.082358
H	2.119463	5.521409	0.932921	-0.054472	0.045690	-0.191850
H	2.048370	5.527019	-0.832363	0.064014	-0.053870	-0.192896
* Frequency(8)	42.6000					
C	-2.779725	-1.354137	0.065622	0.005062	0.001168	0.075312
C	-3.455383	-2.664250	0.080652	0.003214	0.001552	0.061862
C	-2.455821	-3.606837	0.120242	0.002064	-0.001044	-0.070060
C	-1.187204	-2.855933	0.122046	0.003256	-0.003068	-0.103250
N	-1.413014	-1.500309	0.089964	0.005248	-0.002052	-0.019884
C	-3.459299	-0.122181	0.038358	0.004646	0.000838	0.140910
C	0.081916	-3.463039	0.145202	0.002252	-0.006558	-0.167564
C	1.335154	-2.840659	0.128987	0.002136	-0.006636	-0.108958
C	2.641583	-3.470956	0.131802	0.002926	-0.003708	-0.062634
C	3.597553	-2.462364	0.092126	0.000840	-0.000226	0.063852
C	2.897347	-1.192397	0.070328	-0.000692	-0.001326	0.067632
N	1.546757	-1.477086	0.094624	-0.000158	-0.005068	-0.031892

C	3.449241	0.093148	0.037181	-0.003722	0.000314	0.126156
C	2.769822	1.325445	0.031797	-0.004772	-0.001320	0.066432
C	3.445357	2.635693	0.011665	-0.002152	-0.002884	0.062430
C	2.445674	3.578884	0.025384	-0.000266	-0.003172	-0.061398
C	1.177184	2.828022	0.047815	-0.002284	-0.000688	-0.102286
N	1.403068	1.472147	0.051859	-0.004364	-0.000580	-0.027392
C	-0.092047	3.435232	0.056076	-0.000320	0.002532	-0.166856
C	-1.345067	2.812551	0.056373	-0.002108	0.004928	-0.106600
C	-2.651585	3.442912	0.048432	-0.001634	0.001844	-0.072200
C	-3.607619	2.433838	0.032901	0.000050	0.000772	0.064800
C	-2.907384	1.163628	0.038253	0.000248	0.002858	0.082430
N	-1.556717	1.448607	0.052548	-0.000092	0.004830	-0.016148
C	-2.868098	4.930955	0.065434	-0.027958	-0.001764	-0.143690
C	-5.105735	2.568806	0.019122	0.004540	0.026084	0.224150
C	-4.945118	-2.871379	0.051854	0.002714	0.004180	0.185102
C	-2.576431	-5.106020	0.155245	0.000980	-0.001848	-0.157322
C	2.859872	-4.958140	0.178988	0.012364	-0.003706	-0.119266
C	5.095456	-2.599713	0.076987	-0.001174	-0.002282	0.208708
C	4.935161	2.842191	-0.017827	-0.001892	-0.003508	0.184218
C	2.565698	5.078633	0.018852	0.004116	-0.005538	-0.135076
H	-4.546392	-0.166013	0.022675	0.005018	-0.001368	0.214112
H	0.100671	-4.550576	0.170207	0.001096	-0.007108	-0.232216
H	0.808476	-0.775548	0.082159	-0.001988	-0.007382	-0.053788
H	4.536313	0.136382	0.018709	-0.003938	0.003688	0.200488
H	-0.111061	4.522956	0.054774	0.002624	0.002188	-0.234542
H	-0.818830	0.746544	0.055905	0.002024	0.007056	-0.023424
H	-2.328792	5.424810	-0.759360	0.275680	0.019438	0.112602
H	-2.501235	5.377802	1.005781	-0.443442	-0.006222	-0.020860
H	-3.933720	5.181995	-0.030005	0.041558	-0.024438	-0.570014
H	-5.407814	3.626674	-0.053899	-0.016482	-0.092610	-0.366260

H	-5.557255	2.148513	0.942027	0.169118	0.652840	0.478754
H	-5.551196	2.024978	-0.838532	-0.133658	-0.438468	0.713310
H	-5.441534	-2.367278	0.894805	0.092940	-0.106422	0.296420
H	-5.202241	-3.935846	0.104172	0.004304	0.000894	0.076562
H	-5.392466	-2.466742	-0.869010	-0.090418	0.120358	0.289192
H	-3.625732	-5.422925	0.151567	0.001546	-0.001304	-0.206678
H	-2.104524	-5.529277	1.054271	-0.026238	-0.053996	-0.167742
H	-2.085753	-5.573108	-0.711471	0.028642	0.049472	-0.167688
H	2.312124	-5.471093	-0.624400	-0.107244	0.007532	-0.037562
H	2.509545	-5.384586	1.131042	0.164800	-0.020712	-0.075670
H	3.921089	-5.209665	0.073841	-0.007832	0.003226	-0.285190
H	5.397796	-3.651869	0.016822	0.014688	0.028796	-0.039860
H	5.548671	-2.173015	0.986599	-0.122422	-0.264990	0.367264
H	5.538977	-2.072001	-0.781781	0.101270	0.223882	0.429328
H	5.392133	2.369724	-0.900252	0.082618	-0.087618	0.278624
H	5.423412	2.404231	0.866051	-0.090600	0.084156	0.270994
H	5.191107	3.907797	-0.042778	0.002512	-0.007570	0.106556
H	3.614364	5.395562	-0.017868	0.006424	-0.009036	-0.082358
H	2.115212	5.524975	0.917950	-0.054472	0.045690	-0.191850
H	2.053366	5.522816	-0.847415	0.064014	-0.053870	-0.192896
* Frequency(8)	42.6000					
C	-2.779212	-1.354019	0.073253	0.005062	0.001168	0.075312
C	-3.455057	-2.664092	0.086921	0.003214	0.001552	0.061862
C	-2.455612	-3.606942	0.113143	0.002064	-0.001044	-0.070060
C	-1.186874	-2.856244	0.111584	0.003256	-0.003068	-0.103250
N	-1.412482	-1.500517	0.087949	0.005248	-0.002052	-0.019884
C	-3.458828	-0.122096	0.052636	0.004646	0.000838	0.140910
C	0.082144	-3.463704	0.128223	0.002252	-0.006558	-0.167564
C	1.335370	-2.841332	0.117947	0.002136	-0.006636	-0.108958
C	2.641879	-3.471332	0.125455	0.002926	-0.003708	-0.062634

C	3.597639	-2.462387	0.098597	0.000840	-0.000226	0.063852
C	2.897277	-1.192531	0.077181	-0.000692	-0.001326	0.067632
N	1.546741	-1.477599	0.091392	-0.000158	-0.005068	-0.031892
C	3.448864	0.093180	0.049964	-0.003722	0.000314	0.126156
C	2.769338	1.325311	0.038528	-0.004772	-0.001320	0.066432
C	3.445139	2.635401	0.017991	-0.002152	-0.002884	0.062430
C	2.445647	3.578562	0.019163	-0.000266	-0.003172	-0.061398
C	1.176953	2.827952	0.037450	-0.002284	-0.000688	-0.102286
N	1.402626	1.472088	0.049083	-0.004364	-0.000580	-0.027392
C	-0.092080	3.435488	0.039168	-0.000320	0.002532	-0.166856
C	-1.345280	2.813050	0.045572	-0.002108	0.004928	-0.106600
C	-2.651750	3.443098	0.041116	-0.001634	0.001844	-0.072200
C	-3.607614	2.433916	0.039467	0.000050	0.000772	0.064800
C	-2.907359	1.163917	0.046605	0.000248	0.002858	0.082430
N	-1.556727	1.449096	0.050912	-0.000092	0.004830	-0.016148
C	-2.870931	4.930776	0.050874	-0.027958	-0.001764	-0.143690
C	-5.105275	2.571449	0.041836	0.004540	0.026084	0.224150
C	-4.944843	-2.870955	0.070610	0.002714	0.004180	0.185102
C	-2.576331	-5.106207	0.139304	0.000980	-0.001848	-0.157322
C	2.861125	-4.958516	0.166903	0.012364	-0.003706	-0.119266
C	5.095337	-2.599945	0.098135	-0.001174	-0.002282	0.208708
C	4.934969	2.841836	0.000840	-0.001892	-0.003508	0.184218
C	2.566115	5.078071	0.005165	0.004116	-0.005538	-0.135076
H	-4.545883	-0.166152	0.044371	0.005018	-0.001368	0.214112
H	0.100782	-4.551296	0.146676	0.001096	-0.007108	-0.232216
H	0.808275	-0.776296	0.076709	-0.001988	-0.007382	-0.053788
H	4.535914	0.136756	0.039025	-0.003938	0.003688	0.200488
H	-0.110795	4.523177	0.031007	0.002624	0.002188	-0.234542
H	-0.818625	0.747259	0.053531	0.002024	0.007056	-0.023424
H	-2.300858	5.426780	-0.747950	0.275680	0.019438	0.112602

H	-2.546169	5.377171	1.003668	-0.443442	-0.006222	-0.020860
H	-3.929509	5.179518	-0.087764	0.041558	-0.024438	-0.570014
H	-5.409484	3.617290	-0.091012	-0.016482	-0.092610	-0.366260
H	-5.540118	2.214665	0.990539	0.169118	0.652840	0.478754
H	-5.564739	1.980549	-0.766253	-0.133658	-0.438468	0.713310
H	-5.432116	-2.378062	0.924841	0.092940	-0.106422	0.296420
H	-5.201805	-3.935756	0.111930	0.004304	0.000894	0.076562
H	-5.401628	-2.454546	-0.839706	-0.090418	0.120358	0.289192
H	-3.625576	-5.423057	0.130625	0.001546	-0.001304	-0.206678
H	-2.107182	-5.534749	1.037274	-0.026238	-0.053996	-0.167742
H	-2.082851	-5.568095	-0.728463	0.028642	0.049472	-0.167688
H	2.301257	-5.470330	-0.628206	-0.107244	0.007532	-0.037562
H	2.526244	-5.386685	1.123375	0.164800	-0.020712	-0.075670
H	3.920295	-5.209338	0.044942	-0.007832	0.003226	-0.285190
H	5.399285	-3.648952	0.012783	0.014688	0.028796	-0.039860
H	5.536266	-2.199866	1.023813	-0.122422	-0.264990	0.367264
H	5.549238	-2.049315	-0.738277	0.101270	0.223882	0.429328
H	5.400505	2.360845	-0.872019	0.082618	-0.087618	0.278624
H	5.414231	2.412758	0.893511	-0.090600	0.084156	0.270994
H	5.191362	3.907030	-0.031981	0.002512	-0.007570	0.106556
H	3.615015	5.394646	-0.026213	0.006424	-0.009036	-0.082358
H	2.109692	5.529605	0.898510	-0.054472	0.045690	-0.191850
H	2.059852	5.517357	-0.866961	0.064014	-0.053870	-0.192896

* Frequency(8) 42.6000

C	-2.778637	-1.353886	0.081812	0.005062	0.001168	0.075312
C	-3.454692	-2.663916	0.093951	0.003214	0.001552	0.061862
C	-2.455377	-3.607061	0.105181	0.002064	-0.001044	-0.070060
C	-1.186504	-2.856593	0.099850	0.003256	-0.003068	-0.103250
N	-1.411886	-1.500750	0.085689	0.005248	-0.002052	-0.019884
C	-3.458300	-0.122001	0.068650	0.004646	0.000838	0.140910

C	0.082400	-3.464449	0.109180	0.002252	-0.006558	-0.167564
C	1.335613	-2.842086	0.105564	0.002136	-0.006636	-0.108958
C	2.642212	-3.471753	0.118337	0.002926	-0.003708	-0.062634
C	3.597734	-2.462413	0.105853	0.000840	-0.000226	0.063852
C	2.897198	-1.192682	0.084867	-0.000692	-0.001326	0.067632
N	1.546723	-1.478175	0.087768	-0.000158	-0.005068	-0.031892
C	3.448441	0.093216	0.064301	-0.003722	0.000314	0.126156
C	2.768796	1.325161	0.046078	-0.004772	-0.001320	0.066432
C	3.444894	2.635073	0.025086	-0.002152	-0.002884	0.062430
C	2.445617	3.578202	0.012185	-0.000266	-0.003172	-0.061398
C	1.176693	2.827874	0.025826	-0.002284	-0.000688	-0.102286
N	1.402130	1.472022	0.045970	-0.004364	-0.000580	-0.027392
C	-0.092116	3.435776	0.020206	-0.000320	0.002532	-0.166856
C	-1.345520	2.813610	0.033457	-0.002108	0.004928	-0.106600
C	-2.651936	3.443308	0.032911	-0.001634	0.001844	-0.072200
C	-3.607608	2.434004	0.046831	0.000050	0.000772	0.064800
C	-2.907331	1.164242	0.055973	0.000248	0.002858	0.082430
N	-1.556737	1.449645	0.049077	-0.000092	0.004830	-0.016148
C	-2.874108	4.930576	0.034544	-0.027958	-0.001764	-0.143690
C	-5.104759	2.574413	0.067309	0.004540	0.026084	0.224150
C	-4.944535	-2.870480	0.091646	0.002714	0.004180	0.185102
C	-2.576220	-5.106417	0.121425	0.000980	-0.001848	-0.157322
C	2.862530	-4.958937	0.153349	0.012364	-0.003706	-0.119266
C	5.095204	-2.600204	0.121854	-0.001174	-0.002282	0.208708
C	4.934754	2.841437	0.021775	-0.001892	-0.003508	0.184218
C	2.566583	5.077442	-0.010186	0.004116	-0.005538	-0.135076
H	-4.545313	-0.166307	0.068704	0.005018	-0.001368	0.214112
H	0.100907	-4.552104	0.120286	0.001096	-0.007108	-0.232216
H	0.808049	-0.777135	0.070596	-0.001988	-0.007382	-0.053788
H	4.535466	0.137175	0.061809	-0.003938	0.003688	0.200488

H	-0.110497	4.523426	0.004353	0.002624	0.002188	-0.234542
H	-0.818395	0.748061	0.050869	0.002024	0.007056	-0.023424
H	-2.269528	5.428989	-0.735153	0.275680	0.019438	0.112602
H	-2.596564	5.376464	1.001297	-0.443442	-0.006222	-0.020860
H	-3.924786	5.176741	-0.152543	0.041558	-0.024438	-0.570014
H	-5.411357	3.606765	-0.132636	-0.016482	-0.092610	-0.366260
H	-5.520899	2.288857	1.044947	0.169118	0.652840	0.478754
H	-5.579929	1.930719	-0.685189	-0.133658	-0.438468	0.713310
H	-5.421554	-2.390156	0.958528	0.092940	-0.106422	0.296420
H	-5.201316	-3.935654	0.120631	0.004304	0.000894	0.076562
H	-5.411904	-2.440868	-0.806841	-0.090418	0.120358	0.289192
H	-3.625400	-5.423205	0.107137	0.001546	-0.001304	-0.206678
H	-2.110164	-5.540885	1.018211	-0.026238	-0.053996	-0.167742
H	-2.079596	-5.562473	-0.747520	0.028642	0.049472	-0.167688
H	2.289069	-5.469474	-0.632475	-0.107244	0.007532	-0.037562
H	2.544973	-5.389039	1.114775	0.164800	-0.020712	-0.075670
H	3.919405	-5.208971	0.012532	-0.007832	0.003226	-0.285190
H	5.400954	-3.645679	0.008253	0.014688	0.028796	-0.039860
H	5.522353	-2.229981	1.065551	-0.122422	-0.264990	0.367264
H	5.560747	-2.023872	-0.689486	0.101270	0.223882	0.429328
H	5.409894	2.350888	-0.840355	0.082618	-0.087618	0.278624
H	5.403935	2.422322	0.924308	-0.090600	0.084156	0.270994
H	5.191647	3.906170	-0.019871	0.002512	-0.007570	0.106556
H	3.615745	5.393619	-0.035573	0.006424	-0.009036	-0.082358
H	2.103502	5.534797	0.876707	-0.054472	0.045690	-0.191850
H	2.067127	5.511235	-0.888883	0.064014	-0.053870	-0.192896