

Supporting Information

Directed B–H Functionalization of *closo*-Dodecaborate via Concerted Iodination-Deprotonation: Reaction Mechanism and Origins of Regioselectivity

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1. Computational details

All density functional theory (DFT) calculations were conducted with the Gaussian 09 software package.¹ Geometry optimizations of all the minima and transition states were performed at the B3LYP level² of theory with SDD basis set³ for iodine and 6-311+G(d,p) basis set for other atoms, including solvation energy corrections and Grimme's dispersion corrections with Becke-Johnson damping.⁴ Self-consistent reaction field (SCRF) using SMD model⁵ under methanol is used to simulate solvent environment. Frequency analysis was also performed at the same level of geometry optimization to confirm whether each optimized stationary point was local minimum or transition state. For critical transition states, IRC (intrinsic reaction coordinates) analysis was also performed at the same level of theory as geometry optimization to verify the proposed process. We have thoroughly examined the conformational space of each intermediates and transition states, and only the most stable conformers are included in discussions. The 3D diagrams of molecules shown in the article and below in supporting information were generated with CYLview software.⁶

To correct the Gibbs free energies under 1 atm to the standard state in solution (1 mol/L), a correction of $RT\ln(c_s/c_g)$ is added to energies of all species. c_s is the standard molar concentration in solution (1 mol/L), c_g is the standard molar concentration in gas phase (about 0.0446 mol/L), and R is the gas constant. For species at the standard state of 1mol/L at 298.15 K, the correction value equaling to 1.89 kcal/mol was used.

2. Regioselectivity of B–I bond formation with trifluoroacetate leaving group

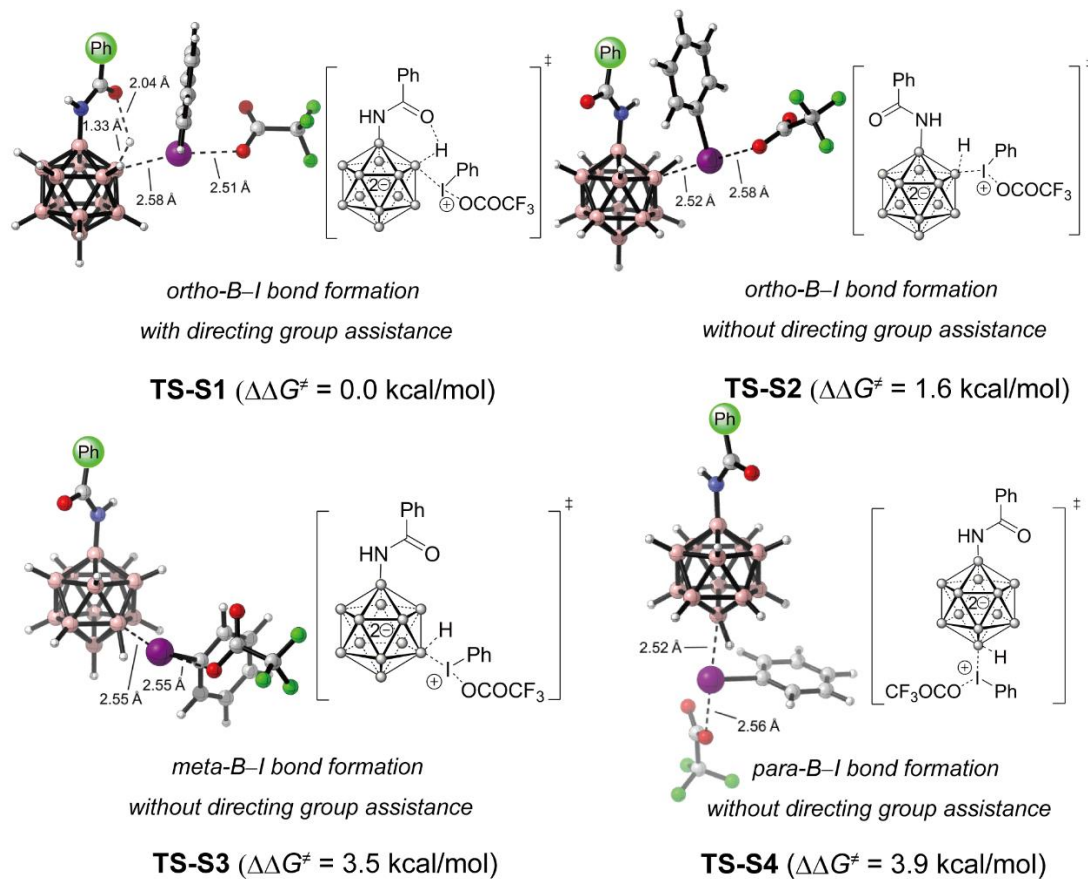


Fig. S1. Relative free energies and optimized structures of competing B–I bond formation transition states with trifluoroacetate leaving group.

3. References

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4. Energies, enthalpies, and free energies of the calculated structures

Zero-point correction (ZPE), thermal correction to enthalpy (ΔH), thermal correction to Gibbs free energy (G), energies (E), enthalpies (H), Gibbs free energies (G) (in Hartree) and imaginary frequencies of the transition states calculated at the B3LYP-D3(BJ)/6-311+G(d,p)-SDD-SMD(Methanol)

Structures	ZPE	TCH	TCG	E	H	G	Imaginary Frequency
INT1	0.277131	0.293768	0.234106	-705.738036	-705.737091	-705.796753	
product	0.270188	0.285665	0.229770	-705.011443	-705.010499	-705.066395	
INT2	0.419328	0.449147	0.356656	-1177.085376	-1177.084432	-1177.176922	
INT4	0.359520	0.383409	0.306551	-948.050217	-948.049273	-948.126130	
PhI(OAc) ₂	0.190450	0.208825	0.140010	-700.017202	-700.016258	-700.085073	
AcO [•]	0.048250	0.053573	0.020763	-228.667753	-228.666809	-228.699618	
INT5	0.468269	0.504102	0.397925	-1405.751193	-1405.750249	-1405.856426	
INT6	0.417536	0.447609	0.355476	-1177.078972	-1177.078028	-1177.170160	
TS1	0.414606	0.444455	0.352511	-1177.073428	-1177.072484	-1177.164427	511.51i
AcOH	0.060984	0.066549	0.033531	-229.117615	-229.116671	-229.149689	
INT7	0.372957	0.396944	0.320569	-948.479454	-948.478510	-948.554885	
TS2	0.357922	0.381699	0.302562	-948.019561	-948.018617	-948.097754	147.22i
PhI	0.089678	0.096509	0.057922	-243.054735	-243.053791	-243.092378	
INT8	0.469056	0.504930	0.397916	-1405.756855	-1405.755911	-1405.862924	
TS6	0.415624	0.445836	0.353688	-1177.068578	-1177.067634	-1177.159783	511.71i
TS7	0.414823	0.445477	0.348509	-1177.063603	-1177.062659	-1177.159627	518.85i
TS8	0.414719	0.445401	0.348879	-1177.062757	-1177.061812	-1177.158335	504.68i
TS-S1	0.392395	0.423984	0.326584	-1474.909952	-1474.909008	-1475.006408	108.5258i
TS-S2	0.392031	0.424069	0.326379	-1474.907125	-1474.906181	-1475.003871	292.9911i
TS-S3	0.391794	0.423934	0.323918	-1474.901831	-1474.900887	-1475.000903	199.0972i
TS-S4	0.39192	0.424099	0.323627	-1474.90061	-1474.899666	-1475.000138	188.6014i

Zero-point correction (ZPE), thermal correction to enthalpy (ΔH), thermal correction to Gibbs free energy (G), energies (E), enthalpies (H), Gibbs free energies (G) (in Hartree) and imaginary frequencies of the transition states in Table 1 calculated at the B3LYP-D3(BJ)/6-311+G(d,p)-SDD-SMD(Methanol)

R	Position	ZPE	TCH	TCG	E	H	G	Imaginary Frequency
4-CN-Ph	<i>Ortho-</i>	0.413344	0.445001	0.349176	-1269.3467	-1269.3458	-1269.4416	487.165i
	<i>Meta</i>	0.413714	0.446036	0.346559	-1269.3366	-1269.3357	-1269.4351	484.588i
	<i>Para-</i>	0.413275	0.445763	0.345249	-1269.3366	-1269.3357	-1269.4362	490.266i
4-OMe-Ph	<i>Ortho-</i>	0.447202	0.479656	0.381244	-1291.6057	-1291.6047	-1291.7031	389.193i
	<i>Meta</i>	0.447496	0.480563	0.379761	-1291.5949	-1291.594	-1291.6948	516.632i
	<i>Para-</i>	0.447378	0.480476	0.379929	-1291.594	-1291.5931	-1291.6936	479.138i
4- <i>t</i> Bu-Ph	<i>Ortho-</i>	0.526213	0.561667	0.45661	-1334.2811	-1334.2802	-1334.3852	505.339i
	<i>Meta</i>	0.527083	0.562984	0.456813	-1334.2697	-1334.2688	-1334.375	476.887i

	<i>Para-</i>	0.52678	0.562838	0.456071	-1334.2688	-1334.2678	-1334.3746	541.473i
Me	<i>Ortho-</i>	0.361364	0.388278	0.303032	-985.32428	-985.32333	-985.40858	313.796i
	<i>Meta</i>	0.361204	0.388954	0.30005	-985.3146	-985.31366	-985.40256	581.935i
	<i>Para-</i>	0.3615	0.389203	0.300991	-985.31373	-985.31279	-985.401	523.187i
tBu	<i>Ortho-</i>	0.44601	0.476688	0.383478	-1103.228	-1103.2271	-1103.3203	260.72i
	<i>Meta</i>	0.44587	0.477328	0.380587	-1103.2163	-1103.2153	-1103.3121	551.488i
	<i>Para-</i>	0.44554	0.477098	0.380723	-1103.2158	-1103.2149	-1103.3113	522.559i
Cy	<i>Ortho-</i>	0.48439	0.515507	0.420023	-1180.6425	-1180.6415	-1180.737	369.572i
	<i>Meta</i>	0.4845	0.516312	0.418385	-1180.6317	-1180.6308	-1180.7287	524.706i
	<i>Para-</i>	0.48451	0.51634	0.418154	-1180.6309	-1180.63	-1180.7282	484.281i
NMe₂	<i>Ortho-</i>	0.40699	0.436697	0.34479	-1079.9777	-1079.9768	-1080.0687	294.072i
	<i>Meta</i>	0.40661	0.437058	0.342437	-1079.9668	-1079.9659	-1080.0605	571.668i
	<i>Para-</i>	0.40623	0.436891	0.340814	-1079.9661	-1079.9651	-1080.0612	516.217i

5. Electronic energies of the stationary points along the intrinsic reaction coordinate of TS1

Electronic energies (*E*) (in Hartree) calculated at the B3LYP-D3(BJ)/6-311+G(d,p)-SDD-SMD(Methanol)

Structures	<i>E</i>	Structures	<i>E</i>	Structures	<i>E</i>
IRC_TS1_point1	-1177.525639	IRC_TS1_point114	-1177.52326	IRC_TS1_point227	-1177.599152
IRC_TS1_point2	-1177.525634	IRC_TS1_point115	-1177.52317	IRC_TS1_point228	-1177.599371
IRC_TS1_point3	-1177.525628	IRC_TS1_point116	-1177.523077	IRC_TS1_point229	-1177.599584
IRC_TS1_point4	-1177.525622	IRC_TS1_point117	-1177.522981	IRC_TS1_point230	-1177.599786
IRC_TS1_point5	-1177.525617	IRC_TS1_point118	-1177.522882	IRC_TS1_point231	-1177.599983
IRC_TS1_point6	-1177.525611	IRC_TS1_point119	-1177.522779	IRC_TS1_point232	-1177.600172
IRC_TS1_point7	-1177.525605	IRC_TS1_point120	-1177.522673	IRC_TS1_point233	-1177.600356
IRC_TS1_point8	-1177.525598	IRC_TS1_point121	-1177.522564	IRC_TS1_point234	-1177.600533
IRC_TS1_point9	-1177.525592	IRC_TS1_point122	-1177.522452	IRC_TS1_point235	-1177.600704
IRC_TS1_point10	-1177.525585	IRC_TS1_point123	-1177.522336	IRC_TS1_point236	-1177.600869
IRC_TS1_point11	-1177.525578	IRC_TS1_point124	-1177.522218	IRC_TS1_point237	-1177.601028
IRC_TS1_point12	-1177.525571	IRC_TS1_point125	-1177.522096	IRC_TS1_point238	-1177.601181
IRC_TS1_point13	-1177.525564	IRC_TS1_point126	-1177.52197	IRC_TS1_point239	-1177.601329
IRC_TS1_point14	-1177.525556	IRC_TS1_point127	-1177.521842	IRC_TS1_point240	-1177.601471
IRC_TS1_point15	-1177.525549	IRC_TS1_point128	-1177.521709	IRC_TS1_point241	-1177.601608
IRC_TS1_point16	-1177.525541	IRC_TS1_point129	-1177.521573	IRC_TS1_point242	-1177.60174
IRC_TS1_point17	-1177.525533	IRC_TS1_point130	-1177.521433	IRC_TS1_point243	-1177.601868
IRC_TS1_point18	-1177.525525	IRC_TS1_point131	-1177.521289	IRC_TS1_point244	-1177.601991
IRC_TS1_point19	-1177.525516	IRC_TS1_point132	-1177.521141	IRC_TS1_point245	-1177.602112
IRC_TS1_point20	-1177.525508	IRC_TS1_point133	-1177.520989	IRC_TS1_point246	-1177.602229
IRC_TS1_point21	-1177.525499	IRC_TS1_point134	-1177.520833	IRC_TS1_point247	-1177.602345
IRC_TS1_point22	-1177.52549	IRC_TS1_point135	-1177.520673	IRC_TS1_point248	-1177.602456

IRC_TS1_point23	-1177.525481	IRC_TS1_point136	-1177.520509	IRC_TS1_point249	-1177.602564
IRC_TS1_point24	-1177.525471	IRC_TS1_point137	-1177.520341	IRC_TS1_point250	-1177.602669
IRC_TS1_point25	-1177.525462	IRC_TS1_point138	-1177.520169	IRC_TS1_point251	-1177.60277
IRC_TS1_point26	-1177.525452	IRC_TS1_point139	-1177.519994	IRC_TS1_point252	-1177.602869
IRC_TS1_point27	-1177.525442	IRC_TS1_point140	-1177.519815	IRC_TS1_point253	-1177.602965
IRC_TS1_point28	-1177.525431	IRC_TS1_point141	-1177.519632	IRC_TS1_point254	-1177.603058
IRC_TS1_point29	-1177.525421	IRC_TS1_point142	-1177.519445	IRC_TS1_point255	-1177.603147
IRC_TS1_point30	-1177.52541	IRC_TS1_point143	-1177.519254	IRC_TS1_point256	-1177.603233
IRC_TS1_point31	-1177.525399	IRC_TS1_point144	-1177.519059	IRC_TS1_point257	-1177.603316
IRC_TS1_point32	-1177.525388	IRC_TS1_point145	-1177.518862	IRC_TS1_point258	-1177.603396
IRC_TS1_point33	-1177.525378	IRC_TS1_point146	-1177.518662	IRC_TS1_point259	-1177.603472
IRC_TS1_point34	-1177.525367	IRC_TS1_point147	-1177.51846	IRC_TS1_point260	-1177.603546
IRC_TS1_point35	-1177.525356	IRC_TS1_point148	-1177.518255	IRC_TS1_point261	-1177.603617
IRC_TS1_point36	-1177.525346	IRC_TS1_point149	-1177.518049	IRC_TS1_point262	-1177.603685
IRC_TS1_point37	-1177.525335	IRC_TS1_point150	-1177.517842	IRC_TS1_point263	-1177.603751
IRC_TS1_point38	-1177.525324	IRC_TS1_point151	-1177.517636	IRC_TS1_point264	-1177.603815
IRC_TS1_point39	-1177.525313	IRC_TS1_point152	-1177.517435	IRC_TS1_point265	-1177.603877
IRC_TS1_point40	-1177.525302	IRC_TS1_point153	-1177.517246	IRC_TS1_point266	-1177.603938
IRC_TS1_point41	-1177.525291	IRC_TS1_point154	-1177.51708	IRC_TS1_point267	-1177.603994
IRC_TS1_point42	-1177.52528	IRC_TS1_point155	-1177.51695	IRC_TS1_point268	-1177.604053
IRC_TS1_point43	-1177.52527	IRC_TS1_point156	-1177.516891	IRC_TS1_point269	-1177.604109
IRC_TS1_point44	-1177.52526	IRC_TS1_point157	-1177.516988	IRC_TS1_point270	-1177.604169
IRC_TS1_point45	-1177.52525	IRC_TS1_point158	-1177.517368	IRC_TS1_point271	-1177.604227
IRC_TS1_point46	-1177.525239	IRC_TS1_point159	-1177.518266	IRC_TS1_point272	-1177.604283
IRC_TS1_point47	-1177.52523	IRC_TS1_point160	-1177.520038	IRC_TS1_point273	-1177.604336
IRC_TS1_point48	-1177.52522	IRC_TS1_point161	-1177.523027	IRC_TS1_point274	-1177.604386
IRC_TS1_point49	-1177.525211	IRC_TS1_point162	-1177.527261	IRC_TS1_point275	-1177.604436
IRC_TS1_point50	-1177.525201	IRC_TS1_point163	-1177.532649	IRC_TS1_point276	-1177.604482
IRC_TS1_point51	-1177.525192	IRC_TS1_point164	-1177.539366	IRC_TS1_point277	-1177.604528
IRC_TS1_point52	-1177.525183	IRC_TS1_point165	-1177.546846	IRC_TS1_point278	-1177.604571
IRC_TS1_point53	-1177.525173	IRC_TS1_point166	-1177.553734	IRC_TS1_point279	-1177.604614
IRC_TS1_point54	-1177.525164	IRC_TS1_point167	-1177.558319	IRC_TS1_point280	-1177.604655
IRC_TS1_point55	-1177.525155	IRC_TS1_point168	-1177.560596	IRC_TS1_point281	-1177.604696
IRC_TS1_point56	-1177.525146	IRC_TS1_point169	-1177.562389	IRC_TS1_point282	-1177.604733
IRC_TS1_point57	-1177.525137	IRC_TS1_point170	-1177.56405	IRC_TS1_point283	-1177.604771
IRC_TS1_point58	-1177.525128	IRC_TS1_point171	-1177.565565	IRC_TS1_point284	-1177.604808
IRC_TS1_point59	-1177.525119	IRC_TS1_point172	-1177.566995	IRC_TS1_point285	-1177.604847
IRC_TS1_point60	-1177.52511	IRC_TS1_point173	-1177.568333	IRC_TS1_point286	-1177.604883
IRC_TS1_point61	-1177.525102	IRC_TS1_point174	-1177.569603	IRC_TS1_point287	-1177.604919
IRC_TS1_point62	-1177.525092	IRC_TS1_point175	-1177.570815	IRC_TS1_point288	-1177.604954
IRC_TS1_point63	-1177.525083	IRC_TS1_point176	-1177.571967	IRC_TS1_point289	-1177.604989
IRC_TS1_point64	-1177.525074	IRC_TS1_point177	-1177.573044	IRC_TS1_point290	-1177.605023
IRC_TS1_point65	-1177.525065	IRC_TS1_point178	-1177.574059	IRC_TS1_point291	-1177.605057
IRC_TS1_point66	-1177.525056	IRC_TS1_point179	-1177.575021	IRC_TS1_point292	-1177.605091

IRC_TS1_point67	-1177.525046	IRC_TS1_point180	-1177.575946	IRC_TS1_point293	-1177.605124
IRC_TS1_point68	-1177.525036	IRC_TS1_point181	-1177.576827	IRC_TS1_point294	-1177.605157
IRC_TS1_point69	-1177.525026	IRC_TS1_point182	-1177.577676	IRC_TS1_point295	-1177.605189
IRC_TS1_point70	-1177.525015	IRC_TS1_point183	-1177.578494	IRC_TS1_point296	-1177.605221
IRC_TS1_point71	-1177.525003	IRC_TS1_point184	-1177.579298	IRC_TS1_point297	-1177.605251
IRC_TS1_point72	-1177.524991	IRC_TS1_point185	-1177.580078	IRC_TS1_point298	-1177.605281
IRC_TS1_point73	-1177.524976	IRC_TS1_point186	-1177.580839	IRC_TS1_point299	-1177.605307
IRC_TS1_point74	-1177.524966	IRC_TS1_point187	-1177.581576	IRC_TS1_point300	-1177.605334
IRC_TS1_point75	-1177.524954	IRC_TS1_point188	-1177.58229	IRC_TS1_point301	-1177.605358
IRC_TS1_point76	-1177.52494	IRC_TS1_point189	-1177.582982	IRC_TS1_point302	-1177.605371
IRC_TS1_point77	-1177.524924	IRC_TS1_point190	-1177.583653	IRC_TS1_point303	-1177.605402
IRC_TS1_point78	-1177.524909	IRC_TS1_point191	-1177.584306	IRC_TS1_point304	-1177.605424
IRC_TS1_point79	-1177.524893	IRC_TS1_point192	-1177.58494	IRC_TS1_point305	-1177.605455
IRC_TS1_point80	-1177.524877	IRC_TS1_point193	-1177.585557	IRC_TS1_point306	-1177.605482
IRC_TS1_point81	-1177.52486	IRC_TS1_point194	-1177.586158	IRC_TS1_point307	-1177.605468
IRC_TS1_point82	-1177.524841	IRC_TS1_point195	-1177.586744	IRC_TS1_point308	-1177.605494
IRC_TS1_point83	-1177.524821	IRC_TS1_point196	-1177.587315	IRC_TS1_point309	-1177.605519
IRC_TS1_point84	-1177.524799	IRC_TS1_point197	-1177.587871	IRC_TS1_point310	-1177.605544
IRC_TS1_point85	-1177.524775	IRC_TS1_point198	-1177.588413	IRC_TS1_point311	-1177.605567
IRC_TS1_point86	-1177.52475	IRC_TS1_point199	-1177.588942	IRC_TS1_point312	-1177.605593
IRC_TS1_point87	-1177.524723	IRC_TS1_point200	-1177.589457	IRC_TS1_point313	-1177.605616
IRC_TS1_point88	-1177.524695	IRC_TS1_point201	-1177.589959	IRC_TS1_point314	-1177.605642
IRC_TS1_point89	-1177.524665	IRC_TS1_point202	-1177.590449	IRC_TS1_point315	-1177.605666
IRC_TS1_point90	-1177.524633	IRC_TS1_point203	-1177.590926	IRC_TS1_point316	-1177.605691
IRC_TS1_point91	-1177.5246	IRC_TS1_point204	-1177.59139	IRC_TS1_point317	-1177.605714
IRC_TS1_point92	-1177.524565	IRC_TS1_point205	-1177.591842	IRC_TS1_point318	-1177.605738
IRC_TS1_point93	-1177.524529	IRC_TS1_point206	-1177.592282	IRC_TS1_point319	-1177.605762
IRC_TS1_point94	-1177.52449	IRC_TS1_point207	-1177.59271	IRC_TS1_point320	-1177.605787
IRC_TS1_point95	-1177.52445	IRC_TS1_point208	-1177.593126	IRC_TS1_point321	-1177.605811
IRC_TS1_point96	-1177.524407	IRC_TS1_point209	-1177.593532	IRC_TS1_point322	-1177.605834
IRC_TS1_point97	-1177.524363	IRC_TS1_point210	-1177.593927	IRC_TS1_point323	-1177.605859
IRC_TS1_point98	-1177.524317	IRC_TS1_point211	-1177.594312	IRC_TS1_point324	-1177.605883
IRC_TS1_point99	-1177.524268	IRC_TS1_point212	-1177.594687	IRC_TS1_point325	-1177.60591
IRC_TS1_point100	-1177.524217	IRC_TS1_point213	-1177.595053	IRC_TS1_point326	-1177.605935
IRC_TS1_point101	-1177.524165	IRC_TS1_point214	-1177.595409	IRC_TS1_point327	-1177.605962
IRC_TS1_point102	-1177.52411	IRC_TS1_point215	-1177.595756	IRC_TS1_point328	-1177.605989
IRC_TS1_point103	-1177.524053	IRC_TS1_point216	-1177.596094	IRC_TS1_point329	-1177.606015
IRC_TS1_point104	-1177.523994	IRC_TS1_point217	-1177.596422	IRC_TS1_point330	-1177.606044
IRC_TS1_point105	-1177.523933	IRC_TS1_point218	-1177.596741	IRC_TS1_point331	-1177.60607
IRC_TS1_point106	-1177.523869	IRC_TS1_point219	-1177.597049	IRC_TS1_point332	-1177.606101
IRC_TS1_point107	-1177.523803	IRC_TS1_point220	-1177.597348	IRC_TS1_point333	-1177.606128
IRC_TS1_point108	-1177.523734	IRC_TS1_point221	-1177.597637	IRC_TS1_point334	-1177.606157
IRC_TS1_point109	-1177.523663	IRC_TS1_point222	-1177.597915		
IRC_TS1_point110	-1177.523588	IRC_TS1_point223	-1177.598183		

IRC_TS1_point111	-1177.523511	IRC_TS1_point224	-1177.598441
IRC_TS1_point112	-1177.52343	IRC_TS1_point225	-1177.598688
IRC_TS1_point113	-1177.523347	IRC_TS1_point226	-1177.598922

6. Cartesian Coordinates for the Optimized Structures

INT1

B	-1.91583700	-0.61658400	-1.28031500
B	-1.97164000	-1.39839800	0.32532400
B	-2.02851700	-0.11807900	1.55888200
B	-1.93858300	1.14375900	-1.03408100
B	-1.99828800	1.44899400	0.71782800
B	-3.44621700	-1.26939100	-0.65950400
B	-3.42723200	0.30052300	-1.49612100
H	-1.33817500	-1.11222400	-2.19730400
B	-3.51745900	-0.95828400	1.09127800
H	-1.44698300	-2.44577300	0.53493800
B	-3.53171300	0.80199700	1.33738400
H	-1.51275200	-0.25808800	2.62544000
B	-3.47470100	1.58154400	-0.26195800
H	-1.35578200	1.88123700	-1.76930200
H	-3.95989400	-2.23158900	-1.14455300
B	-4.41326400	0.08816600	-0.03231200
H	-3.92169200	0.44361900	-2.57275600
H	-4.07698400	-1.70407100	1.83654100
H	-4.09987100	1.30515700	2.25868700
H	-4.00086300	2.63328600	-0.46457800
H	-5.60603500	0.08146300	-0.07670800
B	-1.03757000	0.09446500	0.09125500
H	-1.45638100	2.39869700	1.19781500
N	0.46801500	0.22445700	0.17298600
H	0.81181200	1.11421900	0.50775100
C	1.42114900	-0.65924100	-0.15025700
O	1.18574000	-1.82847100	-0.51645100
C	2.84603100	-0.18482500	-0.05040100
C	3.20298700	1.15373000	-0.25311600
C	3.84753400	-1.12265300	0.22382200
C	4.53742100	1.54639400	-0.17537700
H	2.44733700	1.89159400	-0.49744900
C	5.17903900	-0.72738400	0.31546100
H	3.57489500	-2.16030300	0.37282400
C	5.52767200	0.60853600	0.11451400
H	4.80313700	2.58341900	-0.34674600
H	5.94485600	-1.46095300	0.54120200
H	6.56545900	0.91597500	0.17872300

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B	-2.54618500	1.60047900	0.57155600
B	-2.54157100	1.21517200	-1.18786200
B	-1.61565000	-0.28139900	-1.42401300
B	-1.62153200	0.33953900	1.41480200
B	-1.03577900	-0.77578300	0.17190700
B	-3.93880800	0.78065300	-0.17400600
B	-3.36343400	0.24103800	1.42044600
H	-2.60163700	2.71971200	0.97162500
B	-3.35767200	-0.37472400	-1.39499300
H	-2.59329500	2.06538000	-2.01848700
B	-2.38242500	-1.63312400	-0.56366300
H	-0.91042500	-0.45091100	-2.36762400
B	-2.38517800	-1.24896300	1.19389900
H	-0.92038100	0.58025700	2.34578800
H	-4.99159100	1.32412800	-0.29580800
B	-3.84264900	-0.97028600	0.20948500
H	-3.99796100	0.42236400	2.41178200
H	-3.98819100	-0.62348300	-2.37409800
H	-2.31462700	-2.75185500	-0.96244500
H	-2.32123300	-2.09948400	2.02292800
H	-4.82984000	-1.62192500	0.34955500
B	-1.12077600	0.90486000	-0.19368600
N	0.37716200	1.17925900	-0.25014500
C	1.09576300	0.10097100	-0.01238100
C	2.56050900	0.04715700	-0.00215800
C	3.19618800	-1.19962600	-0.08548300
C	3.32917500	1.21572300	0.09185800
C	4.58426800	-1.27239400	-0.08590900
H	2.60163700	-2.10072400	-0.15900000
C	4.71646200	1.13429700	0.09718700
H	2.85443500	2.18524600	0.18253600
C	5.34590700	-0.10763000	0.00558400
H	5.07165800	-2.23749700	-0.15822000
H	5.30656200	2.03933800	0.17863100
H	6.42829800	-0.16694600	0.00910200
O	0.43874100	-1.01055100	0.22750400
H	0.84519500	2.04768700	-0.47683900

INT2

B	-3.42285700	-1.12341900	-1.35457900
B	-2.72622500	-1.41996300	0.26377900

B	-3.36939800	-0.18469100	1.37521900
B	-4.49439100	0.29672300	-1.23897900
B	-4.45593700	0.87523700	0.44387300
B	-4.09520500	-2.39467200	-0.31323600
B	-5.18610200	-1.33561000	-1.23880100
H	-2.81574800	-1.36554900	-2.34987800
B	-4.06260000	-1.81565800	1.36879500
H	-1.63989500	-1.88201400	0.40542500
B	-5.12984600	-0.39585000	1.48265700
H	-2.71662000	0.24207500	2.27565200
B	-5.82431500	-0.09852400	-0.12930100
H	-4.61642400	1.05563500	-2.15041600
H	-3.96707400	-3.55076300	-0.57779000
B	-5.57984800	-1.76488700	0.44072000
H	-5.82372800	-1.74466300	-2.16010200
H	-3.90893200	-2.56317400	2.28593700
H	-5.72929300	-0.13631300	2.48060000
H	-6.91281000	0.36894500	-0.26734600
H	-6.49781700	-2.47902100	0.70591900
B	-2.98545800	0.23604500	-0.30845900
H	-4.54445200	2.03836800	0.69510900
N	-1.89323600	1.25115900	-0.60452800
H	-2.15478100	2.22217000	-0.47493700
C	-0.65452300	1.07000400	-1.00568000
O	-0.25333600	-0.10235500	-1.34735400
C	0.26551300	2.23249600	-1.07858700
C	0.15208100	3.30085100	-0.18203800
C	1.28832200	2.23263300	-2.03414800
C	1.05237100	4.35890600	-0.24345100
H	-0.60782500	3.28760000	0.58996800
C	2.18171800	3.29605700	-2.09691000
H	1.37417000	1.40288100	-2.72448400
C	2.06730200	4.35871500	-1.19975800
H	0.97230800	5.17443300	0.46569300
H	2.96771500	3.29609800	-2.84324600
H	2.77097300	5.18234900	-1.24306600
I	1.67506800	-1.11536700	-0.50378100
C	1.57417600	0.27369900	1.11715000
C	0.48502000	0.19848400	1.97360000
C	2.57080900	1.23563800	1.21605500
C	0.39663100	1.15249800	2.98707600
H	-0.27584300	-0.55953100	1.85172700
C	2.46850700	2.16478900	2.24806600
H	3.38927100	1.27181600	0.51032700

C	1.38383300	2.12647800	3.12447900
H	-0.44841500	1.12657100	3.66458100
H	3.22889300	2.92991900	2.34940000
H	1.30464500	2.86471000	3.91397600
O	3.37785700	-1.92465000	0.59319200
C	4.03288600	-2.84985200	-0.07965300
O	3.70114300	-3.21090000	-1.20368900
C	5.19745300	-3.41884500	0.68511300
H	4.80875700	-4.08110300	1.46408600
H	5.83632800	-3.98841800	0.01183800
H	5.76364000	-2.62242400	1.16961300

INT4

B	3.72986300	1.95679000	0.99555900
B	4.57273200	1.19994800	-0.38527300
B	3.57123000	-0.13967500	-0.98219000
B	2.20787000	1.08627300	1.26955400
B	2.14407400	-0.14829000	0.02964700
B	3.66204700	2.70917800	-0.61323800
B	2.20163100	2.64425800	0.40245900
H	4.32866300	2.44866000	1.89963900
B	3.55643100	1.42048600	-1.83210500
H	5.76116400	1.16371300	-0.44998600
B	2.02939200	0.54636200	-1.57069500
H	4.01672800	-1.13726900	-1.45054100
B	1.18303900	1.31241300	-0.18318700
H	1.73366400	0.92811600	2.34405500
H	4.20989400	3.74143600	-0.84251400
B	2.09665600	2.30780900	-1.34385000
H	1.71433900	3.61732800	0.88208100
H	4.02265100	1.53603800	-2.92157200
H	1.39981700	0.03799300	-2.44055400
H	1.51543500	3.03916100	-2.08215800
B	3.68261300	0.19224100	0.77536700
I	1.21591100	-2.15558500	0.54072900
C	-0.78709000	-1.94774900	-0.21807400
C	-0.98213600	-1.88510200	-1.59121200
C	-1.83110700	-1.91920900	0.69521400
C	-2.29086200	-1.77485300	-2.06179100
H	-0.14718200	-1.91425000	-2.27734400
C	-3.13314700	-1.82567000	0.20155600
H	-1.64406400	-1.95807300	1.75996500
C	-3.36236700	-1.75023200	-1.16976500

H	-2.46579500	-1.71250900	-3.12974700
H	-3.96244900	-1.79635200	0.89760500
H	-4.37532600	-1.66445400	-1.54399900
H	4.20882000	-0.57241500	1.51859500
N	-0.31801100	1.30856200	-0.20742100
C	-1.18155600	1.69246900	0.74520600
H	-0.74534400	0.93858600	-1.04487500
C	-2.64082100	1.61981600	0.39682000
O	-0.83263400	2.08671600	1.87414900
C	-3.56121900	1.39821800	1.42631600
C	-3.10442200	1.76517100	-0.91473500
C	-4.92035800	1.29835800	1.14676700
H	-3.20166200	1.28726100	2.44197700
C	-4.46643400	1.67989300	-1.19230800
H	-2.41089300	1.96224800	-1.72393400
C	-5.37636600	1.43825200	-0.16438500
H	-5.62361900	1.10825500	1.94977700
H	-4.81577700	1.80068300	-2.21140300
H	-6.43576300	1.36304400	-0.38280800

INT5

B	0.45767900	3.30847000	-1.22729800
B	-0.43796300	2.00257600	-0.43247100
B	-0.29867300	2.13768200	1.31399500
B	1.15454300	4.30106200	0.07003300
B	0.69535400	3.57604400	1.63150500
B	-1.32130400	3.38195700	-1.07762400
B	-0.33403400	4.82668000	-0.74810300
H	0.98950300	3.16735500	-2.27939500
B	-1.78551000	2.66830900	0.48982800
H	-0.43787000	0.94387800	-1.06361000
B	-1.07470800	3.66194800	1.77991600
H	-0.26789100	1.17905700	2.01629600
B	-0.17840800	4.99476200	1.01473700
H	2.20131000	4.85240900	-0.07287900
H	-2.02417000	3.29186900	-2.03413100
B	-1.71076700	4.43249900	0.30643800
H	-0.34875900	5.76853700	-1.47849300
H	-2.81038900	2.07882800	0.62131900
H	-1.60907300	3.78875600	2.83770800
H	-0.07963400	6.06382800	1.53301500
H	-2.69739300	5.10078500	0.32419800
B	1.09339800	2.53016400	0.25560400

H	1.42296400	3.62699300	2.57507500
N	2.35650700	1.71357000	0.32125800
H	2.92564300	1.85230800	1.14405900
C	2.85271500	0.85787100	-0.58505500
O	2.30696900	0.63444900	-1.68199200
C	4.13223600	0.14779900	-0.23459600
C	4.57979500	-0.00815900	1.08219400
C	4.86993600	-0.42853500	-1.27331100
C	5.74316200	-0.72373800	1.35212400
H	4.01048300	0.38855800	1.91413500
C	6.03662400	-1.13830200	-1.00560600
H	4.51721500	-0.32018100	-2.29121100
C	6.47571400	-1.28997900	0.30948200
H	6.06983300	-0.84916700	2.37822700
H	6.60053200	-1.57656600	-1.82139200
H	7.38019200	-1.84929600	0.52129000
I	-1.51321500	-0.83597500	-0.59162800
C	0.38715900	-1.72886300	-0.17643200
C	0.89096900	-1.65539500	1.11713400
C	1.04714400	-2.39110400	-1.20510600
C	2.10522100	-2.28244300	1.38583000
H	0.35310900	-1.12851700	1.89258800
C	2.25964800	-3.01427000	-0.91524500
H	0.63404400	-2.41792100	-2.20465200
C	2.78489600	-2.95980500	0.37444500
H	2.52037300	-2.23241900	2.38519200
H	2.79526700	-3.53002300	-1.70342800
H	3.73480200	-3.43485400	0.58939600
O	-2.41321000	-2.78740800	-0.34712400
C	-2.56619300	-3.25400400	0.88868500
O	-2.21929300	-2.66252100	1.89616800
C	-3.20057900	-4.62145400	0.88121500
H	-2.48488000	-5.33840900	0.46967400
H	-3.46132400	-4.90742400	1.89926200
H	-4.08667200	-4.62505500	0.24463100
O	-4.12504500	-0.31051800	-1.21796300
C	-5.02596400	0.02746100	-0.38375900
O	-6.02007700	0.74060700	-0.68149800
C	-4.89244000	-0.48895300	1.04126500
H	-3.89997600	-0.26365300	1.43573400
H	-5.65185500	-0.05689800	1.69339300
H	-5.00356700	-1.57747100	1.03836900

PhI(OAc)₂

I	-0.39978300	-0.73491600	-0.20050300
C	0.53293000	1.18607500	-0.07143700
C	0.64232100	1.94104000	-1.23135300
C	1.01225900	1.60375900	1.16244000
C	1.26665900	3.18460000	-1.13969300
H	0.25680400	1.57932400	-2.17487900
C	1.63378300	2.85038700	1.22910800
H	0.91048300	0.98355300	2.04217600
C	1.75986300	3.63563300	0.08399600
H	1.36480600	3.79554500	-2.02930900
H	2.01736300	3.20130500	2.17988700
H	2.24489800	4.60283400	0.14530700
O	-2.25117800	0.48175500	0.17658300
C	-3.34561000	-0.23358200	0.14910200
O	-3.34717000	-1.44974500	-0.05369300
C	-4.60025200	0.56004300	0.41128000
H	-5.47751100	-0.02752400	0.14352100
H	-4.64102300	0.80333300	1.47714500
H	-4.58462600	1.49708800	-0.14731400
O	1.62201400	-1.53150300	-0.72220900
C	2.45864200	-1.83090700	0.24749500
O	2.20431100	-1.71223100	1.44269800
C	3.79238500	-2.31718300	-0.26628300
H	4.39441000	-2.70003600	0.55684900
H	3.64894400	-3.09111200	-1.02243600
H	4.31226300	-1.47916400	-0.73923600

AcO⁻

C	0.17700400	0.00001800	-0.01074700
O	0.76370200	-1.12097200	0.00185500
O	0.76383200	1.12089800	0.00185500
C	-1.34936800	0.00006000	-0.00441300
H	-1.74802200	0.89412800	-0.48735400
H	-1.74803200	-0.89347900	-0.48832300
H	-1.69004000	-0.00052300	1.03695600

INT6

B	-1.70479900	4.60607600	0.27874700
B	-0.84960900	4.00345500	1.72249600
B	-0.25377000	2.37240000	1.37085000
B	-1.63143800	3.34354000	-0.97527400

B	-0.71460800	2.02370300	-0.27999600
B	-0.03986000	5.13593200	0.61522500
B	-0.52430400	4.73531800	-1.04619800
H	-2.63224700	5.34858200	0.36355100
B	0.85821800	3.75660100	1.28430800
H	-1.17247900	4.32109400	2.82441100
B	0.94448300	2.49681400	0.03817900
H	-0.14305900	1.51799800	2.18913600
B	0.08622200	3.10875000	-1.41924000
H	-2.49944400	3.16708700	-1.76961400
H	0.20932700	6.25610900	0.93624800
B	1.06158000	4.21277400	-0.42824900
H	-0.62050500	5.56252400	-1.89772700
H	1.74635100	3.88150300	2.06911400
H	0.40424800	2.77489400	-2.51205600
H	2.09084700	4.65333000	-0.83433200
B	-1.83864600	2.89843000	0.74457000
I	-2.02468200	-0.64503800	-0.25268700
C	-0.25407500	-1.69784700	0.32593700
C	0.20813700	-1.54749600	1.62614800
C	0.34520400	-2.52288900	-0.61596100
C	1.33365300	-2.28093000	1.99749200
H	-0.28673800	-0.88867800	2.32544200
C	1.46439700	-3.25079200	-0.21633700
H	-0.03848400	-2.59680000	-1.62396800
C	1.95416000	-3.13006700	1.08275500
H	1.72276200	-2.18015500	3.00362100
H	1.95633000	-3.90056800	-0.92977800
H	2.83245000	-3.69021200	1.37952700
O	-3.00626400	-2.57654100	0.22034700
C	-4.28405800	-2.58305300	-0.08637200
O	-4.85743800	-1.61679400	-0.58214700
C	-4.97297500	-3.87842100	0.25869800
H	-5.90770600	-3.95458000	-0.29537300
H	-4.32834900	-4.73123300	0.04521300
H	-5.19057200	-3.87349300	1.33096200
H	-0.81678600	0.87219900	-0.75917400
H	-2.84971600	2.41042700	1.13740900
N	2.11974300	1.56043000	0.02073000
C	2.34614400	0.51957900	-0.79715400
H	2.80359100	1.69365200	0.75255900
C	3.51853300	-0.36501900	-0.47714600
O	1.63152400	0.26046100	-1.78328800
C	4.02415700	-1.18539400	-1.49099300

C	4.07398200	-0.44927800	0.80428000
C	5.07144100	-2.06452200	-1.23426300
H	3.58593500	-1.13253400	-2.47960700
C	5.11810800	-1.33301300	1.06371900
H	3.67631900	0.14063300	1.62130000
C	5.62035000	-2.14230700	0.04576800
H	5.45598600	-2.69221700	-2.03028900
H	5.52823400	-1.39975200	2.06499400
H	6.43077600	-2.83308700	0.24993300

INT7

B	3.51434400	0.24588900	1.02035700
B	2.11522900	0.15898300	-0.03662200
B	1.33793500	-1.40186600	0.08366200
B	3.64162400	-1.34262800	1.80374900
B	2.29513400	-2.35038400	1.22954300
B	3.70493400	0.00673300	-0.74689300
B	4.66633100	-0.95355700	0.40193500
H	3.83904800	1.26304700	1.54063400
B	2.35603000	-1.01634700	-1.32990200
B	2.49237300	-2.60023100	-0.52795200
B	3.91475300	-2.55985100	0.53717100
H	4.16840300	0.85356300	-1.43975900
B	3.95491700	-1.73149600	-1.03611200
H	5.84045000	-0.79192500	0.50638200
H	1.90293000	-0.87265500	-2.41339300
H	2.10467300	-3.59085300	-1.05941600
H	4.55798200	-3.53939300	0.74409000
H	4.62516300	-2.11417500	-1.94141900
B	2.04256500	-0.61618500	1.53583200
H	1.75842900	-3.16655700	1.90958300
I	1.03972000	2.10853000	-0.47676000
C	-0.93722400	1.82834700	0.32729400
C	-1.08707100	1.55665700	1.67984600
C	-2.01440100	1.99885200	-0.53251500
C	-2.38240200	1.44041700	2.18391300
H	-0.22840300	1.43906900	2.32548100
C	-3.30145000	1.88412000	-0.00532200
H	-1.86385500	2.20984400	-1.58293200
C	-3.48466800	1.60572700	1.34662200
H	-2.52235900	1.21914400	3.23567800
H	-4.15501900	2.00437800	-0.66199100
H	-4.48659400	1.50821700	1.74703200

H	4.08478100	-1.45957800	2.90159700
H	-1.46067500	-0.34041600	-2.34858500
H	1.33929800	-0.22367300	2.40567500
N	-0.16133200	-1.64970800	0.09098000
C	-1.09637300	-1.29333700	-0.73817800
H	-0.49376900	-2.17507700	0.89171400
C	-2.52179100	-1.52345900	-0.46191100
O	-0.71385100	-0.70870900	-1.85317700
C	-3.44811400	-1.55581600	-1.51458500
C	-2.96814500	-1.67030900	0.85849100
C	-4.79934600	-1.73398000	-1.24565900
H	-3.12761500	-1.47274400	-2.54684500
C	-4.32010300	-1.84979200	1.11918400
H	-2.27535200	-1.60848200	1.68807700
C	-5.23771700	-1.87844800	0.07025500
H	-5.50841300	-1.76564500	-2.06407100
H	-4.65895700	-1.94789700	2.14337800
H	-6.29321200	-2.01185500	0.27747600

TS1

B	-2.83898100	3.81344700	0.34197900
B	-1.74102900	3.64224500	1.73922300
B	-0.67915300	2.25998000	1.44299900
B	-2.45194700	2.54130100	-0.83887500
B	-1.11523800	1.62381800	-0.14724800
B	-1.41098100	4.86939600	0.49384200
B	-1.86354300	4.20180500	-1.08651300
H	-3.94899000	4.22092300	0.46986700
B	-0.07988800	3.90963500	1.17105900
H	-2.07887000	3.93131600	2.84255600
B	0.32533000	2.64347100	0.00968900
H	-0.24271600	1.56007500	2.29292500
B	-0.80031500	2.82910600	-1.42967000
H	-3.26748300	2.02412900	-1.53071300
H	-1.50532700	6.03380500	0.72066800
B	-0.14812400	4.24562300	-0.59152800
H	-2.27475900	4.88055600	-1.97224900
H	0.77334800	4.37485500	1.85700800
H	-0.45226500	2.50788300	-2.51427500
H	0.66294300	4.93539600	-1.12100600
B	-2.38706400	2.20265300	0.92950600
I	-1.61954600	-0.85525900	-0.25992600
C	0.20429600	-1.59132900	0.60663400

C	0.48081400	-1.28172600	1.92916400
C	1.04281500	-2.35752700	-0.19007500
C	1.67663400	-1.75539300	2.47141100
H	-0.20238300	-0.69134000	2.52192500
C	2.22547100	-2.82952200	0.37583000
H	0.79687800	-2.56966000	-1.22103600
C	2.54448500	-2.52355300	1.69823900
H	1.92120700	-1.51840500	3.50028000
H	2.90186200	-3.42212400	-0.22819800
H	3.47371700	-2.88213900	2.12486600
O	-2.19862300	-3.23387600	0.09510500
C	-3.39659500	-3.49614800	-0.29374500
O	-4.16151400	-2.66029100	-0.81282500
C	-3.86269900	-4.91944900	-0.05078500
H	-4.20086100	-4.99644200	0.98767100
H	-4.69685500	-5.16688300	-0.70777200
H	-3.04589300	-5.62855800	-0.19227700
H	-0.35248800	0.74830300	-0.81684000
H	-3.15583400	1.45604300	1.43627100
N	1.70379800	2.07260600	-0.10236400
C	2.00722900	0.97318000	-0.80010900
H	2.44057500	2.47347900	0.46220000
C	3.36183400	0.36913800	-0.65517200
O	1.16056800	0.42169900	-1.54416800
C	3.85881500	-0.42272100	-1.69596900
C	4.09919200	0.49697200	0.52647600
C	5.08675600	-1.06196300	-1.56468400
H	3.27694400	-0.53494000	-2.60225800
C	5.32128500	-0.15610100	0.66148200
H	3.70966100	1.06860100	1.36034900
C	5.81831200	-0.93360700	-0.38340000
H	5.46913000	-1.66782800	-2.37817300
H	5.87790000	-0.06772500	1.58731500
H	6.76928500	-1.44301400	-0.27549800

AcOH

C	-0.08500700	0.11822300	-0.00006800
O	-0.62068500	1.21066100	-0.00008300
O	-0.79599500	-1.02510200	0.00008600
C	1.38956200	-0.12868000	0.00000600
H	1.66174300	-0.71338300	0.88261800
H	1.66173800	-0.71452400	-0.88183800
H	1.92723900	0.81714600	-0.00057400

H	-1.74460900	-0.81097500	0.00015000
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TS2

B	0.83948500	3.46476400	1.01975100
B	0.89437600	3.55000700	-0.76920200
B	0.30966700	1.99216100	-1.42248800
B	0.21703200	1.85397800	1.48638400
B	-0.10826900	1.06741500	-0.01896400
B	-0.44387400	4.29765800	0.12126300
B	-0.86689800	3.25952600	1.50538500
H	1.63192400	4.03672000	1.69829800
B	-0.77698800	3.39377000	-1.37643900
H	1.72681600	4.17889700	-1.34105700
B	-1.40221900	1.79151900	-0.92811200
H	0.74672800	1.50438300	-2.41236400
B	-1.45975800	1.70970800	0.87137100
H	0.59530800	1.27537600	2.45121700
H	-0.57142400	5.47983100	0.17204300
B	-1.85963900	3.22451800	0.02698800
H	-1.27788300	3.70337000	2.53014900
H	-1.12612900	3.93247100	-2.37837400
H	-2.17107100	1.18687500	-1.59591500
H	-2.26873000	1.05128800	1.43142800
H	-2.97492700	3.63865300	0.01121800
B	1.31296900	2.05906200	0.07118000
N	2.65519600	1.40689000	0.08371600
C	2.70733800	0.07576500	-0.00205000
C	4.02269600	-0.62425600	0.01384600
C	4.05288600	-1.98263000	0.35024600
C	5.21678800	0.03103900	-0.31007200
C	5.26138400	-2.67140900	0.37894900
H	3.12751600	-2.48869000	0.59539200
C	6.42328600	-0.66282600	-0.28976300
H	5.21283200	1.07523200	-0.59942400
C	6.44883400	-2.01312600	0.05850100
H	5.27720200	-3.72079500	0.65012500
H	7.34202000	-0.15003400	-0.55024500
H	7.38996000	-2.55104100	0.07623100
O	1.64013600	-0.57954500	-0.09037100
I	-1.07430300	-1.70559300	-0.12341200
H	3.51204400	1.92527800	0.21406500
C	-3.18783900	-1.43821300	-0.03005900
C	-3.89827100	-1.20932800	-1.20486100

C	-3.82046900	-1.46418400	1.20996600
C	-5.27591300	-1.00161300	-1.13045900
H	-3.39232100	-1.18831300	-2.16106500
C	-5.19849700	-1.25613500	1.26849900
H	-3.25412800	-1.63708200	2.11581800
C	-5.92634500	-1.02278700	0.10238100
H	-5.83545400	-0.81981400	-2.04117700
H	-5.69798000	-1.27273200	2.23066400
H	-6.99638500	-0.85751900	0.15442400

PhI

C	2.65639500	1.20600700	0.00000200
C	1.26084100	1.21481600	0.00000100
C	0.58146700	0.00000500	0.00000000
C	1.26083800	-1.21481400	0.00000100
C	2.65638600	-1.20601200	0.00000300
C	3.35554300	-0.00000100	0.00000300
H	3.19232900	2.14851300	0.00000300
H	0.71967000	2.15206900	0.00000000
H	0.71965500	-2.15206100	0.00000100
H	3.19232500	-2.14851500	0.00000300
H	4.43940100	-0.00000900	0.00000400
I	-1.56400400	0.00000000	-0.00000100

INT8

B	3.49760900	-0.44222200	0.59748500
B	3.30310000	-0.05112100	-1.13400600
B	4.11947700	1.50187400	-1.44353200
B	4.42736700	0.87408300	1.35599000
B	4.80649400	2.07424600	0.09559900
B	4.53688500	-1.21639000	-0.61610000
B	5.23364800	-0.64479300	0.91811700
H	2.68100600	-1.05568800	1.20225400
B	4.92183800	-0.01836900	-1.87360400
H	2.33018000	-0.37433800	-1.73906300
B	5.85064500	1.29716700	-1.11391400
H	3.70089400	2.26848400	-2.25569900
B	6.04257800	0.90890300	0.61276700
H	4.23134900	1.20196200	2.48562800
H	4.44143700	-2.37906600	-0.86327400
B	6.11217100	-0.38625500	-0.60532200
H	5.62617200	-1.40587600	1.74907800

H	5.09458900	-0.33355700	-3.01140600
H	6.67919500	1.91149100	-1.71395200
H	7.00669300	1.24985200	1.22719600
H	7.12729300	-0.96421600	-0.84792300
B	3.24499900	1.23775200	0.08040700
H	4.86454900	3.23936700	0.34790900
N	2.00074000	2.07669200	0.33288800
H	2.12837400	3.08185000	0.34924400
C	0.75390800	1.67836000	0.49197100
O	0.49040600	0.43564700	0.61529300
C	-0.33550600	2.68813000	0.55270800
C	-0.33080000	3.80682500	-0.28779400
C	-1.39223600	2.49516300	1.45005300
C	-1.38090500	4.71895300	-0.23357000
H	0.47443600	3.94782600	-0.99959600
C	-2.43077500	3.41774100	1.51145700
H	-1.39319000	1.62814100	2.09901900
C	-2.42887400	4.52710300	0.66662000
H	-1.38482800	5.57430600	-0.89926600
H	-3.24433500	3.26629300	2.21064700
H	-3.24655400	5.23772100	0.70443800
I	-1.42285600	-0.63829500	-0.23195500
C	-0.16596800	-2.30780200	0.22737200
C	-0.14676300	-2.78192000	1.53293400
C	0.63282200	-2.83616900	-0.77886900
C	0.72157000	-3.82811800	1.83957000
H	-0.78293800	-2.34685900	2.29203900
C	1.49165600	-3.88476800	-0.45430600
H	0.60168500	-2.43567600	-1.78287800
C	1.53745900	-4.37567500	0.84971200
H	0.75889500	-4.21023500	2.85310400
H	2.13072000	-4.30632100	-1.22094600
H	2.21449700	-5.18527100	1.09668000
O	-2.87287300	-2.01424700	-1.05205900
C	-3.67690900	-2.65205900	-0.20973900
O	-3.59999300	-2.57506400	1.00583400
C	-4.70651200	-3.47486900	-0.94018000
H	-4.24745200	-4.02413800	-1.76326800
H	-5.19009600	-4.16087500	-0.24600800
H	-5.45336400	-2.79561500	-1.36137400
O	-4.66024500	0.74396100	0.56632700
C	-4.32932100	1.38152500	-0.46801000
O	-3.38324600	1.05058300	-1.24872700
C	-5.13865500	2.61685800	-0.84446800

H	-5.53876400	3.10904100	0.04338900
H	-4.54128600	3.32065600	-1.42519300
H	-5.98453100	2.29646700	-1.46295700

TS6

B	-2.09709200	4.37452300	0.02721400
B	-1.26129400	3.83649300	1.51338500
B	-0.63494400	2.18970000	1.29359000
B	-2.04233700	3.04871400	-1.13346100
B	-1.12440900	1.72805000	-0.32555000
B	-0.43436900	4.90176600	0.34358900
B	-0.90675600	4.38677800	-1.29076800
H	-3.01426600	5.12852300	0.06102400
B	0.45939000	3.58844700	1.13922700
H	-1.61323500	4.20564200	2.58680400
B	0.58430300	2.23858900	0.01116800
H	-0.59529700	1.38968000	2.16393400
B	-0.27962700	2.73155500	-1.54392200
H	-2.87185700	2.78413700	-1.93797200
H	-0.17883500	6.04024100	0.57267600
B	0.68568400	3.89738700	-0.59388800
H	-0.96121200	5.13013800	-2.21580600
H	1.31374700	3.79886700	1.93445900
H	0.08692200	2.33576300	-2.59900700
H	1.71044800	4.28711700	-1.05093200
B	-2.25850100	2.69946800	0.58524000
I	-2.03163400	-0.55303500	-0.31314500
C	-0.15041800	-1.58045800	-0.32729000
C	0.39518500	-1.94740400	0.89396700
C	0.42983400	-1.88550900	-1.54928300
C	1.58329100	-2.67678900	0.87847600
H	-0.08292700	-1.67966700	1.82617500
C	1.62435000	-2.60680900	-1.53781600
H	-0.02718400	-1.57855800	-2.48036600
C	2.19257100	-3.00654900	-0.33039800
H	2.03471300	-2.97230800	1.81769900
H	2.10479300	-2.85264700	-2.47751300
H	3.12334800	-3.56051100	-0.33065900
O	-2.74772100	-2.92535500	0.11009800
C	-4.00299700	-3.01854000	0.36219000
O	-4.80039300	-2.05863800	0.33059100
C	-4.49173100	-4.40237700	0.75261900
H	-5.56195700	-4.49885800	0.56719700

H	-3.94344600	-5.17876500	0.21726700
H	-4.31054600	-4.53816600	1.82397100
H	-0.92716700	1.04630900	-1.34368500
H	-3.25690700	2.21975100	1.00812700
N	1.72716200	1.29124600	-0.15110100
C	2.52655200	0.78629900	0.80685100
H	1.96192100	1.03299100	-1.09855500
C	3.70458400	-0.03342000	0.35835800
O	2.32329700	0.97182200	2.01908600
C	4.36267200	-0.81221800	1.31625600
C	4.15415800	-0.06842200	-0.96660000
C	5.43044500	-1.62711200	0.95644100
H	4.01761600	-0.78766200	2.34169900
C	5.22434700	-0.88256600	-1.32795800
H	3.68851400	0.53891100	-1.73359100
C	5.86124600	-1.66914400	-0.36948100
H	5.92207800	-2.23469400	1.70777800
H	5.56021900	-0.90077100	-2.35843400
H	6.69072500	-2.30717800	-0.65323700

TS7

B	0.91609500	-0.80593300	-1.29361600
B	2.00176300	-2.18602200	-1.61143000
B	2.25988300	-3.04401000	-0.08120500
B	0.52619900	-0.81724100	0.49600600
B	1.38862700	-2.19352300	1.21311700
B	0.29138300	-2.29471600	-2.01388700
B	-0.58120700	-1.47435400	-0.67658900
H	0.93095200	0.21687500	-1.88839600
B	1.09041400	-3.67187000	-1.25568300
H	2.83290500	-2.14169300	-2.45598000
B	0.71329600	-3.67918800	0.51562700
H	3.28425200	-3.60486700	0.14096100
B	-0.33800200	-2.31123000	0.88438400
H	0.31568400	0.20320200	1.05761800
H	-0.16654800	-2.31552800	-3.10699100
B	-0.54723400	-3.25215800	-0.67922500
H	-1.72726200	-1.88352900	-0.97553000
H	1.25453000	-4.68748700	-1.85005000
H	0.62273400	-4.69896800	1.11832000
H	-1.19515000	-2.33971900	1.70098400
H	-1.48598400	-3.94452600	-0.88573400
B	2.15038500	-1.25671000	-0.09742600

H	1.81727700	-2.13584700	2.32025000
N	3.33452700	-0.40828000	0.26694500
H	3.59409200	-0.40564000	1.24394100
C	4.10851200	0.34640000	-0.53287800
O	3.87893700	0.51795500	-1.74373200
C	5.30179300	1.00484600	0.10150000
C	5.96833200	0.44967700	1.20045100
C	5.77817500	2.19793200	-0.45349800
C	7.08806600	1.08154500	1.73673700
H	5.63785500	-0.48938800	1.62949500
C	6.88834200	2.83584600	0.09187400
H	5.26817700	2.62479100	-1.30841700
C	7.54751200	2.27783600	1.18760500
H	7.60408100	0.63552300	2.57934200
H	7.24085500	3.76619300	-0.33895200
H	8.41710500	2.77031700	1.60809700
I	-2.44269100	0.12063900	-1.09528300
C	-3.16493200	-0.13387300	0.90775500
C	-2.61850900	0.66207500	1.90327700
C	-4.14406900	-1.08871500	1.13714500
C	-3.08711900	0.48230100	3.20437400
H	-1.85415500	1.39277600	1.68207400
C	-4.59376900	-1.25307500	2.44726800
H	-4.54117000	-1.69112700	0.33149700
C	-4.06766200	-0.47120000	3.47478300
H	-2.67689200	1.08907800	4.00312000
H	-5.35566500	-1.99464000	2.65694800
H	-4.42232500	-0.60607700	4.48999500
O	-4.21970300	1.88784400	-1.11155100
C	-3.90534500	3.04049000	-0.63439100
O	-2.75950500	3.37416100	-0.27709300
C	-5.06208600	4.01314500	-0.48002900
H	-4.70026400	5.04173100	-0.46249800
H	-5.79678300	3.88406500	-1.27598100
H	-5.55666200	3.80227200	0.47407200

TS8

B	1.78440900	1.02031200	-0.92426700
B	2.01050200	-0.59290900	-1.73875100
B	1.87406200	-1.85207400	-0.49455600
B	1.51324500	0.71902300	0.80333000
B	1.53998500	-1.04631900	1.06109700
B	0.46514800	0.28777200	-1.87107500
B	0.15607800	1.09756500	-0.24902700

H	2.32576000	1.99121300	-1.33691700
B	0.52412300	-1.52952700	-1.57382000
H	2.69751600	-0.70100900	-2.69855500
B	0.22269400	-1.80478700	0.14577000
H	2.50553500	-2.85678000	-0.54746800
B	-0.00357900	-0.17660000	0.96865300
H	1.90002800	1.47038000	1.63806800
H	0.08497600	0.75094700	-2.89297000
B	-0.59650100	-0.47501200	-0.65171100
H	-0.49258300	2.08764900	-0.21332900
H	0.10992500	-2.25894600	-2.41144000
H	-0.37810400	-2.74990900	0.53457400
H	-0.74783900	-0.07882200	1.88445900
H	-1.29969200	-0.13055100	-1.62672800
B	2.65874900	-0.29844300	-0.10846400
H	1.92643400	-1.50904300	2.08588100
N	4.12133200	-0.25525100	0.24178300
H	4.35949500	-0.58138300	1.16876800
C	5.15165100	0.21047800	-0.48233400
O	5.02153600	0.71982100	-1.61130200
C	6.51802700	0.10678300	0.13736100
C	6.85582500	-0.89919900	1.05074200
C	7.48909100	1.04272600	-0.23605400
C	8.14112000	-0.96159100	1.58470800
H	6.13104500	-1.65435500	1.33266000
C	8.76859600	0.98801900	0.30872700
H	7.23089900	1.81720500	-0.94786700
C	9.09833100	-0.01573400	1.21980900
H	8.39516400	-1.75244500	2.28128800
H	9.50857100	1.72657500	0.02170700
H	10.09694200	-0.06315300	1.63942100
I	-3.03902000	-0.86368600	-0.61319400
C	-3.38258100	1.17254200	-0.03569800
C	-3.60912900	2.10859900	-1.03319500
C	-3.35017600	1.48123700	1.31567400
C	-3.80727000	3.43357100	-0.64532700
H	-3.62356800	1.82533400	-2.07683800
C	-3.55510600	2.81198000	1.67930600
H	-3.16814200	0.72094300	2.06115400
C	-3.77937100	3.78277800	0.70408900
H	-3.98097500	4.18749100	-1.40417200
H	-3.53271100	3.08322500	2.72826600
H	-3.93230700	4.81509300	0.99651000
O	-5.49981000	-1.01069700	-0.20652500

C	-5.89086300	-1.20743900	1.00376300
O	-5.13461100	-1.42970100	1.96814100
C	-7.39184400	-1.11360200	1.21822000
H	-7.68366100	-1.63120900	2.13249600
H	-7.65605800	-0.05546100	1.31637200
H	-7.93718300	-1.51815500	0.36431100

TS-S1

B	-3.50290200	-3.89476300	0.31768500
B	-3.61523900	-2.77949700	1.70836100
B	-2.54865200	-1.40087800	1.40804600
B	-2.36594500	-3.20735900	-0.86408400
B	-1.84959200	-1.68408600	-0.17174700
B	-4.88177000	-2.77686000	0.45856400
B	-4.11833200	-3.05333800	-1.11797800
H	-3.62081800	-5.07024400	0.45139900
B	-4.29530300	-1.24198500	1.12901800
H	-3.81262500	-3.17246100	2.81313800
B	-3.17286200	-0.52428600	-0.03447500
H	-1.97440000	-0.79837300	2.25044600
B	-3.06116800	-1.67210700	-1.46843100
H	-1.65278700	-3.86000900	-1.55320900
H	-5.98560400	-3.16031900	0.68211000
B	-4.59918000	-1.40116000	-0.63136400
H	-4.66639000	-3.62536200	-2.00455100
H	-4.96344700	-0.53306300	1.81132100
H	-2.83436200	-1.26881300	-2.55594900
H	-5.47154000	-0.79772900	-1.16793700
B	-2.05843600	-3.05025300	0.90385700
I	0.70737400	-1.36909900	-0.30735500
C	0.85834600	0.52172100	0.70542600
C	0.60452400	0.55915100	2.06793300
C	1.23934400	1.62594400	-0.04287700
C	0.73013500	1.79104600	2.71013700
H	0.32124800	-0.32916600	2.61338100
C	1.36529400	2.84242900	0.62483400
H	1.42253100	1.54965900	-1.10435300
C	1.10708200	2.92468700	1.99195200
H	0.53151200	1.85499400	3.77351200
H	1.64862000	3.72532000	0.06483900
H	1.19668100	3.87785400	2.49945400
O	3.16643000	-1.42894400	0.21498500
C	3.95822900	-0.82160800	-0.56365500
O	3.73521600	-0.20664900	-1.60320800

C	5.43535900	-0.89045400	-0.05702000
H	-1.08381600	-0.83665800	-0.84959300
H	-1.13647300	-3.59426800	1.41291400
N	-2.98451300	0.95450900	-0.12640400
C	-2.06874600	1.58511200	-0.88056000
H	-3.51211400	1.53033300	0.51559500
C	-1.85487100	3.04773300	-0.65168900
O	-1.38520800	0.98231100	-1.73149800
C	-1.30019000	3.81024000	-1.68522500
C	-2.10851800	3.65007100	0.58488300
C	-1.02079700	5.15881000	-1.49157900
H	-1.08762300	3.33788900	-2.63627900
C	-1.81822300	4.99756200	0.78130900
H	-2.49191200	3.06788900	1.41412500
C	-1.27649000	5.75497600	-0.25597300
H	-0.59750900	5.74367700	-2.30027800
H	-2.00173600	5.45110300	1.74858900
H	-1.04856900	6.80360100	-0.10100900
F	5.56586400	-0.25459800	1.13122100
F	5.83437200	-2.16874800	0.12863400
F	6.30358900	-0.32116100	-0.91095400

TS-S2

B	-3.40147400	-4.13119500	0.12119200
B	-3.49566400	-3.03061900	1.52744100
B	-2.34466200	-1.69579100	1.31236100
B	-2.16918100	-3.50545000	-0.98257300
B	-1.59254200	-2.01577300	-0.22492100
B	-4.70607800	-2.93290300	0.22212500
B	-3.87853700	-3.21042700	-1.32457900
H	-3.60641100	-5.29720100	0.22135000
B	-4.07834900	-1.44656200	0.96642800
H	-3.75565100	-3.43579000	2.61406400
B	-2.86050900	-0.75771800	-0.11272800
H	-1.75550100	-1.18917100	2.20434500
B	-2.72791700	-1.86919800	-1.57287600
H	-1.45874500	-4.16065000	-1.66947300
H	-5.83954400	-3.25894900	0.37480500
B	-4.29836400	-1.54038600	-0.79629600
H	-4.40937400	-3.70689900	-2.26454900
H	-4.75362300	-0.74844000	1.64653700
H	-2.43838300	-1.43399500	-2.63639500
H	-5.10039600	-0.88222900	-1.37521000
B	-1.92837700	-3.39458600	0.77842800

I	0.89240800	-1.58842300	-0.19888400
C	0.84650100	0.53312500	0.12373100
C	0.64622600	0.98624800	1.41937400
C	1.12562100	1.35998700	-0.95375700
C	0.74935900	2.35837300	1.63989700
H	0.42278200	0.30453900	2.22794700
C	1.22358800	2.72851700	-0.70351700
H	1.27346700	0.96044500	-1.94713300
C	1.04637000	3.22185600	0.58701600
H	0.59270500	2.74534300	2.63955900
H	1.43870800	3.40221000	-1.52402700
H	1.12484100	4.28610900	0.77063700
O	3.34135400	-1.19094200	0.50874000
C	4.11155600	-0.74648900	-0.38703900
O	3.91279800	-0.56336200	-1.58803600
C	5.52279500	-0.37956100	0.17692700
H	-0.83660200	-1.51945600	-1.13918300
H	-1.06101200	-3.98911700	1.32550900
N	-2.55615000	0.68477000	-0.34770500
C	-2.61690700	1.70065700	0.53355800
H	-2.28754000	0.93377800	-1.28812200
C	-2.32343600	3.08395200	0.01890200
O	-2.89261400	1.53239200	1.73354200
C	-2.18269000	4.10892400	0.96082100
C	-2.15307900	3.38674900	-1.33730200
C	-1.85880500	5.40144300	0.56314700
H	-2.30981400	3.87719200	2.01017300
C	-1.82769800	4.68033000	-1.73690200
H	-2.27356200	2.63239300	-2.10580000
C	-1.67302000	5.68991800	-0.78842100
H	-1.74101400	6.18088400	1.30748000
H	-1.69387400	4.89760900	-2.79044300
H	-1.41245200	6.69491300	-1.10105300
F	6.11904600	-1.45471800	0.74317900
F	6.35804400	0.08585900	-0.76890400
F	5.43114500	0.57371000	1.13363200

TS-S3

B	1.61670300	-0.88122600	-1.32912900
B	2.88739400	-2.09692700	-1.64406500
B	3.25845300	-2.90725100	-0.11213000
B	1.22489900	-0.94503400	0.44611100
B	2.26150100	-2.18909700	1.17335300
B	1.20499900	-2.45245800	-2.05255400

B	0.25165500	-1.77837700	-0.72061700
H	1.48661600	0.12860700	-1.93284900
B	2.19374200	-3.70285700	-1.28736500
H	3.70305400	-1.94040800	-2.49051000
B	1.81822000	-3.75991300	0.47508500
H	4.35291400	-3.31241400	0.11513900
B	0.56646900	-2.55797800	0.82607400
H	0.86038000	0.03079300	1.01022800
H	0.76875300	-2.53457600	-3.15139000
B	0.51730700	-3.52178000	-0.71937600
H	-0.90920100	-2.15293900	-1.14841500
H	2.51294700	-4.67834700	-1.88639500
H	1.87838000	-4.77599100	1.08842300
H	-0.27675400	-2.70010500	1.64519200
H	-0.33029100	-4.32043100	-0.93465000
B	2.89971000	-1.15483300	-0.13187300
H	2.66645500	-2.07005900	2.28477000
N	3.94826200	-0.14615200	0.24415400
H	4.19791300	-0.11106700	1.22323800
C	4.59477800	0.73340200	-0.53973000
O	4.35740200	0.87572100	-1.75332600
C	5.64787500	1.57897200	0.12035700
C	6.39859700	1.12345000	1.21072700
C	5.89833700	2.85523800	-0.39587800
C	7.37794400	1.93570500	1.77830900
H	6.24387600	0.12636000	1.60705700
C	6.86621900	3.67165200	0.18171600
H	5.32318300	3.20575900	-1.24428100
C	7.60969700	3.21302800	1.26964400
H	7.96226900	1.56810800	2.61420200
H	7.04174500	4.66453000	-0.21685500
H	8.36834500	3.84621500	1.71588900
I	-1.91605600	-0.49224600	-1.10064700
C	-2.64018300	-1.06477100	0.83452500
C	-2.28787100	-0.27334600	1.91666000
C	-3.41017400	-2.21342900	0.92893100
C	-2.74381700	-0.66788900	3.17378900
H	-1.67901100	0.61074600	1.79380500
C	-3.84631000	-2.59039800	2.19890300
H	-3.65697600	-2.80069700	0.05514200
C	-3.51472400	-1.82125100	3.31356500
H	-2.48526200	-0.07216400	4.04125400
H	-4.44526000	-3.48675900	2.30842400
H	-3.85833300	-2.12273700	4.29618000

O	-3.94479600	1.05132400	-0.96197600
C	-3.81568600	2.14052000	-0.33397900
O	-2.81530400	2.66601800	0.15059000
C	-5.18099700	2.88398100	-0.16770500
F	-5.06096300	4.05550900	0.48109000
F	-5.74715700	3.14682900	-1.36814300
F	-6.06059200	2.12818000	0.53069200

TS-S4

B	2.53360800	1.17613000	-0.77738800
B	2.75720300	-0.30760400	-1.79854400
B	2.53430300	-1.72671300	-0.74855600
B	2.17380700	0.64643200	0.88010200
B	2.15913200	-1.13859300	0.89254400
B	1.24137600	0.62205800	-1.86567600
B	0.87162400	1.20283700	-0.17034300
H	3.11303000	2.18200100	-1.01913700
B	1.23842400	-1.21393800	-1.82716700
H	3.48790100	-0.30965300	-2.73227600
B	0.86122500	-1.72372500	-0.16589100
H	3.14380200	-2.73162900	-0.92128700
B	0.63566800	-0.22881100	0.86220600
H	2.53720800	1.26688600	1.82574900
H	0.89364600	1.22697600	-2.82265600
B	0.13781600	-0.27094100	-0.80712400
H	0.24540400	2.19592300	-0.01448500
H	0.84716000	-1.81504500	-2.77097100
H	0.22308500	-2.69786200	0.05619900
H	-0.15119500	-0.23220800	1.74694800
H	-0.68197100	0.13117300	-1.71437800
B	3.33841500	-0.26666600	-0.11579300
H	2.49892200	-1.74773500	1.85540700
N	4.78735900	-0.32373400	0.28756600
H	4.98612800	-0.82184900	1.14439700
C	5.85521000	0.21356600	-0.32365100
O	5.77505600	0.91643600	-1.34849100
C	7.20032700	-0.05998200	0.29088900
C	7.46668600	-1.21317100	1.03903300
C	8.22720300	0.86695300	0.07927300
C	8.73611500	-1.42894800	1.57090700
H	6.69845100	-1.96276800	1.19126500
C	9.49118300	0.65727900	0.62244900
H	8.02496100	1.75526000	-0.50651600
C	9.74929600	-0.49257200	1.36904400

H	8.93422100	-2.33138500	2.13806500
H	10.27503400	1.38896600	0.46213500
H	10.73560500	-0.66022200	1.78700000
I	-2.36204600	-0.54324000	-0.95770100
C	-2.68439300	1.39053900	-0.08323300
C	-2.89760100	2.46520600	-0.93301900
C	-2.65734100	1.48754700	1.29929400
C	-3.08878300	3.71720800	-0.34948100
H	-2.90920600	2.34118300	-2.00713200
C	-2.85723800	2.74957500	1.85730900
H	-2.48096500	0.62233100	1.92134300
C	-3.06878000	3.85728600	1.03752200
H	-3.25282300	4.57840900	-0.98634400
H	-2.84028200	2.85966000	2.93516100
H	-3.21828000	4.83449200	1.48160100
O	-4.87592000	-0.73891600	-0.53057700
C	-5.24427700	-1.05865500	0.63491000
O	-4.58004400	-1.38022000	1.61903500
C	-6.79860400	-0.99803400	0.79476500
F	-7.24662100	0.26978300	0.63299500
F	-7.42316800	-1.76146500	-0.13062000
F	-7.21606100	-1.41593700	2.00289500

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B	3.98559600	-3.08959500	0.33900500
B	2.87185900	-3.18571800	1.73141800
B	1.52088800	-2.08479600	1.43743900
B	3.32086400	-1.93294100	-0.83636000
B	1.80576400	-1.35133500	-0.14676000
B	2.83921800	-4.44761100	0.47739200
B	3.13163500	-3.68226800	-1.09637200
H	5.15877600	-3.23161700	0.47174600
B	1.32014900	-3.82730700	1.15388400
H	3.26394900	-3.39553300	2.83446600
B	0.63979000	-2.68122400	-0.00167000
H	0.93121800	-1.50858800	2.28779800
B	1.78149400	-2.59000800	-1.43777200
H	3.99711900	-1.23718800	-1.52156300
H	3.19876500	-5.56031100	0.69741000
B	1.47044400	-4.12489200	-0.61059400
H	3.69063000	-4.24174700	-1.98441500
H	0.59466600	-4.48160300	1.83229500
H	1.37085600	-2.35308700	-2.52178000
H	0.84253100	-4.97835700	-1.14988900

B	3.17254200	-1.63091400	0.93344400
I	1.72059900	1.16361400	-0.24002900
C	-0.24034300	1.46950300	0.58898400
C	-0.47406300	1.08163500	1.89892800
C	-1.20477300	2.05789200	-0.21635000
C	-1.75295800	1.28507900	2.41972100
H	0.30522400	0.63541600	2.49912500
C	-2.47123400	2.26158500	0.32820500
H	-0.98842600	2.33764500	-1.23789400
C	-2.74594200	1.87176300	1.63827300
H	-1.96318200	0.98144400	3.43861200
H	-3.24366200	2.71269300	-0.28293900
H	-3.73768400	2.02187000	2.04802700
O	1.73066900	3.62146400	0.10749800
C	2.83338600	4.16261600	-0.27362200
O	3.78569900	3.53392200	-0.77576500
C	2.93868400	5.65904100	-0.04422800
H	3.25583300	5.82499300	0.99050600
H	3.68300000	6.09684400	-0.70995800
H	1.97284000	6.14663100	-0.18322100
H	0.86411400	-0.68762900	-0.83643100

4-CN-Ph-*meta*-ts

B	0.55627700	0.43397000	0.44663100
B	1.17118000	2.04870300	0.92320300
B	1.70392600	2.88861500	-0.55107100
B	0.70892900	0.32786400	-1.38584200
B	1.41318600	1.84233400	-1.95519300
B	-0.57365600	1.82668900	0.81908300
B	-0.83943100	0.78039500	-0.60798900
H	0.65344500	-0.51455500	1.14640800
B	0.15264600	3.30868600	0.19018300
H	1.70950900	2.17929900	1.97087300
B	0.27416800	3.15791400	-1.58172300
H	2.64157200	3.61821600	-0.52309500
B	-0.33478000	1.56750600	-2.08778000
H	0.86346100	-0.73665300	-1.88226700
H	-1.28395200	1.75488800	1.76363400
B	-1.13450100	2.49966300	-0.72296200
H	-0.99581600	-0.33440700	-0.06191600
H	-0.02952400	4.35444000	0.72363900
H	0.16370600	4.10114000	-2.29617900
H	-0.91294400	1.38923300	-3.10748100
H	-2.23435100	2.91993800	-0.85371700

B	1.95670500	1.12714700	-0.41974900
H	2.12930000	1.85719300	-2.90348100
N	3.34360000	0.55465400	-0.35928300
H	3.86479500	0.56893300	-1.22610300
C	3.98795000	0.01489500	0.68719500
O	3.47457300	-0.15890700	1.80486100
C	5.41713000	-0.39878600	0.45468400
C	6.25793900	0.29632100	-0.42174000
C	5.91672500	-1.49071500	1.17211700
C	7.57961900	-0.09483800	-0.58680100
H	5.89608800	1.16219400	-0.96290800
C	7.23013600	-1.90270400	1.00497100
H	5.26698000	-2.01985100	1.85743500
C	8.06529600	-1.20061000	0.12377600
H	8.23518600	0.44917100	-1.25499400
H	7.61432600	-2.75610400	1.54927100
I	-2.91967200	-0.50750500	-0.96934300
C	-3.66685000	0.08108000	0.94904400
C	-4.38745700	1.26271500	1.03377000
C	-3.39007300	-0.73092300	2.03831800
C	-4.85076800	1.64884900	2.29118500
H	-4.57677700	1.86938800	0.15921800
C	-3.85945800	-0.32163300	3.28639100
H	-2.82414200	-1.64550800	1.92738400
C	-4.58539600	0.86201100	3.41125300
H	-5.41471900	2.56910200	2.38846700
H	-3.65358300	-0.93358300	4.15678200
H	-4.94538000	1.17264700	4.38518300
O	-5.31580600	-1.18299200	-1.32324300
C	-5.70638300	-2.27000200	-0.75784900
O	-4.96432400	-3.05283600	-0.13271800
C	-7.19573400	-2.55296700	-0.85684000
H	-7.39482200	-3.61781600	-0.73108600
H	-7.69950100	-2.00813600	-0.05148400
H	-7.60201500	-2.20201900	-1.80648300
C	9.42114800	-1.61176500	-0.04671200
N	10.51926600	-1.94529700	-0.18552300

4-CN-Ph-para-ts

B	1.23708800	1.15901100	-0.89327600
B	1.45986900	-0.36202100	-1.87109700
B	1.39346400	-1.73935000	-0.75042700
B	1.03496300	0.68579700	0.80456200
B	1.10160800	-1.09578200	0.88723100

B	-0.10414200	0.49460000	-1.86129900
B	-0.36686400	1.13530300	-0.15870000
H	1.74308600	2.17712200	-1.22859000
B	0.00034500	-1.34402100	-1.74620200
H	2.11639500	-0.36092800	-2.85837500
B	-0.23386700	-1.78944300	-0.05258800
H	2.04209900	-2.71904700	-0.92349200
B	-0.45921500	-0.25336700	0.93452000
H	1.43842200	1.36040600	1.69484500
H	-0.52919800	1.04780000	-2.81858500
B	-1.10620400	-0.40675300	-0.68598700
H	-1.03063300	2.10341400	-0.00385100
H	-0.43240600	-1.99629000	-2.63612000
H	-0.80300900	-2.78034000	0.26302100
H	-1.17283200	-0.26024200	1.87967700
H	-1.84020000	-0.00739500	-1.61554600
B	2.16108800	-0.21499500	-0.24316900
H	1.53440300	-1.64862100	1.84657600
N	3.63937500	-0.19069100	0.04286400
H	3.93280200	-0.66526300	0.88689000
C	4.62086000	0.38960000	-0.66220400
O	4.43344900	1.06907600	-1.68647100
C	6.02494600	0.19220400	-0.15364900
C	6.43407100	-0.99999900	0.45397800
C	6.94832100	1.22716100	-0.33587400
C	7.74484000	-1.15728600	0.88344500
H	5.73966900	-1.82260200	0.57475400
C	8.25640500	1.09059200	0.10334500
H	6.63259600	2.14408300	-0.81701200
C	8.65665200	-0.10697700	0.71394500
H	8.06544400	-2.08360600	1.34306100
H	8.96797100	1.89673100	-0.02325300
I	-3.52988100	-0.85580600	-0.59731300
C	-3.90015000	1.14885100	0.06619000
C	-4.12553200	2.12451200	-0.89269600
C	-3.87549700	1.40122800	1.42946000
C	-4.33245600	3.43124600	-0.45062300
H	-4.13230000	1.88559000	-1.94747100
C	-4.08999100	2.71434200	1.84742800
H	-3.69079600	0.61174900	2.14359900
C	-4.31424500	3.72386500	0.91235000
H	-4.50556300	4.21568000	-1.17802900
H	-4.07381200	2.94169000	2.90691200
H	-4.47381700	4.74232800	1.24680800

O	-5.97831300	-1.06863700	-0.14469100
C	-6.33881900	-1.33919800	1.06043800
O	-5.55759400	-1.60035900	1.99490600
C	-7.83595100	-1.28428300	1.31238800
H	-8.10009500	-1.86800200	2.19473900
H	-8.11226600	-0.23963200	1.48999300
H	-8.39479300	-1.63686300	0.44437000
C	10.00309500	-0.25903400	1.16125600
N	11.09380500	-0.38167200	1.52425400

4-OMe-Ph-ortho-ts

B	-2.77103700	3.95608800	-0.19923000
B	-1.82260700	3.80005200	1.30251700
B	-0.85690400	2.31811700	1.19373400
B	-2.38467300	2.58555100	-1.26243400
B	-1.20033900	1.61605500	-0.39461500
B	-1.28277200	4.90908200	0.02018200
B	-1.64276800	4.17102800	-1.55585000
H	-3.85325900	4.45044500	-0.20340200
B	-0.10317500	3.89481700	0.87489600
H	-2.23252700	4.19310700	2.34815400
B	0.29989500	2.53062300	-0.17446500
H	-0.55061700	1.64034000	2.11729000
B	-0.67213200	2.69467100	-1.70549500
H	-3.18062500	2.08564400	-1.98894800
H	-1.29860000	6.08970800	0.17141400
B	0.01180500	4.12104700	-0.90466200
H	-1.92031900	4.82261500	-2.51161800
H	0.72701900	4.33408900	1.60551100
H	-0.24391700	2.26133900	-2.72373800
H	0.92213600	4.71234000	-1.39161900
B	-2.50252500	2.35961200	0.52718200
I	-2.02133100	-0.80930500	-0.59166700
C	-1.38353600	-1.16674100	1.42105900
C	-2.28399800	-0.90848000	2.44371300
C	-0.08599200	-1.60724800	1.63491200
C	-1.85034000	-1.10345400	3.75460900
H	-3.28574800	-0.55980300	2.23547400
C	0.32803500	-1.78740200	2.95465000
H	0.58739300	-1.79037400	0.80996800
C	-0.54927300	-1.53555700	4.00846200
H	-2.53281700	-0.90732400	4.57325900
H	1.33932600	-2.12431900	3.15075000
H	-0.21798100	-1.67561100	5.03088100

O	-3.09211500	-2.95255200	-0.20305700
C	-3.66327600	-3.41875800	-1.26141300
O	-3.69193100	-2.82648100	-2.35506700
C	-4.29136800	-4.78931000	-1.10452800
H	-3.50748800	-5.54177700	-1.23855300
H	-4.71407900	-4.91568100	-0.10707900
H	-5.05767600	-4.94558300	-1.86411500
H	-0.45227000	0.53881700	-0.69308800
H	-3.37887100	1.71633100	1.00097400
N	1.66693800	1.92694600	-0.13978600
C	1.98174100	0.68612900	-0.52365300
H	2.42480700	2.50349300	0.19737400
C	3.38324200	0.21371600	-0.37635100
O	1.10996100	-0.08206100	-1.00332600
C	3.78502600	-0.92116800	-1.08586400
C	4.31941700	0.85047500	0.45458200
C	5.08451400	-1.40902600	-0.99802600
H	3.07162300	-1.42509200	-1.72569000
C	5.61315500	0.37041000	0.55976600
H	4.04488300	1.71587800	1.04662100
C	6.00682300	-0.75822300	-0.17249800
H	5.36498800	-2.28251600	-1.56970300
H	6.33452900	0.85494300	1.20703200
O	7.30006300	-1.14752500	-0.01566500
C	7.76937500	-2.27967500	-0.76204600
H	8.81751300	-2.39361100	-0.49128300
H	7.21809600	-3.18312600	-0.48846800
H	7.68350600	-2.09861400	-1.83664000

4-OMe-Ph-meta-ts

B	0.23498500	-1.15333100	-1.32679300
B	1.07736500	-2.71474300	-1.53060000
B	1.24025100	-3.46416200	0.06699900
B	-0.09385600	-0.94324600	0.46268800
B	0.55677800	-2.37201300	1.29000100
B	-0.64013100	-2.57816900	-1.89684600
B	-1.33002400	-1.51019900	-0.62645700
H	0.39490500	-0.20364300	-2.01486100
B	-0.05274600	-3.99460800	-1.02595100
H	1.87583100	-2.88438100	-2.39040200
B	-0.36915500	-3.78259100	0.74389600
H	2.16641500	-4.16485600	0.32181800
B	-1.17685900	-2.23623300	0.99846400
H	-0.12252500	0.14341000	0.93260500

H	-1.12813500	-2.62252500	-2.97592600
B	-1.58266700	-3.26485600	-0.46322500
H	-2.52263400	-1.75528700	-0.91385100
H	-0.07267300	-5.07109900	-1.52839900
H	-0.60414000	-4.71604600	1.44033100
H	-1.99942300	-2.05395000	1.83003300
H	-2.62669100	-3.81016600	-0.58893500
B	1.42075500	-1.69001100	-0.11362100
H	1.02062000	-2.28567800	2.38100300
N	2.73162000	-1.00830200	0.14911600
H	3.00865300	-0.94035600	1.11856300
C	3.58148200	-0.45006200	-0.73424200
O	3.33904600	-0.37764700	-1.95401300
C	4.86244200	0.10619300	-0.19320600
C	5.45111600	-0.34541900	0.99820400
C	5.51869800	1.10213900	-0.92038800
C	6.65041900	0.18608600	1.44424600
H	4.99290900	-1.13924000	1.57667600
C	6.71711300	1.65579100	-0.47938200
H	5.07983800	1.45655000	-1.84495000
C	7.28847800	1.19396200	0.71008400
H	7.11293100	-0.17336800	2.35598000
H	7.19057200	2.43391000	-1.06187500
I	-2.92476900	0.33598000	-1.08606100
C	-3.71718900	0.15595000	0.89650700
C	-3.10963100	0.87952700	1.91132100
C	-4.78784800	-0.70193300	1.09762200
C	-3.61210600	0.72728100	3.20319100
H	-2.27152900	1.53145000	1.71160400
C	-5.26937800	-0.84179600	2.39928600
H	-5.22976800	-1.25172300	0.27783700
C	-4.68388800	-0.13073900	3.44592200
H	-3.15494100	1.27756600	4.01720800
H	-6.10190100	-1.50949500	2.58772000
H	-5.06290400	-0.24706400	4.45460100
O	-4.45736400	2.32034200	-1.14229300
C	-4.03232400	3.41917000	-0.62498300
O	-2.87776300	3.60283200	-0.19473100
C	-5.06808200	4.52597500	-0.52079200
H	-5.66560800	4.34779600	0.37944700
H	-4.58489300	5.49927700	-0.43025100
H	-5.74217300	4.51686900	-1.37855200
O	8.45985800	1.65870400	1.22747900
C	9.16586700	2.67829600	0.50748700

H	8.56205700	3.58572000	0.42282000
H	10.05888200	2.88633500	1.09435200
H	9.45302100	2.32561400	-0.48675700

4-OMe-Ph-para-ts

B	1.08422600	1.17546600	-0.82239300
B	1.31764500	-0.31536100	-1.84328800
B	1.24793400	-1.72449000	-0.76408500
B	0.87219900	0.65249900	0.85848300
B	0.94460200	-1.13026800	0.88919700
B	-0.24892400	0.53609500	-1.81672100
B	-0.52558900	1.12491300	-0.10012700
H	1.58762200	2.20513500	-1.12554000
B	-0.14018000	-1.30470200	-1.75596400
H	1.97696400	-0.28370100	-2.82820600
B	-0.38360500	-1.80010300	-0.07794100
H	1.90094000	-2.69681700	-0.96176900
B	-0.61875000	-0.29413700	0.95320500
H	1.26685800	1.30207900	1.77131200
H	-0.67136000	1.11518600	-2.75987600
B	-1.25638900	-0.40238700	-0.67498000
H	-1.19332000	2.08616200	0.07910900
H	-0.56598000	-1.93126600	-2.66760800
H	-0.95116500	-2.80145900	0.20658900
H	-1.33827000	-0.33055300	1.89320800
H	-1.98976800	0.00686900	-1.60042600
B	2.01191400	-0.21351000	-0.20676900
H	1.37220700	-1.71013100	1.83502000
N	3.48537500	-0.19889500	0.09171500
H	3.76863000	-0.69865200	0.92331800
C	4.48445800	0.37247500	-0.60365200
O	4.28968600	1.08592300	-1.60756700
C	5.88027200	0.12169400	-0.12104500
C	6.23276300	-0.99887500	0.64756000
C	6.88556600	1.02521600	-0.47259800
C	7.54213800	-1.20032200	1.05266200
H	5.49187500	-1.74283600	0.91638400
C	8.20372700	0.84401200	-0.06356400
H	6.63157000	1.89166600	-1.07070200
C	8.53576500	-0.27696700	0.70330500
H	7.81581100	-2.07272100	1.63449000
H	8.95274200	1.57129100	-0.34471000
I	-3.68231200	-0.85111600	-0.60852100
C	-4.05503500	1.15185400	0.05916000

C	-4.28369100	2.12848500	-0.89788400
C	-4.02803100	1.40200100	1.42274700
C	-4.49234100	3.43412700	-0.45337400
H	-4.29192800	1.89134700	-1.95307700
C	-4.24410700	2.71405900	1.84313300
H	-3.83866400	0.61191000	2.13503000
C	-4.47205600	3.72461800	0.91004800
H	-4.66820500	4.21940200	-1.17924200
H	-4.22592300	2.93992900	2.90290700
H	-4.63270800	4.74229400	1.24637500
O	-6.13479200	-1.05618300	-0.18187700
C	-6.51720400	-1.31342600	1.01952200
O	-5.75415000	-1.57595000	1.96822600
C	-8.01756600	-1.24006800	1.24647400
H	-8.30134900	-1.80526000	2.13475000
H	-8.28704500	-0.18986400	1.40009400
H	-8.56552600	-1.60355100	0.37594700
O	9.79233500	-0.55620500	1.14951400
C	10.85397000	0.34607500	0.81027800
H	10.66651100	1.34135300	1.22194500
H	11.75081000	-0.07437300	1.26198700
H	10.98177400	0.40748400	-0.27380200

4-*t*Bu-Ph-ortho-ts

B	4.58524200	-2.99717700	0.33060100
B	3.46685500	-3.12313700	1.71609000
B	2.09020000	-2.05715700	1.41527000
B	3.89784000	-1.85520400	-0.84687500
B	2.36470800	-1.31726000	-0.16469500
B	3.47292200	-4.38369000	0.46060200
B	3.75411600	-3.60882700	-1.11046600
H	5.76103800	-3.10991500	0.47025200
B	1.93394300	-3.80250600	1.12808100
H	3.85755100	-3.32502900	2.82137900
B	1.23016300	-2.67175800	-0.03091700
H	1.48125500	-1.49966500	2.26387700
B	2.37804300	-2.55127600	-1.45688300
H	4.56083300	-1.14239900	-1.52782500
H	3.86075200	-5.48684900	0.68189100
B	2.10267700	-4.09498100	-0.63436000
H	4.33322600	-4.15252200	-1.99575700
H	1.22255600	-4.47607300	1.80304600
H	1.96992000	-2.32395900	-2.54402000
H	1.50102600	-4.96475300	-1.17804700

B	3.73193100	-1.55958300	0.92165900
I	2.18057400	1.21455900	-0.24362200
C	0.24676700	1.42046000	0.67324100
C	0.09482600	1.03092300	1.99484500
C	-0.78250400	1.95310400	-0.08951800
C	-1.16981100	1.16614800	2.57012900
H	0.92352200	0.63490200	2.56278100
C	-2.03295400	2.09117800	0.50977900
H	-0.62653600	2.23656900	-1.12091600
C	-2.22792100	1.69114400	1.83072900
H	-1.31833400	0.85833300	3.59862400
H	-2.85546400	2.49419200	-0.06826700
H	-3.20828300	1.78525800	2.28245400
O	2.09720700	3.65493300	0.13784200
C	3.15130900	4.24848800	-0.30057500
O	4.11174500	3.66242000	-0.83641500
C	3.15564200	5.75906100	-0.15941100
H	4.17786300	6.13847300	-0.15195400
H	2.63325700	6.18430500	-1.02261800
H	2.62859900	6.07180500	0.74279300
H	1.41835900	-0.65015600	-0.84482300
H	4.27992200	-0.64660900	1.44325800
N	-0.24614500	-2.46267600	-0.15352400
C	-0.80961700	-1.46651700	-0.84722800
H	-0.86217600	-3.02117000	0.42172000
C	-2.26348400	-1.19814200	-0.68840500
O	-0.12218100	-0.72786300	-1.59476900
C	-2.93489900	-0.49326800	-1.68845300
C	-2.95781900	-1.52800800	0.48092700
C	-4.26832500	-0.13055700	-1.52858100
H	-2.40578600	-0.21834600	-2.59260700
C	-4.28367600	-1.14902700	0.63977300
H	-2.45907700	-2.03896500	1.29614000
C	-4.96928800	-0.43771000	-0.35670200
H	-4.75216100	0.41317500	-2.32837700
H	-4.78406400	-1.39497700	1.56827900
C	-6.41977300	-0.00529600	-0.12080600
C	-6.46589500	0.93577500	1.10177200
H	-5.85549000	1.82685900	0.92878200
H	-7.49515500	1.25808100	1.28688600
H	-6.09963100	0.44218000	2.00503100
C	-7.00986600	0.73859700	-1.32761800
H	-7.01420100	0.11542100	-2.22630200
H	-8.04467900	1.01679800	-1.11038200

H	-6.45888400	1.65671800	-1.54968700
C	-7.28824200	-1.24943100	0.15675800
H	-7.26466800	-1.93822900	-0.69294300
H	-6.94921300	-1.79097200	1.04294300
H	-8.32744200	-0.95004300	0.32331300

4-*t*Bu-Ph-*meta*-ts

B	0.41740500	1.31894400	-1.32167700
B	-0.38514300	2.90926100	-1.44962100
B	-0.65430000	3.52207600	0.19228800
B	0.61561800	0.95005700	0.45921200
B	-0.07432100	2.31506300	1.36123000
B	1.35188900	2.77140000	-1.70177900
B	1.93381700	1.58554600	-0.48448000
H	0.29328100	0.43563300	-2.09964200
B	0.71992600	4.11934900	-0.75575500
H	-1.11856700	3.16540700	-2.34553200
B	0.90535500	3.74983900	1.00653500
H	-1.58919000	4.21296100	0.44163200
B	1.67263300	2.17063200	1.18268900
H	0.59240300	-0.17280100	0.83431500
H	1.91739200	2.89769600	-2.73579200
B	2.19461000	3.31365100	-0.15184100
H	3.15173800	1.82738800	-0.64755000
H	0.78950500	5.23451300	-1.15994500
H	1.10123600	4.61558400	1.79632300
H	2.43125200	1.90159300	2.05128200
H	3.25242300	3.84722300	-0.15653800
B	-0.84296600	1.77518400	-0.15420100
H	-0.61840100	2.14503000	2.40425800
N	-2.18227400	1.10880900	-0.03204700
H	-2.53214100	0.99336000	0.90913600
C	-3.00094600	0.66004500	-1.00090700
O	-2.69249800	0.65295000	-2.20733000
C	-4.34036500	0.14537000	-0.56312500
C	-4.99021200	0.61386400	0.58611600
C	-4.98295900	-0.81985300	-1.33990900
C	-6.23900600	0.12090400	0.94209400
H	-4.53978700	1.38766000	1.19797700
C	-6.22878600	-1.32126200	-0.96916500
H	-4.49885400	-1.18926200	-2.23609200
C	-6.88592800	-0.86272900	0.17812600
H	-6.71755800	0.51616900	1.82993700
H	-6.68365800	-2.07953900	-1.59189300

I	3.55560800	-0.22203300	-1.03071600
C	4.12067100	-0.34589200	1.03121900
C	3.38170700	-1.17608900	1.86047800
C	5.18919000	0.42332200	1.46669800
C	3.74112100	-1.22978500	3.20684900
H	2.55320900	-1.75605700	1.48062100
C	5.52735900	0.35562000	2.81810500
H	5.73629100	1.06118000	0.78590400
C	4.80621200	-0.46641400	3.68299300
H	3.17982000	-1.86773700	3.87946700
H	6.35485600	0.94970200	3.18797300
H	5.07453700	-0.51144900	4.73207300
O	5.07976400	-2.19195700	-1.20127700
C	4.60658600	-3.34952100	-0.89810000
O	3.41018300	-3.58451000	-0.64352700
C	5.63328800	-4.46675900	-0.82253500
H	5.15665200	-5.43736600	-0.96376500
H	6.42741500	-4.32478500	-1.55676800
H	6.08599100	-4.44353600	0.17437000
C	-8.26071900	-1.38177900	0.61378200
C	-9.26042000	-0.20649200	0.63591600
H	-10.24995800	-0.56128200	0.93998000
H	-8.95253200	0.57246800	1.33739100
H	-9.35091800	0.24609600	-0.35601000
C	-8.80402900	-2.46295900	-0.33153800
H	-8.14690400	-3.33626000	-0.37009200
H	-9.78163400	-2.79780800	0.02582800
H	-8.93368600	-2.08551400	-1.34959400
C	-8.15018400	-1.98506000	2.02963900
H	-7.44294200	-2.81972000	2.04259200
H	-7.81459400	-1.24481200	2.75970600
H	-9.12568600	-2.35972700	2.35438600

4-*t*Bu-Ph-*para*-ts

B	0.45061300	1.35269900	-0.81117300
B	0.71016800	-0.07348600	-1.91400200
B	0.71241400	-1.53881600	-0.90953800
B	0.29257300	0.73618700	0.84360400
B	0.42575200	-1.04238500	0.77879500
B	-0.88224800	0.71958500	-1.81212400
B	-1.14096800	1.20813100	-0.06168700
H	0.90822800	2.41501800	-1.06826400
B	-0.70944100	-1.11721000	-1.85140800
H	1.35180300	0.03387600	-2.90589800

B	-0.89971900	-1.70708700	-0.19682300
H	1.39459700	-2.47525100	-1.17144100
B	-1.16359200	-0.26662800	0.91645200
H	0.68292500	1.35077500	1.78213600
H	-1.34489600	1.33236700	-2.71412900
B	-1.83146000	-0.31153800	-0.70163300
H	-1.83771600	2.13461900	0.18088500
H	-1.13282800	-1.71045300	-2.78613500
H	-1.42644200	-2.74151800	0.04473500
H	-1.86098600	-0.37856300	1.86735500
H	-2.59918400	0.11222000	-1.59158400
B	1.43678000	-0.03370700	-0.28945400
H	0.89326600	-1.65603600	1.68345500
N	2.91939400	0.00031600	-0.03696900
H	3.25122000	-0.59593400	0.70937500
C	3.87529300	0.67803400	-0.69490500
O	3.63183600	1.50489700	-1.59487900
C	5.29599100	0.39981300	-0.30192200
C	5.71750100	-0.85140300	0.16434700
C	6.24926300	1.40915400	-0.44498100
C	7.05280300	-1.07592100	0.47572900
H	5.01133900	-1.66872200	0.25938700
C	7.58318400	1.18341700	-0.11285700
H	5.94263700	2.38189000	-0.81098600
C	8.01698500	-0.06408000	0.35054800
H	7.34569500	-2.06223100	0.81481800
H	8.28549000	1.99829300	-0.22577300
I	-4.23651200	-0.85481200	-0.61667500
C	-4.68463000	1.09368100	0.15951200
C	-4.96341400	2.11385200	-0.73738400
C	-4.66124600	1.26373800	1.53541300
C	-5.22939500	3.37956500	-0.21473200
H	-4.96794600	1.93897800	-1.80463900
C	-4.93573600	2.53680800	2.03425700
H	-4.43152700	0.44229800	2.19883700
C	-5.21589800	3.58896400	1.16362000
H	-5.44591300	4.19762800	-0.89171000
H	-4.92248300	2.69984600	3.10557100
H	-5.42276600	4.57602100	1.56052000
O	-6.67287700	-1.19585100	-0.20217800
C	-7.04698400	-1.53872700	0.98005000
O	-6.27575100	-1.80240200	1.92183800
C	-8.55048500	-1.57150700	1.19536200
H	-8.80461200	-2.21323500	2.03960300

H	-8.88371000	-0.55276400	1.41959300
H	-9.07041000	-1.90548100	0.29638300
C	9.47985800	-0.35885800	0.69988500
C	9.56973600	-0.85398000	2.15818300
H	8.99309800	-1.76903000	2.31192700
H	10.61155300	-1.06606500	2.41692900
H	9.19400500	-0.09526500	2.85114200
C	10.37532300	0.87996300	0.55327400
H	11.40200000	0.61831100	0.82353800
H	10.38703600	1.25439100	-0.47390900
H	10.05422100	1.69269800	1.21088400
C	10.00937900	-1.45769900	-0.24567100
H	9.94827300	-1.13484800	-1.28919900
H	11.05701900	-1.67651000	-0.01713600
H	9.44119400	-2.38528900	-0.14337700

Me-ortho-ts

B	-2.78004600	-1.03136300	-1.22214900
B	-1.37777000	-0.62536300	-0.20769100
B	-1.88284000	-0.06996600	1.39430000
B	-4.20602400	-0.73104500	-0.21192200
B	-3.65828000	-0.14232100	1.39604200
B	-1.82283500	-2.30959200	-0.45342400
B	-3.59538900	-2.38783000	-0.42318700
H	-2.76872400	-0.83615500	-2.39258800
B	-1.27313900	-1.72218000	1.16623900
H	-0.81464800	0.32811500	-0.95818300
B	-2.71313600	-1.43749900	2.15706600
H	-1.27804400	0.76645000	1.97872000
B	-4.14252500	-1.83694100	1.17525600
H	-5.22203100	-0.34451400	-0.69549300
H	-1.14143600	-3.04177400	-1.09464600
B	-2.66284500	-2.81661600	1.02831800
H	-4.19446500	-3.20146500	-1.05147500
H	-0.22983500	-2.06410800	1.61320500
H	-2.69386800	-1.59123400	3.33669100
H	-5.13972600	-2.25828200	1.67045500
H	-2.59637800	-3.93851200	1.41873600
B	-2.83052600	0.38066600	-0.07523500
H	-4.30146600	0.64450000	2.01520600
N	-2.92993100	1.79838200	-0.54451200
H	-3.71138900	2.35511100	-0.22484000
C	-2.06977900	2.41946900	-1.35402600
O	-1.05495600	1.83720000	-1.80591400

I	1.08247900	-0.48597400	-0.93230200
C	1.45998700	0.86622400	0.68862200
C	1.81294800	0.32448800	1.91566600
C	1.31314500	2.22669400	0.46271500
C	2.02900000	1.20624000	2.97411100
H	1.91087900	-0.74298100	2.05038300
C	1.52762100	3.08797600	1.53872600
H	1.02993100	2.60694700	-0.50833100
C	1.88307800	2.58013200	2.78748300
H	2.30362600	0.81046600	3.94487000
H	1.41495100	4.15590100	1.39217800
H	2.04605600	3.25720600	3.61793200
O	3.47997900	-0.42056600	-1.17821600
C	4.18903700	-1.23991100	-0.46988100
O	3.72428000	-2.10453500	0.28786100
C	5.68731900	-1.04345800	-0.60135300
H	5.97838200	-0.20564100	0.04048600
H	6.21973000	-1.93690800	-0.27472900
H	5.96148400	-0.79235600	-1.62689700
C	-2.32964600	3.85620400	-1.71425700
H	-2.34907000	3.95291200	-2.80243400
H	-3.26720300	4.22696200	-1.29925100
H	-1.50253400	4.46640400	-1.34115400

Me-meta-ts

B	-3.18170500	-0.55289400	1.91733500
B	-2.34080500	-1.01099800	0.43912900
B	-2.19257200	0.49345000	-0.62416800
B	-3.58276600	1.17374100	1.80185900
B	-2.95563200	1.83313900	0.27362000
B	-1.41897100	-0.70262300	1.92265600
B	-2.18786300	0.64407200	2.78063800
H	-3.89082200	-1.32248900	2.47958200
B	-0.84876500	-0.02004000	0.41436600
H	-2.35673800	-2.07855200	-0.06939600
B	-1.20171100	1.73266300	0.31244600
H	-2.20276100	0.44209400	-1.80649800
B	-2.08297800	2.12303500	1.78905700
H	-4.59075700	1.59708700	2.27082100
H	-0.81822600	-1.56955400	2.46391900
B	-0.71800600	0.98607500	1.84136400
H	-2.17465600	0.69590700	3.96802500
H	-0.53632200	-0.22165900	-0.78596800
H	-0.48417000	2.46008300	-0.28617100

H	-2.01322100	3.20246400	2.28060000
H	0.33187400	1.21542700	2.33895700
B	-3.65981000	0.15443100	0.34834600
H	-3.52529500	2.67624600	-0.33948100
N	-5.00191800	-0.10014500	-0.27275000
H	-5.78165700	0.40230100	0.13076800
C	-5.32695100	-0.89663000	-1.30658800
O	-4.49282200	-1.57168900	-1.93881500
I	1.33225600	-1.02315400	-0.19110600
C	2.13846400	0.91139000	-0.64710700
C	2.72206800	1.63518300	0.38154300
C	2.03094400	1.37513500	-1.94974500
C	3.22510100	2.89983400	0.07656700
H	2.78132500	1.23822300	1.38457600
C	2.53711000	2.64447400	-2.22897900
H	1.56440400	0.77895500	-2.72215600
C	3.13087000	3.40221000	-1.22055900
H	3.68520000	3.48928700	0.86096400
H	2.46274200	3.03434800	-3.23739500
H	3.52061900	4.38802300	-1.44616200
O	3.71756700	-1.70394500	-0.57149400
C	4.53461900	-1.59972600	0.41601400
O	4.21301900	-1.27243200	1.57477200
C	5.99105500	-1.87177800	0.07918300
H	6.41507900	-0.96245800	-0.35953200
H	6.55576200	-2.11984700	0.97842700
H	6.08116000	-2.67267400	-0.65621100
C	-6.78727700	-0.94896500	-1.69542000
H	-7.42506800	-0.33534700	-1.05786000
H	-6.88847700	-0.61506400	-2.73159700
H	-7.12635000	-1.98712000	-1.64877200

Me-para-ts

B	2.97775900	1.03274400	-0.50406000
B	3.30230500	-0.57253700	-1.29941300
B	3.07249000	-1.83853000	-0.07386000
B	2.54574800	0.72247400	1.18606700
B	2.57737500	-1.04386900	1.44286200
B	1.76396800	0.28506400	-1.57477300
B	1.28912200	1.08062800	0.00820700
H	3.53800600	2.01414300	-0.86302200
B	1.82577600	-1.53754900	-1.27683800
H	4.07840400	-0.66692200	-2.19046700
B	1.36569300	-1.82043900	0.40353300

H	3.72260000	-2.83269000	-0.06877600
B	1.03642200	-0.19823400	1.20617700
H	2.83584100	1.47747600	2.05626200
H	1.47471900	0.74581500	-2.62697800
B	0.60224300	-0.50115500	-0.46284300
H	0.62673300	2.06174200	-0.01521000
H	1.50511400	-2.26933900	-2.15238200
H	0.74740900	-2.77699700	0.73329100
H	0.20505200	-0.11603700	2.04548600
H	0.00197200	-0.21934800	-1.51937600
B	3.79171700	-0.27486800	0.38709400
H	2.87095200	-1.50490500	2.49874800
N	5.21843100	-0.21540700	0.86217900
H	5.40052700	-0.60302200	1.77850600
C	6.29824600	0.28876600	0.24312000
O	6.25708400	0.80869200	-0.88890000
C	7.61434600	0.20533600	0.98356600
I	-1.83252900	-0.90580600	-0.61463000
C	-2.21696700	1.16278700	-0.20986800
C	-2.31896600	2.03594400	-1.28265900
C	-2.32699600	1.55617500	1.11508400
C	-2.53873900	3.38419800	-1.00089300
H	-2.22333200	1.68793800	-2.30215600
C	-2.55182600	2.90842500	1.37140700
H	-2.23459600	0.84358600	1.92213600
C	-2.65392600	3.81748700	0.31931200
H	-2.61804800	4.09053300	-1.81898900
H	-2.63964100	3.24504400	2.39779300
H	-2.82309500	4.86725400	0.52899300
O	-4.32175300	-1.02902200	-0.41684500
C	-4.80540000	-1.20010500	0.76325100
O	-4.12578000	-1.40533600	1.78673400
C	-6.31780400	-1.09756500	0.86069900
H	-6.68152100	-1.60536700	1.75450800
H	-6.58258000	-0.03724700	0.92971700
H	-6.79849600	-1.50709900	-0.02885800
H	8.01589800	1.21510700	1.10297900
H	7.52726000	-0.26351600	1.96452200
H	8.32454600	-0.36257900	0.37662300
<i>t</i>Bu-ortho-ts			
B	2.05645100	1.95521900	-1.31647800
B	0.74637700	1.35095500	-0.28091100
B	1.20132600	1.38720200	1.42500400

B	3.37105300	2.39979400	-0.21155900
B	2.84767200	2.05334000	1.47246600
B	0.65695300	2.97780500	-0.94406600
B	2.29702600	3.65456000	-0.87017800
H	2.24838800	1.50010200	-2.39549400
B	0.13021900	2.63498700	0.75138600
H	0.59394200	0.11950100	-0.77089800
B	1.45532200	3.09302600	1.83405800
H	0.82696300	0.55726700	2.18504000
B	2.79229300	3.71028700	0.83575300
H	4.50778000	2.27717000	-0.54075100
H	-0.13815700	3.26640600	-1.77852100
B	1.10734000	4.07019600	0.38423900
H	2.67878400	4.45090600	-1.66741000
H	-1.01359100	2.69943400	1.05612000
H	1.24623600	3.50220700	2.93163500
H	3.53621800	4.54741900	1.23918600
H	0.64239300	5.16214700	0.46787700
B	2.41383100	0.95341800	0.15844100
H	3.62750300	1.69878400	2.29848900
N	3.02471700	-0.40960600	0.07806100
H	3.90835600	-0.54980500	0.54627700
C	2.51719400	-1.46311400	-0.56347800
O	1.42342800	-1.38388700	-1.17021300
I	-1.43899100	0.18594600	-1.00866200
C	-1.54963000	-0.75060100	0.91602600
C	-2.21908700	-0.07925800	1.92816700
C	-0.92227100	-1.97497700	1.08741100
C	-2.25454500	-0.67950600	3.18639800
H	-2.69017300	0.87685200	1.75205800
C	-0.96476600	-2.55132700	2.35665900
H	-0.40625800	-2.45907000	0.27146200
C	-1.62660500	-1.90606500	3.40045200
H	-2.76753500	-0.17716400	3.99815100
H	-0.47663900	-3.50479900	2.52160900
H	-1.65223100	-2.35978700	4.38442900
O	-3.63670300	-0.76562200	-1.27583800
C	-4.65205300	-0.08697000	-0.84639900
O	-4.59041700	1.06135200	-0.38267300
C	-5.97244600	-0.83078400	-0.90958400
H	-6.03489600	-1.48417000	-0.03315500
H	-6.80716400	-0.13001100	-0.88348800
H	-6.02969100	-1.45682600	-1.80089900
C	3.26382800	-2.80407700	-0.53789900

C	4.66104100	-2.70452400	0.08819900
H	5.29531000	-1.99059700	-0.44528600
H	4.62122800	-2.42014100	1.14397400
H	5.14703500	-3.68192900	0.03513300
C	3.38859300	-3.30571900	-1.98768700
H	3.88819300	-4.27821700	-1.99674000
H	2.40777200	-3.41807000	-2.45273300
H	3.98027500	-2.61277300	-2.59331100
C	2.40146100	-3.78341700	0.28391300
H	1.41776200	-3.91918800	-0.16956900
H	2.89667700	-4.75739500	0.32820000
H	2.26495900	-3.42278000	1.30726000

***t*Bu-*meta*-ts**

B	-2.27227800	-0.03461100	2.35387500
B	-1.59616600	-0.71201900	0.87621400
B	-1.49212700	0.63895700	-0.37809900
B	-2.61274600	1.68347900	2.05816700
B	-2.10875000	2.11676400	0.40807800
B	-0.52495600	-0.27256200	2.21932100
B	-1.15238100	1.20662600	2.96633700
H	-2.95424100	-0.69205700	3.07094400
B	-0.07537800	0.18836300	0.59188700
H	-1.70011400	-1.83214600	0.51172500
B	-0.36464800	1.93217700	0.30069200
H	-1.61708900	0.44399700	-1.53843300
B	-1.08385900	2.54529900	1.78974400
H	-3.55257700	2.21426000	2.55854400
H	0.09063300	-1.09764600	2.80731200
B	0.23279600	1.35464600	1.86117200
H	-1.02268100	1.40313700	4.13129400
H	0.11529900	-0.16337400	-0.59784700
H	0.32093500	2.54190900	-0.44816100
H	-0.92518000	3.67216100	2.13151800
H	1.33469100	1.58820700	2.22745900
B	-2.87077900	0.49925900	0.75823500
H	-2.70014800	2.90687400	-0.25324700
N	-4.27567500	0.24583800	0.29776900
H	-4.98206800	0.83633700	0.71266400
C	-4.72703200	-0.63925500	-0.60658700
O	-3.97149600	-1.41693700	-1.21871800
I	1.98184500	-1.01604400	-0.05354600
C	2.82867400	0.76603200	-0.88329100
C	3.50746000	1.62690700	-0.03415300

C	2.65149800	1.00395800	-2.23821800
C	4.03719100	2.79351200	-0.58499600
H	3.61872200	1.40587800	1.01749800
C	3.18785800	2.17854300	-2.76551000
H	2.11214300	0.30711300	-2.86530700
C	3.87674100	3.06825100	-1.94240800
H	4.57108000	3.48604100	0.05519500
H	3.06257600	2.39149400	-3.82071300
H	4.28964300	3.97900300	-2.36027900
O	4.28484700	-1.92056100	-0.50392100
C	5.16756000	-1.73980500	0.41348700
O	4.95886400	-1.15990000	1.49679600
C	6.54006500	-2.31911200	0.11314700
H	6.51732900	-3.39126100	0.33394000
H	6.79216900	-2.19946900	-0.94173200
H	7.30128500	-1.85096200	0.73793500
C	-6.24357000	-0.68802500	-0.88880800
C	-6.72866700	-2.10716600	-0.53586600
H	-7.79676300	-2.19830100	-0.75303700
H	-6.19473800	-2.86221300	-1.11626800
H	-6.57825400	-2.32008500	0.52694700
C	-7.05920500	0.33659300	-0.08860900
H	-6.96692400	0.18163200	0.99055900
H	-6.76795300	1.36509700	-0.32261000
H	-8.11734300	0.23216900	-0.34231500
C	-6.44340600	-0.42807400	-2.39367100
H	-5.90461300	-1.16196300	-2.99616000
H	-7.50651500	-0.49330200	-2.64273100
H	-6.08971500	0.57010000	-2.66961400

***t*Bu-*para*-ts**

B	2.16088900	0.99096300	-0.70109200
B	2.42863600	-0.59939300	-1.54552000
B	2.26339600	-1.88903200	-0.33330300
B	1.82292400	0.64728900	1.00410700
B	1.86066600	-1.12434200	1.22400700
B	0.88239000	0.27070200	-1.71508000
B	0.50369100	1.03298100	-0.09430200
H	2.70265300	1.97808600	-1.07132500
B	0.95194300	-1.56088900	-1.45780000
H	3.15450100	-0.68115800	-2.47958100
B	0.58695200	-1.87534500	0.24121800
H	2.90856300	-2.88512400	-0.38614000
B	0.31253000	-0.26885900	1.09249000

H	2.16444700	1.38362100	1.87151900
H	0.53387700	0.75312100	-2.73924000
B	-0.21584900	-0.53457800	-0.55448100
H	-0.15325700	2.01727200	-0.05788900
H	0.57854100	-2.27442400	-2.32725800
H	-0.01625200	-2.83643300	0.58572900
H	-0.47056600	-0.19742100	1.97834100
H	-0.87237600	-0.26017200	-1.58125600
B	3.01636600	-0.33826400	0.11532900
H	2.21247300	-1.60772500	2.25175500
N	4.46680600	-0.30660600	0.51275500
H	4.68855400	-0.75790900	1.38841700
C	5.50925400	0.23369500	-0.13560000
O	5.38734500	0.81813700	-1.22932100
C	6.90799100	0.12815400	0.50894500
I	-2.65668900	-0.90582000	-0.58409500
C	-2.99331100	1.17248300	-0.19031400
C	-3.10060400	2.03766000	-1.26902000
C	-3.06529500	1.57991500	1.13279600
C	-3.28424100	3.39299300	-0.99548900
H	-3.03488700	1.67827200	-2.28694600
C	-3.25511400	2.93906100	1.38101300
H	-2.97136300	0.87223600	1.94416900
C	-3.36047300	3.84063400	0.32274700
H	-3.36596700	4.09339500	-1.81843400
H	-3.31267700	3.28689900	2.40577400
H	-3.50152000	4.89579400	0.52606200
O	-5.13896100	-0.99333300	-0.26654800
C	-5.58240200	-1.14304400	0.93181100
O	-4.87032600	-1.34606900	1.93374200
C	-7.08903700	-1.01765700	1.08054400
H	-7.42729000	-1.49633200	2.00000700
H	-7.33876100	0.04743500	1.12865900
H	-7.60566700	-1.44508200	0.21990300
C	7.39561600	1.56395000	0.78239200
H	8.40312800	1.53833300	1.20759500
H	7.42617600	2.15253600	-0.13687100
H	6.73825800	2.07185000	1.49476500
C	6.92931200	-0.66772300	1.82129800
H	6.31291800	-0.20017000	2.59511900
H	6.59393100	-1.69970100	1.68000000
H	7.95308900	-0.70673000	2.20269600
C	7.83943000	-0.55492500	-0.50946800
H	7.87866200	0.00383700	-1.44649500

H	8.85280300	-0.61475800	-0.10221300
H	7.50100000	-1.57205600	-0.72989400

Cy-ortho-ts

B	-0.95171400	4.37349400	0.41927300
B	-0.01403100	3.68096400	1.76815900
B	0.37237400	1.99943000	1.36562600
B	-1.13612300	3.13453700	-0.84115200
B	-0.30083400	1.70386200	-0.24453800
B	0.78456500	4.73508400	0.57704100
B	0.08435700	4.41059500	-1.02402000
H	-1.79518800	5.19228900	0.60397800
B	1.59968500	3.26687800	1.15601400
H	-0.19081600	4.01906600	2.89517700
B	1.43345900	2.02704100	-0.09119700
H	0.48846600	1.12728500	2.16040600
B	0.47513500	2.73841900	-1.46517500
H	-2.10383600	3.04578500	-1.52472800
H	1.18591600	5.81636900	0.87205900
B	1.66130300	3.71666100	-0.58194000
H	-0.01583500	5.25670600	-1.85426400
H	2.57872900	3.28825700	1.83238400
H	0.65803500	2.35095800	-2.57158800
H	2.68317300	4.04128400	-1.09765700
B	-1.20042000	2.68639700	0.90722600
I	-1.92911900	-0.25227200	-0.61937400
C	-1.33958000	-1.03397000	1.28602900
C	-2.07180900	-0.65733900	2.40220500
C	-0.22680500	-1.85824400	1.34061200
C	-1.65428600	-1.13883300	3.64248500
H	-2.93061000	-0.00614800	2.31859200
C	0.17786100	-2.32034500	2.59271800
H	0.31810600	-2.12149500	0.44611000
C	-0.53251800	-1.96176800	3.73746500
H	-2.20621500	-0.85960700	4.53240800
H	1.04887900	-2.96114900	2.66480300
H	-0.21115400	-2.32407200	4.70709800
O	-3.66377600	-1.91977600	-0.32095700
C	-4.46009500	-1.97858700	-1.33435400
O	-4.33212200	-1.28456400	-2.35845500
C	-5.61735000	-2.94636500	-1.19130700
H	-6.42686800	-2.43344500	-0.66191100
H	-5.98193300	-3.24938900	-2.17313200
H	-5.33020900	-3.82071600	-0.60619000

H	-0.00607800	0.49940700	-0.76071000
H	-2.20922200	2.30727700	1.40183900
N	2.50781200	1.00689900	-0.30105600
C	2.35995400	-0.16842100	-0.91212900
H	3.43072700	1.21323800	0.05552800
O	1.24663900	-0.52613800	-1.37158900
C	3.54235700	-1.11153000	-1.03497500
C	4.91711800	-0.48598900	-0.76588200
C	3.31587300	-2.33997500	-0.12546500
H	3.51816100	-1.46151800	-2.07398000
C	6.03441200	-1.51875600	-0.95555700
H	4.96127900	-0.11682900	0.26645700
H	5.07879100	0.37100000	-1.42686900
C	4.44011100	-3.36647200	-0.29467500
H	3.27462300	-2.00315800	0.91750300
H	2.35111700	-2.79635800	-0.35757900
C	5.81980200	-2.74354100	-0.05993000
H	7.00282800	-1.05583600	-0.74174700
H	6.05865800	-1.83478700	-2.00598400
H	4.27853800	-4.20330000	0.39252000
H	4.39699900	-3.77733700	-1.31121000
H	6.60493000	-3.48549200	-0.23823800
H	5.90367500	-2.43836800	0.99109500

Cy-meta-ts

B	-1.57708800	0.98382300	2.51931300
B	-1.06524300	-0.18511400	1.30458100
B	-0.97330000	0.68484400	-0.32347600
B	-1.82865200	2.54008100	1.70173900
B	-1.43191500	2.38187400	-0.02425500
B	0.13623400	0.56488000	2.37274400
B	-0.33518200	2.25300300	2.63470700
H	-2.24031300	0.64987600	3.44658200
B	0.48069500	0.44604100	0.66155400
H	-1.26870900	-1.34980000	1.32799300
B	0.28252300	2.02048300	-0.16177200
H	-1.20076000	0.14140200	-1.34997900
B	-0.27425900	3.13633200	1.08561500
H	-2.68965700	3.28075100	2.05586000
H	0.74122500	-0.07962300	3.16295600
B	0.96491000	1.92145500	1.46851000
H	-0.10214600	2.79738200	3.66515800
H	0.55551200	-0.30598900	-0.34288900
H	0.94507100	2.30195900	-1.10191000

H	-0.01707700	4.29547000	1.03705500
H	2.10526200	2.16295100	1.67756600
B	-2.26514500	1.03137700	0.87011700
H	-2.02272800	2.96927500	-0.87119600
N	-3.71282400	0.76442700	0.58488400
H	-4.35430900	1.52104500	0.78379600
C	-4.28908200	-0.32730300	0.04852400
O	-3.64713400	-1.34345800	-0.27648400
I	2.42520100	-1.05096600	0.27293000
C	3.27392700	0.36493900	-1.09462500
C	4.08417100	1.36471500	-0.57828300
C	2.96482300	0.24354800	-2.44087500
C	4.61064700	2.29581800	-1.47310000
H	4.29602500	1.42584600	0.47914600
C	3.49960900	1.18921300	-3.31567600
H	2.32499100	-0.55025700	-2.80159800
C	4.31766000	2.20988600	-2.83339300
H	5.24522400	3.09012100	-1.09777200
H	3.27075700	1.12225100	-4.37283900
H	4.72751700	2.94158000	-3.51990000
O	4.60911000	-2.22076800	-0.11143400
C	5.63345500	-1.82064800	0.55554900
O	5.60419800	-0.95728900	1.45357700
C	6.95418100	-2.45192900	0.14880900
H	7.32571300	-1.92256200	-0.73489000
H	7.69062800	-2.35592100	0.94721800
H	6.82224100	-3.50122500	-0.11936800
C	-5.79336200	-0.26186300	-0.17166000
C	-6.10178900	-0.25300300	-1.68187300
C	-6.50440100	-1.43622200	0.52286400
H	-6.17257600	0.67167400	0.25863800
C	-7.61161700	-0.22404000	-1.94067300
H	-5.66959300	-1.15285100	-2.13395100
H	-5.61717800	0.60881700	-2.15234400
C	-8.01402300	-1.40484500	0.26091900
H	-6.08629400	-2.37551900	0.14480600
H	-6.30336700	-1.40509000	1.59882400
C	-8.32319800	-1.38655800	-1.24003400
H	-7.80199800	-0.25589900	-3.01848000
H	-8.02332200	0.72543700	-1.57516700
H	-8.48928700	-2.26941700	0.73582100
H	-8.44465400	-0.51079300	0.72982700
H	-9.40410900	-1.32150700	-1.40272600
H	-7.99126100	-2.33268300	-1.68668800

Cy-para-ts

B	1.62967800	0.77557000	-0.96683900
B	1.83451500	-0.96760300	-1.44945000
B	1.62576100	-1.96239100	0.00382900
B	1.30441700	0.81532800	0.77846700
B	1.27346700	-0.86692600	1.36784000
B	0.31844200	-0.09591100	-1.79902700
B	-0.01285700	1.01945500	-0.36876000
H	2.21032000	1.63821900	-1.53777000
B	0.31596700	-1.81844100	-1.16003300
H	2.54097000	-1.27444900	-2.35009500
B	-0.03875200	-1.75562200	0.57214600
H	2.22810800	-2.97392900	0.16198000
B	-0.24247800	0.00418900	1.06060300
H	1.68914200	1.70405500	1.46654300
H	-0.02116000	0.17198100	-2.90191600
B	-0.79695800	-0.58636400	-0.49087400
H	-0.63602300	2.01140000	-0.54180100
H	-0.09569500	-2.68531000	-1.85643300
H	-0.67792600	-2.59527900	1.11224700
H	-1.00787100	0.29374700	1.91695200
H	-1.47479100	-0.37398000	-1.52271700
B	2.44686300	-0.38202600	0.11487200
H	1.61687600	-1.13477800	2.47427600
N	3.89903500	-0.29758200	0.49848600
H	4.11016600	-0.43922900	1.47764100
C	4.96996600	-0.03407000	-0.26950600
O	4.89269900	0.17165300	-1.49610400
I	-3.23981800	-0.93891400	-0.48470200
C	-3.57889600	1.16296000	-0.24801900
C	-3.73641200	1.93356700	-1.38998700
C	-3.61928800	1.67775300	1.03898700
C	-3.93907700	3.30356700	-1.22388100
H	-3.69655800	1.49179800	-2.37633900
C	-3.82767400	3.04950700	1.17977400
H	-3.49240900	1.04058800	1.90218100
C	-3.98396900	3.85784200	0.05460600
H	-4.06043300	3.93135300	-2.09884500
H	-3.86225600	3.48007900	2.17368800
H	-4.14139700	4.92341700	0.17461200
O	-5.72425100	-0.99520300	-0.15144000
C	-6.16185000	-1.01086100	1.05805200
O	-5.44480900	-1.10896200	2.07227200

C	-7.66627900	-0.85680100	1.20153800
H	-7.90473000	0.21079200	1.15009300
H	-8.19295400	-1.35831800	0.38834300
H	-8.00355500	-1.24183700	2.16437000
C	6.31769900	0.01577000	0.43579100
C	7.27917700	-1.03531900	-0.14742100
C	6.92337800	1.42764100	0.32593700
H	6.16873300	-0.20964800	1.49754100
C	8.65277900	-0.96423900	0.52880000
H	7.38967800	-0.85461000	-1.22229100
H	6.84805200	-2.03523100	-0.03151400
C	8.29754900	1.49673400	1.00046900
H	7.02214600	1.68650400	-0.73409700
H	6.24122100	2.15780700	0.77373100
C	9.25426600	0.44217000	0.43328400
H	9.32722000	-1.69733600	0.07423700
H	8.54981700	-1.24240200	1.58554500
H	8.72037200	2.49915500	0.87669000
H	8.17936900	1.33467300	2.07953400
H	10.21328300	0.47928200	0.96060800
H	9.46172300	0.67350200	-0.61942200

NMe₂-ortho-ts

B	-2.33518100	-1.64886700	-1.32877800
B	-1.01741000	-1.15336400	-0.24711600
B	-1.56551100	-1.01252300	1.42413100
B	-3.75526800	-1.83913200	-0.28972800
B	-3.28648100	-1.44835200	1.40081600
B	-1.10878200	-2.81787000	-0.80276800
B	-2.82474400	-3.26839100	-0.79632700
H	-2.39921600	-1.25160000	-2.44516600
B	-0.63717700	-2.43277200	0.89995200
H	-0.67651500	-0.00162200	-0.82841100
B	-2.07106600	-2.63621800	1.91805100
H	-1.12435300	-0.19029900	2.15696000
B	-3.41980800	-3.13836700	0.87192900
H	-4.84559400	-1.59417600	-0.69890100
H	-0.31204700	-3.26193200	-1.56425600
B	-1.77693800	-3.74891100	0.55624000
H	-3.26480000	-4.06189900	-1.56613700
H	0.46962000	-2.62177900	1.28133400
H	-1.98403400	-2.99227900	3.05026300
H	-4.29259500	-3.83977700	1.27672200
H	-1.47148800	-4.88490200	0.73529800

B	-2.63532500	-0.49963600	0.05483800
H	-4.05779400	-0.94033100	2.15189700
N	-3.03624400	0.92555000	-0.12341500
H	-3.84730500	1.24064300	0.38692200
C	-2.34821800	1.85146000	-0.82850100
O	-1.28104000	1.54068400	-1.42424200
I	1.33296500	-0.34822700	-0.93781900
C	1.47187800	0.78542600	0.87598200
C	1.96637400	0.14832600	2.00458000
C	1.04193200	2.10349300	0.86271300
C	2.02970300	0.88530900	3.18661500
H	2.28544200	-0.88354500	1.97312700
C	1.10779800	2.81746500	2.05910900
H	0.65739800	2.55823000	-0.03885900
C	1.59888100	2.21113100	3.21455800
H	2.40971800	0.41297300	4.08489500
H	0.77356400	3.84822700	2.07923000
H	1.64540400	2.77332800	4.13996800
O	3.65246100	0.25609000	-1.18224100
C	4.54113300	-0.53310900	-0.66927600
O	4.28768900	-1.59323600	-0.07789100
C	5.96936400	-0.04293100	-0.81246100
H	6.14403600	0.73000000	-0.05726100
H	6.67171300	-0.86037600	-0.64876700
H	6.13137500	0.40446900	-1.79426900
N	-2.83830800	3.12366000	-0.89318900
C	-1.97775400	4.18944400	-1.39938700
H	-2.59883700	4.95624100	-1.86485600
H	-1.39640900	4.65249600	-0.59246000
H	-1.29329200	3.79384000	-2.14517200
C	-3.97272800	3.53904800	-0.07277600
H	-3.73309400	3.53250600	0.99737300
H	-4.24811900	4.55363800	-0.35679800
H	-4.84268300	2.90284600	-0.25020700

NMe₂-meta-ts

B	-2.54070800	0.06675700	2.25802200
B	-1.83427600	-0.70832600	0.84571300
B	-1.72616900	0.54354100	-0.50433800
B	-2.90203500	1.75118600	1.82508100
B	-2.37433700	2.06736400	0.15618000
B	-0.78881100	-0.15142000	2.17003500
B	-1.45084200	1.36889600	2.79124500
H	-3.22404600	-0.54451500	3.01410500

B	-0.32345800	0.18985100	0.51849700
H	-1.91583700	-1.85556400	0.56791700
B	-0.62729900	1.90275600	0.09179100
H	-1.82562000	0.26067400	-1.64898600
B	-1.38033400	2.61463800	1.51703900
H	-3.85616500	2.30618300	2.26979500
H	-0.17128300	-0.92046000	2.82811300
B	-0.04813500	1.45245900	1.70002900
H	-1.34473600	1.65505700	3.94016300
H	-0.08526300	-0.24276700	-0.63759400
H	0.06441800	2.46222800	-0.69007400
H	-1.24320700	3.76650300	1.77571000
H	1.04506300	1.72820500	2.06341900
B	-3.12897500	0.46716300	0.61525400
H	-2.96573300	2.79660700	-0.57218700
N	-4.52222300	0.17155100	0.16199300
H	-5.23042800	0.79281600	0.52285700
C	-4.94151400	-0.76537600	-0.72962200
O	-4.15532400	-1.58178400	-1.25826600
I	1.76954700	-1.03096100	0.00052000
C	2.62806100	0.71138400	-0.89987800
C	3.30129100	1.60535000	-0.08097400
C	2.46669800	0.89164400	-2.26578100
C	3.84108500	2.74582300	-0.67498200
H	3.40170000	1.42750300	0.97988800
C	3.01159800	2.04190400	-2.83618700
H	1.93158100	0.17036800	-2.86847000
C	3.69467600	2.96379300	-2.04421800
H	4.37109000	3.46294200	-0.05910700
H	2.89737800	2.21083100	-3.90057300
H	4.11427300	3.85520000	-2.49578300
O	4.09584600	-1.92553900	-0.31817900
C	4.95540800	-1.67003700	0.60356700
O	4.70686900	-1.05450800	1.65847100
C	6.37037100	-2.14389700	0.31629300
H	6.85907200	-1.39491400	-0.31560800
H	6.93927100	-2.24177300	1.24148200
H	6.36584200	-3.09027800	-0.22647200
N	-6.28101800	-0.76821000	-1.04894100
C	-7.24803200	0.01270000	-0.28165000
H	-8.23184900	-0.12132600	-0.72931300
H	-7.30194100	-0.30539300	0.76682500
H	-7.01988100	1.08080900	-0.32013900
C	-6.81538900	-1.91700600	-1.77373900

H	-7.09264500	-2.73400100	-1.09453000
H	-7.70418400	-1.60679100	-2.32526700
H	-6.07790500	-2.28799200	-2.48103800

NMe₂-para-ts

B	2.42436200	1.00191200	-0.65752500
B	2.70093600	-0.58001000	-1.51579900
B	2.50846700	-1.88166600	-0.32523300
B	2.05648000	0.64106900	1.03571600
B	2.08583000	-1.13211700	1.23440500
B	1.16190800	0.29930100	-1.70180000
B	0.75656400	1.04498300	-0.07797600
H	2.97421500	1.99199800	-1.00853700
B	1.21570500	-1.53302800	-1.46532700
H	3.43852600	-0.65393700	-2.44138300
B	0.82410200	-1.86674700	0.22314700
H	3.14823700	-2.88157100	-0.37873600
B	0.54221300	-0.26868900	1.08846900
H	2.38617200	1.36609700	1.91758400
H	0.83281400	0.79513000	-2.72613600
B	0.03803000	-0.51391400	-0.56992300
H	0.10283600	2.03176800	-0.04302000
H	0.85412900	-2.23460300	-2.34982100
H	0.21124800	-2.82865200	0.54823400
H	-0.25293800	-0.20665200	1.96419000
H	-0.61031900	-0.20542600	-1.59103500
B	3.26892600	-0.33925900	0.15770100
H	2.41580900	-1.62953000	2.26312400
N	4.70546000	-0.31355100	0.58750500
H	4.89610700	-0.74098000	1.48113500
C	5.75561300	0.28024800	-0.03417200
O	5.64709700	0.81634600	-1.15944900
I	-2.40594200	-0.88724000	-0.63050700
C	-2.74889200	1.17288400	-0.15297700
C	-2.88280100	2.07737300	-1.19572700
C	-2.80022300	1.52959200	1.18573000
C	-3.07114900	3.41996300	-0.86816600
H	-2.83320800	1.75730400	-2.22759600
C	-2.99411200	2.87710000	1.48842100
H	-2.68794200	0.79283500	1.96793200
C	-3.12517300	3.81715700	0.46716200
H	-3.17364200	4.14985200	-1.66268400
H	-3.03529500	3.18572000	2.52643700
H	-3.26947800	4.86285700	0.71263300

O	-4.88374900	-0.99575700	-0.32418300
C	-5.32813600	-1.15940600	0.87255500
O	-4.61655200	-1.36918900	1.87291500
C	-6.83551800	-1.04232400	1.01923600
H	-7.09249300	0.02134000	1.05886400
H	-7.34804900	-1.47943800	0.16093600
H	-7.17163700	-1.51700900	1.94149400
N	6.96129700	0.29040100	0.63429600
C	8.16053500	0.63825000	-0.12197100
H	8.92499600	0.99277600	0.57088600
H	8.56109200	-0.22331500	-0.67275800
H	7.93845100	1.43173700	-0.83142700
C	7.17239000	-0.51400300	1.83429100
H	7.11907300	-1.59110800	1.63045500
H	8.16242800	-0.29050400	2.22993400
H	6.44927600	-0.26229900	2.61374800

IRC_TS1_point1

B	-2.67896500	4.00128600	0.21580700
B	-1.64091500	3.70868700	1.63520100
B	-0.64451500	2.28084900	1.30582000
B	-2.31806700	2.75155700	-1.00115800
B	-1.05697000	1.75390800	-0.31064200
B	-1.20443700	4.96746500	0.45671300
B	-1.62702200	4.38344300	-1.16734600
H	-3.76726300	4.47297100	0.32293700
B	0.05363100	3.90607300	1.12397300
H	-1.99476600	3.97621000	2.74087200
B	0.42598500	2.66285700	-0.08499900
H	-0.27599600	1.52362500	2.14336400
B	-0.61750800	2.96265500	-1.51841100
H	-3.13638200	2.31738900	-1.74768500
H	-1.25067400	6.12603200	0.73199200
B	0.06323200	4.32721200	-0.60950200
H	-1.97384600	5.11886600	-2.03790100
H	0.90434200	4.29568600	1.86206800
H	-0.26239800	2.67770200	-2.61385400
H	0.92067900	5.00783200	-1.07839600
B	-2.33371400	2.33994500	0.73966400
I	-1.66823600	-1.15628700	-0.18402700
C	0.29979900	-1.69485600	0.46160700
C	0.67810100	-1.37177000	1.75769300
C	1.11442500	-2.37730300	-0.43162800
C	1.94713600	-1.76804000	2.17574200

H	0.01319400	-0.83628400	2.41997700
C	2.37528700	-2.76959300	0.01419500
H	0.78560400	-2.59441000	-1.43838900
C	2.78773000	-2.46634000	1.31031600
H	2.27342400	-1.52483200	3.17993500
H	3.03458400	-3.30067700	-0.66128200
H	3.77389700	-2.76566400	1.64360600
O	-2.15443600	-3.24164900	0.38947500
C	-3.39646900	-3.55779900	0.09981400
O	-4.17849200	-2.77452300	-0.43265600
C	-3.76700800	-4.95920400	0.51121800
H	-3.98051700	-4.95397000	1.58421400
H	-4.65840100	-5.27551800	-0.02887300
H	-2.94229400	-5.64890600	0.33080800
H	-0.86652700	0.59428900	-0.74356500
H	-3.16162200	1.61799800	1.19529200
N	1.80313900	2.06382100	-0.12648700
C	2.24322600	1.04861700	-0.88778900
H	2.46026300	2.41109600	0.55778800
C	3.59863600	0.48593000	-0.56590400
O	1.57951500	0.56164800	-1.82221600
C	4.27032800	-0.23289700	-1.56015300
C	4.17527900	0.59117100	0.70459900
C	5.50160300	-0.82433000	-1.29607600
H	3.81723200	-0.32812400	-2.53902300
C	5.40422300	-0.00680300	0.97156000
H	3.65872600	1.10282800	1.50807000
C	6.07095300	-0.71461000	-0.02716400
H	6.01438800	-1.37491000	-2.07677500
H	5.83261500	0.06768000	1.96458000
H	7.02591500	-1.18298500	0.18355400

IRC_TS1_point2

B	-2.67773600	4.00214700	0.21906700
B	-1.63900300	3.70881500	1.63782600
B	-0.64305200	2.28091700	1.30741800
B	-2.31771600	2.75277500	-0.99852600
B	-1.05644800	1.75464000	-0.30898300
B	-1.20286900	4.96793000	0.45956600
B	-1.62642000	4.38458900	-1.16446800
H	-3.76588100	4.47403700	0.32690100
B	0.05532800	3.90606500	1.12580500
H	-1.99223800	3.97601000	2.74377000
B	0.42682200	2.66320100	-0.08376900

H	-0.27427400	1.52329700	2.14450400
B	-0.61739100	2.96371300	-1.51658000
H	-3.13649300	2.31904700	-1.74480200
H	-1.24873400	6.12640800	0.73526800
B	0.06413900	4.32779300	-0.60752500
H	-1.97352500	5.12040800	-2.03458800
H	0.90647500	4.29526000	1.86360000
H	-0.26291300	2.67910600	-2.61232300
H	0.92146000	5.00841100	-1.07664000
B	-2.33256600	2.34052700	0.74214600
I	-1.66839000	-1.15558300	-0.18455300
C	0.29914800	-1.69448900	0.46268000
C	0.67600900	-1.37254900	1.75947800
C	1.11476500	-2.37615300	-0.43024100
C	1.94450000	-1.76927600	2.17865300
H	0.01030400	-0.83772600	2.42151300
C	2.37504100	-2.76892300	0.01669800
H	0.78701100	-2.59243900	-1.43753100
C	2.78601400	-2.46686400	1.31356400
H	2.26963800	-1.52699700	3.18343500
H	3.03502600	-3.29950600	-0.65845400
H	3.77164300	-2.76668800	1.64778400
O	-2.15440000	-3.24125000	0.38553400
C	-3.39597900	-3.55823300	0.09408500
O	-4.17790900	-2.77542100	-0.43920200
C	-3.76633300	-4.96020400	0.50474900
H	-3.97941300	-4.95562500	1.57807000
H	-4.65786800	-5.27657200	-0.03539500
H	-2.94158800	-5.64965400	0.32366700
H	-0.86621200	0.59529600	-0.74256900
H	-3.16040800	1.61861100	1.19794400
N	1.80375600	2.06373500	-0.12620100
C	2.24300900	1.04846600	-0.88791100
H	2.46133000	2.41050100	0.55786900
C	3.59817400	0.48489900	-0.56655400
O	1.57874300	0.56209200	-1.82218100
C	4.26964200	-0.23317200	-1.56149700
C	4.17475200	0.58853800	0.70410100
C	5.50065300	-0.82538100	-1.29796900
H	3.81660200	-0.32717100	-2.54051900
C	5.40339500	-0.01028700	0.97054700
H	3.65855300	1.09965200	1.50800900
C	6.06991800	-0.71730500	-0.02885600
H	6.01319000	-1.37534300	-2.07920400

H	5.83167100	0.06291400	1.96374600
H	7.02466900	-1.18630100	0.18148200

IRC_TS1_point3

B	-2.67652100	4.00293600	0.22232200
B	-1.63708700	3.70892700	1.64040200
B	-0.64158700	2.28095400	1.30894500
B	-2.31737000	2.75394000	-0.99592100
B	-1.05594500	1.75537300	-0.30744000
B	-1.20135800	4.96838100	0.46235800
B	-1.62587700	4.38569200	-1.16165100
H	-3.76451900	4.47498100	0.33090100
B	0.05700800	3.90603200	1.12752200
H	-1.98964100	3.97580300	2.74663900
B	0.42762100	2.66355700	-0.08272300
H	-0.27241700	1.52304000	2.14556800
B	-0.61728700	2.96480000	-1.51482000
H	-3.13663000	2.32062500	-1.74191100
H	-1.24686300	6.12676300	0.73853300
B	0.06496500	4.32843100	-0.60565800
H	-1.97336300	5.12186700	-2.03130700
H	0.90863000	4.29476800	1.86502800
H	-0.26347500	2.68044200	-2.61083400
H	0.92216500	5.00907800	-1.07496400
B	-2.33136100	2.34106100	0.74463100
I	-1.66842000	-1.15481800	-0.18540800
C	0.29826600	-1.69419800	0.46391400
C	0.67358100	-1.37354600	1.76149800
C	1.11492800	-2.37497200	-0.42872100
C	1.94163900	-1.77068900	2.18178400
H	0.00710700	-0.83936100	2.42325100
C	2.37477700	-2.76811100	0.01929500
H	0.78837100	-2.59023300	-1.43662600
C	2.78422800	-2.46736200	1.31697400
H	2.26560400	-1.52944600	3.18722000
H	3.03562200	-3.29794300	-0.65564400
H	3.76962500	-2.76743500	1.65198400
O	-2.15528600	-3.24108700	0.38457400
C	-3.39563200	-3.55882400	0.08936300
O	-4.17671100	-2.77628300	-0.44553100
C	-3.76535700	-4.96142100	0.49727700
H	-3.97822000	-4.95954500	1.57030700
H	-4.65666400	-5.27668600	-0.04336800
H	-2.94024000	-5.65007000	0.31440800

H	-0.86581800	0.59609700	-0.74145900
H	-3.15907400	1.61911400	1.20060700
N	1.80437100	2.06370800	-0.12602800
C	2.24281500	1.04834100	-0.88808100
H	2.46232500	2.40993600	0.55800300
C	3.59770100	0.48384600	-0.56722400
O	1.57802300	0.56263200	-1.82237200
C	4.26901000	-0.23338500	-1.56291300
C	4.17411800	0.58585100	0.70363700
C	5.49977400	-0.82634400	-1.29987300
H	3.81605600	-0.32612300	-2.54209000
C	5.40254300	-0.01369200	0.96953900
H	3.65775800	1.09612300	1.50810300
C	6.06893800	-0.71983400	-0.03059100
H	6.01231300	-1.37559800	-2.08167100
H	5.83077000	0.05825500	1.96281700
H	7.02350400	-1.18940100	0.17929200

IRC_TS1_point4

B	-2.67536200	4.00374200	0.22535100
B	-1.63523600	3.70914200	1.64281700
B	-0.64013600	2.28112100	1.31043300
B	-2.31705000	2.75503200	-0.99343000
B	-1.05541500	1.75609000	-0.30586400
B	-1.19989900	4.96885700	0.46490800
B	-1.62536600	4.38671300	-1.15903200
H	-3.76322300	4.47595500	0.33458800
B	0.05863300	3.90613100	1.12912800
H	-1.98719500	3.97576100	2.74930300
B	0.42842600	2.66392800	-0.08162600
H	-0.27068000	1.52286900	2.14663500
B	-0.61721400	2.96574100	-1.51314900
H	-3.13674000	2.32205900	-1.73913800
H	-1.24507900	6.12716800	0.74141400
B	0.06578300	4.32898400	-0.60394000
H	-1.97315300	5.12320200	-2.02831000
H	0.91066800	4.29454400	1.86630200
H	-0.26402700	2.68167400	-2.60944600
H	0.92282300	5.00962100	-1.07352700
B	-2.33022600	2.34164500	0.74699900
I	-1.66850800	-1.15407000	-0.18581400
C	0.29771500	-1.69376400	0.46507200
C	0.67138500	-1.37436600	1.76342000
C	1.11548500	-2.37365800	-0.42721100

C	1.93872500	-1.77208400	2.18498900
H	0.00403600	-0.84088300	2.42486100
C	2.37457900	-2.76740200	0.02208900
H	0.79022300	-2.58797800	-1.43569600
C	2.78229700	-2.46803100	1.32059300
H	2.26134400	-1.53188500	3.19106500
H	3.03619400	-3.29668300	-0.65248700
H	3.76695800	-2.76878900	1.65669800
O	-2.15524900	-3.24076200	0.38055300
C	-3.39510200	-3.55940900	0.08357000
O	-4.17609500	-2.77741700	-0.45225400
C	-3.76455300	-4.96262600	0.49120500
H	-3.97656300	-4.96091000	1.56484900
H	-4.65631000	-5.27848800	-0.04908100
H	-2.93944200	-5.65102000	0.30780100
H	-0.86540800	0.59705700	-0.74055500
H	-3.15784400	1.61973300	1.20319300
N	1.80495800	2.06364500	-0.12579600
C	2.24259600	1.04822300	-0.88826000
H	2.46336900	2.40941900	0.55795800
C	3.59725000	0.48289800	-0.56795500
O	1.57727000	0.56307300	-1.82245000
C	4.26832100	-0.23358900	-1.56430400
C	4.17359900	0.58332500	0.70304400
C	5.49880300	-0.82733000	-1.30177200
H	3.81546000	-0.32509000	-2.54365800
C	5.40170900	-0.01706600	0.96846400
H	3.65750500	1.09303600	1.50794000
C	6.06787000	-0.72245300	-0.03230200
H	6.01111000	-1.37598000	-2.08407500
H	5.82980000	0.05360500	1.96192700
H	7.02219800	-1.19265900	0.17722600

IRC_TS1_point5

B	-2.67418600	4.00452600	0.22836400
B	-1.63333100	3.70934500	1.64515800
B	-0.63868300	2.28122900	1.31181200
B	-2.31676100	2.75610600	-0.99098600
B	-1.05495900	1.75676300	-0.30441100
B	-1.19841400	4.96932400	0.46736900
B	-1.62487600	4.38772800	-1.15649800
H	-3.76189900	4.47690500	0.33833700
B	0.06029600	3.90616200	1.13057300
H	-1.98458400	3.97571500	2.75192600

B	0.42919500	2.66427900	-0.08077300
H	-0.26883000	1.52272400	2.14760100
B	-0.61717200	2.96671500	-1.51159200
H	-3.13696500	2.32351200	-1.73636200
H	-1.24322400	6.12755800	0.74426800
B	0.06656600	4.32957100	-0.60237700
H	-1.97305700	5.12452400	-2.02535500
H	0.91282800	4.29416200	1.86741300
H	-0.26466300	2.68282400	-2.60814300
H	0.92348800	5.01020800	-1.07220900
B	-2.32905100	2.34220800	0.74935600
I	-1.66854300	-1.15337300	-0.18656900
C	0.29678800	-1.69347700	0.46657800
C	0.66888400	-1.37538100	1.76574200
C	1.11567000	-2.37241200	-0.42541300
C	1.93591700	-1.77335800	2.18841300
H	0.00067600	-0.84265800	2.42693900
C	2.37444200	-2.76637100	0.02495000
H	0.79153700	-2.58575300	-1.43451600
C	2.78067700	-2.46824300	1.32427000
H	2.25736700	-1.53419200	3.19516500
H	3.03695300	-3.29485500	-0.64938200
H	3.76522300	-2.76907700	1.66113800
O	-2.15610500	-3.24056900	0.37977400
C	-3.39470900	-3.56002700	0.07903800
O	-4.17503300	-2.77824600	-0.45803200
C	-3.76328800	-4.96401200	0.48312200
H	-3.97516800	-4.96590400	1.55624700
H	-4.65458200	-5.27818600	-0.05795500
H	-2.93769500	-5.65140700	0.29731500
H	-0.86499300	0.59780100	-0.73931800
H	-3.15654100	1.62029400	1.20579500
N	1.80556300	2.06368300	-0.12585800
C	2.24239200	1.04810400	-0.88857900
H	2.46432900	2.40893400	0.55791200
C	3.59677000	0.48187600	-0.56870800
O	1.57651300	0.56352000	-1.82261400
C	4.26777100	-0.23373400	-1.56579300
C	4.17287400	0.58065200	0.70254200
C	5.49801800	-0.82819500	-1.30371900
H	3.81501800	-0.32398600	-2.54529300
C	5.40075800	-0.02046200	0.96747500
H	3.65671100	1.08957400	1.50793200
C	6.06688600	-0.72492800	-0.03401000

H	6.01036100	-1.37610300	-2.08658600
H	5.82875200	0.04894600	1.96103100
H	7.02104500	-1.19568300	0.17511300

IRC_TS1_point6

B	-2.67307500	4.00527800	0.23127600
B	-1.63149100	3.70960800	1.64743600
B	-0.63720700	2.28146600	1.31319300
B	-2.31647200	2.75711400	-0.98857300
B	-1.05441400	1.75749700	-0.30292200
B	-1.19704600	4.96981100	0.46972400
B	-1.62446600	4.38867300	-1.15404000
H	-3.76065900	4.47778800	0.34193200
B	0.06188200	3.90634300	1.13198600
H	-1.98211600	3.97575900	2.75445600
B	0.42997100	2.66468900	-0.07982900
H	-0.26698200	1.52269300	2.14856800
B	-0.61715100	2.96761100	-1.51004700
H	-3.13710100	2.32479000	-1.73362100
H	-1.24156200	6.12798200	0.74693100
B	0.06728800	4.33014000	-0.60086300
H	-1.97301000	5.12573600	-2.02252300
H	0.91483100	4.29407300	1.86846500
H	-0.26529300	2.68396800	-2.60687400
H	0.92400900	5.01078500	-1.07101500
B	-2.32788800	2.34277600	0.75166400
I	-1.66857000	-1.15261900	-0.18696300
C	0.29622600	-1.69301500	0.46783100
C	0.66649700	-1.37626700	1.76781700
C	1.11633500	-2.37096700	-0.42376400
C	1.93268500	-1.77490500	2.19191700
H	-0.00262600	-0.84424000	2.42860400
C	2.37426900	-2.76557200	0.02801500
H	0.79372300	-2.58322000	-1.43351700
C	2.77852800	-2.46900500	1.32825000
H	2.25261700	-1.53690200	3.19937500
H	3.03771200	-3.29335300	-0.64596800
H	3.76227500	-2.77059500	1.66632100
O	-2.15601900	-3.24039700	0.37580200
C	-3.39411800	-3.56071200	0.07332000
O	-4.17426700	-2.77947200	-0.46477000
C	-3.76242300	-4.96526700	0.47749800
H	-3.97296000	-4.96697200	1.55145300
H	-4.65457300	-5.28034400	-0.06271100

H	-2.93698400	-5.65245000	0.29106100
H	-0.86459500	0.59868800	-0.73850000
H	-3.15522700	1.62088800	1.20838500
N	1.80611900	2.06362100	-0.12566600
C	2.24218000	1.04801100	-0.88880800
H	2.46533800	2.40843200	0.55778700
C	3.59631500	0.48096400	-0.56947500
O	1.57584000	0.56403600	-1.82296800
C	4.26709000	-0.23388800	-1.56721100
C	4.17233100	0.57816300	0.70190400
C	5.49703900	-0.82913700	-1.30560500
H	3.81449000	-0.32287800	-2.54693700
C	5.39991900	-0.02374800	0.96634800
H	3.65617100	1.08636900	1.50778900
C	6.06582500	-0.72745000	-0.03576500
H	6.00920200	-1.37644200	-2.08896000
H	5.82773600	0.04435100	1.96010900
H	7.01972200	-1.19885900	0.17298000

IRC_TS1_point7

B	-2.67192400	4.00604000	0.23411000
B	-1.62962100	3.70983400	1.64962900
B	-0.63577500	2.28159100	1.31449200
B	-2.31619900	2.75811700	-0.98625300
B	-1.05397200	1.75809700	-0.30151900
B	-1.19557900	4.97026300	0.47199300
B	-1.62398300	4.38961900	-1.15168100
H	-3.75936400	4.47872400	0.34546500
B	0.06351900	3.90639300	1.13330500
H	-1.97956400	3.97577100	2.75691400
B	0.43073800	2.66502200	-0.07903900
H	-0.26520000	1.52255800	2.14948700
B	-0.61712200	2.96848900	-1.50860400
H	-3.13733800	2.32615200	-1.73096300
H	-1.23972900	6.12836700	0.74952900
B	0.06806600	4.33066700	-0.59944800
H	-1.97289100	5.12696400	-2.01978200
H	0.91695200	4.29375400	1.86943300
H	-0.26591500	2.68501200	-2.60567800
H	0.92467500	5.01129200	-1.06987000
B	-2.32675000	2.34333400	0.75390700
I	-1.66859900	-1.15192800	-0.18762800
C	0.29537100	-1.69269100	0.46942600
C	0.66396100	-1.37730600	1.77026200

C	1.11667700	-2.36962100	-0.42185100
C	1.92984700	-1.77614500	2.19551700
H	-0.00616800	-0.84621100	2.43085100
C	2.37424000	-2.76443800	0.03106700
H	0.79520800	-2.58091600	-1.43222500
C	2.77695300	-2.46911200	1.33213100
H	2.24850900	-1.53923000	3.20368100
H	3.03855600	-3.29148900	-0.64256300
H	3.76048000	-2.77082100	1.67106900
O	-2.15679700	-3.24011100	0.37469700
C	-3.39373600	-3.56131300	0.06877200
O	-4.17348800	-2.78026800	-0.47018300
C	-3.76102800	-4.96678900	0.46913400
H	-3.97177200	-4.97233400	1.54247200
H	-4.65238200	-5.28014200	-0.07227700
H	-2.93492200	-5.65284000	0.28039200
H	-0.86402400	0.59945600	-0.73726600
H	-3.15397800	1.62146700	1.21089200
N	1.80674000	2.06371800	-0.12586300
C	2.24199300	1.04792200	-0.88920800
H	2.46629400	2.40801200	0.55764400
C	3.59586400	0.48000500	-0.57029800
O	1.57504400	0.56440200	-1.82294300
C	4.26657800	-0.23399000	-1.56873900
C	4.17160900	0.57555300	0.70135700
C	5.49627100	-0.82998700	-1.30757300
H	3.81406400	-0.32173600	-2.54857200
C	5.39890800	-0.02718300	0.96538800
H	3.65564400	1.08315700	1.50762500
C	6.06477200	-0.73000800	-0.03739900
H	6.00842100	-1.37656600	-2.09147700
H	5.82662100	0.03964500	1.95923700
H	7.01847100	-1.20201900	0.17102600

IRC_TS1_point8

B	-2.67081300	4.00675300	0.23701300
B	-1.62776300	3.71009100	1.65187400
B	-0.63427700	2.28183400	1.31583200
B	-2.31590400	2.75909200	-0.98385300
B	-1.05340500	1.75885400	-0.30007100
B	-1.19423100	4.97074300	0.47430600
B	-1.62360200	4.39054100	-1.14925600
H	-3.75812700	4.47954900	0.34907900
B	0.06511000	3.90658000	1.13464900

H	-1.97704500	3.97581100	2.75942100
B	0.43150900	2.66544200	-0.07817400
H	-0.26325800	1.52257400	2.15040200
B	-0.61710300	2.96939600	-1.50710100
H	-3.13748000	2.32738400	-1.72821600
H	-1.23809500	6.12878200	0.75217000
B	0.06876100	4.33125900	-0.59799900
H	-1.97292000	5.12814200	-2.01696800
H	0.91897800	4.29366000	1.87041100
H	-0.26657100	2.68613000	-2.60444000
H	0.92515900	5.01190500	-1.06873900
B	-2.32554800	2.34387500	0.75621200
I	-1.66859800	-1.15120200	-0.18814200
C	0.29468600	-1.69226600	0.47081900
C	0.66138100	-1.37828200	1.77252000
C	1.11728500	-2.36813800	-0.42004500
C	1.92644100	-1.77776700	2.19925600
H	-0.00964500	-0.84784000	2.43262500
C	2.37408200	-2.76351600	0.03431200
H	0.79742100	-2.57825800	-1.43111700
C	2.77474000	-2.46982700	1.33634200
H	2.24356200	-1.54205100	3.20816100
H	3.03949300	-3.28965900	-0.63904100
H	3.75763000	-2.77213500	1.67643400
O	-2.15683400	-3.24004000	0.37122700
C	-3.39314600	-3.56196600	0.06323400
O	-4.17253000	-2.78135000	-0.47679300
C	-3.76015500	-4.96793700	0.46332300
H	-3.96938100	-4.97366800	1.53740200
H	-4.65252300	-5.28187300	-0.07706100
H	-2.93429200	-5.65374800	0.27354200
H	-0.86369300	0.60025100	-0.73639200
H	-3.15259500	1.62201600	1.21349900
N	1.80728300	2.06362300	-0.12565100
C	2.24179700	1.04782300	-0.88945800
H	2.46726400	2.40743600	0.55758200
C	3.59539500	0.47904700	-0.57102900
O	1.57448000	0.56502500	-1.82359700
C	4.26592900	-0.23416300	-1.57012900
C	4.17100800	0.57300300	0.70075500
C	5.49533200	-0.83092400	-1.30940600
H	3.81363500	-0.32063000	-2.55024400
C	5.39806200	-0.03043600	0.96426900
H	3.65476900	1.07970900	1.50759600

C	6.06377100	-0.73244100	-0.03917200
H	6.00738400	-1.37687400	-2.09379900
H	5.82555300	0.03507500	1.95834600
H	7.01723400	-1.20505500	0.16882100

IRC_TS1_point9

B	-2.66968300	4.00747400	0.23976600
B	-1.62592100	3.71030800	1.65401200
B	-0.63283200	2.28196700	1.31710600
B	-2.31561900	2.76003700	-0.98158600
B	-1.05293500	1.75940700	-0.29867800
B	-1.19280400	4.97117500	0.47650700
B	-1.62313000	4.39143500	-1.14695900
H	-3.75686100	4.48042900	0.35249700
B	0.06672000	3.90665500	1.13594100
H	-1.97456300	3.97582300	2.76180500
B	0.43229700	2.66578300	-0.07737900
H	-0.26150000	1.52243200	2.15130900
B	-0.61706600	2.97021600	-1.50568800
H	-3.13767500	2.32865700	-1.72561700
H	-1.23633400	6.12915200	0.75465900
B	0.06952600	4.33175900	-0.59662000
H	-1.97279100	5.12930200	-2.01431400
H	0.92103500	4.29342300	1.87134900
H	-0.26715500	2.68715000	-2.60327900
H	0.92579000	5.01239300	-1.06764700
B	-2.32441300	2.34440500	0.75839800
I	-1.66858500	-1.15046700	-0.18878200
C	0.29392900	-1.69188800	0.47240200
C	0.65873600	-1.37937900	1.77500500
C	1.11784900	-2.36666800	-0.41808200
C	1.92336100	-1.77912900	2.20304800
H	-0.01344900	-0.85000300	2.43490000
C	2.37409700	-2.76238300	0.03759100
H	0.79928300	-2.57577900	-1.42980500
C	2.77299000	-2.47004600	1.34050700
H	2.23900400	-1.54461000	3.21270700
H	3.04037700	-3.28787700	-0.63527600
H	3.75540200	-2.77268800	1.68167600
O	-2.15738500	-3.23973000	0.36929000
C	-3.39273800	-3.56256900	0.05847700
O	-4.17193400	-2.78220700	-0.48227000
C	-3.75883200	-4.96944900	0.45547800
H	-3.96847200	-4.97824400	1.52907400

H	-4.65031800	-5.28220200	-0.08616600
H	-2.93226200	-5.65423400	0.26409500
H	-0.86292000	0.60108500	-0.73528600
H	-3.15134700	1.62257000	1.21594800
N	1.80793400	2.06377200	-0.12591800
C	2.24162700	1.04778000	-0.88988700
H	2.46825600	2.40706300	0.55735300
C	3.59496800	0.47814900	-0.57191200
O	1.57364000	0.56536500	-1.82338900
C	4.26540700	-0.23424800	-1.57168600
C	4.17031600	0.57046700	0.70015400
C	5.49451500	-0.83181600	-1.31137900
H	3.81315900	-0.31948300	-2.55185800
C	5.39700800	-0.03391200	0.96332200
H	3.65448000	1.07674900	1.50728900
C	6.06261300	-0.73512300	-0.04073700
H	6.00650800	-1.37708300	-2.09629500
H	5.82442000	0.03033900	1.95746100
H	7.01582900	-1.20841700	0.16702000

IRC_TS1_point10

B	-2.66857500	4.00814500	0.24260200
B	-1.62406600	3.71055600	1.65618800
B	-0.63133600	2.28220300	1.31839700
B	-2.31531300	2.76096600	-0.97924200
B	-1.05235900	1.76016100	-0.29728000
B	-1.19146600	4.97163700	0.47873400
B	-1.62275400	4.39232100	-1.14461400
H	-3.75563400	4.48119500	0.35604000
B	0.06830700	3.90683300	1.13720400
H	-1.97203800	3.97586300	2.76424100
B	0.43306300	2.66619100	-0.07658800
H	-0.25952500	1.52246800	2.15217600
B	-0.61703800	2.97111100	-1.50425100
H	-3.13781200	2.32982900	-1.72291700
H	-1.23471400	6.12955100	0.75721100
B	0.07021200	4.33234500	-0.59525700
H	-1.97285200	5.13042500	-2.01158200
H	0.92307200	4.29330900	1.87224300
H	-0.26780700	2.68820300	-2.60208700
H	0.92627600	5.01299800	-1.06659800
B	-2.32319700	2.34491600	0.76066300
I	-1.66857600	-1.14978500	-0.18939100
C	0.29312700	-1.69150000	0.47397900

C	0.65599000	-1.38042000	1.77747900
C	1.11839500	-2.36516300	-0.41607600
C	1.91987000	-1.78072700	2.20701700
H	-0.01709600	-0.85169100	2.43685300
C	2.37398300	-2.76130600	0.04103300
H	0.80144300	-2.57308200	-1.42851900
C	2.77081100	-2.47059800	1.34493200
H	2.23399100	-1.54739200	3.21742800
H	3.04147800	-3.28573500	-0.63160100
H	3.75278200	-2.77361400	1.68717300
O	-2.15755800	-3.23972200	0.36636200
C	-3.39217200	-3.56314700	0.05316500
O	-4.17088400	-2.78303300	-0.48849000
C	-3.75790100	-4.97054300	0.44912300
H	-3.96608100	-4.98025000	1.52326400
H	-4.65032400	-5.28336500	-0.09164300
H	-2.93154700	-5.65496800	0.25623300
H	-0.86263000	0.60178400	-0.73427700
H	-3.14994400	1.62307700	1.21851800
N	1.80847100	2.06365600	-0.12570000
C	2.24145700	1.04767800	-0.89018500
H	2.46918400	2.40643700	0.55736500
C	3.59450200	0.47715800	-0.57262400
O	1.57317800	0.56604700	-1.82427400
C	4.26478900	-0.23446200	-1.57304200
C	4.16969000	0.56788800	0.69956700
C	5.49361300	-0.83277500	-1.31316700
H	3.81282100	-0.31841400	-2.55355000
C	5.39616800	-0.03713200	0.96219600
H	3.65345100	1.07319500	1.50730500
C	6.06167300	-0.73750100	-0.04252700
H	6.00551100	-1.37742000	-2.09855800
H	5.82331200	0.02581400	1.95660000
H	7.01467700	-1.21134100	0.16475700

IRC_TS1_point11

B	-2.66747300	4.00881300	0.24527900
B	-1.62223800	3.71076300	1.65825000
B	-0.62985900	2.28235300	1.31960700
B	-2.31503300	2.76184300	-0.97702800
B	-1.05185900	1.76067400	-0.29592800
B	-1.19009700	4.97205100	0.48084300
B	-1.62233000	4.39315600	-1.14239400
H	-3.75440600	4.48200000	0.35937300

B	0.06989200	3.90694500	1.13841700
H	-1.96958600	3.97587300	2.76654400
B	0.43386100	2.66655600	-0.07585100
H	-0.25773300	1.52235300	2.15302800
B	-0.61701900	2.97187700	-1.50289600
H	-3.13799200	2.33100000	-1.72036700
H	-1.23305000	6.12990800	0.75957800
B	0.07093200	4.33283500	-0.59395900
H	-1.97277700	5.13150600	-2.00901900
H	0.92507800	4.29316800	1.87309100
H	-0.26839900	2.68920500	-2.60099600
H	0.92682200	5.01349500	-1.06561500
B	-2.32204600	2.34541000	0.76278800
I	-1.66850700	-1.14903300	-0.19003500
C	0.29243700	-1.69108400	0.47557600
C	0.65320600	-1.38157100	1.78003100
C	1.11916200	-2.36357900	-0.41402300
C	1.91651200	-1.78220500	2.21104900
H	-0.02116200	-0.85398900	2.43913600
C	2.37404800	-2.76014500	0.04458400
H	0.80369600	-2.57042200	-1.42716000
C	2.76887000	-2.47091100	1.34943700
H	2.22895500	-1.55016000	3.22226700
H	3.04247200	-3.28393200	-0.62747200
H	3.75016000	-2.77442400	1.69295000
O	-2.15788700	-3.23942300	0.36378400
C	-3.39171500	-3.56374600	0.04832700
O	-4.17039400	-2.78392800	-0.49395500
C	-3.75663300	-4.97199700	0.44191800
H	-3.96518600	-4.98404900	1.51574100
H	-4.64828200	-5.28410300	-0.09993200
H	-2.92963000	-5.65552800	0.24789700
H	-0.86169700	0.60265200	-0.73334800
H	-3.14865700	1.62359100	1.22092500
N	1.80914300	2.06385700	-0.12609700
C	2.24128700	1.04766500	-0.89066400
H	2.47021300	2.40612200	0.55696300
C	3.59407600	0.47630200	-0.57358000
O	1.57228900	0.56637400	-1.82398100
C	4.26426100	-0.23454500	-1.57464300
C	4.16898900	0.56544000	0.69890200
C	5.49276800	-0.83369500	-1.31513400
H	3.81230100	-0.31731300	-2.55514800
C	5.39506100	-0.04057900	0.96126200

H	3.65321100	1.07042400	1.50687700
C	6.06042900	-0.74022900	-0.04402300
H	6.00466700	-1.37767900	-2.10102900
H	5.82216400	0.02115700	1.95567600
H	7.01315500	-1.21480000	0.16310300
IRC_TS1_point12			
B	-2.66639000	4.00942900	0.24799900
B	-1.62040900	3.71100200	1.66031700
B	-0.62837800	2.28258400	1.32082400
B	-2.31473200	2.76270900	-0.97478200
B	-1.05128300	1.76141200	-0.29460700
B	-1.18879400	4.97249100	0.48293600
B	-1.62198100	4.39399300	-1.14017400
H	-3.75321300	4.48269100	0.36279000
B	0.07145300	3.90712000	1.13956700
H	-1.96708700	3.97591900	2.76886400
B	0.43461500	2.66695200	-0.07515300
H	-0.25574800	1.52240100	2.15382500
B	-0.61699700	2.97274600	-1.50156300
H	-3.13813400	2.33208300	-1.71775200
H	-1.23147200	6.13028700	0.76198200
B	0.07159100	4.33340500	-0.59272200
H	-1.97288500	5.13255700	-2.00642200
H	0.92710000	4.29305500	1.87386400
H	-0.26905300	2.69017500	-2.59988400
H	0.92729200	5.01408400	-1.06469000
B	-2.32083300	2.34588100	0.76497700
I	-1.66848200	-1.14840500	-0.19071100
C	0.29156600	-1.69070600	0.47732200
C	0.65028100	-1.38266600	1.78271500
C	1.11972600	-2.36201500	-0.41181000
C	1.91290100	-1.78375800	2.21527400
H	-0.02506200	-0.85579800	2.44128200
C	2.37400300	-2.75890500	0.04827600
H	0.80590800	-2.56766000	-1.42569000
C	2.76670400	-2.47128400	1.35413200
H	2.22377000	-1.55290900	3.22726800
H	3.04373200	-3.28154200	-0.62351600
H	3.74766200	-2.77501300	1.69870400
O	-2.15810800	-3.23948800	0.36118900
C	-3.39116700	-3.56426700	0.04324800
O	-4.16931800	-2.78453000	-0.49970400
C	-3.75566700	-4.97305900	0.43523500
H	-3.96286400	-4.98653700	1.50945200

H	-4.64813700	-5.28485600	-0.10591700
H	-2.92884000	-5.65614600	0.23941400
H	-0.86143200	0.60326500	-0.73221900
H	-3.14725300	1.62404800	1.22342300
N	1.80967400	2.06375000	-0.12589000
C	2.24115400	1.04758800	-0.89103600
H	2.47109000	2.40549100	0.55703900
C	3.59363500	0.47533300	-0.57430000
O	1.57193300	0.56709300	-1.82505000
C	4.26365700	-0.23478900	-1.57596700
C	4.16838800	0.56289900	0.69828900
C	5.49187000	-0.83468600	-1.31688900
H	3.81203300	-0.31626900	-2.55687100
C	5.39425600	-0.04373700	0.96008900
H	3.65220200	1.06691500	1.50686400
C	6.05953400	-0.74256900	-0.04584700
H	6.00355000	-1.37812000	-2.10321600
H	5.82103100	0.01669400	1.95482800
H	7.01205300	-1.21766200	0.16078100

IRC_TS1_point13

B	-2.66532400	4.01003300	0.25058600
B	-1.61859600	3.71119700	1.66228400
B	-0.62686900	2.28275000	1.32194400
B	-2.31446400	2.76350400	-0.97263300
B	-1.05075400	1.76187600	-0.29331500
B	-1.18749400	4.97288200	0.48492800
B	-1.62161900	4.39475700	-1.13805400
H	-3.75203100	4.48340800	0.36603200
B	0.07301000	3.90726800	1.14066700
H	-1.96465400	3.97592600	2.77106800
B	0.43541300	2.66733900	-0.07451200
H	-0.25390300	1.52233400	2.15460000
B	-0.61700300	2.97345200	-1.50028700
H	-3.13831300	2.33314000	-1.71525900
H	-1.22991900	6.13062500	0.76420500
B	0.07225200	4.33388600	-0.59153600
H	-1.97289100	5.13354000	-2.00397100
H	0.92905400	4.29300600	1.87458700
H	-0.26966900	2.69114700	-2.59888500
H	0.92773400	5.01459300	-1.06385100
B	-2.31966500	2.34633300	0.76702900
I	-1.66835500	-1.14766000	-0.19137200
C	0.29090500	-1.69027500	0.47896900

C	0.64737000	-1.38384500	1.78535500
C	1.12064200	-2.36035400	-0.40963200
C	1.90930800	-1.78529500	2.21954400
H	-0.02931600	-0.85813300	2.44355500
C	2.37413100	-2.75768500	0.05209600
H	0.80848400	-2.56487200	-1.42424500
C	2.76462000	-2.47162400	1.35896400
H	2.21835600	-1.55578100	3.23238200
H	3.04489700	-3.27960800	-0.61908700
H	3.74478900	-2.77591500	1.70494200
O	-2.15827900	-3.23919000	0.35824400
C	-3.39066800	-3.56483900	0.03843800
O	-4.16890700	-2.78541000	-0.50504200
C	-3.75440600	-4.97444900	0.42850500
H	-3.96188500	-4.98983800	1.50251700
H	-4.64623100	-5.28582800	-0.11355100
H	-2.92698600	-5.65672200	0.23179700
H	-0.86036100	0.60413600	-0.73146800
H	-3.14591800	1.62451100	1.22578400
N	1.81035800	2.06399400	-0.12644900
C	2.24097200	1.04758400	-0.89157300
H	2.47215700	2.40523900	0.55640500
C	3.59319600	0.47449100	-0.57532500
O	1.57098700	0.56739400	-1.82472700
C	4.26313500	-0.23489600	-1.57761500
C	4.16765200	0.56055300	0.69757100
C	5.49102900	-0.83562300	-1.31883600
H	3.81146700	-0.31528000	-2.55843600
C	5.39309400	-0.04709700	0.95918700
H	3.65189300	1.06430900	1.50633800
C	6.05823200	-0.74527700	-0.04726300
H	6.00289100	-1.37837600	-2.10567000
H	5.81989200	0.01222500	1.95385000
H	7.01046300	-1.22111200	0.15927100

IRC_TS1_point14

B	-2.66427700	4.01058700	0.25317800
B	-1.61680500	3.71141300	1.66423400
B	-0.62541200	2.28296800	1.32307700
B	-2.31417700	2.76430400	-0.97050100
B	-1.05018700	1.76259600	-0.29208600
B	-1.18623800	4.97329400	0.48688500
B	-1.62130600	4.39554300	-1.13596700
H	-3.75088500	4.48401400	0.36930800

B	0.07453200	3.90743500	1.14170400
H	-1.96219900	3.97595900	2.77326600
B	0.43614800	2.66772500	-0.07390500
H	-0.25192600	1.52236500	2.15531300
B	-0.61699700	2.97429200	-1.49906900
H	-3.13846400	2.33412900	-1.71274800
H	-1.22839700	6.13098000	0.76646000
B	0.07287500	4.33443700	-0.59042600
H	-1.97305100	5.13452900	-2.00151500
H	0.93104600	4.29289400	1.87524000
H	-0.27032900	2.69204600	-2.59786800
H	0.92817800	5.01516600	-1.06304800
B	-2.31846700	2.34675300	0.76912200
I	-1.66830700	-1.14709100	-0.19210600
C	0.29000600	-1.68988300	0.48085500
C	0.64425600	-1.38498000	1.78822200
C	1.12128500	-2.35870900	-0.40722500
C	1.90555100	-1.78678300	2.22402200
H	-0.03354900	-0.86012200	2.44589500
C	2.37415800	-2.75629700	0.05607100
H	0.81082400	-2.56203800	-1.42259800
C	2.76244300	-2.47182000	1.36395700
H	2.21291900	-1.55849300	3.23766500
H	3.04627000	-3.27707700	-0.61474000
H	3.74230400	-2.77623300	1.71104400
O	-2.15849900	-3.23934000	0.35583400
C	-3.39013800	-3.56533000	0.03357600
O	-4.16782600	-2.78585000	-0.51036900
C	-3.75345800	-4.97548100	0.42171600
H	-3.95968800	-4.99258300	1.49601800
H	-4.64599400	-5.28629700	-0.11979200
H	-2.92619400	-5.65727800	0.22306400
H	-0.86011600	0.60467500	-0.73024700
H	-3.14452500	1.62490600	1.22819000
N	1.81088300	2.06392300	-0.12626900
C	2.24088400	1.04755500	-0.89202500
H	2.47297700	2.40463500	0.55655100
C	3.59279800	0.47359100	-0.57606700
O	1.57073400	0.56813500	-1.82592100
C	4.26252600	-0.23516600	-1.57889300
C	4.16712600	0.55811800	0.69689800
C	5.49010100	-0.83666600	-1.32054900
H	3.81124800	-0.31426200	-2.56018700
C	5.39236000	-0.05014800	0.95793200

H	3.65104300	1.06097100	1.50624000
C	6.05737400	-0.74759000	-0.04912600
H	6.00148900	-1.37902300	-2.10772800
H	5.81876200	0.00785700	1.95300800
H	7.00938700	-1.22395400	0.15691000

IRC_TS1_point15

B	-2.66325100	4.01112000	0.25567500
B	-1.61501000	3.71159600	1.66610000
B	-0.62387400	2.28314900	1.32410400
B	-2.31391900	2.76501100	-0.96841700
B	-1.04962900	1.76300700	-0.29085700
B	-1.18501400	4.97365900	0.48875400
B	-1.62101100	4.39623000	-1.13394900
H	-3.74975300	4.48463400	0.37246200
B	0.07605600	3.90761600	1.14268300
H	-1.95978400	3.97596300	2.77536700
B	0.43694000	2.66812600	-0.07337200
H	-0.25002000	1.52236400	2.15601100
B	-0.61702900	2.97493700	-1.49787400
H	-3.13864500	2.33506500	-1.71030800
H	-1.22696400	6.13129300	0.76853700
B	0.07347100	4.33490800	-0.58936000
H	-1.97315100	5.13540200	-1.99917600
H	0.93294500	4.29292800	1.87583000
H	-0.27097200	2.69297500	-2.59695800
H	0.92851000	5.01568700	-1.06235700
B	-2.31727800	2.34715900	0.77110600
I	-1.66812800	-1.14636800	-0.19279000
C	0.28933600	-1.68945800	0.48257700
C	0.64123100	-1.38616200	1.79095600
C	1.12229400	-2.35700900	-0.40489700
C	1.90175700	-1.78833200	2.22851600
H	-0.03791000	-0.86238200	2.44812600
C	2.37435300	-2.75499200	0.06014400
H	0.81364900	-2.55917300	-1.42103700
C	2.76025100	-2.47213400	1.36908800
H	2.20721300	-1.56137700	3.24302300
H	3.04766200	-3.27491000	-0.61008700
H	3.73930200	-2.77708900	1.71765500
O	-2.15855100	-3.23903600	0.35268700
C	-3.38959500	-3.56585000	0.02883000
O	-4.16745300	-2.78667100	-0.51555000

C	-3.75218200	-4.97679000	0.41532600
H	-3.95858800	-4.99553000	1.48950400
H	-4.64420200	-5.28738000	-0.12692100
H	-2.92437500	-5.65782400	0.21591800
H	-0.85893500	0.60552700	-0.72965900
H	-3.14313600	1.62531100	1.23050700
N	1.81157100	2.06418300	-0.12697100
C	2.24068100	1.04753400	-0.89261200
H	2.47408300	2.40443500	0.55566600
C	3.59233300	0.47273300	-0.57714400
O	1.56973800	0.56840400	-1.82562500
C	4.26201800	-0.23532100	-1.58058500
C	4.16633700	0.55586800	0.69614900
C	5.48929100	-0.83760700	-1.32247700
H	3.81062800	-0.31344200	-2.56169500
C	5.39114200	-0.05339200	0.95707900
H	3.65058700	1.05850000	1.50565200
C	6.05604500	-0.75022400	-0.05046400
H	6.00115300	-1.37920300	-2.11020700
H	5.81765800	0.00365500	1.95196000
H	7.00778000	-1.22729700	0.15550600

IRC_TS1_point16

B	-2.66224700	4.01161200	0.25813900
B	-1.61326500	3.71177400	1.66793900
B	-0.62244500	2.28334000	1.32514900
B	-2.31365200	2.76575100	-0.96640500
B	-1.04907600	1.76370200	-0.28972600
B	-1.18380800	4.97403700	0.49058900
B	-1.62073600	4.39697300	-1.13198700
H	-3.74865800	4.48515900	0.37559900
B	0.07753300	3.90776800	1.14362200
H	-1.95738700	3.97596100	2.77744700
B	0.43765600	2.66850500	-0.07284900
H	-0.24807000	1.52234700	2.15663200
B	-0.61704400	2.97574900	-1.49676700
H	-3.13880800	2.33597200	-1.70791500
H	-1.22549900	6.13161800	0.77065900
B	0.07405600	4.33543900	-0.58836000
H	-1.97335200	5.13634500	-1.99685100
H	0.93489600	4.29281100	1.87638100
H	-0.27163600	2.69382500	-2.59603800
H	0.92892800	5.01624400	-1.06165700
B	-2.31610600	2.34752100	0.77309100

I	-1.66804900	-1.14585600	-0.19357500
C	0.28844500	-1.68903200	0.48456800
C	0.63793600	-1.38731400	1.79396800
C	1.12305500	-2.35527600	-0.40231700
C	1.89784800	-1.78972300	2.23322200
H	-0.04252500	-0.86459000	2.45064600
C	2.37444300	-2.75348600	0.06441300
H	0.81616300	-2.55628100	-1.41922600
C	2.75804500	-2.47215200	1.37437900
H	2.20148900	-1.56402200	3.24856600
H	3.04908200	-3.27236100	-0.60527600
H	3.73673800	-2.77719500	1.72416000
O	-2.15874700	-3.23927200	0.35036200
C	-3.38908500	-3.56633800	0.02416600
O	-4.16639100	-2.78700900	-0.52052200
C	-3.75128300	-4.97780900	0.40857100
H	-3.95657800	-4.99840600	1.48295000
H	-4.64389400	-5.28766600	-0.13327900
H	-2.92361600	-5.65836600	0.20718400
H	-0.85868900	0.60601100	-0.72838400
H	-3.14176900	1.62563900	1.23280300
N	1.81209600	2.06418200	-0.12685700
C	2.24064200	1.04757100	-0.89314300
H	2.47484600	2.40389400	0.55586800
C	3.59199200	0.47193800	-0.57792200
O	1.56956400	0.56914300	-1.82685100
C	4.26138100	-0.23562100	-1.58180700
C	4.16593300	0.55360800	0.69538100
C	5.48829900	-0.83873200	-1.32412800
H	3.81042500	-0.31246700	-2.56346400
C	5.39051700	-0.05629000	0.95571900
H	3.65000600	1.05545000	1.50541700
C	6.05521100	-0.75253100	-0.05235400
H	5.99932100	-1.38017800	-2.11206400
H	5.81656300	-0.00057900	1.95111700
H	7.00669700	-1.23018000	0.15316300

IRC_TS1_point17

B	-2.66125900	4.01207000	0.26055100
B	-1.61149300	3.71194200	1.66970700
B	-0.62089000	2.28353200	1.32608800
B	-2.31340400	2.76637000	-0.96438400
B	-1.04849100	1.76406500	-0.28856300
B	-1.18266000	4.97437300	0.49234000

B	-1.62050600	4.39758300	-1.13006700
H	-3.74757600	4.48567500	0.37867100
B	0.07902100	3.90797100	1.14447900
H	-1.95499100	3.97595900	2.77945000
B	0.43843500	2.66890800	-0.07242100
H	-0.24610100	1.52241600	2.15725400
B	-0.61709900	2.97634200	-1.49565400
H	-3.13899200	2.33678800	-1.70552500
H	-1.22418500	6.13190400	0.77260300
B	0.07458800	4.33590000	-0.58741100
H	-1.97355300	5.13710600	-1.99461800
H	0.93674400	4.29290900	1.87684200
H	-0.27230700	2.69470000	-2.59521100
H	0.92915400	5.01677800	-1.06110600
B	-2.31489900	2.34787800	0.77501100
I	-1.66782800	-1.14517400	-0.19429000
C	0.28773000	-1.68862700	0.48638800
C	0.63480000	-1.38846700	1.79680200
C	1.12410400	-2.35356600	-0.39981900
C	1.89389000	-1.79122500	2.23791900
H	-0.04693900	-0.86668100	2.45282000
C	2.37470400	-2.75207000	0.06872300
H	0.81915700	-2.55339200	-1.41752000
C	2.75578100	-2.47237900	1.37978100
H	2.19556300	-1.56682000	3.25413000
H	3.05073300	-3.26988700	-0.60044400
H	3.73372300	-2.77786300	1.73105900
O	-2.15870100	-3.23897100	0.34713400
C	-3.38849400	-3.56678800	0.01949900
O	-4.16600200	-2.78772800	-0.52552700
C	-3.74998100	-4.97901400	0.40242400
H	-3.95533500	-5.00106800	1.47674700
H	-4.64221200	-5.28877200	-0.14000600
H	-2.92182100	-5.65884400	0.20034200
H	-0.85745100	0.60682000	-0.72792100
H	-3.14032700	1.62597900	1.23508200
N	1.81277400	2.06441700	-0.12763800
C	2.24041600	1.04751100	-0.89377200
H	2.47598300	2.40371800	0.55476500
C	3.59149600	0.47103500	-0.57902600
O	1.56854800	0.56938800	-1.82667100
C	4.26089300	-0.23584500	-1.58353000
C	4.16508200	0.55143000	0.69463200
C	5.48754300	-0.83966000	-1.32604900

H	3.80975500	-0.31184900	-2.56490200
C	5.38925000	-0.05940800	0.95492100
H	3.64936600	1.05307300	1.50480900
C	6.05388900	-0.75504400	-0.05364000
H	5.99939700	-1.38020400	-2.11462100
H	5.81551900	-0.00447100	1.94998500
H	7.00513500	-1.23331500	0.15178400

IRC_TS1_point18

B	-2.66029900	4.01250500	0.26290000
B	-1.60979700	3.71207000	1.67144700
B	-0.61948800	2.28368600	1.32704400
B	-2.31316100	2.76705700	-0.96248500
B	-1.04795800	1.76472400	-0.28752400
B	-1.18150500	4.97471400	0.49407800
B	-1.62026600	4.39828800	-1.12821000
H	-3.74653200	4.48612700	0.38167900
B	0.08045100	3.90810100	1.14534000
H	-1.95265900	3.97590100	2.78142600
B	0.43913300	2.66928600	-0.07197400
H	-0.24419100	1.52233400	2.15778300
B	-0.61713400	2.97712300	-1.49464200
H	-3.13916600	2.33763000	-1.70325200
H	-1.22277800	6.13219300	0.77462000
B	0.07513300	4.33641100	-0.58649700
H	-1.97378100	5.13801700	-1.99240200
H	0.93864200	4.29278200	1.87731400
H	-0.27296900	2.69552900	-2.59438400
H	0.92954000	5.01732000	-1.06048500
B	-2.31375900	2.34818100	0.77688400
I	-1.66770900	-1.14471200	-0.19512300
C	0.28687800	-1.68815400	0.48843900
C	0.63135200	-1.38960200	1.79990900
C	1.12501400	-2.35175200	-0.39709400
C	1.88982600	-1.79249300	2.24281800
H	-0.05192100	-0.86907800	2.45545700
C	2.37485200	-2.75048100	0.07328100
H	0.82189400	-2.55046200	-1.41557000
C	2.75352500	-2.47223600	1.38535900
H	2.18953800	-1.56936100	3.25989500
H	3.05216700	-3.26740400	-0.59515800
H	3.73098700	-2.77783600	1.73800200
O	-2.15886100	-3.23927400	0.34481100
C	-3.38800500	-3.56729900	0.01501500

O	-4.16500300	-2.78803200	-0.53021400
C	-3.74914400	-4.98004600	0.39580000
H	-3.95359000	-5.00400400	1.47023800
H	-4.64181000	-5.28897600	-0.14641800
H	-2.92109200	-5.65940900	0.19182000
H	-0.85716300	0.60727400	-0.72665300
H	-3.13899300	1.62623800	1.23725800
N	1.81330900	2.06452300	-0.12766000
C	2.24041500	1.04761900	-0.89437300
H	2.47670800	2.40327600	0.55496000
C	3.59121300	0.47036700	-0.57985800
O	1.56839600	0.57008900	-1.82780200
C	4.26021100	-0.23618400	-1.58469900
C	4.16482700	0.54940500	0.69373700
C	5.48646200	-0.84089900	-1.32761800
H	3.80952800	-0.31095200	-2.56667300
C	5.38875100	-0.06211400	0.95344800
H	3.64910700	1.05040700	1.50439300
C	6.05305800	-0.75736600	-0.05552700
H	5.99707000	-1.38160600	-2.11622100
H	5.81448200	-0.00852900	1.94913800
H	7.00400200	-1.23631100	0.14954300

IRC_TS1_point19

B	-2.65934800	4.01289100	0.26523900
B	-1.60805100	3.71221700	1.67313000
B	-0.61793300	2.28387700	1.32790900
B	-2.31292100	2.76760100	-0.96052700
B	-1.04735400	1.76505900	-0.28643000
B	-1.18042100	4.97501800	0.49572900
B	-1.62009300	4.39883400	-1.12637700
H	-3.74549700	4.48654700	0.38468400
B	0.08190500	3.90831000	1.14609400
H	-1.95028000	3.97588500	2.78334400
B	0.43989200	2.66967300	-0.07163300
H	-0.24217400	1.52244500	2.15833400
B	-0.61721000	2.97768100	-1.49360800
H	-3.13935700	2.33834300	-1.70090700
H	-1.22155800	6.13244800	0.77646200
B	0.07561200	4.33685700	-0.58565100
H	-1.97407500	5.13869000	-1.99025500
H	0.94045200	4.29290500	1.87766500
H	-0.27366800	2.69634400	-2.59362600
H	0.92968700	5.01786100	-1.06004500

B	-2.31254100	2.34848700	0.77875000
I	-1.66746300	-1.14408800	-0.19588000
C	0.28609100	-1.68776400	0.49037200
C	0.62809000	-1.39069200	1.80284300
C	1.12606100	-2.35005400	-0.39440400
C	1.88573700	-1.79386900	2.24769700
H	-0.05641200	-0.87097800	2.45760100
C	2.37516400	-2.74893900	0.07783000
H	0.82497000	-2.54761100	-1.41368400
C	2.75122400	-2.47229700	1.39100800
H	2.18344800	-1.57195900	3.26562800
H	3.05404500	-3.26463600	-0.59011400
H	3.72806200	-2.77816300	1.74512300
O	-2.15873700	-3.23900100	0.34160100
C	-3.38736700	-3.56766900	0.01043100
O	-4.16453800	-2.78860900	-0.53502900
C	-3.74782800	-4.98112400	0.38980100
H	-3.95224900	-5.00641900	1.46423200
H	-4.64022900	-5.29003300	-0.15287500
H	-2.91932700	-5.65978800	0.18516700
H	-0.85595500	0.60801500	-0.72624800
H	-3.13751300	1.62651200	1.23950000
N	1.81396100	2.06468300	-0.12841500
C	2.24017900	1.04751000	-0.89503300
H	2.47784500	2.40308400	0.55375000
C	3.59069600	0.46940800	-0.58096100
O	1.56742300	0.57033300	-1.82784600
C	4.25973700	-0.23648800	-1.58643000
C	4.16392900	0.54726800	0.69301400
C	5.48576300	-0.84180600	-1.32954600
H	3.80881600	-0.31052800	-2.56804500
C	5.38746100	-0.06511600	0.95269000
H	3.64831200	1.04808200	1.50380000
C	6.05177700	-0.75973600	-0.05680700
H	5.99752700	-1.38144500	-2.11889100
H	5.81353100	-0.01211600	1.94790600
H	7.00254000	-1.23916900	0.14808200
IRC_TS1_point20			
B	-2.65842600	4.01327700	0.26749700
B	-1.60640000	3.71229200	1.67479300
B	-0.61654900	2.28399100	1.32878500
B	-2.31270000	2.76824300	-0.95871700
B	-1.04683900	1.76566000	-0.28546600
B	-1.17931700	4.97532200	0.49740000

B	-1.61988300	4.39950400	-1.12459400
H	-3.74449500	4.48694000	0.38759000
B	0.08329000	3.90841800	1.14689900
H	-1.94801200	3.97576100	2.78523900
B	0.44057700	2.67005700	-0.07125400
H	-0.24030300	1.52231000	2.15878500
B	-0.61726300	2.97842700	-1.49266300
H	-3.13953800	2.33914100	-1.69874000
H	-1.22021500	6.13270000	0.77840400
B	0.07611900	4.33735200	-0.58479100
H	-1.97431800	5.13957100	-1.98811900
H	0.94228900	4.29277700	1.87808700
H	-0.27432300	2.69718000	-2.59287500
H	0.93003200	5.01839400	-1.05947400
B	-2.31142900	2.34873700	0.78052300
I	-1.66729000	-1.14365900	-0.19676200
C	0.28529200	-1.68724600	0.49244200
C	0.62453600	-1.39176300	1.80598300
C	1.12712500	-2.34818600	-0.39156800
C	1.88151800	-1.79500700	2.25274800
H	-0.06164600	-0.87341300	2.46022200
C	2.37536700	-2.74730000	0.08264900
H	0.82796600	-2.54466800	-1.41162700
C	2.74888800	-2.47203800	1.39685100
H	2.17712900	-1.57436600	3.27156800
H	3.05552600	-3.26221500	-0.58443100
H	3.72507800	-2.77809300	1.75250900
O	-2.15885200	-3.23933200	0.33919600
C	-3.38689300	-3.56821200	0.00609300
O	-4.16364400	-2.78894100	-0.53952200
C	-3.74704100	-4.98218600	0.38339100
H	-3.95088300	-5.00932200	1.45784300
H	-4.63965400	-5.29028100	-0.15933300
H	-2.91856800	-5.66038400	0.17712100
H	-0.85555000	0.60847300	-0.72507400
H	-3.13620600	1.62671100	1.24156800
N	1.81451800	2.06491700	-0.12864900
C	2.24019100	1.04767300	-0.89568000
H	2.47856900	2.40276900	0.55382200
C	3.59045100	0.46884800	-0.58185400
O	1.56720800	0.57095600	-1.82874500
C	4.25900600	-0.23688100	-1.58756200
C	4.16381000	0.54549900	0.69198600
C	5.48459400	-0.84317300	-1.33102600

H	3.80852100	-0.30976500	-2.56978300
C	5.38707300	-0.06761700	0.95113000
H	3.64833900	1.04582500	1.50319800
C	6.05092800	-0.76208800	-0.05864900
H	5.99479200	-1.38328300	-2.12023100
H	5.81255400	-0.01597200	1.94706500
H	7.00132300	-1.24232300	0.14602800

IRC_TS1_point21

B	-2.65750600	4.01360200	0.26977000
B	-1.60468700	3.71240800	1.67640900
B	-0.61502100	2.28416400	1.32959900
B	-2.31246700	2.76873400	-0.95682200
B	-1.04623100	1.76599900	-0.28443800
B	-1.17827700	4.97559400	0.49897700
B	-1.61974700	4.40000800	-1.12283200
H	-3.74349900	4.48727700	0.39053200
B	0.08470800	3.90860700	1.14758200
H	-1.94566300	3.97571600	2.78709000
B	0.44130900	2.67041000	-0.07096400
H	-0.23827900	1.52240900	2.15927500
B	-0.61735100	2.97897200	-1.49169900
H	-3.13973400	2.33977700	-1.69644500
H	-1.21905100	6.13292000	0.78018300
B	0.07656500	4.33777800	-0.58401800
H	-1.97467600	5.14019100	-1.98603700
H	0.94407100	4.29287600	1.87836600
H	-0.27503900	2.69793500	-2.59216700
H	0.93014300	5.01892700	-1.05909700
B	-2.31021800	2.34899200	0.78233800
I	-1.66703400	-1.14311200	-0.19758100
C	0.28443100	-1.68685300	0.49449200
C	0.62112900	-1.39276000	1.80901900
C	1.12814700	-2.34651300	-0.38867200
C	1.87733700	-1.79616300	2.25777900
H	-0.06631900	-0.87519800	2.46241500
C	2.37570600	-2.74564200	0.08744900
H	0.83104700	-2.54192700	-1.40952500
C	2.74659000	-2.47184900	1.40272200
H	2.17092200	-1.57664600	3.27743000
H	3.05751600	-3.25929100	-0.57907200
H	3.72230800	-2.77795600	1.75981200
O	-2.15867200	-3.23913500	0.33606900
C	-3.38622200	-3.56851200	0.00158700

O	-4.16305100	-2.78935100	-0.54415000
C	-3.74576700	-4.98312300	0.37746700
H	-3.94957800	-5.01149700	1.45193500
H	-4.63820000	-5.29121200	-0.16565500
H	-2.91689700	-5.66066800	0.17059800
H	-0.85447700	0.60912500	-0.72463600
H	-3.13471900	1.62692000	1.24376100
N	1.81512600	2.06497500	-0.12926800
C	2.23996800	1.04752600	-0.89636600
H	2.47965900	2.40252300	0.55267400
C	3.58993700	0.46785300	-0.58293200
O	1.56635600	0.57122700	-1.82909700
C	4.25852600	-0.23726900	-1.58926200
C	4.16291700	0.54339800	0.69129200
C	5.48392300	-0.84407900	-1.33295600
H	3.80777700	-0.30949900	-2.57110600
C	5.38581800	-0.07050800	0.95037100
H	3.64750500	1.04356200	1.50262300
C	6.04971500	-0.76432200	-0.05997200
H	5.99543900	-1.38301300	-2.12298200
H	5.81174400	-0.01927600	1.94571300
H	6.99999800	-1.24489600	0.14439500

IRC_TS1_point22

B	-2.65661500	4.01395100	0.27196600
B	-1.60307000	3.71244000	1.67801600
B	-0.61364300	2.28424600	1.33040400
B	-2.31226300	2.76933700	-0.95507200
B	-1.04572800	1.76652000	-0.28352600
B	-1.17721900	4.97586600	0.50060700
B	-1.61956100	4.40064400	-1.12109500
H	-3.74252900	4.48763300	0.39336700
B	0.08605700	3.90870000	1.14834700
H	-1.94344400	3.97554000	2.78892500
B	0.44198500	2.67080000	-0.07064700
H	-0.23643200	1.52226000	2.15967000
B	-0.61741900	2.97967300	-1.49079100
H	-3.13992300	2.34054900	-1.69436000
H	-1.21777400	6.13314000	0.78207400
B	0.07703500	4.33825700	-0.58319000
H	-1.97492700	5.14104000	-1.98395300
H	0.94584700	4.29275600	1.87875700
H	-0.27568700	2.69878800	-2.59147200
H	0.93043500	5.01945800	-1.05856100

B	-2.30912500	2.34920300	0.78403500
I	-1.66680400	-1.14270000	-0.19851700
C	0.28367300	-1.68630500	0.49655700
C	0.61752700	-1.39371500	1.81214000
C	1.12934000	-2.34463500	-0.38574000
C	1.87297400	-1.79716800	2.26294600
H	-0.07160900	-0.87743100	2.46486400
C	2.37596100	-2.74398000	0.09249400
H	0.83430400	-2.53900700	-1.40738400
C	2.74415000	-2.47152300	1.40880800
H	2.16435600	-1.57887000	3.28348800
H	3.05912700	-3.25684400	-0.57311900
H	3.71906000	-2.77789700	1.76760500
O	-2.15872200	-3.23944900	0.33350900
C	-3.38574100	-3.56908000	-0.00264800
O	-4.16228100	-2.78975400	-0.54854100
C	-3.74498600	-4.98420900	0.37134000
H	-3.94865400	-5.01424500	1.44573100
H	-4.63734900	-5.29162300	-0.17214600
H	-2.91600300	-5.66127300	0.16328600
H	-0.85388700	0.60961300	-0.72363200
H	-3.13342600	1.62707500	1.24574800
N	1.81571000	2.06531900	-0.12975600
C	2.23995900	1.04770100	-0.89702200
H	2.48042500	2.40233100	0.55250300
C	3.58969400	0.46734600	-0.58387500
O	1.56599600	0.57173200	-1.82967300
C	4.25775700	-0.23773000	-1.59038400
C	4.16288000	0.54185300	0.69016100
C	5.48269900	-0.84555000	-1.33436000
H	3.80737300	-0.30893700	-2.57276300
C	5.38549500	-0.07281300	0.94877400
H	3.64769200	1.04165300	1.50188000
C	6.04884000	-0.76668200	-0.06173200
H	5.99252600	-1.38516100	-2.12413400
H	5.81080500	-0.02290600	1.94489600
H	6.99869900	-1.24817100	0.14257100

IRC_TS1_point23

B	-2.65572400	4.01422400	0.27417700
B	-1.60140500	3.71252000	1.67957900
B	-0.61216500	2.28439000	1.33119200
B	-2.31203800	2.76979400	-0.95324200
B	-1.04513100	1.76689000	-0.28255500

B	-1.17621000	4.97610300	0.50213100
B	-1.61944500	4.40111900	-1.11939000
H	-3.74157000	4.48789900	0.39623800
B	0.08743300	3.90885400	1.14899300
H	-1.94115300	3.97545400	2.79072100
B	0.44268800	2.67111200	-0.07037100
H	-0.23444900	1.52229900	2.16011200
B	-0.61751100	2.98021900	-1.48988400
H	-3.14011300	2.34112300	-1.69212000
H	-1.21664100	6.13332400	0.78381300
B	0.07746400	4.33865800	-0.58246100
H	-1.97531600	5.14162900	-1.98192400
H	0.94759600	4.29280500	1.87900100
H	-0.27640200	2.69948600	-2.59079300
H	0.93054800	5.01996200	-1.05820500
B	-2.30794100	2.34941100	0.78579800
I	-1.66654100	-1.14224100	-0.19940900
C	0.28276200	-1.68587700	0.49871100
C	0.61397400	-1.39458500	1.81526600
C	1.13034700	-2.34298900	-0.38264400
C	1.86873700	-1.79802000	2.26809300
H	-0.07658000	-0.87920300	2.46717900
C	2.37630400	-2.74223600	0.09755600
H	0.83735500	-2.53643300	-1.40504700
C	2.74188300	-2.47102600	1.41487300
H	2.15806400	-1.58073200	3.28944100
H	3.06108500	-3.25396900	-0.56733200
H	3.71644600	-2.77724800	1.77507900
O	-2.15850700	-3.23937200	0.33048200
C	-3.38506000	-3.56934000	-0.00707600
O	-4.16154500	-2.79000700	-0.55299400
C	-3.74382600	-4.98501700	0.36546500
H	-3.94751500	-5.01620000	1.43987400
H	-4.63606700	-5.29238000	-0.17840300
H	-2.91451900	-5.66150800	0.15687800
H	-0.85303200	0.61017200	-0.72309000
H	-3.13196900	1.62722500	1.24787800
N	1.81626600	2.06528200	-0.13018700
C	2.23976700	1.04754400	-0.89773600
H	2.48142400	2.40201800	0.55155800
C	3.58921200	0.46635900	-0.58492400
O	1.56531200	0.57205000	-1.83034700
C	4.25723500	-0.23821300	-1.59200700
C	4.16206200	0.53982400	0.68947100

C	5.48200400	-0.84650100	-1.33627000
H	3.80660800	-0.30879200	-2.57407100
C	5.38433500	-0.07558100	0.94796900
H	3.64698200	1.03953700	1.50128200
C	6.04769900	-0.76881600	-0.06312700
H	5.99309800	-1.38495200	-2.12687600
H	5.81019600	-0.02593700	1.94339900
H	6.99750400	-1.25052000	0.14074300

IRC_TS1_point24

B	-2.65485400	4.01455500	0.27633000
B	-1.59981000	3.71252800	1.68114100
B	-0.61079200	2.28444900	1.33193600
B	-2.31185100	2.77036600	-0.95153000
B	-1.04464200	1.76731700	-0.28167800
B	-1.17518400	4.97635400	0.50372700
B	-1.61927500	4.40172400	-1.11768700
H	-3.74061900	4.48825000	0.39902500
B	0.08875900	3.90893400	1.14972000
H	-1.93895800	3.97525500	2.79251100
B	0.44334800	2.67149700	-0.07011200
H	-0.23261400	1.52217400	2.16047100
B	-0.61759700	2.98086800	-1.48899800
H	-3.14032300	2.34189400	-1.69009400
H	-1.21541100	6.13352400	0.78566100
B	0.07790600	4.33911900	-0.58166000
H	-1.97556900	5.14245000	-1.97987700
H	0.94932900	4.29269000	1.87936400
H	-0.27705300	2.70034600	-2.59014200
H	0.93078800	5.02048900	-1.05770400
B	-2.30686300	2.34960200	0.78744200
I	-1.66626200	-1.14184500	-0.20040200
C	0.28201700	-1.68531700	0.50077300
C	0.61036400	-1.39536300	1.81833700
C	1.13161000	-2.34116200	-0.37960400
C	1.86425900	-1.79885200	2.27334600
H	-0.08174800	-0.88099700	2.46934500
C	2.37659800	-2.74056600	0.10280700
H	0.84081300	-2.53361100	-1.40280600
C	2.73933800	-2.47063800	1.42118100
H	2.15133600	-1.58266600	3.29556000
H	3.06289000	-3.25140900	-0.56120400
H	3.71299300	-2.77715700	1.78321200
O	-2.15846900	-3.23965100	0.32774900

C	-3.38454400	-3.56991600	-0.01123800
O	-4.16087900	-2.79048500	-0.55732800
C	-3.74300200	-4.98610400	0.35964300
H	-3.94696900	-5.01871200	1.43389300
H	-4.63490600	-5.29299200	-0.18487800
H	-2.91342400	-5.66208800	0.15036800
H	-0.85223600	0.61069100	-0.72228200
H	-3.13068300	1.62736200	1.24981400
N	1.81686500	2.06568200	-0.13090000
C	2.23970900	1.04767600	-0.89836800
H	2.48225300	2.40191300	0.55108100
C	3.58894100	0.46584400	-0.58590300
O	1.56476700	0.57240800	-1.83059800
C	4.25645500	-0.23873800	-1.59315800
C	4.16204600	0.53844300	0.68827600
C	5.48077800	-0.84802200	-1.33763400
H	3.80605800	-0.30847700	-2.57559200
C	5.38404100	-0.07770200	0.94636500
H	3.64718400	1.03785400	1.50046300
C	6.04681500	-0.77113300	-0.06480800
H	5.99025500	-1.38722300	-2.12795200
H	5.80926500	-0.02932800	1.94262400
H	6.99616500	-1.25381200	0.13911400

IRC_TS1_point25

B	-2.65399500	4.01478400	0.27848100
B	-1.59819800	3.71257500	1.68266300
B	-0.60937000	2.28456900	1.33271300
B	-2.31163500	2.77079400	-0.94975600
B	-1.04406700	1.76773400	-0.28074600
B	-1.17420900	4.97655800	0.50520700
B	-1.61917600	4.40217400	-1.11603200
H	-3.73969700	4.48844700	0.40181900
B	0.09008700	3.90905900	1.15034600
H	-1.93674200	3.97513200	2.79425700
B	0.44402500	2.67177900	-0.06983200
H	-0.23069600	1.52214200	2.16088300
B	-0.61769200	2.98141600	-1.48813400
H	-3.14049700	2.34239800	-1.68790000
H	-1.21431100	6.13367400	0.78735700
B	0.07831800	4.33949300	-0.58095900
H	-1.97597700	5.14300100	-1.97790300
H	0.95103200	4.29270200	1.87958800
H	-0.27776000	2.70099000	-2.58947700

H	0.93091000	5.02095500	-1.05735800
B	-2.30571500	2.34976700	0.78916000
I	-1.66598400	-1.14147600	-0.20136600
C	0.28109400	-1.68483100	0.50300300
C	0.60669300	-1.39607100	1.82152500
C	1.13262900	-2.33954200	-0.37633400
C	1.86000000	-1.79935100	2.27856800
H	-0.08705900	-0.88280300	2.47179500
C	2.37693800	-2.73877200	0.10811600
H	0.84383600	-2.53124200	-1.40024700
C	2.73711900	-2.46981700	1.42740300
H	2.14498400	-1.58405700	3.30156000
H	3.06472200	-3.24874300	-0.55495200
H	3.71048600	-2.77603500	1.79085400
O	-2.15823100	-3.23970600	0.32479700
C	-3.38387400	-3.57017300	-0.01557900
O	-4.16003300	-2.79063000	-0.56161700
C	-3.74199200	-4.98682100	0.35385300
H	-3.94605700	-5.02048900	1.42811200
H	-4.63380800	-5.29359400	-0.19105500
H	-2.91217200	-5.66233200	0.14411800
H	-0.85161700	0.61117200	-0.72161200
H	-3.12926900	1.62746200	1.25188300
N	1.81737300	2.06559200	-0.13118400
C	2.23954800	1.04753700	-0.89912100
H	2.48314400	2.40154700	0.55038500
C	3.58849500	0.46489500	-0.58692300
O	1.56424100	0.57277400	-1.83154100
C	4.25584700	-0.23933300	-1.59466800
C	4.16134900	0.53652900	0.68756100
C	5.48000400	-0.84906200	-1.33949800
H	3.80528900	-0.30842200	-2.57694600
C	5.38300900	-0.08033900	0.94548800
H	3.64672000	1.03597700	1.49979500
C	6.04573000	-0.77320700	-0.06627400
H	5.99054200	-1.38722300	-2.13060400
H	5.80890300	-0.03209100	1.94094900
H	6.99506700	-1.25601600	0.13712400

IRC_TS1_point26

B	-2.65313800	4.01511600	0.28059800
B	-1.59661800	3.71258100	1.68418700
B	-0.60801300	2.28461300	1.33341100
B	-2.31146700	2.77134600	-0.94807300

B	-1.04359900	1.76806700	-0.27989500
B	-1.17319500	4.97680100	0.50676800
B	-1.61901400	4.40275600	-1.11436000
H	-3.73875400	4.48882600	0.40456700
B	0.09140100	3.90912500	1.15103600
H	-1.93455500	3.97494000	2.79601000
B	0.44466000	2.67213700	-0.06961800
H	-0.22887900	1.52205500	2.16122200
B	-0.61779700	2.98201200	-1.48726500
H	-3.14074600	2.34319200	-1.68592600
H	-1.21309600	6.13386800	0.78916900
B	0.07874400	4.33993100	-0.58018600
H	-1.97622200	5.14381200	-1.97588900
H	0.95274400	4.29257500	1.87992700
H	-0.27842500	2.70183900	-2.58886100
H	0.93111700	5.02147300	-1.05688900
B	-2.30465600	2.34995600	0.79076700
I	-1.66567300	-1.14110700	-0.20241500
C	0.28032800	-1.68427900	0.50508500
C	0.60310100	-1.39662300	1.82453700
C	1.13389600	-2.33783100	-0.37315200
C	1.85545900	-1.79994400	2.28387700
H	-0.09201100	-0.88402100	2.47365300
C	2.37724600	-2.73711300	0.11357000
H	0.84740100	-2.52861700	-1.39786200
C	2.73449300	-2.46933900	1.43391200
H	2.13819700	-1.58557000	3.30768300
H	3.06671600	-3.24605800	-0.54867200
H	3.70693800	-2.77580600	1.79924500
O	-2.15810000	-3.23996300	0.32192600
C	-3.38330900	-3.57074200	-0.01967700
O	-4.15942500	-2.79116000	-0.56589800
C	-3.74110700	-4.98788100	0.34831400
H	-3.94569100	-5.02276100	1.42237600
H	-4.63243100	-5.29434200	-0.19739800
H	-2.91090700	-5.66287000	0.13823500
H	-0.85063200	0.61170200	-0.72096200
H	-3.12800100	1.62760300	1.25379000
N	1.81796500	2.06597000	-0.13202200
C	2.23943000	1.04758100	-0.89970200
H	2.48403300	2.40148300	0.54960800
C	3.58819100	0.46434500	-0.58794500
O	1.56352000	0.57296800	-1.83152100
C	4.25508700	-0.23989900	-1.59589300

C	4.16132200	0.53526300	0.68632000
C	5.47882500	-0.85057700	-1.34087500
H	3.80453900	-0.30838500	-2.57825700
C	5.38273600	-0.08227900	0.94387300
H	3.64684100	1.03440800	1.49894900
C	6.04487400	-0.77542200	-0.06791700
H	5.98792600	-1.38947100	-2.13170500
H	5.80795100	-0.03524600	1.94023500
H	6.99375000	-1.25921500	0.13559400

IRC_TS1_point27

B	-2.65230800	4.01530600	0.28270400
B	-1.59505300	3.71260900	1.68567900
B	-0.60662700	2.28472700	1.33419000
B	-2.31126100	2.77174600	-0.94633200
B	-1.04304300	1.76853500	-0.27897500
B	-1.17225900	4.97698100	0.50821000
B	-1.61893400	4.40317800	-1.11274300
H	-3.73786700	4.48895700	0.40729600
B	0.09268600	3.90924000	1.15165100
H	-1.93241300	3.97479900	2.79771400
B	0.44531900	2.67241700	-0.06933400
H	-0.22701400	1.52198100	2.16162400
B	-0.61789700	2.98255900	-1.48642300
H	-3.14089500	2.34361700	-1.68375200
H	-1.21204000	6.13399200	0.79081100
B	0.07913200	4.34028900	-0.57950500
H	-1.97665100	5.14430700	-1.97396800
H	0.95439500	4.29258900	1.88013300
H	-0.27912200	2.70243400	-2.58819300
H	0.93123800	5.02189900	-1.05656100
B	-2.30353500	2.35008900	0.79245700
I	-1.66536900	-1.14082000	-0.20344400
C	0.27942700	-1.68372900	0.50737000
C	0.59937100	-1.39713500	1.82775400
C	1.13495800	-2.33623400	-0.36974500
C	1.85120900	-1.80008100	2.28913700
H	-0.09758800	-0.88580700	2.47619000
C	2.37759100	-2.73529600	0.11908500
H	0.85041600	-2.52646000	-1.39510900
C	2.73232800	-2.46821900	1.44025000
H	2.13182100	-1.58648300	3.31369500
H	3.06840300	-3.24365400	-0.54201300
H	3.70446900	-2.77431200	1.80704700

O	-2.15784200	-3.24013300	0.31899100
C	-3.38266200	-3.57103100	-0.02392700
O	-4.15853300	-2.79127100	-0.57004800
C	-3.74022700	-4.98856000	0.34267100
H	-3.94490900	-5.02441800	1.41673700
H	-4.63151800	-5.29484000	-0.20337900
H	-2.90988000	-5.66317900	0.13215000
H	-0.85021700	0.61213400	-0.72016300
H	-3.12661700	1.62766700	1.25582200
N	1.81844100	2.06589600	-0.13227700
C	2.23927900	1.04747700	-0.90050500
H	2.48482500	2.40108600	0.54914000
C	3.58775100	0.46342600	-0.58891900
O	1.56308800	0.57337200	-1.83264300
C	4.25434100	-0.24062700	-1.59726100
C	4.16075400	0.53347800	0.68556600
C	5.47791900	-0.85173800	-1.34266800
H	3.80381700	-0.30836700	-2.57977500
C	5.38183000	-0.08479000	0.94291300
H	3.64668700	1.03282800	1.49817200
C	6.04380400	-0.77747800	-0.06944000
H	5.98781300	-1.38975300	-2.13422100
H	5.80788100	-0.03773800	1.93832200
H	6.99269900	-1.26134800	0.13350200

IRC_TS1_point28

B	-2.65146000	4.01565000	0.28478200
B	-1.59348900	3.71262400	1.68716700
B	-0.60530300	2.28476100	1.33485900
B	-2.31111000	2.77228500	-0.94468100
B	-1.04259700	1.76878900	-0.27814600
B	-1.17124200	4.97722000	0.50973500
B	-1.61876800	4.40374400	-1.11110500
H	-3.73692700	4.48938200	0.40999800
B	0.09398900	3.90929000	1.15231200
H	-1.93023400	3.97463000	2.79943300
B	0.44592400	2.67272500	-0.06913800
H	-0.22523200	1.52192100	2.16195600
B	-0.61801700	2.98310600	-1.48557500
H	-3.14118700	2.34444400	-1.68182600
H	-1.21081700	6.13419000	0.79258900
B	0.07955900	4.34069400	-0.57875900
H	-1.97687700	5.14512300	-1.97198400
H	0.95609900	4.29243500	1.88045600

H	-0.27979900	2.70325400	-2.58760700
H	0.93143200	5.02240100	-1.05611100
B	-2.30250200	2.35028800	0.79403600
I	-1.66505000	-1.14048800	-0.20454400
C	0.27860100	-1.68320100	0.50950900
C	0.59580100	-1.39744600	1.83073100
C	1.13615500	-2.33469000	-0.36637600
C	1.84666400	-1.80037900	2.29448300
H	-0.10233700	-0.88646700	2.47782300
C	2.37787900	-2.73366400	0.12474700
H	0.85396400	-2.52412200	-1.39251900
C	2.72966500	-2.46760200	1.44692900
H	2.12508700	-1.58746500	3.31977600
H	3.07050700	-3.24091100	-0.53555100
H	3.70096100	-2.77381300	1.81559300
O	-2.15762200	-3.24040800	0.31601100
C	-3.38205100	-3.57158600	-0.02797500
O	-4.15794000	-2.79181700	-0.57425800
C	-3.73928800	-4.98956400	0.33737500
H	-3.94440100	-5.02648700	1.41127300
H	-4.63012600	-5.29559700	-0.20937700
H	-2.90855800	-5.66368200	0.12655300
H	-0.84907900	0.61264700	-0.71959900
H	-3.12538200	1.62782600	1.25770000
N	1.81900200	2.06616900	-0.13308500
C	2.23910800	1.04740600	-0.90102400
H	2.48576800	2.40104200	0.54808700
C	3.58744600	0.46285800	-0.59003400
O	1.56223600	0.57339000	-1.83243400
C	4.25363800	-0.24120800	-1.59861200
C	4.16071600	0.53231200	0.68426500
C	5.47683400	-0.85319700	-1.34413500
H	3.80276500	-0.30867700	-2.58073900
C	5.38158900	-0.08654900	0.94126700
H	3.64667200	1.03130300	1.49732100
C	6.04302700	-0.77953300	-0.07111500
H	5.98550500	-1.39190200	-2.13543200
H	5.80686000	-0.04067700	1.93772500
H	6.99147300	-1.26435500	0.13194900

IRC_TS1_point29

B	-2.65065400	4.01581200	0.28685400
B	-1.59195700	3.71264400	1.68863700
B	-0.60393000	2.28488200	1.33563600

B	-2.31091200	2.77266000	-0.94295500
B	-1.04205900	1.76930000	-0.27722000
B	-1.17034400	4.97738500	0.51114700
B	-1.61871000	4.40413900	-1.10951600
H	-3.73607100	4.48945600	0.41266700
B	0.09524200	3.90941200	1.15291300
H	-1.92815800	3.97448600	2.80109900
B	0.44657400	2.67303400	-0.06887500
H	-0.22339700	1.52184500	2.16235300
B	-0.61812300	2.98364900	-1.48473700
H	-3.14130400	2.34479700	-1.67966900
H	-1.20981300	6.13429900	0.79416900
B	0.07991500	4.34105200	-0.57809300
H	-1.97732200	5.14555300	-1.97011700
H	0.95770200	4.29247800	1.88064400
H	-0.28048500	2.70381000	-2.58692600
H	0.93154300	5.02279200	-1.05581200
B	-2.30139500	2.35039800	0.79570700
I	-1.66471300	-1.14027200	-0.20561100
C	0.27775900	-1.68258700	0.51183900
C	0.59208900	-1.39775000	1.83395300
C	1.13728900	-2.33308800	-0.36288000
C	1.84245700	-1.80018900	2.29974800
H	-0.10800200	-0.88810900	2.48035600
C	2.37824500	-2.73181700	0.13039800
H	0.85700500	-2.52211800	-1.38962500
C	2.72754800	-2.46623300	1.45333200
H	2.11874800	-1.58794900	3.32576200
H	3.07209600	-3.23868300	-0.52864400
H	3.69845400	-2.77206700	1.82351800
O	-2.15731800	-3.24066000	0.31300900
C	-3.38141500	-3.57193900	-0.03213600
O	-4.15707200	-2.79196600	-0.57826700
C	-3.73846100	-4.99026000	0.33193600
H	-3.94343500	-5.02810200	1.40586900
H	-4.62942200	-5.29603200	-0.21491700
H	-2.90771900	-5.66412100	0.12051000
H	-0.84882700	0.61306000	-0.71869700
H	-3.12401200	1.62786700	1.25970900
N	1.81947200	2.06621100	-0.13351200
C	2.23892600	1.04734400	-0.90188600
H	2.48649000	2.40064100	0.54778700
C	3.58694600	0.46192000	-0.59091900
O	1.56179000	0.57381200	-1.83362100

C	4.25270000	-0.24209200	-1.59982700
C	4.16026300	0.53065900	0.68345800
C	5.47573200	-0.85452600	-1.34581000
H	3.80222100	-0.30857900	-2.58265500
C	5.38080300	-0.08891600	0.94018900
H	3.64688400	1.03008400	1.49638500
C	6.04191100	-0.78162400	-0.07266100
H	5.98493700	-1.39248700	-2.13778000
H	5.80717800	-0.04281700	1.93542000
H	6.99040100	-1.26648600	0.12982600
IRC_TS1_point30			
B	-2.64981900	4.01616100	0.28887600
B	-1.59042200	3.71267100	1.69007300
B	-0.60265800	2.28490600	1.33627600
B	-2.31077600	2.77318100	-0.94135300
B	-1.04163300	1.76949500	-0.27643000
B	-1.16932600	4.97761600	0.51261300
B	-1.61854400	4.40468400	-1.10793200
H	-3.73514000	4.48990900	0.41530100
B	0.09652400	3.90943600	1.15353300
H	-1.92600500	3.97434000	2.80276700
B	0.44714500	2.67326200	-0.06867800
H	-0.22168500	1.52177700	2.16266900
B	-0.61826300	2.98414900	-1.48393800
H	-3.14163500	2.34562800	-1.67778400
H	-1.20858800	6.13449400	0.79588900
B	0.08034700	4.34140600	-0.57739300
H	-1.97754100	5.14636100	-1.96818400
H	0.95938400	4.29229300	1.88093200
H	-0.28117800	2.70457900	-2.58639000
H	0.93172600	5.02326900	-1.05539300
B	-2.30039700	2.35060900	0.79724700
I	-1.66441200	-1.13998400	-0.20671900
C	0.27683900	-1.68208800	0.51409800
C	0.58853300	-1.39785200	1.83695800
C	1.13834200	-2.33171700	-0.35928500
C	1.83799000	-1.80016200	2.30511000
H	-0.11265600	-0.88840900	2.48197700
C	2.37848800	-2.73019100	0.13624000
H	0.86037100	-2.52011300	-1.38676200
C	2.72493900	-2.46539800	1.46010700
H	2.11220500	-1.58836600	3.33176400
H	3.07417800	-3.23594800	-0.52198700
H	3.69518400	-2.77113500	1.83204100

O	-2.15702000	-3.24101400	0.30997200
C	-3.38077300	-3.57247800	-0.03612100
O	-4.15646900	-2.79246000	-0.58228900
C	-3.73745500	-4.99121900	0.32678800
H	-3.94232500	-5.03012100	1.40066200
H	-4.62824200	-5.29669100	-0.22033900
H	-2.90644200	-5.66461900	0.11469900
H	-0.84764200	0.61352900	-0.71817300
H	-3.12282400	1.62804100	1.26153500
N	1.81997900	2.06628600	-0.13411100
C	2.23873500	1.04715500	-0.90239700
H	2.48749500	2.40065200	0.54641200
C	3.58672200	0.46141600	-0.59226100
O	1.56088400	0.57364100	-1.83336100
C	4.25209300	-0.24268500	-1.60136400
C	4.16022800	0.52961900	0.68204500
C	5.47480200	-0.85587800	-1.34748000
H	3.80066700	-0.30942900	-2.58301100
C	5.38057600	-0.09051500	0.93851700
H	3.64666200	1.02856900	1.49551900
C	6.04126600	-0.78345000	-0.07445600
H	5.98297600	-1.39453400	-2.13917000
H	5.80594000	-0.04564300	1.93510800
H	6.98933100	-1.26920300	0.12814800

IRC_TS1_point31

B	-2.64904000	4.01632100	0.29091300
B	-1.58890100	3.71268900	1.69150700
B	-0.60128000	2.28502600	1.33700600
B	-2.31061800	2.77354900	-0.93964900
B	-1.04114200	1.77000800	-0.27551700
B	-1.16846100	4.97778200	0.51398200
B	-1.61852000	4.40506900	-1.10638400
H	-3.73431600	4.48997600	0.41791200
B	0.09776400	3.90956400	1.15408200
H	-1.92396200	3.97421500	2.80438100
B	0.44777000	2.67362200	-0.06852600
H	-0.21985300	1.52173500	2.16303300
B	-0.61840600	2.98467800	-1.48311300
H	-3.14177000	2.34596700	-1.67568400
H	-1.20761200	6.13461100	0.79739200
B	0.08065200	4.34177800	-0.57677600
H	-1.97800600	5.14675900	-1.96638700
H	0.96097000	4.29235300	1.88106800

H	-0.28188700	2.70510900	-2.58572000
H	0.93181300	5.02362700	-1.05517000
B	-2.29930700	2.35071000	0.79889000
I	-1.66405100	-1.13983900	-0.20775300
C	0.27609400	-1.68139400	0.51644600
C	0.58495200	-1.39792700	1.84014100
C	1.13957900	-2.33005100	-0.35576600
C	1.83386600	-1.79970400	2.31033400
H	-0.11809700	-0.88969600	2.48434800
C	2.37888800	-2.72827600	0.14192500
H	0.86351600	-2.51811300	-1.38382200
C	2.72282800	-2.46386800	1.46651900
H	2.10598300	-1.58849900	3.33767100
H	3.07575600	-3.23371000	-0.51506900
H	3.69251900	-2.76931700	1.84004800
O	-2.15661300	-3.24131500	0.30690600
C	-3.38009900	-3.57292200	-0.04011900
O	-4.15568300	-2.79267900	-0.58602400
C	-3.73654100	-4.99204400	0.32150900
H	-3.94068900	-5.03201200	1.39550500
H	-4.62775100	-5.29706500	-0.22528800
H	-2.90571300	-5.66524400	0.10824700
H	-0.84753700	0.61392500	-0.71724800
H	-3.12147200	1.62807700	1.26351700
N	1.82047500	2.06657100	-0.13501300
C	2.23848300	1.04713400	-0.90331300
H	2.48816700	2.40027700	0.54619800
C	3.58607500	0.46038300	-0.59298800
O	1.56029100	0.57402700	-1.83445000
C	4.25095000	-0.24370200	-1.60246600
C	4.15988900	0.52811100	0.68114500
C	5.47344300	-0.85743400	-1.34897300
H	3.80057800	-0.30897000	-2.58574700
C	5.37996100	-0.09263800	0.93719700
H	3.64734900	1.02782400	1.49432500
C	6.04005800	-0.78563400	-0.07600400
H	5.98193400	-1.39541100	-2.14134200
H	5.80685200	-0.04716300	1.93209800
H	6.98817500	-1.27140700	0.12602500

IRC_TS1_point32

B	-2.64822600	4.01664100	0.29288000
B	-1.58737500	3.71272400	1.69286400
B	-0.60004900	2.28505800	1.33759400

B	-2.31052100	2.77403600	-0.93809200
B	-1.04074700	1.77020300	-0.27480300
B	-1.16745700	4.97798800	0.51532900
B	-1.61841100	4.40556700	-1.10488600
H	-3.73340400	4.49037900	0.42050400
B	0.09901900	3.90957900	1.15458700
H	-1.92179400	3.97407100	2.80597900
B	0.44830900	2.67375900	-0.06834300
H	-0.21817400	1.52164100	2.16328700
B	-0.61860700	2.98514500	-1.48243000
H	-3.14215200	2.34671300	-1.67375700
H	-1.20641300	6.13477300	0.79898600
B	0.08106300	4.34206500	-0.57620100
H	-1.97831900	5.14748200	-1.96453300
H	0.96263300	4.29217500	1.88120400
H	-0.28267700	2.70580200	-2.58528500
H	0.93193700	5.02406400	-1.05488900
B	-2.29833100	2.35091800	0.80039600
I	-1.66378900	-1.13960800	-0.20879900
C	0.27508900	-1.68088400	0.51882000
C	0.58138700	-1.39785600	1.84319800
C	1.14048600	-2.32879600	-0.35199600
C	1.82956500	-1.79932100	2.31564800
H	-0.12292300	-0.88999700	2.48619900
C	2.37912200	-2.72658400	0.14785000
H	0.86655300	-2.51647400	-1.38068300
C	2.72043700	-2.46267400	1.47323500
H	2.09970000	-1.58839300	3.34355800
H	3.07772800	-3.23103600	-0.50823200
H	3.68973200	-2.76775100	1.84833800
O	-2.15627400	-3.24177000	0.30407800
C	-3.37943900	-3.57344000	-0.04390700
O	-4.15503400	-2.79301600	-0.58955900
C	-3.73539000	-4.99306600	0.31623400
H	-3.93868800	-5.03451700	1.39031700
H	-4.62679600	-5.29762300	-0.23039400
H	-2.90443000	-5.66571900	0.10154800
H	-0.84653700	0.61434600	-0.71676100
H	-3.12029600	1.62825300	1.26533300
N	1.82088900	2.06635600	-0.13521500
C	2.23831800	1.04687300	-0.90396600
H	2.48923600	2.40043100	0.54440300
C	3.58602600	0.46007100	-0.59471300
O	1.55946900	0.57370200	-1.83443600

C	4.25039800	-0.24435300	-1.60419200
C	4.15983700	0.52721500	0.67959900
C	5.47268700	-0.85863400	-1.35096800
H	3.79818200	-0.31077100	-2.58514200
C	5.37962700	-0.09422800	0.93561800
H	3.64678800	1.02623800	1.49346400
C	6.03952000	-0.78720100	-0.07797200
H	5.98026900	-1.39744200	-2.14296600
H	5.80513000	-0.05028400	1.93232900
H	6.98725100	-1.27381100	0.12419600
IRC_TS1_point33			
B	-2.64746700	4.01688400	0.29492100
B	-1.58581200	3.71274900	1.69427200
B	-0.59866300	2.28513900	1.33820300
B	-2.31047900	2.77446300	-0.93641700
B	-1.04036300	1.77061400	-0.27396200
B	-1.16657300	4.97819100	0.51669100
B	-1.61843100	4.40601400	-1.10336400
H	-3.73257300	4.49061700	0.42318700
B	0.10029100	3.90967400	1.15505100
H	-1.91961400	3.97397600	2.80759300
B	0.44885700	2.67414900	-0.06840900
H	-0.21629700	1.52163000	2.16355800
B	-0.61885900	2.98565500	-1.48164500
H	-3.14249200	2.34724500	-1.67173900
H	-1.20533800	6.13494300	0.80051300
B	0.08130300	4.34247400	-0.57565700
H	-1.97881900	5.14804000	-1.96272600
H	0.96431500	4.29215000	1.88124900
H	-0.28354000	2.70639500	-2.58471500
H	0.93197400	5.02444900	-1.05475800
B	-2.29728000	2.35104900	0.80200100
I	-1.66343600	-1.13954100	-0.20977000
C	0.27445500	-1.68013700	0.52101800
C	0.57801600	-1.39766200	1.84614200
C	1.14184200	-2.32713300	-0.34853700
C	1.82545900	-1.79867700	2.32077700
H	-0.12780800	-0.89057300	2.48800300
C	2.37956100	-2.72468400	0.15356000
H	0.87003100	-2.51437800	-1.37786700
C	2.71818800	-2.46120800	1.47973500
H	2.09344200	-1.58823700	3.34935400
H	3.07951600	-3.22867500	-0.50134900
H	3.68667800	-2.76619300	1.85665500

O	-2.15578800	-3.24206600	0.30110700
C	-3.37871000	-3.57395500	-0.04762100
O	-4.15438500	-2.79333100	-0.59295600
C	-3.73435000	-4.99409000	0.31103800
H	-3.93670000	-5.03704000	1.38525300
H	-4.62626600	-5.29791500	-0.23523200
H	-2.90363000	-5.66643300	0.09460500
H	-0.84636400	0.61470500	-0.71598000
H	-3.11898400	1.62833000	1.26731800
N	1.82142600	2.06695500	-0.13680100
C	2.23798600	1.04683600	-0.90477500
H	2.48983100	2.40009300	0.54420200
C	3.58523000	0.45890900	-0.59522700
O	1.55860500	0.57396000	-1.83506600
C	4.24922100	-0.24533600	-1.60526100
C	4.15969300	0.52588600	0.67856700
C	5.47115400	-0.86039000	-1.35226700
H	3.79884200	-0.30947400	-2.58885500
C	5.37936800	-0.09592400	0.93388700
H	3.64803100	1.02600400	1.49199600
C	6.03834500	-0.78947000	-0.07956900
H	5.97882500	-1.39855700	-2.14498900
H	5.80676200	-0.05084500	1.92856400
H	6.98606000	-1.27619800	0.12195900

IRC_TS1_point34

B	-2.64666700	4.01711300	0.29690200
B	-1.58427700	3.71277800	1.69560300
B	-0.59741900	2.28521600	1.33881500
B	-2.31038000	2.77488800	-0.93481700
B	-1.03995900	1.77095300	-0.27324000
B	-1.16560300	4.97835300	0.51795400
B	-1.61838900	4.40643400	-1.10189200
H	-3.73168300	4.49083800	0.42583600
B	0.10152500	3.90972300	1.15548200
H	-1.91741200	3.97381100	2.80916900
B	0.44941100	2.67426300	-0.06815400
H	-0.21452900	1.52154300	2.16378100
B	-0.61907800	2.98613400	-1.48100700
H	-3.14282700	2.34776300	-1.66963700
H	-1.20419800	6.13504100	0.80199700
B	0.08170000	4.34271100	-0.57516500
H	-1.97927400	5.14857300	-1.96091400
H	0.96597400	4.29205000	1.88123000

H	-0.28438800	2.70696900	-2.58426900
H	0.93206800	5.02479800	-1.05462100
B	-2.29627300	2.35121600	0.80355600
I	-1.66317700	-1.13936400	-0.21079300
C	0.27351600	-1.67957900	0.52335900
C	0.57438600	-1.39747100	1.84917100
C	1.14284500	-2.32588500	-0.34480100
C	1.82128200	-1.79789700	2.32596300
H	-0.13318000	-0.89128400	2.49007500
C	2.37992100	-2.72287800	0.15944900
H	0.87301000	-2.51302500	-1.37465800
C	2.71607400	-2.45951800	1.48627800
H	2.08717500	-1.58770000	3.35513900
H	3.08143500	-3.22620500	-0.49428100
H	3.68428100	-2.76385200	1.86476400
O	-2.15547900	-3.24255600	0.29858100
C	-3.37806700	-3.57444600	-0.05125300
O	-4.15363700	-2.79350100	-0.59611100
C	-3.73318900	-4.99510700	0.30553600
H	-3.93505200	-5.03966900	1.37978000
H	-4.62516500	-5.29856800	-0.24087600
H	-2.90226000	-5.66681200	0.08787000
H	-0.84586300	0.61512800	-0.71537500
H	-3.11770600	1.62845300	1.26926500
N	1.82173800	2.06647300	-0.13648300
C	2.23784900	1.04659200	-0.90563900
H	2.49091900	2.40030600	0.54232000
C	3.58526100	0.45873300	-0.59712700
O	1.55804000	0.57369200	-1.83566100
C	4.24849900	-0.24611700	-1.60701300
C	4.15953900	0.52495700	0.67707100
C	5.47035300	-0.86151900	-1.35445000
H	3.79567600	-0.31211000	-2.58770100
C	5.37875400	-0.09783400	0.93255800
H	3.64725100	1.02427500	1.49119000
C	6.03765900	-0.79101100	-0.08155000
H	5.97722400	-1.40055200	-2.14681500
H	5.80477400	-0.05467700	1.92893200
H	6.98501600	-1.27856900	0.12016000

IRC_TS1_point35

B	-2.64586200	4.01749900	0.29903800
B	-1.58268200	3.71276500	1.69709600
B	-0.59607400	2.28520600	1.33937400

B	-2.31036800	2.77548300	-0.93314900
B	-1.03962100	1.77123600	-0.27246200
B	-1.16462100	4.97859500	0.51951600
B	-1.61833200	4.40704900	-1.10023700
H	-3.73076000	4.49133900	0.42868700
B	0.10284000	3.90971700	1.15605300
H	-1.91512400	3.97361400	2.81091700
B	0.44991500	2.67462800	-0.06826400
H	-0.21274200	1.52142000	2.16400300
B	-0.61934600	2.98671100	-1.48018200
H	-3.14330800	2.34869600	-1.66768400
H	-1.20294800	6.13524100	0.80385400
B	0.08198200	4.34317100	-0.57447800
H	-1.97964800	5.14948200	-1.95886500
H	0.96772800	4.29180300	1.88143900
H	-0.28528300	2.70782000	-2.58373900
H	0.93214600	5.02531300	-1.05424700
B	-2.29526700	2.35141300	0.80512300
I	-1.66283800	-1.13929400	-0.21187300
C	0.27277600	-1.67892400	0.52546400
C	0.57111000	-1.39701200	1.85187500
C	1.14401900	-2.32459700	-0.34120400
C	1.81713900	-1.79712600	2.33103100
H	-0.13759600	-0.89097800	2.49133100
C	2.38022700	-2.72129300	0.16535900
H	0.87640300	-2.51141300	-1.37169400
C	2.71366200	-2.45828400	1.49296100
H	2.08093000	-1.58712200	3.36078400
H	3.08334900	-3.22399200	-0.48725700
H	3.68109100	-2.76255500	1.87335700
O	-2.15499200	-3.24277100	0.29555900
C	-3.37731700	-3.57491700	-0.05497400
O	-4.15308300	-2.79390500	-0.59964800
C	-3.73202900	-4.99610800	0.30047000
H	-3.93367800	-5.04204200	1.37465900
H	-4.62394800	-5.29911200	-0.24619600
H	-2.90093100	-5.66732100	0.08179200
H	-0.84518500	0.61551800	-0.71480300
H	-3.11649400	1.62861000	1.27116100
N	1.82231000	2.06716200	-0.13836400
C	2.23745000	1.04642100	-0.90617000
H	2.49152600	2.39995400	0.54200200
C	3.58444800	0.45749400	-0.59760500
O	1.55686000	0.57369700	-1.83559800

C	4.24741700	-0.24711200	-1.60807400
C	4.15952700	0.52372900	0.67595700
C	5.46891800	-0.86329500	-1.35575100
H	3.79635700	-0.31083300	-2.59115800
C	5.37877800	-0.09920600	0.93063100
H	3.64849500	1.02402000	1.48980500
C	6.03674900	-0.79312900	-0.08329300
H	5.97565000	-1.40187600	-2.14873400
H	5.80625400	-0.05496800	1.92561300
H	6.98407100	-1.28084400	0.11770100

IRC_TS1_point36

B	-2.64504400	4.01772300	0.30112000
B	-1.58115500	3.71279900	1.69854700
B	-0.59483700	2.28529800	1.34014600
B	-2.31023300	2.77592600	-0.93143600
B	-1.03922400	1.77172300	-0.27160200
B	-1.16363100	4.97875700	0.52089500
B	-1.61824500	4.40747800	-1.09865000
H	-3.72986100	4.49153700	0.43139900
B	0.10408100	3.90977200	1.15663700
H	-1.91297600	3.97347200	2.81258700
B	0.45049700	2.67475900	-0.06783500
H	-0.21097500	1.52134000	2.16436200
B	-0.61951000	2.98723900	-1.47940100
H	-3.14354500	2.34917200	-1.66550300
H	-1.20177000	6.13534500	0.80543700
B	0.08242700	4.34341000	-0.57383900
H	-1.98003100	5.14999100	-1.95697700
H	0.96939400	4.29169500	1.88158300
H	-0.28604300	2.70834300	-2.58310100
H	0.93234600	5.02558700	-1.05397300
B	-2.29425100	2.35156800	0.80679900
I	-1.66253200	-1.13916700	-0.21301700
C	0.27203300	-1.67819400	0.52769900
C	0.56753100	-1.39665000	1.85481800
C	1.14524300	-2.32316300	-0.33758600
C	1.81295100	-1.79614200	2.33614800
H	-0.14303000	-0.89165000	2.49330200
C	2.38061200	-2.71944700	0.17123300
H	0.87964700	-2.50986600	-1.36861400
C	2.71147800	-2.45648600	1.49949300
H	2.07453100	-1.58646300	3.36654600
H	3.08499900	-3.22188200	-0.47998000

H	3.67832200	-2.76032300	1.88163300
O	-2.15468300	-3.24333600	0.29283100
C	-3.37672200	-3.57542600	-0.05874800
O	-4.15221800	-2.79404600	-0.60309500
C	-3.73128900	-4.99695700	0.29514100
H	-3.93266000	-5.04407900	1.36936000
H	-4.62338100	-5.29947300	-0.25162800
H	-2.90024600	-5.66788200	0.07549200
H	-0.84514900	0.61596500	-0.71394200
H	-3.11520100	1.62872000	1.27322100
N	1.82259300	2.06664000	-0.13780000
C	2.23731500	1.04624700	-0.90706400
H	2.49255200	2.40004400	0.54050400
C	3.58439100	0.45721800	-0.59926200
O	1.55645700	0.57362900	-1.83649500
C	4.24651100	-0.24794600	-1.60968600
C	4.15938600	0.52268800	0.67460800
C	5.46782600	-0.86465600	-1.35775200
H	3.79355400	-0.31290800	-2.59070000
C	5.37811900	-0.10131900	0.92934000
H	3.64817400	1.02257700	1.48889400
C	6.03577200	-0.79502400	-0.08511800
H	5.97390500	-1.40385800	-2.15056900
H	5.80510300	-0.05843700	1.92497400
H	6.98273600	-1.28355600	0.11600300
IRC_TS1_point37			
B	-2.64417300	4.01814900	0.30335600
B	-1.57954800	3.71277900	1.70015100
B	-0.59349800	2.28527200	1.34081200
B	-2.31013800	2.77658000	-0.92967500
B	-1.03883200	1.77198200	-0.27073500
B	-1.16257900	4.97899700	0.52260700
B	-1.61808300	4.40812800	-1.09685300
H	-3.72887000	4.49206900	0.43432000
B	0.10542500	3.90973300	1.15736300
H	-1.91072300	3.97322900	2.81444100
B	0.45103900	2.67508100	-0.06778700
H	-0.20928200	1.52115500	2.16469800
B	-0.61969300	2.98783600	-1.47844900
H	-3.14392500	2.35017400	-1.66344200
H	-1.20048500	6.13552000	0.80745300
B	0.08280100	4.34385700	-0.57297500
H	-1.98027600	5.15092100	-1.95478100
H	0.97112400	4.29141800	1.88197100

H	-0.28683200	2.70926300	-2.58245000
H	0.93250300	5.02611400	-1.05338400
B	-2.29323200	2.35181100	0.80843300
I	-1.66220600	-1.13902800	-0.21422300
C	0.27104200	-1.67769800	0.52993800
C	0.56417900	-1.39612900	1.85755700
C	1.14609700	-2.32222600	-0.33379200
C	1.80889900	-1.79520500	2.34113700
H	-0.14753500	-0.89123600	2.49470100
C	2.38080800	-2.71801400	0.17717400
H	0.88254800	-2.50885600	-1.36535200
C	2.70920800	-2.45511000	1.50605900
H	2.06860900	-1.58541900	3.37197600
H	3.08694500	-3.21965600	-0.47308900
H	3.67566900	-2.75849100	1.88981700
O	-2.15418100	-3.24352100	0.28967900
C	-3.37592400	-3.57581500	-0.06269100
O	-4.15158300	-2.79440100	-0.60689700
C	-3.73004400	-4.99781700	0.28998600
H	-3.93170700	-5.04598500	1.36407500
H	-4.62174700	-5.30023500	-0.25737500
H	-2.89856500	-5.66816800	0.07005400
H	-0.84421700	0.61642100	-0.71346500
H	-3.11400600	1.62892500	1.27512800
N	1.82316900	2.06717400	-0.13950700
C	2.23686300	1.04591400	-0.90745000
H	2.49323600	2.39960500	0.54015400
C	3.58362100	0.45597800	-0.59991400
O	1.55513100	0.57343700	-1.83620700
C	4.24543500	-0.24909100	-1.61080100
C	4.15927900	0.52138200	0.67348000
C	5.46654900	-0.86634200	-1.35922300
H	3.79343300	-0.31266200	-2.59316000
C	5.37802600	-0.10281300	0.92756100
H	3.64886500	1.02179700	1.48776800
C	6.03499900	-0.79698700	-0.08692500
H	5.97234800	-1.40534800	-2.15246600
H	5.80555500	-0.05962900	1.92285900
H	6.98192600	-1.28570500	0.11359400

IRC_TS1_point38

B	-2.64330600	4.01850400	0.30558800
B	-1.57797400	3.71282600	1.70175200
B	-0.59227700	2.28534000	1.34165900

B	-2.31002400	2.77718600	-0.92788700
B	-1.03850200	1.77255000	-0.26982400
B	-1.16148700	4.97922800	0.52420100
B	-1.61792700	4.40872500	-1.09510100
H	-3.72790000	4.49248500	0.43718700
B	0.10672900	3.90975300	1.15811200
H	-1.90850900	3.97308800	2.81627000
B	0.45161800	2.67524400	-0.06729300
H	-0.20753800	1.52103500	2.16510100
B	-0.61985800	2.98849400	-1.47756100
H	-3.14422000	2.35094700	-1.66128400
H	-1.19911500	6.13570600	0.80931600
B	0.08330400	4.34417100	-0.57216400
H	-1.98053400	5.15171600	-1.95269100
H	0.97290500	4.29116200	1.88232600
H	-0.28759100	2.70994200	-2.58172100
H	0.93281800	5.02644700	-1.05289300
B	-2.29223000	2.35202200	0.81018400
I	-1.66188200	-1.13893800	-0.21546800
C	0.27045000	-1.67682300	0.53205100
C	0.56084300	-1.39548700	1.86030700
C	1.14733200	-2.32080700	-0.33021700
C	1.80476800	-1.79412900	2.34613700
H	-0.15235700	-0.89118100	2.49622800
C	2.38101300	-2.71639400	0.18308100
H	0.88581400	-2.50732000	-1.36231500
C	2.70679100	-2.45357900	1.51264500
H	2.06231000	-1.58462700	3.37759100
H	3.08813200	-3.21811500	-0.46564700
H	3.67232500	-2.75692400	1.89832500
O	-2.15386000	-3.24407600	0.28674000
C	-3.37534500	-3.57637900	-0.06657300
O	-4.15074000	-2.79466600	-0.61062200
C	-3.72941800	-4.99867400	0.28483300
H	-3.93088700	-5.04785300	1.35891200
H	-4.62126900	-5.30054900	-0.26262000
H	-2.89805700	-5.66886200	0.06403700
H	-0.84431900	0.61690100	-0.71241500
H	-3.11277800	1.62910300	1.27721100
N	1.82345700	2.06672300	-0.13898000
C	2.23668400	1.04575900	-0.90826400
H	2.49426800	2.39970400	0.53867500
C	3.58342900	0.45553100	-0.60130500
O	1.55464600	0.57340400	-1.83691400

C	4.24437100	-0.25002300	-1.61225200
C	4.15925600	0.52035000	0.67217300
C	5.46519300	-0.86797900	-1.36102800
H	3.79116800	-0.31405900	-2.59344300
C	5.37756800	-0.10478500	0.92606600
H	3.64911700	1.02079100	1.48669900
C	6.03393400	-0.79905800	-0.08877400
H	5.97041800	-1.40740100	-2.15427300
H	5.80546700	-0.06211300	1.92109900
H	6.98057200	-1.28844900	0.11166300

IRC_TS1_point39

B	-2.64241000	4.01888800	0.30789500
B	-1.57635100	3.71284300	1.70342100
B	-0.59089600	2.28536400	1.34245600
B	-2.30986800	2.77777600	-0.92598200
B	-1.03804000	1.77282000	-0.26880300
B	-1.16043900	4.97944100	0.52592400
B	-1.61774800	4.40927600	-1.09324100
H	-3.72690000	4.49290600	0.44014200
B	0.10808000	3.90975300	1.15888900
H	-1.90629000	3.97290200	2.81816400
B	0.45219500	2.67554400	-0.06711500
H	-0.20584200	1.52089300	2.16559200
B	-0.61999600	2.98901800	-1.47649300
H	-3.14448300	2.35175800	-1.65900200
H	-1.19790800	6.13584200	0.81126300
B	0.08369900	4.34456100	-0.57124600
H	-1.98078600	5.15241500	-1.95048900
H	0.97458100	4.29102200	1.88272500
H	-0.28833500	2.71073800	-2.58092800
H	0.93296500	5.02688700	-1.05230600
B	-2.29117000	2.35228600	0.81195200
I	-1.66156900	-1.13874700	-0.21665600
C	0.26931900	-1.67643500	0.53439500
C	0.55737900	-1.39508200	1.86314800
C	1.14808800	-2.31992700	-0.32641800
C	1.80081500	-1.79313500	2.35102600
H	-0.15727300	-0.89126700	2.49802900
C	2.38128600	-2.71486300	0.18883500
H	0.88849300	-2.50645200	-1.35899500
C	2.70478300	-2.45193500	1.51891900
H	2.05658400	-1.58348000	3.38288100
H	3.09024300	-3.21562900	-0.45909200

H	3.67025000	-2.75448000	1.90594700
O	-2.15334700	-3.24430700	0.28355700
C	-3.37451800	-3.57670900	-0.07065200
O	-4.14997900	-2.79488900	-0.61451800
C	-3.72821700	-4.99941900	0.27950300
H	-3.92984500	-5.04954900	1.35353400
H	-4.61982200	-5.30124800	-0.26840600
H	-2.89648300	-5.66907400	0.05843900
H	-0.84342500	0.61739500	-0.71197700
H	-3.11151500	1.62932900	1.27927200
N	1.82402400	2.06715000	-0.14054400
C	2.23620300	1.04535000	-0.90864600
H	2.49493500	2.39910800	0.53859900
C	3.58270000	0.45433100	-0.60214300
O	1.55330200	0.57317600	-1.83678300
C	4.24326400	-0.25123000	-1.61350900
C	4.15906700	0.51896900	0.67100200
C	5.46395800	-0.86962300	-1.36270500
H	3.79041400	-0.31448800	-2.59531800
C	5.37730200	-0.10651200	0.92441200
H	3.64948100	1.01968800	1.48567200
C	6.03310900	-0.80107100	-0.09059900
H	5.96880200	-1.40902700	-2.15626000
H	5.80517100	-0.06415000	1.91975800
H	6.97964900	-1.29078800	0.10942400
IRC_TS1_point40			
B	-2.64149300	4.01941300	0.31026900
B	-1.57470400	3.71291900	1.70514400
B	-0.58969800	2.28541400	1.34332200
B	-2.30981300	2.77857900	-0.92415100
B	-1.03781200	1.77344100	-0.26789400
B	-1.15922400	4.97976600	0.52770300
B	-1.61754600	4.41008200	-1.09135200
H	-3.72584400	4.49359300	0.44319600
B	0.10946400	3.90973700	1.15974200
H	-1.90393300	3.97276400	2.82014500
B	0.45275300	2.67572700	-0.06661600
H	-0.20411100	1.52073100	2.16597700
B	-0.62021100	2.98982400	-1.47556500
H	-3.14492200	2.35289400	-1.65686200
H	-1.19630100	6.13613100	0.81339800
B	0.08425500	4.34496400	-0.57032600
H	-1.98096400	5.15357300	-1.94819000
H	0.97652500	4.29059400	1.88321200

H	-0.28917700	2.71161400	-2.58019500
H	0.93337200	5.02732800	-1.05165000
B	-2.29019100	2.35258100	0.81374900
I	-1.66125900	-1.13868200	-0.21791900
C	0.26880600	-1.67548100	0.53639900
C	0.55439000	-1.39413600	1.86565500
C	1.14916500	-2.31868900	-0.32284700
C	1.79688900	-1.79195000	2.35581600
H	-0.16123600	-0.89031900	2.49905800
C	2.38124300	-2.71356200	0.19473300
H	0.89151000	-2.50517800	-1.35591500
C	2.70221300	-2.45070400	1.52546000
H	2.05066400	-1.58241000	3.38818900
H	3.09096900	-3.21464800	-0.45161700
H	3.66655700	-2.75349500	1.91449200
O	-2.15299700	-3.24480500	0.28060200
C	-3.37389300	-3.57732100	-0.07455000
O	-4.14916900	-2.79526900	-0.61831000
C	-3.72744700	-5.00040000	0.27428700
H	-3.92903500	-5.05168200	1.34821800
H	-4.61902200	-5.30163500	-0.27388600
H	-2.89573500	-5.66981500	0.05235700
H	-0.84354700	0.61789300	-0.71072600
H	-3.11036400	1.62960600	1.28136600
N	1.82430200	2.06672200	-0.14005500
C	2.23595400	1.04517200	-0.90939200
H	2.49607700	2.39939000	0.53667900
C	3.58239400	0.45376200	-0.60342700
O	1.55263700	0.57303900	-1.83713200
C	4.24203700	-0.25233200	-1.61485900
C	4.15913600	0.51800300	0.66963800
C	5.46242000	-0.87146700	-1.36443500
H	3.78837000	-0.31567900	-2.59601900
C	5.37704300	-0.10825100	0.92265300
H	3.65005000	1.01898000	1.48446400
C	6.03207900	-0.80312400	-0.09261500
H	5.96669700	-1.41122600	-2.15807200
H	5.80578400	-0.06583900	1.91722700
H	6.97842600	-1.29332700	0.10707700

IRC_TS1_point41

B	-2.64057900	4.01975200	0.31265900
B	-1.57302800	3.71299100	1.70686800
B	-0.58823200	2.28550900	1.34422600

B	-2.30963500	2.77909000	-0.92208400
B	-1.03729000	1.77374200	-0.26673000
B	-1.15818900	4.97996600	0.52940200
B	-1.61739800	4.41052300	-1.08945000
H	-3.72483800	4.49391900	0.44624000
B	0.11084100	3.90980600	1.16051400
H	-1.90166000	3.97267500	2.82208000
B	0.45335100	2.67603700	-0.06637100
H	-0.20231200	1.52067900	2.16658800
B	-0.62035200	2.99026700	-1.47440500
H	-3.14513000	2.35350700	-1.65434300
H	-1.19515200	6.13625200	0.81524500
B	0.08463100	4.34530900	-0.56941700
H	-1.98128300	5.15403900	-1.94600200
H	0.97820400	4.29061700	1.88354300
H	-0.28994700	2.71226500	-2.57928700
H	0.93347000	5.02767200	-1.05116700
B	-2.28906900	2.35286300	0.81567600
I	-1.66095700	-1.13845200	-0.21900400
C	0.26767600	-1.67514200	0.53872600
C	0.55083700	-1.39392700	1.86853700
C	1.14999500	-2.31771100	-0.31921000
C	1.79298300	-1.79101000	2.36057500
H	-0.16657500	-0.89106000	2.50116600
C	2.38166500	-2.71185500	0.20018800
H	0.89423200	-2.50416800	-1.35275600
C	2.70041000	-2.44885400	1.53141200
H	2.04492500	-1.58145300	3.39340100
H	3.09322500	-3.21192000	-0.44540000
H	3.66480600	-2.75065400	1.92165900
O	-2.15251500	-3.24509400	0.27744900
C	-3.37307400	-3.57764500	-0.07869900
O	-4.14832800	-2.79540500	-0.62224100
C	-3.72630200	-5.00112000	0.26878000
H	-3.92777100	-5.05339500	1.34276300
H	-4.61786400	-5.30228900	-0.27963700
H	-2.89433300	-5.67001400	0.04636600
H	-0.84279400	0.61842600	-0.71033900
H	-3.10898200	1.62985400	1.28365900
N	1.82485800	2.06713300	-0.14158100
C	2.23545200	1.04475100	-0.90981800
H	2.49663400	2.39856700	0.53710200
C	3.58168400	0.45259900	-0.60436300
O	1.55132400	0.57287300	-1.83730200

C	4.24086700	-0.25352200	-1.61624300
C	4.15892900	0.51656600	0.66842600
C	5.46111400	-0.87312100	-1.36627900
H	3.78714100	-0.31641300	-2.59754000
C	5.37664900	-0.11022500	0.92106100
H	3.65035300	1.01773200	1.48345200
C	6.03111600	-0.80530200	-0.09446300
H	5.96490900	-1.41296800	-2.16017900
H	5.80511300	-0.06850500	1.91623100
H	6.97725800	-1.29605200	0.10500600

IRC_TS1_point42

B	-2.63961800	4.02041400	0.31516500
B	-1.57132800	3.71311600	1.70870200
B	-0.58705300	2.28557200	1.34513700
B	-2.30961000	2.78004700	-0.92018000
B	-1.03712800	1.77439100	-0.26577200
B	-1.15688000	4.98036700	0.53133100
B	-1.61715400	4.41148100	-1.08743600
H	-3.72371000	4.49479400	0.44946500
B	0.11228400	3.90978100	1.16145800
H	-1.89920100	3.97255600	2.82419600
B	0.45390100	2.67623700	-0.06583400
H	-0.20061400	1.52050700	2.16700600
B	-0.62059500	2.99117500	-1.47341500
H	-3.14565800	2.35488600	-1.65212400
H	-1.19340000	6.13661000	0.81758200
B	0.08523200	4.34577800	-0.56839600
H	-1.98142100	5.15542900	-1.94351400
H	0.98024200	4.29010700	1.88412900
H	-0.29085200	2.71328800	-2.57852300
H	0.93393000	5.02820900	-1.05036900
B	-2.28810400	2.35325000	0.81754200
I	-1.66066700	-1.13837600	-0.22024300
C	0.26709400	-1.67424500	0.54068500
C	0.54811200	-1.39278800	1.87084600
C	1.15079800	-2.31677200	-0.31563500
C	1.78931000	-1.78975900	2.36510700
H	-0.16991000	-0.88948800	2.50190600
C	2.38140900	-2.71089500	0.20597800
H	0.89679600	-2.50334200	-1.34958400
C	2.69784900	-2.44785400	1.53774800
H	2.03951800	-1.58007400	3.39831500
H	3.09372600	-3.21130700	-0.43814100

H	3.66118400	-2.74996300	1.92992100
O	-2.15212600	-3.24546700	0.27456300
C	-3.37235200	-3.57821100	-0.08265900
O	-4.14749100	-2.79579300	-0.62609400
C	-3.72530600	-5.00216400	0.26327500
H	-3.92696200	-5.05583300	1.33706300
H	-4.61659900	-5.30271400	-0.28568700
H	-2.89319100	-5.67067700	0.04002900
H	-0.84280400	0.61894700	-0.70887700
H	-3.10788500	1.63023900	1.28580100
N	1.82513400	2.06668600	-0.14110600
C	2.23511500	1.04450200	-0.91046900
H	2.49793700	2.39904900	0.53466100
C	3.58126700	0.45191100	-0.60564200
O	1.55042500	0.57257600	-1.83723200
C	4.23949600	-0.25482500	-1.61757700
C	4.15901700	0.51562100	0.66699000
C	5.45947200	-0.87512100	-1.36803700
H	3.78523200	-0.31761100	-2.59862400
C	5.37652400	-0.11177400	0.91908400
H	3.65101400	1.01713900	1.48216800
C	6.03014500	-0.80730200	-0.09665100
H	5.96268500	-1.41531900	-2.16207300
H	5.80604900	-0.06970300	1.91334000
H	6.97620500	-1.29834600	0.10225400

IRC_TS1_point43

B	-2.63865900	4.02081000	0.31771600
B	-1.56955000	3.71323600	1.71055500
B	-0.58552000	2.28570200	1.34615000
B	-2.30945600	2.78060300	-0.91795700
B	-1.03660900	1.77478400	-0.26450100
B	-1.15577100	4.98061200	0.53313100
B	-1.61701000	4.41196200	-1.08541300
H	-3.72264300	4.49522000	0.45271800
B	0.11374100	3.90988000	1.16230100
H	-1.89676200	3.97254200	2.82627100
B	0.45450800	2.67656400	-0.06551300
H	-0.19869800	1.52048600	2.16769600
B	-0.62077200	2.99165100	-1.47216200
H	-3.14592900	2.35556600	-1.64944600
H	-1.19210700	6.13679300	0.81953700
B	0.08562900	4.34613800	-0.56742600
H	-1.98173900	5.15596200	-1.94120700

H	0.98206600	4.29012900	1.88449700
H	-0.29169900	2.71393600	-2.57751900
H	0.93406800	5.02852200	-1.04986800
B	-2.28694100	2.35357600	0.81963500
I	-1.66036200	-1.13811800	-0.22125400
C	0.26613300	-1.67381200	0.54284600
C	0.54466900	-1.39263700	1.87360500
C	1.15171500	-2.31566400	-0.31223700
C	1.78546100	-1.78891600	2.36968100
H	-0.17514700	-0.89040000	2.50392300
C	2.38180400	-2.70917700	0.21117700
H	0.89960100	-2.50208900	-1.34668400
C	2.69599800	-2.44609300	1.54347500
H	2.03375400	-1.57940700	3.40340800
H	3.09566900	-3.20881400	-0.43204200
H	3.65917900	-2.74738300	1.93693800
O	-2.15172600	-3.24585600	0.27141800
C	-3.37158400	-3.57862900	-0.08690600
O	-4.14660000	-2.79598000	-0.63019900
C	-3.72428100	-5.00294600	0.25764800
H	-3.92564100	-5.05763800	1.33152700
H	-4.61572700	-5.30333900	-0.29139600
H	-2.89204000	-5.67099500	0.03372700
H	-0.84228200	0.61952100	-0.70839900
H	-3.10643900	1.63054200	1.28831200
N	1.82566500	2.06709800	-0.14252000
C	2.23460600	1.04412700	-0.91094000
H	2.49837900	2.39806500	0.53550500
C	3.58056700	0.45078700	-0.60657600
O	1.54918100	0.57254100	-1.83767000
C	4.23820100	-0.25602700	-1.61896200
C	4.15886700	0.51417700	0.66574400
C	5.45798400	-0.87688800	-1.36994000
H	3.78348900	-0.31858700	-2.59969800
C	5.37608300	-0.11394100	0.91746400
H	3.65146100	1.01592100	1.48111500
C	6.02903700	-0.80967000	-0.09857600
H	5.96060500	-1.41727200	-2.16420000
H	5.80542000	-0.07267000	1.91221200
H	6.97478800	-1.30145800	0.10019900
IRC_TS1_point44			
B	-2.63765500	4.02148700	0.32035700
B	-1.56781200	3.71342700	1.71250500

B	-0.58428800	2.28583200	1.34719900
B	-2.30937800	2.78155800	-0.91587600
B	-1.03639900	1.77541800	-0.26335800
B	-1.15444700	4.98102700	0.53514500
B	-1.61673900	4.41289000	-1.08327800
H	-3.72148000	4.49605100	0.45606800
B	0.11521500	3.90991200	1.16333100
H	-1.89428800	3.97249800	2.82849100
B	0.45509300	2.67679500	-0.06486800
H	-0.19697700	1.52039200	2.16827600
B	-0.62098300	2.99253200	-1.47102000
H	-3.14637700	2.35686400	-1.64697300
H	-1.19041700	6.13714500	0.82190500
B	0.08624900	4.34661200	-0.56630900
H	-1.98189500	5.15722500	-1.93861600
H	0.98407900	4.28975300	1.88513500
H	-0.29258200	2.71492100	-2.57660300
H	0.93449900	5.02907000	-1.04901100
B	-2.28591900	2.35402600	0.82166500
I	-1.66009300	-1.13796000	-0.22243000
C	0.26534400	-1.67313500	0.54485300
C	0.54195000	-1.39164100	1.87589500
C	1.15229200	-2.31495700	-0.30873100
C	1.78198500	-1.78774200	2.37397600
H	-0.17853600	-0.88906000	2.50485400
C	2.38156100	-2.70831100	0.21664000
H	0.90177100	-2.50157400	-1.34351700
C	2.69370200	-2.44506100	1.54937900
H	2.02876000	-1.57797400	3.40799400
H	3.09642600	-3.20796500	-0.42541600
H	3.65618300	-2.74636200	1.94445400
O	-2.15129500	-3.24604100	0.26848900
C	-3.37075100	-3.57903400	-0.09108300
O	-4.14567800	-2.79624100	-0.63427500
C	-3.72311100	-5.00387600	0.25178000
H	-3.92485800	-5.06001000	1.32543600
H	-4.61413600	-5.30374000	-0.29801000
H	-2.89057500	-5.67144900	0.02721100
H	-0.84207500	0.62009900	-0.70684400
H	-3.10527500	1.63099800	1.29063300
N	1.82596600	2.06662200	-0.14207700
C	2.23416200	1.04376000	-0.91145300
H	2.49981900	2.39855200	0.53286700
C	3.58002500	0.44993800	-0.60789300

O	1.54802600	0.57209600	-1.83727100
C	4.23672200	-0.25746000	-1.62040700
C	4.15887800	0.51307700	0.66428000
C	5.45627800	-0.87897700	-1.37183200
H	3.78175600	-0.31968400	-2.60127700
C	5.37594300	-0.11556300	0.91540700
H	3.65203000	1.01512500	1.47987000
C	6.02802900	-0.81177500	-0.10084900
H	5.95831200	-1.41965800	-2.16629800
H	5.80620200	-0.07400300	1.90946400
H	6.97374900	-1.30378800	0.09728800

IRC_TS1_point45

B	-2.63663200	4.02206600	0.32311400
B	-1.56593300	3.71359100	1.71454500
B	-0.58276100	2.28596000	1.34831100
B	-2.30928300	2.78232100	-0.91353700
B	-1.03596700	1.77594900	-0.26202800
B	-1.15318300	4.98137800	0.53717900
B	-1.61654300	4.41358900	-1.08105900
H	-3.72031000	4.49678300	0.45957700
B	0.11677800	3.90998500	1.16434000
H	-1.89167100	3.97251000	2.83078100
B	0.45569300	2.67713200	-0.06445300
H	-0.19505400	1.52031800	2.16901200
B	-0.62120700	2.99317600	-1.46967500
H	-3.14679000	2.35790400	-1.64424300
H	-1.18881500	6.13745500	0.82418100
B	0.08672100	4.34705000	-0.56517700
H	-1.98210600	5.15813200	-1.93605400
H	0.98611300	4.28960000	1.88568900
H	-0.29351700	2.71575500	-2.57552600
H	0.93477800	5.02944000	-1.04830800
B	-2.28477600	2.35444800	0.82388400
I	-1.65978700	-1.13767700	-0.22339700
C	0.26460300	-1.67254300	0.54681400
C	0.53889700	-1.39128700	1.87838700
C	1.15311200	-2.31392700	-0.30549600
C	1.77835300	-1.78693900	2.37827700
H	-0.18296100	-0.88936200	2.50643800
C	2.38166200	-2.70695300	0.22169300
H	0.90435000	-2.50040600	-1.34074100
C	2.69165200	-2.44371900	1.55494600
H	2.02332300	-1.57735700	3.41278100

H	3.09758900	-3.20633700	-0.41927600
H	3.65364000	-2.74463700	1.95144300
O	-2.15097400	-3.24655400	0.26536500
C	-3.37001700	-3.57960200	-0.09545500
O	-4.14473100	-2.79655900	-0.63861500
C	-3.72215500	-5.00481600	0.24598400
H	-3.92362300	-5.06204600	1.31968400
H	-4.61331300	-5.30442300	-0.30390400
H	-2.88954000	-5.67194900	0.02067500
H	-0.84178700	0.62071100	-0.70612200
H	-3.10389100	1.63141100	1.29324400
N	1.82646400	2.06702700	-0.14334000
C	2.23363300	1.04344300	-0.91197100
H	2.50020600	2.39754100	0.53387800
C	3.57930700	0.44882400	-0.60879700
O	1.54679200	0.57216600	-1.83780600
C	4.23522500	-0.25882900	-1.62168900
C	4.15883300	0.51172600	0.66296500
C	5.45455800	-0.88096400	-1.37373700
H	3.77944300	-0.32110100	-2.60184000
C	5.37557600	-0.11770900	0.91362600
H	3.65273100	1.01415300	1.47869900
C	6.02686500	-0.81420200	-0.10295900
H	5.95590600	-1.42195400	-2.16838300
H	5.80598300	-0.07671600	1.90781500
H	6.97227400	-1.30695900	0.09495500

IRC_TS1_point46

B	-2.63560400	4.02268300	0.32587200
B	-1.56414600	3.71386000	1.71658300
B	-0.58142500	2.28618900	1.34951400
B	-2.30915200	2.78316700	-0.91123900
B	-1.03566400	1.77655100	-0.26065900
B	-1.15189300	4.98178100	0.53919000
B	-1.61629800	4.41437400	-1.07885200
H	-3.71914600	4.49745800	0.46302900
B	0.11827300	3.91011800	1.16539100
H	-1.88917500	3.97259300	2.83306600
B	0.45631500	2.67740000	-0.06370800
H	-0.19322000	1.52036800	2.16978500
B	-0.62140000	2.99394000	-1.46837900
H	-3.14713900	2.35894600	-1.64145300
H	-1.18727300	6.13778200	0.82643300
B	0.08731600	4.34749000	-0.56403800

H	-1.98235700	5.15908800	-1.93345300
H	0.98808600	4.28946900	1.88627900
H	-0.29440100	2.71657200	-2.57444200
H	0.93511300	5.02993500	-1.04753200
B	-2.28366200	2.35492600	0.82612500
I	-1.65954200	-1.13742900	-0.22443300
C	0.26366300	-1.67209800	0.54883400
C	0.53609200	-1.39063900	1.88071300
C	1.15363400	-2.31326400	-0.30219800
C	1.77502700	-1.78594600	2.38234300
H	-0.18672500	-0.88878600	2.50773300
C	2.38160600	-2.70594800	0.22667300
H	0.90637600	-2.49987800	-1.33777000
C	2.68970800	-2.44252500	1.56032000
H	2.01856800	-1.57616200	3.41713200
H	3.09878000	-3.20495400	-0.41342600
H	3.65135200	-2.74309300	1.95810400
O	-2.15051100	-3.24655200	0.26237700
C	-3.36909400	-3.57982900	-0.09984200
O	-4.14372200	-2.79664000	-0.64289900
C	-3.72088200	-5.00558900	0.23976800
H	-3.92265400	-5.06432000	1.31330600
H	-4.61171300	-5.30467500	-0.31082000
H	-2.88796200	-5.67220500	0.01373500
H	-0.84142600	0.62134000	-0.70454300
H	-3.10258300	1.63190000	1.29584300
N	1.82678500	2.06653800	-0.14293000
C	2.23309900	1.04298900	-0.91237300
H	2.50174200	2.39799800	0.53115300
C	3.57866900	0.44787700	-0.61019200
O	1.54544700	0.57163600	-1.83725500
C	4.23366700	-0.26027100	-1.62332800
C	4.15876000	0.51044800	0.66145000
C	5.45275800	-0.88312800	-1.37578900
H	3.77786100	-0.32194500	-2.60392700
C	5.37533500	-0.11955900	0.91154300
H	3.65319900	1.01309800	1.47747800
C	6.02570500	-0.81656600	-0.10525400
H	5.95347300	-1.42438200	-2.17069500
H	5.80641800	-0.07853500	1.90536400
H	6.97103100	-1.30967600	0.09211300
IRC_TS1_point47			
B	-2.63453000	4.02345700	0.32881700

B	-1.56217900	3.71408200	1.71878500
B	-0.57991900	2.28632700	1.35069200
B	-2.30912800	2.78415700	-0.90881000
B	-1.03534500	1.77721100	-0.25929600
B	-1.15049500	4.98224700	0.54143800
B	-1.61606900	4.41530700	-1.07645900
H	-3.71788100	4.49849100	0.46678900
B	0.11992400	3.91017400	1.16653000
H	-1.88638500	3.97263300	2.83555200
B	0.45689800	2.67776100	-0.06324300
H	-0.19130900	1.52025700	2.17053700
B	-0.62169000	2.99477000	-1.46697500
H	-3.14770400	2.36034500	-1.63865900
H	-1.18540200	6.13821700	0.82901200
B	0.08784000	4.34802500	-0.56277600
H	-1.98250700	5.16037000	-1.93064400
H	0.99030100	4.28916500	1.88697600
H	-0.29545200	2.71761600	-2.57333000
H	0.93549200	5.03040300	-1.04665100
B	-2.28254700	2.35546300	0.82844400
I	-1.65924200	-1.13711800	-0.22532600
C	0.26307600	-1.67141500	0.55062800
C	0.53349700	-1.39003700	1.88291500
C	1.15424800	-2.31246000	-0.29909800
C	1.77172500	-1.78514900	2.38630700
H	-0.19019500	-0.88832500	2.50887500
C	2.38139400	-2.70505400	0.23154200
H	0.90853600	-2.49903100	-1.33504800
C	2.68755200	-2.44162000	1.56563700
H	2.01368900	-1.57543900	3.42148700
H	3.09926100	-3.20418300	-0.40739500
H	3.64849700	-2.74215900	1.96488300
O	-2.15024600	-3.24717600	0.25937500
C	-3.36835400	-3.58051500	-0.10430000
O	-4.14269300	-2.79704200	-0.64736900
C	-3.71989700	-5.00671100	0.23368900
H	-3.92165900	-5.06669600	1.30715400
H	-4.61060800	-5.30551600	-0.31728500
H	-2.88680400	-5.67280600	0.00704200
H	-0.84131000	0.62198800	-0.70355100
H	-3.10127100	1.63244500	1.29853000
N	1.82725100	2.06694600	-0.14410200
C	2.23252500	1.04270800	-0.91293600
H	2.50208200	2.39695600	0.53228000

C	3.57789500	0.44672100	-0.61105900
O	1.54415000	0.57176400	-1.83776600
C	4.23193600	-0.26189900	-1.62447800
C	4.15879400	0.50918500	0.66008600
C	5.45082600	-0.88533400	-1.37771500
H	3.77500400	-0.32391900	-2.60403700
C	5.37506500	-0.12159800	0.90957200
H	3.65411400	1.01236900	1.47622100
C	6.02454200	-0.81895500	-0.10759400
H	5.95077900	-1.42700400	-2.17278400
H	5.80664400	-0.08083100	1.90317500
H	6.96963000	-1.31267300	0.08934200

IRC_TS1_point48

B	-2.63349000	4.02404500	0.33168100
B	-1.56034300	3.71443000	1.72090400
B	-0.57850000	2.28663900	1.35203500
B	-2.30898300	2.78491300	-0.90631400
B	-1.03497600	1.77779000	-0.25772700
B	-1.14921800	4.98265500	0.54344200
B	-1.61585500	4.41597900	-1.07419000
H	-3.71671800	4.49910100	0.47034700
B	0.12144700	3.91039700	1.16760400
H	-1.88383200	3.97285400	2.83790200
B	0.45753200	2.67805300	-0.06240200
H	-0.18937900	1.52043400	2.17149100
B	-0.62189400	2.99542200	-1.46554100
H	-3.14803500	2.36121500	-1.63561500
H	-1.18391800	6.13855300	0.83116900
B	0.08841300	4.34842700	-0.56162200
H	-1.98281900	5.16111200	-1.92803700
H	0.99228300	4.28921600	1.88752900
H	-0.29637100	2.71827900	-2.57210200
H	0.93576800	5.03082600	-1.04595300
B	-2.28137600	2.35597100	0.83087700
I	-1.65901300	-1.13680600	-0.22618600
C	0.26213900	-1.67109400	0.55254700
C	0.53072000	-1.38967400	1.88518200
C	1.15479700	-2.31177500	-0.29608900
C	1.76857000	-1.78433900	2.39010600
H	-0.19415500	-0.88839000	2.51036000
C	2.38148400	-2.70395600	0.23604300
H	0.91052900	-2.49838700	-1.33237200
C	2.68586600	-2.44037000	1.57051700

H	2.00912200	-1.57455200	3.42560100
H	3.10063000	-3.20255800	-0.40215500
H	3.64661900	-2.74039500	1.97086600
O	-2.14978800	-3.24702000	0.25635400
C	-3.36738400	-3.58060900	-0.10884400
O	-4.14163500	-2.79697500	-0.65183200
C	-3.71858800	-5.00736800	0.22716500
H	-3.92035700	-5.06902900	1.30056800
H	-4.60925100	-5.30551500	-0.32429400
H	-2.88529100	-5.67294200	-0.00057600
H	-0.84088100	0.62265900	-0.70197400
H	-3.09986300	1.63297400	1.30139800
N	1.82757300	2.06647200	-0.14371100
C	2.23192300	1.04222200	-0.91325400
H	2.50366400	2.39743000	0.52952700
C	3.57719500	0.44575800	-0.61253400
O	1.54268500	0.57121500	-1.83718000
C	4.23030800	-0.26328000	-1.62629600
C	4.15868600	0.50781200	0.65848200
C	5.44888500	-0.88759500	-1.37988300
H	3.77348300	-0.32448000	-2.60648700
C	5.37472500	-0.12367500	0.90745600
H	3.65456000	1.01118300	1.47495100
C	6.02318900	-0.82162500	-0.10989200
H	5.94811800	-1.42956600	-2.17522200
H	5.80677900	-0.08314600	1.90094400
H	6.96806300	-1.31595700	0.08665300

IRC_TS1_point49

B	-2.63237700	4.02493000	0.33481100
B	-1.55830600	3.71471300	1.72325500
B	-0.57698500	2.28682800	1.35330000
B	-2.30898900	2.78604800	-0.90376000
B	-1.03471900	1.77855800	-0.25628500
B	-1.14775700	4.98320300	0.54586100
B	-1.61562700	4.41705800	-1.07163700
H	-3.71539200	4.50026000	0.47435400
B	0.12315200	3.91048200	1.16884300
H	-1.88091500	3.97292800	2.84056200
B	0.45811700	2.67846500	-0.06187400
H	-0.18742200	1.52035400	2.17228900
B	-0.62222900	2.99639500	-1.46405900
H	-3.14866300	2.36278700	-1.63265400
H	-1.18194900	6.13905900	0.83397000

B	0.08895100	4.34905400	-0.56025700
H	-1.98300800	5.16258400	-1.92500900
H	0.99459200	4.28888900	1.88830900
H	-0.29751100	2.71946200	-2.57092000
H	0.93615600	5.03140500	-1.04495300
B	-2.28024300	2.35659400	0.83333200
I	-1.65872100	-1.13645300	-0.22701000
C	0.26159200	-1.67045800	0.55421800
C	0.52846800	-1.38896900	1.88715100
C	1.15521300	-2.31122800	-0.29316200
C	1.76560200	-1.78360200	2.39371400
H	-0.19696400	-0.88749200	2.51124500
C	2.38110500	-2.70343400	0.24059700
H	0.91227600	-2.49788900	-1.32974400
C	2.68378300	-2.43977900	1.57544200
H	2.00481900	-1.57376700	3.42950400
H	3.10084200	-3.20225900	-0.39653400
H	3.64384900	-2.73990700	1.97715100
O	-2.14956300	-3.24766700	0.25350700
C	-3.36661500	-3.58127600	-0.11340600
O	-4.14047000	-2.79731000	-0.65643200
C	-3.71759600	-5.00851200	0.22075500
H	-3.91997100	-5.07146100	1.29390500
H	-4.60766600	-5.30645900	-0.33164700
H	-2.88391500	-5.67347900	-0.00710900
H	-0.84082800	0.62334700	-0.70066700
H	-3.09854000	1.63361600	1.30422800
N	1.82801200	2.06684300	-0.14474300
C	2.23128300	1.04193200	-0.91380000
H	2.50403100	2.39637100	0.53059600
C	3.57633600	0.44450900	-0.61335500
O	1.54128400	0.57134500	-1.83755400
C	4.22833800	-0.26516400	-1.62735700
C	4.15874100	0.50653300	0.65712700
C	5.44675600	-0.88999300	-1.38187000
H	3.77020800	-0.32688800	-2.60637100
C	5.37452100	-0.12568000	0.90534300
H	3.65560000	1.01051700	1.47371700
C	6.02200600	-0.82401300	-0.11243300
H	5.94515600	-1.43243000	-2.17740500
H	5.80734300	-0.08517300	1.89836300
H	6.96674400	-1.31878300	0.08346000

IRC_TS1_point50

B	-2.63130800	4.02559100	0.33783500
B	-1.55641300	3.71511600	1.72552500
B	-0.57552900	2.28717000	1.35479100
B	-2.30886400	2.78683700	-0.90108200
B	-1.03433900	1.77915500	-0.25454500
B	-1.14641900	4.98365400	0.54799300
B	-1.61539600	4.41775400	-1.06922100
H	-3.71418400	4.50100300	0.47808400
B	0.12473000	3.91073100	1.17004400
H	-1.87827300	3.97323300	2.84306400
B	0.45874500	2.67876700	-0.06091000
H	-0.18548200	1.52055600	2.17341000
B	-0.62245100	2.99703100	-1.46246500
H	-3.14905300	2.36373600	-1.62944500
H	-1.18034700	6.13945600	0.83624100
B	0.08954700	4.34945400	-0.55897500
H	-1.98326500	5.16337400	-1.92226900
H	0.99665500	4.28895900	1.88897700
H	-0.29847400	2.72012800	-2.56954900
H	0.93647300	5.03178900	-1.04415600
B	-2.27906800	2.35716500	0.83593600
I	-1.65848100	-1.13607600	-0.22773500
C	0.26079600	-1.67013500	0.55593900
C	0.52593400	-1.38870500	1.88922300
C	1.15573500	-2.31059200	-0.29044300
C	1.76269000	-1.78295800	2.39718700
H	-0.20063800	-0.88771500	2.51263600
C	2.38113800	-2.70250300	0.24470400
H	0.91412900	-2.49724300	-1.32734100
C	2.68217700	-2.43874600	1.57990600
H	2.00055700	-1.57314200	3.43330200
H	3.10188900	-3.20100700	-0.39165800
H	3.64197900	-2.73849100	1.98266800
O	-2.14915900	-3.24744000	0.25039400
C	-3.36565900	-3.58132200	-0.11813000
O	-4.13939200	-2.79719900	-0.66119000
C	-3.71635400	-5.00911100	0.21407200
H	-3.91835800	-5.07383600	1.28726000
H	-4.60669800	-5.30626000	-0.33850300
H	-2.88263200	-5.67361500	-0.01526100
H	-0.84038200	0.62407700	-0.69909200
H	-3.09712900	1.63421900	1.30728800
N	1.82833000	2.06642900	-0.14439700
C	2.23061900	1.04146200	-0.91407100

H	2.50553300	2.39673000	0.52820600
C	3.57556900	0.44352900	-0.61485600
O	1.53971900	0.57088300	-1.83701900
C	4.22660500	-0.26655200	-1.62923900
C	4.15862200	0.50511200	0.65544300
C	5.44465000	-0.89239000	-1.38409300
H	3.76855100	-0.32740400	-2.60884400
C	5.37410300	-0.12794000	0.90317200
H	3.65608500	1.00931000	1.47236500
C	6.02049400	-0.82693400	-0.11477200
H	5.94225300	-1.43520000	-2.17987800
H	5.80728900	-0.08784600	1.89621300
H	6.96490300	-1.32253800	0.08082500
IRC_TS1_point51			
B	-2.63017500	4.02647300	0.34113500
B	-1.55434200	3.71546100	1.72801900
B	-0.57397300	2.28743900	1.35621500
B	-2.30884300	2.78797800	-0.89834700
B	-1.03406500	1.77998300	-0.25293000
B	-1.14496700	4.98423200	0.55052200
B	-1.61518700	4.41883500	-1.06653200
H	-3.71284900	4.50209000	0.48227100
B	0.12645400	3.91089000	1.17138200
H	-1.87532000	3.97337600	2.84586100
B	0.45935800	2.67923400	-0.06024400
H	-0.18343500	1.52057700	2.17435400
B	-0.62278800	2.99804400	-1.46084700
H	-3.14963300	2.36523200	-1.62623200
H	-1.17844600	6.13997900	0.83912800
B	0.09007800	4.35012500	-0.55751800
H	-1.98354000	5.16478500	-1.91910100
H	0.99897300	4.28874700	1.88981900
H	-0.29962600	2.72129100	-2.56820800
H	0.93681500	5.03243000	-1.04309300
B	-2.27787300	2.35782100	0.83858800
I	-1.65819500	-1.13566000	-0.22850100
C	0.26020400	-1.66966800	0.55752200
C	0.52385000	-1.38812800	1.89104800
C	1.15603500	-2.31022800	-0.28776000
C	1.76000400	-1.78236300	2.40045100
H	-0.20321400	-0.88691100	2.51350200
C	2.38078700	-2.70214300	0.24880200
H	0.91560700	-2.49694100	-1.32491700
C	2.68032900	-2.43827900	1.58431600

H	1.99673300	-1.57244000	3.43679700
H	3.10224000	-3.20068700	-0.38672100
H	3.63963000	-2.73802900	1.98821600
O	-2.14894500	-3.24801300	0.24763700
C	-3.36484900	-3.58181400	-0.12283700
O	-4.13805100	-2.79729300	-0.66598200
C	-3.71545700	-5.01005000	0.20736100
H	-3.91858700	-5.07600400	1.28017800
H	-4.60489100	-5.30697900	-0.34658300
H	-2.88123200	-5.67396800	-0.02168300
H	-0.84026100	0.62478700	-0.69743300
H	-3.09572300	1.63489300	1.31034100
N	1.82874900	2.06671100	-0.14517600
C	2.22990200	1.04112400	-0.91450400
H	2.50607400	2.39579500	0.52888100
C	3.57462400	0.44219500	-0.61566400
O	1.53818800	0.57094500	-1.83714700
C	4.22442300	-0.26857800	-1.63032500
C	4.15867100	0.50372800	0.65409200
C	5.44230500	-0.89496500	-1.38618700
H	3.76505900	-0.32988700	-2.60883200
C	5.37390900	-0.13005200	0.90094900
H	3.65719400	1.00854700	1.47119000
C	6.01920100	-0.82947200	-0.11746100
H	5.93899100	-1.43824000	-2.18222400
H	5.80803900	-0.08988300	1.89339100
H	6.96351600	-1.32545800	0.07736300

IRC_TS1_point52

B	-2.62908100	4.02724700	0.34434700
B	-1.55239500	3.71590200	1.73046700
B	-0.57250100	2.28779600	1.35783500
B	-2.30875900	2.78887600	-0.89550900
B	-1.03371400	1.78063500	-0.25105600
B	-1.14356000	4.98474700	0.55285600
B	-1.61493900	4.41963900	-1.06392600
H	-3.71159200	4.50302300	0.48621600
B	0.12808700	3.91114600	1.17274600
H	-1.87259100	3.97370900	2.84855500
B	0.45997400	2.67955900	-0.05917500
H	-0.18151800	1.52076300	2.17559700
B	-0.62304600	2.99874700	-1.45910400
H	-3.15010800	2.36637600	-1.62289900
H	-1.17670200	6.14045100	0.84162800

B	0.09069400	4.35057000	-0.55606300
H	-1.98373800	5.16575000	-1.91615400
H	1.00112000	4.28877600	1.89066000
H	-0.30065600	2.72207800	-2.56671800
H	0.93717500	5.03283800	-1.04212000
B	-2.27671900	2.35846700	0.84133700
I	-1.65791800	-1.13522000	-0.22911800
C	0.25960200	-1.66929300	0.55903700
C	0.52173100	-1.38778800	1.89286100
C	1.15643800	-2.30977800	-0.28526900
C	1.75743900	-1.78183200	2.40356300
H	-0.20620700	-0.88683700	2.51463100
C	2.38062000	-2.70161800	0.25259700
H	0.91715000	-2.49652300	-1.32268400
C	2.67873300	-2.43764400	1.58841400
H	1.99297400	-1.57193000	3.44019400
H	3.10268700	-3.20023200	-0.38208000
H	3.63762800	-2.73728400	1.99334400
O	-2.14859800	-3.24777800	0.24439500
C	-3.36393100	-3.58184900	-0.12774000
O	-4.13695500	-2.79717200	-0.67103900
C	-3.71432100	-5.01061700	0.20062900
H	-3.91705900	-5.07824100	1.27349100
H	-4.60407000	-5.30680800	-0.35342900
H	-2.88009800	-5.67412200	-0.02978000
H	-0.83983300	0.62559800	-0.69581700
H	-3.09434700	1.63557500	1.31353300
N	1.82905700	2.06638700	-0.14493100
C	2.22915400	1.04068100	-0.91478900
H	2.50739800	2.39589600	0.52711400
C	3.57375000	0.44114400	-0.61715600
O	1.53650000	0.57062000	-1.83670700
C	4.22252200	-0.27011800	-1.63218100
C	4.15851800	0.50228100	0.65236100
C	5.44003500	-0.89752400	-1.38844300
H	3.76308800	-0.33069300	-2.61110900
C	5.37343900	-0.13238900	0.89871500
H	3.65770600	1.00738900	1.46977500
C	6.01759500	-0.83251500	-0.11987700
H	5.93588500	-1.44124600	-2.18470700
H	5.80790600	-0.09266500	1.89122800
H	6.96156100	-1.32938100	0.07463900

IRC_TS1_point53

B	-2.62795200	4.02810000	0.34775300
B	-1.55032000	3.71631600	1.73305500
B	-0.57092100	2.28814700	1.35941100
B	-2.30871800	2.78996400	-0.89262000
B	-1.03341100	1.78148900	-0.24926600
B	-1.14214200	4.98534400	0.55542200
B	-1.61476100	4.42066600	-1.06116100
H	-3.71027800	4.50402200	0.49049100
B	0.12980500	3.91138700	1.17414800
H	-1.86964600	3.97396100	2.85143000
B	0.46059700	2.68006800	-0.05837700
H	-0.17940800	1.52089200	2.17670000
B	-0.62338500	2.99973400	-1.45736600
H	-3.15064500	2.36773300	-1.61948100
H	-1.17489300	6.14099100	0.84449400
B	0.09120300	4.35125200	-0.55455900
H	-1.98409200	5.16703300	-1.91293600
H	1.00342100	4.28870600	1.89152700
H	-0.30180800	2.72314500	-2.56523100
H	0.93746100	5.03349600	-1.04105100
B	-2.27548000	2.35914000	0.84416100
I	-1.65762800	-1.13475000	-0.22980800
C	0.25897200	-1.66901300	0.56054100
C	0.51976300	-1.38741800	1.89458300
C	1.15670000	-2.30951700	-0.28285800
C	1.75501600	-1.78138900	2.40651100
H	-0.20872600	-0.88636700	2.51557500
C	2.38038200	-2.70129700	0.25620800
H	0.91847700	-2.49628400	-1.32051500
C	2.67717400	-2.43720200	1.59229600
H	1.98956300	-1.57136700	3.44333500
H	3.10328600	-3.19971600	-0.37786000
H	3.63575900	-2.73670100	1.99814400
O	-2.14836400	-3.24827100	0.24169400
C	-3.36307700	-3.58214800	-0.13254000
O	-4.13545900	-2.79699500	-0.67596200
C	-3.71353900	-5.01131600	0.19372100
H	-3.91743500	-5.08021300	1.26620900
H	-4.60241000	-5.30709300	-0.36173700
H	-2.87887600	-5.67432900	-0.03647300
H	-0.83960000	0.62629900	-0.69385800
H	-3.09287800	1.63626800	1.31678700
N	1.82944900	2.06659100	-0.14546000
C	2.22835700	1.04029800	-0.91507300

H	2.50814300	2.39519300	0.52726400
C	3.57273000	0.43976800	-0.61796300
O	1.53483000	0.57058600	-1.83656100
C	4.22013000	-0.27223000	-1.63330100
C	4.15859700	0.50085100	0.65095700
C	5.43742500	-0.90029800	-1.39060900
H	3.75940500	-0.33313400	-2.61122000
C	5.37325100	-0.13460400	0.89635500
H	3.65895000	1.00661200	1.46857900
C	6.01613900	-0.83526100	-0.12269500
H	5.93223500	-1.44452100	-2.18714900
H	5.80881500	-0.09474400	1.88815400
H	6.95999000	-1.33256500	0.07100600

IRC_TS1_point54

B	-2.62688200	4.02891300	0.35109600
B	-1.54836100	3.71679200	1.73562300
B	-0.56943300	2.28854700	1.36112900
B	-2.30868400	2.79089300	-0.88965300
B	-1.03308300	1.78218100	-0.24727400
B	-1.14075500	4.98589900	0.55786800
B	-1.61456800	4.42150700	-1.05843400
H	-3.70904000	4.50500800	0.49458600
B	0.13144100	3.91168400	1.17560000
H	-1.86688700	3.97432500	2.85424900
B	0.46119300	2.68043400	-0.05725100
H	-0.17748400	1.52113300	2.17804600
B	-0.62370600	3.00047300	-1.45552000
H	-3.15118300	2.36891600	-1.61601600
H	-1.17315500	6.14150900	0.84710400
B	0.09176900	4.35173600	-0.55301300
H	-1.98434700	5.16804100	-1.90986800
H	1.00557500	4.28878300	1.89244900
H	-0.30292700	2.72398700	-2.56365200
H	0.93776400	5.03393600	-1.04000800
B	-2.27433900	2.35982000	0.84703700
I	-1.65729100	-1.13425900	-0.23030000
C	0.25858400	-1.66858700	0.56189700
C	0.51812600	-1.38692100	1.89615400
C	1.15697400	-2.30931600	-0.28052000
C	1.75287200	-1.78088200	2.40928100
H	-0.21090500	-0.88581900	2.51642500
C	2.38003300	-2.70120800	0.25975800
H	0.91967100	-2.49621600	-1.31835900

C	2.67564000	-2.43693000	1.59606900
H	1.98642400	-1.57081300	3.44632500
H	3.10317000	-3.20008300	-0.37339800
H	3.63371800	-2.73654600	2.00290500
O	-2.14803800	-3.24806300	0.23835700
C	-3.36218400	-3.58213100	-0.13756500
O	-4.13430300	-2.79676400	-0.68116700
C	-3.71254100	-5.01179000	0.18694500
H	-3.91628700	-5.08217300	1.25943400
H	-4.60159500	-5.30693600	-0.36877200
H	-2.87785200	-5.67444400	-0.04425000
H	-0.83919400	0.62717700	-0.69215900
H	-3.09150300	1.63697400	1.32011000
N	1.82973600	2.06636200	-0.14536000
C	2.22750500	1.03987900	-0.91543700
H	2.50929000	2.39504900	0.52604300
C	3.57172900	0.43864000	-0.61949500
O	1.53299500	0.57037000	-1.83624800
C	4.21807300	-0.27394400	-1.63518500
C	4.15834100	0.49937500	0.64920800
C	5.43503400	-0.90299200	-1.39292400
H	3.75719400	-0.33425100	-2.61344300
C	5.37268300	-0.13698000	0.89411800
H	3.65936700	1.00548400	1.46714600
C	6.01443900	-0.83837400	-0.12514300
H	5.92903000	-1.44770300	-2.18969200
H	5.80853100	-0.09757000	1.88608500
H	6.95796200	-1.33653100	0.06823700

IRC_TS1_point55

B	-2.62578000	4.02977000	0.35452800
B	-1.54630200	3.71728600	1.73823600
B	-0.56786000	2.28896800	1.36278200
B	-2.30866200	2.79194300	-0.88669500
B	-1.03278200	1.78304500	-0.24538400
B	-1.13937400	4.98653300	0.56040300
B	-1.61443300	4.42250400	-1.05567300
H	-3.70776300	4.50599700	0.49886500
B	0.13313700	3.91200300	1.17700300
H	-1.86396000	3.97470500	2.85713200
B	0.46178900	2.68098400	-0.05639100
H	-0.17535600	1.52133400	2.17923000
B	-0.62407500	3.00142800	-1.45373800
H	-3.15174300	2.37020200	-1.61251200

H	-1.17140600	6.14209800	0.84988900
B	0.09224300	4.35243300	-0.55152800
H	-1.98476600	5.16926500	-1.90667500
H	1.00786600	4.28882900	1.89328500
H	-0.30410500	2.72497600	-2.56210800
H	0.93799500	5.03461700	-1.03898600
B	-2.27309800	2.36052500	0.84994700
I	-1.65698200	-1.13376900	-0.23089400
C	0.25794300	-1.66848900	0.56333800
C	0.51626600	-1.38675000	1.89780300
C	1.15725800	-2.30912700	-0.27836500
C	1.75070300	-1.78055100	2.41195500
H	-0.21343700	-0.88573100	2.51748800
C	2.37995700	-2.70088300	0.26291600
H	0.92093800	-2.49600500	-1.31644300
C	2.67438900	-2.43645700	1.59947000
H	1.98337700	-1.57035600	3.44917000
H	3.10406500	-3.19934200	-0.36984700
H	3.63232400	-2.73579400	2.00702500
O	-2.14775600	-3.24846800	0.23568000
C	-3.36128400	-3.58227800	-0.14238500
O	-4.13272900	-2.79639100	-0.68613700
C	-3.71181000	-5.01232800	0.17998300
H	-3.91659100	-5.08405500	1.25211500
H	-4.60011800	-5.30688800	-0.37702100
H	-2.87678000	-5.67456800	-0.05119000
H	-0.83884500	0.62784100	-0.68996700
H	-3.09002700	1.63770300	1.32346800
N	1.83008600	2.06653500	-0.14570000
C	2.22662700	1.03946400	-0.91554700
H	2.51019600	2.39464300	0.52565600
C	3.57062500	0.43724300	-0.62024100
O	1.53118000	0.57022300	-1.83579400
C	4.21538600	-0.27623500	-1.63619600
C	4.15854000	0.49806300	0.64768200
C	5.43206500	-0.90605200	-1.39504600
H	3.75310600	-0.33689300	-2.61336300
C	5.37259100	-0.13912400	0.89152500
H	3.66093400	1.00497300	1.46579600
C	6.01283300	-0.84126600	-0.12811500
H	5.92481800	-1.45140800	-2.19203800
H	5.80978700	-0.09938600	1.88254500
H	6.95621400	-1.33990200	0.06439200

IRC_TS1_point56

B	-2.62481100	4.03049900	0.35791200
B	-1.54439100	3.71780400	1.74082700
B	-0.56634800	2.28946300	1.36456400
B	-2.30869700	2.79276200	-0.88363200
B	-1.03246400	1.78374700	-0.24328800
B	-1.13814500	4.98708900	0.56280700
B	-1.61440900	4.42325100	-1.05294400
H	-3.70664700	4.50682900	0.50300700
B	0.13470100	3.91240000	1.17842100
H	-1.86125000	3.97513100	2.85996900
B	0.46235200	2.68140900	-0.05528200
H	-0.17337000	1.52176300	2.18068100
B	-0.62450200	3.00212400	-1.45185200
H	-3.15231100	2.37115300	-1.60889100
H	-1.16989100	6.14262100	0.85239700
B	0.09264900	4.35293500	-0.55002700
H	-1.98525000	5.17008100	-1.90364200
H	1.00991500	4.28910300	1.89414000
H	-0.30534800	2.72573000	-2.56047500
H	0.93809200	5.03507200	-1.03805800
B	-2.27195800	2.36117700	0.85293700
I	-1.65655200	-1.13323400	-0.23123900
C	0.25779800	-1.66798800	0.56460700
C	0.51518900	-1.38596700	1.89916400
C	1.15739700	-2.30922600	-0.27605900
C	1.74906200	-1.77991600	2.41443300
H	-0.21465500	-0.88448300	2.51804100
C	2.37942200	-2.70125100	0.26636000
H	0.92173800	-2.49642800	-1.31421000
C	2.67295800	-2.43647400	1.60302200
H	1.98099100	-1.56950900	3.45176200
H	3.10336800	-3.20059900	-0.36539100
H	3.63029200	-2.73612700	2.01153200
O	-2.14740400	-3.24843300	0.23237800
C	-3.36039300	-3.58219100	-0.14742400
O	-4.13141500	-2.79590200	-0.69123600
C	-3.71099800	-5.01266200	0.17307300
H	-3.91584700	-5.08579300	1.24517500
H	-4.59935500	-5.30655600	-0.38438300
H	-2.87593000	-5.67459800	-0.05886400
H	-0.83846200	0.62875200	-0.68819600
H	-3.08859300	1.63835400	1.32695300
N	1.83034300	2.06643100	-0.14584000
C	2.22566600	1.03908600	-0.91610200

H	2.51118000	2.39429900	0.52486000
C	3.56950400	0.43608300	-0.62190900
O	1.52919800	0.57009400	-1.83570200
C	4.21327000	-0.27801700	-1.63826000
C	4.15807200	0.49652800	0.64596700
C	5.42963400	-0.90879800	-1.39747600
H	3.75090100	-0.33810000	-2.61588200
C	5.37179200	-0.14159600	0.88943400
H	3.66104500	1.00377800	1.46443500
C	6.01099000	-0.84446500	-0.13047700
H	5.92168300	-1.45462100	-2.19474800
H	5.80908600	-0.10241700	1.88086900
H	6.95404100	-1.34396700	0.06178400
IRC_TS1_point57			
B	-2.62376900	4.03140300	0.36124700
B	-1.54238100	3.71838700	1.74336100
B	-0.56483300	2.28993900	1.36619100
B	-2.30874600	2.79378700	-0.88073100
B	-1.03220600	1.78458400	-0.24139300
B	-1.13680100	4.98778300	0.56520800
B	-1.61433000	4.42424500	-1.05029900
H	-3.70542600	4.50791400	0.50716400
B	0.13635000	3.91280000	1.17974100
H	-1.85835500	3.97565600	2.86276200
B	0.46287500	2.68199100	-0.05442800
H	-0.17129300	1.52198500	2.18184400
B	-0.62493500	3.00303400	-1.45013100
H	-3.15299500	2.37246400	-1.60547200
H	-1.16815600	6.14329600	0.85500700
B	0.09308100	4.35364300	-0.54865000
H	-1.98570900	5.17133100	-1.90058100
H	1.01219500	4.28924100	1.89487200
H	-0.30659100	2.72666900	-2.55900200
H	0.93827200	5.03578300	-1.03715800
B	-2.27077900	2.36192400	0.85580300
I	-1.65621100	-1.13280700	-0.23168800
C	0.25718500	-1.66807000	0.56598100
C	0.51339300	-1.38600700	1.90076800
C	1.15780500	-2.30907000	-0.27415200
C	1.74710000	-1.77965800	2.41689100
H	-0.21733500	-0.88487000	2.51925200
C	2.37961500	-2.70082800	0.26909900
H	0.92312600	-2.49617900	-1.31257200
C	2.67204300	-2.43588100	1.60600600

H	1.97815900	-1.56916500	3.45441700
H	3.10469800	-3.19951800	-0.36244900
H	3.62939900	-2.73507600	2.01506700
O	-2.14705700	-3.24853100	0.22961600
C	-3.35945700	-3.58216200	-0.15219000
O	-4.12996000	-2.79540800	-0.69614100
C	-3.71017300	-5.01312400	0.16617500
H	-3.91598200	-5.08773300	1.23791100
H	-4.59790600	-5.30640900	-0.39248300
H	-2.87481900	-5.67463200	-0.06588300
H	-0.83797700	0.62936700	-0.68582500
H	-3.08719800	1.63913600	1.33028300
N	1.83062600	2.06659700	-0.14600600
C	2.22471300	1.03864800	-0.91599000
H	2.51220300	2.39431400	0.52385100
C	3.56831600	0.43469900	-0.62254500
O	1.52725500	0.56979900	-1.83487900
C	4.21017800	-0.28065500	-1.63896800
C	4.15851300	0.49558200	0.64422300
C	5.42621600	-0.91227100	-1.39939200
H	3.74614500	-0.34135700	-2.61523800
C	5.37194600	-0.14336900	0.88647700
H	3.66314800	1.00394200	1.46274300
C	6.00928000	-0.84738900	-0.13361200
H	5.91670000	-1.45909300	-2.19671600
H	5.81095500	-0.10346600	1.87660600
H	6.95218700	-1.34737200	0.05767100

IRC_TS1_point58

B	-2.62296100	4.03195400	0.36463700
B	-1.54053400	3.71895700	1.74591300
B	-0.56326400	2.29057400	1.36799100
B	-2.30887800	2.79440200	-0.87758300
B	-1.03188900	1.78530300	-0.23923300
B	-1.13584500	4.98832100	0.56746300
B	-1.61459400	4.42481300	-1.04764900
H	-3.70450400	4.50841800	0.51137300
B	0.13779400	3.91335100	1.18100200
H	-1.85566600	3.97618500	2.86556100
B	0.46338900	2.68252500	-0.05344500
H	-0.16911700	1.52271400	2.18336400
B	-0.62552700	3.00365500	-1.44827300
H	-3.15360200	2.37296900	-1.60160900
H	-1.16703700	6.14379900	0.85729000

B	0.09321400	4.35418400	-0.54733100
H	-1.98663700	5.17181700	-1.89765000
H	1.01409600	4.28983200	1.89548500
H	-0.30803500	2.72724400	-2.55736400
H	0.93800200	5.03630200	-1.03651500
B	-2.26960300	2.36250600	0.85892100
I	-1.65565700	-1.13219800	-0.23195000
C	0.25724900	-1.66754400	0.56720500
C	0.51285300	-1.38487900	1.90193300
C	1.15782500	-2.30953000	-0.27183500
C	1.74596700	-1.77880800	2.41910100
H	-0.21764900	-0.88283200	2.51951700
C	2.37893900	-2.70168200	0.27249500
H	0.92354200	-2.49723900	-1.31020000
C	2.67076700	-2.43612300	1.60937300
H	1.97656600	-1.56781700	3.45660200
H	3.10358500	-3.20164700	-0.35796500
H	3.62746000	-2.73579700	2.01937300
O	-2.14668600	-3.24903600	0.22676900
C	-3.35855600	-3.58206500	-0.15703500
O	-4.12827100	-2.79452000	-0.70085200
C	-3.70970600	-5.01332000	0.15897700
H	-3.91578700	-5.08949900	1.23063500
H	-4.59729200	-5.30561000	-0.40045500
H	-2.87431200	-5.67457200	-0.07384700
H	-0.83754300	0.63022700	-0.68396700
H	-3.08559700	1.63967700	1.33402300
N	1.83084800	2.06668700	-0.14645300
C	2.22365500	1.03834400	-0.91672900
H	2.51301600	2.39380300	0.52344900
C	3.56709800	0.43354800	-0.62425900
O	1.52515400	0.56974200	-1.83498200
C	4.20804100	-0.28235400	-1.64119000
C	4.15782600	0.49392500	0.64265200
C	5.42373700	-0.91497100	-1.40193600
H	3.74396700	-0.34240900	-2.61801200
C	5.37086200	-0.14607100	0.88462300
H	3.66297300	1.00255600	1.46159500
C	6.00725000	-0.85070500	-0.13587400
H	5.91359500	-1.46216300	-2.19966200
H	5.80981500	-0.10694400	1.87535000
H	6.94976300	-1.35165600	0.05522900

IRC_TS1_point59

B	-2.62199900	4.03286300	0.36790200
B	-1.53863200	3.71955600	1.74841300
B	-0.56184400	2.29106000	1.36963800
B	-2.30898600	2.79537500	-0.87472000
B	-1.03165500	1.78607600	-0.23728600
B	-1.13456400	4.98902200	0.56981400
B	-1.61455600	4.42578500	-1.04504700
H	-3.70335900	4.50957200	0.51543200
B	0.13935500	3.91378600	1.18234200
H	-1.85289400	3.97673900	2.86831400
B	0.46384400	2.68309400	-0.05249000
H	-0.16717500	1.52293500	2.18457300
B	-0.62599900	3.00450900	-1.44654700
H	-3.15439600	2.37431400	-1.59828800
H	-1.16533900	6.14450000	0.85983400
B	0.09361300	4.35486000	-0.54594000
H	-1.98708100	5.17307500	-1.89465000
H	1.01628400	4.29000400	1.89626400
H	-0.30929700	2.72816400	-2.55590000
H	0.93815600	5.03698200	-1.03559300
B	-2.26852300	2.36323800	0.86173900
I	-1.65524200	-1.13187300	-0.23222900
C	0.25682600	-1.66766200	0.56845000
C	0.51135800	-1.38497000	1.90339800
C	1.15832600	-2.30946000	-0.27010100
C	1.74433400	-1.77858700	2.42132400
H	-0.22002300	-0.88333200	2.52066200
C	2.37925100	-2.70135000	0.27496300
H	0.92494000	-2.49707200	-1.30872000
C	2.67008500	-2.43560000	1.61206100
H	1.97408400	-1.56757200	3.45903500
H	3.10487300	-3.20076900	-0.35528500
H	3.62680400	-2.73483000	2.02254800
O	-2.14630200	-3.24841000	0.22357900
C	-3.35764800	-3.58167500	-0.16187200
O	-4.12715100	-2.79387400	-0.70583200
C	-3.70879200	-5.01354000	0.15227600
H	-3.91577000	-5.09116200	1.22357900
H	-4.59598500	-5.30530800	-0.40816100
H	-2.87324300	-5.67446400	-0.08069600
H	-0.83697800	0.63089400	-0.68144200
H	-3.08432600	1.64045300	1.33729900
N	1.83105300	2.06680100	-0.14643800
C	2.22260700	1.03788600	-0.91652100

H	2.51410700	2.39411900	0.52201000
C	3.56581600	0.43219500	-0.62497900
O	1.52308200	0.56937500	-1.83399200
C	4.20466700	-0.28527600	-1.64184100
C	4.15835100	0.49328900	0.64069500
C	5.42002600	-0.91878100	-1.40375800
H	3.73886700	-0.34614000	-2.61732700
C	5.37112400	-0.14751700	0.88145700
H	3.66524500	1.00324100	1.45962100
C	6.00542900	-0.85367900	-0.13903200
H	5.90814000	-1.46730600	-2.20138500
H	5.81187300	-0.10744900	1.87087700
H	6.94778100	-1.35517000	0.05111400

IRC_TS1_point60

B	-2.62131200	4.03331200	0.37132700
B	-1.53686400	3.72013800	1.75099100
B	-0.56027600	2.29175500	1.37148400
B	-2.30917600	2.79589900	-0.87151600
B	-1.03135200	1.78684300	-0.23508900
B	-1.13379900	4.98956300	0.57206000
B	-1.61499300	4.42629100	-1.04239700
H	-3.70258700	4.50987600	0.51968600
B	0.14069700	3.91441800	1.18358400
H	-1.85028000	3.97731100	2.87112900
B	0.46431000	2.68373800	-0.05154800
H	-0.16491800	1.52373800	2.18612000
B	-0.62667400	3.00513500	-1.44466500
H	-3.15500200	2.37459300	-1.59431200
H	-1.16449700	6.14500500	0.86208700
B	0.09357000	4.35548400	-0.54466000
H	-1.98827000	5.17346100	-1.89171300
H	1.01807100	4.29076100	1.89682100
H	-0.31081000	2.72870300	-2.55421500
H	0.93765200	5.03765400	-1.03499600
B	-2.26734700	2.36377700	0.86494200
I	-1.65456500	-1.13111900	-0.23253900
C	0.25692900	-1.66732200	0.56960800
C	0.51096900	-1.38395600	1.90446600
C	1.15838000	-2.31010200	-0.26800500
C	1.74346400	-1.77781800	2.42327800
H	-0.22020900	-0.88141500	2.52094400
C	2.37873300	-2.70233700	0.27798300
H	0.92533200	-2.49831500	-1.30656600

C	2.66910400	-2.43589000	1.61501600
H	1.97289100	-1.56620500	3.46091700
H	3.10410600	-3.20281900	-0.35139200
H	3.62531500	-2.73547900	2.02627800
O	-2.14593700	-3.24962200	0.22131800
C	-3.35674800	-3.58160600	-0.16650100
O	-4.12497800	-2.79259400	-0.71032200
C	-3.70879800	-5.01355400	0.14498900
H	-3.91643400	-5.09270200	1.21611200
H	-4.59548900	-5.30408800	-0.41664200
H	-2.87311000	-5.67428200	-0.08845100
H	-0.83627800	0.63162400	-0.67946200
H	-3.08266000	1.64090000	1.34114400
N	1.83124600	2.06703900	-0.14694000
C	2.22143000	1.03758800	-0.91709500
H	2.51485900	2.39361100	0.52174600
C	3.56445000	0.43093600	-0.62644400
O	1.52077900	0.56929500	-1.83383300
C	4.20214700	-0.28723200	-1.64377900
C	4.15776200	0.49165100	0.63915600
C	5.41714000	-0.92175800	-1.40623000
H	3.73597900	-0.34762900	-2.61945900
C	5.37011800	-0.15024300	0.87942900
H	3.66548800	1.00206700	1.45845800
C	6.00325800	-0.85710900	-0.14149200
H	5.90441800	-1.47073000	-2.20425500
H	5.81119500	-0.11070900	1.86905800
H	6.94524300	-1.35950800	0.04828600

IRC_TS1_point61

B	-2.62049300	4.03403500	0.37460300
B	-1.53508800	3.72069500	1.75350400
B	-0.55888100	2.29226800	1.37321200
B	-2.30934500	2.79665200	-0.86858700
B	-1.03109300	1.78751800	-0.23300300
B	-1.13273000	4.99018600	0.57436800
B	-1.61513700	4.42708600	-1.03979400
H	-3.70161900	4.51077000	0.52372700
B	0.14212300	3.91491000	1.18493000
H	-1.84767600	3.97782100	2.87388300
B	0.46470800	2.68430500	-0.05051300
H	-0.16297600	1.52409200	2.18746300
B	-0.62724400	3.00588500	-1.44288900
H	-3.15583800	2.37563900	-1.59090700

H	-1.16309500	6.14563500	0.86451800
B	0.09379900	4.35610300	-0.54327000
H	-1.98893800	5.17443300	-1.88876700
H	1.02007900	4.29108200	1.89759600
H	-0.31215600	2.72947600	-2.55268200
H	0.93759800	5.03825900	-1.03414100
B	-2.26629700	2.36436600	0.86783700
I	-1.65401000	-1.13088400	-0.23261800
C	0.25682700	-1.66733200	0.57079700
C	0.51015300	-1.38366900	1.90573600
C	1.15880500	-2.31036300	-0.26621600
C	1.74243500	-1.77738200	2.42524700
H	-0.22152000	-0.88112200	2.52179900
C	2.37888400	-2.70253100	0.28045800
H	0.92634900	-2.49874200	-1.30489600
C	2.66857100	-2.43566300	1.61757500
H	1.97126000	-1.56556500	3.46299200
H	3.10469500	-3.20308100	-0.34851500
H	3.62466200	-2.73507700	2.02932600
O	-2.14548100	-3.24825000	0.21752700
C	-3.35588800	-3.58072000	-0.17152900
O	-4.12412800	-2.79158500	-0.71540600
C	-3.70798300	-5.01333200	0.13842700
H	-3.91633700	-5.09374900	1.20926800
H	-4.59463900	-5.30331000	-0.42386600
H	-2.87244800	-5.67402200	-0.09522100
H	-0.83579200	0.63239900	-0.67675700
H	-3.08137900	1.64150500	1.34451900
N	1.83138300	2.06718200	-0.14697000
C	2.22027700	1.03718500	-0.91709000
H	2.51587900	2.39391500	0.52037300
C	3.56306700	0.42964600	-0.62744800
O	1.51861600	0.56900500	-1.83309300
C	4.19877900	-0.29006700	-1.64477800
C	4.15800100	0.49096500	0.63716000
C	5.41341400	-0.92555200	-1.40820100
H	3.73118100	-0.35106700	-2.61948900
C	5.37005300	-0.15181300	0.87643900
H	3.66722200	1.00258300	1.45651600
C	6.00121300	-0.86022400	-0.14448800
H	5.89910900	-1.47580700	-2.20616200
H	5.81253700	-0.11162600	1.86522200
H	6.94297100	-1.36329000	0.04453400

IRC_TS1_point62

B	-2.61996500	4.03445000	0.37788000
B	-1.53349100	3.72130200	1.75598300
B	-0.55741400	2.29300100	1.37501800
B	-2.30961800	2.79710600	-0.86548400
B	-1.03083800	1.78829200	-0.23086000
B	-1.13214900	4.99075000	0.57649400
B	-1.61570100	4.42754800	-1.03727400
H	-3.70102400	4.51104400	0.52777800
B	0.14331000	3.91561600	1.18611600
H	-1.84527100	3.97846200	2.87657400
B	0.46509300	2.68502100	-0.04960300
H	-0.16082900	1.52489100	2.18896900
B	-0.62797600	3.00646000	-1.44106400
H	-3.15647800	2.37581800	-1.58709100
H	-1.16247300	6.14618300	0.86662500
B	0.09362400	4.35677200	-0.54206600
H	-1.99022800	5.17480700	-1.88597900
H	1.02168100	4.29197700	1.89811200
H	-0.31368100	2.73001600	-2.55106700
H	0.93692500	5.03905900	-1.03359300
B	-2.26523200	2.36489800	0.87094200
I	-1.65319600	-1.12997800	-0.23293800
C	0.25696400	-1.66719500	0.57189500
C	0.50979500	-1.38289500	1.90676700
C	1.15898100	-2.31107100	-0.26435400
C	1.74174800	-1.77671000	2.42700800
H	-0.22185900	-0.87967000	2.52221200
C	2.37864900	-2.70342500	0.28308600
H	0.92690300	-2.49994900	-1.30302300
C	2.66793500	-2.43582400	1.62013700
H	1.97027600	-1.56429000	3.46468700
H	3.10449200	-3.20466500	-0.34526400
H	3.62373100	-2.73534500	2.03247700
O	-2.14509300	-3.25021400	0.21573600
C	-3.35498800	-3.58080200	-0.17588500
O	-4.12161900	-2.79008000	-0.71958100
C	-3.70831000	-5.01330700	0.13118800
H	-3.91751700	-5.09520300	1.20179700
H	-4.59424500	-5.30193600	-0.43253700
H	-2.87251900	-5.67377600	-0.10275400
H	-0.83468700	0.63297400	-0.67493500
H	-3.07980400	1.64190300	1.34823300
N	1.83151500	2.06747700	-0.14741600

C	2.21896500	1.03683400	-0.91737500
H	2.51668900	2.39368200	0.51970300
C	3.56154600	0.42828500	-0.62866800
O	1.51602600	0.56877000	-1.83243000
C	4.19576200	-0.29252500	-1.64628500
C	4.15767400	0.48967200	0.63548200
C	5.41001800	-0.92903100	-1.41042400
H	3.72741800	-0.35344000	-2.62079800
C	5.36933300	-0.15414900	0.87405700
H	3.66815900	1.00215000	1.45508500
C	5.99896600	-0.86366100	-0.14713700
H	5.89458300	-1.48003100	-2.20865300
H	5.81270100	-0.11391000	1.86250800
H	6.94042700	-1.36750400	0.04134000

IRC_TS1_point63

B	-2.61939000	4.03480500	0.38100100
B	-1.53192200	3.72179800	1.75834900
B	-0.55604900	2.29357200	1.37673400
B	-2.30986400	2.79746100	-0.86261000
B	-1.03055300	1.78882600	-0.22872400
B	-1.13147900	4.99124100	0.57853400
B	-1.61617200	4.42802300	-1.03487500
H	-3.70036800	4.51135500	0.53163200
B	0.14449100	3.91621600	1.18727100
H	-1.84292200	3.97894700	2.87915600
B	0.46539300	2.68563000	-0.04866400
H	-0.15878700	1.52548900	2.19037400
B	-0.62869300	3.00705000	-1.43937600
H	-3.15732000	2.37622100	-1.58363200
H	-1.16166600	6.14667900	0.86867100
B	0.09352300	4.35734500	-0.54090200
H	-1.99138000	5.17524200	-1.88330900
H	1.02339100	4.29258000	1.89864800
H	-0.31513000	2.73044500	-2.54953700
H	0.93647800	5.03962200	-1.03304600
B	-2.26418800	2.36522700	0.87384800
I	-1.65250400	-1.12991500	-0.23280800
C	0.25715500	-1.66714100	0.57312600
C	0.50962700	-1.38215000	1.90791900
C	1.15938600	-2.31168600	-0.26242000
C	1.74132700	-1.77590800	2.42880600
H	-0.22216300	-0.87847300	2.52283900
C	2.37873100	-2.70408400	0.28566400

H	0.92761100	-2.50106000	-1.30106600
C	2.66762100	-2.43574500	1.62265600
H	1.96951200	-1.56301000	3.46646200
H	3.10459800	-3.20593400	-0.34211900
H	3.62318700	-2.73528300	2.03549400
O	-2.14453200	-3.24805700	0.21158400
C	-3.35415900	-3.57931300	-0.18091100
O	-4.12099000	-2.78854000	-0.72443800
C	-3.70751700	-5.01261200	0.12474500
H	-3.91744500	-5.09580200	1.19507500
H	-4.59352700	-5.30063900	-0.43958500
H	-2.87201900	-5.67315800	-0.10941100
H	-0.83432500	0.63374400	-0.67179500
H	-3.07844000	1.64220000	1.35169600
N	1.83159100	2.06781100	-0.14762700
C	2.21778000	1.03658200	-0.91762500
H	2.51750900	2.39397800	0.51871500
C	3.56012900	0.42714600	-0.62982800
O	1.51393500	0.56861400	-1.83205800
C	4.19236800	-0.29527500	-1.64747000
C	4.15773900	0.48906300	0.63354200
C	5.40621900	-0.93281700	-1.41245000
H	3.72270400	-0.35673300	-2.62120200
C	5.36902200	-0.15576300	0.87129700
H	3.66957800	1.00272300	1.45323100
C	5.99670800	-0.86686300	-0.14994100
H	5.88922500	-1.48515100	-2.21063400
H	5.81349800	-0.11512400	1.85927400
H	6.93785500	-1.37151600	0.03792000

IRC_TS1_point64

B	-2.61906800	4.03522000	0.38401500
B	-1.53053400	3.72243300	1.76061700
B	-0.55471000	2.29433300	1.37838900
B	-2.31028500	2.79782200	-0.85971600
B	-1.03035400	1.78953400	-0.22673100
B	-1.13110300	4.99183500	0.58043200
B	-1.61690000	4.42843000	-1.03258500
H	-3.69998000	4.51174100	0.53539800
B	0.14549100	3.91700700	1.18831900
H	-1.84072400	3.97966200	2.88163200
B	0.46568000	2.68638500	-0.04782700
H	-0.15680600	1.52629300	2.19176600
B	-0.62952600	3.00751500	-1.43771400

H	-3.15812000	2.37635700	-1.58011700
H	-1.16121700	6.14730000	0.87053300
B	0.09320000	4.35801700	-0.53985400
H	-1.99275700	5.17564500	-1.88077000
H	1.02477600	4.29363300	1.89905700
H	-0.31675100	2.73103700	-2.54815700
H	0.93560100	5.04051200	-1.03264700
B	-2.26330000	2.36575500	0.87671700
I	-1.65151900	-1.12887500	-0.23307500
C	0.25741400	-1.66711000	0.57413400
C	0.50941900	-1.38146100	1.90885700
C	1.15967100	-2.31251400	-0.26071800
C	1.74087900	-1.77521400	2.43037700
H	-0.22246200	-0.87721500	2.52324800
C	2.37871400	-2.70497800	0.28802700
H	0.92827100	-2.50239000	-1.29936800
C	2.66728900	-2.43580200	1.62492700
H	1.96877700	-1.56166400	3.46796900
H	3.10472900	-3.20737700	-0.33925100
H	3.62270000	-2.73526600	2.03823400
O	-2.14417200	-3.25074300	0.21029700
C	-3.35329100	-3.57964900	-0.18487100
O	-4.11831600	-2.78693600	-0.72809600
C	-3.70821000	-5.01272300	0.11741600
H	-3.91875100	-5.09769200	1.18754200
H	-4.59372200	-5.29899600	-0.44823800
H	-2.87268200	-5.67316000	-0.11750000
H	-0.83271100	0.63421300	-0.67055600
H	-3.07701400	1.64255600	1.35517300
N	1.83165200	2.06813100	-0.14805600
C	2.21635200	1.03618300	-0.91765800
H	2.51842300	2.39417200	0.51730800
C	3.55849600	0.42577800	-0.63091700
O	1.51106300	0.56817600	-1.83086600
C	4.18904700	-0.29808200	-1.64864800
C	4.15759300	0.48819300	0.63170600
C	5.40251000	-0.93664900	-1.41437800
H	3.71843500	-0.35979400	-2.62197200
C	5.36851600	-0.15760500	0.86867300
H	3.67096500	1.00304700	1.45150400
C	5.99442500	-0.87022100	-0.15260400
H	5.88418700	-1.49005500	-2.21267400
H	5.81424800	-0.11640300	1.85593500
H	6.93529400	-1.37561100	0.03467000

IRC_TS1_point65

B	-2.61879600	4.03509900	0.38695300
B	-1.52926800	3.72281600	1.76283700
B	-0.55341200	2.29496200	1.38012000
B	-2.31056800	2.79772900	-0.85691900
B	-1.03002400	1.78998100	-0.22456000
B	-1.13095200	4.99215600	0.58222100
B	-1.61772900	4.42854200	-1.03039700
H	-3.69973100	4.51122900	0.53903300
B	0.14634000	3.91772000	1.18932000
H	-1.83876800	3.98006400	2.88402900
B	0.46587800	2.68708200	-0.04695500
H	-0.15465100	1.52714600	2.19325500
B	-0.63034400	3.00796100	-1.43608600
H	-3.15885500	2.37594900	-1.57659600
H	-1.16123400	6.14760400	0.87223600
B	0.09271800	4.35859100	-0.53888000
H	-1.99449300	5.17547000	-1.87836700
H	1.02605200	4.29458000	1.89940400
H	-0.31820300	2.73109200	-2.54656100
H	0.93467100	5.04115500	-1.03233100
B	-2.26226300	2.36576600	0.87962600
I	-1.65067400	-1.12889900	-0.23288400
C	0.25786200	-1.66707100	0.57537000
C	0.50975200	-1.38039700	1.90989200
C	1.16014100	-2.31344300	-0.25872800
C	1.74094300	-1.77417000	2.43201800
H	-0.22201500	-0.87534100	2.52368700
C	2.37883200	-2.70604100	0.29064100
H	0.92885900	-2.50409200	-1.29725100
C	2.66720500	-2.43587400	1.62737900
H	1.96870700	-1.55987400	3.46947800
H	3.10464800	-3.20942900	-0.33596100
H	3.62231100	-2.73550300	2.04121300
O	-2.14358200	-3.24814600	0.20627200
C	-3.35253700	-3.57757700	-0.18968500
O	-4.11767700	-2.78474600	-0.73261000
C	-3.70748100	-5.01144800	0.11118800
H	-3.91905800	-5.09772100	1.18092200
H	-4.59268400	-5.29714800	-0.45545000
H	-2.87198800	-5.67181000	-0.12371800
H	-0.83233600	0.63485700	-0.66680200
H	-3.07551200	1.64244100	1.35872700

N	1.83166200	2.06866200	-0.14830500
C	2.21514600	1.03609100	-0.91800500
H	2.51901300	2.39440500	0.51691000
C	3.55706000	0.42476600	-0.63204400
O	1.50907100	0.56819000	-1.83077400
C	4.18549600	-0.30078700	-1.64986500
C	4.15765900	0.48763700	0.62988300
C	5.39849100	-0.94049800	-1.41647200
H	3.71346600	-0.36304500	-2.62242300
C	5.36812300	-0.15933400	0.86603800
H	3.67244000	1.00370600	1.44982100
C	5.99198200	-0.87356500	-0.15538600
H	5.87842900	-1.49536100	-2.21477600
H	5.81489000	-0.11796200	1.85299400
H	6.93243000	-1.37995900	0.03125200
IRC_TS1_point66			
B	-2.61862200	4.03552300	0.38987700
B	-1.52806400	3.72337300	1.76504600
B	-0.55223900	2.29563400	1.38169900
B	-2.31111700	2.79807600	-0.85415300
B	-1.02990500	1.79057900	-0.22264900
B	-1.13069400	4.99272000	0.58413100
B	-1.61854800	4.42897100	-1.02813200
H	-3.69946500	4.51176500	0.54272400
B	0.14718700	3.91845700	1.19040400
H	-1.83674500	3.98067300	2.88646400
B	0.46605200	2.68779800	-0.04608900
H	-0.15290300	1.52781800	2.19457000
B	-0.63126500	3.00840600	-1.43447800
H	-3.15984600	2.37622900	-1.57329800
H	-1.16083200	6.14821100	0.87416300
B	0.09230900	4.35923100	-0.53778200
H	-1.99586900	5.17601200	-1.87582000
H	1.02727500	4.29554600	1.89990800
H	-0.31990400	2.73182000	-2.54529600
H	0.93371700	5.04204800	-1.03182200
B	-2.26155800	2.36623800	0.88232900
I	-1.64950800	-1.12785400	-0.23304500
C	0.25831900	-1.66708400	0.57629400
C	0.50986200	-1.37975100	1.91072400
C	1.16053900	-2.31439300	-0.25712900
C	1.74083800	-1.77352900	2.43341100
H	-0.22196400	-0.87412500	2.52403300
C	2.37897600	-2.70705200	0.29281100

H	0.92954300	-2.50557400	-1.29562900
C	2.66715300	-2.43601200	1.62942300
H	1.96836700	-1.55858800	3.47079800
H	3.10486500	-3.21103300	-0.33331300
H	3.62214500	-2.73555000	2.04365000
O	-2.14316900	-3.25056600	0.20480000
C	-3.35167500	-3.57771200	-0.19357900
O	-4.11510000	-2.78295200	-0.73623800
C	-3.70850400	-5.01136500	0.10407300
H	-3.91989300	-5.09951900	1.17378300
H	-4.59403600	-5.29495500	-0.46310000
H	-2.87364800	-5.67205300	-0.13226800
H	-0.83046800	0.63538900	-0.66590900
H	-3.07430500	1.64274300	1.36198600
N	1.83162200	2.06896800	-0.14872800
C	2.21356900	1.03564200	-0.91793700
H	2.51996200	2.39487200	0.51501400
C	3.55528100	0.42338100	-0.63316800
O	1.50593700	0.56760300	-1.82921600
C	4.18190700	-0.30381500	-1.65095400
C	4.15751200	0.48698900	0.62787800
C	5.39452300	-0.94454700	-1.41830800
H	3.70880400	-0.36656100	-2.62297000
C	5.36765300	-0.16089300	0.86321800
H	3.67392200	1.00443200	1.44783300
C	5.98958800	-0.87689200	-0.15810000
H	5.87301100	-1.50071000	-2.21659600
H	5.81584800	-0.11866900	1.84930300
H	6.92976200	-1.38402300	0.02795100

IRC_TS1_point67

B	-2.61862400	4.03509500	0.39271400
B	-1.52712200	3.72361400	1.76723800
B	-0.55107000	2.29625000	1.38349500
B	-2.31144600	2.79772300	-0.85140700
B	-1.02955700	1.79103000	-0.22046400
B	-1.13095300	4.99292200	0.58589500
B	-1.61961500	4.42888100	-1.02599000
H	-3.69956800	4.51076100	0.54617800
B	0.14773100	3.91921000	1.19147100
H	-1.83524100	3.98091500	2.88879600
B	0.46617300	2.68856900	-0.04513100
H	-0.15083900	1.52869100	2.19614000
B	-0.63212000	3.00879100	-1.43280600

H	-3.16045700	2.37535500	-1.56986200
H	-1.16144200	6.14838800	0.87582200
B	0.09156800	4.35983500	-0.53675600
H	-1.99789400	5.17556200	-1.87350100
H	1.02812800	4.29667300	1.90037700
H	-0.32128100	2.73180500	-2.54361100
H	0.93246000	5.04283000	-1.03141900
B	-2.26062800	2.36602800	0.88520300
I	-1.64840700	-1.12766100	-0.23293200
C	0.25900000	-1.66708000	0.57745200
C	0.51050900	-1.37867000	1.91165400
C	1.16111200	-2.31549300	-0.25526400
C	1.74122300	-1.77256100	2.43487500
H	-0.22112600	-0.87212200	2.52439800
C	2.37919300	-2.70838900	0.29524700
H	0.93017800	-2.50745700	-1.29362800
C	2.66728400	-2.43629800	1.63166100
H	1.96872000	-1.55680800	3.47209600
H	3.10484500	-3.21342400	-0.33025500
H	3.62198700	-2.73605900	2.04635700
O	-2.14264100	-3.24864400	0.20152600
C	-3.35099500	-3.57555800	-0.19800700
O	-4.11398000	-2.78021100	-0.74036600
C	-3.70838200	-5.00972600	0.09778300
H	-3.92093600	-5.09933800	1.16702800
H	-4.59338300	-5.29212500	-0.47065300
H	-2.87357600	-5.67049500	-0.13884300
H	-0.82976400	0.63589800	-0.66224600
H	-3.07281900	1.64229000	1.36546000
N	1.83154400	2.06953900	-0.14885000
C	2.21219600	1.03554500	-0.91813400
H	2.52045700	2.39502800	0.51485800
C	3.55367200	0.42229200	-0.63420100
O	1.50372000	0.56767500	-1.82908000
C	4.17805600	-0.30662200	-1.65215200
C	4.15756500	0.48634900	0.62605500
C	5.39019100	-0.94854900	-1.42052100
H	3.70346900	-0.36984500	-2.62340100
C	5.36723400	-0.16276600	0.86045000
H	3.67554400	1.00504900	1.44619600
C	5.98697900	-0.88040600	-0.16107900
H	5.86682900	-1.50616400	-2.21888400
H	5.81659300	-0.12039000	1.84615100
H	6.92673500	-1.38856400	0.02423800

IRC_TS1_point68

B	-2.61867500	4.03525600	0.39555100
B	-1.52621300	3.72400300	1.76941800
B	-0.55007700	2.29682800	1.38511500
B	-2.31205900	2.79782900	-0.84871800
B	-1.02947000	1.79145700	-0.21849800
B	-1.13100400	4.99333100	0.58779400
B	-1.62061100	4.42913300	-1.02375600
H	-3.69956800	4.51094700	0.54971100
B	0.14830800	3.91989700	1.19262200
H	-1.83361400	3.98133700	2.89117500
B	0.46620900	2.68924500	-0.04417400
H	-0.14926600	1.52932200	2.19752200
B	-0.63311200	3.00915000	-1.43117400
H	-3.16146800	2.37535400	-1.56667600
H	-1.16147800	6.14882900	0.87772100
B	0.09095500	4.36041100	-0.53559100
H	-1.99946700	5.17586100	-1.87101300
H	1.02901000	4.29765000	1.90099300
H	-0.32294600	2.73240300	-2.54227300
H	0.93129400	5.04369300	-1.03079500
B	-2.26005800	2.36625800	0.88784400
I	-1.64703700	-1.12671200	-0.23296600
C	0.25971700	-1.66712400	0.57837100
C	0.51109000	-1.37792300	1.91241200
C	1.16164700	-2.31663800	-0.25365600
C	1.74158000	-1.77189700	2.43614000
H	-0.22045300	-0.87064200	2.52466400
C	2.37947600	-2.70966600	0.29736000
H	0.93085300	-2.50924500	-1.29193600
C	2.66752000	-2.43661400	1.63359000
H	1.96896500	-1.55543300	3.47324000
H	3.10501900	-3.21549400	-0.32763600
H	3.62207200	-2.73639300	2.04864700
O	-2.14209300	-3.24992500	0.19925600
C	-3.35016400	-3.57494400	-0.20210000
O	-4.11172900	-2.77800200	-0.74430800
C	-3.70936100	-5.00895100	0.09148800
H	-3.92164700	-5.09975100	1.16079900
H	-4.59488400	-5.28991400	-0.47712200
H	-2.87526800	-5.67015300	-0.14586600
H	-0.82781900	0.63650100	-0.66103200
H	-3.07175300	1.64231400	1.36859800

N	1.83138400	2.06986400	-0.14923400
C	2.21046800	1.03510800	-0.91809500
H	2.52130000	2.39552800	0.51302600
C	3.55174300	0.42090400	-0.63540900
O	1.50042400	0.56704900	-1.82740400
C	4.17417500	-0.30976400	-1.65330800
C	4.15733800	0.48572900	0.62397000
C	5.38593000	-0.95272600	-1.42246800
H	3.69838900	-0.37356400	-2.62392500
C	5.36668600	-0.16431700	0.85751500
H	3.67696500	1.00582300	1.44415100
C	5.98439800	-0.88379000	-0.16392800
H	5.86103400	-1.51170700	-2.22081000
H	5.81749500	-0.12110000	1.84239400
H	6.92388000	-1.39268900	0.02075500

IRC_TS1_point69

B	-2.61894300	4.03467300	0.39817200
B	-1.52561200	3.72411100	1.77148100
B	-0.54913100	2.29737000	1.38684800
B	-2.31250200	2.79733300	-0.84616900
B	-1.02920100	1.79188300	-0.21643800
B	-1.13157600	4.99343900	0.58947900
B	-1.62185200	4.42893500	-1.02174000
H	-3.69996400	4.50977700	0.55287200
B	0.14855600	3.92061400	1.19370400
H	-1.83254800	3.98142000	2.89335900
B	0.46620800	2.69001500	-0.04319600
H	-0.14747900	1.53008700	2.19903100
B	-0.63402900	3.00946700	-1.42956600
H	-3.16208400	2.37430100	-1.56354800
H	-1.16243900	6.14892200	0.87931200
B	0.09002100	4.36098700	-0.53455400
H	-2.00158900	5.17533900	-1.86884300
H	1.02947900	4.29879400	1.90156200
H	-0.32430000	2.73242400	-2.54066700
H	0.92983400	5.04450500	-1.03032100
B	-2.25935400	2.36590600	0.89050700
I	-1.64566700	-1.12627600	-0.23288500
C	0.26061400	-1.66713200	0.57946400
C	0.51199800	-1.37688500	1.91327300
C	1.16232900	-2.31782500	-0.25190400
C	1.74225900	-1.77100500	2.43745400
H	-0.21933900	-0.86867900	2.52501000

C	2.37983400	-2.71112300	0.29960900
H	0.93155000	-2.51118300	-1.29004700
C	2.66790000	-2.43699100	1.63561100
H	1.96968000	-1.55372000	3.47437100
H	3.10513600	-3.21797500	-0.32484300
H	3.62223300	-2.73695700	2.05104600
O	-2.14157600	-3.24885000	0.19678700
C	-3.34948600	-3.57293100	-0.20604800
O	-4.11012000	-2.77492900	-0.74796800
C	-3.70990800	-5.00717500	0.08511300
H	-3.92259800	-5.09985600	1.15403500
H	-4.59542100	-5.28586100	-0.48428200
H	-2.87645600	-5.66890500	-0.15379600
H	-0.82680500	0.63690800	-0.65790700
H	-3.07047000	1.64165100	1.37177700
N	1.83117200	2.07040500	-0.14930600
C	2.20888300	1.03490200	-0.91811300
H	2.52172000	2.39572600	0.51274800
C	3.54993800	0.41971300	-0.63635500
O	1.49788700	0.56699500	-1.82704800
C	4.17004600	-0.31276300	-1.65439200
C	4.15738200	0.48518100	0.62207500
C	5.38135200	-0.95688400	-1.42463500
H	3.69272600	-0.37710600	-2.62421600
C	5.36630300	-0.16603000	0.85458800
H	3.67873700	1.00667600	1.44239400
C	5.98170200	-0.88729100	-0.16699400
H	5.85454300	-1.51738300	-2.22302400
H	5.81848000	-0.12241800	1.83890400
H	6.92081900	-1.39714600	0.01693000

IRC_TS1_point70

B	-2.61930800	4.03446300	0.40071300
B	-1.52513000	3.72432400	1.77347100
B	-0.54839300	2.29786800	1.38844100
B	-2.31317300	2.79707700	-0.84370300
B	-1.02914500	1.79212200	-0.21450400
B	-1.13207200	4.99364900	0.59117100
B	-1.62307500	4.42889100	-1.01973200
H	-3.70034700	4.50943700	0.55596900
B	0.14874700	3.92126800	1.19480800
H	-1.83151100	3.98168500	2.89549000
B	0.46608300	2.69064000	-0.04221100
H	-0.14616000	1.53071900	2.20044900

B	-0.63506700	3.00966400	-1.42801300
H	-3.16303700	2.37379600	-1.56062100
H	-1.16310900	6.14915600	0.88094300
B	0.08913500	4.36147300	-0.53345700
H	-2.00341800	5.17522000	-1.86664700
H	1.02986000	4.29985800	1.90219700
H	-0.32584700	2.73274500	-2.53931100
H	0.92837500	5.04535100	-1.02969600
B	-2.25896400	2.36584000	0.89296400
I	-1.64407300	-1.12536800	-0.23281200
C	0.26160900	-1.66717500	0.58040900
C	0.51301500	-1.37601100	1.91400100
C	1.16304900	-2.31910000	-0.25027000
C	1.74303900	-1.77028000	2.43864600
H	-0.21811700	-0.86694600	2.52524500
C	2.38029100	-2.71259600	0.30170100
H	0.93231900	-2.51317600	-1.28829500
C	2.66842100	-2.43741600	1.63747600
H	1.97043500	-1.55222900	3.47541100
H	3.10536300	-3.22037900	-0.32223500
H	3.62256300	-2.73749700	2.05325300
O	-2.14098300	-3.24931800	0.19407300
C	-3.34875300	-3.57168400	-0.21013300
O	-4.10813500	-2.77228700	-0.75191300
C	-3.71088100	-5.00581800	0.07964900
H	-3.92329300	-5.09922300	1.14877300
H	-4.59682300	-5.28382600	-0.48978700
H	-2.87786100	-5.66783500	-0.15929800
H	-0.82472600	0.63747500	-0.65647600
H	-3.06958100	1.64131700	1.37466100
N	1.83087800	2.07072900	-0.14959500
C	2.20703700	1.03446600	-0.91805000
H	2.52239200	2.39620400	0.51112600
C	3.54790200	0.41832700	-0.63755600
O	1.49449400	0.56633500	-1.82531200
C	4.16594900	-0.31597800	-1.65554100
C	4.15712800	0.48461000	0.61999300
C	5.37689900	-0.96109500	-1.42663900
H	3.68735000	-0.38094800	-2.62467400
C	5.36574500	-0.16751400	0.85160800
H	3.68014000	1.00747600	1.44039900
C	5.97903700	-0.89062200	-0.16993500
H	5.84851100	-1.52294700	-2.22503600
H	5.81938500	-0.12309100	1.83516100

H	6.91791000	-1.40116500	0.01327200
IRC_TS1_point71			
B	-2.61984900	4.03367900	0.40301400
B	-1.52488700	3.72427700	1.77531100
B	-0.54768300	2.29831000	1.39003700
B	-2.31373700	2.79636000	-0.84143200
B	-1.02895100	1.79243500	-0.21261200
B	-1.13296900	4.99361100	0.59266200
B	-1.62449400	4.42850500	-1.01794300
H	-3.70103500	4.50807900	0.55874800
B	0.14867600	3.92191900	1.19581500
H	-1.83088900	3.98160100	2.89743400
B	0.46594000	2.69135600	-0.04126700
H	-0.14465700	1.53138500	2.20183500
B	-0.63606200	3.00981500	-1.42654500
H	-3.16368300	2.37251300	-1.55787700
H	-1.16442700	6.14911300	0.88233600
B	0.08800200	4.36193200	-0.53250100
H	-2.00563000	5.17453500	-1.86473700
H	1.02992800	4.30098700	1.90275600
H	-0.32718300	2.73270900	-2.53787300
H	0.92672400	5.04605300	-1.02926600
B	-2.25850100	2.36530800	0.89533700
I	-1.64249000	-1.12475100	-0.23270600
C	0.26268000	-1.66720700	0.58146500
C	0.51418100	-1.37494400	1.91479300
C	1.16379600	-2.32041800	-0.24855600
C	1.74402500	-1.76931500	2.43982500
H	-0.21672900	-0.86496100	2.52554700
C	2.38077200	-2.71413700	0.30384600
H	0.93299600	-2.51528900	-1.28641400
C	2.66905900	-2.43775900	1.63933500
H	1.97154700	-1.55036100	3.47636500
H	3.10558500	-3.22292300	-0.31958100
H	3.62305900	-2.73793100	2.05541500
O	-2.14034800	-3.24868400	0.19201900
C	-3.34802400	-3.56974300	-0.21366400
O	-4.10629600	-2.76906500	-0.75514800
C	-3.71181900	-5.00385000	0.07348600
H	-3.92437400	-5.09901900	1.14206100
H	-4.59822600	-5.27862100	-0.49630600
H	-2.88031100	-5.66711400	-0.16763100
H	-0.82353000	0.63780500	-0.65387000

H	-3.06852100	1.64045100	1.37749300
N	1.83053400	2.07125800	-0.14968500
C	2.20528800	1.03417100	-0.91793700
H	2.52270200	2.39647500	0.51070500
C	3.54596700	0.41710600	-0.63842500
O	1.49174500	0.56612100	-1.82474000
C	4.16162700	-0.31916500	-1.65646600
C	4.15720300	0.48430000	0.61804600
C	5.37216500	-0.96538900	-1.42863700
H	3.68151700	-0.38474500	-2.62479600
C	5.36545100	-0.16890100	0.84861900
H	3.68206400	1.00875200	1.43849800
C	5.97632200	-0.89402400	-0.17292900
H	5.84189900	-1.52881600	-2.22698200
H	5.82062700	-0.12378400	1.83146100
H	6.91488900	-1.40543600	0.00956000
IRC_TS1_point72			
B	-2.62055200	4.03303900	0.40503900
B	-1.52492100	3.72430800	1.77697700
B	-0.54727300	2.29870100	1.39159100
B	-2.31443400	2.79564700	-0.83934800
B	-1.02895100	1.79245700	-0.21076300
B	-1.13394300	4.99359000	0.59397200
B	-1.62590100	4.42807100	-1.01634900
H	-3.70181900	4.50715900	0.56106800
B	0.14841500	3.92251800	1.19681800
H	-1.83061200	3.98172900	2.89915100
B	0.46567000	2.69189400	-0.04025600
H	-0.14372600	1.53198900	2.20330900
B	-0.63708800	3.00975900	-1.42513900
H	-3.16445500	2.37137000	-1.55543700
H	-1.16573300	6.14912500	0.88345400
B	0.08684700	4.36226200	-0.53156800
H	-2.00757700	5.17386900	-1.86310000
H	1.02971800	4.30210900	1.90339500
H	-0.32848200	2.73259000	-2.53651700
H	0.92505700	5.04673000	-1.02873000
B	-2.25834700	2.36488400	0.89749700
I	-1.64068400	-1.12388300	-0.23253400
C	0.26387000	-1.66723000	0.58252000
C	0.51553200	-1.37390900	1.91557800
C	1.16459800	-2.32178900	-0.24686700
C	1.74515900	-1.76846700	2.44097700
H	-0.21507300	-0.86298100	2.52585700

C	2.38131000	-2.71574700	0.30590600
H	0.93373900	-2.51735600	-1.28458900
C	2.66978400	-2.43822400	1.64112700
H	1.97275200	-1.54877000	3.47734200
H	3.10575800	-3.22553800	-0.31707100
H	3.62359000	-2.73857000	2.05745400
O	-2.13991000	-3.24864400	0.18917500
C	-3.34759800	-3.56796400	-0.21762500
O	-4.10459700	-2.76593500	-0.75894500
C	-3.71276600	-5.00201300	0.06877900
H	-3.92426500	-5.09775800	1.13823400
H	-4.59956900	-5.27734700	-0.50082400
H	-2.88055300	-5.66481300	-0.17235800
H	-0.82135100	0.63823000	-0.65223300
H	-3.06791200	1.63972700	1.37996900
N	1.83014400	2.07161300	-0.14982000
C	2.20345300	1.03380700	-0.91780800
H	2.52319800	2.39692900	0.50945000
C	3.54394900	0.41579600	-0.63951700
O	1.48845100	0.56551500	-1.82297900
C	4.15737500	-0.32244900	-1.65748600
C	4.15710800	0.48395000	0.61600000
C	5.36757600	-0.96961200	-1.43059700
H	3.67588900	-0.38870000	-2.62501600
C	5.36506400	-0.17012400	0.84560800
H	3.68369900	1.00980300	1.43656600
C	5.97369900	-0.89717200	-0.17592700
H	5.83568400	-1.53431000	-2.22898000
H	5.82177400	-0.12411600	1.82766700
H	6.91213000	-1.40905800	0.00577000

IRC_TS1_point73

B	-2.62138100	4.03215500	0.40689000
B	-1.52495800	3.72429800	1.77841500
B	-0.54672100	2.29917200	1.39291200
B	-2.31517400	2.79466200	-0.83738400
B	-1.02876100	1.79255900	-0.20907800
B	-1.13514500	4.99350800	0.59496400
B	-1.62756100	4.42743000	-1.01501500
H	-3.70277800	4.50589800	0.56330900
B	0.14808600	3.92325500	1.19745500
H	-1.83021700	3.98183900	2.90067500
B	0.46535500	2.69254200	-0.03951200
H	-0.14241600	1.53272100	2.20451100

B	-0.63819500	3.00958300	-1.42397000
H	-3.16529000	2.36986400	-1.55310500
H	-1.16728800	6.14910600	0.88425700
B	0.08549200	4.36261000	-0.53099100
H	-2.00989500	5.17300000	-1.86171100
H	1.02953500	4.30343400	1.90357200
H	-0.32993200	2.73238300	-2.53543900
H	0.92312400	5.04744600	-1.02865300
B	-2.25809400	2.36431400	0.89953700
I	-1.63900500	-1.12318900	-0.23233700
C	0.26495100	-1.66726200	0.58354100
C	0.51677200	-1.37261100	1.91627400
C	1.16529700	-2.32329400	-0.24512400
C	1.74625600	-1.76714600	2.44205100
H	-0.21368900	-0.86073100	2.52604000
C	2.38182400	-2.71731600	0.30804600
H	0.93436600	-2.51977500	-1.28267500
C	2.67054200	-2.43830800	1.64291100
H	1.97395900	-1.54635700	3.47816600
H	3.10610000	-3.22807800	-0.31447500
H	3.62430700	-2.73854300	2.05947500
O	-2.13903100	-3.24854000	0.18737700
C	-3.34660900	-3.56632900	-0.22069600
O	-4.10255200	-2.76279800	-0.76152000
C	-3.71402600	-5.00026200	0.06288000
H	-3.93017200	-5.09630900	1.12925300
H	-4.59821500	-5.27330700	-0.50964600
H	-2.88401900	-5.66448700	-0.17568200
H	-0.81968400	0.63833400	-0.65068500
H	-3.06704700	1.63877100	1.38244800
N	1.82971200	2.07199700	-0.14973200
C	2.20172300	1.03347200	-0.91742000
H	2.52349100	2.39751100	0.50845400
C	3.54206800	0.41463400	-0.64033900
O	1.48557100	0.56537700	-1.82247400
C	4.15322700	-0.32581700	-1.65826800
C	4.15734100	0.48414200	0.61406000
C	5.36303700	-0.97404700	-1.43222900
H	3.67049300	-0.39281400	-2.62535100
C	5.36493600	-0.17093100	0.84282500
H	3.68572600	1.01174600	1.43463700
C	5.97115300	-0.90038200	-0.17849800
H	5.82948500	-1.54044800	-2.23054500
H	5.82306400	-0.12396800	1.82432700

H	6.90928000	-1.41307700	0.00273800
IRC_TS1_point74			
B	-2.62242000	4.03083400	0.40821400
B	-1.52540600	3.72411800	1.77953400
B	-0.54634100	2.29958100	1.39421600
B	-2.31577500	2.79328200	-0.83585300
B	-1.02870200	1.79232000	-0.20750300
B	-1.13676100	4.99322700	0.59562600
B	-1.62929400	4.42648200	-1.01405700
H	-3.70412700	4.50368300	0.56487900
B	0.14739900	3.92399700	1.19808300
H	-1.83061300	3.98171600	2.90179100
B	0.46517600	2.69316200	-0.03873100
H	-0.14129000	1.53366900	2.20590600
B	-0.63917600	3.00928600	-1.42295900
H	-3.16572100	2.36742500	-1.55103600
H	-1.16977300	6.14884200	0.88457000
B	0.08398100	4.36285700	-0.53052400
H	-2.01253500	5.17136800	-1.86085600
H	1.02864300	4.30513300	1.90386600
H	-0.33102500	2.73174100	-2.53436100
H	0.92094300	5.04809100	-1.02871100
B	-2.25789700	2.36337600	0.90125500
I	-1.63741400	-1.12253200	-0.23219700
C	0.26620800	-1.66716500	0.58455200
C	0.51830800	-1.37114000	1.91691100
C	1.16609700	-2.32477600	-0.24331100
C	1.74754200	-1.76588400	2.44315000
H	-0.21161700	-0.85786100	2.52604900
C	2.38229100	-2.71911300	0.31036500
H	0.93495300	-2.52249500	-1.28055800
C	2.67128200	-2.43871400	1.64486700
H	1.97549700	-1.54390200	3.47895100
H	3.10595300	-3.23151400	-0.31134900
H	3.62474400	-2.73927600	2.06187500
O	-2.13857000	-3.24807100	0.18520200
C	-3.34621900	-3.56429700	-0.22386300
O	-4.10096700	-2.75944900	-0.76434800
C	-3.71506000	-4.99825500	0.05811900
H	-3.92329000	-5.09818500	1.12828500
H	-4.60524900	-5.26748400	-0.50976500
H	-2.88585600	-5.66315500	-0.18942600
H	-0.81778200	0.63876900	-0.64835200

H	-3.06613300	1.63740000	1.38466000
N	1.82954800	2.07299800	-0.15029300
C	2.20043500	1.03359400	-0.91757400
H	2.52366900	2.39802500	0.50863100
C	3.54063600	0.41394300	-0.64102300
O	1.48325600	0.56464500	-1.82008600
C	4.14901700	-0.32899500	-1.65854700
C	4.15802600	0.48457700	0.61229800
C	5.35836900	-0.97832300	-1.43365800
H	3.66384900	-0.39750400	-2.62395400
C	5.36528600	-0.17154000	0.83990600
H	3.68872600	1.01420700	1.43274000
C	5.96881900	-0.90327300	-0.18128100
H	5.82222200	-1.54697900	-2.23169900
H	5.82560100	-0.12328000	1.82007400
H	6.90657500	-1.41689100	-0.00106700

IRC_TS1_point75

B	-2.62348300	4.02986300	0.40971500
B	-1.52592500	3.72401300	1.78077600
B	-0.54623400	2.29993800	1.39550000
B	-2.31655100	2.79219300	-0.83418400
B	-1.02852400	1.79236000	-0.20595300
B	-1.13822200	4.99302700	0.59650000
B	-1.63094200	4.42571600	-1.01292700
H	-3.70532700	4.50241200	0.56665100
B	0.14669800	3.92459500	1.19879300
H	-1.83087000	3.98176800	2.90307500
B	0.46464900	2.69365900	-0.03787000
H	-0.14060600	1.53432500	2.20717400
B	-0.64020200	3.00897300	-1.42181400
H	-3.16655100	2.36588800	-1.54912200
H	-1.17164900	6.14869400	0.88534300
B	0.08254900	4.36310700	-0.52987300
H	-2.01474100	5.17048400	-1.85964400
H	1.02792900	4.30630000	1.90433100
H	-0.33224000	2.73140700	-2.53324200
H	0.91894800	5.04883300	-1.02834300
B	-2.25797600	2.36272800	0.90299800
I	-1.63551500	-1.12160200	-0.23200100
C	0.26750900	-1.66721100	0.58548800
C	0.51982200	-1.37008300	1.91755700
C	1.16695900	-2.32625600	-0.24170800
C	1.74885700	-1.76500800	2.44414900

H	-0.20982100	-0.85581600	2.52621500
C	2.38294600	-2.72080800	0.31231700
H	0.93577800	-2.52471700	-1.27882000
C	2.67217600	-2.43920000	1.64651400
H	1.97695300	-1.54213900	3.47972800
H	3.10641900	-3.23411200	-0.30899200
H	3.62551900	-2.73986100	2.06375900
O	-2.13774200	-3.24816800	0.18332700
C	-3.34536200	-3.56255400	-0.22686000
O	-4.09894300	-2.75619800	-0.76691900
C	-3.71662400	-4.99612400	0.05351600
H	-3.93566200	-5.09355600	1.12069300
H	-4.60060800	-5.26659400	-0.52215500
H	-2.88597000	-5.66153900	-0.18405800
H	-0.81557600	0.63857800	-0.64739300
H	-3.06570000	1.63637600	1.38671500
N	1.82887300	2.07289700	-0.14956400
C	2.19849100	1.03290600	-0.91652000
H	2.52416400	2.39900500	0.50645100
C	3.53860100	0.41261900	-0.64176100
O	1.48007500	0.56444600	-1.81973000
C	4.14491000	-0.33211100	-1.65944400
C	4.15815700	0.48452100	0.61027100
C	5.35400900	-0.98229800	-1.43548000
H	3.65877800	-0.40118000	-2.62461700
C	5.36516700	-0.17238500	0.83696500
H	3.69041100	1.01555200	1.43078900
C	5.96643800	-0.90619200	-0.18408600
H	5.81627700	-1.55244700	-2.23347800
H	5.82668200	-0.12347200	1.81674000
H	6.90394300	-1.42056300	-0.00441800

IRC_TS1_point76

B	-2.62470400	4.02840000	0.41104700
B	-1.52659000	3.72363100	1.78195900
B	-0.54605400	2.30014500	1.39688400
B	-2.31730500	2.79068200	-0.83265200
B	-1.02863300	1.79202900	-0.20430500
B	-1.13998700	4.99257500	0.59725200
B	-1.63278600	4.42464000	-1.01190300
H	-3.70680000	4.50021200	0.56813300
B	0.14583000	3.92515200	1.19956400
H	-1.83148800	3.98143600	2.90424100
B	0.46434100	2.69413400	-0.03693300

H	-0.13977100	1.53491900	2.20856200
B	-0.64128900	3.00854600	-1.42073400
H	-3.16707100	2.36345100	-1.54720600
H	-1.17413000	6.14827200	0.88573000
B	0.08092400	4.36318500	-0.52925900
H	-2.01727000	5.16882300	-1.85875000
H	1.02688800	4.30774000	1.90477400
H	-0.33338000	2.73076000	-2.53213200
H	0.91675400	5.04925900	-1.02819200
B	-2.25801100	2.36162900	0.90470300
I	-1.63364800	-1.12068300	-0.23183700
C	0.26887500	-1.66714200	0.58650900
C	0.52143400	-1.36883500	1.91825400
C	1.16781100	-2.32773600	-0.24002300
C	1.75023900	-1.76404200	2.44520000
H	-0.20780900	-0.85343900	2.52642300
C	2.38347900	-2.72268000	0.31439500
H	0.93640300	-2.52713100	-1.27689700
C	2.67302900	-2.43977900	1.64825500
H	1.97853600	-1.54022400	3.48053100
H	3.10641200	-3.23731300	-0.30633700
H	3.62617000	-2.74067700	2.06577400
O	-2.13693600	-3.24760800	0.18114500
C	-3.34463700	-3.56044700	-0.22987100
O	-4.09715600	-2.75275900	-0.76954400
C	-3.71799400	-4.99377500	0.04905800
H	-3.94077400	-5.09098800	1.11542800
H	-4.60059200	-5.26300500	-0.52931400
H	-2.88754800	-5.66031400	-0.18597000
H	-0.81372000	0.63905400	-0.64521900
H	-3.06508900	1.63484900	1.38877700
N	1.82858100	2.07380500	-0.15010100
C	2.19695900	1.03298900	-0.91688200
H	2.52412300	2.39910600	0.50710900
C	3.53695400	0.41179300	-0.64269300
O	1.47734300	0.56362300	-1.81712400
C	4.14060400	-0.33532500	-1.66008200
C	4.15857000	0.48470200	0.60844800
C	5.34930000	-0.98656000	-1.43724500
H	3.65239900	-0.40546400	-2.62387700
C	5.36529400	-0.17319200	0.83398400
H	3.69299500	1.01751000	1.42900500
C	5.96400100	-0.90915300	-0.18705900
H	5.80944600	-1.55840300	-2.23517800

H	5.82884800	-0.12307300	1.81260000
H	6.90129900	-1.42415900	-0.00835400

IRC_TS1_point77

B	-2.62605700	4.02693800	0.41213900
B	-1.52749000	3.72334900	1.78292700
B	-0.54608500	2.30044200	1.39814800
B	-2.31807500	2.78903200	-0.83123900
B	-1.02834200	1.79178200	-0.20277900
B	-1.14190800	4.99211500	0.59775000
B	-1.63466600	4.42339200	-1.01113200
H	-3.70835500	4.49829300	0.56933700
B	0.14476100	3.92575700	1.20012800
H	-1.83227900	3.98138900	2.90518600
B	0.46375600	2.69456900	-0.03603700
H	-0.13921500	1.53563800	2.20991300
B	-0.64231300	3.00788300	-1.41973200
H	-3.16773800	2.36115700	-1.54558300
H	-1.17663300	6.14787100	0.88600000
B	0.07922200	4.36323600	-0.52880600
H	-2.01970600	5.16729800	-1.85801100
H	1.02570000	4.30906800	1.90512300
H	-0.33442300	2.72994400	-2.53104800
H	0.91446600	5.04982200	-1.02801700
B	-2.25818900	2.36060400	0.90625800
I	-1.63165400	-1.11962900	-0.23160400
C	0.27020900	-1.66718100	0.58749800
C	0.52309700	-1.36764400	1.91890400
C	1.16856600	-2.32940900	-0.23830900
C	1.75167700	-1.76309700	2.44619000
H	-0.20578000	-0.85115000	2.52656500
C	2.38400800	-2.72463600	0.31644700
H	0.93705900	-2.52956400	-1.27503000
C	2.67391200	-2.44039400	1.64993900
H	1.98019100	-1.53834000	3.48126400
H	3.10662400	-3.24029600	-0.30385900
H	3.62690700	-2.74145000	2.06767800
O	-2.13617100	-3.24739000	0.17903600
C	-3.34395500	-3.55839400	-0.23277800
O	-4.09535000	-2.74923800	-0.77195800
C	-3.71943200	-4.99142600	0.04498700
H	-3.94707800	-5.08790300	1.11096000
H	-4.59981300	-5.26073700	-0.53722800
H	-2.88774700	-5.65845800	-0.18572900

H	-0.81125100	0.63875900	-0.64445200
H	-3.06471800	1.63340500	1.39062200
N	1.82790300	2.07375400	-0.14910200
C	2.19512300	1.03231000	-0.91541900
H	2.52450800	2.40016900	0.50537100
C	3.53503200	0.41049500	-0.64305900
O	1.47439900	0.56367000	-1.81709600
C	4.13634500	-0.33853300	-1.66063700
C	4.15915300	0.48496000	0.60646500
C	5.34480000	-0.99060800	-1.43894600
H	3.64693500	-0.40938000	-2.62393500
C	5.36563000	-0.17371800	0.83088800
H	3.69535100	1.01939800	1.42697600
C	5.96176400	-0.91196000	-0.18995400
H	5.80322500	-1.56399800	-2.23680100
H	5.83067800	-0.12271800	1.80882500
H	6.89886600	-1.42763000	-0.01190400

IRC_TS1_point78

B	-2.62744300	4.02526200	0.41302700
B	-1.52841600	3.72294800	1.78379500
B	-0.54602100	2.30063400	1.39942800
B	-2.31878000	2.78721800	-0.83002500
B	-1.02846600	1.79128700	-0.20122000
B	-1.14392100	4.99157600	0.59812400
B	-1.63654400	4.42204500	-1.01050100
H	-3.71002500	4.49591200	0.57025100
B	0.14368700	3.92635000	1.20074000
H	-1.83323900	3.98111500	2.90600100
B	0.46346000	2.69498900	-0.03517600
H	-0.13847600	1.53631800	2.21127900
B	-0.64327800	3.00721200	-1.41878200
H	-3.16811900	2.35833500	-1.54408200
H	-1.17939800	6.14741500	0.88592100
B	0.07749900	4.36323400	-0.52840800
H	-2.02221700	5.16533200	-1.85760200
H	1.02437900	4.31068300	1.90545500
H	-0.33533400	2.72905100	-2.53005900
H	0.91220200	5.05018400	-1.02804800
B	-2.25829900	2.35935300	0.90770200
I	-1.62987000	-1.11863200	-0.23147500
C	0.27145500	-1.66715100	0.58846500
C	0.52464600	-1.36636100	1.91950000
C	1.16923900	-2.33100300	-0.23669900

C	1.75301200	-1.76210800	2.44711600
H	-0.20380400	-0.84866700	2.52666000
C	2.38435900	-2.72664600	0.31843100
H	0.93746900	-2.53212400	-1.27317300
C	2.67465300	-2.44103400	1.65156100
H	1.98176700	-1.53632500	3.48191500
H	3.10645000	-3.24363900	-0.30133900
H	3.62749300	-2.74227200	2.06952300
O	-2.13532600	-3.24700800	0.17718400
C	-3.34315400	-3.55649600	-0.23537300
O	-4.09365300	-2.74602800	-0.77401500
C	-3.72088400	-4.98919300	0.04087000
H	-3.95705300	-5.08391900	1.10467300
H	-4.59705200	-5.25837200	-0.54729800
H	-2.88869500	-5.65739100	-0.18267000
H	-0.80896900	0.63904300	-0.64219100
H	-3.06418100	1.63171000	1.39239900
N	1.82776000	2.07482200	-0.14975300
C	2.19390000	1.03266300	-0.91589900
H	2.52450300	2.40037100	0.50601300
C	3.53371300	0.41001100	-0.64415200
O	1.47189200	0.56259700	-1.81324000
C	4.13235400	-0.34163500	-1.66121400
C	4.15981900	0.48548000	0.60464900
C	5.34042800	-0.99473600	-1.44052000
H	3.64092400	-0.41356300	-2.62325400
C	5.36606200	-0.17413400	0.82802300
H	3.69815800	1.02159000	1.42531900
C	5.95969500	-0.91459400	-0.19276500
H	5.79677300	-1.56984700	-2.23830700
H	5.83305500	-0.12190800	1.80497200
H	6.89663200	-1.43081900	-0.01563900

IRC_TS1_point79

B	-2.62897700	4.02339600	0.41368700
B	-1.52958200	3.72256600	1.78447500
B	-0.54604900	2.30099700	1.40065600
B	-2.31942900	2.78509100	-0.82886600
B	-1.02792300	1.79085600	-0.19975700
B	-1.14619100	4.99095300	0.59822600
B	-1.63856200	4.42040400	-1.01008200
H	-3.71188300	4.49327900	0.57087300
B	0.14236700	3.92710600	1.20116800
H	-1.83451500	3.98098300	2.90659400
B	0.46296200	2.69545600	-0.03415400

H	-0.13793700	1.53723400	2.21273700
B	-0.64418900	3.00629300	-1.41796800
H	-3.16847900	2.35520000	-1.54265300
H	-1.18257800	6.14684000	0.88562200
B	0.07569100	4.36315800	-0.52813700
H	-2.02486600	5.16312300	-1.85737500
H	1.02273600	4.31242500	1.90573200
H	-0.33618300	2.72790700	-2.52911700
H	0.90967100	5.05068800	-1.02813000
B	-2.25847200	2.35805600	0.90901900
I	-1.62797400	-1.11752100	-0.23126400
C	0.27273100	-1.66715600	0.58940600
C	0.52630800	-1.36502900	1.92008300
C	1.16983200	-2.33284400	-0.23494800
C	1.75439100	-1.76113000	2.44806700
H	-0.20164800	-0.84601600	2.52670000
C	2.38469600	-2.72885300	0.32055100
H	0.93786900	-2.53493200	-1.27119600
C	2.67539600	-2.44181400	1.65327000
H	1.98342700	-1.53428100	3.48257200
H	3.10630000	-3.24717900	-0.29866300
H	3.62802400	-2.74333100	2.07151200
O	-2.13461700	-3.24649800	0.17537200
C	-3.34252400	-3.55441400	-0.23785800
O	-4.09209100	-2.74261100	-0.77589500
C	-3.72197900	-4.98693200	0.03707900
H	-3.96387400	-5.08101600	1.10030900
H	-4.59543200	-5.25638600	-0.55562200
H	-2.88812600	-5.65531700	-0.18159900
H	-0.80631800	0.63875300	-0.64163400
H	-3.06365600	1.62988700	1.39406500
N	1.82712100	2.07472000	-0.14819900
C	2.19222800	1.03199500	-0.91412500
H	2.52479900	2.40137200	0.50520900
C	3.53199400	0.40877000	-0.64394300
O	1.46948600	0.56319200	-1.81444000
C	4.12810200	-0.34475000	-1.66134000
C	4.16092900	0.48604900	0.60294400
C	5.33592000	-0.99867500	-1.44207300
H	3.63504000	-0.41770300	-2.62252300
C	5.36693000	-0.17433100	0.82492300
H	3.70138500	1.02418700	1.42341200
C	5.95768400	-0.91722400	-0.19566600
H	5.79013800	-1.57563300	-2.23973500

H	5.83584200	-0.12094100	1.80081300
H	6.89433300	-1.43426600	-0.01935800

IRC_TS1_point80

B	-2.63050300	4.02156500	0.41427100
B	-1.53076100	3.72216200	1.78514000
B	-0.54613500	2.30117300	1.40188900
B	-2.32006800	2.78308800	-0.82789400
B	-1.02798100	1.79029000	-0.19824800
B	-1.14842800	4.99035700	0.59839600
B	-1.64044600	4.41890100	-1.00971600
H	-3.71374000	4.49076300	0.57140200
B	0.14109800	3.92768900	1.20170400
H	-1.83580900	3.98083900	2.90716100
B	0.46262400	2.69587700	-0.03341900
H	-0.13734600	1.53802000	2.21417300
B	-0.64503400	3.00547200	-1.41703600
H	-3.16877800	2.35216800	-1.54148900
H	-1.18563500	6.14636200	0.88537000
B	0.07384100	4.36318200	-0.52784500
H	-2.02741200	5.16107300	-1.85722000
H	1.02115300	4.31412000	1.90606700
H	-0.33677700	2.72671600	-2.52803500
H	0.90728100	5.05120000	-1.02812100
B	-2.25863900	2.35670000	0.91029500
I	-1.62623700	-1.11647700	-0.23118800
C	0.27391700	-1.66717600	0.59031300
C	0.52783500	-1.36378300	1.92058700
C	1.17044600	-2.33450000	-0.23340000
C	1.75566300	-1.76030400	2.44894300
H	-0.19962200	-0.84340700	2.52664500
C	2.38494300	-2.73104100	0.32250100
H	0.93827700	-2.53752800	-1.26942200
C	2.67600700	-2.44272400	1.65488800
H	1.98497600	-1.53238600	3.48315100
H	3.10606200	-3.25075900	-0.29617000
H	3.62843600	-2.74456000	2.07339200
O	-2.13382600	-3.24602000	0.17379600
C	-3.34174700	-3.55245300	-0.24013900
O	-4.09049700	-2.73940800	-0.77763200
C	-3.72327800	-4.98471900	0.03326300
H	-3.97368100	-5.07714700	1.09429500
H	-4.59217400	-5.25460700	-0.56555700
H	-2.88848400	-5.65379400	-0.17797800

H	-0.80315500	0.63858900	-0.63890800
H	-3.06323800	1.62808000	1.39562100
N	1.82708200	2.07597600	-0.14911300
C	2.19120000	1.03246300	-0.91438000
H	2.52500500	2.40209900	0.50485600
C	3.53087800	0.40848900	-0.64524000
O	1.46695900	0.56176800	-1.80932600
C	4.12438800	-0.34768700	-1.66203200
C	4.16169800	0.48667800	0.60099300
C	5.33190900	-1.00256800	-1.44363700
H	3.62939900	-0.42180300	-2.62213100
C	5.36750800	-0.17460800	0.82207900
H	3.70414600	1.02640400	1.42161900
C	5.95593500	-0.91959900	-0.19843700
H	5.78407400	-1.58135700	-2.24117700
H	5.83818400	-0.12012000	1.79720100
H	6.89248100	-1.43715300	-0.02296400
IRC_TS1_point81			
B	-2.63222000	4.01936600	0.41468000
B	-1.53214800	3.72163200	1.78566600
B	-0.54618400	2.30152100	1.40310000
B	-2.32068000	2.78062900	-0.82690200
B	-1.02742600	1.78966000	-0.19684100
B	-1.15099800	4.98959600	0.59829300
B	-1.64261700	4.41699800	-1.00947300
H	-3.71591600	4.48748400	0.57164800
B	0.13957500	3.92853100	1.20211300
H	-1.83751400	3.98046300	2.90756500
B	0.46217900	2.69630000	-0.03223900
H	-0.13676300	1.53900500	2.21565600
B	-0.64590300	3.00444200	-1.41634800
H	-3.16889600	2.34830400	-1.54017900
H	-1.18944100	6.14565500	0.88469400
B	0.07194700	4.36301000	-0.52763500
H	-2.03032900	5.15829600	-1.85733400
H	1.01910800	4.31623600	1.90638800
H	-0.33758000	2.72550900	-2.52724600
H	0.90452700	5.05167900	-1.02836600
B	-2.25883600	2.35515000	0.91145100
I	-1.62430700	-1.11518400	-0.23103600
C	0.27526600	-1.66704200	0.59119700
C	0.52954100	-1.36242700	1.92114800
C	1.17103800	-2.33631700	-0.23167900
C	1.75698800	-1.75953500	2.44991900

H	-0.19730600	-0.84055700	2.52665100
C	2.38518100	-2.73345300	0.32465000
H	0.93859800	-2.54045100	-1.26741900
C	2.67663500	-2.44382100	1.65664300
H	1.98657700	-1.53060600	3.48384800
H	3.10561800	-3.25485500	-0.29333300
H	3.62872400	-2.74621300	2.07552500
O	-2.13301900	-3.24542300	0.17234000
C	-3.34101600	-3.55037000	-0.24218300
O	-4.08889500	-2.73604600	-0.77908200
C	-3.72438400	-4.98240000	0.02965600
H	-3.97940700	-5.07447600	1.08959300
H	-4.59107900	-5.25161000	-0.57266500
H	-2.88931600	-5.65214400	-0.17815600
H	-0.80050500	0.63864900	-0.63865100
H	-3.06254600	1.62582700	1.39713800
N	1.82640600	2.07570700	-0.14714000
C	2.18954400	1.03181000	-0.91274800
H	2.52500100	2.40241000	0.50552300
C	3.52918800	0.40725100	-0.64473200
O	1.46482000	0.56255400	-1.81087400
C	4.12004500	-0.35063300	-1.66196200
C	4.16295600	0.48711400	0.59959400
C	5.32734200	-1.00626300	-1.44533500
H	3.62292100	-0.42589700	-2.62082600
C	5.36863200	-0.17483000	0.81890900
H	3.70782600	1.02882400	1.42019100
C	5.95405400	-0.92206400	-0.20162200
H	5.77701100	-1.58693800	-2.24289400
H	5.84165100	-0.11905800	1.79266700
H	6.89031900	-1.44044200	-0.02736000

IRC_TS1_point82

B	-2.63396100	4.01726000	0.41511400
B	-1.53363800	3.72109100	1.78625500
B	-0.54643600	2.30163800	1.40438500
B	-2.32135000	2.77832400	-0.82599500
B	-1.02731300	1.78911300	-0.19529200
B	-1.15354400	4.98882000	0.59837900
B	-1.64465200	4.41522400	-1.00921400
H	-3.71803500	4.48460200	0.57197200
B	0.13803400	3.92906100	1.20266400
H	-1.83923400	3.98024300	2.90801500
B	0.46173000	2.69671800	-0.03146200

H	-0.13641500	1.53979500	2.21724300
B	-0.64676000	3.00340800	-1.41537800
H	-3.16917600	2.34490900	-1.53911500
H	-1.19296000	6.14497200	0.88439400
B	0.06989000	4.36295300	-0.52732900
H	-2.03305900	5.15598700	-1.85727000
H	1.01712500	4.31795000	1.90683300
H	-0.33805200	2.72400500	-2.52605600
H	0.90186400	5.05221900	-1.02826800
B	-2.25913400	2.35359100	0.91266000
I	-1.62241000	-1.11391900	-0.23099000
C	0.27653000	-1.66708600	0.59211800
C	0.53114200	-1.36132500	1.92169800
C	1.17169400	-2.33804400	-0.23009200
C	1.75824400	-1.75906400	2.45089000
H	-0.19514700	-0.83803500	2.52663900
C	2.38541900	-2.73587400	0.32666400
H	0.93911200	-2.54300500	-1.26563900
C	2.67718800	-2.44513700	1.65836600
H	1.98808800	-1.52920100	3.48455700
H	3.10538700	-3.25866000	-0.29077400
H	3.62899400	-2.74805000	2.07757000
O	-2.13213000	-3.24455200	0.17074500
C	-3.34019000	-3.54808100	-0.24431100
O	-4.08729500	-2.73262800	-0.78073300
C	-3.72527800	-4.97992500	0.02623900
H	-3.98418300	-5.07168200	1.08541200
H	-4.59011000	-5.24871700	-0.57907500
H	-2.88974900	-5.65017500	-0.17849500
H	-0.79685500	0.63803100	-0.63597900
H	-3.06225500	1.62379600	1.39861400
N	1.82628600	2.07692300	-0.14794300
C	2.18833200	1.03200900	-0.91246100
H	2.52548100	2.40379800	0.50418100
C	3.52795700	0.40682500	-0.64592600
O	1.46198800	0.56095600	-1.80597900
C	4.11628000	-0.35344300	-1.66277400
C	4.16371300	0.48759600	0.59752600
C	5.32333800	-1.00996500	-1.44711400
H	3.61735300	-0.42979900	-2.62064800
C	5.36918900	-0.17525400	0.81589100
H	3.71048000	1.03092400	1.41814400
C	5.95229600	-0.92444300	-0.20459500
H	5.77097400	-1.59243800	-2.24452500

H	5.84387900	-0.11858200	1.78890000
H	6.88841400	-1.44344900	-0.03113800

IRC_TS1_point83

B	-2.63584100	4.01483300	0.41537900
B	-1.53524600	3.72040100	1.78671800
B	-0.54668500	2.30180000	1.40564000
B	-2.32204400	2.77564700	-0.82514200
B	-1.02702700	1.78815600	-0.19386000
B	-1.15630400	4.98788000	0.59820100
B	-1.64691600	4.41312600	-1.00907200
H	-3.72037500	4.48111100	0.57199300
B	0.13631000	3.92972800	1.20311400
H	-1.84122500	3.97972900	2.90832300
B	0.46120500	2.69694100	-0.03023600
H	-0.13602300	1.54060900	2.21875900
B	-0.64770000	3.00221600	-1.41470600
H	-3.16930000	2.34079000	-1.53798800
H	-1.19692800	6.14410600	0.88359300
B	0.06786200	4.36259300	-0.52713300
H	-2.03601000	5.15297900	-1.85753800
H	1.01487700	4.31991600	1.90719000
H	-0.33879800	2.72253500	-2.52520600
H	0.89906600	5.05245400	-1.02848200
B	-2.25948800	2.35182400	0.91377100
I	-1.62032600	-1.11232400	-0.23089800
C	0.27794700	-1.66689500	0.59300200
C	0.53289200	-1.36011000	1.92229000
C	1.17230200	-2.33979700	-0.22844000
C	1.75955800	-1.75864200	2.45189200
H	-0.19276800	-0.83535600	2.52671100
C	2.38558500	-2.73844800	0.32874100
H	0.93945300	-2.54565600	-1.26374900
C	2.67774000	-2.44658500	1.66009700
H	1.98965200	-1.52795700	3.48532200
H	3.10481600	-3.26289400	-0.28807300
H	3.62915800	-2.75020300	2.07965500
O	-2.13119700	-3.24387500	0.16935700
C	-3.33934900	-3.54589600	-0.24613500
O	-4.08564500	-2.72922200	-0.78201500
C	-3.72635400	-4.97743100	0.02308000
H	-3.98939500	-5.06862100	1.08106500
H	-4.58916700	-5.24555500	-0.58522600
H	-2.89096700	-5.64854800	-0.17843800

H	-0.79379100	0.63837300	-0.63551800
H	-3.06177100	1.62134600	1.40000900
N	1.82558200	2.07667200	-0.14616700
C	2.18666200	1.03139300	-0.91106800
H	2.52529400	2.40381800	0.50513000
C	3.52626900	0.40564100	-0.64568500
O	1.45965400	0.56121300	-1.80618200
C	4.11198000	-0.35622700	-1.66293300
C	4.16480700	0.48776000	0.59609700
C	5.31892100	-1.01336800	-1.44909800
H	3.61091500	-0.43352500	-2.61956100
C	5.37026500	-0.17563600	0.81263100
H	3.71385800	1.03267800	1.41689700
C	5.95055700	-0.92669900	-0.20805200
H	5.76426900	-1.59732400	-2.24669200
H	5.84724900	-0.11784500	1.78436300
H	6.88659200	-1.44622700	-0.03594700

IRC_TS1_point84

B	-2.63777800	4.01244400	0.41565600
B	-1.53697000	3.71971300	1.78720000
B	-0.54703500	2.30187300	1.40693100
B	-2.32277500	2.77299800	-0.82427400
B	-1.02675700	1.78764300	-0.19230900
B	-1.15910900	4.98690900	0.59810800
B	-1.64912300	4.41101800	-1.00895100
H	-3.72270900	4.47790300	0.57207600
B	0.13455400	3.93024800	1.20360600
H	-1.84323200	3.97937900	2.90864800
B	0.46066100	2.69728500	-0.02933200
H	-0.13579500	1.54135500	2.22037000
B	-0.64858200	3.00092400	-1.41378900
H	-3.16955500	2.33695100	-1.53699600
H	-1.20078500	6.14322900	0.88302600
B	0.06567200	4.36235700	-0.52688800
H	-2.03886900	5.15027000	-1.85767600
H	1.01259800	4.32170700	1.90761000
H	-0.33932600	2.72086100	-2.52411500
H	0.89620500	5.05284100	-1.02848700
B	-2.25990500	2.35005800	0.91489500
I	-1.61826400	-1.11079000	-0.23086600
C	0.27925300	-1.66690400	0.59392300
C	0.53452200	-1.35912200	1.92288700
C	1.17291400	-2.34156800	-0.22684400

C	1.76077500	-1.75845300	2.45291300
H	-0.19056600	-0.83298000	2.52678600
C	2.38574200	-2.74104400	0.33075500
H	0.93992100	-2.54813700	-1.26198100
C	2.67822000	-2.44818300	1.66183200
H	1.99110200	-1.52697900	3.48611600
H	3.10447900	-3.26683200	-0.28555800
H	3.62933600	-2.75239700	2.08169700
O	-2.13020500	-3.24271900	0.16778500
C	-3.33845300	-3.54346800	-0.24804500
O	-4.08408200	-2.72577300	-0.78344400
C	-3.72697200	-4.97483900	0.02009200
H	-3.99215300	-5.06605500	1.07768500
H	-4.58889600	-5.24229400	-0.58990100
H	-2.89152400	-5.64648400	-0.17991100
H	-0.79025300	0.63753400	-0.63359900
H	-3.06152000	1.61904400	1.40141200
N	1.82527100	2.07749000	-0.14634200
C	2.18521700	1.03123300	-0.91030700
H	2.52565200	2.40491900	0.50426400
C	3.52485000	0.40491600	-0.64645800
O	1.45674700	0.55986300	-1.80239700
C	4.10808100	-0.35894600	-1.66362800
C	4.16561300	0.48801900	0.59418600
C	5.31488400	-1.01680300	-1.45106500
H	3.60522000	-0.43717000	-2.61925500
C	5.37097000	-0.17610000	0.80945800
H	3.71659900	1.03443800	1.41506000
C	5.94887400	-0.92894200	-0.21129800
H	5.75826000	-1.60227600	-2.24865300
H	5.84975200	-0.11742500	1.78029900
H	6.88483200	-1.44898200	-0.04017200

IRC_TS1_point85

B	-2.63977100	4.00981100	0.41575500
B	-1.53874100	3.71892300	1.78757000
B	-0.54741300	2.30190500	1.40821700
B	-2.32350300	2.77009500	-0.82355500
B	-1.02663600	1.78636400	-0.19083300
B	-1.16202000	4.98581300	0.59780500
B	-1.65144700	4.40871500	-1.00895300
H	-3.72515200	4.47424400	0.57189000
B	0.13267900	3.93077900	1.20403300
H	-1.84542200	3.97884600	2.90882800

B	0.46009900	2.69737100	-0.02814700
H	-0.13553000	1.54209500	2.22195300
B	-0.64956200	2.99953800	-1.41313800
H	-3.16968100	2.33260500	-1.53603000
H	-1.20487400	6.14222400	0.88208400
B	0.06351500	4.36184100	-0.52676500
H	-2.04184000	5.14706700	-1.85810400
H	1.01020100	4.32356500	1.90793000
H	-0.33994000	2.71903700	-2.52318200
H	0.89334300	5.05290200	-1.02871600
B	-2.26034500	2.34811700	0.91597700
I	-1.61613000	-1.10894800	-0.23083000
C	0.28062500	-1.66674000	0.59480800
C	0.53621600	-1.35805300	1.92349000
C	1.17345100	-2.34331400	-0.22524700
C	1.76200900	-1.75828700	2.45391900
H	-0.18824600	-0.83048300	2.52689000
C	2.38580300	-2.74371800	0.33276400
H	0.94022200	-2.55061300	-1.26018600
C	2.67866300	-2.44985700	1.66352800
H	1.99257100	-1.52609400	3.48691000
H	3.10383000	-3.27105700	-0.28300100
H	3.62939100	-2.75481500	2.08371600
O	-2.12919600	-3.24194000	0.16643100
C	-3.33753900	-3.54122900	-0.24969000
O	-4.08247700	-2.72241600	-0.78458100
C	-3.72781100	-4.97229900	0.01733100
H	-3.99612400	-5.06311100	1.07408400
H	-4.58826800	-5.23911300	-0.59493300
H	-2.89253600	-5.64473800	-0.18024100
H	-0.78654500	0.63798600	-0.63268200
H	-3.06118500	1.61647500	1.40274300
N	1.82464700	2.07743900	-0.14498200
C	2.18362700	1.03065500	-0.90902000
H	2.52560100	2.40532100	0.50461300
C	3.52329900	0.40388600	-0.64650900
O	1.45422400	0.55942200	-1.80117100
C	4.10400300	-0.36155700	-1.66398800
C	4.16664400	0.48814400	0.59264900
C	5.31074700	-1.01996700	-1.45314300
H	3.59913100	-0.44061000	-2.61845300
C	5.37201000	-0.17650300	0.80621300
H	3.71971400	1.03596700	1.41372700
C	5.94730200	-0.93101600	-0.21477800

H	5.75205200	-1.60673000	-2.25092400
H	5.85289300	-0.11687400	1.77593100
H	6.88325100	-1.45145900	-0.04492800
IRC_TS1_point86			
B	-2.64183000	4.00717600	0.41582900
B	-1.54062900	3.71813600	1.78790500
B	-0.54781800	2.30194700	1.40949500
B	-2.32423900	2.76712800	-0.82276500
B	-1.02622000	1.78588700	-0.18929800
B	-1.16499900	4.98467800	0.59747700
B	-1.65374400	4.40629100	-1.00902400
H	-3.72763300	4.47074000	0.57167900
B	0.13078000	3.93129200	1.20442700
H	-1.84764600	3.97843300	2.90898300
B	0.45952100	2.69762500	-0.02716400
H	-0.13536700	1.54283500	2.22358500
B	-0.65041100	2.99798800	-1.41229800
H	-3.16985500	2.32832100	-1.53513100
H	-1.20897600	6.14119400	0.88117100
B	0.06125800	4.36142800	-0.52663900
H	-2.04476500	5.14395200	-1.85851400
H	1.00771300	4.32544600	1.90827000
H	-0.34045900	2.71713500	-2.52219300
H	0.89037800	5.05310700	-1.02888900
B	-2.26082200	2.34617600	0.91700000
I	-1.61402600	-1.10721600	-0.23082500
C	0.28189000	-1.66670400	0.59570300
C	0.53780700	-1.35711700	1.92409100
C	1.17396100	-2.34508600	-0.22367900
C	1.76314400	-1.75826100	2.45493600
H	-0.18605600	-0.82816000	2.52699400
C	2.38582900	-2.74641000	0.33474000
H	0.94057000	-2.55303100	-1.25845400
C	2.67902700	-2.45162400	1.66523200
H	1.99393800	-1.52536500	3.48771800
H	3.10331100	-3.27510300	-0.28053900
H	3.62943200	-2.75724100	2.08571600
O	-2.12814800	-3.24056800	0.16493000
C	-3.33659300	-3.53878900	-0.25136700
O	-4.08100300	-2.71908800	-0.78575800
C	-3.72823400	-4.96971800	0.01473300
H	-3.99878900	-5.06039300	1.07098500
H	-4.58769300	-5.23603500	-0.59921300
H	-2.89293100	-5.64267600	-0.18113700

H	-0.78305200	0.63689600	-0.63125200
H	-3.06093400	1.61395700	1.40406900
N	1.82424200	2.07795900	-0.14467400
C	2.18211300	1.03027300	-0.90793800
H	2.52582900	2.40609300	0.50432600
C	3.52184900	0.40300900	-0.64694400
O	1.45139900	0.55822500	-1.79801100
C	4.10012800	-0.36414400	-1.66453500
C	4.16755900	0.48828700	0.59092900
C	5.30683000	-1.02310500	-1.45518100
H	3.59341400	-0.44404500	-2.61795500
C	5.37292500	-0.17690600	0.80300900
H	3.72258400	1.03748300	1.41215400
C	5.94581700	-0.93302600	-0.21815900
H	5.74620200	-1.61117600	-2.25306900
H	5.85571600	-0.11638600	1.77173300
H	6.88176800	-1.45385000	-0.04943900

IRC_TS1_point87

B	-2.64388100	4.00436600	0.41575000
B	-1.54249300	3.71729200	1.78816000
B	-0.54825300	2.30190600	1.41079200
B	-2.32495300	2.76400500	-0.82217000
B	-1.02618800	1.78426900	-0.18779900
B	-1.16801000	4.98345900	0.59700400
B	-1.65609400	4.40378400	-1.00919000
H	-3.73013500	4.46692300	0.57127800
B	0.12880900	3.93175000	1.20479100
H	-1.84997000	3.97792200	2.90901700
B	0.45896300	2.69759300	-0.02600400
H	-0.13515600	1.54357400	2.22522900
B	-0.65139200	2.99640400	-1.41170300
H	-3.16994800	2.32373400	-1.53429100
H	-1.21316700	6.14008300	0.88002100
B	0.05903400	4.36076200	-0.52662700
H	-2.04773800	5.14052800	-1.85913800
H	1.00520500	4.32728500	1.90851100
H	-0.34095500	2.71500300	-2.52124000
H	0.88747300	5.05301600	-1.02920500
B	-2.26129200	2.34410800	0.91805000
I	-1.61191800	-1.10517300	-0.23084100
C	0.28316900	-1.66655100	0.59656000
C	0.53939800	-1.35614800	1.92467600
C	1.17438800	-2.34681700	-0.22214000

C	1.76426000	-1.75826100	2.45592300
H	-0.18383800	-0.82579000	2.52709700
C	2.38576700	-2.74912200	0.33667800
H	0.94078600	-2.55538800	-1.25674400
C	2.67934400	-2.45342500	1.66688000
H	1.99528100	-1.52471000	3.48850600
H	3.10257800	-3.27927400	-0.27810700
H	3.62937000	-2.75979600	2.08766500
O	-2.12709700	-3.23976700	0.16366300
C	-3.33562300	-3.53658900	-0.25281400
O	-4.07947500	-2.71587500	-0.78672600
C	-3.72883200	-4.96722700	0.01231700
H	-4.00203000	-5.05756700	1.06789900
H	-4.58705800	-5.23301600	-0.60355200
H	-2.89364400	-5.64086800	-0.18147500
H	-0.77875500	0.63753700	-0.63010400
H	-3.06065300	1.61129700	1.40536100
N	1.82369100	2.07798800	-0.14348900
C	2.18062600	1.02968400	-0.90663300
H	2.52588900	2.40675500	0.50431700
C	3.52044500	0.40207300	-0.64707500
O	1.44883100	0.55737600	-1.79600900
C	4.09628700	-0.36659600	-1.66494100
C	4.16861800	0.48841000	0.58940200
C	5.30298300	-1.02602600	-1.45725400
H	3.58764700	-0.44726500	-2.61725000
C	5.37402800	-0.17725600	0.79983000
H	3.72559300	1.03889200	1.41083400
C	5.94445500	-0.93489100	-0.22159500
H	5.74042500	-1.61526000	-2.25534000
H	5.85880100	-0.11586800	1.76751100
H	6.88044600	-1.45603500	-0.05410900

IRC_TS1_point88

B	-2.64601100	4.00152100	0.41564200
B	-1.54449200	3.71643500	1.78836000
B	-0.54868300	2.30192300	1.41207300
B	-2.32566300	2.76075600	-0.82144000
B	-1.02561800	1.78388400	-0.18624700
B	-1.17110300	4.98218200	0.59645300
B	-1.65843100	4.40107300	-1.00945000
H	-3.73271100	4.46314900	0.57080200
B	0.12682100	3.93224800	1.20508300
H	-1.85235300	3.97749200	2.90901100

B	0.45838800	2.69777300	-0.02498500
H	-0.13502200	1.54432500	2.22690700
B	-0.65218100	2.99461100	-1.41091300
H	-3.17001200	2.31903000	-1.53344500
H	-1.21744900	6.13892000	0.87877900
B	0.05673800	4.36019300	-0.52662600
H	-2.05070500	5.13702400	-1.85980900
H	1.00257300	4.32923700	1.90875800
H	-0.34142100	2.71281600	-2.52029900
H	0.88444800	5.05304200	-1.02955100
B	-2.26178700	2.34201600	0.91899700
I	-1.60983900	-1.10330100	-0.23087200
C	0.28435100	-1.66648200	0.59742600
C	0.54091000	-1.35524500	1.92526500
C	1.17478300	-2.34856100	-0.22061900
C	1.76528700	-1.75834700	2.45692000
H	-0.18169800	-0.82349600	2.52720700
C	2.38565000	-2.75185600	0.33859900
H	0.94100000	-2.55773100	-1.25506100
C	2.67957200	-2.45530100	1.66853900
H	1.99654200	-1.52415900	3.48930700
H	3.10186600	-3.28338500	-0.27570500
H	3.62924900	-2.76239300	2.08961600
O	-2.12601600	-3.23814200	0.16222600
C	-3.33463600	-3.53415900	-0.25429500
O	-4.07810800	-2.71271400	-0.78768900
C	-3.72904500	-4.96470400	0.01004100
H	-4.00464400	-5.05478600	1.06504500
H	-4.58615400	-5.23015700	-0.60756900
H	-2.89380600	-5.63883700	-0.18184500
H	-0.77533700	0.63604600	-0.62888500
H	-3.06038400	1.60861600	1.40665100
N	1.82327400	2.07835100	-0.14290800
C	2.17913000	1.02917500	-0.90534300
H	2.52606800	2.40735400	0.50440300
C	3.51905600	0.40115100	-0.64730000
O	1.44611200	0.55618200	-1.79304300
C	4.09253000	-0.36903800	-1.66538200
C	4.16964000	0.48850900	0.58782700
C	5.29925400	-1.02889500	-1.45930300
H	3.58201800	-0.45052200	-2.61661100
C	5.37512000	-0.17758300	0.79665700
H	3.72854900	1.04026100	1.40944500
C	5.94318000	-0.93668100	-0.22501100

H	5.73480300	-1.61930100	-2.25755700
H	5.86184200	-0.11531800	1.76329400
H	6.87922700	-1.45811400	-0.05874500

IRC_TS1_point89

B	-2.64808400	3.99857200	0.41539900
B	-1.54640300	3.71556900	1.78850500
B	-0.54914100	2.30183200	1.41337500
B	-2.32634800	2.75744200	-0.82095000
B	-1.02565900	1.78186300	-0.18473600
B	-1.17417000	4.98086700	0.59580500
B	-1.66078600	4.39838700	-1.00976900
H	-3.73523000	4.45923500	0.57021300
B	0.12479000	3.93266000	1.20537500
H	-1.85474400	3.97703500	2.90891000
B	0.45784400	2.69761500	-0.02382800
H	-0.13483300	1.54509300	2.22861000
B	-0.65316000	2.99283100	-1.41038600
H	-3.17009100	2.31426600	-1.53271500
H	-1.22167900	6.13773300	0.87742000
B	0.05448800	4.35937300	-0.52673100
H	-2.05364700	5.13342400	-1.86061100
H	1.00000200	4.33108000	1.90890400
H	-0.34183000	2.71044100	-2.51936900
H	0.88153100	5.05280200	-1.02996700
B	-2.26226200	2.33986700	0.92003200
I	-1.60778500	-1.10107300	-0.23093400
C	0.28552900	-1.66631600	0.59823500
C	0.54239200	-1.35434500	1.92581500
C	1.17509100	-2.35026400	-0.21914200
C	1.76628000	-1.75846300	2.45787100
H	-0.17959900	-0.82122400	2.52729000
C	2.38546700	-2.75457500	0.34046400
H	0.94112500	-2.55997700	-1.25343800
C	2.67976400	-2.45718200	1.67013000
H	1.99775400	-1.52366700	3.49007200
H	3.10105800	-3.28746700	-0.27339800
H	3.62908300	-2.76501300	2.09148500
O	-2.12494400	-3.23742200	0.16107400
C	-3.33361700	-3.53205200	-0.25555400
O	-4.07665400	-2.70967200	-0.78850400
C	-3.72943200	-4.96230600	0.00792000
H	-4.00751600	-5.05204200	1.06231600
H	-4.58533500	-5.22741800	-0.61150000

H	-2.89418400	-5.63698300	-0.18193600
H	-0.77043600	0.63707000	-0.62773200
H	-3.06012600	1.60590500	1.40792100
N	1.82278300	2.07837800	-0.14176300
C	2.17775200	1.02856000	-0.90397000
H	2.52619200	2.40813700	0.50422000
C	3.51777900	0.40025800	-0.64742000
O	1.44356300	0.55513200	-1.79062000
C	4.08891000	-0.37135900	-1.66576900
C	4.17074600	0.48861900	0.58636300
C	5.29568400	-1.03159000	-1.46133700
H	3.57654800	-0.45355500	-2.61593500
C	5.37631600	-0.17786400	0.79356000
H	3.73150300	1.04155000	1.40819700
C	5.94203600	-0.93834100	-0.22838900
H	5.72942500	-1.62304100	-2.25980200
H	5.86493600	-0.11478800	1.75920600
H	6.87817000	-1.46001100	-0.06332700

IRC_TS1_point90

B	-2.65025300	3.99552500	0.41512900
B	-1.54847700	3.71465800	1.78858500
B	-0.54955800	2.30184300	1.41467700
B	-2.32699800	2.75392300	-0.82025200
B	-1.02491500	1.78164800	-0.18312900
B	-1.17735100	4.97946500	0.59504200
B	-1.66313300	4.39539700	-1.01020800
H	-3.73788200	4.45515600	0.56948700
B	0.12275300	3.93315800	1.20556600
H	-1.85726400	3.97659800	2.90875200
B	0.45731000	2.69775500	-0.02278600
H	-0.13467700	1.54588000	2.23035800
B	-0.65384800	2.99082300	-1.40961500
H	-3.16997300	2.30908300	-1.53186900
H	-1.22615100	6.13644600	0.87584700
B	0.05217400	4.35868200	-0.52685400
H	-2.05665800	5.12948400	-1.86155100
H	0.99725200	4.33313200	1.90906300
H	-0.34220100	2.70792000	-2.51841800
H	0.87846200	5.05267200	-1.03050300
B	-2.26273200	2.33762600	0.92092600
I	-1.60577000	-1.09911100	-0.23100000
C	0.28661700	-1.66621100	0.59907200
C	0.54381400	-1.35344700	1.92638300

C	1.17536800	-2.35195300	-0.21767900
C	1.76719200	-1.75862800	2.45883900
H	-0.17750900	-0.81891500	2.52739100
C	2.38520400	-2.75732100	0.34232100
H	0.94119400	-2.56223200	-1.25181000
C	2.67984600	-2.45913900	1.67173900
H	1.99890400	-1.52325600	3.49085600
H	3.10013200	-3.29164400	-0.27105000
H	3.62876800	-2.76778300	2.09339600
O	-2.12384800	-3.23548800	0.15970500
C	-3.33260600	-3.52963000	-0.25687200
O	-4.07539600	-2.70668600	-0.78928800
C	-3.72943800	-4.95985300	0.00589700
H	-4.01009400	-5.04925600	1.05964500
H	-4.58411900	-5.22472500	-0.61534700
H	-2.89413200	-5.63501400	-0.18189300
H	-0.76731100	0.63502000	-0.62654100
H	-3.05979100	1.60306900	1.40921600
N	1.82239200	2.07864200	-0.14097500
C	2.17630400	1.02797000	-0.90254300
H	2.52635800	2.40859800	0.50462600
C	3.51647600	0.39932900	-0.64748100
O	1.44099600	0.55391900	-1.78774200
C	4.08528700	-0.37366400	-1.66611500
C	4.17186400	0.48869500	0.58491600
C	5.29214700	-1.03421500	-1.46337400
H	3.57100600	-0.45667400	-2.61515300
C	5.37755900	-0.17811500	0.79044000
H	3.73452400	1.04281300	1.40695900
C	5.94095800	-0.93991900	-0.23180600
H	5.72401400	-1.62674500	-2.26205100
H	5.86815500	-0.11417400	1.75500400
H	6.87719400	-1.46179600	-0.06804700

IRC_TS1_point91

B	-2.65232200	3.99247100	0.41474200
B	-1.55040300	3.71380200	1.78863500
B	-0.55001700	2.30172400	1.41599500
B	-2.32764000	2.75044000	-0.81984400
B	-1.02498600	1.77921400	-0.18161700
B	-1.18043900	4.97807800	0.59422900
B	-1.66547500	4.39255400	-1.01066000
H	-3.74039000	4.45119800	0.56873900
B	0.12069000	3.93354400	1.20579800

H	-1.85968000	3.97624600	2.90853400
B	0.45678200	2.69746600	-0.02161700
H	-0.13450400	1.54671000	2.23215100
B	-0.65482700	2.98884700	-1.40915000
H	-3.17007700	2.30421900	-1.53123100
H	-1.23036900	6.13521700	0.87429300
B	0.04992100	4.35771000	-0.52706700
H	-2.05955500	5.12577400	-1.86249500
H	0.99465500	4.33499800	1.90911500
H	-0.34255200	2.70535400	-2.51753600
H	0.87555200	5.05229400	-1.03100400
B	-2.26319000	2.33543100	0.92196600
I	-1.60378700	-1.09672500	-0.23110200
C	0.28769100	-1.66600700	0.59981400
C	0.54518900	-1.35259600	1.92688300
C	1.17557000	-2.35360600	-0.21626900
C	1.76806100	-1.75883700	2.45974900
H	-0.17552800	-0.81672100	2.52744000
C	2.38491100	-2.76002400	0.34411200
H	0.94125000	-2.56436700	-1.25027700
C	2.67991900	-2.46107900	1.67327400
H	1.99998200	-1.52289600	3.49159100
H	3.09926900	-3.29562800	-0.26885600
H	3.62850800	-2.77044900	2.09519500
O	-2.12276700	-3.23488900	0.15866800
C	-3.33154100	-3.52762300	-0.25796300
O	-4.07401300	-2.70381400	-0.78997400
C	-3.72961500	-4.95756100	0.00402700
H	-4.01262700	-5.04661100	1.05720900
H	-4.58307400	-5.22231900	-0.61894900
H	-2.89412900	-5.63307500	-0.18174400
H	-0.76159900	0.63655200	-0.62556900
H	-3.05953900	1.60034400	1.41048700
N	1.82195800	2.07863700	-0.13985100
C	2.17503500	1.02733400	-0.90109200
H	2.52653000	2.40941300	0.50436800
C	3.51529700	0.39843700	-0.64757100
O	1.43846100	0.55277600	-1.78503700
C	4.08187000	-0.37588700	-1.66646700
C	4.17299400	0.48876900	0.58352800
C	5.28884200	-1.03670500	-1.46535200
H	3.56580800	-0.45958100	-2.61448700
C	5.37883000	-0.17833300	0.78743500
H	3.73741300	1.04397400	1.40579300

C	5.94002000	-0.94138300	-0.23511000
H	5.71900800	-1.63019300	-2.26424000
H	5.87125600	-0.11361400	1.75104500
H	6.87638800	-1.46342200	-0.07252500

IRC_TS1_point92

B	-2.65450600	3.98922100	0.41432000
B	-1.55252500	3.71284500	1.78861100
B	-0.55039100	2.30174500	1.41734200
B	-2.32820000	2.74665700	-0.81916500
B	-1.02410600	1.77910200	-0.17990500
B	-1.18369300	4.97656300	0.59326900
B	-1.66780500	4.38929000	-1.01126500
H	-3.74311700	4.44675800	0.56776200
B	0.11862900	3.93405900	1.20590900
H	-1.86235000	3.97579100	2.90823300
B	0.45631700	2.69757700	-0.02053300
H	-0.13427200	1.54756600	2.23398900
B	-0.65538700	2.98663900	-1.40837400
H	-3.16969300	2.29845400	-1.53035000
H	-1.23508400	6.13381500	0.87238300
B	0.04761900	4.35691200	-0.52729500
H	-2.06261000	5.12132100	-1.86373600
H	0.99178400	4.33720000	1.90921600
H	-0.34276400	2.70244800	-2.51651300
H	0.87244400	5.05203100	-1.03173900
B	-2.26360900	2.33305000	0.92283400
I	-1.60184800	-1.09467900	-0.23120200
C	0.28869400	-1.66584900	0.60062100
C	0.54652800	-1.35168400	1.92742900
C	1.17573300	-2.35520600	-0.21487700
C	1.76886600	-1.75906600	2.46068000
H	-0.17346800	-0.81436000	2.52753000
C	2.38450500	-2.76275500	0.34589200
H	0.94116600	-2.56651000	-1.24871100
C	2.67985600	-2.46310800	1.67482300
H	2.00103000	-1.52262200	3.49235300
H	3.09811000	-3.29988500	-0.26656700
H	3.62797500	-2.77343700	2.09707100
O	-2.12166400	-3.23267900	0.15738900
C	-3.33051100	-3.52521300	-0.25912900
O	-4.07285100	-2.70099300	-0.79060800
C	-3.72943200	-4.95516700	0.00221400
H	-4.01504400	-5.04387200	1.05470800

H	-4.58165800	-5.21967700	-0.62257700
H	-2.89395000	-5.63118400	-0.18151300
H	-0.75884800	0.63399900	-0.62417000
H	-3.05908200	1.59733500	1.41182100
N	1.82159000	2.07877900	-0.13886300
C	2.17362100	1.02665000	-0.89958500
H	2.52670200	2.40973500	0.50496700
C	3.51406700	0.39749900	-0.64749200
O	1.43606900	0.55154300	-1.78228400
C	4.07838300	-0.37805900	-1.66672700
C	4.17416800	0.48880900	0.58220300
C	5.28549800	-1.03908600	-1.46737200
H	3.56033000	-0.46258900	-2.61355900
C	5.38018700	-0.17851800	0.78437900
H	3.74045500	1.04511900	1.40470200
C	5.93912600	-0.94274700	-0.23851900
H	5.71378900	-1.63357400	-2.26652000
H	5.87462100	-0.11293700	1.74686900
H	6.87564900	-1.46490200	-0.07733100

IRC_TS1_point93

B	-2.65656400	3.98606600	0.41381500
B	-1.55447600	3.71197900	1.78858200
B	-0.55086300	2.30158900	1.41868400
B	-2.32880200	2.74300700	-0.81880600
B	-1.02411900	1.77646500	-0.17838400
B	-1.18678000	4.97508700	0.59232000
B	-1.67011900	4.38628100	-1.01182700
H	-3.74561700	4.44273300	0.56686700
B	0.11654600	3.93439400	1.20609300
H	-1.86480700	3.97551900	2.90791200
B	0.45579700	2.69717300	-0.01935200
H	-0.13415600	1.54843400	2.23589100
B	-0.65634800	2.98446100	-1.40794000
H	-3.16982500	2.29348700	-1.52976500
H	-1.23928500	6.13251900	0.87064900
B	0.04537200	4.35578700	-0.52759200
H	-2.06546900	5.11748000	-1.86479000
H	0.98915600	4.33906100	1.90920400
H	-0.34308400	2.69968500	-2.51567000
H	0.86955200	5.05148700	-1.03231800
B	-2.26405900	2.33079900	0.92386300
I	-1.59993000	-1.09215400	-0.23133800
C	0.28967900	-1.66559700	0.60130400

C	0.54781300	-1.35087100	1.92789000
C	1.17585600	-2.35678500	-0.21353100
C	1.76962400	-1.75936600	2.46156000
H	-0.17157400	-0.81222400	2.52755900
C	2.38412000	-2.76542800	0.34761600
H	0.94117100	-2.56853400	-1.24725700
C	2.67982200	-2.46510600	1.67631300
H	2.00198700	-1.52240600	3.49307300
H	3.09718500	-3.30380100	-0.26445600
H	3.62761000	-2.77618400	2.09882600
O	-2.12056400	-3.23204000	0.15642800
C	-3.32939700	-3.52325900	-0.26007600
O	-4.07154100	-2.69828300	-0.79118200
C	-3.72935500	-4.95296600	0.00058300
H	-4.01700200	-5.04136300	1.05258400
H	-4.58045700	-5.21753500	-0.62572700
H	-2.89358000	-5.62915000	-0.18133200
H	-0.75229600	0.63570200	-0.62332500
H	-3.05885200	1.59459300	1.41309900
N	1.82119600	2.07872900	-0.13778700
C	2.17241100	1.02596400	-0.89807700
H	2.52688800	2.41044900	0.50482400
C	3.51294300	0.39657000	-0.64755000
O	1.43351300	0.55030700	-1.77937100
C	4.07513900	-0.38020400	-1.66705500
C	4.17527700	0.48880900	0.58088700
C	5.28243100	-1.04138000	-1.46930800
H	3.55535100	-0.46543000	-2.61289100
C	5.38149400	-0.17869700	0.78145800
H	3.74324400	1.04611900	1.40361000
C	5.93836100	-0.94402800	-0.24176100
H	5.70909900	-1.63676500	-2.26866200
H	5.87770900	-0.11235600	1.74301200
H	6.87505900	-1.46627000	-0.08174200

IRC_TS1_point94

B	-2.65874100	3.98266300	0.41326500
B	-1.55661900	3.71097700	1.78847600
B	-0.55124000	2.30156800	1.42006400
B	-2.32930500	2.73902300	-0.81818000
B	-1.02325500	1.77613200	-0.17660900
B	-1.19005400	4.97346300	0.59120900
B	-1.67242200	4.38281500	-1.01255600
H	-3.74837200	4.43805600	0.56569900

B	0.11446200	3.93485800	1.20614800
H	-1.86757600	3.97504700	2.90749800
B	0.45536100	2.69715800	-0.01822700
H	-0.13390400	1.54930500	2.23779400
B	-0.65686300	2.98206700	-1.40719900
H	-3.16929200	2.28733800	-1.52889400
H	-1.24410800	6.13101300	0.86849600
B	0.04309300	4.35482800	-0.52791000
H	-2.06851000	5.11267300	-1.86625600
H	0.98622000	4.34128500	1.90924600
H	-0.34318800	2.69645400	-2.51460800
H	0.86645400	5.05104000	-1.03319200
B	-2.26446200	2.32831500	0.92473100
I	-1.59804300	-1.08994400	-0.23147100
C	0.29062300	-1.66536600	0.60207200
C	0.54908900	-1.34996500	1.92841200
C	1.17593200	-2.35828500	-0.21220600
C	1.77034500	-1.75967000	2.46245800
H	-0.16954600	-0.80986200	2.52764800
C	2.38360800	-2.76812600	0.34931600
H	0.94098100	-2.57052300	-1.24576300
C	2.67965100	-2.46719400	1.67780100
H	2.00294900	-1.52228200	3.49381900
H	3.09587200	-3.30805600	-0.26226000
H	3.62692500	-2.77933700	2.10064800
O	-2.11944100	-3.22978500	0.15526700
C	-3.32832400	-3.52090600	-0.26108300
O	-4.07043000	-2.69561000	-0.79169100
C	-3.72900500	-4.95063400	-0.00101400
H	-4.01895400	-5.03874600	1.05035600
H	-4.57902900	-5.21492600	-0.62891400
H	-2.89330200	-5.62730600	-0.18117000
H	-0.74941200	0.63316300	-0.62171800
H	-3.05834700	1.59147400	1.41445300
N	1.82081300	2.07868300	-0.13661000
C	2.17101700	1.02515700	-0.89651300
H	2.52706700	2.41071900	0.50532700
C	3.51176100	0.39559600	-0.64740100
O	1.43119400	0.54901300	-1.77668400
C	4.07180100	-0.38226900	-1.66727800
C	4.17643800	0.48877800	0.57965200
C	5.27930000	-1.04353100	-1.47131700
H	3.55002500	-0.46831700	-2.61191600
C	5.38289800	-0.17884000	0.77847400

H	3.74618400	1.04708200	1.40262900
C	5.93763300	-0.94518800	-0.24514200
H	5.70417100	-1.63979400	-2.27097000
H	5.88109800	-0.11165700	1.73891100
H	6.87454900	-1.46743600	-0.08656600

IRC_TS1_point95

B	-2.66080600	3.97939700	0.41266700
B	-1.55861800	3.71005100	1.78837600
B	-0.55174600	2.30135400	1.42142000
B	-2.32989200	2.73520800	-0.81783100
B	-1.02316400	1.77361800	-0.17505400
B	-1.19314400	4.97186800	0.59014100
B	-1.67470600	4.37961200	-1.01322100
H	-3.75087900	4.43391600	0.56466300
B	0.11236000	3.93510700	1.20627400
H	-1.87009800	3.97477000	2.90708600
B	0.45483500	2.69666800	-0.01705800
H	-0.13386200	1.55013100	2.23975300
B	-0.65777300	2.97969000	-1.40675900
H	-3.16938100	2.28216600	-1.52831400
H	-1.24832100	6.12959800	0.86658300
B	0.04085100	4.35356200	-0.52827700
H	-2.07133100	5.10860200	-1.86743900
H	0.98354200	4.34308500	1.90918100
H	-0.34347900	2.69344700	-2.51376600
H	0.86358100	5.05030100	-1.03386900
B	-2.26493600	2.32597400	0.92571900
I	-1.59616200	-1.08730900	-0.23163100
C	0.29154500	-1.66506200	0.60272800
C	0.55031000	-1.34917000	1.92886400
C	1.17598900	-2.35977700	-0.21091500
C	1.77101800	-1.76004900	2.46332300
H	-0.16769900	-0.80776200	2.52768700
C	2.38313500	-2.77076800	0.35097800
H	0.94092200	-2.57240900	-1.24437200
C	2.67952000	-2.46924700	1.67925000
H	2.00381400	-1.52221500	3.49454100
H	3.09484200	-3.31193200	-0.26022100
H	3.62643900	-2.78219300	2.10236400
O	-2.11831000	-3.22886500	0.15434700
C	-3.32715900	-3.51893900	-0.26191100
O	-4.06920000	-2.69304700	-0.79216100
C	-3.72866700	-4.94849300	-0.00242900

H	-4.02029500	-5.03637100	1.04852700
H	-4.57773800	-5.21290000	-0.63158200
H	-2.89267900	-5.62525300	-0.18107100
H	-0.74277200	0.63441200	-0.62086400
H	-3.05815400	1.58868000	1.41573100
N	1.82042000	2.07855600	-0.13557700
C	2.16980100	1.02436500	-0.89497000
H	2.52719200	2.41114400	0.50555300
C	3.51065600	0.39459700	-0.64740800
O	1.42863300	0.54765800	-1.77367400
C	4.06869200	-0.38434800	-1.66758300
C	4.17750900	0.48868600	0.57840300
C	5.27643300	-1.04563700	-1.47323400
H	3.54522100	-0.47109300	-2.61123500
C	5.38422500	-0.17899000	0.77561700
H	3.74885400	1.04788500	1.40161900
C	5.93701200	-0.94629600	-0.24834900
H	5.69976500	-1.64270000	-2.27311000
H	5.88416500	-0.11105800	1.73512100
H	6.87415300	-1.46853400	-0.09096300
IRC_TS1_point96			
B	-2.66296200	3.97592600	0.41202000
B	-1.56076100	3.70901000	1.78820300
B	-0.55218500	2.30123800	1.42279800
B	-2.33040500	2.73112200	-0.81729100
B	-1.02244200	1.77284300	-0.17329000
B	-1.19637600	4.97014600	0.58892600
B	-1.67698100	4.37603800	-1.01403100
H	-3.75358800	4.42923900	0.56339200
B	0.11025700	3.93544700	1.20628300
H	-1.87286700	3.97430700	2.90658900
B	0.45437300	2.69644000	-0.01591400
H	-0.13369200	1.55094600	2.24167600
B	-0.65834400	2.97713500	-1.40610400
H	-3.16890900	2.27598800	-1.52751600
H	-1.25302900	6.12801100	0.86431100
B	0.03860100	4.35239400	-0.52867800
H	-2.07428300	5.10371400	-1.86899600
H	0.98062900	4.34515800	1.90913900
H	-0.34358900	2.69002800	-2.51275100
H	0.86055700	5.04961300	-1.03481000
B	-2.26537900	2.32344400	0.92658600
I	-1.59430500	-1.08488100	-0.23178800
C	0.29244500	-1.66475700	0.60344800

C	0.55153100	-1.34828900	1.92936000
C	1.17599800	-2.36119600	-0.20964700
C	1.77167000	-1.76042200	2.46419300
H	-0.16573500	-0.80546500	2.52777400
C	2.38255100	-2.77342600	0.35261200
H	0.94068500	-2.57424200	-1.24295700
C	2.67927800	-2.47136700	1.68068600
H	2.00469400	-1.52221300	3.49527400
H	3.09347900	-3.31607700	-0.25813600
H	3.62569400	-2.78537800	2.10411500
O	-2.11716300	-3.22675600	0.15331100
C	-3.32602700	-3.51669100	-0.26276500
O	-4.06810800	-2.69052300	-0.79256700
C	-3.72815800	-4.94625800	-0.00381200
H	-4.02172800	-5.03391400	1.04660800
H	-4.57630800	-5.21046800	-0.63430300
H	-2.89221500	-5.62341200	-0.18096000
H	-0.73926300	0.63237700	-0.61933500
H	-3.05773300	1.58556700	1.41706500
N	1.81999500	2.07828900	-0.13425700
C	2.16843600	1.02342800	-0.89336400
H	2.52737200	2.41146500	0.50574700
C	3.50951600	0.39356900	-0.64725600
O	1.42630200	0.54625600	-1.77095800
C	4.06552900	-0.38635200	-1.66780500
C	4.17862300	0.48857800	0.57722000
C	5.27354100	-1.04760700	-1.47521000
H	3.54016800	-0.47387700	-2.61031200
C	5.38563600	-0.17909700	0.77271600
H	3.75161200	1.04865700	1.40069300
C	5.93643800	-0.94728500	-0.25166100
H	5.69522400	-1.64542100	-2.27539300
H	5.88746800	-0.11035600	1.73115200
H	6.87385000	-1.46942900	-0.09568000
IRC_TS1_point97			
B	-2.66503400	3.97256300	0.41133800
B	-1.56280200	3.70801500	1.78803200
B	-0.55272400	2.30096900	1.42415400
B	-2.33098500	2.72716500	-0.81694400
B	-1.02226300	1.77055600	-0.17169500
B	-1.19946500	4.96843400	0.58774400
B	-1.67923100	4.37264800	-1.01479600
H	-3.75610400	4.42498000	0.56222300
B	0.10814600	3.93560900	1.20633900

H	-1.87545000	3.97398700	2.90609300
B	0.45384200	2.69587900	-0.01477100
H	-0.13370500	1.55170500	2.24364200
B	-0.65918700	2.97457800	-1.40565200
H	-3.16890900	2.27056500	-1.52693100
H	-1.25726200	6.12647300	0.86222100
B	0.03637100	4.35100300	-0.52911400
H	-2.07705800	5.09938000	-1.87033100
H	0.97790500	4.34689200	1.90901900
H	-0.34384000	2.68677300	-2.51189500
H	0.85770600	5.04869400	-1.03559700
B	-2.26588400	2.32101900	0.92752700
I	-1.59246400	-1.08215800	-0.23196200
C	0.29331900	-1.66440200	0.60409100
C	0.55270600	-1.34748600	1.92980700
C	1.17599300	-2.36260200	-0.20840300
C	1.77227800	-1.76084900	2.46504300
H	-0.16391100	-0.80336100	2.52782700
C	2.38199000	-2.77603900	0.35421900
H	0.94054800	-2.57599100	-1.24161800
C	2.67905500	-2.47346100	1.68209700
H	2.00549600	-1.52225300	3.49599300
H	3.09232300	-3.31993100	-0.25616200
H	3.62508600	-2.78833900	2.10579000
O	-2.11601300	-3.22551900	0.15243800
C	-3.32482400	-3.51470400	-0.26349300
O	-4.06695800	-2.68809800	-0.79294700
C	-3.72760700	-4.94416700	-0.00505400
H	-4.02269500	-5.03163500	1.04497800
H	-4.57489700	-5.20850500	-0.63665900
H	-2.89141900	-5.62139800	-0.18085000
H	-0.73302400	0.63299200	-0.61837800
H	-3.05756300	1.58270700	1.41833400
N	1.81958600	2.07806200	-0.13325700
C	2.16720300	1.02250400	-0.89179300
H	2.52740400	2.41152800	0.50641800
C	3.50843300	0.39249100	-0.64718900
O	1.42378800	0.54478200	-1.76794800
C	4.06255300	-0.38837600	-1.66806700
C	4.17967800	0.48840500	0.57604600
C	5.27086900	-1.04953900	-1.47709900
H	3.53553000	-0.47659200	-2.60959200
C	5.38700400	-0.17920900	0.76992300
H	3.75419900	1.04927700	1.39978100

C	5.93596500	-0.94822900	-0.25482700
H	5.69109800	-1.64804300	-2.27753400
H	5.89054300	-0.10971600	1.72742400
H	6.87365300	-1.47026000	-0.10006500

IRC_TS1_point98

B	-2.66715900	3.96907000	0.41061300
B	-1.56493400	3.70694000	1.78779700
B	-0.55323500	2.30075300	1.42550700
B	-2.33152900	2.72303600	-0.81648800
B	-1.02169200	1.76940800	-0.16997800
B	-1.20262600	4.96663000	0.58644900
B	-1.68147000	4.36901200	-1.01567000
H	-3.75874200	4.42038600	0.56088800
B	0.10603800	3.93580800	1.20629900
H	-1.87818200	3.97353900	2.90552800
B	0.45334200	2.69544000	-0.01363400
H	-0.13364600	1.55243900	2.24555800
B	-0.65982600	2.97189100	-1.40509100
H	-3.16855400	2.26448200	-1.52621400
H	-1.26178500	6.12481600	0.85987700
B	0.03415800	4.34964100	-0.52959100
H	-2.07990200	5.09450800	-1.87192900
H	0.97504600	4.34876500	1.90889000
H	-0.34399500	2.68322800	-2.51095500
H	0.85477500	5.04777500	-1.03658100
B	-2.26638100	2.31847200	0.92837700
I	-1.59064800	-1.07953900	-0.23213700
C	0.29418200	-1.66402300	0.60476400
C	0.55387700	-1.34661300	1.93027400
C	1.17594700	-2.36394300	-0.20718400
C	1.77286700	-1.76126400	2.46588700
H	-0.16201000	-0.80111600	2.52790300
C	2.38134600	-2.77864900	0.35579800
H	0.94028300	-2.57768700	-1.24027300
C	2.67875400	-2.47559000	1.68348900
H	2.00630200	-1.52233000	3.49671100
H	3.09093700	-3.32395100	-0.25417100
H	3.62430200	-2.79151200	2.10747800
O	-2.11485500	-3.22353500	0.15151600
C	-3.32364200	-3.51255900	-0.26421700
O	-4.06589300	-2.68572200	-0.79327100
C	-3.72694200	-4.94203700	-0.00625500
H	-4.02374100	-5.02932200	1.04330700

H	-4.57338200	-5.20631100	-0.63904200
H	-2.89071800	-5.61954200	-0.18069200
H	-0.72895200	0.63145100	-0.61700900
H	-3.05725800	1.57964300	1.41962900
N	1.81911900	2.07757900	-0.13183200
C	2.16588100	1.02143900	-0.89016400
H	2.52758100	2.41193500	0.50623800
C	3.50735100	0.39140900	-0.64704300
O	1.42146400	0.54323600	-1.76517900
C	4.05958000	-0.39034600	-1.66828100
C	4.18075700	0.48823400	0.57490900
C	5.26822200	-1.05136500	-1.47901600
H	3.53077400	-0.47931500	-2.60872000
C	5.38842700	-0.17927600	0.76711600
H	3.75679400	1.04989000	1.39889600
C	5.93554800	-0.94906700	-0.25804500
H	5.68694400	-1.65052100	-2.27974900
H	5.89375700	-0.10899800	1.72360500
H	6.87354800	-1.47092200	-0.10462800
IRC_TS1_point99			
B	-2.66922500	3.96564300	0.40985900
B	-1.56699800	3.70588200	1.78756100
B	-0.55380800	2.30041900	1.42684600
B	-2.33211000	2.71898600	-0.81615600
B	-1.02147800	1.76726700	-0.16836200
B	-1.20568900	4.96481800	0.58517300
B	-1.68367800	4.36548300	-1.01652000
H	-3.76125000	4.41605200	0.55961200
B	0.10393000	3.93587200	1.20628800
H	-1.88079800	3.97317200	2.90495700
B	0.45280200	2.69479100	-0.01253100
H	-0.13371700	1.55312100	2.24751100
B	-0.66062400	2.96918800	-1.40464300
H	-3.16848800	2.25887900	-1.52563500
H	-1.26599800	6.12317200	0.85764800
B	0.03195200	4.34812800	-0.53009000
H	-2.08261800	5.08997200	-1.87339000
H	0.97230200	4.35040600	1.90871200
H	-0.34422000	2.67976200	-2.51009700
H	0.85196600	5.04668100	-1.03746700
B	-2.26692000	2.31598900	0.92927000
I	-1.58885600	-1.07672700	-0.23231800
C	0.29502000	-1.66360100	0.60539000
C	0.55501600	-1.34578000	1.93071200

C	1.17588400	-2.36526100	-0.20598300
C	1.77342100	-1.76171300	2.46671900
H	-0.16020000	-0.79898300	2.52796000
C	2.38070500	-2.78122400	0.35735600
H	0.94007300	-2.57930600	-1.23897900
C	2.67845100	-2.47770600	1.68486500
H	2.00705100	-1.52243800	3.49742200
H	3.08966500	-3.32778000	-0.25225400
H	3.62358400	-2.79455500	2.10911800
O	-2.11370500	-3.22207200	0.15070700
C	-3.32241500	-3.51058000	-0.26485400
O	-4.06481500	-2.68343300	-0.79357900
C	-3.72622400	-4.94000700	-0.00736000
H	-4.02449400	-5.02712800	1.04181500
H	-4.57183200	-5.20443400	-0.64120700
H	-2.88977200	-5.61757600	-0.18050400
H	-0.72311200	0.63160700	-0.61601700
H	-3.05712200	1.57674000	1.42087500
N	1.81868900	2.07725000	-0.13089400
C	2.16465000	1.02037000	-0.88856900
H	2.52751400	2.41162300	0.50737300
C	3.50630900	0.39025600	-0.64689800
O	1.41902100	0.54162400	-1.76220100
C	4.05675500	-0.39232700	-1.66848900
C	4.18181100	0.48799400	0.57381400
C	5.26575400	-1.05314400	-1.48085600
H	3.52632100	-0.48198900	-2.60795100
C	5.38984500	-0.17934400	0.76440200
H	3.75931800	1.05035300	1.39808000
C	5.93522900	-0.94986100	-0.26114600
H	5.68310300	-1.65289500	-2.28186200
H	5.89684700	-0.10830600	1.71995600
H	6.87354800	-1.47151200	-0.10896200

IRC_TS1_point100

B	-2.67131700	3.96214900	0.40906900
B	-1.56911300	3.70477100	1.78726400
B	-0.55438600	2.30011000	1.42815500
B	-2.33268500	2.71484500	-0.81577400
B	-1.02103000	1.76586900	-0.16669700
B	-1.20877100	4.96294500	0.58381200
B	-1.68587400	4.36181100	-1.01744900
H	-3.76381700	4.41155000	0.55822700
B	0.10182900	3.93593900	1.20619100

H	-1.88348600	3.97271900	2.90432800
B	0.45226700	2.69417200	-0.01142100
H	-0.13376100	1.55377000	2.24939300
B	-0.66131800	2.96640600	-1.40416500
H	-3.16823100	2.25290400	-1.52499300
H	-1.27034000	6.12145200	0.85525500
B	0.02978300	4.34660600	-0.53063700
H	-2.08535800	5.08513200	-1.87502000
H	0.96949900	4.35208200	1.90849900
H	-0.34442200	2.67612400	-2.50922900
H	0.84912900	5.04556600	-1.03849400
B	-2.26747000	2.31343000	0.93008500
I	-1.58708900	-1.07395800	-0.23250100
C	0.29585400	-1.66314100	0.60602200
C	0.55615000	-1.34489200	1.93115300
C	1.17579200	-2.36651800	-0.20481200
C	1.77395900	-1.76214600	2.46753900
H	-0.15834800	-0.79675800	2.52802600
C	2.38000700	-2.78378000	0.35888400
H	0.93977900	-2.58086900	-1.23769600
C	2.67809400	-2.47983000	1.68621800
H	2.00779700	-1.52256800	3.49812600
H	3.08824800	-3.33168700	-0.25034300
H	3.62275500	-2.79771400	2.11075200
O	-2.11255200	-3.22013600	0.14988400
C	-3.32120000	-3.50851600	-0.26547400
O	-4.06379700	-2.68120500	-0.79384000
C	-3.72541500	-4.93797800	-0.00841400
H	-4.02528100	-5.02493600	1.04032200
H	-4.57019000	-5.20246300	-0.64336500
H	-2.88885000	-5.61572000	-0.18024800
H	-0.71871900	0.63040100	-0.61485100
H	-3.05692900	1.57373300	1.42212000
N	1.81817700	2.07654600	-0.12937000
C	2.16337100	1.01917000	-0.88693300
H	2.52770400	2.41218500	0.50667000
C	3.50529400	0.38912400	-0.64674900
O	1.41673800	0.53989300	-1.75938000
C	4.05397000	-0.39427100	-1.66868200
C	4.18286800	0.48777200	0.57272800
C	5.26334500	-1.05484300	-1.48270300
H	3.52184700	-0.48467100	-2.60710700
C	5.39128800	-0.17937100	0.76169300
H	3.76177100	1.05083900	1.39723300

C	5.93496700	-0.95056000	-0.26426100
H	5.67931100	-1.65516500	-2.28399900
H	5.89999200	-0.10756300	1.71628100
H	6.87363100	-1.47195900	-0.11337300
IRC_TS1_point101			
B	-2.67336800	3.95869400	0.40825500
B	-1.57118300	3.70366200	1.78696900
B	-0.55499800	2.29970500	1.42946000
B	-2.33327800	2.71075000	-0.81547000
B	-1.02082500	1.76377900	-0.16509900
B	-1.21179000	4.96105500	0.58246300
B	-1.68804000	4.35819600	-1.01836400
H	-3.76629800	4.40719800	0.55687400
B	0.09973200	3.93589800	1.20611800
H	-1.88610800	3.97231100	2.90369400
B	0.45170400	2.69342100	-0.01037100
H	-0.13390100	1.55437100	2.25131500
B	-0.66209700	2.96359200	-1.40373800
H	-3.16814600	2.24722600	-1.52443600
H	-1.27448900	6.11972700	0.85293000
B	0.02760700	4.34498300	-0.53119500
H	-2.08800600	5.08047800	-1.87657100
H	0.96675900	4.35360400	1.90826300
H	-0.34464800	2.67250800	-2.50838900
H	0.84637600	5.04430900	-1.03945500
B	-2.26804800	2.31091500	0.93093000
I	-1.58534800	-1.07105700	-0.23268200
C	0.29666800	-1.66263500	0.60662600
C	0.55726100	-1.34401900	1.93157700
C	1.17568000	-2.36774700	-0.20365000
C	1.77446600	-1.76260300	2.46835500
H	-0.15654900	-0.79459100	2.52808200
C	2.37929700	-2.78631200	0.36039900
H	0.93950900	-2.58236500	-1.23644500
C	2.67772000	-2.48195600	1.68756300
H	2.00850000	-1.52272800	3.49883000
H	3.08687800	-3.33548100	-0.24847700
H	3.62194400	-2.80081800	2.11236000
O	-2.11141500	-3.21853900	0.14914000
C	-3.31996000	-3.50657000	-0.26603400
O	-4.06279000	-2.67905000	-0.79409500
C	-3.72456200	-4.93602000	-0.00940800
H	-4.02590100	-5.02282300	1.03893200
H	-4.56849300	-5.20071300	-0.64540800

H	-2.88775000	-5.61379300	-0.17994800
H	-0.71313800	0.63030500	-0.61396700
H	-3.05684500	1.57082200	1.42332800
N	1.81772900	2.07613500	-0.12853800
C	2.16215500	1.01796100	-0.88531200
H	2.52750400	2.41141300	0.50846000
C	3.50430000	0.38789300	-0.64652600
O	1.41436800	0.53813100	-1.75644100
C	4.05130000	-0.39622300	-1.66883300
C	4.18393200	0.48746700	0.57171400
C	5.26108200	-1.05649300	-1.48448200
H	3.51759100	-0.48731900	-2.60629100
C	5.39276200	-0.17940200	0.75906500
H	3.76424900	1.05114900	1.39652100
C	5.93480000	-0.95122400	-0.26728400
H	5.67575400	-1.65732800	-2.28606400
H	5.90309700	-0.10682700	1.71272600
H	6.87382000	-1.47234200	-0.11763100

IRC_TS1_point102

B	-2.67543000	3.95521000	0.40741100
B	-1.57328100	3.70252000	1.78661400
B	-0.55563000	2.29932400	1.43071600
B	-2.33388400	2.70661700	-0.81515000
B	-1.02048400	1.76223400	-0.16348700
B	-1.21480000	4.95913100	0.58104400
B	-1.69019600	4.35450200	-1.01934200
H	-3.76880000	4.40278900	0.55544900
B	0.09764300	3.93585800	1.20596300
H	-1.88874900	3.97184600	2.90300800
B	0.45114600	2.69266000	-0.00929100
H	-0.13402700	1.55494300	2.25314500
B	-0.66283000	2.96074700	-1.40333300
H	-3.16796300	2.24135500	-1.52386100
H	-1.27867300	6.11795700	0.85049700
B	0.02548400	4.34333800	-0.53180100
H	-2.09064900	5.07567500	-1.87823000
H	0.96400900	4.35511300	1.90797600
H	-0.34488700	2.66880600	-2.50758700
H	0.84362300	5.04304600	-1.04052400
B	-2.26864400	2.30835300	0.93170100
I	-1.58363200	-1.06817800	-0.23286500
C	0.29748200	-1.66208800	0.60722200
C	0.55836500	-1.34309800	1.93199400

C	1.17554800	-2.36891600	-0.20252500
C	1.77495900	-1.76304000	2.46915100
H	-0.15473500	-0.79236300	2.52813500
C	2.37854500	-2.78881400	0.36188000
H	0.93918600	-2.58379700	-1.23521900
C	2.67730700	-2.48407300	1.68887900
H	2.00919400	-1.52289400	3.49951800
H	3.08542100	-3.33929000	-0.24663700
H	3.62106300	-2.80397100	2.11394600
O	-2.11028200	-3.21659700	0.14839500
C	-3.31873400	-3.50457100	-0.26657700
O	-4.06183400	-2.67696000	-0.79431300
C	-3.72362800	-4.93408300	-0.01035000
H	-4.02653200	-5.02073000	1.03756000
H	-4.56670600	-5.19894600	-0.64742800
H	-2.88663200	-5.61194600	-0.17956700
H	-0.70868900	0.62933600	-0.61298300
H	-3.05674800	1.56787000	1.42452500
N	1.81717100	2.07520300	-0.12690100
C	2.16092300	1.01662600	-0.88367700
H	2.52776400	2.41230000	0.50689900
C	3.50335600	0.38671500	-0.64636400
O	1.41216800	0.53620100	-1.75357500
C	4.04869200	-0.39814900	-1.66899400
C	4.18497900	0.48720000	0.57068500
C	5.25889100	-1.05808000	-1.48626300
H	3.51337100	-0.48996600	-2.60545500
C	5.39423400	-0.17939200	0.75645000
H	3.76657700	1.05154900	1.39569800
C	5.93468700	-0.95179900	-0.27030500
H	5.67228800	-1.65941000	-2.28813200
H	5.90619800	-0.10605900	1.70918000
H	6.87408400	-1.47259300	-0.12190800
IRC_TS1_point103			
B	-2.67746100	3.95174600	0.40654800
B	-1.57534700	3.70137700	1.78626800
B	-0.55627300	2.29886300	1.43198200
B	-2.33448600	2.70250300	-0.81487400
B	-1.02029100	1.76016500	-0.16192600
B	-1.21777200	4.95718600	0.57963600
B	-1.69232100	4.35083200	-1.02031200
H	-3.77125200	4.39843800	0.55403700
B	0.09556200	3.93573000	1.20583300
H	-1.89136300	3.97141200	2.90232000

B	0.45055900	2.69181600	-0.00830000
H	-0.13422700	1.55548300	2.25503600
B	-0.66359600	2.95785000	-1.40293100
H	-3.16787300	2.23564500	-1.52332400
H	-1.28275100	6.11617200	0.84809800
B	0.02333700	4.34162600	-0.53241100
H	-2.09323800	5.07094800	-1.87984900
H	0.96128100	4.35653400	1.90768300
H	-0.34511400	2.66507900	-2.50676900
H	0.84092500	5.04165700	-1.04154500
B	-2.26925100	2.30582700	0.93250300
I	-1.58194300	-1.06520300	-0.23304100
C	0.29827600	-1.66149000	0.60779900
C	0.55945500	-1.34217500	1.93240100
C	1.17539300	-2.37005400	-0.20140000
C	1.77542500	-1.76349800	2.46994800
H	-0.15294000	-0.79015000	2.52818700
C	2.37777200	-2.79130100	0.36335500
H	0.93886300	-2.58517500	-1.23400800
C	2.67686900	-2.48620600	1.69019500
H	2.00985400	-1.52309600	3.50021400
H	3.08396200	-3.34305300	-0.24481700
H	3.62016200	-2.80713400	2.11552800
O	-2.10917500	-3.21491300	0.14770900
C	-3.31749700	-3.50266600	-0.26707800
O	-4.06090600	-2.67493500	-0.79453200
C	-3.72265700	-4.93220000	-0.01125400
H	-4.02708200	-5.01868600	1.03624100
H	-4.56484200	-5.19735400	-0.64940600
H	-2.88536600	-5.61004000	-0.17912100
H	-0.70324600	0.62909200	-0.61226800
H	-3.05670500	1.56496400	1.42569300
N	1.81671100	2.07473600	-0.12618400
C	2.15973100	1.01528700	-0.88202000
H	2.52735600	2.41086300	0.50975500
C	3.50241100	0.38540900	-0.64605600
O	1.40987900	0.53429800	-1.75068900
C	4.04616700	-0.40007900	-1.66908300
C	4.18606100	0.48682600	0.56975700
C	5.25682100	-1.05961700	-1.48798000
H	3.50929200	-0.49260100	-2.60458400
C	5.39576800	-0.17939300	0.75390400
H	3.76903500	1.05167300	1.39512400
C	5.93466700	-0.95234800	-0.27325500

H	5.66898800	-1.66139400	-2.29014500
H	5.90932800	-0.10528900	1.70571600
H	6.87445300	-1.47279200	-0.12609600
IRC_TS1_point104			
B	-2.67949400	3.94827800	0.40566300
B	-1.57742600	3.70021100	1.78586800
B	-0.55694200	2.29842800	1.43319600
B	-2.33511400	2.69839100	-0.81460500
B	-1.02004300	1.75852000	-0.16035600
B	-1.22071600	4.95522300	0.57817600
B	-1.69443600	4.34712900	-1.02132600
H	-3.77370400	4.39409400	0.55257700
B	0.09349000	3.93560800	1.20563900
H	-1.89397700	3.97093000	2.90158800
B	0.44999600	2.69095000	-0.00724000
H	-0.13442000	1.55599500	2.25682600
B	-0.66435300	2.95496500	-1.40258200
H	-3.16773200	2.22983700	-1.52280000
H	-1.28682000	6.11436600	0.84563100
B	0.02126200	4.33988700	-0.53306000
H	-2.09580300	5.06616300	-1.88153900
H	0.95857100	4.35792000	1.90734800
H	-0.34537800	2.66131700	-2.50601300
H	0.83823900	5.04028100	-1.04265400
B	-2.26988200	2.30326700	0.93323800
I	-1.58028100	-1.06224500	-0.23322500
C	0.29907500	-1.66085400	0.60836200
C	0.56053300	-1.34121400	1.93279500
C	1.17522500	-2.37112800	-0.20032000
C	1.77587500	-1.76393600	2.47072200
H	-0.15115000	-0.78789600	2.52822800
C	2.37696700	-2.79374600	0.36478800
H	0.93850800	-2.58647900	-1.23283500
C	2.67639700	-2.48831800	1.69147700
H	2.01050300	-1.52329800	3.50088900
H	3.08245000	-3.34679400	-0.24303800
H	3.61921300	-2.81031500	2.11707800
O	-2.10807700	-3.21293900	0.14702400
C	-3.31627800	-3.50071600	-0.26756600
O	-4.06003400	-2.67297500	-0.79472800
C	-3.72160500	-4.93034100	-0.01210900
H	-4.02762000	-5.01666900	1.03494500
H	-4.56288600	-5.19577500	-0.65135900
H	-2.88405300	-5.60818700	-0.17860200

H	-0.69884100	0.62835700	-0.61140400
H	-3.05667400	1.56205300	1.42684900
N	1.81611800	2.07361000	-0.12449100
C	2.15854400	1.01382400	-0.88039000
H	2.52779000	2.41227600	0.50696600
C	3.50153800	0.38418600	-0.64586300
O	1.40777800	0.53216200	-1.74776800
C	4.04372000	-0.40198900	-1.66919900
C	4.18710400	0.48652100	0.56879400
C	5.25483000	-1.06110100	-1.48969700
H	3.50528000	-0.49523200	-2.60372500
C	5.39727500	-0.17935900	0.75138700
H	3.77125800	1.05205500	1.39429900
C	5.93469400	-0.95281200	-0.27618600
H	5.66580300	-1.66330700	-2.29215200
H	5.91241800	-0.10449700	1.70228500
H	6.87489100	-1.47286400	-0.13026700

IRC_TS1_point105

B	-2.68150000	3.94481300	0.40476400
B	-1.57947800	3.69903500	1.78547600
B	-0.55761000	2.29791600	1.43441000
B	-2.33572300	2.69427700	-0.81435400
B	-1.01986000	1.75650100	-0.15884700
B	-1.22363800	4.95323300	0.57671900
B	-1.69652400	4.34342300	-1.02234000
H	-3.77614100	4.38971600	0.55111200
B	0.09143200	3.93540100	1.20545000
H	-1.89658700	3.97046400	2.90084900
B	0.44938200	2.69002300	-0.00630900
H	-0.13467300	1.55648400	2.25867700
B	-0.66510700	2.95201000	-1.40220900
H	-3.16763300	2.22407700	-1.52226500
H	-1.29085800	6.11253000	0.84316300
B	0.01914800	4.33810500	-0.53372000
H	-2.09836500	5.06135700	-1.88322500
H	0.95585500	4.35925600	1.90700000
H	-0.34561200	2.65747600	-2.50521700
H	0.83558500	5.03878500	-1.04374200
B	-2.27050700	2.30074100	0.93399700
I	-1.57863800	-1.05920700	-0.23340100
C	0.29985000	-1.66016100	0.60891400
C	0.56160500	-1.34023900	1.93318900
C	1.17503200	-2.37215800	-0.19923900

C	1.77630500	-1.76438900	2.47149900
H	-0.14934700	-0.78562000	2.52827700
C	2.37613900	-2.79616800	0.36621300
H	0.93812800	-2.58773900	-1.23166200
C	2.67590100	-2.49044500	1.69275600
H	2.01112800	-1.52354900	3.50157600
H	3.08089400	-3.35054000	-0.24126200
H	3.61821500	-2.81355800	2.11863700
O	-2.10701300	-3.21116300	0.14638400
C	-3.31506100	-3.49884800	-0.26801900
O	-4.05920100	-2.67107900	-0.79492200
C	-3.72051500	-4.92852900	-0.01292500
H	-4.02807900	-5.01468700	1.03369900
H	-4.56085100	-5.19435000	-0.65327100
H	-2.88260300	-5.60627200	-0.17802100
H	-0.69350400	0.62797300	-0.61086100
H	-3.05664900	1.55914600	1.42797900
N	1.81563800	2.07304100	-0.12378200
C	2.15737300	1.01235500	-0.87869300
H	2.52708200	2.41008700	0.51096000
C	3.50064200	0.38281700	-0.64548200
O	1.40556500	0.53011100	-1.74493100
C	4.04133500	-0.40389000	-1.66923400
C	4.18819900	0.48606700	0.56795100
C	5.25293900	-1.06253000	-1.49136100
H	3.50134600	-0.49787100	-2.60279100
C	5.39886100	-0.17934600	0.74891600
H	3.77370200	1.05194500	1.39389400
C	5.93481200	-0.95325700	-0.27907500
H	5.66272000	-1.66513500	-2.29412700
H	5.91558800	-0.10370500	1.69889200
H	6.87543400	-1.47289100	-0.13442100

IRC_TS1_point106

B	-2.68350300	3.94135400	0.40385600
B	-1.58153400	3.69782600	1.78505000
B	-0.55831400	2.29740400	1.43558700
B	-2.33637700	2.69018900	-0.81412400
B	-1.01971300	1.75473800	-0.15733000
B	-1.22651500	4.95122100	0.57524200
B	-1.69860100	4.33971300	-1.02337100
H	-3.77855600	4.38539600	0.54963400
B	0.08938200	3.93517500	1.20523600
H	-1.89919000	3.96993300	2.90008700

B	0.44881300	2.68905000	-0.00528100
H	-0.13494500	1.55691200	2.26043600
B	-0.66589200	2.94908800	-1.40190700
H	-3.16753300	2.21830600	-1.52176900
H	-1.29483400	6.11067100	0.84068000
B	0.01711400	4.33626900	-0.53439400
H	-2.10087400	5.05656800	-1.88493300
H	0.95317400	4.36050900	1.90664100
H	-0.34590400	2.65362600	-2.50448800
H	0.83296200	5.03728000	-1.04488100
B	-2.27117100	2.29818100	0.93470500
I	-1.57701400	-1.05615900	-0.23358700
C	0.30062900	-1.65943700	0.60945200
C	0.56265400	-1.33925200	1.93357300
C	1.17483100	-2.37312500	-0.19820200
C	1.77671400	-1.76483700	2.47225600
H	-0.14757400	-0.78335100	2.52832400
C	2.37528800	-2.79853900	0.36759100
H	0.93773700	-2.58890800	-1.23053700
C	2.67537900	-2.49254300	1.69399900
H	2.01173100	-1.52381200	3.50224700
H	3.07932000	-3.35421800	-0.23954300
H	3.61719300	-2.81677900	2.12015200
O	-2.10596100	-3.20917300	0.14574600
C	-3.31385800	-3.49694800	-0.26845900
O	-4.05842800	-2.66925300	-0.79510800
C	-3.71935500	-4.92674500	-0.01369700
H	-4.02843500	-5.01275900	1.03250000
H	-4.55878400	-5.19293200	-0.65509700
H	-2.88111800	-5.60440300	-0.17745700
H	-0.68905700	0.62753400	-0.61018400
H	-3.05667300	1.55624800	1.42909100
N	1.81503300	2.07182700	-0.12221100
C	2.15622200	1.01076400	-0.87706500
H	2.52767600	2.41179400	0.50753900
C	3.49983200	0.38153700	-0.64524400
O	1.40351300	0.52775300	-1.74194000
C	4.03904800	-0.40577900	-1.66930500
C	4.18923500	0.48570500	0.56706400
C	5.25114300	-1.06391300	-1.49301300
H	3.49753000	-0.50049300	-2.60190300
C	5.40038800	-0.17931200	0.74650600
H	3.77584300	1.05229500	1.39308700
C	5.93496200	-0.95363600	-0.28190800

H	5.65979700	-1.66688800	-2.29607700
H	5.91866600	-0.10290600	1.69557700
H	6.87602800	-1.47281200	-0.13849300
IRC_TS1_point107			
B	-2.68548500	3.93788500	0.40293900
B	-1.58356500	3.69659500	1.78462000
B	-0.55901500	2.29682000	1.43674200
B	-2.33701600	2.68608100	-0.81389600
B	-1.01956500	1.75280600	-0.15588600
B	-1.22937400	4.94917200	0.57375200
B	-1.70065600	4.33597300	-1.02441600
H	-3.78096100	4.38102400	0.54814800
B	0.08735000	3.93486500	1.20499400
H	-1.90177000	3.96940400	2.89931200
B	0.44817600	2.68802000	-0.00439000
H	-0.13525100	1.55730000	2.26221200
B	-0.66665400	2.94608100	-1.40157500
H	-3.16745100	2.21252800	-1.52124400
H	-1.29879100	6.10877000	0.83817300
B	0.01504500	4.33439800	-0.53509600
H	-2.10339500	5.05171500	-1.88665700
H	0.95049500	4.36170800	1.90623800
H	-0.34617300	2.64968900	-2.50373200
H	0.83036000	5.03566700	-1.04602900
B	-2.27182600	2.29563800	0.93542000
I	-1.57540100	-1.05303500	-0.23376900
C	0.30138600	-1.65866000	0.60998500
C	0.56369900	-1.33825000	1.93396100
C	1.17460500	-2.37404000	-0.19717000
C	1.77711100	-1.76528900	2.47300800
H	-0.14578800	-0.78106800	2.52838800
C	2.37441900	-2.80086800	0.36894900
H	0.93730900	-2.59002100	-1.22941600
C	2.67484200	-2.49463200	1.69522400
H	2.01232200	-1.52411500	3.50292300
H	3.07769800	-3.35787500	-0.23784600
H	3.61613700	-2.82002600	2.12165200
O	-2.10494100	-3.20729000	0.14513800
C	-3.31266500	-3.49512100	-0.26886400
O	-4.05770300	-2.66750500	-0.79528100
C	-3.71815500	-4.92501500	-0.01441000
H	-4.02867400	-5.01088100	1.03137900
H	-4.55667800	-5.19164700	-0.65682400
H	-2.87953500	-5.60251300	-0.17685700

H	-0.68397900	0.62702900	-0.60985900
H	-3.05668800	1.55333900	1.43018200
N	1.81450500	2.07104200	-0.12136900
C	2.15506000	1.00914100	-0.87533500
H	2.52689100	2.40954700	0.51129000
C	3.49899100	0.38012400	-0.64483200
O	1.40136300	0.52548600	-1.73907800
C	4.03681300	-0.40764000	-1.66931500
C	4.19031700	0.48518300	0.56628700
C	5.24943200	-1.06523400	-1.49463400
H	3.49378400	-0.50309500	-2.60095400
C	5.40198900	-0.17930500	0.74412200
H	3.77819100	1.05202600	1.39276500
C	5.93519100	-0.95399600	-0.28472500
H	5.65696000	-1.66854100	-2.29802000
H	5.92180900	-0.10213600	1.69228300
H	6.87670900	-1.47269700	-0.14257700

IRC_TS1_point108

B	-2.68745200	3.93442800	0.40202100
B	-1.58558400	3.69532900	1.78417600
B	-0.55974500	2.29620800	1.43787700
B	-2.33769600	2.68200500	-0.81369400
B	-1.01950400	1.75089700	-0.15442900
B	-1.23217800	4.94709600	0.57226300
B	-1.70269900	4.33224400	-1.02545700
H	-3.78331700	4.37674700	0.54668200
B	0.08532700	3.93451300	1.20475300
H	-1.90431800	3.96881800	2.89853300
B	0.44758500	2.68692800	-0.00341500
H	-0.13558500	1.55761800	2.26392800
B	-0.66746700	2.94310100	-1.40131300
H	-3.16741000	2.20682700	-1.52076600
H	-1.30263000	6.10684500	0.83569500
B	0.01304000	4.33245300	-0.53579900
H	-2.10584100	5.04694000	-1.88835600
H	0.94786700	4.36279300	1.90583600
H	-0.34649500	2.64576600	-2.50303200
H	0.82780900	5.03400900	-1.04718400
B	-2.27251700	2.29307400	0.93611100
I	-1.57380300	-1.04987200	-0.23396100
C	0.30213700	-1.65785900	0.61050600
C	0.56471300	-1.33725600	1.93434300
C	1.17436900	-2.37490100	-0.19617400

C	1.77748400	-1.76574500	2.47374700
H	-0.14405400	-0.77883200	2.52845700
C	2.37353500	-2.80314300	0.37026400
H	0.93688300	-2.59103600	-1.22834100
C	2.67428700	-2.49668800	1.69641500
H	2.01288700	-1.52443400	3.50358800
H	3.07609400	-3.36141600	-0.23621700
H	3.61508700	-2.82320300	2.12309800
O	-2.10394200	-3.20531100	0.14453400
C	-3.31148600	-3.49329600	-0.26925700
O	-4.05703900	-2.66583400	-0.79545700
C	-3.71691200	-4.92332600	-0.01508700
H	-4.02879500	-5.00907800	1.03031400
H	-4.55458400	-5.19039400	-0.65844700
H	-2.87793500	-5.60067400	-0.17630500
H	-0.67941200	0.62684500	-0.60950800
H	-3.05676900	1.55046300	1.43126000
N	1.81390000	2.06981300	-0.11999300
C	2.15393300	1.00742500	-0.87368600
H	2.52733500	2.41074000	0.50874000
C	3.49823100	0.37877700	-0.64453400
O	1.39932300	0.52293200	-1.73603800
C	4.03468400	-0.40949100	-1.66935100
C	4.19134500	0.48473900	0.56548200
C	5.24782100	-1.06651800	-1.49622400
H	3.49020000	-0.50565300	-2.60006900
C	5.40352900	-0.17928600	0.74181500
H	3.78027100	1.05219300	1.39207600
C	5.93544600	-0.95431300	-0.28745900
H	5.65430800	-1.67012000	-2.29991700
H	5.92483400	-0.10137600	1.68910200
H	6.87741900	-1.47252000	-0.14652000

IRC_TS1_point109

B	-2.68940300	3.93096200	0.40109800
B	-1.58758600	3.69403900	1.78372100
B	-0.56047300	2.29554300	1.43898600
B	-2.33836600	2.67790900	-0.81348200
B	-1.01940000	1.74900200	-0.15302700
B	-1.23496400	4.94498600	0.57075600
B	-1.70471700	4.32847600	-1.02651700
H	-3.78566600	4.37242800	0.54520400
B	0.08332500	3.93409500	1.20447300
H	-1.90684100	3.96822200	2.89774200

B	0.44693500	2.68579000	-0.00254400
H	-0.13593600	1.55789300	2.26563800
B	-0.66824600	2.94004300	-1.40101800
H	-3.16736200	2.20108700	-1.52025700
H	-1.30645500	6.10487800	0.83318600
B	0.01101900	4.33048100	-0.53652800
H	-2.10828700	5.04209000	-1.89008200
H	0.94524500	4.36383100	1.90538900
H	-0.34680300	2.64176800	-2.50231600
H	0.82527500	5.03227200	-1.04836300
B	-2.27320200	2.29051700	0.93679800
I	-1.57221600	-1.04665500	-0.23415400
C	0.30287000	-1.65701400	0.61102200
C	0.56572000	-1.33624500	1.93472700
C	1.17411100	-2.37570700	-0.19519300
C	1.77784700	-1.76619600	2.47447300
H	-0.14231400	-0.77658600	2.52854400
C	2.37263500	-2.80536600	0.37154700
H	0.93642100	-2.59198800	-1.22728000
C	2.67372000	-2.49872100	1.69757700
H	2.01344300	-1.52478100	3.50424800
H	3.07444800	-3.36491500	-0.23462600
H	3.61401100	-2.82638300	2.12451200
O	-2.10297500	-3.20335600	0.14394200
C	-3.31032700	-3.49152800	-0.26962600
O	-4.05643100	-2.66424600	-0.79562200
C	-3.71563700	-4.92169300	-0.01571100
H	-4.02884600	-5.00732300	1.02931100
H	-4.55245700	-5.18925200	-0.65999200
H	-2.87626900	-5.59884600	-0.17570500
H	-0.67460800	0.62631000	-0.60945800
H	-3.05684100	1.54757400	1.43232400
N	1.81333600	2.06882100	-0.11903200
C	2.15279300	1.00566300	-0.87193700
H	2.52676600	2.40911500	0.51116800
C	3.49745800	0.37734500	-0.64411400
O	1.39722700	0.52041400	-1.73308500
C	4.03260800	-0.41130600	-1.66934500
C	4.19240800	0.48418300	0.56475800
C	5.24628400	-1.06774400	-1.49779200
H	3.48668000	-0.50817800	-2.59913900
C	5.40512300	-0.17928800	0.73953200
H	3.78248500	1.05189400	1.39174700
C	5.93576400	-0.95461100	-0.29017600

H	5.65173500	-1.67160700	-2.30181200
H	5.92789900	-0.10065100	1.68594500
H	6.87819500	-1.47231400	-0.15047000

IRC_TS1_point110

B	-2.69133200	3.92750800	0.40017200
B	-1.58956400	3.69272100	1.78325800
B	-0.56121300	2.29484200	1.44008000
B	-2.33905900	2.67384500	-0.81330000
B	-1.01940500	1.74697700	-0.15161700
B	-1.23769800	4.94285400	0.56925500
B	-1.70672100	4.32472800	-1.02756800
H	-3.78796200	4.36819200	0.54375100
B	0.08133500	3.93363400	1.20420000
H	-1.90932300	3.96758400	2.89694800
B	0.44632900	2.68459400	-0.00161900
H	-0.13630700	1.55811500	2.26731200
B	-0.66907400	2.93700900	-1.40078700
H	-3.16736300	2.19545400	-1.51979200
H	-1.31016300	6.10289400	0.83071400
B	0.00904700	4.32844400	-0.53726000
H	-2.11066600	5.03732600	-1.89177500
H	0.94267600	4.36476700	1.90493800
H	-0.34714300	2.63778200	-2.50164200
H	0.82279600	5.03048100	-1.04953500
B	-2.27390800	2.28795300	0.93747400
I	-1.57064800	-1.04339400	-0.23435400
C	0.30359300	-1.65613900	0.61152200
C	0.56670000	-1.33524000	1.93510400
C	1.17384200	-2.37645700	-0.19424500
C	1.77818900	-1.76664800	2.47518400
H	-0.14062200	-0.77438600	2.52863300
C	2.37172600	-2.80752900	0.37278700
H	0.93596200	-2.59284400	-1.22626400
C	2.67314000	-2.50071800	1.69870500
H	2.01397400	-1.52514300	3.50489600
H	3.07282500	-3.36829300	-0.23310300
H	3.61294700	-2.82949000	2.12587200
O	-2.10203800	-3.20139200	0.14335300
C	-3.30918500	-3.48979000	-0.26998400
O	-4.05588600	-2.66273900	-0.79579400
C	-3.71434200	-4.92011100	-0.01630200
H	-4.02881800	-5.00563800	1.02835600

H	-4.55034400	-5.18817200	-0.66145300
H	-2.87459200	-5.59706500	-0.17512500
H	-0.67000000	0.62629900	-0.60945200
H	-3.05696500	1.54472300	1.43337400
N	1.81274000	2.06758100	-0.11779600
C	2.15169400	1.00384000	-0.87025100
H	2.52697500	2.40963900	0.50972800
C	3.49675400	0.37595300	-0.64375500
O	1.39520800	0.51768700	-1.72998900
C	4.03063000	-0.41310200	-1.66934800
C	4.19344000	0.48367000	0.56403500
C	5.24483900	-1.06893300	-1.49932500
H	3.48331400	-0.51064800	-2.59825600
C	5.40667900	-0.17929000	0.73732400
H	3.78452400	1.05186000	1.39120100
C	5.93610900	-0.95488000	-0.29281700
H	5.64932200	-1.67302400	-2.30366100
H	5.93087200	-0.09994800	1.68289600
H	6.87899500	-1.47207400	-0.15428900

IRC_TS1_point111

B	-2.69324600	3.92404600	0.39924400
B	-1.59153000	3.69137700	1.78278200
B	-0.56195100	2.29409900	1.44114800
B	-2.33974300	2.66976700	-0.81310400
B	-1.01933600	1.74507400	-0.15025000
B	-1.24041000	4.94069200	0.56774100
B	-1.70869800	4.32094400	-1.02863600
H	-3.79025300	4.36391900	0.54228500
B	0.07936800	3.93311900	1.20389100
H	-1.91178800	3.96692500	2.89614300
B	0.44567700	2.68336400	-0.00077100
H	-0.13669000	1.55829200	2.26896900
B	-0.66986200	2.93390900	-1.40052200
H	-3.16733800	2.18976200	-1.51930000
H	-1.31386500	6.10087200	0.82821500
B	0.00707500	4.32638900	-0.53800900
H	-2.11304100	5.03249200	-1.89349500
H	0.94011200	4.36566300	1.90445700
H	-0.34747600	2.63373700	-2.50095900
H	0.82033000	5.02864100	-1.05073000
B	-2.27460800	2.28538600	0.93813600
I	-1.56909200	-1.04009700	-0.23455400
C	0.30430100	-1.65522200	0.61201400

C	0.56766900	-1.33422000	1.93548000
C	1.17355500	-2.37714700	-0.19332000
C	1.77851900	-1.76709500	2.47588000
H	-0.13893100	-0.77218200	2.52873800
C	2.37080200	-2.80963400	0.37398800
H	0.93547200	-2.59363200	-1.22526900
C	2.67254900	-2.50268600	1.69979900
H	2.01449500	-1.52553100	3.50553700
H	3.07116400	-3.37162400	-0.23162400
H	3.61185600	-2.83259600	2.12719700
O	-2.10113500	-3.19941100	0.14276300
C	-3.30807300	-3.48809700	-0.27033200
O	-4.05540100	-2.66131300	-0.79596200
C	-3.71302400	-4.91858300	-0.01685400
H	-4.02875300	-5.00399600	1.02744300
H	-4.54820100	-5.18718700	-0.66286500
H	-2.87286400	-5.59530500	-0.17449800
H	-0.66542000	0.62578500	-0.60970400
H	-3.05707700	1.54185100	1.43440700
N	1.81216700	2.06645700	-0.11678700
C	2.15058900	1.00196900	-0.86847300
H	2.52661400	2.40855900	0.51110000
C	3.49605600	0.37451700	-0.64331800
O	1.39315500	0.51493400	-1.72691900
C	4.02870500	-0.41486200	-1.66932200
C	4.19449700	0.48309100	0.56337000
C	5.24345900	-1.07007200	-1.50083700
H	3.48000800	-0.51308400	-2.59734000
C	5.40826500	-0.17930700	0.73514600
H	3.78663600	1.05154800	1.39087600
C	5.93649900	-0.95513500	-0.29543200
H	5.64697900	-1.67436600	-2.30550400
H	5.93386600	-0.09927500	1.67987600
H	6.87984000	-1.47181400	-0.15810000

IRC_TS1_point112

B	-2.69513400	3.92059300	0.39831000
B	-1.59346400	3.69000700	1.78229900
B	-0.56268900	2.29332000	1.44219800
B	-2.34043900	2.66572100	-0.81294300
B	-1.01938400	1.74297400	-0.14888200
B	-1.24307600	4.93851100	0.56623100
B	-1.71066300	4.31718500	-1.02969600
H	-3.79249300	4.35970500	0.54084300

B	0.07741400	3.93256400	1.20358800
H	-1.91420900	3.96622700	2.89533300
B	0.44507200	2.68208700	0.00011100
H	-0.13707900	1.55842700	2.27059500
B	-0.67069000	2.93084000	-1.40032500
H	-3.16735500	2.18417700	-1.51884900
H	-1.31746200	6.09883300	0.82575000
B	0.00514200	4.32427800	-0.53876600
H	-2.11536100	5.02773400	-1.89518600
H	0.93759800	4.36647200	1.90396600
H	-0.34782100	2.62969800	-2.50031000
H	0.81791900	5.02674400	-1.05192000
B	-2.27531400	2.28281400	0.93878800
I	-1.56755400	-1.03675600	-0.23475600
C	0.30500000	-1.65427200	0.61248800
C	0.56861500	-1.33320500	1.93584600
C	1.17326000	-2.37777900	-0.19242900
C	1.77883100	-1.76754100	2.47655900
H	-0.13728300	-0.77001900	2.52884400
C	2.36987400	-2.81167400	0.37514400
H	0.93498500	-2.59432500	-1.22431800
C	2.67194900	-2.50461400	1.70085500
H	2.01499300	-1.52593600	3.50616500
H	3.06952500	-3.37483600	-0.23021300
H	3.61077600	-2.83563000	2.12846700
O	-2.10026800	-3.19746600	0.14217200
C	-3.30698300	-3.48644900	-0.27067000
O	-4.05498200	-2.65997200	-0.79613700
C	-3.71170500	-4.91711000	-0.01737500
H	-4.02864100	-5.00241700	1.02657400
H	-4.54608300	-5.18627000	-0.66420400
H	-2.87114800	-5.59360000	-0.17387700
H	-0.66089300	0.62591900	-0.61003700
H	-3.05722100	1.53900800	1.43542000
N	1.81158900	2.06520100	-0.11564000
C	2.14952400	1.00005400	-0.86674500
H	2.52669500	2.40870100	0.51029100
C	3.49541300	0.37310800	-0.64290900
O	1.39115900	0.51202400	-1.72372600
C	4.02686700	-0.41659200	-1.66929600
C	4.19553600	0.48253200	0.56272100
C	5.24215800	-1.07117300	-1.50231500
H	3.47683800	-0.51545500	-2.59645800
C	5.40982700	-0.17933000	0.73303500

H	3.78863400	1.05137500	1.39044100
C	5.93691200	-0.95537100	-0.29797900
H	5.64477000	-1.67564100	-2.30730600
H	5.93678400	-0.09863500	1.67695400
H	6.88070100	-1.47154000	-0.16179800

IRC_TS1_point113

B	-2.69700600	3.91713300	0.39738100
B	-1.59538900	3.68861000	1.78180300
B	-0.56342600	2.29250500	1.44322200
B	-2.34112800	2.66166300	-0.81276500
B	-1.01933500	1.74106500	-0.14756600
B	-1.24571700	4.93630200	0.56471100
B	-1.71259500	4.31339000	-1.03077100
H	-3.79472500	4.35547000	0.53938900
B	0.07548600	3.93196100	1.20325300
H	-1.91661400	3.96550600	2.89451500
B	0.44442300	2.68078000	0.00093000
H	-0.13748100	1.55851400	2.27219700
B	-0.67147700	2.92770800	-1.40009000
H	-3.16734300	2.17853500	-1.51837600
H	-1.32104900	6.09676100	0.82326400
B	0.00321900	4.32215100	-0.53953200
H	-2.11766700	5.02291900	-1.89689700
H	0.93509100	4.36724400	1.90345400
H	-0.34816600	2.62561900	-2.49966100
H	0.81552100	5.02481500	-1.05312800
B	-2.27601600	2.28023400	0.93942200
I	-1.56602600	-1.03338800	-0.23495700
C	0.30568400	-1.65328300	0.61295200
C	0.56954400	-1.33218000	1.93621000
C	1.17295100	-2.37834900	-0.19156700
C	1.77912900	-1.76798300	2.47722000
H	-0.13564500	-0.76786500	2.52896500
C	2.36893500	-2.81365200	0.37625700
H	0.93447300	-2.59494600	-1.22339400
C	2.67133800	-2.50651000	1.70187600
H	2.01547600	-1.52636900	3.50678300
H	3.06785800	-3.37799200	-0.22885000
H	3.60967400	-2.83865600	2.12969800
O	-2.09943300	-3.19550000	0.14156700
C	-3.30592600	-3.48484700	-0.27100700
O	-4.05462500	-2.65871200	-0.79631500
C	-3.71037600	-4.91569200	-0.01786400

H	-4.02850700	-5.00088200	1.02573900
H	-4.54394800	-5.18544700	-0.66550400
H	-2.86938900	-5.59192100	-0.17321600
H	-0.65646900	0.62543700	-0.61061900
H	-3.05735600	1.53614100	1.43641600
N	1.81102600	2.06400400	-0.11462700
C	2.14845700	0.99809700	-0.86492700
H	2.52647000	2.40795800	0.51103300
C	3.49478700	0.37168100	-0.64245100
O	1.38912400	0.50905600	-1.72051700
C	4.02508100	-0.41828300	-1.66925400
C	4.19659000	0.48193700	0.56211500
C	5.24091400	-1.07222900	-1.50377400
H	3.47372700	-0.51778900	-2.59555700
C	5.41140200	-0.17936800	0.73095900
H	3.79066800	1.05103700	1.39014200
C	5.93735400	-0.95559900	-0.30049400
H	5.64262500	-1.67685400	-2.30909800
H	5.93970700	-0.09802500	1.67406700
H	6.88158600	-1.47125900	-0.16547300

IRC_TS1_point114

B	-2.69884600	3.91368000	0.39644200
B	-1.59727500	3.68719000	1.78130300
B	-0.56415300	2.29165600	1.44423000
B	-2.34182100	2.65763600	-0.81262400
B	-1.01942100	1.73890000	-0.14624300
B	-1.24831100	4.93407900	0.56319500
B	-1.71451500	4.30962300	-1.03183700
H	-3.79690600	4.35127100	0.53795700
B	0.07357200	3.93132500	1.20292700
H	-1.91897600	3.96474600	2.89369100
B	0.44383000	2.67943700	0.00178200
H	-0.13787800	1.55856800	2.27377600
B	-0.67230000	2.92460900	-1.39992600
H	-3.16736700	2.17299400	-1.51793800
H	-1.32453800	6.09467500	0.82080300
B	0.00133200	4.31997200	-0.54030900
H	-2.11992600	5.01816200	-1.89858700
H	0.93263600	4.36793600	1.90293100
H	-0.34850600	2.62153200	-2.49903400
H	0.81318300	5.02281600	-1.05433800
B	-2.27671600	2.27764600	0.94005000

I	-1.56451200	-1.02997800	-0.23515700
C	0.30635700	-1.65226000	0.61339400
C	0.57045100	-1.33116200	1.93656500
C	1.17263300	-2.37886000	-0.19073900
C	1.77940900	-1.76842100	2.47786300
H	-0.13404700	-0.76575100	2.52908700
C	2.36799200	-2.81556200	0.37732400
H	0.93396100	-2.59547400	-1.22251400
C	2.67072000	-2.50836200	1.70285700
H	2.01593700	-1.52681600	3.50738800
H	3.06620900	-3.38103100	-0.22755400
H	3.60858400	-2.84160800	2.13087400
O	-2.09863800	-3.19359200	0.14095400
C	-3.30489600	-3.48330000	-0.27133600
O	-4.05433300	-2.65753900	-0.79650000
C	-3.70906700	-4.91433400	-0.01832500
H	-4.02835500	-4.99940900	1.02494300
H	-4.54186100	-5.18467900	-0.66673600
H	-2.86768300	-5.59031900	-0.17255900
H	-0.65202900	0.62572400	-0.61123500
H	-3.05751200	1.53329900	1.43739600
N	1.81047200	2.06274000	-0.11354500
C	2.14742600	0.99610900	-0.86316200
H	2.52650700	2.40794100	0.51049900
C	3.49421000	0.37028100	-0.64200800
O	1.38714600	0.50596500	-1.71720000
C	4.02337300	-0.41993400	-1.66920900
C	4.19763100	0.48135400	0.56153000
C	5.23973500	-1.07324800	-1.50520100
H	3.47073800	-0.52004600	-2.59468400
C	5.41295300	-0.17941500	0.72894400
H	3.79261700	1.05077700	1.38978700
C	5.93781100	-0.95581500	-0.30294600
H	5.64058900	-1.67800200	-2.31085400
H	5.94255600	-0.09745400	1.67127200
H	6.88247500	-1.47097700	-0.16904500
IRC_TS1_point115			
B	-2.70066800	3.91022500	0.39551200
B	-1.59915200	3.68575000	1.78079200
B	-0.56488200	2.29077600	1.44521600
B	-2.34250500	2.65359500	-0.81246000
B	-1.01938600	1.73697000	-0.14497800
B	-1.25087500	4.93183200	0.56167100
B	-1.71639600	4.30581800	-1.03291700

H	-3.79907200	4.34707300	0.53651600
B	0.07168800	3.93064400	1.20257000
H	-1.92131700	3.96397500	2.89286300
B	0.44318400	2.67806000	0.00257500
H	-0.13828900	1.55857800	2.27533600
B	-0.67307800	2.92144300	-1.39971200
H	-3.16736400	2.16740400	-1.51747900
H	-1.32801100	6.09256100	0.81832800
B	-0.00053900	4.31778100	-0.54109000
H	-2.12216100	5.01336400	-1.90028900
H	0.93019200	4.36859400	1.90239000
H	-0.34885200	2.61742100	-2.49841100
H	0.81085800	5.02080000	-1.05555800
B	-2.27741200	2.27505200	0.94066300
I	-1.56300700	-1.02654700	-0.23535600
C	0.30701200	-1.65120400	0.61382600
C	0.57133800	-1.33014100	1.93691700
C	1.17230100	-2.37931200	-0.18993900
C	1.77967500	-1.76885600	2.47848800
H	-0.13246900	-0.76365900	2.52922600
C	2.36704100	-2.81740900	0.37834700
H	0.93342800	-2.59593400	-1.22166200
C	2.67009500	-2.51017800	1.70380100
H	2.01638300	-1.52729100	3.50798400
H	3.06454200	-3.38400600	-0.22630900
H	3.60747800	-2.84454100	2.13200900
O	-2.09787400	-3.19167000	0.14031900
C	-3.30390100	-3.48180200	-0.27166900
O	-4.05410200	-2.65644900	-0.79668900
C	-3.70775700	-4.91303600	-0.01875700
H	-4.02818900	-4.99798000	1.02417900
H	-4.53976600	-5.18401400	-0.66793500
H	-2.86593200	-5.58874000	-0.17186300
H	-0.64764300	0.62523600	-0.61211900
H	-3.05766400	1.53044200	1.43836700
N	1.80993000	2.06150600	-0.11254800
C	2.14639800	0.99409300	-0.86130100
H	2.52637300	2.40741100	0.51086600
C	3.49365100	0.36888000	-0.64153300
O	1.38511400	0.50280900	-1.71384100
C	4.02171300	-0.42154500	-1.66915600
C	4.19868200	0.48075100	0.56097800
C	5.23860400	-1.07422700	-1.50660900
H	3.46780700	-0.52226300	-2.59380500

C	5.41450700	-0.17947600	0.72696600
H	3.79458400	1.05041300	1.38952200
C	5.93828400	-0.95602900	-0.30536400
H	5.63860900	-1.67909800	-2.31259700
H	5.94539800	-0.09691700	1.66851400
H	6.88337100	-1.47070200	-0.17258600

IRC_TS1_point116

B	-2.70245600	3.90677500	0.39456800
B	-1.60098500	3.68428900	1.78027600
B	-0.56559200	2.28986600	1.44619400
B	-2.34318500	2.64958300	-0.81233300
B	-1.01950900	1.73472200	-0.14368400
B	-1.25339400	4.92957200	0.56014800
B	-1.71826600	4.30204200	-1.03398700
H	-3.80119000	4.34289000	0.53509000
B	0.06981600	3.92993800	1.20222700
H	-1.92362000	3.96316600	2.89202600
B	0.44261200	2.67666000	0.00341000
H	-0.13868600	1.55856700	2.27688400
B	-0.67389200	2.91831600	-1.39957500
H	-3.16738500	2.16190000	-1.51705000
H	-1.33139400	6.09043500	0.81586700
B	-0.00237500	4.31553700	-0.54188400
H	-2.12435300	5.00860400	-1.90198000
H	0.92779800	4.36918400	1.90183900
H	-0.34917900	2.61328000	-2.49779800
H	0.80859700	5.01870000	-1.05678700
B	-2.27810000	2.27245100	0.94127500
I	-1.56151400	-1.02307400	-0.23555200
C	0.30765600	-1.65012000	0.61424200
C	0.57220300	-1.32912800	1.93726300
C	1.17196000	-2.37970800	-0.18917000
C	1.77992600	-1.76928600	2.47909700
H	-0.13092600	-0.76160400	2.52936800
C	2.36608700	-2.81919000	0.37932700
H	0.93289200	-2.59630600	-1.22084800
C	2.66946600	-2.51194900	1.70470600
H	2.01681100	-1.52777600	3.50856600
H	3.06288800	-3.38687200	-0.22512700
H	3.60638600	-2.84740100	2.13308800
O	-2.09714900	-3.18982700	0.13967100
C	-3.30293300	-3.48036800	-0.27199600
O	-4.05393300	-2.65544400	-0.79688400

C	-3.70648600	-4.91179700	-0.01916600
H	-4.02803200	-4.99661100	1.02344700
H	-4.53774200	-5.18338200	-0.66907100
H	-2.86427900	-5.58726200	-0.17117600
H	-0.64326100	0.62572900	-0.61298600
H	-3.05782600	1.52760900	1.43932700
N	1.80940700	2.06024600	-0.11151700
C	2.14540600	0.99205600	-0.85950500
H	2.52641100	2.40735000	0.51043300
C	3.49313600	0.36750800	-0.64106600
O	1.38315700	0.49956000	-1.71039800
C	4.02011900	-0.42311100	-1.66910100
C	4.19972100	0.48015800	0.56044700
C	5.23752500	-1.07517000	-1.50799100
H	3.46498000	-0.52439700	-2.59294700
C	5.41603700	-0.17954800	0.72504100
H	3.79648400	1.05009800	1.38922700
C	5.93876300	-0.95623700	-0.30772500
H	5.63671600	-1.68013600	-2.31430900
H	5.94817000	-0.09642000	1.66583900
H	6.88426000	-1.47043600	-0.17603500
IRC_TS1_point117			
B	-2.70422300	3.90332400	0.39363600
B	-1.60281300	3.68281400	1.77975000
B	-0.56630600	2.28892800	1.44715100
B	-2.34385300	2.64555100	-0.81217600
B	-1.01946900	1.73277900	-0.14245700
B	-1.25588100	4.92729000	0.55861800
B	-1.72008900	4.29822300	-1.03507300
H	-3.80328900	4.33872600	0.53365400
B	0.06797900	3.92918800	1.20185100
H	-1.92589500	3.96235900	2.89118600
B	0.44197000	2.67522300	0.00418100
H	-0.13909900	1.55851300	2.27841500
B	-0.67465000	2.91511000	-1.39937000
H	-3.16737800	2.15635100	-1.51660000
H	-1.33475400	6.08828500	0.81339500
B	-0.00419300	4.31328700	-0.54267700
H	-2.12651200	5.00381300	-1.90367800
H	0.92541700	4.36974400	1.90127300
H	-0.34951600	2.60913500	-2.49719000
H	0.80634800	5.01659800	-1.05801900
B	-2.27878400	2.26984500	0.94187300
I	-1.56003000	-1.01958300	-0.23574900

C	0.30827700	-1.64901200	0.61465200
C	0.57304600	-1.32811900	1.93761000
C	1.17160600	-2.38005000	-0.18842700
C	1.78016500	-1.76971400	2.47968900
H	-0.12940800	-0.75958200	2.52953300
C	2.36512600	-2.82091000	0.38026400
H	0.93233700	-2.59661600	-1.22006100
C	2.66883100	-2.51368500	1.70557600
H	2.01722600	-1.52828500	3.50913800
H	3.06122300	-3.38966800	-0.22399800
H	3.60528700	-2.85023300	2.13412500
O	-2.09645100	-3.18797700	0.13899100
C	-3.30200300	-3.47898900	-0.27233000
O	-4.05382000	-2.65452400	-0.79708400
C	-3.70522700	-4.91062500	-0.01955000
H	-4.02786900	-4.99529000	1.02274500
H	-4.53572200	-5.18286400	-0.67017900
H	-2.86258200	-5.58581000	-0.17045100
H	-0.63888400	0.62518200	-0.61417600
H	-3.05799300	1.52476900	1.44028200
N	1.80889600	2.05900500	-0.11054800
C	2.14441900	0.99000600	-0.85760500
H	2.52635300	2.40698700	0.51054000
C	3.49263800	0.36614400	-0.64058000
O	1.38113100	0.49624800	-1.70689500
C	4.01856600	-0.42463600	-1.66904400
C	4.20076500	0.47955700	0.55994400
C	5.23648200	-1.07607900	-1.50935700
H	3.46220500	-0.52648500	-2.59209300
C	5.41755800	-0.17963400	0.72315200
H	3.79838800	1.04971400	1.38899600
C	5.93924500	-0.95644600	-0.31005300
H	5.63486900	-1.68112900	-2.31600900
H	5.95092400	-0.09596000	1.66320200
H	6.88514100	-1.47018600	-0.17944800
IRC_TS1_point118			
B	-2.70595100	3.89988000	0.39268300
B	-1.60458800	3.68132300	1.77922300
B	-0.56699100	2.28796800	1.44810600
B	-2.34450800	2.64155100	-0.81206400
B	-1.01962600	1.73041500	-0.14118000
B	-1.25832200	4.92500100	0.55708800
B	-1.72190300	4.29444100	-1.03614700
H	-3.80533800	4.33456200	0.53223100

B	0.06615400	3.92842400	1.20149800
H	-1.92813600	3.96151100	2.89033700
B	0.44143300	2.67377800	0.00500900
H	-0.13948800	1.55845100	2.27994200
B	-0.67544800	2.91195600	-1.39926200
H	-3.16738400	2.15088800	-1.51618000
H	-1.33802600	6.08612800	0.81093200
B	-0.00597200	4.31098400	-0.54348500
H	-2.12862800	4.99905000	-1.90537100
H	0.92309000	4.37024300	1.90070000
H	-0.34981700	2.60495000	-2.49658800
H	0.80417200	5.01440200	-1.05926500
B	-2.27945800	2.26724100	0.94247400
I	-1.55855700	-1.01604900	-0.23594300
C	0.30888800	-1.64788100	0.61504600
C	0.57387000	-1.32712200	1.93795300
C	1.17124200	-2.38034200	-0.18771200
C	1.78039200	-1.77013400	2.48026600
H	-0.12792000	-0.75759400	2.52969900
C	2.36416500	-2.82256700	0.38116100
H	0.93177800	-2.59684300	-1.21930900
C	2.66819800	-2.51537400	1.70640800
H	2.01763000	-1.52879800	3.50969700
H	3.05957100	-3.39236200	-0.22292700
H	3.60420400	-2.85298900	2.13510800
O	-2.09579300	-3.18623600	0.13829700
C	-3.30109600	-3.47768300	-0.27265700
O	-4.05376600	-2.65369000	-0.79729000
C	-3.70402800	-4.90951500	-0.01991500
H	-4.02774400	-4.99402900	1.02206800
H	-4.53380000	-5.18235700	-0.67122700
H	-2.86102900	-5.58448400	-0.16974400
H	-0.63450700	0.62595500	-0.61527800
H	-3.05815900	1.52195500	1.44122700
N	1.80841200	2.05777000	-0.10956300
C	2.14346500	0.98793600	-0.85577500
H	2.52642500	2.40695600	0.51011600
C	3.49218200	0.36481500	-0.64009700
O	1.37919300	0.49285900	-1.70332200
C	4.01707000	-0.42611000	-1.66898600
C	4.20179500	0.47896900	0.55945900
C	5.23547800	-1.07695100	-1.51069800
H	3.45952100	-0.52848500	-2.59125900
C	5.41905200	-0.17972900	0.72131200

H	3.80023000	1.04937000	1.38874400
C	5.93972100	-0.95665100	-0.31232800
H	5.63309100	-1.68206800	-2.31768100
H	5.95360400	-0.09553900	1.66064300
H	6.88600100	-1.46995100	-0.18277400
IRC_TS1_point119			
B	-2.70765800	3.89643800	0.39174800
B	-1.60636400	3.67982100	1.77868400
B	-0.56768400	2.28698200	1.44903900
B	-2.34514700	2.63752300	-0.81191400
B	-1.01955900	1.72848400	-0.13998300
B	-1.26072900	4.92269300	0.55555400
B	-1.72365700	4.29060800	-1.03723800
H	-3.80736400	4.33043400	0.53079500
B	0.06436900	3.92761400	1.20110500
H	-1.93034500	3.96067600	2.88948900
B	0.44079800	2.67229400	0.00575700
H	-0.13989500	1.55834400	2.28145100
B	-0.67617200	2.90871200	-1.39905600
H	-3.16736000	2.14537700	-1.51574100
H	-1.34127600	6.08394900	0.80846500
B	-0.00773200	4.30868600	-0.54428500
H	-2.13070300	4.99426600	-1.90706500
H	0.92077500	4.37071600	1.90011400
H	-0.35012700	2.60078000	-2.49598900
H	0.80200600	5.01222600	-1.06050200
B	-2.28012600	2.26463500	0.94306000
I	-1.55708900	-1.01250400	-0.23613900
C	0.30947200	-1.64674100	0.61544300
C	0.57467100	-1.32613100	1.93829900
C	1.17086600	-2.38058700	-0.18702100
C	1.78061000	-1.77055300	2.48082500
H	-0.12646000	-0.75564700	2.52989300
C	2.36319800	-2.82416800	0.38201700
H	0.93120100	-2.59701800	-1.21858100
C	2.66756200	-2.51702800	1.70720500
H	2.01802600	-1.52933000	3.51024400
H	3.05791300	-3.39498700	-0.22190800
H	3.60312200	-2.85571200	2.13604600
O	-2.09515900	-3.18448100	0.13756300
C	-3.30023200	-3.47643900	-0.27299700
O	-4.05375900	-2.65294400	-0.79749700
C	-3.70285100	-4.90848100	-0.02025800
H	-4.02762600	-4.99282100	1.02141900

H	-4.53189300	-5.18197300	-0.67225500
H	-2.85944000	-5.58319500	-0.16899600
H	-0.63012200	0.62518900	-0.61672300
H	-3.05833500	1.51914200	1.44217300
N	1.80794000	2.05654600	-0.10862900
C	2.14251500	0.98587500	-0.85383900
H	2.52644700	2.40676000	0.50999500
C	3.49173300	0.36350200	-0.63961000
O	1.37715500	0.48940100	-1.69965000
C	4.01560400	-0.42754400	-1.66893400
C	4.20282100	0.47838100	0.55899400
C	5.23449800	-1.07779100	-1.51202800
H	3.45687900	-0.53043900	-2.59043800
C	5.42052700	-0.17983600	0.71950400
H	3.80206500	1.04897900	1.38853900
C	5.94018900	-0.95686000	-0.31457200
H	5.63134600	-1.68296700	-2.31934200
H	5.95625600	-0.09515400	1.65811800
H	6.88683800	-1.46973900	-0.18606500
IRC_TS1_point120			
B	-2.70932200	3.89300300	0.39078200
B	-1.60807700	3.67830400	1.77814700
B	-0.56833400	2.28598100	1.44997400
B	-2.34576300	2.63353400	-0.81182300
B	-1.01974600	1.72597400	-0.13871600
B	-1.26308900	4.92038000	0.55402200
B	-1.72541000	4.28682700	-1.03831200
H	-3.80933500	4.32630100	0.52937200
B	0.06259300	3.92680400	1.20075100
H	-1.93251900	3.95979700	2.88863000
B	0.44031100	2.67081800	0.00658700
H	-0.14026700	1.55823900	2.28295700
B	-0.67694600	2.90554100	-1.39898300
H	-3.16734200	2.13996800	-1.51533800
H	-1.34443100	6.08176700	0.80600900
B	-0.00945000	4.30633400	-0.54510200
H	-2.13272900	4.98952100	-1.90875200
H	0.91851800	4.37113800	1.89952500
H	-0.35038600	2.59658000	-2.49540500
H	0.79991900	5.00995400	-1.06175100
B	-2.28077900	2.26203900	0.94365100
I	-1.55563300	-1.00891500	-0.23633200
C	0.31004700	-1.64557300	0.61582000
C	0.57545600	-1.32515400	1.93864100

C	1.17048100	-2.38078800	-0.18635100
C	1.78082100	-1.77096200	2.48137100
H	-0.12502900	-0.75373400	2.53008500
C	2.36223200	-2.82571300	0.38283700
H	0.93062000	-2.59711700	-1.21788300
C	2.66693000	-2.51863700	1.70796700
H	2.01841700	-1.52985800	3.51077800
H	3.05627200	-3.39751400	-0.22094300
H	3.60206300	-2.85835500	2.13693100
O	-2.09456400	-3.18289000	0.13681900
C	-3.29938200	-3.47527700	-0.27332300
O	-4.05381200	-2.65228100	-0.79771300
C	-3.70175400	-4.90750700	-0.02058600
H	-4.02756400	-4.99167300	1.02079200
H	-4.53010500	-5.18158600	-0.67322900
H	-2.85801700	-5.58203700	-0.16827600
H	-0.62567000	0.62639600	-0.61799400
H	-3.05849500	1.51635500	1.44309500
N	1.80750700	2.05535600	-0.10769200
C	2.14159900	0.98378800	-0.85197000
H	2.52657600	2.40680000	0.50954200
C	3.49132500	0.36222700	-0.63911900
O	1.37521600	0.48589200	-1.69594200
C	4.01418500	-0.42892200	-1.66888100
C	4.20383300	0.47781100	0.55854600
C	5.23354400	-1.07859600	-1.51333500
H	3.45431900	-0.53229700	-2.58963700
C	5.42197000	-0.17995000	0.71774200
H	3.80384200	1.04862300	1.38832100
C	5.94064200	-0.95706500	-0.31676700
H	5.62965800	-1.68381600	-2.32097600
H	5.95882800	-0.09480900	1.65567100
H	6.88764400	-1.46954500	-0.18926800

IRC_TS1_point121

B	-2.71096300	3.88956200	0.38984300
B	-1.60980000	3.67677000	1.77759500
B	-0.56899600	2.28495200	1.45088500
B	-2.34635800	2.62951300	-0.81168400
B	-1.01962100	1.72410900	-0.13754400
B	-1.26541700	4.91804600	0.55248800
B	-1.72708400	4.28298200	-1.03941000
H	-3.81128700	4.32218500	0.52793100
B	0.06086600	3.92594100	1.20034200

H	-1.93466600	3.95892200	2.88777200
B	0.43968600	2.66930600	0.00731000
H	-0.14065000	1.55808000	2.28444200
B	-0.67761500	2.90226600	-1.39876500
H	-3.16727900	2.13448800	-1.51491900
H	-1.34758000	6.07955700	0.80355000
B	-0.01114900	4.30400200	-0.54590400
H	-2.13471600	4.98473900	-1.91044200
H	0.91626900	4.37153300	1.89892500
H	-0.35065100	2.59238300	-2.49480700
H	0.79783800	5.00771400	-1.06298800
B	-2.28141400	2.25942100	0.94421400
I	-1.55417700	-1.00532100	-0.23652700
C	0.31059500	-1.64442100	0.61621800
C	0.57621900	-1.32418200	1.93899400
C	1.17007900	-2.38094800	-0.18570600
C	1.78102400	-1.77136800	2.48190100
H	-0.12361900	-0.75185600	2.53031500
C	2.36125700	-2.82720600	0.38361800
H	0.93001100	-2.59717400	-1.21720400
C	2.66629500	-2.52021100	1.70869400
H	2.01880500	-1.53040100	3.51129800
H	3.05461200	-3.39998300	-0.22002800
H	3.60100300	-2.86096600	2.13777000
O	-2.09398800	-3.18124600	0.13602300
C	-3.29859200	-3.47418700	-0.27367500
O	-4.05389200	-2.65171200	-0.79792100
C	-3.70069600	-4.90662400	-0.02089800
H	-4.02754900	-4.99059000	1.02017800
H	-4.52835600	-5.18131200	-0.67419200
H	-2.85661500	-5.58096600	-0.16751200
H	-0.62138500	0.62514200	-0.61957100
H	-3.05866400	1.51355300	1.44402000
N	1.80708100	2.05417400	-0.10679200
C	2.14067500	0.98174000	-0.85000900
H	2.52668600	2.40678700	0.50919200
C	3.49091300	0.36097800	-0.63863900
O	1.37315700	0.48230900	-1.69208400
C	4.01278200	-0.43025800	-1.66883900
C	4.20482900	0.47724700	0.55811200
C	5.23260100	-1.07936800	-1.51463400
H	3.45178100	-0.53410800	-2.58885100
C	5.42338300	-0.18007200	0.71600600
H	3.80559700	1.04824100	1.38813000

C	5.94107300	-0.95727200	-0.31893500
H	5.62798000	-1.68462800	-2.32260400
H	5.96136400	-0.09449600	1.65325000
H	6.88841300	-1.46937400	-0.19244800

IRC_TS1_point122

B	-2.71255700	3.88613400	0.38886100
B	-1.61144600	3.67522700	1.77704900
B	-0.56960000	2.28391600	1.45180000
B	-2.34692000	2.62555100	-0.81162100
B	-1.01982900	1.72141500	-0.13629000
B	-1.26769500	4.91570900	0.55095700
B	-1.72877500	4.27921000	-1.04048300
H	-3.81316600	4.31811000	0.52651300
B	0.05913700	3.92509200	1.19999800
H	-1.93676100	3.95802300	2.88690500
B	0.43926800	2.66780700	0.00814900
H	-0.14099700	1.55793600	2.28592200
B	-0.67836100	2.89907800	-1.39874300
H	-3.16723100	2.12916900	-1.51454200
H	-1.35060000	6.07735300	0.80111300
B	-0.01279800	4.30160500	-0.54673100
H	-2.13663500	4.98004700	-1.91211200
H	0.91408800	4.37188600	1.89832500
H	-0.35085800	2.58822000	-2.49426600
H	0.79584400	5.00539000	-1.06422000
B	-2.28203300	2.25683700	0.94479000
I	-1.55273700	-1.00168200	-0.23671600
C	0.31112600	-1.64321600	0.61657800
C	0.57697000	-1.32323000	1.93933700
C	1.16966600	-2.38107300	-0.18507000
C	1.78122800	-1.77176200	2.48241700
H	-0.12224400	-0.75002800	2.53053900
C	2.36028500	-2.82865100	0.38436800
H	0.92940700	-2.59716700	-1.21654800
C	2.66567100	-2.52174300	1.70939000
H	2.01919800	-1.53093000	3.51180400
H	3.05299100	-3.40234600	-0.21916500
H	3.59998300	-2.86348400	2.13855800
O	-2.09345500	-3.17986600	0.13522900
C	-3.29778800	-3.47318700	-0.27399300
O	-4.05404400	-2.65122200	-0.79814700
C	-3.69973500	-4.90579500	-0.02119700
H	-4.02758200	-4.98955900	1.01959200

H	-4.52672300	-5.18105400	-0.67511400
H	-2.85532800	-5.57997100	-0.16677300
H	-0.61661000	0.62710700	-0.62103000
H	-3.05880600	1.51079200	1.44490100
N	1.80671100	2.05305200	-0.10590200
C	2.13980300	0.97965900	-0.84809100
H	2.52688100	2.40690500	0.50873100
C	3.49054200	0.35976800	-0.63814700
O	1.37119100	0.47872500	-1.68824600
C	4.01142100	-0.43153800	-1.66879700
C	4.20581400	0.47670600	0.55769700
C	5.23167500	-1.08010900	-1.51591200
H	3.44933000	-0.53581900	-2.58809400
C	5.42476200	-0.18019900	0.71431700
H	3.80730400	1.04788400	1.38794300
C	5.94148300	-0.95747600	-0.32105600
H	5.62636500	-1.68539500	-2.32419600
H	5.96381400	-0.09422400	1.65091100
H	6.88914400	-1.46922300	-0.19552300

IRC_TS1_point123

B	-2.71412100	3.88268100	0.38791500
B	-1.61311200	3.67365400	1.77648200
B	-0.57021900	2.28283800	1.45268700
B	-2.34745500	2.62153300	-0.81149700
B	-1.01962000	1.71965000	-0.13514100
B	-1.26994300	4.91335000	0.54942600
B	-1.73035400	4.27534600	-1.04159200
H	-3.81505500	4.31393700	0.52505100
B	0.05747500	3.92417600	1.19957300
H	-1.93886700	3.95707300	2.88603400
B	0.43865700	2.66628700	0.00884300
H	-0.14133900	1.55772300	2.28738400
B	-0.67895200	2.89578300	-1.39850400
H	-3.16709000	2.12366900	-1.51414200
H	-1.35368600	6.07510700	0.79865600
B	-0.01443000	4.29924700	-0.54752800
H	-2.13854600	4.97522000	-1.91381700
H	0.91190400	4.37220200	1.89772200
H	-0.35105100	2.58394800	-2.49364100
H	0.79385800	5.00307500	-1.06546900
B	-2.28261600	2.25419100	0.94532000
I	-1.55128900	-0.99804300	-0.23691000
C	0.31164000	-1.64207700	0.61699800

C	0.57769700	-1.32227000	1.93970600
C	1.16923300	-2.38116100	-0.18446600
C	1.78142400	-1.77214900	2.48291900
H	-0.12086500	-0.74819000	2.53080700
C	2.35929600	-2.83004300	0.38507800
H	0.92874200	-2.59712400	-1.21590700
C	2.66503800	-2.52323800	1.71004700
H	2.01959400	-1.53147300	3.51229700
H	3.05130300	-3.40469100	-0.21834600
H	3.59893800	-2.86600100	2.13929900
O	-2.09293300	-3.17835000	0.13437400
C	-3.29708300	-3.47227400	-0.27436000
O	-4.05419000	-2.65083200	-0.79834600
C	-3.69884300	-4.90508200	-0.02149200
H	-4.02775900	-4.98862000	1.01898900
H	-4.52519000	-5.18084400	-0.67603800
H	-2.85423000	-5.57920100	-0.16601100
H	-0.61268600	0.62499100	-0.62255400
H	-3.05894000	1.50797500	1.44579900
N	1.80633700	2.05193900	-0.10503900
C	2.13889300	0.97765300	-0.84612400
H	2.52709100	2.40710900	0.50812300
C	3.49015400	0.35860100	-0.63767500
O	1.36912700	0.47505200	-1.68420900
C	4.01005700	-0.43276700	-1.66876500
C	4.20676700	0.47617900	0.55728800
C	5.23074000	-1.08080800	-1.51718500
H	3.44684900	-0.53748700	-2.58733000
C	5.42609800	-0.18032900	0.71264900
H	3.80897000	1.04753300	1.38775900
C	5.94185800	-0.95767500	-0.32315700
H	5.62470700	-1.68612000	-2.32580200
H	5.96623100	-0.09397100	1.64858000
H	6.88982400	-1.46908700	-0.19861900

IRC_TS1_point124

B	-2.71563500	3.87926500	0.38691500
B	-1.61468300	3.67208100	1.77592800
B	-0.57077200	2.28176500	1.45357300
B	-2.34795100	2.61759700	-0.81146800
B	-1.01981900	1.71676600	-0.13392500
B	-1.27212600	4.91099000	0.54790200
B	-1.73197500	4.27159200	-1.04265800
H	-3.81683400	4.30993500	0.52363300

B	0.05580000	3.92328800	1.19924600
H	-1.94087700	3.95615900	2.88515700
B	0.43831100	2.66476700	0.00969400
H	-0.14166600	1.55753600	2.28883200
B	-0.67966800	2.89258300	-1.39854000
H	-3.16701600	2.11845200	-1.51379400
H	-1.35655300	6.07288700	0.79623900
B	-0.01600200	4.29680900	-0.54835900
H	-2.14034700	4.97060200	-1.91546000
H	0.90980200	4.37248800	1.89711700
H	-0.35120900	2.57987100	-2.49316800
H	0.79196200	5.00070800	-1.06667700
B	-2.28319500	2.25162900	0.94587300
I	-1.54986600	-0.99435600	-0.23709300
C	0.31211800	-1.64083300	0.61734200
C	0.57841700	-1.32134800	1.94005400
C	1.16878900	-2.38122000	-0.18385500
C	1.78162600	-1.77252700	2.48340600
H	-0.11954500	-0.74645100	2.53106900
C	2.35831800	-2.83139500	0.38576100
H	0.92811200	-2.59702900	-1.21528400
C	2.66442900	-2.52469200	1.71067600
H	2.01999800	-1.53200200	3.51277500
H	3.04970200	-3.40690900	-0.21757500
H	3.59796100	-2.86839900	2.13999000
O	-2.09246200	-3.17724600	0.13353200
C	-3.29632100	-3.47146000	-0.27466300
O	-4.05442600	-2.65052200	-0.79857500
C	-3.69805100	-4.90441600	-0.02176900
H	-4.02790200	-4.98771400	1.01844400
H	-4.52373300	-5.18074600	-0.67692900
H	-2.85307400	-5.57835800	-0.16524900
H	-0.60716600	0.62795600	-0.62439700
H	-3.05905900	1.50524800	1.44662800
N	1.80604000	2.05090100	-0.10419500
C	2.13807300	0.97561500	-0.84415900
H	2.52735100	2.40729700	0.50768500
C	3.48980900	0.35746600	-0.63719200
O	1.36709700	0.47144400	-1.68024300
C	4.00873500	-0.43394400	-1.66873900
C	4.20770900	0.47567300	0.55690500
C	5.22982300	-1.08148400	-1.51843300
H	3.44448900	-0.53905400	-2.58662200
C	5.42739400	-0.18046700	0.71103100

H	3.81060300	1.04718000	1.38760800
C	5.94220600	-0.95787600	-0.32520200
H	5.62314400	-1.68681300	-2.32734900
H	5.96855200	-0.09376600	1.64634500
H	6.89046800	-1.46897300	-0.20157100

IRC_TS1_point125

B	-2.71710900	3.87580300	0.38596000
B	-1.61627400	3.67046000	1.77535000
B	-0.57133800	2.28062700	1.45442600
B	-2.34841100	2.61358400	-0.81137300
B	-1.01956800	1.71500600	-0.13280500
B	-1.27428100	4.90861000	0.54638700
B	-1.73345200	4.26772600	-1.04377200
H	-3.81867600	4.30562600	0.52213200
B	0.05421200	3.92231300	1.19882000
H	-1.94296600	3.95508700	2.88427200
B	0.43773600	2.66324500	0.01036400
H	-0.14196700	1.55725600	2.29026500
B	-0.68017900	2.88928000	-1.39829800
H	-3.16676000	2.11285800	-1.51340200
H	-1.35961600	6.07060300	0.79378000
B	-0.01755500	4.29443000	-0.54914800
H	-2.14220200	4.96567300	-1.91721500
H	0.90768800	4.37271000	1.89652800
H	-0.35131000	2.57546500	-2.49250100
H	0.79008500	4.99829100	-1.06796100
B	-2.28371700	2.24896500	0.94636500
I	-1.54841800	-0.99066300	-0.23728300
C	0.31259800	-1.63971600	0.61779400
C	0.57910900	-1.32040500	1.94044700
C	1.16831900	-2.38124400	-0.18328300
C	1.78182300	-1.77289000	2.48388200
H	-0.11817200	-0.74462600	2.53138100
C	2.35731600	-2.83268900	0.38640200
H	0.92736600	-2.59690700	-1.21466500
C	2.66380600	-2.52609900	1.71126200
H	2.02041600	-1.53254400	3.51324300
H	3.04796100	-3.40917800	-0.21684000
H	3.59692600	-2.87084600	2.14063800
O	-2.09199000	-3.17593000	0.13262900
C	-3.29569100	-3.47075900	-0.27503300
O	-4.05462300	-2.65032200	-0.79875800
C	-3.69738600	-4.90389000	-0.02205900

H	-4.02831500	-4.98694600	1.01784300
H	-4.52251500	-5.18053800	-0.67780800
H	-2.85239800	-5.57796800	-0.16454900
H	-0.60367600	0.62516000	-0.62576600
H	-3.05912800	1.50239500	1.44748400
N	1.80572200	2.04988100	-0.10337500
C	2.13717500	0.97366500	-0.84219200
H	2.52767900	2.40775500	0.50680100
C	3.48943400	0.35639700	-0.63673200
O	1.36503000	0.46772400	-1.67605100
C	4.00739300	-0.43505300	-1.66871900
C	4.20860300	0.47519300	0.55652200
C	5.22887700	-1.08210200	-1.51968200
H	3.44201800	-0.54059300	-2.58586200
C	5.42863300	-0.18060100	0.70943400
H	3.81217200	1.04687900	1.38742600
C	5.94250200	-0.95806200	-0.32723500
H	5.62146700	-1.68745100	-2.32893800
H	5.97085500	-0.09355700	1.64409100
H	6.89104700	-1.46885800	-0.20460700

IRC_TS1_point126

B	-2.71853100	3.87239900	0.38495400
B	-1.61776600	3.66883800	1.77478800
B	-0.57184600	2.27949200	1.45526500
B	-2.34884200	2.60967300	-0.81138000
B	-1.01970300	1.71208900	-0.13166400
B	-1.27635400	4.90622300	0.54488500
B	-1.73498100	4.26399100	-1.04482900
H	-3.82035800	4.30165400	0.52071000
B	0.05260700	3.92136000	1.19850000
H	-1.94490000	3.95411000	2.88338700
B	0.43742500	2.66170300	0.01119800
H	-0.14227800	1.55698700	2.29166200
B	-0.68084600	2.88607700	-1.39836800
H	-3.16664800	2.10771300	-1.51309000
H	-1.36234100	6.06835100	0.79139200
B	-0.01904300	4.29195700	-0.54997300
H	-2.14389300	4.96110500	-1.91883100
H	0.90566900	4.37289600	1.89592400
H	-0.35142300	2.57144900	-2.49208300
H	0.78830000	4.99586000	-1.06915300
B	-2.28425100	2.24641000	0.94687300
I	-1.54699700	-0.98691200	-0.23746100

C	0.31302300	-1.63847300	0.61814400
C	0.57979000	-1.31952500	1.94081200
C	1.16783800	-2.38125800	-0.18269500
C	1.78202500	-1.77324900	2.48434300
H	-0.11690500	-0.74298200	2.53169200
C	2.35633400	-2.83394900	0.38702200
H	0.92668700	-2.59675500	-1.21406400
C	2.66322000	-2.52745800	1.71182100
H	2.02083500	-1.53306900	3.51369600
H	3.04636200	-3.41127100	-0.21615200
H	3.59600200	-2.87310400	2.14122700
O	-2.09156800	-3.17511100	0.13174000
C	-3.29498300	-3.47017800	-0.27532100
O	-4.05491200	-2.65022200	-0.79896800
C	-3.69681200	-4.90343500	-0.02231400
H	-4.02857700	-4.98622300	1.01734900
H	-4.52134000	-5.18057400	-0.67862900
H	-2.85150000	-5.57739300	-0.16382900
H	-0.59758500	0.62837500	-0.62805000
H	-3.05922500	1.49968300	1.44824900
N	1.80548800	2.04892400	-0.10256800
C	2.13638400	0.97169400	-0.84019700
H	2.52800200	2.40804600	0.50632300
C	3.48909300	0.35534500	-0.63627300
O	1.36291700	0.46410600	-1.67193100
C	4.00609500	-0.43612300	-1.66871900
C	4.20947200	0.47472500	0.55616200
C	5.22795300	-1.08270700	-1.52090000
H	3.43972400	-0.54201900	-2.58520600
C	5.42981700	-0.18074800	0.70789200
H	3.81369800	1.04653600	1.38729700
C	5.94276300	-0.95825700	-0.32920100
H	5.61993000	-1.68806600	-2.33044400
H	5.97302200	-0.09341500	1.64195600
H	6.89157600	-1.46877800	-0.20744500
IRC_TS1_point127			
B	-2.71990600	3.86894500	0.38398500
B	-1.61926200	3.66716000	1.77420300
B	-0.57235100	2.27828500	1.45606800
B	-2.34923100	2.60569300	-0.81134000
B	-1.01947400	1.71012600	-0.13059400
B	-1.27839400	4.90381600	0.54339700
B	-1.73637000	4.26016000	-1.04592900
H	-3.82210200	4.29733500	0.51920900

B	0.05109000	3.92032000	1.19809200
H	-1.94691000	3.95293300	2.88249800
B	0.43692700	2.66016800	0.01186700
H	-0.14253600	1.55661700	2.29302500
B	-0.68131600	2.88279100	-1.39819600
H	-3.16633200	2.10218000	-1.51274500
H	-1.36526800	6.06603500	0.78897900
B	-0.02050400	4.28954000	-0.55075900
H	-2.14564000	4.95621300	-1.92057000
H	0.90366100	4.37298900	1.89534000
H	-0.35145000	2.56706200	-2.49146000
H	0.78655600	4.99335900	-1.07042700
B	-2.28472200	2.24374800	0.94732000
I	-1.54554500	-0.98313800	-0.23764600
C	0.31344900	-1.63737400	0.61861000
C	0.58044300	-1.31863000	1.94122500
C	1.16732500	-2.38125200	-0.18213800
C	1.78222600	-1.77359000	2.48479500
H	-0.11557900	-0.74123900	2.53204900
C	2.35532900	-2.83515500	0.38760300
H	0.92587800	-2.59659200	-1.21345800
C	2.66262600	-2.52876300	1.71233800
H	2.02127800	-1.53358800	3.51413400
H	3.04462600	-3.41341100	-0.21550200
H	3.59503400	-2.87538600	2.14176700
O	-2.09114200	-3.17414800	0.13080000
C	-3.29439700	-3.46973900	-0.27566400
O	-4.05515600	-2.65024300	-0.79912900
C	-3.69642200	-4.90313100	-0.02259400
H	-4.02916500	-4.98567500	1.01678800
H	-4.52052400	-5.18040000	-0.67941400
H	-2.85125300	-5.57739100	-0.16325500
H	-0.59387600	0.62610300	-0.62958200
H	-3.05924900	1.49682700	1.44902900
N	1.80523800	2.04800200	-0.10178500
C	2.13551200	0.96980400	-0.83821500
H	2.52842200	2.40868300	0.50531500
C	3.48872000	0.35436600	-0.63583700
O	1.36079700	0.46039400	-1.66761000
C	4.00477200	-0.43711600	-1.66872700
C	4.21028500	0.47429300	0.55579800
C	5.22699100	-1.08324800	-1.52211900
H	3.43731000	-0.54340300	-2.58449800
C	5.43093300	-0.18088200	0.70637200

H	3.81513500	1.04626900	1.38711900
C	5.94296200	-0.95843000	-0.33115000
H	5.61827100	-1.68861600	-2.33199300
H	5.97514800	-0.09325900	1.63981200
H	6.89202800	-1.46869500	-0.21035600

IRC_TS1_point128

B	-2.72122400	3.86554500	0.38298200
B	-1.62066800	3.66547400	1.77362900
B	-0.57280900	2.27707100	1.45684500
B	-2.34959400	2.60180200	-0.81138500
B	-1.01950200	1.70733400	-0.12954300
B	-1.28034800	4.90139800	0.54192800
B	-1.73778200	4.25643800	-1.04698100
H	-3.82368100	4.29335100	0.51779000
B	0.04957400	3.91928300	1.19776100
H	-1.94875700	3.95184200	2.88161300
B	0.43662500	2.65861500	0.01264800
H	-0.14279800	1.55623100	2.29433200
B	-0.68189800	2.87958800	-1.39826900
H	-3.16615400	2.09707900	-1.51248400
H	-1.36786300	6.06374000	0.78664600
B	-0.02190300	4.28705000	-0.55157100
H	-2.14721900	4.95167900	-1.92215800
H	0.90175000	4.37303300	1.89473800
H	-0.35149400	2.56307200	-2.49106900
H	0.78489800	4.99086600	-1.07160100
B	-2.28519500	2.24117000	0.94776800
I	-1.54410900	-0.97931000	-0.23781800
C	0.31382300	-1.63618600	0.61899600
C	0.58107500	-1.31779800	1.94161800
C	1.16679800	-2.38125100	-0.18156900
C	1.78242800	-1.77392600	2.48523300
H	-0.11436500	-0.73968300	2.53241200
C	2.35434200	-2.83632900	0.38816400
H	0.92512400	-2.59641900	-1.21286800
C	2.66206700	-2.53001400	1.71282700
H	2.02172000	-1.53408700	3.51455600
H	3.04302700	-3.41537400	-0.21490200
H	3.59418000	-2.87746300	2.14224000
O	-2.09075800	-3.17362800	0.12986600
C	-3.29375600	-3.46944300	-0.27593900
O	-4.05546400	-2.65037900	-0.79929800

C	-3.69614000	-4.90293300	-0.02284200
H	-4.02964500	-4.98520100	1.01632500
H	-4.51978000	-5.18047900	-0.68014700
H	-2.85084400	-5.57727600	-0.16265700
H	-0.58789100	0.62852300	-0.63204300
H	-3.05931100	1.49410400	1.44972500
N	1.80505700	2.04713600	-0.10100900
C	2.13472000	0.96791700	-0.83620500
H	2.52881900	2.40915400	0.50468200
C	3.48836200	0.35340700	-0.63541400
O	1.35860300	0.45678200	-1.66331600
C	4.00347900	-0.43806900	-1.66875900
C	4.21105700	0.47387500	0.55544900
C	5.22604100	-1.08377400	-1.52330900
H	3.43506100	-0.54467500	-2.58390200
C	5.43198000	-0.18102300	0.70490200
H	3.81650800	1.04596000	1.38698200
C	5.94311700	-0.95861000	-0.33303500
H	5.61673800	-1.68914100	-2.33346300
H	5.97712000	-0.09316700	1.63778400
H	6.89241400	-1.46864900	-0.21307300

IRC_TS1_point129

B	-2.72248600	3.86211600	0.38200400
B	-1.62205100	3.66374400	1.77304200
B	-0.57324700	2.27579900	1.45758600
B	-2.34991000	2.59787700	-0.81141300
B	-1.01929700	1.70512800	-0.12855700
B	-1.28225200	4.89896700	0.54047600
B	-1.73907900	4.25266600	-1.04805700
H	-3.82527800	4.28913000	0.51632300
B	0.04813700	3.91818000	1.19737800
H	-1.95063300	3.95059300	2.88073000
B	0.43621900	2.65707200	0.01332100
H	-0.14300700	1.55576200	2.29559700
B	-0.68233600	2.87634000	-1.39820100
H	-3.16582600	2.09173800	-1.51221400
H	-1.37056200	6.06140100	0.78431200
B	-0.02326000	4.28459400	-0.55235600
H	-2.14881100	4.94694400	-1.92382200
H	0.89987700	4.37299000	1.89415400
H	-0.35145900	2.55884300	-2.49055400
H	0.78330100	4.98831300	-1.07282600
B	-2.28560800	2.23852800	0.94816800

I	-1.54265100	-0.97545100	-0.23799500
C	0.31418600	-1.63511400	0.61946600
C	0.58168100	-1.31696600	1.94204600
C	1.16623800	-2.38124500	-0.18102000
C	1.78262900	-1.77424300	2.48565800
H	-0.11312100	-0.73807100	2.53280700
C	2.35334000	-2.83745200	0.38868800
H	0.92426600	-2.59624900	-1.21227300
C	2.66150800	-2.53120700	1.71327400
H	2.02218300	-1.53456800	3.51496000
H	3.04134000	-3.41734600	-0.21434100
H	3.59331400	-2.87951700	2.14265900
O	-2.09037700	-3.17312100	0.12889700
C	-3.29320300	-3.46931100	-0.27624400
O	-4.05573400	-2.65063900	-0.79942600
C	-3.69606700	-4.90288800	-0.02311400
H	-4.03042600	-4.98490200	1.01581100
H	-4.51939600	-5.18039300	-0.68085100
H	-2.85102300	-5.57766600	-0.16219800
H	-0.58347300	0.62728200	-0.63396200
H	-3.05930100	1.49128500	1.45041500
N	1.80488000	2.04631900	-0.10025400
C	2.13387300	0.96610800	-0.83420400
H	2.52930300	2.40989600	0.50367200
C	3.48797600	0.35251600	-0.63501300
O	1.35638700	0.45313900	-1.65887400
C	4.00216700	-0.43895000	-1.66880200
C	4.21177200	0.47349600	0.55509800
C	5.22505900	-1.08424200	-1.52449200
H	3.43273600	-0.54588900	-2.58328100
C	5.43295600	-0.18114900	0.70346100
H	3.81779100	1.04571800	1.38680700
C	5.94320800	-0.95876800	-0.33489200
H	5.61512000	-1.68960700	-2.33495300
H	5.97902400	-0.09306500	1.63577200
H	6.89272100	-1.46860200	-0.21581300
IRC_TS1_point130			
B	-2.72368400	3.85872400	0.38101000
B	-1.62335300	3.66199700	1.77246300
B	-0.57364100	2.27451300	1.45829900
B	-2.35019200	2.59401700	-0.81150200
B	-1.01922400	1.70244800	-0.12761000
B	-1.28407000	4.89652600	0.53904700
B	-1.74036200	4.24897200	-1.04909700

H	-3.82674100	4.28513000	0.51491300
B	0.04672400	3.91706400	1.19704600
H	-1.95238100	3.94938200	2.87985300
B	0.43594600	2.65552200	0.01405600
H	-0.14320400	1.55525800	2.29680200
B	-0.68282500	2.87314900	-1.39829300
H	-3.16557000	2.08668900	-1.51200600
H	-1.37301400	6.05907200	0.78204500
B	-0.02455500	4.28209300	-0.55315300
H	-2.15026700	4.94245400	-1.92537700
H	0.89809500	4.37288900	1.89355900
H	-0.35142000	2.55488800	-2.49019800
H	0.78178700	4.98576000	-1.07398100
B	-2.28600300	2.23593800	0.94855700
I	-1.54120500	-0.97155100	-0.23816200
C	0.31450200	-1.63399800	0.61988800
C	0.58226000	-1.31618400	1.94246300
C	1.16565600	-2.38124600	-0.18046700
C	1.78282700	-1.77455000	2.48606700
H	-0.11196600	-0.73659800	2.53321400
C	2.35234800	-2.83854000	0.38918900
H	0.92342500	-2.59608200	-1.21168800
C	2.66097500	-2.53234400	1.71368900
H	2.02264500	-1.53502800	3.51534600
H	3.03974300	-3.41918100	-0.21382500
H	3.59253300	-2.88140200	2.14301600
O	-2.09002800	-3.17298300	0.12793000
C	-3.29262700	-3.46934100	-0.27649800
O	-4.05603300	-2.65101900	-0.79954600
C	-3.69614600	-4.90297200	-0.02337200
H	-4.03121400	-4.98470500	1.01535500
H	-4.51915900	-5.18048000	-0.68152800
H	-2.85121300	-5.57808700	-0.16174500
H	-0.57753800	0.62893400	-0.63641100
H	-3.05929900	1.48854700	1.45103400
N	1.80476000	2.04556100	-0.09950500
C	2.13307800	0.96433000	-0.83219000
H	2.52978200	2.41056000	0.50288700
C	3.48759200	0.35165900	-0.63462900
O	1.35410300	0.44959500	-1.65443100
C	4.00087000	-0.43978200	-1.66886600
C	4.21243900	0.47313900	0.55475600
C	5.22407400	-1.08468400	-1.52565000
H	3.43052200	-0.54700600	-2.58274200

C	5.43385800	-0.18127400	0.70206600
H	3.81900500	1.04546200	1.38665700
C	5.94324600	-0.95892500	-0.33669100
H	5.61357800	-1.69004200	-2.33638000
H	5.98079200	-0.09300600	1.63385300
H	6.89295600	-1.46858100	-0.21840400
IRC_TS1_point131			
B	-2.72481300	3.85532800	0.38003400
B	-1.62461000	3.66021500	1.77187700
B	-0.57400400	2.27317700	1.45897800
B	-2.35042300	2.59015600	-0.81159500
B	-1.01900600	1.70007900	-0.12671900
B	-1.28581800	4.89408100	0.53764400
B	-1.74154600	4.24527100	-1.05014200
H	-3.82818100	4.28099200	0.51348300
B	0.04538500	3.91589500	1.19668800
H	-1.95411500	3.94805300	2.87897900
B	0.43562300	2.65397800	0.01472100
H	-0.14335100	1.55468500	2.29796400
B	-0.68322000	2.86994300	-1.39831400
H	-3.16521600	2.08153800	-1.51180600
H	-1.37547900	6.05671700	0.77980100
B	-0.02579700	4.27960800	-0.55393100
H	-2.15169900	4.93787500	-1.92696200
H	0.89637400	4.37269900	1.89297600
H	-0.35132200	2.55081600	-2.48978500
H	0.78035300	4.98315100	-1.07516200
B	-2.28634000	2.23330900	0.94890300
I	-1.53974700	-0.96761700	-0.23833200
C	0.31479200	-1.63297000	0.62036400
C	0.58281000	-1.31541400	1.94290000
C	1.16504300	-2.38125000	-0.17992900
C	1.78302200	-1.77483600	2.48646100
H	-0.11080900	-0.73511000	2.53364200
C	2.35135000	-2.83957800	0.38965600
H	0.92250600	-2.59592500	-1.21110300
C	2.66044900	-2.53341800	1.71406500
H	2.02312000	-1.53546300	3.51571100
H	3.03810300	-3.42098700	-0.21335000
H	3.59176100	-2.88322700	2.14331700
O	-2.08968800	-3.17298400	0.12694800
C	-3.29211600	-3.46955300	-0.27675700
O	-4.05629700	-2.65152200	-0.79962800
C	-3.69644800	-4.90321600	-0.02365000

H	-4.03226800	-4.98468200	1.01486700
H	-4.51926600	-5.18047000	-0.68218100
H	-2.85190600	-5.57893400	-0.16141100
H	-0.57240100	0.62837900	-0.63850600
H	-3.05924000	1.48575700	1.45163000
N	1.80465900	2.04486100	-0.09877300
C	2.13225200	0.96263300	-0.83018200
H	2.53032700	2.41141200	0.50187800
C	3.48718500	0.35086900	-0.63426800
O	1.35178400	0.44607800	-1.64989100
C	3.99956100	-0.44054400	-1.66894200
C	4.21304900	0.47282300	0.55441600
C	5.22306200	-1.08507400	-1.52679200
H	3.42827300	-0.54805400	-2.58220200
C	5.43468500	-0.18138300	0.70070600
H	3.82013300	1.04526000	1.38648400
C	5.94322200	-0.95906200	-0.33845100
H	5.61198500	-1.69042400	-2.33780500
H	5.98247400	-0.09294300	1.63197000
H	6.89311300	-1.46856300	-0.22097600

IRC_TS1_point132

B	-2.72587000	3.85196900	0.37905200
B	-1.62578600	3.65841400	1.77129400
B	-0.57432300	2.27181900	1.45962100
B	-2.35061100	2.58635800	-0.81173700
B	-1.01884900	1.69739900	-0.12587100
B	-1.28747500	4.89163600	0.53626800
B	-1.74269200	4.24164200	-1.05115600
H	-3.82950600	4.27700100	0.51209900
B	0.04408500	3.91470600	1.19636100
H	-1.95573900	3.94672200	2.87811200
B	0.43539400	2.65243200	0.01541400
H	-0.14347400	1.55407200	2.29906700
B	-0.68363100	2.86678700	-1.39844300
H	-3.16489400	2.07660800	-1.51165600
H	-1.37774500	6.05437100	0.77762200
B	-0.02697400	4.27710000	-0.55471400
H	-2.15301600	4.93347400	-1.92846700
H	0.89474600	4.37243800	1.89238700
H	-0.35120900	2.54694000	-2.48948200
H	0.77900900	4.98053400	-1.07629500
B	-2.28664400	2.23071100	0.94922300
I	-1.53829800	-0.96365000	-0.23849600
C	0.31503800	-1.63193100	0.62081200

C	0.58333000	-1.31468500	1.94332900
C	1.16440600	-2.38126300	-0.17939300
C	1.78321100	-1.77510800	2.48683800
H	-0.10972200	-0.73372200	2.53407800
C	2.35036100	-2.84057200	0.39009500
H	0.92158500	-2.59577700	-1.21052700
C	2.65994400	-2.53443100	1.71440700
H	2.02359300	-1.53587300	3.51605500
H	3.03652600	-3.42267600	-0.21291800
H	3.59105400	-2.88490600	2.14356100
O	-2.08937600	-3.17333000	0.12597600
C	-3.29160100	-3.46994500	-0.27697400
O	-4.05656100	-2.65214400	-0.79969000
C	-3.69693800	-4.90360400	-0.02392700
H	-4.03340900	-4.98478800	1.01441100
H	-4.51958700	-5.18057000	-0.68281800
H	-2.85274500	-5.57991500	-0.16111600
H	-0.56625000	0.62960000	-0.64095500
H	-3.05917300	1.48302500	1.45216300
N	1.80460800	2.04422900	-0.09804900
C	2.13146000	0.96098700	-0.82817100
H	2.53088200	2.41225500	0.50099200
C	3.48677200	0.35012400	-0.63392500
O	1.34940100	0.44266800	-1.64533000
C	3.99826100	-0.44125000	-1.66903600
C	4.21360700	0.47253700	0.55408500
C	5.22204100	-1.08543100	-1.52790800
H	3.42609900	-0.54901200	-2.58172300
C	5.43543800	-0.18148600	0.69939300
H	3.82118800	1.04506500	1.38632500
C	5.94314200	-0.95919200	-0.34015400
H	5.61043700	-1.69077100	-2.33917800
H	5.98403100	-0.09290900	1.63016900
H	6.89319600	-1.46856200	-0.22342600
IRC_TS1_point133			
B	-2.72685400	3.84863000	0.37808700
B	-1.62690200	3.65658700	1.77070600
B	-0.57460700	2.27041800	1.46022000
B	-2.35075300	2.58259100	-0.81189300
B	-1.01859200	1.69487600	-0.12509100
B	-1.28905100	4.88919800	0.53492200
B	-1.74375100	4.23804200	-1.05216400
H	-3.83078400	4.27294800	0.51071500
B	0.04285600	3.91347500	1.19602000

H	-1.95731900	3.94529900	2.87725100
B	0.43514100	2.65089500	0.01605500
H	-0.14355200	1.55339900	2.30011800
B	-0.68397800	2.86364000	-1.39854200
H	-3.16451300	2.07167600	-1.51152600
H	-1.37996500	6.05201900	0.77548100
B	-0.02809200	4.27460600	-0.55548300
H	-2.15428900	4.92906200	-1.92997400
H	0.89319300	4.37209300	1.89180600
H	-0.35105600	2.54303400	-2.48916600
H	0.77775400	4.97786900	-1.07744100
B	-2.28689400	2.22809600	0.94950000
I	-1.53684300	-0.95965600	-0.23865900
C	0.31525000	-1.63096500	0.62129200
C	0.58381800	-1.31397300	1.94376900
C	1.16374200	-2.38127900	-0.17887100
C	1.78339400	-1.77536000	2.48719700
H	-0.10865000	-0.73234000	2.53452500
C	2.34937200	-2.84151500	0.39050100
H	0.92060900	-2.59563700	-1.20995500
C	2.65944800	-2.53538200	1.71471100
H	2.02407100	-1.53625700	3.51637700
H	3.03493500	-3.42431400	-0.21252800
H	3.59036800	-2.88650600	2.14375200
O	-2.08907900	-3.17389300	0.12501000
C	-3.29113800	-3.47052900	-0.27718000
O	-4.05678300	-2.65288600	-0.79971300
C	-3.69765600	-4.90415500	-0.02422200
H	-4.03479100	-4.98506800	1.01393300
H	-4.52024000	-5.18061400	-0.68343400
H	-2.85403200	-5.58127400	-0.16093000
H	-0.56041100	0.62945300	-0.64333600
H	-3.05906300	1.48027600	1.45266200
N	1.80458200	2.04365900	-0.09733800
C	2.13065300	0.95942500	-0.82616000
H	2.53148400	2.41323800	0.49997400
C	3.48634100	0.34944500	-0.63360500
O	1.34697100	0.43931700	-1.64069300
C	3.99695300	-0.44188700	-1.66914300
C	4.21411000	0.47229100	0.55375800
C	5.22099800	-1.08574000	-1.52900400
H	3.42391300	-0.54989800	-2.58125500
C	5.43611500	-0.18157300	0.69811900
H	3.82216000	1.04491400	1.38615200

C	5.94300200	-0.95930400	-0.34181200
H	5.60885700	-1.69107100	-2.34053500
H	5.98549400	-0.09287700	1.62841600
H	6.89320100	-1.46856700	-0.22583300

IRC_TS1_point134

B	-2.72776400	3.84533700	0.37712500
B	-1.62793900	3.65474600	1.77012000
B	-0.57484700	2.26899300	1.46077800
B	-2.35085600	2.57889400	-0.81208900
B	-1.01836800	1.69212800	-0.12436900
B	-1.29053300	4.88677100	0.53360400
B	-1.74476300	4.23451500	-1.05314500
H	-3.83195800	4.26901300	0.50937400
B	0.04167400	3.91222400	1.19570000
H	-1.95879700	3.94386000	2.87639600
B	0.43496300	2.64935900	0.01670900
H	-0.14360200	1.55268400	2.30110800
B	-0.68432800	2.86054600	-1.39872800
H	-3.16415200	2.06693500	-1.51143600
H	-1.38201200	6.04968200	0.77340000
B	-0.02914500	4.27210100	-0.55625400
H	-2.15546000	4.92480100	-1.93141600
H	0.89173300	4.37167600	1.89122000
H	-0.35088400	2.53928800	-2.48893900
H	0.77659000	4.97519300	-1.07855200
B	-2.28710500	2.22550800	0.94974700
I	-1.53539800	-0.95563900	-0.23881600
C	0.31541900	-1.63000100	0.62175200
C	0.58427600	-1.31329400	1.94420000
C	1.16305800	-2.38129900	-0.17835500
C	1.78356800	-1.77559500	2.48753700
H	-0.10763700	-0.73103500	2.53497500
C	2.34839200	-2.84241100	0.39087800
H	0.91962700	-2.59550100	-1.20939500
C	2.65896900	-2.53627300	1.71498300
H	2.02454400	-1.53661400	3.51667800
H	3.03339600	-3.42584400	-0.21218100
H	3.58973300	-2.88798100	2.14389000
O	-2.08881000	-3.17479400	0.12407000
C	-3.29068000	-3.47130200	-0.27734600
O	-4.05698600	-2.65374100	-0.79971000
C	-3.69858200	-4.90485700	-0.02452400
H	-4.03629800	-4.98548900	1.01347400

H	-4.52114000	-5.18073100	-0.68403800
H	-2.85553600	-5.58281800	-0.16080200
H	-0.55384200	0.63055700	-0.64604200
H	-3.05893600	1.47757600	1.45310200
N	1.80460100	2.04315700	-0.09663500
C	2.12987600	0.95792600	-0.82415500
H	2.53209900	2.41424100	0.49903200
C	3.48590500	0.34881900	-0.63330400
O	1.34449600	0.43607400	-1.63603200
C	3.99564900	-0.44246700	-1.66926500
C	4.21456200	0.47208000	0.55343800
C	5.21994100	-1.08601400	-1.53007500
H	3.42178200	-0.55069800	-2.58083600
C	5.43671800	-0.18165000	0.69689000
H	3.82305900	1.04478200	1.38598700
C	5.94280400	-0.95940400	-0.34341700
H	5.60730400	-1.69133600	-2.34184500
H	5.98684100	-0.09286500	1.62673800
H	6.89313400	-1.46858300	-0.22813700

IRC_TS1_point135

B	-2.72859900	3.84207800	0.37618000
B	-1.62891000	3.65289000	1.76953100
B	-0.57505000	2.26753200	1.46129100
B	-2.35091900	2.57524500	-0.81229700
B	-1.01807300	1.68948900	-0.12372500
B	-1.29193000	4.88435900	0.53231400
B	-1.74569500	4.23102900	-1.05411500
H	-3.83307400	4.26506200	0.50804500
B	0.04056200	3.91094000	1.19537200
H	-1.96021700	3.94235200	2.87555100
B	0.43477100	2.64783000	0.01732300
H	-0.14361200	1.55191800	2.30204600
B	-0.68462700	2.85747100	-1.39890000
H	-3.16375100	2.06223500	-1.51136400
H	-1.38398400	6.04734900	0.77135800
B	-0.03013500	4.26960700	-0.55701400
H	-2.15657600	4.92056300	-1.93284900
H	0.89035400	4.37118400	1.89063900
H	-0.35068400	2.53555300	-2.48871900
H	0.77551700	4.97247700	-1.07967100
B	-2.28726600	2.22291800	0.94995400
I	-1.53395200	-0.95160200	-0.23897000
C	0.31554800	-1.62910100	0.62223300

C	0.58470300	-1.31263300	1.94463200
C	1.16235200	-2.38131900	-0.17785600
C	1.78373400	-1.77581000	2.48785700
H	-0.10664500	-0.72974200	2.53542800
C	2.34741900	-2.84325400	0.39122300
H	0.91860800	-2.59536700	-1.20884600
C	2.65849900	-2.53710700	1.71522000
H	2.02501700	-1.53694300	3.51695400
H	3.03186000	-3.42731000	-0.21187600
H	3.58911900	-2.88937700	2.14398300
O	-2.08855400	-3.17595600	0.12315000
C	-3.29026300	-3.47227100	-0.27749400
O	-4.05713900	-2.65470900	-0.79966800
C	-3.69974000	-4.90572100	-0.02484300
H	-4.03803200	-4.98607800	1.01299900
H	-4.52236800	-5.18081400	-0.68462400
H	-2.85745800	-5.58471100	-0.16077900
H	-0.54740200	0.63069300	-0.64888100
H	-3.05877200	1.47488000	1.45351100
N	1.80464900	2.04271800	-0.09594200
C	2.12910400	0.95651800	-0.82214700
H	2.53275000	2.41535600	0.49801100
C	3.48545400	0.34825500	-0.63302500
O	1.34198400	0.43290700	-1.63131800
C	3.99433700	-0.44298200	-1.66940100
C	4.21495700	0.47190800	0.55312500
C	5.21885900	-1.08624300	-1.53112600
H	3.41964600	-0.55142400	-2.58043300
C	5.43724500	-0.18171000	0.69570100
H	3.82387600	1.04468900	1.38581500
C	5.94254500	-0.95948500	-0.34497700
H	5.60572600	-1.69155900	-2.34313500
H	5.98809000	-0.09285600	1.62511100
H	6.89299000	-1.46859900	-0.23038900
IRC_TS1_point136			
B	-2.72936000	3.83887100	0.37524100
B	-1.62980100	3.65103000	1.76894500
B	-0.57520900	2.26605400	1.46177000
B	-2.35094200	2.57167000	-0.81253600
B	-1.01779900	1.68665600	-0.12313600
B	-1.29323300	4.88196500	0.53105000
B	-1.74657700	4.22761700	-1.05505800
H	-3.83409200	4.26121400	0.50675500
B	0.03950000	3.90964500	1.19506300

H	-1.96153900	3.94083200	2.87471400
B	0.43464800	2.64630900	0.01794800
H	-0.14359100	1.55112000	2.30293300
B	-0.68492600	2.85445000	-1.39914400
H	-3.16336000	2.05770600	-1.51132100
H	-1.38579300	6.04503900	0.76936800
B	-0.03106000	4.26710800	-0.55777500
H	-2.15759800	4.91645700	-1.93422700
H	0.88906900	4.37062900	1.89005300
H	-0.35046300	2.53194800	-2.48856900
H	0.77453600	4.96974300	-1.08076500
B	-2.28738500	2.22035800	0.95013700
I	-1.53251800	-0.94755300	-0.23911800
C	0.31563400	-1.62821200	0.62269300
C	0.58510200	-1.31199800	1.94505000
C	1.16163300	-2.38133600	-0.17736900
C	1.78389100	-1.77600600	2.48815600
H	-0.10570400	-0.72850700	2.53587400
C	2.34645800	-2.84404700	0.39153800
H	0.91759200	-2.59523000	-1.20831500
C	2.65804400	-2.53788600	1.71542600
H	2.02548100	-1.53724300	3.51720700
H	3.03037400	-3.42867300	-0.21161200
H	3.58854500	-2.89066600	2.14403200
O	-2.08832200	-3.17745800	0.12226200
C	-3.28985500	-3.47343200	-0.27760400
O	-4.05725900	-2.65578100	-0.79959400
C	-3.70111200	-4.90673300	-0.02517300
H	-4.03990800	-4.98680600	1.01253800
H	-4.52386100	-5.18094800	-0.68519700
H	-2.85963400	-5.58681100	-0.16082400
H	-0.54045200	0.63186300	-0.65202600
H	-3.05858600	1.47223400	1.45387000
N	1.80473700	2.04234900	-0.09525700
C	2.12836100	0.95517700	-0.82015600
H	2.53341400	2.41650600	0.49704200
C	3.48499400	0.34774600	-0.63276400
O	1.33945800	0.42985400	-1.62658800
C	3.99302100	-0.44344000	-1.66955200
C	4.21529700	0.47177200	0.55281900
C	5.21775900	-1.08643600	-1.53215300
H	3.41754800	-0.55206900	-2.58007300
C	5.43769500	-0.18175600	0.69455600
H	3.82461300	1.04462100	1.38564700

C	5.94222600	-0.95954800	-0.34648600
H	5.60416300	-1.69174500	-2.34438200
H	5.98922500	-0.09285900	1.62355200
H	6.89277200	-1.46861800	-0.23254800

IRC_TS1_point137

B	-2.73004700	3.83571100	0.37432100
B	-1.63062500	3.64916700	1.76836000
B	-0.57532800	2.26455200	1.46220900
B	-2.35092600	2.56815200	-0.81278100
B	-1.01745500	1.68392200	-0.12261700
B	-1.29444600	4.87959600	0.52981200
B	-1.74738200	4.22425400	-1.05599100
H	-3.83504600	4.25738300	0.50548300
B	0.03850900	3.90832800	1.19474800
H	-1.96279500	3.93926800	2.87388800
B	0.43451100	2.64480000	0.01854000
H	-0.14353200	1.55028500	2.30377600
B	-0.68517900	2.85144900	-1.39937500
H	-3.16293900	2.05323900	-1.51129100
H	-1.38751300	6.04274500	0.76741400
B	-0.03192200	4.26462400	-0.55852600
H	-2.15856000	4.91239400	-1.93559100
H	0.88786700	4.37001600	1.88947000
H	-0.35021900	2.52837000	-2.48843000
H	0.77364700	4.96697700	-1.08186600
B	-2.28745700	2.21781100	0.95028700
I	-1.53108700	-0.94349700	-0.23926100
C	0.31568000	-1.62738100	0.62316100
C	0.58547400	-1.31137700	1.94545900
C	1.16090600	-2.38134600	-0.17690200
C	1.78403900	-1.77618300	2.48843300
H	-0.10478200	-0.72728300	2.53631100
C	2.34551200	-2.84478700	0.39182200
H	0.91656300	-2.59508600	-1.20780100
C	2.65759900	-2.53861200	1.71560300
H	2.02593900	-1.53751500	3.51743500
H	3.02890700	-3.42996600	-0.21138600
H	3.58799200	-2.89188400	2.14404500
O	-2.08809900	-3.17924400	0.12139700
C	-3.28948200	-3.47478600	-0.27769600
O	-4.05732200	-2.65695300	-0.79948000
C	-3.70271200	-4.90789800	-0.02552000
H	-4.04199600	-4.98769300	1.01206500

H	-4.52567100	-5.18105700	-0.68574900
H	-2.86220300	-5.58923100	-0.16096900
H	-0.53346400	0.63223200	-0.65547800
H	-3.05836900	1.46961200	1.45420600
N	1.80485300	2.04204300	-0.09458400
C	2.12762700	0.95393000	-0.81815000
H	2.53410900	2.41775100	0.49601800
C	3.48451500	0.34729500	-0.63252700
O	1.33689700	0.42688400	-1.62182400
C	3.99169300	-0.44383800	-1.66971900
C	4.21557500	0.47167600	0.55251800
C	5.21663200	-1.08658400	-1.53316100
H	3.41544500	-0.55264400	-2.57973500
C	5.43806400	-0.18178100	0.69344900
H	3.82526200	1.04459000	1.38547000
C	5.94184200	-0.95958800	-0.34795000
H	5.60258000	-1.69188900	-2.34560500
H	5.99025600	-0.09285900	1.62204500
H	6.89247500	-1.46863100	-0.23465100

IRC_TS1_point138

B	-2.73065800	3.83260900	0.37340700
B	-1.63136800	3.64731100	1.76778000
B	-0.57540200	2.26304400	1.46262100
B	-2.35087100	2.56471200	-0.81305500
B	-1.01713600	1.68099400	-0.12213900
B	-1.29556300	4.87725200	0.52860000
B	-1.74813700	4.22096900	-1.05689600
H	-3.83590300	4.25365300	0.50424900
B	0.03757000	3.90700700	1.19445300
H	-1.96395400	3.93770200	2.87307100
B	0.43445000	2.64330800	0.01914800
H	-0.14344000	1.54942900	2.30457700
B	-0.68543300	2.84850800	-1.39967800
H	-3.16252400	2.04893600	-1.51128100
H	-1.38907100	6.04047900	0.76550600
B	-0.03271800	4.26213700	-0.55928200
H	-2.15943000	4.90845800	-1.93690500
H	0.88676100	4.36934800	1.88888000
H	-0.34995200	2.52490200	-2.48835000
H	0.77285200	4.96419000	-1.08295000
B	-2.28748600	2.21530200	0.95041800
I	-1.52966900	-0.93944100	-0.23939800
C	0.31569000	-1.62655500	0.62360000

C	0.58582400	-1.31077500	1.94584500
C	1.16017700	-2.38134800	-0.17645200
C	1.78417700	-1.77634200	2.48868800
H	-0.10390300	-0.72610500	2.53673000
C	2.34458600	-2.84547700	0.39207900
H	0.91555300	-2.59493400	-1.20731100
C	2.65716900	-2.53929000	1.71575500
H	2.02638100	-1.53776200	3.51764000
H	3.02749400	-3.43116300	-0.21119600
H	3.58747100	-2.89301200	2.14402700
O	-2.08789400	-3.18137000	0.12056400
C	-3.28912300	-3.47632500	-0.27775200
O	-4.05734200	-2.65821400	-0.79933100
C	-3.70452500	-4.90920300	-0.02587600
H	-4.04422300	-4.98871000	1.01160600
H	-4.52774400	-5.18120300	-0.68628500
H	-2.86503200	-5.59185200	-0.16118600
H	-0.52609600	0.63368100	-0.65906700
H	-3.05812200	1.46704200	1.45449800
N	1.80500600	2.04181300	-0.09391900
C	2.12690700	0.95274500	-0.81617300
H	2.53482000	2.41904100	0.49502600
C	3.48401700	0.34689700	-0.63231100
O	1.33433600	0.42402700	-1.61704600
C	3.99035600	-0.44418100	-1.66990200
C	4.21578800	0.47161800	0.55221800
C	5.21548100	-1.08669300	-1.53414500
H	3.41337300	-0.55314500	-2.57944000
C	5.43835000	-0.18178600	0.69238300
H	3.82582100	1.04458600	1.38529000
C	5.94139400	-0.95960500	-0.34936400
H	5.60100900	-1.69199500	-2.34678600
H	5.99116700	-0.09286100	1.62060300
H	6.89210300	-1.46863800	-0.23666300
IRC_TS1_point139			
B	-2.73119200	3.82956600	0.37251600
B	-1.63204200	3.64546100	1.76720300
B	-0.57544100	2.26151900	1.46299500
B	-2.35077700	2.56133200	-0.81333100
B	-1.01673600	1.67820900	-0.12172100
B	-1.29658700	4.87493700	0.52741500
B	-1.74881100	4.21773800	-1.05779200
H	-3.83669100	4.24996000	0.50303600
B	0.03670500	3.90566700	1.19415100

H	-1.96503900	3.93611100	2.87226900
B	0.43436100	2.64183200	0.01972000
H	-0.14331300	1.54853900	2.30533300
B	-0.68564200	2.84557800	-1.39996000
H	-3.16208700	2.04471200	-1.51128200
H	-1.39052800	6.03823800	0.76363600
B	-0.03345000	4.25966800	-0.56002900
H	-2.16023300	4.90458100	-1.93820000
H	0.88574400	4.36862700	1.88829300
H	-0.34966900	2.52147300	-2.48828700
H	0.77214900	4.96137800	-1.08403800
B	-2.28747000	2.21281800	0.95051900
I	-1.52825700	-0.93539400	-0.23953200
C	0.31566900	-1.62577300	0.62403300
C	0.58615500	-1.31018100	1.94621100
C	1.15945500	-2.38133600	-0.17602700
C	1.78430700	-1.77648300	2.48891800
H	-0.10304200	-0.72493900	2.53713200
C	2.34368400	-2.84611600	0.39230800
H	0.91455300	-2.59477100	-1.20684500
C	2.65675300	-2.53992200	1.71588200
H	2.02680800	-1.53798800	3.51782300
H	3.02611100	-3.43229300	-0.21103800
H	3.58696800	-2.89408300	2.14398500
O	-2.08769400	-3.18378200	0.11975100
C	-3.28879600	-3.47804300	-0.27779000
O	-4.05730100	-2.65955800	-0.79914300
C	-3.70655300	-4.91064900	-0.02624800
H	-4.04664400	-4.98987700	1.01113900
H	-4.53011800	-5.18133000	-0.68679700
H	-2.86822500	-5.59476300	-0.16150000
H	-0.51847800	0.63421700	-0.66299000
H	-3.05785200	1.46451200	1.45477100
N	1.80518900	2.04165000	-0.09327100
C	2.12619300	0.95166400	-0.81416300
H	2.53556600	2.42042700	0.49398200
C	3.48349200	0.34655400	-0.63212400
O	1.33169800	0.42125900	-1.61223100
C	3.98900300	-0.44446800	-1.67010600
C	4.21593400	0.47160000	0.55191900
C	5.21430400	-1.08675800	-1.53510700
H	3.41129900	-0.55358500	-2.57917500
C	5.43855000	-0.18176600	0.69135500
H	3.82628400	1.04462100	1.38509600

C	5.94088000	-0.95959500	-0.35073100
H	5.59942000	-1.69205800	-2.34794100
H	5.99196500	-0.09285200	1.61921500
H	6.89165200	-1.46863500	-0.23861300

IRC_TS1_point140

B	-2.73165000	3.82658700	0.37163200
B	-1.63262800	3.64362100	1.76663400
B	-0.57543400	2.25999200	1.46334600
B	-2.35064500	2.55805100	-0.81364500
B	-1.01637700	1.67516700	-0.12134100
B	-1.29751400	4.87265000	0.52625600
B	-1.74943600	4.21459500	-1.05865900
H	-3.83738000	4.24637500	0.50186500
B	0.03588900	3.90432600	1.19387200
H	-1.96602200	3.93452200	2.87147700
B	0.43437200	2.64037700	0.02031300
H	-0.14315300	1.54763200	2.30604500
B	-0.68586100	2.84271800	-1.40033100
H	-3.16166500	2.04067700	-1.51130400
H	-1.39181600	6.03602800	0.76181400
B	-0.03411900	4.25719500	-0.56078400
H	-2.16094200	4.90084100	-1.93944300
H	0.88482700	4.36784900	1.88769200
H	-0.34936100	2.51814700	-2.48828400
H	0.77154000	4.95854200	-1.08510900
B	-2.28741300	2.21038400	0.95060700
I	-1.52686100	-0.93136100	-0.23965900
C	0.31562600	-1.62497600	0.62442000
C	0.58647000	-1.30960000	1.94654500
C	1.15874700	-2.38131000	-0.17562300
C	1.78442800	-1.77660800	2.48912700
H	-0.10221900	-0.72381800	2.53750700
C	2.34281100	-2.84670600	0.39251400
H	0.91359700	-2.59459400	-1.20640900
C	2.65635300	-2.54051200	1.71599000
H	2.02721200	-1.53819700	3.51798600
H	3.02479200	-3.43333300	-0.21090800
H	3.58649300	-2.89507900	2.14392500
O	-2.08751500	-3.18653800	0.11897400
C	-3.28848600	-3.47993600	-0.27779200
O	-4.05721300	-2.66097000	-0.79892100
C	-3.70878000	-4.91221900	-0.02662800
H	-4.04918300	-4.99116200	1.01068900

H	-4.53273600	-5.18149900	-0.68728900
H	-2.87165100	-5.59783800	-0.16188400
H	-0.51062200	0.63610800	-0.66670400
H	-3.05755000	1.46203700	1.45499400
N	1.80541000	2.04157800	-0.09263300
C	2.12547700	0.95063400	-0.81220100
H	2.53632900	2.42187100	0.49296300
C	3.48294300	0.34626300	-0.63196300
O	1.32906700	0.41861600	-1.60738600
C	3.98764000	-0.44470100	-1.67032800
C	4.21600900	0.47162100	0.55161500
C	5.21310500	-1.08678500	-1.53604500
H	3.40925900	-0.55395600	-2.57895600
C	5.43866200	-0.18172300	0.69036800
H	3.82664800	1.04468500	1.38489200
C	5.94030300	-0.95956100	-0.35204500
H	5.59784800	-1.69208500	-2.34904900
H	5.99263500	-0.09283900	1.61789400
H	6.89112600	-1.46862000	-0.24046500

IRC_TS1_point141

B	-2.73203200	3.82367500	0.37077700
B	-1.63314800	3.64179000	1.76606600
B	-0.57539500	2.25844300	1.46364700
B	-2.35047500	2.55485000	-0.81395200
B	-1.01592700	1.67237800	-0.12102200
B	-1.29834700	4.87039800	0.52512400
B	-1.74997400	4.21150500	-1.05952100
H	-3.83800000	4.24284600	0.50072100
B	0.03515500	3.90296600	1.19357200
H	-1.96692500	3.93291700	2.87070300
B	0.43431100	2.63893500	0.02085500
H	-0.14295600	1.54668600	2.30670700
B	-0.68602200	2.83985300	-1.40065300
H	-3.16122500	2.03674300	-1.51133700
H	-1.39300300	6.03384800	0.76003500
B	-0.03472300	4.25474600	-0.56153000
H	-2.16158800	4.89717100	-1.94066400
H	0.88399700	4.36702500	1.88709400
H	-0.34905000	2.51486700	-2.48829600
H	0.77101800	4.95569800	-1.08618400
B	-2.28731100	2.20797900	0.95065900
I	-1.52547300	-0.92735500	-0.23978300
C	0.31557200	-1.62421800	0.62479200

C	0.58677500	-1.30902300	1.94685000
C	1.15806400	-2.38126300	-0.17525100
C	1.78454200	-1.77671900	2.48931200
H	-0.10141000	-0.72270700	2.53785400
C	2.34197200	-2.84724800	0.39269400
H	0.91267200	-2.59440100	-1.20600400
C	2.65597100	-2.54106300	1.71607900
H	2.02759200	-1.53839400	3.51813100
H	3.02351200	-3.43431500	-0.21080300
H	3.58603300	-2.89603100	2.14385400
O	-2.08733900	-3.18956200	0.11822100
C	-3.28821600	-3.48198700	-0.27777900
O	-4.05705900	-2.66244500	-0.79866300
C	-3.71119900	-4.91391300	-0.02702000
H	-4.05188900	-4.99258200	1.01023500
H	-4.53562200	-5.18165000	-0.68775300
H	-2.87540300	-5.60116400	-0.16236000
H	-0.50230600	0.63649200	-0.67097700
H	-3.05724000	1.45962500	1.45521000
N	1.80566900	2.04157400	-0.09201800
C	2.12477200	0.94973500	-0.81016800
H	2.53713500	2.42341500	0.49188800
C	3.48236300	0.34602700	-0.63184200
O	1.32628400	0.41605300	-1.60248400
C	3.98626300	-0.44488500	-1.67057400
C	4.21601400	0.47168300	0.55130800
C	5.21188600	-1.08676900	-1.53695800
H	3.40722500	-0.55427800	-2.57877400
C	5.43868600	-0.18165300	0.68942000
H	3.82691300	1.04478500	1.38467100
C	5.93966400	-0.95949700	-0.35330900
H	5.59626500	-1.69207400	-2.35012500
H	5.99318500	-0.09281000	1.61663000
H	6.89052700	-1.46859100	-0.24224900
IRC_TS1_point142			
B	-2.73233700	3.82083100	0.36992200
B	-1.63356700	3.63996900	1.76550700
B	-0.57529600	2.25689700	1.46393000
B	-2.35026700	2.55175900	-0.81430900
B	-1.01555500	1.66912600	-0.12074700
B	-1.29908400	4.86817600	0.52401600
B	-1.75047900	4.20851600	-1.06034500
H	-3.83851100	4.23943500	0.49962800
B	0.03445800	3.90161600	1.19330800

H	-1.96771300	3.93131300	2.86993400
B	0.43441800	2.63751900	0.02144200
H	-0.14271900	1.54573900	2.30732900
B	-0.68621600	2.83708700	-1.40111000
H	-3.16080800	2.03302300	-1.51138600
H	-1.39401000	6.03170000	0.75830800
B	-0.03527000	4.25229100	-0.56229000
H	-2.16213300	4.89365200	-1.94182400
H	0.88327200	4.36614700	1.88647100
H	-0.34870500	2.51170400	-2.48837800
H	0.77058600	4.95283000	-1.08723600
B	-2.28716900	2.20563600	0.95071100
I	-1.52410900	-0.92337800	-0.23990400
C	0.31550900	-1.62341000	0.62509700
C	0.58707200	-1.30845500	1.94711700
C	1.15740800	-2.38119500	-0.17490100
C	1.78464900	-1.77681700	2.48947800
H	-0.10063900	-0.72164500	2.53816500
C	2.34117100	-2.84774500	0.39285600
H	0.91181600	-2.59419100	-1.20563400
C	2.65560800	-2.54157500	1.71615600
H	2.02794300	-1.53858300	3.51826300
H	3.02230900	-3.43521100	-0.21071600
H	3.58560500	-2.89691200	2.14377400
O	-2.08719800	-3.19292300	0.11752400
C	-3.28796400	-3.48418900	-0.27772600
O	-4.05686600	-2.66396400	-0.79837700
C	-3.71379500	-4.91570100	-0.02742000
H	-4.05466700	-4.99409400	1.00980700
H	-4.53871300	-5.18185700	-0.68819200
H	-2.87932300	-5.60457400	-0.16290100
H	-0.49409700	0.63935200	-0.67475800
H	-3.05688400	1.45727000	1.45536600
N	1.80596900	2.04168900	-0.09141000
C	2.12404700	0.94885300	-0.80823600
H	2.53795500	2.42502400	0.49085400
C	3.48176100	0.34584500	-0.63174700
O	1.32355200	0.41363400	-1.59751700
C	3.98488100	-0.44501700	-1.67083700
C	4.21594500	0.47178200	0.55099100
C	5.21064800	-1.08671700	-1.53784200
H	3.40524200	-0.55453800	-2.57864500
C	5.43862100	-0.18155800	0.68851300
H	3.82707400	1.04491300	1.38443200

C	5.93896700	-0.95940500	-0.35451500
H	5.59471600	-1.69202900	-2.35114500
H	5.99359900	-0.09277400	1.61544000
H	6.88986100	-1.46854200	-0.24392300
IRC_TS1_point143			
B	-2.73257000	3.81805700	0.36910800
B	-1.63393200	3.63816200	1.76494600
B	-0.57516500	2.25532200	1.46414500
B	-2.35002300	2.54873300	-0.81462900
B	-1.01504100	1.66641100	-0.12052400
B	-1.29973500	4.86599400	0.52293600
B	-1.75087900	4.20555900	-1.06118000
H	-3.83895700	4.23611600	0.49857200
B	0.03386600	3.90024300	1.19299400
H	-1.96842100	3.92971800	2.86919000
B	0.43434700	2.63611700	0.02193600
H	-0.14244200	1.54475200	2.30790000
B	-0.68631200	2.83427300	-1.40143800
H	-3.16037100	2.02939500	-1.51144700
H	-1.39494000	6.02959500	0.75663700
B	-0.03575000	4.24987800	-0.56303500
H	-2.16263100	4.89022000	-1.94295300
H	0.88262000	4.36525600	1.88586500
H	-0.34837900	2.50859900	-2.48846600
H	0.77022300	4.95001300	-1.08828300
B	-2.28697500	2.20332500	0.95071200
I	-1.52275300	-0.91945000	-0.24002800
C	0.31546800	-1.62265100	0.62539600
C	0.58736800	-1.30788800	1.94735800
C	1.15679300	-2.38110400	-0.17459000
C	1.78475100	-1.77690600	2.48962600
H	-0.09988500	-0.72059800	2.53844600
C	2.34040800	-2.84820000	0.39299700
H	0.91099900	-2.59396700	-1.20529800
C	2.65526700	-2.54205300	1.71621700
H	2.02826500	-1.53877300	3.51838400
H	3.02114800	-3.43606000	-0.21064600
H	3.58519400	-2.89775500	2.14368900
O	-2.08705600	-3.19649100	0.11685500
C	-3.28776100	-3.48651500	-0.27766600
O	-4.05660600	-2.66552500	-0.79806100
C	-3.71655500	-4.91758700	-0.02783100
H	-4.05756800	-4.99570800	1.00938000
H	-4.54203600	-5.18201900	-0.68860700

H	-2.88351700	-5.60817900	-0.16353600
H	-0.48509900	0.63891800	-0.67998500
H	-3.05654700	1.45501300	1.45554500
N	1.80631600	2.04185000	-0.09083400
C	2.12336200	0.94818400	-0.80615600
H	2.53883100	2.42671900	0.48976000
C	3.48112700	0.34571800	-0.63170700
O	1.32051600	0.41126900	-1.59246200
C	3.98348900	-0.44510900	-1.67112700
C	4.21581000	0.47192000	0.55067300
C	5.20940100	-1.08662600	-1.53869700
H	3.40327700	-0.55476100	-2.57855900
C	5.43847300	-0.18143600	0.68764700
H	3.82714400	1.04507300	1.38418300
C	5.93821700	-0.95928400	-0.35566900
H	5.59316800	-1.69195000	-2.35212600
H	5.99389800	-0.09272100	1.61430800
H	6.88913400	-1.46847300	-0.24552400

IRC_TS1_point144

B	-2.73271700	3.81533200	0.36827500
B	-1.63417200	3.63635600	1.76439300
B	-0.57495300	2.25376300	1.46435300
B	-2.34972000	2.54580600	-0.81503100
B	-1.01467400	1.66283200	-0.12033400
B	-1.30028900	4.86384200	0.52187800
B	-1.75128100	4.20272300	-1.06195200
H	-3.83929800	4.23281400	0.49754200
B	0.03328000	3.89890100	1.19275000
H	-1.96901200	3.92806200	2.86843900
B	0.43460100	2.63474400	0.02253700
H	-0.14210400	1.54378600	2.30843800
B	-0.68649200	2.83160400	-1.40201800
H	-3.15993900	2.02594400	-1.51151000
H	-1.39567400	6.02751200	0.75497900
B	-0.03618000	4.24743800	-0.56380800
H	-2.16302400	4.88687100	-1.94405500
H	0.88209700	4.36427600	1.88520300
H	-0.34797600	2.50560200	-2.48864900
H	0.76996500	4.94707800	-1.08934400
B	-2.28673000	2.20108100	0.95072800
I	-1.52144000	-0.91556600	-0.24014600
C	0.31541500	-1.62177200	0.62559400
C	0.58765700	-1.30733000	1.94755900

C	1.15620200	-2.38098700	-0.17428900
C	1.78485100	-1.77698400	2.48976000
H	-0.09915600	-0.71960000	2.53870700
C	2.33968300	-2.84861100	0.39312700
H	0.91025100	-2.59372900	-1.20498400
C	2.65495100	-2.54249400	1.71627400
H	2.02856500	-1.53896000	3.51849800
H	3.02005000	-3.43684400	-0.21058300
H	3.58481400	-2.89854100	2.14360500
O	-2.08696900	-3.20038200	0.11626200
C	-3.28756600	-3.48896700	-0.27755600
O	-4.05631700	-2.66710200	-0.79771900
C	-3.71949600	-4.91953500	-0.02825400
H	-4.06054700	-4.99741000	1.00897300
H	-4.54558800	-5.18222000	-0.68898300
H	-2.88790400	-5.61185600	-0.16425800
H	-0.47703200	0.64391800	-0.68376800
H	-3.05609000	1.45275300	1.45562200
N	1.80670400	2.04218000	-0.09023900
C	2.12262900	0.94744600	-0.80429400
H	2.53972400	2.42854700	0.48870000
C	3.48047900	0.34564600	-0.63167700
O	1.31771300	0.40912200	-1.58735800
C	3.98209700	-0.44514500	-1.67142700
C	4.21559900	0.47209400	0.55033800
C	5.20813600	-1.08649700	-1.53952100
H	3.40135300	-0.55492300	-2.57851300
C	5.43823800	-0.18128600	0.68682400
H	3.82710000	1.04526700	1.38390300
C	5.93741600	-0.95912700	-0.35676400
H	5.59164800	-1.69183800	-2.35305200
H	5.99406500	-0.09265100	1.61324800
H	6.88835000	-1.46837200	-0.24702400

IRC_TS1_point145

B	-2.73280100	3.81269100	0.36751300
B	-1.63438300	3.63458000	1.76384200
B	-0.57472200	2.25216600	1.46447000
B	-2.34938900	2.54293900	-0.81535600
B	-1.01402600	1.66014600	-0.12025000
B	-1.30076200	4.86175500	0.52086000
B	-1.75154000	4.19990400	-1.06276000
H	-3.83960100	4.22963800	0.49656800
B	0.03284200	3.89753000	1.19241400

H	-1.96955100	3.92645200	2.86773200
B	0.43447800	2.63340000	0.02296100
H	-0.14173600	1.54275900	2.30890900
B	-0.68650600	2.82883300	-1.40232600
H	-3.15946100	2.02252500	-1.51158200
H	-1.39643200	6.02549300	0.75342500
B	-0.03653700	4.24509100	-0.56454900
H	-2.16341700	4.88362500	-1.94511700
H	0.88161500	4.36333300	1.88460400
H	-0.34763300	2.50260000	-2.48877900
H	0.76975100	4.94431300	-1.09038800
B	-2.28642100	2.19886300	0.95066900
I	-1.52013500	-0.91174500	-0.24027000
C	0.31541600	-1.62101600	0.62583400
C	0.58795000	-1.30677900	1.94774900
C	1.15566400	-2.38085500	-0.17402800
C	1.78494800	-1.77706100	2.48988200
H	-0.09843700	-0.71859800	2.53892700
C	2.33900500	-2.84898500	0.39323900
H	0.90952200	-2.59348900	-1.20469700
C	2.65466200	-2.54290000	1.71631500
H	2.02883700	-1.53916100	3.51861000
H	3.01898900	-3.43760400	-0.21053300
H	3.58445000	-2.89930100	2.14351700
O	-2.08686500	-3.20438300	0.11568800
C	-3.28742500	-3.49150900	-0.27745400
O	-4.05595700	-2.66870600	-0.79735100
C	-3.72255600	-4.92155600	-0.02868700
H	-4.06363500	-4.99918500	1.00855900
H	-4.54934400	-5.18229600	-0.68933500
H	-2.89255900	-5.61575000	-0.16508400
H	-0.46716300	0.64158200	-0.69013400
H	-3.05569100	1.45063800	1.45577400
N	1.80712300	2.04249600	-0.08969300
C	2.12197200	0.94706100	-0.80216400
H	2.54068900	2.43044500	0.48751900
C	3.47978500	0.34562600	-0.63173200
O	1.31439000	0.40700000	-1.58215900
C	3.98069800	-0.44515600	-1.67176000
C	4.21532300	0.47230100	0.55000800
C	5.20687800	-1.08633200	-1.54031000
H	3.39945000	-0.55507800	-2.57851300
C	5.43792200	-0.18110900	0.68604400
H	3.82698000	1.04548800	1.38361900

C	5.93657500	-0.95894000	-0.35780400
H	5.59012900	-1.69169300	-2.35394200
H	5.99412700	-0.09255100	1.61224400
H	6.88752200	-1.46824400	-0.24846200

IRC_TS1_point146

B	-2.73278700	3.81006200	0.36670500
B	-1.63444300	3.63277800	1.76329700
B	-0.57439900	2.25059700	1.46458400
B	-2.34898600	2.54016300	-0.81581400
B	-1.01365500	1.65634600	-0.12015200
B	-1.30113200	4.85968200	0.51986100
B	-1.75185000	4.19723200	-1.06347800
H	-3.83984300	4.22621700	0.49556200
B	0.03237200	3.89619100	1.19218100
H	-1.96997900	3.92461700	2.86701500
B	0.43481900	2.63207700	0.02356100
H	-0.14126200	1.54175400	2.30932500
B	-0.68669100	2.82627000	-1.40302600
H	-3.15897500	2.01920300	-1.51164300
H	-1.39689500	6.02348200	0.75176800
B	-0.03685800	4.24265700	-0.56534300
H	-2.16371100	4.88032600	-1.94623600
H	0.88134200	4.36218700	1.88387400
H	-0.34717200	2.49967000	-2.48905400
H	0.76973500	4.94111000	-1.09158000
B	-2.28604400	2.19668800	0.95062700
I	-1.51889000	-0.90796400	-0.24037800
C	0.31538300	-1.62007200	0.62593400
C	0.58823100	-1.30625500	1.94789900
C	1.15514300	-2.38070300	-0.17376400
C	1.78504300	-1.77713400	2.48999400
H	-0.09772100	-0.71766100	2.53915800
C	2.33836000	-2.84932600	0.39335300
H	0.90886100	-2.59324300	-1.20441700
C	2.65440700	-2.54327000	1.71635900
H	2.02908600	-1.53937600	3.51872300
H	3.01795000	-3.43835400	-0.21047100
H	3.58412300	-2.90001800	2.14343700
O	-2.08682100	-3.20869500	0.11519300
C	-3.28728200	-3.49416100	-0.27729700
O	-4.05557800	-2.67032200	-0.79695900
C	-3.72576500	-4.92364800	-0.02911500
H	-4.06686900	-5.00111400	1.00815100

H	-4.55334200	-5.18243100	-0.68960000
H	-2.89749400	-5.61983700	-0.16599000
H	-0.45856100	0.64858100	-0.69416800
H	-3.05503800	1.44833700	1.45573400
N	1.80760000	2.04302500	-0.08909100
C	2.12125400	0.94651500	-0.80033100
H	2.54167600	2.43257600	0.48636700
C	3.47909200	0.34564400	-0.63178300
O	1.31149500	0.40518000	-1.57696700
C	3.97930900	-0.44511900	-1.67210500
C	4.21496500	0.47252700	0.54964900
C	5.20560900	-1.08613700	-1.54106900
H	3.39755400	-0.55518500	-2.57853500
C	5.43752000	-0.18091000	0.68530600
H	3.82670200	1.04573700	1.38327100
C	5.93568900	-0.95872100	-0.35878200
H	5.58861600	-1.69152500	-2.35479100
H	5.99405000	-0.09242800	1.61130800
H	6.88664100	-1.46808400	-0.24981800

IRC_TS1_point147

B	-2.73270600	3.80753000	0.36598000
B	-1.63447600	3.63101800	1.76274400
B	-0.57407000	2.24897400	1.46458700
B	-2.34856700	2.53743500	-0.81620600
B	-1.01294500	1.65329200	-0.12024700
B	-1.30142700	4.85768300	0.51891000
B	-1.75201100	4.19458900	-1.06422600
H	-3.83998300	4.22310900	0.49467600
B	0.03204500	3.89482000	1.19184100
H	-1.97032200	3.92292600	2.86633000
B	0.43475400	2.63076300	0.02395000
H	-0.14078300	1.54067900	2.30965600
B	-0.68670600	2.82359100	-1.40345200
H	-3.15851600	2.01606400	-1.51175700
H	-1.39742500	6.02153700	0.75032700
B	-0.03711900	4.24034400	-0.56610100
H	-2.16399700	4.87728300	-1.94720800
H	0.88107100	4.36110900	1.88322400
H	-0.34680900	2.49684800	-2.48931100
H	0.76967300	4.93830800	-1.09263500
B	-2.28559800	2.19452700	0.95049400
I	-1.51765100	-0.90421600	-0.24049100
C	0.31540600	-1.61928800	0.62608900

C	0.58850800	-1.30576600	1.94804400
C	1.15467100	-2.38056800	-0.17352900
C	1.78513600	-1.77721600	2.49009900
H	-0.09705900	-0.71678000	2.53934600
C	2.33777100	-2.84964000	0.39345400
H	0.90822800	-2.59303500	-1.20415900
C	2.65418500	-2.54361000	1.71639300
H	2.02930700	-1.53959800	3.51883300
H	3.01700800	-3.43902400	-0.21042700
H	3.58384200	-2.90066100	2.14334900
O	-2.08677600	-3.21312400	0.11472700
C	-3.28718300	-3.49688700	-0.27714400
O	-4.05514200	-2.67194800	-0.79655100
C	-3.72899100	-4.92579200	-0.02953500
H	-4.07004800	-5.00305000	1.00777600
H	-4.55733000	-5.18261500	-0.68986000
H	-2.90237900	-5.62389500	-0.16688500
H	-0.44781000	0.64695400	-0.70073000
H	-3.05453300	1.44631600	1.45581000
N	1.80808700	2.04352200	-0.08853500
C	2.12059200	0.94633200	-0.79822100
H	2.54266300	2.43463200	0.48524800
C	3.47833500	0.34569600	-0.63194300
O	1.30798200	0.40339200	-1.57163900
C	3.97792100	-0.44508100	-1.67249800
C	4.21453300	0.47277200	0.54927500
C	5.20436300	-1.08592200	-1.54179000
H	3.39575900	-0.55531100	-2.57865900
C	5.43703200	-0.18068900	0.68460500
H	3.82635200	1.04598000	1.38291800
C	5.93477600	-0.95848000	-0.35969900
H	5.58716800	-1.69133400	-2.35557900
H	5.99383900	-0.09227500	1.61043900
H	6.88573200	-1.46789800	-0.25106400

IRC_TS1_point148

B	-2.73252300	3.80500400	0.36522100
B	-1.63436600	3.62924100	1.76218500
B	-0.57365800	2.24736700	1.46455600
B	-2.34807300	2.53479100	-0.81672200
B	-1.01246700	1.64937900	-0.12035600
B	-1.30162400	4.85572100	0.51797800
B	-1.75221400	4.19209300	-1.06489400
H	-3.84006200	4.21978300	0.49378200

B	0.03170000	3.89347900	1.19157300
H	-1.97055200	3.92103800	2.86563900
B	0.43500700	2.62945700	0.02447100
H	-0.14019200	1.53965300	2.30993300
B	-0.68688600	2.82108800	-1.40419300
H	-3.15810300	2.01311600	-1.51188100
H	-1.39765600	6.01963500	0.74881000
B	-0.03735400	4.23794900	-0.56691000
H	-2.16421100	4.87427600	-1.94819000
H	0.88099800	4.35986400	1.88245100
H	-0.34636100	2.49419700	-2.48972600
H	0.76980200	4.93510000	-1.09383000
B	-2.28505600	2.19239300	0.95035500
I	-1.51646800	-0.90050500	-0.24058600
C	0.31539700	-1.61838500	0.62613700
C	0.58877400	-1.30531900	1.94815400
C	1.15421900	-2.38043500	-0.17328800
C	1.78522900	-1.77730400	2.49019300
H	-0.09641400	-0.71599400	2.53954900
C	2.33721800	-2.84993700	0.39356400
H	0.90767300	-2.59284100	-1.20390700
C	2.65400300	-2.54392200	1.71643400
H	2.02950200	-1.53982900	3.51894100
H	3.01610200	-3.43968600	-0.21036600
H	3.58361200	-2.90124800	2.14327200
O	-2.08678200	-3.21784500	0.11433100
C	-3.28710900	-3.49970100	-0.27695300
O	-4.05467800	-2.67356900	-0.79612400
C	-3.73230400	-4.92799400	-0.02993500
H	-4.07327100	-5.00509700	1.00743300
H	-4.56145000	-5.18291000	-0.69003200
H	-2.90737900	-5.62801800	-0.16781800
H	-0.43785600	0.65261200	-0.70551300
H	-3.05380700	1.44416600	1.45572500
N	1.80863000	2.04420300	-0.08792700
C	2.11988800	0.94607100	-0.79631700
H	2.54364400	2.43683800	0.48423800
C	3.47756800	0.34577000	-0.63212700
O	1.30474900	0.40191100	-1.56630700
C	3.97655300	-0.44502000	-1.67291500
C	4.21402100	0.47301900	0.54886200
C	5.20312800	-1.08569300	-1.54247700
H	3.39402000	-0.55541500	-2.57883900
C	5.43646400	-0.18045000	0.68394000

H	3.82584800	1.04622200	1.38249700
C	5.93383600	-0.95821500	-0.36055200
H	5.58577000	-1.69113800	-2.35631100
H	5.99348300	-0.09209800	1.60964300
H	6.88479400	-1.46768000	-0.25220600
IRC_TS1_point149			
B	-2.73225200	3.80257400	0.36451800
B	-1.63419100	3.62752700	1.76161600
B	-0.57321900	2.24573800	1.46441500
B	-2.34752600	2.53221800	-0.81722800
B	-1.01176300	1.64558500	-0.12069100
B	-1.30174000	4.85387300	0.51709700
B	-1.75233200	4.18970300	-1.06554100
H	-3.84003800	4.21665900	0.49299300
B	0.03144400	3.89216200	1.19125700
H	-1.97068900	3.91923600	2.86496700
B	0.43501800	2.62816200	0.02488500
H	-0.13958000	1.53864500	2.31016100
B	-0.68702100	2.81857200	-1.40481800
H	-3.15776100	2.01045300	-1.51204900
H	-1.39787500	6.01784200	0.74746200
B	-0.03754600	4.23564300	-0.56769700
H	-2.16441800	4.87153300	-1.94902700
H	0.88096100	4.35867100	1.88172100
H	-0.34598700	2.49177100	-2.49018800
H	0.76992700	4.93213100	-1.09493900
B	-2.28440100	2.19028900	0.95014200
I	-1.51531700	-0.89685600	-0.24067700
C	0.31540600	-1.61758400	0.62619600
C	0.58903200	-1.30492600	1.94825100
C	1.15381100	-2.38033000	-0.17305600
C	1.78532700	-1.77740000	2.49027900
H	-0.09581400	-0.71528700	2.53971800
C	2.33672800	-2.85021300	0.39367400
H	0.90716800	-2.59270100	-1.20366200
C	2.65386600	-2.54420800	1.71647600
H	2.02967800	-1.54005100	3.51904200
H	3.01530300	-3.44027000	-0.21031200
H	3.58344500	-2.90175500	2.14320000
O	-2.08681900	-3.22272000	0.11398900
C	-3.28707600	-3.50254400	-0.27675900
O	-4.05417700	-2.67514800	-0.79569800
C	-3.73558900	-4.93020100	-0.03031800
H	-4.07637400	-5.00712200	1.00713600

H	-4.56550000	-5.18331100	-0.69017600
H	-2.91222300	-5.63199400	-0.16872100
H	-0.42557900	0.65361600	-0.71206300
H	-3.05315300	1.44228500	1.45572000
N	1.80919000	2.04491100	-0.08734000
C	2.11922100	0.94609100	-0.79425400
H	2.54459600	2.43897300	0.48335100
C	3.47674900	0.34587000	-0.63241700
O	1.30105800	0.40057700	-1.56087300
C	3.97521300	-0.44496600	-1.67338200
C	4.21343700	0.47327300	0.54841700
C	5.20194100	-1.08545300	-1.54311600
H	3.39241900	-0.55555200	-2.57913100
C	5.43582000	-0.18019100	0.68331200
H	3.82526500	1.04644500	1.38205300
C	5.93289500	-0.95792900	-0.36133300
H	5.58446800	-1.69093400	-2.35696900
H	5.99299200	-0.09188200	1.60891900
H	6.88385600	-1.46743100	-0.25322000
IRC_TS1_point150			
B	-2.73187900	3.80022000	0.36380900
B	-1.63388900	3.62587300	1.76104500
B	-0.57271300	2.24415400	1.46420300
B	-2.34688900	2.52974700	-0.81781100
B	-1.01112500	1.64093000	-0.12117800
B	-1.30176600	4.85215700	0.51625300
B	-1.75248300	4.18751800	-1.06610000
H	-3.83996600	4.21340100	0.49222800
B	0.03118400	3.89093900	1.19100300
H	-1.97072700	3.91732400	2.86431000
B	0.43515800	2.62689800	0.02540100
H	-0.13887200	1.53778500	2.31038300
B	-0.68732400	2.81623900	-1.40563700
H	-3.15751600	2.00810900	-1.51221800
H	-1.39785800	6.01618500	0.74609500
B	-0.03771800	4.23333200	-0.56850800
H	-2.16459800	4.86893400	-1.94982300
H	0.88107900	4.35742700	1.88091900
H	-0.34557600	2.48964100	-2.49078400
H	0.77021200	4.92889600	-1.09615200
B	-2.28361200	2.18824100	0.94989900
I	-1.51423300	-0.89329800	-0.24075300
C	0.31537200	-1.61676000	0.62618500
C	0.58927800	-1.30459800	1.94831600

C	1.15343500	-2.38024900	-0.17280900
C	1.78543500	-1.77750000	2.49035200
H	-0.09522800	-0.71467300	2.53988600
C	2.33629600	-2.85047500	0.39379700
H	0.90675200	-2.59259400	-1.20341600
C	2.65378200	-2.54447400	1.71653100
H	2.02984700	-1.54025400	3.51912900
H	3.01457400	-3.44082700	-0.21024400
H	3.58334200	-2.90220700	2.14315000
O	-2.08691200	-3.22781800	0.11372500
C	-3.28708700	-3.50538600	-0.27654400
O	-4.05366300	-2.67665800	-0.79528000
C	-3.73884600	-4.93238800	-0.03067200
H	-4.07939700	-5.00917800	1.00688400
H	-4.56953700	-5.18382700	-0.69022600
H	-2.91699200	-5.63587500	-0.16963100
H	-0.41224700	0.65897300	-0.71814100
H	-3.05234500	1.44044400	1.45564100
N	1.80978500	2.04575900	-0.08672900
C	2.11852700	0.94615900	-0.79229300
H	2.54552100	2.44114900	0.48261400
C	3.47591700	0.34598700	-0.63277200
O	1.29739900	0.39955300	-1.55543000
C	3.97392600	-0.44491100	-1.67388400
C	4.21278900	0.47352000	0.54792900
C	5.20081100	-1.08521300	-1.54370600
H	3.39094200	-0.55570600	-2.57950800
C	5.43511500	-0.17991700	0.68272300
H	3.82455700	1.04664100	1.38155200
C	5.93196700	-0.95762800	-0.36203700
H	5.58325900	-1.69074100	-2.35755300
H	5.99236600	-0.09163200	1.60827600
H	6.88293200	-1.46715400	-0.25411000
IRC_TS1_point151			
B	-2.73144000	3.79804400	0.36314600
B	-1.63351000	3.62436900	1.76048900
B	-0.57217200	2.24265100	1.46390400
B	-2.34619100	2.52742700	-0.81838000
B	-1.01034100	1.63570700	-0.12193400
B	-1.30172400	4.85064000	0.51546700
B	-1.75262600	4.18555600	-1.06659300
H	-3.83983300	4.21032600	0.49156000
B	0.03096700	3.88984900	1.19077200
H	-1.97067200	3.91552600	2.86369400

B	0.43516600	2.62570900	0.02592500
H	-0.13813500	1.53709900	2.31061500
B	-0.68771100	2.81406400	-1.40645500
H	-3.15739300	2.00618500	-1.51238000
H	-1.39773800	6.01473200	0.74483300
B	-0.03785900	4.23113900	-0.56930400
H	-2.16478000	4.86665700	-1.95049000
H	0.88125600	4.35631100	1.88013700
H	-0.34521700	2.48785700	-2.49145400
H	0.77053900	4.92580000	-1.09732800
B	-2.28271000	2.18631300	0.94961100
I	-1.51322600	-0.88989900	-0.24081900
C	0.31528700	-1.61606200	0.62616900
C	0.58951700	-1.30435200	1.94836000
C	1.15311400	-2.38020800	-0.17255300
C	1.78555800	-1.77759800	2.49041400
H	-0.09467500	-0.71414200	2.54000800
C	2.33594500	-2.85072100	0.39392700
H	0.90643000	-2.59252100	-1.20317600
C	2.65375000	-2.54472800	1.71659800
H	2.03002900	-1.54041300	3.51919800
H	3.01398000	-3.44130700	-0.21017200
H	3.58330500	-2.90259700	2.14312100
O	-2.08706300	-3.23300500	0.11354700
C	-3.28712700	-3.50813500	-0.27632000
O	-4.05316100	-2.67806000	-0.79489800
C	-3.74194100	-4.93447600	-0.03099100
H	-4.08218000	-5.01115000	1.00668800
H	-4.57335100	-5.18446100	-0.69021900
H	-2.92141200	-5.63943800	-0.17048500
H	-0.39453300	0.66364900	-0.72649000
H	-3.05154500	1.43888200	1.45561400
N	1.81040100	2.04663100	-0.08614900
C	2.11791400	0.94649500	-0.79027900
H	2.54640200	2.44317400	0.48207200
C	3.47507300	0.34612100	-0.63323600
O	1.29337100	0.39876600	-1.54998000
C	3.97272100	-0.44487700	-1.67443000
C	4.21210000	0.47375800	0.54741700
C	5.19977900	-1.08498300	-1.54423200
H	3.38966700	-0.55590300	-2.58000300
C	5.43437100	-0.17963500	0.68218400
H	3.82379500	1.04679100	1.38104400
C	5.93108500	-0.95732000	-0.36265400

H	5.58218800	-1.69056300	-2.35804700
H	5.99163200	-0.09135200	1.60772000
H	6.88205500	-1.46685500	-0.25485800
IRC_TS1_point152			
B	-2.73096500	3.79606100	0.36251700
B	-1.63305500	3.62303300	1.75996200
B	-0.57158900	2.24129800	1.46356400
B	-2.34545200	2.52530500	-0.81893400
B	-1.00954900	1.62968000	-0.12286400
B	-1.30163800	4.84933000	0.51472800
B	-1.75282800	4.18384300	-1.06699100
H	-3.83968800	4.20733000	0.49094100
B	0.03074000	3.88893600	1.19059700
H	-1.97051400	3.91379100	2.86312800
B	0.43525700	2.62460400	0.02652700
H	-0.13733000	1.53662000	2.31083800
B	-0.68824100	2.81214300	-1.40741400
H	-3.15736000	2.00460700	-1.51247400
H	-1.39742200	6.01349600	0.74355700
B	-0.03798700	4.22905800	-0.57010100
H	-2.16493500	4.86457400	-1.95112000
H	0.88155400	4.35527100	1.87928600
H	-0.34485000	2.48643700	-2.49222700
H	0.77095000	4.92266200	-1.09855300
B	-2.28173400	2.18457700	0.94933400
I	-1.51233000	-0.88674500	-0.24086800
C	0.31512000	-1.61550100	0.62614500
C	0.58975200	-1.30417700	1.94837800
C	1.15285700	-2.38018600	-0.17228700
C	1.78570100	-1.77768400	2.49046300
H	-0.09414800	-0.71369800	2.54010100
C	2.33566800	-2.85096300	0.39406300
H	0.90621600	-2.59242000	-1.20295200
C	2.65375900	-2.54497600	1.71668000
H	2.03023900	-1.54052600	3.51924600
H	3.01349400	-3.44176300	-0.21007700
H	3.58330800	-2.90296400	2.14312900
O	-2.08728800	-3.23818600	0.11346400
C	-3.28716200	-3.51073100	-0.27607000
O	-4.05270700	-2.67933300	-0.79456600
C	-3.74483500	-4.93642400	-0.03127000
H	-4.08471800	-5.01304800	1.00654400
H	-4.57693500	-5.18520600	-0.69012400
H	-2.92548500	-5.64268800	-0.17129500

H	-0.37267900	0.67367700	-0.73671800
H	-3.05060800	1.43743400	1.45554500
N	1.81105600	2.04755700	-0.08557600
C	2.11743200	0.94699500	-0.78838600
H	2.54724400	2.44513500	0.48170900
C	3.47425600	0.34626100	-0.63376800
O	1.28925100	0.39832300	-1.54464400
C	3.97161800	-0.44485600	-1.67499600
C	4.21139000	0.47397600	0.54689700
C	5.19885100	-1.08476700	-1.54469200
H	3.38858900	-0.55611900	-2.58058100
C	5.43361300	-0.17935400	0.68169700
H	3.82297500	1.04688600	1.38053300
C	5.93026500	-0.95701200	-0.36318600
H	5.58124200	-1.69040700	-2.35845800
H	5.99081700	-0.09105500	1.60725400
H	6.88124200	-1.46654200	-0.25547600

IRC_TS1_point153

B	-2.73045400	3.79424800	0.36194600
B	-1.63255300	3.62188000	1.75944000
B	-0.57096200	2.24006300	1.46315700
B	-2.34467000	2.52328200	-0.81942000
B	-1.00868100	1.62330700	-0.12393900
B	-1.30153900	4.84823000	0.51401900
B	-1.75304900	4.18229200	-1.06732700
H	-3.83952500	4.20447300	0.49038700
B	0.03052800	3.88818700	1.19039500
H	-1.97025900	3.91218900	2.86259900
B	0.43526300	2.62354100	0.02709400
H	-0.13646400	1.53636000	2.31107500
B	-0.68881100	2.81031500	-1.40836100
H	-3.15740900	2.00329700	-1.51249100
H	-1.39706200	6.01247400	0.74231600
B	-0.03811900	4.22712200	-0.57088900
H	-2.16510900	4.86263500	-1.95170800
H	0.88190700	4.35435800	1.87838800
H	-0.34454200	2.48536600	-2.49309100
H	0.77133600	4.91968300	-1.09978300
B	-2.28065000	2.18298900	0.94905300
I	-1.51149500	-0.88380300	-0.24091800
C	0.31492400	-1.61504500	0.62611500
C	0.58998900	-1.30404500	1.94835900
C	1.15266900	-2.38015100	-0.17202800

C	1.78586200	-1.77774800	2.49048700
H	-0.09366200	-0.71334900	2.54016700
C	2.33544300	-2.85121800	0.39421200
H	0.90609800	-2.59227100	-1.20275100
C	2.65379900	-2.54523100	1.71677700
H	2.03045400	-1.54059900	3.51926900
H	3.01307200	-3.44224300	-0.20994800
H	3.58332400	-2.90334600	2.14318200
O	-2.08758500	-3.24333900	0.11347300
C	-3.28719800	-3.51319300	-0.27579800
O	-4.05229900	-2.68048800	-0.79428600
C	-3.74753400	-4.93823800	-0.03151300
H	-4.08699800	-5.01486000	1.00645600
H	-4.58027600	-5.18606300	-0.68995500
H	-2.92918600	-5.64560200	-0.17204900
H	-0.34802900	0.68384600	-0.74910900
H	-3.04959900	1.43620300	1.45554700
N	1.81174200	2.04850200	-0.08499500
C	2.11705300	0.94773100	-0.78648200
H	2.54805600	2.44702600	0.48150900
C	3.47344000	0.34640900	-0.63438400
O	1.28479300	0.39819200	-1.53929500
C	3.97060000	-0.44484800	-1.67559000
C	4.21065700	0.47417300	0.54636800
C	5.19801800	-1.08456800	-1.54509500
H	3.38769800	-0.55636800	-2.58125000
C	5.43284000	-0.17907800	0.68125200
H	3.82211400	1.04691500	1.38003200
C	5.92950600	-0.95670300	-0.36364800
H	5.58041000	-1.69027900	-2.35879100
H	5.98992200	-0.09075500	1.60686700
H	6.88048800	-1.46622100	-0.25597900

IRC_TS1_point154

B	-2.72992500	3.79264900	0.36141900
B	-1.63199400	3.62096500	1.75890700
B	-0.57024600	2.23902100	1.46267700
B	-2.34376500	2.52133800	-0.81981500
B	-1.00773200	1.61591900	-0.12522800
B	-1.30146600	4.84744800	0.51333300
B	-1.75335700	4.18096100	-1.06757400
H	-3.83938700	4.20168400	0.48987400
B	0.03027700	3.88771600	1.19017300
H	-1.96988400	3.91066100	2.86212400

B	0.43529000	2.62256400	0.02766900
H	-0.13540700	1.53653100	2.31140000
B	-0.68949700	2.80870500	-1.40937500
H	-3.15754500	2.00237300	-1.51237700
H	-1.39658100	6.01176700	0.74116100
B	-0.03829300	4.22538700	-0.57169700
H	-2.16529100	4.86085000	-1.95227700
H	0.88232300	4.35358600	1.87743800
H	-0.34411900	2.48487100	-2.49404500
H	0.77178000	4.91681800	-1.10098100
B	-2.27936100	2.18157700	0.94879000
I	-1.51073700	-0.88112400	-0.24097200
C	0.31470200	-1.61452000	0.62597600
C	0.59021600	-1.30396100	1.94827700
C	1.15255700	-2.38006200	-0.17175700
C	1.78605500	-1.77776200	2.49045500
H	-0.09327700	-0.71321200	2.54023400
C	2.33525100	-2.85151700	0.39440200
H	0.90611800	-2.59202300	-1.20257400
C	2.65389000	-2.54549800	1.71689600
H	2.03061200	-1.54068900	3.51926600
H	3.01258200	-3.44290100	-0.20977000
H	3.58331200	-2.90387100	2.14331200
O	-2.08796500	-3.24840900	0.11359900
C	-3.28725500	-3.51545100	-0.27550200
O	-4.05197000	-2.68150000	-0.79407400
C	-3.74995800	-4.93985100	-0.03168300
H	-4.08899700	-5.01653900	1.00641100
H	-4.58327500	-5.18696800	-0.68974500
H	-2.93242800	-5.64806800	-0.17283600
H	-0.32192900	0.69585900	-0.76100800
H	-3.04836900	1.43513000	1.45556300
N	1.81244100	2.04945500	-0.08439200
C	2.11670600	0.94861100	-0.78466900
H	2.54885800	2.44880700	0.48145600
C	3.47265300	0.34658300	-0.63507500
O	1.28009000	0.39842600	-1.53393900
C	3.96970200	-0.44485200	-1.67619700
C	4.20991800	0.47434800	0.54585000
C	5.19730000	-1.08440800	-1.54543400
H	3.38703100	-0.55661900	-2.58199700
C	5.43207600	-0.17881200	0.68085300
H	3.82118300	1.04676300	1.37962700
C	5.92883600	-0.95639200	-0.36404400

H	5.57970500	-1.69022000	-2.35902700
H	5.98892700	-0.09057700	1.60660800
H	6.87979700	-1.46593500	-0.25632700

IRC_TS1_point155

B	-2.72961000	3.79160900	0.36103700
B	-1.63149000	3.62025300	1.75826600
B	-0.56950800	2.23833500	1.46217300
B	-2.34282300	2.51976600	-0.81979100
B	-1.00652500	1.60807800	-0.12672300
B	-1.30151400	4.84737900	0.51285500
B	-1.75380200	4.17988800	-1.06770400
H	-3.83942900	4.19963400	0.48913700
B	0.03001800	3.88767800	1.18972600
H	-1.96942400	3.90970200	2.86152000
B	0.43531600	2.62191900	0.02819500
H	-0.13309700	1.53760500	2.31146700
B	-0.69022000	2.80759600	-1.41009800
H	-3.15753900	2.00156000	-1.51184000
H	-1.39646800	6.01172100	0.74008000
B	-0.03851700	4.22418800	-0.57244200
H	-2.16550600	4.85884400	-1.95314300
H	0.88258500	4.35340400	1.87630800
H	-0.34308400	2.48487700	-2.49455900
H	0.77215600	4.91462200	-1.10186900
B	-2.27802000	2.18066000	0.94871400
I	-1.51020200	-0.87909500	-0.24103300
C	0.31439100	-1.61394900	0.62575800
C	0.59039100	-1.30398200	1.94818500
C	1.15258400	-2.37984700	-0.17144800
C	1.78626800	-1.77766800	2.49027700
H	-0.09287100	-0.71357500	2.54079100
C	2.33513700	-2.85184400	0.39462400
H	0.90656400	-2.59196900	-1.20234900
C	2.65406100	-2.54582700	1.71704600
H	2.03083800	-1.54061000	3.51910900
H	3.01152000	-3.44440000	-0.20942300
H	3.58328100	-2.90441300	2.14367800
O	-2.08848800	-3.25270000	0.11380000
C	-3.28719400	-3.51720600	-0.27519900
O	-4.05181500	-2.68220000	-0.79400700
C	-3.75173000	-4.94101700	-0.03175600
H	-4.09014500	-5.01778300	1.00659800
H	-4.58559600	-5.18820700	-0.68911500

H	-2.93469100	-5.64981900	-0.17309800
H	-0.28686000	0.71038100	-0.77623400
H	-3.04677200	1.43406600	1.45554700
N	1.81300300	2.05008100	-0.08382100
C	2.11663000	0.94975200	-0.78304400
H	2.54979800	2.45039700	0.48095800
C	3.47214800	0.34687600	-0.63575400
O	1.27511000	0.39881500	-1.52920700
C	3.96904200	-0.44489200	-1.67670800
C	4.20933300	0.47452700	0.54560700
C	5.19678000	-1.08436400	-1.54571400
H	3.38678800	-0.55684100	-2.58276300
C	5.43142200	-0.17864800	0.68055400
H	3.81983200	1.04639600	1.37936900
C	5.92834500	-0.95611300	-0.36437600
H	5.57917600	-1.69021200	-2.35924400
H	5.98821400	-0.09039700	1.60632000
H	6.87932300	-1.46554300	-0.25651100

IRC_TS1_point156

B	-2.72926745	3.79111444	0.36083124
B	-1.63131545	3.61991244	1.75807524
B	-0.56943945	2.23764744	1.46185124
B	-2.34223345	2.51896844	-0.82002276
B	-1.00552445	1.60148544	-0.12839576
B	-1.30126745	4.84706344	0.51269424
B	-1.75382945	4.17947244	-1.06766076
H	-3.83927645	4.19859044	0.48871924
B	0.02982555	3.88730244	1.18991124
H	-1.96915645	3.90898344	2.86140824
B	0.43504355	2.62113844	0.02854124
H	-0.13300245	1.53774244	2.31177724
B	-0.69060145	2.80677344	-1.41081776
H	-3.15776945	2.00179644	-1.51186076
H	-1.39561345	6.01147244	0.73952024
B	-0.03841045	4.22329044	-0.57267576
H	-2.16504545	4.85822344	-1.95339676
H	0.88306155	4.35252244	1.87586024
H	-0.34255145	2.48555044	-2.49542276
H	0.77265655	4.91306344	-1.10215376
B	-2.27735045	2.18032044	0.94835824
I	-1.50983245	-0.87759156	-0.24107376
C	0.31400955	-1.61366156	0.62548624
C	0.59052755	-1.30405856	1.94801624

C	1.15252855	-2.37985956	-0.17122276
C	1.78634755	-1.77772556	2.49026324
H	-0.09266945	-0.71367256	2.54077724
C	2.33518455	-2.85185456	0.39468224
H	0.90659155	-2.59199256	-1.20218376
C	2.65419855	-2.54588556	1.71709124
H	2.03092055	-1.54073756	3.51913224
H	3.01157555	-3.44445656	-0.20934576
H	3.58343055	-2.90447156	2.14371824
O	-2.08890945	-3.25620856	0.11395724
C	-3.28688145	-3.51848056	-0.27489276
O	-4.05180045	-2.68262356	-0.79397276
C	-3.75298545	-4.94178156	-0.03193276
H	-4.09114745	-5.01877456	1.00652324
H	-4.58714145	-5.18921556	-0.68891976
H	-2.93617945	-5.65089056	-0.17342476
H	-0.24277445	0.72597044	-0.79798776
H	-3.04612045	1.43371044	1.45512324
N	1.81351155	2.05027344	-0.08351176
C	2.11694255	0.95084744	-0.78125676
H	2.55028855	2.45114644	0.48105224
C	3.47154755	0.34680544	-0.63631976
O	1.27028155	0.39936644	-1.52531576
C	3.96852855	-0.44505356	-1.67711676
C	4.20890555	0.47463944	0.54532824
C	5.19646955	-1.08429556	-1.54583176
H	3.38665755	-0.55727256	-2.58340576
C	5.43099855	-0.17843356	0.68033424
H	3.81937455	1.04626844	1.37920124
C	5.92802555	-0.95593956	-0.36454776
H	5.57884355	-1.69016056	-2.35932076
H	5.98761355	-0.09005756	1.60616724
H	6.87899855	-1.46534656	-0.25664576
IRC_TS1_point157			
B	-2.72892500	3.79062000	0.36062600
B	-1.63114100	3.61957200	1.75788400
B	-0.56937100	2.23696000	1.46152900
B	-2.34164400	2.51817100	-0.82025400
B	-1.00452400	1.59489300	-0.13006800
B	-1.30102000	4.84674800	0.51253400
B	-1.75385700	4.17905700	-1.06761800
H	-3.83912400	4.19754700	0.48830100
B	0.02963300	3.88692700	1.19009700
H	-1.96888900	3.90826500	2.86129600

B	0.43477100	2.62035800	0.02888800
H	-0.13290800	1.53788000	2.31208800
B	-0.69098300	2.80595100	-1.41153800
H	-3.15800000	2.00203300	-1.51188100
H	-1.39475900	6.01122400	0.73896000
B	-0.03830300	4.22239300	-0.57291000
H	-2.16458500	4.85760200	-1.95365100
H	0.88353900	4.35164100	1.87541300
H	-0.34201900	2.48622400	-2.49628600
H	0.77315800	4.91150500	-1.10243800
B	-2.27668100	2.17998100	0.94800300
I	-1.50946300	-0.87608900	-0.24111500
C	0.31362800	-1.61337400	0.62521500
C	0.59066400	-1.30413500	1.94784700
C	1.15247300	-2.37987200	-0.17099700
C	1.78642700	-1.77778300	2.49025000
H	-0.09246800	-0.71377000	2.54076300
C	2.33523200	-2.85186500	0.39474100
H	0.90662000	-2.59201600	-1.20201900
C	2.65433600	-2.54594400	1.71713700
H	2.03100300	-1.54086500	3.51915500
H	3.01163100	-3.44451300	-0.20926800
H	3.58358000	-2.90453000	2.14375900
O	-2.08933100	-3.25971700	0.11411500
C	-3.28656900	-3.51975500	-0.27458600
O	-4.05178600	-2.68304700	-0.79393900
C	-3.75424000	-4.94254600	-0.03210900
H	-4.09215000	-5.01976600	1.00644900
H	-4.58868700	-5.19022500	-0.68872500
H	-2.93766800	-5.65196200	-0.17375200
H	-0.19868900	0.74155900	-0.81974200
H	-3.04546900	1.43335500	1.45470000
N	1.81402100	2.05046600	-0.08320300
C	2.11725500	0.95194300	-0.77947000
H	2.55077900	2.45189500	0.48114600
C	3.47094700	0.34673500	-0.63688600
O	1.26545300	0.39991800	-1.52142500
C	3.96801500	-0.44521500	-1.67752600
C	4.20847800	0.47475200	0.54504900
C	5.19615900	-1.08422700	-1.54595000
H	3.38652700	-0.55770400	-2.58404900
C	5.43057600	-0.17821900	0.68011400
H	3.81891700	1.04614100	1.37903400
C	5.92770600	-0.95576600	-0.36471900

H	5.57851100	-1.69010900	-2.35939800
H	5.98701300	-0.08971800	1.60601500
H	6.87867400	-1.46515000	-0.25678000

IRC_TS1_point158

B	-2.72855500	3.79038400	0.36054900
B	-1.63117000	3.61949800	1.75796900
B	-0.56965300	2.23627800	1.46133900
B	-2.34130900	2.51773200	-0.82062300
B	-1.00379300	1.58971800	-0.13156500
B	-1.30063700	4.84620900	0.51248500
B	-1.75361800	4.17896300	-1.06752600
H	-3.83885000	4.19703400	0.48817300
B	0.02950700	3.88636000	1.19059100
H	-1.96869200	3.90769800	2.86150500
B	0.43423600	2.61946300	0.02900300
H	-0.13429900	1.53737900	2.31262900
B	-0.69105600	2.80514900	-1.41218700
H	-3.15837700	2.00275900	-1.51222400
H	-1.39352200	6.01078600	0.73872300
B	-0.03803400	4.22169600	-0.57287500
H	-2.16383000	4.85776200	-1.95352200
H	0.88416700	4.35034600	1.87533300
H	-0.34200800	2.48719000	-2.49740500
H	0.77361700	4.91041200	-1.10248500
B	-2.27639500	2.17992500	0.94750400
I	-1.50917200	-0.87489500	-0.24115100
C	0.31323500	-1.61329200	0.62496100
C	0.59078000	-1.30422000	1.94765400
C	1.15235400	-2.38002000	-0.17082700
C	1.78644400	-1.77792900	2.49035400
H	-0.09244800	-0.71362400	2.54029800
C	2.33533600	-2.85173300	0.39472000
H	0.90627000	-2.59203800	-1.20188500
C	2.65442200	-2.54585000	1.71712100
H	2.03101500	-1.54110600	3.51929800
H	3.01244600	-3.44363000	-0.20933600
H	3.58379900	-2.90438600	2.14358400
O	-2.08968000	-3.26265800	0.11424900
C	-3.28612300	-3.52076500	-0.27426600
O	-4.05185400	-2.68331800	-0.79391100
C	-3.75523800	-4.94309500	-0.03232600
H	-4.09315200	-5.02062400	1.00620600
H	-4.58983800	-5.19102300	-0.68882100

H	-2.93877900	-5.65266200	-0.17421100
H	-0.15019000	0.75398900	-0.84473100
H	-3.04544400	1.43351300	1.45420200
N	1.81451500	2.05038500	-0.08308400
C	2.11785000	0.95303200	-0.77752800
H	2.55099600	2.45218000	0.48156500
C	3.47025900	0.34646000	-0.63739100
O	1.26084400	0.40063700	-1.51818200
C	3.96758800	-0.44541900	-1.67787500
C	4.20812500	0.47481300	0.54472000
C	5.19595400	-1.08413800	-1.54597600
H	3.38640500	-0.55823200	-2.58458700
C	5.43028300	-0.17798300	0.67994200
H	3.81916800	1.04616500	1.37897000
C	5.92746900	-0.95566700	-0.36480400
H	5.57825200	-1.69005500	-2.35938800
H	5.98642400	-0.08935800	1.60598300
H	6.87841600	-1.46510800	-0.25692700

IRC_TS1_point159

B	-2.72836300	3.79028300	0.36057200
B	-1.63121900	3.61943100	1.75793100
B	-0.56984000	2.23579700	1.46117400
B	-2.34104400	2.51735800	-0.82066200
B	-1.00349700	1.58598600	-0.13246500
B	-1.30042300	4.84601700	0.51247500
B	-1.75348500	4.17877400	-1.06747700
H	-3.83871300	4.19690600	0.48793200
B	0.02944800	3.88603100	1.19074800
H	-1.96848300	3.90758000	2.86155000
B	0.43361700	2.61880100	0.02897300
H	-0.13457500	1.53735600	2.31286400
B	-0.69105600	2.80443700	-1.41244400
H	-3.15858900	2.00306500	-1.51227300
H	-1.39290400	6.01064100	0.73843800
B	-0.03787400	4.22127600	-0.57288500
H	-2.16333200	4.85753000	-1.95365100
H	0.88455400	4.34963300	1.87509700
H	-0.34174300	2.48793500	-2.49813500
H	0.77383400	4.90986500	-1.10243200
B	-2.27608600	2.17999700	0.94719900
I	-1.50897400	-0.87404200	-0.24119100
C	0.31285000	-1.61324500	0.62482000
C	0.59087300	-1.30430600	1.94752700

C	1.15229900	-2.38007800	-0.17065400
C	1.78647000	-1.77799200	2.49037900
H	-0.09231200	-0.71367600	2.54025800
C	2.33542300	-2.85166500	0.39472400
H	0.90623200	-2.59226200	-1.20172600
C	2.65451100	-2.54584700	1.71713400
H	2.03111400	-1.54119200	3.51934700
H	3.01271300	-3.44342700	-0.20929800
H	3.58395000	-2.90428800	2.14358100
O	-2.09006100	-3.26490300	0.11436800
C	-3.28565400	-3.52154800	-0.27395200
O	-4.05197300	-2.68347300	-0.79394500
C	-3.75595800	-4.94345600	-0.03248100
H	-4.09372200	-5.02130000	1.00616400
H	-4.59076600	-5.19193600	-0.68859600
H	-2.93954100	-5.65318400	-0.17430700
H	-0.09729300	0.75702200	-0.87295400
H	-3.04525400	1.43360400	1.45396100
N	1.81492700	2.05014200	-0.08303000
C	2.11880700	0.95438500	-0.77572200
H	2.55141500	2.45249000	0.48148400
C	3.46979300	0.34632000	-0.63784700
O	1.25641000	0.40128300	-1.51562600
C	3.96727600	-0.44558700	-1.67815300
C	4.20788400	0.47489200	0.54458400
C	5.19580100	-1.08409900	-1.54601300
H	3.38647100	-0.55865600	-2.58510000
C	5.43003500	-0.17783900	0.67981000
H	3.81900400	1.04610700	1.37890100
C	5.92729400	-0.95558500	-0.36488700
H	5.57802600	-1.68999500	-2.35942400
H	5.98602300	-0.08901700	1.60587400
H	6.87823100	-1.46499900	-0.25701100

IRC_TS1_point160

B	-2.72825300	3.79026200	0.36064600
B	-1.63129600	3.61943200	1.75789100
B	-0.56998200	2.23545100	1.46104100
B	-2.34087900	2.51707100	-0.82057800
B	-1.00374600	1.58370500	-0.13275500
B	-1.30030000	4.84592600	0.51246500
B	-1.75336900	4.17859400	-1.06746500
H	-3.83861900	4.19702500	0.48778500
B	0.02943800	3.88581900	1.19077900

H	-1.96829100	3.90764500	2.86161000
B	0.43291600	2.61830900	0.02883500
H	-0.13464900	1.53735900	2.31300300
B	-0.69096300	2.80380000	-1.41247200
H	-3.15874500	2.00326400	-1.51227300
H	-1.39254600	6.01059500	0.73829100
B	-0.03776100	4.22104900	-0.57288600
H	-2.16296500	4.85734600	-1.95376800
H	0.88482500	4.34918400	1.87493200
H	-0.34155200	2.48853600	-2.49870000
H	0.77392800	4.90971500	-1.10231800
B	-2.27584100	2.18011500	0.94697600
I	-1.50883300	-0.87344200	-0.24122800
C	0.31254700	-1.61326600	0.62477800
C	0.59095600	-1.30437700	1.94744800
C	1.15227300	-2.38011400	-0.17050600
C	1.78650100	-1.77802300	2.49039300
H	-0.09223200	-0.71374500	2.54022800
C	2.33549500	-2.85162900	0.39473500
H	0.90618700	-2.59245100	-1.20159400
C	2.65458100	-2.54585600	1.71714700
H	2.03120600	-1.54126700	3.51938000
H	3.01287500	-3.44336100	-0.20925600
H	3.58403900	-2.90427400	2.14359300
O	-2.09040200	-3.26658400	0.11447100
C	-3.28520900	-3.52212600	-0.27367300
O	-4.05210900	-2.68355900	-0.79399700
C	-3.75646700	-4.94369200	-0.03258500
H	-4.09412500	-5.02178000	1.00612600
H	-4.59144500	-5.19268600	-0.68841800
H	-2.94005100	-5.65350300	-0.17441700
H	-0.04318600	0.75227300	-0.90411700
H	-3.04517300	1.43379200	1.45391800
N	1.81527600	2.04980100	-0.08308000
C	2.11988900	0.95576700	-0.77401800
H	2.55183400	2.45268000	0.48130900
C	3.46942400	0.34622900	-0.63825500
O	1.25238000	0.40181600	-1.51362600
C	3.96705500	-0.44572100	-1.67837200
C	4.20771100	0.47496800	0.54451500
C	5.19569600	-1.08407400	-1.54603900
H	3.38659800	-0.55898300	-2.58553200
C	5.42984500	-0.17773200	0.67971300
H	3.81888200	1.04599900	1.37892100

C	5.92716900	-0.95552200	-0.36495500
H	5.57784700	-1.68994500	-2.35944600
H	5.98569300	-0.08879600	1.60580800
H	6.87808600	-1.46493000	-0.25705400

IRC_TS1_point161

B	-2.72818800	3.79028000	0.36074000
B	-1.63138200	3.61946600	1.75785900
B	-0.57009800	2.23519100	1.46093500
B	-2.34078200	2.51685800	-0.82044700
B	-1.00442900	1.58245300	-0.13254700
B	-1.30022500	4.84588200	0.51246000
B	-1.75326200	4.17843400	-1.06747200
H	-3.83855200	4.19726700	0.48770200
B	0.02945800	3.88567000	1.19075400
H	-1.96812800	3.90779900	2.86167400
B	0.43219900	2.61794200	0.02865900
H	-0.13465200	1.53734300	2.31307900
B	-0.69082700	2.80324200	-1.41238300
H	-3.15887300	2.00340000	-1.51226400
H	-1.39233700	6.01058900	0.73821500
B	-0.03767100	4.22093000	-0.57287100
H	-2.16269000	4.85721400	-1.95386800
H	0.88501800	4.34889400	1.87481900
H	-0.34143300	2.48899900	-2.49916300
H	0.77395100	4.90976200	-1.10219500
B	-2.27565400	2.18024700	0.94679700
I	-1.50873300	-0.87300900	-0.24125700
C	0.31231800	-1.61330400	0.62475900
C	0.59103100	-1.30443700	1.94739700
C	1.15226400	-2.38014000	-0.17038300
C	1.78652800	-1.77804000	2.49040600
H	-0.09217600	-0.71380200	2.54019900
C	2.33555700	-2.85160800	0.39474500
H	0.90612900	-2.59259400	-1.20148600
C	2.65463600	-2.54586900	1.71715600
H	2.03129200	-1.54132800	3.51941000
H	3.01299900	-3.44334000	-0.20921200
H	3.58410000	-2.90428500	2.14361000
O	-2.09069800	-3.26788200	0.11455100
C	-3.28479400	-3.52256500	-0.27342800
O	-4.05224500	-2.68360400	-0.79405600
C	-3.75684100	-4.94385100	-0.03266500
H	-4.09441700	-5.02214800	1.00610300

H	-4.59195900	-5.19331100	-0.68826500
H	-2.94040000	-5.65370700	-0.17450400
H	0.01099400	0.74349300	-0.93703300
H	-3.04517500	1.43402700	1.45398300
N	1.81556100	2.04940900	-0.08318900
C	2.12098800	0.95709000	-0.77240300
H	2.55222800	2.45278500	0.48110000
C	3.46911200	0.34616300	-0.63861400
O	1.24877600	0.40220600	-1.51206700
C	3.96689300	-0.44583100	-1.67854800
C	4.20758300	0.47503700	0.54448400
C	5.19562200	-1.08405600	-1.54605700
H	3.38674300	-0.55925100	-2.58589500
C	5.42969700	-0.17765000	0.67964000
H	3.81880100	1.04588400	1.37897600
C	5.92707500	-0.95547600	-0.36500800
H	5.57769900	-1.68990000	-2.35946100
H	5.98541600	-0.08863500	1.60576400
H	6.87797000	-1.46488300	-0.25708000

IRC_TS1_point162

B	-2.72814600	3.79031800	0.36084400
B	-1.63147400	3.61951600	1.75783300
B	-0.57020400	2.23497100	1.46084200
B	-2.34072200	2.51668500	-0.82029000
B	-1.00533300	1.58168300	-0.13209600
B	-1.30017400	4.84585900	0.51245900
B	-1.75315700	4.17828500	-1.06748900
H	-3.83849600	4.19757900	0.48765400
B	0.02949300	3.88554800	1.19070300
H	-1.96798200	3.90800300	2.86174200
B	0.43146100	2.61764300	0.02846600
H	-0.13463700	1.53732000	2.31314800
B	-0.69066800	2.80271900	-1.41223000
H	-3.15899400	2.00351000	-1.51225200
H	-1.39220200	6.01060300	0.73817400
B	-0.03759200	4.22086400	-0.57284500
H	-2.16245600	4.85711400	-1.95395800
H	0.88517400	4.34868300	1.87473500
H	-0.34134700	2.48937800	-2.49957600
H	0.77394200	4.90990600	-1.10207200
B	-2.27549600	2.18038900	0.94663600
I	-1.50865800	-0.87265500	-0.24127600
C	0.31211200	-1.61333100	0.62472700

C	0.59110400	-1.30449300	1.94736000
C	1.15226400	-2.38016000	-0.17027500
C	1.78655200	-1.77805000	2.49041900
H	-0.09212900	-0.71385000	2.54016500
C	2.33561400	-2.85159300	0.39475400
H	0.90606600	-2.59271600	-1.20139100
C	2.65468500	-2.54588300	1.71716400
H	2.03137800	-1.54138500	3.51944000
H	3.01311100	-3.44333800	-0.20916600
H	3.58414900	-2.90430300	2.14362900
O	-2.09097500	-3.26900400	0.11461900
C	-3.28439000	-3.52293700	-0.27319800
O	-4.05238200	-2.68362900	-0.79412000
C	-3.75715100	-4.94397500	-0.03273200
H	-4.09465900	-5.02246400	1.00608800
H	-4.59239700	-5.19387800	-0.68812500
H	-2.94067400	-5.65385900	-0.17458000
H	0.06510800	0.73330900	-0.97065700
H	-3.04522500	1.43429400	1.45410400
N	1.81580400	2.04897100	-0.08332700
C	2.12213500	0.95839900	-0.77080300
H	2.55261000	2.45285600	0.48086200
C	3.46882300	0.34610800	-0.63894900
O	1.24543600	0.40248800	-1.51078400
C	3.96676000	-0.44593000	-1.67870300
C	4.20747900	0.47510300	0.54447200
C	5.19556300	-1.08404100	-1.54607000
H	3.38690000	-0.55949400	-2.58622700
C	5.42956800	-0.17757900	0.67957900
H	3.81874000	1.04576600	1.37904800
C	5.92699800	-0.95543600	-0.36505400
H	5.57756500	-1.68985600	-2.35947300
H	5.98516400	-0.08849900	1.60573000
H	6.87786800	-1.46484800	-0.25709900

IRC_TS1_point163

B	-2.72811600	3.79037200	0.36096100
B	-1.63157500	3.61958000	1.75781100
B	-0.57031100	2.23476000	1.46075200
B	-2.34068100	2.51652700	-0.82010600
B	-1.00632200	1.58106300	-0.13157800
B	-1.30013400	4.84584800	0.51246100
B	-1.75304400	4.17813200	-1.06751400
H	-3.83844200	4.19795700	0.48762500

B	0.02954100	3.88543500	1.19063300
H	-1.96783900	3.90825000	2.86181800
B	0.43065700	2.61736900	0.02825100
H	-0.13462800	1.53730800	2.31324800
B	-0.69048300	2.80218300	-1.41202300
H	-3.15912600	2.00361700	-1.51223900
H	-1.39210300	6.01063100	0.73815300
B	-0.03751500	4.22082500	-0.57280800
H	-2.16223100	4.85703000	-1.95404900
H	0.88531800	4.34850500	1.87466500
H	-0.34127200	2.48970700	-2.49996800
H	0.77391400	4.91011600	-1.10194100
B	-2.27534900	2.18054300	0.94647500
I	-1.50858700	-0.87231800	-0.24129200
C	0.31190400	-1.61336100	0.62468800
C	0.59118100	-1.30454900	1.94732700
C	1.15227100	-2.38017900	-0.17017100
C	1.78657400	-1.77805700	2.49043400
H	-0.09208100	-0.71389200	2.54012500
C	2.33567300	-2.85158200	0.39476300
H	0.90600400	-2.59284100	-1.20129800
C	2.65473200	-2.54589800	1.71717000
H	2.03146800	-1.54144300	3.51947200
H	3.01322400	-3.44334500	-0.20911500
H	3.58419500	-2.90432700	2.14364800
O	-2.09125400	-3.27009400	0.11468300
C	-3.28397300	-3.52328900	-0.27296600
O	-4.05252700	-2.68364600	-0.79419000
C	-3.75744400	-4.94408800	-0.03279600
H	-4.09488600	-5.02276900	1.00607500
H	-4.59281600	-5.19444000	-0.68798500
H	-2.94092400	-5.65399000	-0.17465300
H	0.11882700	0.72173800	-1.00449300
H	-3.04531200	1.43460500	1.45427000
N	1.81603600	2.04848800	-0.08348800
C	2.12343500	0.95978200	-0.76914600
H	2.55300200	2.45293300	0.48058700
C	3.46852900	0.34605900	-0.63928400
O	1.24213400	0.40271400	-1.50964000
C	3.96663700	-0.44603100	-1.67885600
C	4.20738500	0.47516900	0.54446800
C	5.19550700	-1.08402500	-1.54608300
H	3.38707400	-0.55973800	-2.58655900
C	5.42944300	-0.17750900	0.67952300

H	3.81868600	1.04564100	1.37913600
C	5.92692400	-0.95539700	-0.36509800
H	5.57743200	-1.68980900	-2.35948700
H	5.98491300	-0.08837300	1.60570000
H	6.87776700	-1.46481700	-0.25711400

IRC_TS1_point164

B	-2.72809500	3.79043500	0.36108200
B	-1.63167600	3.61965300	1.75779100
B	-0.57041400	2.23456200	1.46066600
B	-2.34065500	2.51638500	-0.81991200
B	-1.00733400	1.58058100	-0.13103700
B	-1.30010300	4.84584700	0.51246600
B	-1.75292900	4.17798300	-1.06754300
H	-3.83839000	4.19836300	0.48761200
B	0.02959500	3.88533100	1.19055100
H	-1.96770400	3.90851400	2.86189500
B	0.42983600	2.61712400	0.02803200
H	-0.13463500	1.53731700	2.31338600
B	-0.69029000	2.80165700	-1.41178600
H	-3.15926200	2.00372200	-1.51222100
H	-1.39203600	6.01066700	0.73814800
B	-0.03744100	4.22080900	-0.57276300
H	-2.16202100	4.85696200	-1.95413300
H	0.88544700	4.34835500	1.87460900
H	-0.34120200	2.48996300	-2.50031000
H	0.77387800	4.91036200	-1.10181400
B	-2.27521500	2.18069900	0.94631900
I	-1.50851800	-0.87200300	-0.24130800
C	0.31170100	-1.61339900	0.62465000
C	0.59125700	-1.30460300	1.94730000
C	1.15228200	-2.38019800	-0.17007300
C	1.78659400	-1.77806100	2.49044900
H	-0.09203500	-0.71393100	2.54008300
C	2.33572900	-2.85157300	0.39477200
H	0.90594900	-2.59297200	-1.20120800
C	2.65477800	-2.54591400	1.71717500
H	2.03155600	-1.54149900	3.51950300
H	3.01333000	-3.44335800	-0.20906300
H	3.58423800	-2.90435100	2.14366800
O	-2.09151900	-3.27112000	0.11474200
C	-3.28357600	-3.52361200	-0.27274700
O	-4.05266700	-2.68366100	-0.79425800
C	-3.75771400	-4.94419100	-0.03285400

H	-4.09509400	-5.02305300	1.00606400
H	-4.59320200	-5.19496500	-0.68785300
H	-2.94115200	-5.65410500	-0.17472100
H	0.17242800	0.70850400	-1.03804400
H	-3.04542300	1.43494000	1.45446100
N	1.81624600	2.04799300	-0.08366300
C	2.12477500	0.96113900	-0.76753100
H	2.55337700	2.45303300	0.48029400
C	3.46823800	0.34601700	-0.63960300
O	1.23883800	0.40295300	-1.50854800
C	3.96652300	-0.44613000	-1.67900300
C	4.20730300	0.47523300	0.54447000
C	5.19545500	-1.08401000	-1.54609400
H	3.38725000	-0.55997100	-2.58687900
C	5.42932400	-0.17744200	0.67947100
H	3.81863900	1.04551600	1.37923000
C	5.92685600	-0.95536200	-0.36513900
H	5.57730600	-1.68976300	-2.35950100
H	5.98467400	-0.08825800	1.60567600
H	6.87767200	-1.46479000	-0.25712600

IRC_TS1_point165

B	-2.72808000	3.79050300	0.36120400
B	-1.63177500	3.61972900	1.75777400
B	-0.57051300	2.23437400	1.46058400
B	-2.34063900	2.51625400	-0.81971500
B	-1.00840300	1.58023100	-0.13044700
B	-1.30007900	4.84585200	0.51247200
B	-1.75281000	4.17783600	-1.06757600
H	-3.83833900	4.19878300	0.48760900
B	0.02965400	3.88523500	1.19046100
H	-1.96757700	3.90878200	2.86197000
B	0.42901100	2.61690500	0.02781600
H	-0.13465300	1.53734400	2.31355100
B	-0.69009400	2.80114000	-1.41153200
H	-3.15939900	2.00382500	-1.51220000
H	-1.39199400	6.01070700	0.73815700
B	-0.03737200	4.22080900	-0.57271100
H	-2.16182400	4.85690400	-1.95421200
H	0.88556400	4.34822700	1.87456500
H	-0.34112900	2.49014200	-2.50060000
H	0.77383500	4.91062500	-1.10169100
B	-2.27509700	2.18085100	0.94617100
I	-1.50845400	-0.87170700	-0.24132200

C	0.31150300	-1.61344500	0.62462000
C	0.59133300	-1.30465400	1.94727700
C	1.15229700	-2.38021700	-0.16998200
C	1.78661200	-1.77806400	2.49046300
H	-0.09198900	-0.71396900	2.54004400
C	2.33578400	-2.85156700	0.39478000
H	0.90590000	-2.59310400	-1.20112100
C	2.65482100	-2.54593000	1.71718000
H	2.03164000	-1.54155300	3.51953200
H	3.01343100	-3.44337300	-0.20901200
H	3.58427800	-2.90437600	2.14368600
O	-2.09176900	-3.27209400	0.11479600
C	-3.28320300	-3.52390900	-0.27254200
O	-4.05280100	-2.68367600	-0.79432300
C	-3.75796700	-4.94428900	-0.03290700
H	-4.09528500	-5.02331700	1.00605400
H	-4.59356000	-5.19545400	-0.68772900
H	-2.94136400	-5.65421000	-0.17478500
H	0.22601800	0.69472800	-1.07166200
H	-3.04554800	1.43529300	1.45466700
N	1.81642900	2.04749300	-0.08384900
C	2.12611000	0.96243900	-0.76595700
H	2.55372600	2.45315700	0.47998300
C	3.46794500	0.34598100	-0.63990700
O	1.23562700	0.40319200	-1.50750400
C	3.96641600	-0.44622700	-1.67914600
C	4.20723100	0.47529300	0.54447200
C	5.19540500	-1.08399500	-1.54610500
H	3.38742100	-0.56019300	-2.58718300
C	5.42921100	-0.17737700	0.67942300
H	3.81859500	1.04539300	1.37932600
C	5.92679300	-0.95532800	-0.36517900
H	5.57718600	-1.68971900	-2.35951800
H	5.98444800	-0.08815400	1.60565400
H	6.87758100	-1.46476700	-0.25713700

IRC_TS1_point166

B	-2.72806800	3.79058900	0.36134800
B	-1.63188900	3.61982400	1.75775600
B	-0.57062300	2.23415800	1.46048800
B	-2.34063100	2.51611000	-0.81947900
B	-1.00971400	1.57991000	-0.12972200
B	-1.30005700	4.84586300	0.51248100
B	-1.75266500	4.17766500	-1.06761700

H	-3.83827500	4.19928600	0.48761500
B	0.02972900	3.88512700	1.19034700
H	-1.96743400	3.90909900	2.86205500
B	0.42803100	2.61666700	0.02756300
H	-0.13468500	1.53739100	2.31376500
B	-0.68985700	2.80052900	-1.41121400
H	-3.15956100	2.00394900	-1.51216500
H	-1.39196700	6.01075700	0.73817800
B	-0.03729300	4.22082000	-0.57264300
H	-2.16159900	4.85684200	-1.95429700
H	0.88568900	4.34809000	1.87452200
H	-0.34103900	2.49027300	-2.50087800
H	0.77378100	4.91094700	-1.10154900
B	-2.27497500	2.18102900	0.94600500
I	-1.50838400	-0.87137300	-0.24133500
C	0.31126600	-1.61349900	0.62459200
C	0.59142200	-1.30471200	1.94725400
C	1.15231800	-2.38023900	-0.16988000
C	1.78663400	-1.77806700	2.49048100
H	-0.09193500	-0.71401800	2.54000700
C	2.33584800	-2.85156100	0.39478900
H	0.90584700	-2.59325500	-1.20101800
C	2.65487200	-2.54594900	1.71718400
H	2.03173600	-1.54161600	3.51956400
H	3.01354500	-3.44339200	-0.20895300
H	3.58432400	-2.90440400	2.14370700
O	-2.09204900	-3.27320900	0.11485900
C	-3.28279300	-3.52424000	-0.27231600
O	-4.05295000	-2.68369800	-0.79439600
C	-3.75825300	-4.94440400	-0.03296500
H	-4.09549900	-5.02361300	1.00604200
H	-4.59395800	-5.19599400	-0.68759000
H	-2.94160700	-5.65432800	-0.17485700
H	0.27841900	0.68156300	-1.10704400
H	-3.04570600	1.43573500	1.45492200
N	1.81661600	2.04691800	-0.08406200
C	2.12766800	0.96388000	-0.76415600
H	2.55409100	2.45333900	0.47958300
C	3.46760800	0.34594500	-0.64024200
O	1.23263500	0.40329400	-1.50660400
C	3.96629300	-0.44633900	-1.67931300
C	4.20715400	0.47535900	0.54447200
C	5.19534600	-1.08397600	-1.54611900
H	3.38761300	-0.56044400	-2.58752900

C	5.42908000	-0.17730100	0.67937000
H	3.81854200	1.04525100	1.37944100
C	5.92672000	-0.95528800	-0.36522400
H	5.57705000	-1.68966800	-2.35954000
H	5.98419200	-0.08804100	1.60563400
H	6.87747800	-1.46474300	-0.25714800

IRC_TS1_point167

B	-2.72805500	3.79073400	0.36156400
B	-1.63205200	3.61997600	1.75773200
B	-0.57078100	2.23383100	1.46034500
B	-2.34063900	2.51590200	-0.81912000
B	-1.01171600	1.57947200	-0.12861800
B	-1.30002800	4.84588900	0.51249500
B	-1.75243500	4.17740200	-1.06768300
H	-3.83815900	4.20005400	0.48763300
B	0.02984600	3.88497000	1.19016300
H	-1.96722200	3.90956500	2.86216200
B	0.42654400	2.61631500	0.02718000
H	-0.13477300	1.53749100	2.31410300
B	-0.68948800	2.79959400	-1.41071000
H	-3.15979800	2.00415200	-1.51208200
H	-1.39194700	6.01082900	0.73821700
B	-0.03717300	4.22084800	-0.57252900
H	-2.16125800	4.85672900	-1.95441700
H	0.88585900	4.34787600	1.87445800
H	-0.34091300	2.49036500	-2.50116300
H	0.77369200	4.91142000	-1.10134100
B	-2.27483300	2.18129600	0.94577300
I	-1.50827600	-0.87087300	-0.24135300
C	0.31090700	-1.61357100	0.62454200
C	0.59155000	-1.30479600	1.94721900
C	1.15234600	-2.38027400	-0.16973000
C	1.78666800	-1.77807300	2.49050700
H	-0.09184500	-0.71409400	2.53996200
C	2.33594400	-2.85155300	0.39480500
H	0.90577900	-2.59347600	-1.20085300
C	2.65495000	-2.54597800	1.71719200
H	2.03187200	-1.54170500	3.51960600
H	3.01370700	-3.44341800	-0.20886600
H	3.58439300	-2.90444700	2.14373900
O	-2.09244100	-3.27488000	0.11496000
C	-3.28224800	-3.52472200	-0.27200800
O	-4.05315500	-2.68374900	-0.79449300

C	-3.75868500	-4.94458600	-0.03304700
H	-4.09581000	-5.02404500	1.00602100
H	-4.59453200	-5.19674900	-0.68738900
H	-2.94198900	-5.65451700	-0.17496000
H	0.32586000	0.67005400	-1.14732400
H	-3.04594300	1.43646300	1.45531200
N	1.81684900	2.04611900	-0.08433500
C	2.12995700	0.96585400	-0.76165500
H	2.55449600	2.45371400	0.47892200
C	3.46713600	0.34589700	-0.64069500
O	1.23022800	0.40297000	-1.50604000
C	3.96610000	-0.44651000	-1.67956900
C	4.20704400	0.47544800	0.54445700
C	5.19525400	-1.08394700	-1.54613800
H	3.38788400	-0.56080700	-2.58803800
C	5.42888100	-0.17718500	0.67929400
H	3.81844600	1.04504600	1.37960500
C	5.92660800	-0.95522800	-0.36529100
H	5.57685600	-1.68959700	-2.35958000
H	5.98382400	-0.08788500	1.60561300
H	6.87732700	-1.46470800	-0.25716300

IRC_TS1_point168

B	-2.72804200	3.79111400	0.36201900
B	-1.63236800	3.62032100	1.75769300
B	-0.57109500	2.23310500	1.46005500
B	-2.34077000	2.51550800	-0.81832000
B	-1.01604800	1.57843200	-0.12634700
B	-1.29998200	4.84594800	0.51253500
B	-1.75192600	4.17681300	-1.06780700
H	-3.83781100	4.20172100	0.48770200
B	0.03009100	3.88464000	1.18974100
H	-1.96676500	3.91046300	2.86230700
B	0.42343000	2.61548000	0.02637000
H	-0.13512200	1.53775000	2.31478000
B	-0.68870400	2.79750800	-1.40960600
H	-3.16026400	2.00464700	-1.51175300
H	-1.39189800	6.01094100	0.73825700
B	-0.03690800	4.22089600	-0.57223900
H	-2.16045700	4.85628400	-1.95467300
H	0.88618500	4.34725300	1.87426100
H	-0.34073100	2.49033000	-2.50125900
H	0.77347800	4.91222800	-1.10092000
B	-2.27473000	2.18189000	0.94537000

I	-1.50802600	-0.86974700	-0.24139000
C	0.31016200	-1.61366800	0.62439800
C	0.59179200	-1.30496700	1.94713100
C	1.15237600	-2.38034900	-0.16941100
C	1.78676200	-1.77810200	2.49055800
H	-0.09160000	-0.71425100	2.53990500
C	2.33614600	-2.85153400	0.39485000
H	0.90569200	-2.59395100	-1.20046300
C	2.65512300	-2.54603500	1.71722200
H	2.03212100	-1.54187700	3.51967500
H	3.01400800	-3.44344700	-0.20870200
H	3.58455200	-2.90452900	2.14380800
O	-2.09315700	-3.27855900	0.11523100
C	-3.28142800	-3.52576700	-0.27148000
O	-4.05348900	-2.68396100	-0.79463100
C	-3.75966900	-4.94505800	-0.03321400
H	-4.09649700	-5.02497400	1.00596600
H	-4.59576400	-5.19819200	-0.68698600
H	-2.94295300	-5.65503700	-0.17517800
H	0.34062200	0.67108200	-1.19745900
H	-3.04642000	1.43823400	1.45613700
N	1.81715100	2.04483400	-0.08460100
C	2.13402500	0.96910200	-0.75729700
H	2.55475300	2.45508400	0.47746400
C	3.46637300	0.34581700	-0.64142300
O	1.23143300	0.40087700	-1.50684600
C	3.96563200	-0.44686700	-1.68014900
C	4.20680000	0.47559900	0.54433700
C	5.19501700	-1.08387600	-1.54618400
H	3.38839100	-0.56151500	-2.58913400
C	5.42844000	-0.17692600	0.67913300
H	3.81814000	1.04465100	1.37985400
C	5.92634400	-0.95507700	-0.36543100
H	5.57646700	-1.68946700	-2.35968900
H	5.98307800	-0.08757300	1.60558700
H	6.87700100	-1.46461200	-0.25720200

IRC_TS1_point169

B	-2.72802300	3.79165200	0.36250200
B	-1.63264800	3.62074500	1.75767000
B	-0.57149600	2.23229900	1.45979300
B	-2.34108600	2.51511800	-0.81741800
B	-1.02088800	1.57691300	-0.12376800
B	-1.29992300	4.84600200	0.51258400

B	-1.75129600	4.17608400	-1.06791700
H	-3.83732700	4.20363500	0.48780900
B	0.03031200	3.88423800	1.18924800
H	-1.96627100	3.91141400	2.86238900
B	0.42020800	2.61431400	0.02548800
H	-0.13568500	1.53795400	2.31544700
B	-0.68792200	2.79507700	-1.40827900
H	-3.16087300	2.00529000	-1.51119000
H	-1.39176000	6.01103600	0.73818900
B	-0.03662900	4.22086700	-0.57187800
H	-2.15945200	4.85542400	-1.95504100
H	0.88663100	4.34619000	1.87392400
H	-0.34049700	2.48976600	-2.50079600
H	0.77331700	4.91273400	-1.10050500
B	-2.27492200	2.18263200	0.94514200
I	-1.50771300	-0.86834700	-0.24142900
C	0.30943500	-1.61365600	0.62418800
C	0.59200700	-1.30515500	1.94699800
C	1.15235000	-2.38043500	-0.16904900
C	1.78690500	-1.77816900	2.49060100
H	-0.09124800	-0.71440900	2.53991700
C	2.33636300	-2.85150400	0.39492800
H	0.90567400	-2.59448100	-1.20000700
C	2.65534300	-2.54609500	1.71728200
H	2.03233600	-1.54204000	3.51973300
H	3.01428200	-3.44344000	-0.20856200
H	3.58476600	-2.90461000	2.14389700
O	-2.09374600	-3.28293100	0.11562400
C	-3.28106100	-3.52706200	-0.27108500
O	-4.05369300	-2.68436300	-0.79467900
C	-3.76093200	-4.94575800	-0.03339700
H	-4.09738200	-5.02608500	1.00590200
H	-4.59730500	-5.19963200	-0.68659000
H	-2.94433400	-5.65588400	-0.17546600
H	0.32834900	0.68769900	-1.24067000
H	-3.04710300	1.44045700	1.45715800
N	1.81710900	2.04426800	-0.08428100
C	2.13668000	0.97128000	-0.75379500
H	2.55436100	2.45774900	0.47596200
C	3.46594500	0.34568900	-0.64188700
O	1.23633400	0.39778000	-1.50861900
C	3.96502800	-0.44724300	-1.68082400
C	4.20649800	0.47570600	0.54408800
C	5.19468600	-1.08378900	-1.54625100

H	3.38880400	-0.56218000	-2.59036900
C	5.42794100	-0.17662800	0.67895400
H	3.81760300	1.04429000	1.37987400
C	5.92599900	-0.95486800	-0.36557600
H	5.57607900	-1.68934700	-2.35980000
H	5.98228300	-0.08723600	1.60556100
H	6.87661300	-1.46444600	-0.25726000

IRC_TS1_point170

B	-2.72796100	3.79229800	0.36293600
B	-1.63283500	3.62124800	1.75764800
B	-0.57206900	2.23153600	1.45961800
B	-2.34151500	2.51469400	-0.81658000
B	-1.02570300	1.57498800	-0.12090700
B	-1.29980800	4.84603900	0.51259400
B	-1.75050000	4.17523700	-1.06806200
H	-3.83682700	4.20550800	0.48786800
B	0.03048000	3.88374200	1.18870000
H	-1.96584600	3.91243800	2.86241200
B	0.41720300	2.61289000	0.02458800
H	-0.13636300	1.53799300	2.31603800
B	-0.68725500	2.79248100	-1.40672000
H	-3.16175100	2.00600500	-1.51051800
H	-1.39149800	6.01113600	0.73796600
B	-0.03638800	4.22071100	-0.57154200
H	-2.15839200	4.85422200	-1.95555500
H	0.88727900	4.34469800	1.87345200
H	-0.34005100	2.48825300	-2.49988500
H	0.77338800	4.91272900	-1.10020100
B	-2.27538400	2.18348300	0.94521500
I	-1.50733200	-0.86675800	-0.24147800
C	0.30886200	-1.61353600	0.62395600
C	0.59219500	-1.30535100	1.94682900
C	1.15228900	-2.38053300	-0.16867600
C	1.78708000	-1.77827000	2.49062500
H	-0.09083200	-0.71455000	2.53998300
C	2.33657800	-2.85147300	0.39504700
H	0.90573900	-2.59496300	-1.19958500
C	2.65561000	-2.54616500	1.71737700
H	2.03247300	-1.54216600	3.51978100
H	3.01449500	-3.44340300	-0.20846900
H	3.58503200	-2.90468300	2.14401100
O	-2.09416200	-3.28768300	0.11606800
C	-3.28110800	-3.52860100	-0.27083300

O	-4.05373300	-2.68491900	-0.79466700
C	-3.76243200	-4.94667800	-0.03360100
H	-4.09844700	-5.02727800	1.00583500
H	-4.59911100	-5.20090400	-0.68629300
H	-2.94606300	-5.65705100	-0.17584800
H	0.34037600	0.70511500	-1.28374800
H	-3.04818100	1.44283400	1.45837800
N	1.81666500	2.04437500	-0.08351000
C	2.13785700	0.97252600	-0.75125400
H	2.55355400	2.46132200	0.47463200
C	3.46575000	0.34545900	-0.64210300
O	1.24077600	0.39488900	-1.51056200
C	3.96438800	-0.44761200	-1.68149400
C	4.20618000	0.47574900	0.54378700
C	5.19430000	-1.08372100	-1.54633800
H	3.38897100	-0.56265500	-2.59148900
C	5.42746900	-0.17633500	0.67878400
H	3.81686300	1.04404800	1.37958200
C	5.92561100	-0.95463800	-0.36569700
H	5.57578700	-1.68927600	-2.35985300
H	5.98157800	-0.08691800	1.60551600
H	6.87620800	-1.46423100	-0.25732400

IRC_TS1_point171

B	-2.72791900	3.79306300	0.36331900
B	-1.63296800	3.62177400	1.75764800
B	-0.57272500	2.23074700	1.45949300
B	-2.34217300	2.51433400	-0.81566700
B	-1.03045000	1.57286100	-0.11818100
B	-1.29968300	4.84606400	0.51257900
B	-1.74970900	4.17431300	-1.06818400
H	-3.83644600	4.20717200	0.48791000
B	0.03057400	3.88317800	1.18810000
H	-1.96552600	3.91326600	2.86244400
B	0.41436000	2.61130500	0.02384400
H	-0.13704600	1.53793600	2.31645400
B	-0.68675500	2.78979700	-1.40509600
H	-3.16272900	2.00660300	-1.50988400
H	-1.39114600	6.01123100	0.73760100
B	-0.03619600	4.22039000	-0.57117800
H	-2.15742700	4.85282100	-1.95614900
H	0.88791800	4.34306600	1.87292100
H	-0.33978500	2.48621800	-2.49873100
H	0.77360200	4.91213600	-1.10011900

B	-2.27625100	2.18443400	0.94553600
I	-1.50691900	-0.86499200	-0.24153000
C	0.30841400	-1.61322300	0.62368000
C	0.59235400	-1.30552800	1.94665000
C	1.15218800	-2.38063200	-0.16833900
C	1.78725100	-1.77838800	2.49061000
H	-0.09043900	-0.71463700	2.54003000
C	2.33674400	-2.85142700	0.39516200
H	0.90580500	-2.59527100	-1.19926000
C	2.65589500	-2.54622400	1.71746200
H	2.03251900	-1.54225000	3.51978900
H	3.01459300	-3.44333000	-0.20846100
H	3.58532200	-2.90471400	2.14408700
O	-2.09452600	-3.29270400	0.11654200
C	-3.28140500	-3.53036200	-0.27063800
O	-4.05366000	-2.68560200	-0.79456600
C	-3.76417700	-4.94779900	-0.03381300
H	-4.09962500	-5.02843500	1.00579900
H	-4.60109900	-5.20200100	-0.68612300
H	-2.94796200	-5.65835600	-0.17627600
H	0.34082300	0.72540300	-1.32225300
H	-3.04949600	1.44494500	1.45963900
N	1.81583200	2.04455000	-0.08270600
C	2.13892400	0.97321100	-0.74943400
H	2.55259600	2.46429000	0.47359100
C	3.46561200	0.34528400	-0.64213900
O	1.24702200	0.39169200	-1.51248300
C	3.96370900	-0.44792700	-1.68213600
C	4.20583900	0.47576800	0.54345400
C	5.19382000	-1.08364400	-1.54650300
H	3.38879900	-0.56288100	-2.59236700
C	5.42701800	-0.17603800	0.67858800
H	3.81609800	1.04400200	1.37910100
C	5.92515500	-0.95436600	-0.36585500
H	5.57554500	-1.68921700	-2.35990400
H	5.98104800	-0.08662800	1.60537700
H	6.87577400	-1.46396000	-0.25746800

IRC_TS1_point172

B	-2.72786400	3.79389900	0.36364300
B	-1.63302900	3.62233500	1.75767900
B	-0.57353600	2.22999200	1.45946100
B	-2.34295400	2.51396700	-0.81476900
B	-1.03501100	1.57059400	-0.11561700

B	-1.29949800	4.84607700	0.51252400
B	-1.74885500	4.17331600	-1.06832800
H	-3.83602900	4.20906100	0.48789100
B	0.03061300	3.88251900	1.18749800
H	-1.96517600	3.91428100	2.86248100
B	0.41173500	2.60957700	0.02324200
H	-0.13789200	1.53783900	2.31697500
B	-0.68644500	2.78709900	-1.40340600
H	-3.16398500	2.00730900	-1.50912800
H	-1.39062400	6.01135400	0.73707500
B	-0.03603700	4.21988700	-0.57084100
H	-2.15631200	4.85110300	-1.95690000
H	0.88870700	4.34106400	1.87226100
H	-0.33958800	2.48325500	-2.49728800
H	0.77399500	4.91107100	-1.10012000
B	-2.27739200	2.18546100	0.94613800
I	-1.50646000	-0.86310700	-0.24158000
C	0.30805000	-1.61288600	0.62343800
C	0.59251000	-1.30569000	1.94648000
C	1.15207800	-2.38072500	-0.16801300
C	1.78741600	-1.77852400	2.49058900
H	-0.08999600	-0.71469900	2.54009200
C	2.33688300	-2.85138700	0.39530500
H	0.90590800	-2.59555800	-1.19893700
C	2.65620500	-2.54628800	1.71756800
H	2.03254000	-1.54234900	3.51980200
H	3.01466500	-3.44325000	-0.20845000
H	3.58567300	-2.90473100	2.14417700
O	-2.09483500	-3.29790900	0.11700000
C	-3.28182600	-3.53234100	-0.27047400
O	-4.05346400	-2.68638900	-0.79441600
C	-3.76615000	-4.94911400	-0.03404800
H	-4.10113400	-5.02984800	1.00573000
H	-4.60352800	-5.20322400	-0.68592200
H	-2.95035700	-5.66007300	-0.17683300
H	0.35431600	0.74427500	-1.35904600
H	-3.05127200	1.44736600	1.46121400
N	1.81475100	2.04469100	-0.08191900
C	2.13974900	0.97364200	-0.74799400
H	2.55127900	2.46741400	0.47251600
C	3.46555300	0.34507600	-0.64202600
O	1.25270600	0.38888000	-1.51474400
C	3.96305000	-0.44820300	-1.68268200
C	4.20552600	0.47576100	0.54319100

C	5.19330300	-1.08358100	-1.54668000
H	3.38849800	-0.56301800	-2.59315200
C	5.42662500	-0.17575600	0.67842800
H	3.81524700	1.04402000	1.37855900
C	5.92467100	-0.95408600	-0.36599900
H	5.57528400	-1.68916700	-2.35995200
H	5.98056500	-0.08630300	1.60523500
H	6.87529400	-1.46364400	-0.25764300

IRC_TS1_point173

B	-2.72783800	3.79479400	0.36390300
B	-1.63305300	3.62290300	1.75774000
B	-0.57445800	2.22924500	1.45949800
B	-2.34389500	2.51363400	-0.81384200
B	-1.03925800	1.56823600	-0.11330400
B	-1.29928400	4.84607800	0.51241900
B	-1.74804700	4.17228500	-1.06848000
H	-3.83569700	4.21078800	0.48781200
B	0.03059200	3.88179000	1.18689800
H	-1.96486800	3.91523000	2.86252400
B	0.40929900	2.60776600	0.02282700
H	-0.13878200	1.53774800	2.31748500
B	-0.68634700	2.78443400	-1.40174100
H	-3.16530600	2.00794300	-1.50841900
H	-1.39001300	6.01147100	0.73645500
B	-0.03592600	4.21920000	-0.57053800
H	-2.15531600	4.84940300	-1.95766300
H	0.88942500	4.33911600	1.87158600
H	-0.33962700	2.47998200	-2.49581700
H	0.77447100	4.90959500	-1.10027500
B	-2.27881300	2.18652900	0.94694900
I	-1.50598900	-0.86111900	-0.24162800
C	0.30775500	-1.61253700	0.62322800
C	0.59265600	-1.30581800	1.94631900
C	1.15194900	-2.38079900	-0.16773500
C	1.78756500	-1.77866700	2.49054400
H	-0.08959900	-0.71470800	2.54013400
C	2.33697400	-2.85134500	0.39543400
H	0.90600200	-2.59572300	-1.19870400
C	2.65651500	-2.54634100	1.71765200
H	2.03252000	-1.54243300	3.51978900
H	3.01465600	-3.44316900	-0.20848000
H	3.58602000	-2.90471200	2.14422100
O	-2.09513100	-3.30316600	0.11742700

C	-3.28232500	-3.53448600	-0.27031800
O	-4.05317800	-2.68726800	-0.79420300
C	-3.76831900	-4.95059300	-0.03429000
H	-4.10272300	-5.03124900	1.00567400
H	-4.60604100	-5.20429700	-0.68580200
H	-2.95287000	-5.66191300	-0.17741300
H	0.36264500	0.76544800	-1.39404500
H	-3.05320300	1.44954200	1.46280600
N	1.81348200	2.04464900	-0.08127800
C	2.14078700	0.97383000	-0.74690400
H	2.54979900	2.46970800	0.47169300
C	3.46554800	0.34489600	-0.64179000
O	1.25902500	0.38601400	-1.51689400
C	3.96240300	-0.44841200	-1.68314400
C	4.20524400	0.47574900	0.54298900
C	5.19273700	-1.08351700	-1.54690900
H	3.38801300	-0.56297300	-2.59367000
C	5.42628400	-0.17548300	0.67826600
H	3.81452500	1.04414500	1.37805600
C	5.92415400	-0.95379400	-0.36618700
H	5.57501600	-1.68912200	-2.36003600
H	5.98028700	-0.08601900	1.60503700
H	6.87482700	-1.46331500	-0.25788900

IRC_TS1_point174

B	-2.72781600	3.79574100	0.36412200
B	-1.63304900	3.62350700	1.75783100
B	-0.57553800	2.22849200	1.45962400
B	-2.34494200	2.51326500	-0.81289100
B	-1.04323400	1.56572200	-0.11110500
B	-1.29900300	4.84606600	0.51225700
B	-1.74721700	4.17119000	-1.06867000
H	-3.83531700	4.21279600	0.48765000
B	0.03053900	3.88096000	1.18630800
H	-1.96448300	3.91641700	2.86258000
B	0.40695800	2.60582400	0.02252900
H	-0.13991000	1.53767300	2.31818500
B	-0.68642900	2.78159200	-1.39997500
H	-3.16691300	2.00869100	-1.50758600
H	-1.38921200	6.01160400	0.73568000
B	-0.03583500	4.21831600	-0.57027700
H	-2.15417300	4.84746600	-1.95857000
H	0.89024700	4.33688300	1.87081300
H	-0.33983300	2.47627700	-2.49425700

H	0.77508400	4.90768900	-1.10050200
B	-2.28043100	2.18764100	0.94795800
I	-1.50547400	-0.85901200	-0.24167700
C	0.30753700	-1.61213500	0.62302200
C	0.59280500	-1.30592400	1.94618100
C	1.15181800	-2.38085600	-0.16746700
C	1.78770400	-1.77881900	2.49050800
H	-0.08916800	-0.71469300	2.54020000
C	2.33703800	-2.85131400	0.39558200
H	0.90610800	-2.59590000	-1.19846300
C	2.65682800	-2.54639300	1.71774500
H	2.03249400	-1.54253800	3.51978700
H	3.01462600	-3.44309100	-0.20849800
H	3.58640200	-2.90467700	2.14426800
O	-2.09542200	-3.30855800	0.11781800
C	-3.28284600	-3.53683400	-0.27015100
O	-4.05280000	-2.68824200	-0.79394700
C	-3.77072200	-4.95225200	-0.03455300
H	-4.10467300	-5.03294400	1.00557700
H	-4.60901400	-5.20549100	-0.68563000
H	-2.95593200	-5.66422400	-0.17811700
H	0.37758600	0.78372100	-1.42754300
H	-3.05557000	1.45205900	1.46472300
N	1.81211900	2.04439600	-0.08074600
C	2.14188600	0.97392700	-0.74595800
H	2.54801600	2.47203100	0.47089100
C	3.46562500	0.34468400	-0.64142000
O	1.26481800	0.38370500	-1.51947800
C	3.96178400	-0.44858300	-1.68350100
C	4.20502300	0.47572500	0.54291200
C	5.19215000	-1.08346600	-1.54713600
H	3.38744500	-0.56284700	-2.59408300
C	5.42600400	-0.17522300	0.67815000
H	3.81379900	1.04429700	1.37761000
C	5.92362100	-0.95350800	-0.36637300
H	5.57468000	-1.68907700	-2.36013800
H	5.98009300	-0.08571600	1.60483500
H	6.87432300	-1.46296100	-0.25818100

IRC_TS1_point175

B	-2.72782100	3.79671200	0.36428900
B	-1.63303700	3.62411600	1.75794500
B	-0.57671900	2.22773700	1.45982300
B	-2.34609300	2.51289400	-0.81190700

B	-1.04678500	1.56318100	-0.10909800
B	-1.29868000	4.84603700	0.51203400
B	-1.74645000	4.17006900	-1.06887900
H	-3.83500200	4.21467000	0.48743700
B	0.03045300	3.88006400	1.18574100
H	-1.96410500	3.91758300	2.86264600
B	0.40476400	2.60381400	0.02237400
H	-0.14110000	1.53762000	2.31893500
B	-0.68668700	2.77864800	-1.39820900
H	-3.16853700	2.00935600	-1.50677800
H	-1.38833300	6.01172200	0.73485100
B	-0.03578300	4.21724800	-0.57007100
H	-2.15314100	4.84563500	-1.95945200
H	0.89095800	4.33480200	1.87006900
H	-0.34029000	2.47285900	-2.49275800
H	0.77572300	4.90552200	-1.10084100
B	-2.28220000	2.18874500	0.94908600
I	-1.50494600	-0.85682200	-0.24173000
C	0.30739800	-1.61166900	0.62281200
C	0.59295300	-1.30599300	1.94605700
C	1.15168400	-2.38088400	-0.16724900
C	1.78783000	-1.77897100	2.49046100
H	-0.08878600	-0.71464100	2.54025000
C	2.33706500	-2.85128800	0.39571000
H	0.90620000	-2.59601400	-1.19828800
C	2.65712400	-2.54643300	1.71781000
H	2.03245300	-1.54264300	3.51977300
H	3.01453700	-3.44303500	-0.20853700
H	3.58675700	-2.90462200	2.14427000
O	-2.09570500	-3.31390700	0.11815700
C	-3.28339100	-3.53929800	-0.26998400
O	-4.05235200	-2.68929800	-0.79364100
C	-3.77327600	-4.95403800	-0.03482100
H	-4.10666700	-5.03462200	1.00548900
H	-4.61201800	-5.20651000	-0.68554500
H	-2.95907900	-5.66662900	-0.17882700
H	0.38862500	0.80326600	-1.46143200
H	-3.05796000	1.45435300	1.46661100
N	1.81071200	2.04394800	-0.08035300
C	2.14304400	0.97386300	-0.74521300
H	2.54615800	2.47358100	0.47035600
C	3.46577200	0.34448000	-0.64094800
O	1.27071300	0.38141900	-1.52186100
C	3.96119900	-0.44869600	-1.68376500

C	4.20486700	0.47570200	0.54293800
C	5.19154700	-1.08341700	-1.54739100
H	3.38679000	-0.56258800	-2.59427500
C	5.42579500	-0.17497900	0.67804700
H	3.81326200	1.04449000	1.37730800
C	5.92308600	-0.95322800	-0.36659900
H	5.57432100	-1.68903400	-2.36027900
H	5.98010600	-0.08547300	1.60459600
H	6.87385200	-1.46262300	-0.25853200

IRC_TS1_point176

B	-2.72783000	3.79770800	0.36443300
B	-1.63302800	3.62475800	1.75808000
B	-0.57803000	2.22696700	1.46011700
B	-2.34730800	2.51246600	-0.81088700
B	-1.05005400	1.56067400	-0.10718000
B	-1.29828600	4.84598400	0.51175100
B	-1.74568300	4.16888700	-1.06912300
H	-3.83463400	4.21681800	0.48714800
B	0.03035400	3.87907600	1.18519900
H	-1.96364200	3.91899800	2.86272400
B	0.40263400	2.60169200	0.02229900
H	-0.14255100	1.53757400	2.31989200
B	-0.68707500	2.77552400	-1.39639000
H	-3.17041800	2.01009400	-1.50581300
H	-1.38725800	6.01184500	0.73387500
B	-0.03574400	4.21599100	-0.56991200
H	-2.15196100	4.84360000	-1.96047200
H	0.89175300	4.33249100	1.86926200
H	-0.34082900	2.46911500	-2.49119700
H	0.77646600	4.90296400	-1.10125300
B	-2.28405600	2.18985100	0.95032200
I	-1.50438900	-0.85455100	-0.24177900
C	0.30731600	-1.61115600	0.62262500
C	0.59311000	-1.30603200	1.94595700
C	1.15155600	-2.38088500	-0.16704400
C	1.78794600	-1.77912700	2.49043300
H	-0.08837300	-0.71456400	2.54032400
C	2.33706800	-2.85127500	0.39584800
H	0.90629300	-2.59616800	-1.19809800
C	2.65740800	-2.54647300	1.71787800
H	2.03241400	-1.54278000	3.51978100
H	3.01442600	-3.44300100	-0.20855700
H	3.58712500	-2.90455900	2.14426800

O	-2.09599000	-3.31931200	0.11844900
C	-3.28392100	-3.54191400	-0.26980000
O	-4.05183600	-2.69043900	-0.79330200
C	-3.77602300	-4.95596300	-0.03510900
H	-4.10901400	-5.03658500	1.00535200
H	-4.61544700	-5.20759900	-0.68540600
H	-2.96277100	-5.66951100	-0.17966100
H	0.40468700	0.81985900	-1.49414500
H	-3.06069300	1.45697200	1.46878400
N	1.80929300	2.04331100	-0.08004100
C	2.14417100	0.97375600	-0.74457100
H	2.54411200	2.47513200	0.46987800
C	3.46597000	0.34424000	-0.64035700
O	1.27607400	0.37970800	-1.52472100
C	3.96065600	-0.44877700	-1.68392200
C	4.20478600	0.47567100	0.54311000
C	5.19095000	-1.08338100	-1.54762600
H	3.38608400	-0.56225700	-2.59436000
C	5.42566000	-0.17475600	0.67799500
H	3.81275800	1.04467100	1.37712600
C	5.92256000	-0.95296600	-0.36681900
H	5.57389300	-1.68899100	-2.36043600
H	5.98022800	-0.08523300	1.60436100
H	6.87336800	-1.46228200	-0.25892500

IRC_TS1_point177

B	-2.72786200	3.79874200	0.36454300
B	-1.63303100	3.62542600	1.75822900
B	-0.57946000	2.22616500	1.46049900
B	-2.34863600	2.51200400	-0.80979900
B	-1.05308400	1.55830500	-0.10546500
B	-1.29783300	4.84589900	0.51139100
B	-1.74496400	4.16763700	-1.06939700
H	-3.83432800	4.21881400	0.48681800
B	0.03023300	3.87799400	1.18466800
H	-1.96319300	3.92039200	2.86280500
B	0.40056100	2.59944200	0.02232900
H	-0.14408400	1.53751400	2.32090100
B	-0.68764200	2.77227600	-1.39457200
H	-3.17227700	2.01069200	-1.50484400
H	-1.38610400	6.01193300	0.73284800
B	-0.03573700	4.21451400	-0.56981100
H	-2.15088800	4.84167500	-1.96144200
H	0.89241800	4.33035400	1.86849100

H	-0.34149300	2.46532100	-2.48970200
H	0.77719500	4.90018200	-1.10177200
B	-2.28603700	2.19095500	0.95164900
I	-1.50379000	-0.85214300	-0.24183400
C	0.30729300	-1.61056000	0.62242900
C	0.59327400	-1.30602900	1.94586600
C	1.15142200	-2.38084700	-0.16688200
C	1.78805700	-1.77928500	2.49039500
H	-0.08800100	-0.71445000	2.54038200
C	2.33703700	-2.85126800	0.39596100
H	0.90635200	-2.59626600	-1.19796000
C	2.65767300	-2.54650300	1.71791400
H	2.03236900	-1.54292800	3.51978000
H	3.01425400	-3.44300400	-0.20859900
H	3.58745600	-2.90449200	2.14422100
O	-2.09627200	-3.32481200	0.11869400
C	-3.28448300	-3.54470300	-0.26961100
O	-4.05125300	-2.69170100	-0.79291000
C	-3.77897700	-4.95804700	-0.03540900
H	-4.11140600	-5.03852700	1.00522900
H	-4.61892600	-5.20849800	-0.68538500
H	-2.96655700	-5.67247100	-0.18049800
H	0.41645700	0.83637400	-1.52621400
H	-3.06334900	1.45933100	1.47086900
N	1.80783100	2.04249800	-0.07981100
C	2.14533900	0.97352200	-0.74412900
H	2.54204800	2.47592300	0.46968000
C	3.46621400	0.34399100	-0.63965900
O	1.28158200	0.37794800	-1.52742500
C	3.96013500	-0.44880900	-1.68399500
C	4.20477200	0.47563700	0.54339200
C	5.19033700	-1.08334700	-1.54788800
H	3.38532100	-0.56181600	-2.59425900
C	5.42560400	-0.17454800	0.67795300
H	3.81246400	1.04485300	1.37712900
C	5.92204000	-0.95271400	-0.36708400
H	5.57344800	-1.68894700	-2.36062900
H	5.98056000	-0.08506800	1.60409000
H	6.87292100	-1.46197200	-0.25937800

IRC_TS1_point178

B	-2.72789400	3.79981300	0.36464000
B	-1.63305000	3.62615100	1.75839100
B	-0.58104000	2.22533200	1.46099800

B	-2.35004500	2.51146600	-0.80865100
B	-1.05604100	1.55601200	-0.10371900
B	-1.29728900	4.84577600	0.51095100
B	-1.74422900	4.16628900	-1.06972000
H	-3.83394100	4.22117600	0.48640000
B	0.03010600	3.87679100	1.18415300
H	-1.96264900	3.92211100	2.86288400
B	0.39847700	2.59703300	0.02241800
H	-0.14598400	1.53742100	2.32216500
B	-0.68835700	2.76885600	-1.39266200
H	-3.17445800	2.01133600	-1.50363900
H	-1.38468200	6.01201600	0.73160700
B	-0.03573200	4.21281100	-0.56976700
H	-2.14961800	4.83945300	-1.96260400
H	0.89321400	4.32788300	1.86762300
H	-0.34240400	2.46034400	-2.48782500
H	0.77806400	4.89689100	-1.10239300
B	-2.28808900	2.19207000	0.95307200
I	-1.50312700	-0.84961200	-0.24188900
C	0.30732400	-1.60991200	0.62225900
C	0.59345300	-1.30598600	1.94580300
C	1.15129100	-2.38077100	-0.16672200
C	1.78815800	-1.77944500	2.49038200
H	-0.08757600	-0.71429200	2.54047600
C	2.33698200	-2.85127100	0.39608900
H	0.90639400	-2.59640100	-1.19779100
C	2.65792200	-2.54653200	1.71795700
H	2.03232200	-1.54312000	3.51981100
H	3.01404300	-3.44303900	-0.20861900
H	3.58779600	-2.90442600	2.14417300
O	-2.09655900	-3.33047300	0.11889700
C	-3.28504100	-3.54769400	-0.26940000
O	-4.05060300	-2.69308000	-0.79248000
C	-3.78218800	-4.96029700	-0.03573500
H	-4.11427700	-5.04084200	1.00503600
H	-4.62297100	-5.20946900	-0.68528200
H	-2.97108400	-5.67606900	-0.18150500
H	0.43197300	0.84766200	-1.55465300
H	-3.06640400	1.46211700	1.47329400
N	1.80635500	2.04148300	-0.07961000
C	2.14651200	0.97330700	-0.74379300
H	2.53974100	2.47674200	0.46963400
C	3.46649300	0.34370400	-0.63884600
O	1.28663700	0.37688300	-1.53094500

C	3.95965100	-0.44882200	-1.68395700
C	4.20483400	0.47559300	0.54383400
C	5.18973400	-1.08332800	-1.54811700
H	3.38450900	-0.56130500	-2.59405200
C	5.42563100	-0.17436400	0.67797000
H	3.81220200	1.04500400	1.37728100
C	5.92153800	-0.95248400	-0.36733600
H	5.57292000	-1.68890200	-2.36083500
H	5.98101600	-0.08490500	1.60382300
H	6.87246500	-1.46166400	-0.25988100

IRC_TS1_point179

B	-2.72794800	3.80088900	0.36470200
B	-1.63309200	3.62688800	1.75855000
B	-0.58269000	2.22449000	1.46159400
B	-2.35154300	2.51091300	-0.80745000
B	-1.05887800	1.55385700	-0.10195900
B	-1.29669300	4.84560400	0.51043000
B	-1.74357800	4.16489200	-1.07007100
H	-3.83363600	4.22326200	0.48598500
B	0.02996700	3.87551100	1.18366100
H	-1.96216900	3.92373200	2.86294900
B	0.39648000	2.59454800	0.02261600
H	-0.14788700	1.53729200	2.32343300
B	-0.68923200	2.76547300	-1.39083000
H	-3.17648200	2.01173500	-1.50246900
H	-1.38323600	6.01204000	0.73035800
B	-0.03575000	4.21090500	-0.56980100
H	-2.14853800	4.83744800	-1.96364200
H	0.89382300	4.32572000	1.86682600
H	-0.34338000	2.45548200	-2.48597800
H	0.77886100	4.89353500	-1.10309600
B	-2.29019500	2.19314800	0.95452900
I	-1.50242700	-0.84698500	-0.24195300
C	0.30741900	-1.60919500	0.62208400
C	0.59363900	-1.30589200	1.94574900
C	1.15115800	-2.38064900	-0.16661500
C	1.78825600	-1.77959900	2.49035900
H	-0.08719900	-0.71409200	2.54054800
C	2.33689200	-2.85128000	0.39617900
H	0.90638500	-2.59642400	-1.19768700
C	2.65814100	-2.54655300	1.71796000
H	2.03227900	-1.54331900	3.51983300
H	3.01377300	-3.44312100	-0.20866200

H	3.58807400	-2.90437500	2.14407900
O	-2.09682400	-3.33610600	0.11904300
C	-3.28563100	-3.55079400	-0.26919400
O	-4.04990400	-2.69457300	-0.79200400
C	-3.78552800	-4.96265100	-0.03606400
H	-4.11706000	-5.04301500	1.00487800
H	-4.62689700	-5.21017700	-0.68534200
H	-2.97550600	-5.67955800	-0.18246500
H	0.44219600	0.86017700	-1.58367900
H	-3.06917500	1.46445900	1.47548000
N	1.80487400	2.04032200	-0.07945300
C	2.14764100	0.97297600	-0.74368500
H	2.53748900	2.47665800	0.46998000
C	3.46680600	0.34342500	-0.63797600
O	1.29176700	0.37559700	-1.53418000
C	3.95920400	-0.44879400	-1.68383700
C	4.20495900	0.47554300	0.54436600
C	5.18914300	-1.08331300	-1.54836300
H	3.38371700	-0.56074000	-2.59369600
C	5.42574500	-0.17420500	0.67798800
H	3.81218400	1.04512700	1.37762800
C	5.92107500	-0.95227500	-0.36762800
H	5.57241000	-1.68885900	-2.36106400
H	5.98166000	-0.08483600	1.60353400
H	6.87208100	-1.46140600	-0.26042000
IRC_TS1_point180			
B	-2.72799700	3.80196900	0.36476000
B	-1.63315500	3.62767600	1.75871700
B	-0.58444000	2.22365000	1.46232000
B	-2.35307200	2.51029300	-0.80622000
B	-1.06173100	1.55178400	-0.10007600
B	-1.29601600	4.84538700	0.50983900
B	-1.74291800	4.16342600	-1.07046600
H	-3.83322300	4.22577700	0.48549300
B	0.02983300	3.87414000	1.18319900
H	-1.96160400	3.92574300	2.86299600
B	0.39448100	2.59196300	0.02285400
H	-0.15019200	1.53713600	2.32500000
B	-0.69017400	2.76198300	-1.38891700
H	-3.17885800	2.01217200	-1.50101100
H	-1.38149500	6.01205900	0.72886800
B	-0.03575700	4.20882400	-0.56989400
H	-2.14724700	4.83510300	-1.96490800
H	0.89461500	4.32316900	1.86592500

H	-0.34432400	2.44923500	-2.48354300
H	0.77983500	4.88965800	-1.10390200
B	-2.29230000	2.19422000	0.95604900
I	-1.50168700	-0.84431100	-0.24200500
C	0.30755800	-1.60844900	0.62194400
C	0.59384500	-1.30575800	1.94573000
C	1.15103600	-2.38048500	-0.16650100
C	1.78834600	-1.77974700	2.49037100
H	-0.08675300	-0.71384100	2.54066800
C	2.33678600	-2.85129500	0.39628700
H	0.90635900	-2.59646900	-1.19754500
C	2.65833600	-2.54657700	1.71797900
H	2.03224300	-1.54356900	3.51989800
H	3.01347000	-3.44323700	-0.20867600
H	3.58835500	-2.90433900	2.14399300
O	-2.09709300	-3.34178200	0.11914400
C	-3.28617700	-3.55401300	-0.26896400
O	-4.04917300	-2.69614800	-0.79151300
C	-3.78904500	-4.96509800	-0.03641400
H	-4.12036200	-5.04559400	1.00462600
H	-4.63140300	-5.21095700	-0.68526400
H	-2.98072200	-5.68374600	-0.18361700
H	0.45748700	0.86778800	-1.60767500
H	-3.07238400	1.46732100	1.47805400
N	1.80340300	2.03899200	-0.07928500
C	2.14870800	0.97270800	-0.74369100
H	2.53500400	2.47665500	0.47054200
C	3.46711900	0.34312200	-0.63703100
O	1.29636200	0.37514900	-1.53850000
C	3.95881400	-0.44876100	-1.68361200
C	4.20514700	0.47547600	0.54503100
C	5.18859400	-1.08331300	-1.54854600
H	3.38290800	-0.56012900	-2.59325200
C	5.42593600	-0.17407500	0.67807000
H	3.81217300	1.04519400	1.37811200
C	5.92066200	-0.95209700	-0.36787800
H	5.57182700	-1.68881500	-2.36128700
H	5.98240000	-0.08475800	1.60326600
H	6.87171000	-1.46115400	-0.26099000

IRC_TS1_point181

B	-2.72807300	3.80302700	0.36478600
B	-1.63324200	3.62845700	1.75887500
B	-0.58620500	2.22282700	1.46313400

B	-2.35466800	2.50968400	-0.80495200
B	-1.06444800	1.54992000	-0.09829200
B	-1.29530800	4.84511700	0.50917600
B	-1.74237400	4.16193700	-1.07087800
H	-3.83292100	4.22786400	0.48505600
B	0.02969200	3.87272600	1.18276400
H	-1.96116000	3.92754800	2.86301700
B	0.39259200	2.58935700	0.02321100
H	-0.15236600	1.53695600	2.32650100
B	-0.69125400	2.75853800	-1.38713600
H	-3.18093500	2.01230100	-1.49965900
H	-1.37982300	6.01200300	0.72743900
B	-0.03578400	4.20658400	-0.57006200
H	-2.14624100	4.83309600	-1.96596600
H	0.89516200	4.32107400	1.86513700
H	-0.34538200	2.44374700	-2.48145900
H	0.78066800	4.88591500	-1.10474800
B	-2.29442300	2.19524600	0.95757200
I	-1.50094000	-0.84159200	-0.24206200
C	0.30775200	-1.60763300	0.62178400
C	0.59406100	-1.30557200	1.94571000
C	1.15091300	-2.38027200	-0.16645000
C	1.78843900	-1.77988700	2.49036400
H	-0.08636900	-0.71355400	2.54075800
C	2.33664600	-2.85131200	0.39633900
H	0.90628900	-2.59636000	-1.19749000
C	2.65849600	-2.54659600	1.71794400
H	2.03222500	-1.54381600	3.51994300
H	3.01312100	-3.44339300	-0.20872500
H	3.58855500	-2.90433700	2.14385800
O	-2.09732700	-3.34733100	0.11918400
C	-3.28675700	-3.55726800	-0.26875100
O	-4.04842200	-2.69781500	-0.79098800
C	-3.79259900	-4.96758200	-0.03675700
H	-4.12338400	-5.04787100	1.00444000
H	-4.63556400	-5.21141100	-0.68539500
H	-2.98555200	-5.68756100	-0.18465900
H	0.46693400	0.88020200	-1.63432200
H	-3.07511700	1.46955100	1.48024300
N	1.80192400	2.03755600	-0.07914300
C	2.14970400	0.97227500	-0.74394700
H	2.53266200	2.47565400	0.47148800
C	3.46744900	0.34284200	-0.63607500
O	1.30113900	0.37422100	-1.54209300

C	3.95846800	-0.44869100	-1.68333200
C	4.20538000	0.47539700	0.54572900
C	5.18807600	-1.08331400	-1.54875100
H	3.38218900	-0.55951400	-2.59271500
C	5.42620200	-0.17397100	0.67813100
H	3.81240500	1.04521300	1.37874800
C	5.92031000	-0.95194200	-0.36817500
H	5.57130900	-1.68877500	-2.36152300
H	5.98327600	-0.08477700	1.60297800
H	6.87144300	-1.46096000	-0.26157000
IRC_TS1_point182			
B	-2.72813700	3.80409700	0.36482000
B	-1.63335400	3.62930800	1.75903600
B	-0.58807300	2.22200000	1.46408200
B	-2.35629100	2.50899000	-0.80365600
B	-1.06713700	1.54811100	-0.09635600
B	-1.29451300	4.84480100	0.50843900
B	-1.74179100	4.16036500	-1.07133800
H	-3.83249600	4.23045800	0.48452300
B	0.02956200	3.87122200	1.18234300
H	-1.96062600	3.92981700	2.86301400
B	0.39064800	2.58662200	0.02356800
H	-0.15501100	1.53675000	2.32835400
B	-0.69235100	2.75491000	-1.38525000
H	-3.18344800	2.01248500	-1.49796600
H	-1.37780400	6.01194300	0.72571100
B	-0.03579200	4.20418000	-0.57028100
H	-2.14497700	4.83064600	-1.96731000
H	0.89594400	4.31849100	1.86421300
H	-0.34657200	2.43738500	-2.47913900
H	0.78172500	4.88153700	-1.10573500
B	-2.29654700	2.19628700	0.95916900
I	-1.50015700	-0.83883300	-0.24210400
C	0.30798200	-1.60680700	0.62167200
C	0.59429700	-1.30534600	1.94572700
C	1.15080100	-2.38001400	-0.16637700
C	1.78852500	-1.78001800	2.49040100
H	-0.08589600	-0.71320800	2.54090500
C	2.33649500	-2.85133200	0.39642500
H	0.90620800	-2.59627700	-1.19738200
C	2.65863500	-2.54662500	1.71794200
H	2.03221100	-1.54411600	3.52004100
H	3.01273300	-3.44357900	-0.20874200
H	3.58876100	-2.90436300	2.14374200

O	-2.09757800	-3.35297500	0.11919300
C	-3.28727200	-3.56065100	-0.26850000
O	-4.04766000	-2.69955600	-0.79045600
C	-3.79634700	-4.97015200	-0.03712300
H	-4.12702700	-5.05062500	1.00414300
H	-4.64042700	-5.21196800	-0.68534400
H	-2.99132700	-5.69221000	-0.18592900
H	0.48183500	0.88464800	-1.65293700
H	-3.07839600	1.47241500	1.48290500
N	1.80044500	2.03593700	-0.07895500
C	2.15072600	0.97191300	-0.74424900
H	2.53002000	2.47476400	0.47271900
C	3.46777400	0.34252600	-0.63504000
O	1.30534100	0.37452800	-1.54716100
C	3.95818100	-0.44863300	-1.68295100
C	4.20566500	0.47528800	0.54654800
C	5.18761100	-1.08333600	-1.54887100
H	3.38143900	-0.55885000	-2.59208900
C	5.42653300	-0.17389600	0.67826500
H	3.81262000	1.04516300	1.37950600
C	5.92001600	-0.95182000	-0.36840500
H	5.57071700	-1.68873700	-2.36173800
H	5.98424000	-0.08477200	1.60271500
H	6.87119300	-1.46076400	-0.26217400
IRC_TS1_point183			
B	-2.72823300	3.80513700	0.36482400
B	-1.63348600	3.63014100	1.75918500
B	-0.58991500	2.22121500	1.46510000
B	-2.35796900	2.50833800	-0.80232400
B	-1.06971600	1.54652200	-0.09449300
B	-1.29370600	4.84443600	0.50764300
B	-1.74134600	4.15878500	-1.07178800
H	-3.83216700	4.23264500	0.48407100
B	0.02942500	3.86970900	1.18194800
H	-1.96021000	3.93187100	2.86298000
B	0.38884100	2.58391100	0.02405000
H	-0.15749300	1.53654100	2.33012300
B	-0.69360100	2.75141400	-1.38356800
H	-3.18565000	2.01238100	-1.49637100
H	-1.37587200	6.01181800	0.72405200
B	-0.03582400	4.20165300	-0.57056400
H	-2.14398500	4.82851500	-1.96846300
H	0.89650800	4.31635700	1.86339700
H	-0.34792300	2.43186700	-2.47700100

H	0.78263100	4.87734800	-1.10675300
B	-2.29867100	2.19728200	0.96074100
I	-1.49938200	-0.83606300	-0.24215400
C	0.30825700	-1.60589600	0.62152000
C	0.59454600	-1.30506900	1.94573100
C	1.15069000	-2.37970200	-0.16638000
C	1.78862300	-1.78013500	2.49040500
H	-0.08547300	-0.71282200	2.54101500
C	2.33631500	-2.85134600	0.39643600
H	0.90609500	-2.59602000	-1.19737400
C	2.65874200	-2.54664900	1.71787300
H	2.03222300	-1.54440900	3.52010700
H	3.01231300	-3.44379100	-0.20880300
H	3.58888500	-2.90442900	2.14357300
O	-2.09777700	-3.35842600	0.11913800
C	-3.28784500	-3.56401300	-0.26828900
O	-4.04689100	-2.70137600	-0.78990000
C	-3.80007100	-4.97271300	-0.03747900
H	-4.13033600	-5.05304400	1.00390500
H	-4.64487100	-5.21216800	-0.68547300
H	-2.99666700	-5.69642700	-0.18709200
H	0.48979000	0.89623600	-1.67746400
H	-3.08117200	1.47469200	1.48518000
N	1.79895600	2.03424200	-0.07877200
C	2.15161300	0.97141300	-0.74477400
H	2.52750200	2.47297900	0.47432900
C	3.46812000	0.34223900	-0.63404700
O	1.30990300	0.37400600	-1.55105300
C	3.95794200	-0.44853800	-1.68255000
C	4.20597800	0.47516600	0.54735200
C	5.18718800	-1.08334900	-1.54902500
H	3.38082900	-0.55821500	-2.59143100
C	5.42692400	-0.17384000	0.67835200
H	3.81303400	1.04505500	1.38036100
C	5.91979400	-0.95171000	-0.36869200
H	5.57021300	-1.68869900	-2.36196600
H	5.98528500	-0.08483700	1.60243200
H	6.87106300	-1.46060900	-0.26277600

IRC_TS1_point184

B	-2.72831100	3.80617800	0.36483300
B	-1.63363700	3.63103900	1.75933000
B	-0.59183700	2.22043900	1.46623700
B	-2.35964800	2.50760200	-0.80098200

B	-1.07229600	1.54493800	-0.09244700
B	-1.29281900	4.84402700	0.50677700
B	-1.74085300	4.15713000	-1.07228800
H	-3.83177200	4.23510300	0.48356900
B	0.02930600	3.86812500	1.18156300
H	-1.95976300	3.93420500	2.86292400
B	0.38698000	2.58108000	0.02451200
H	-0.16021000	1.53632000	2.33210000
B	-0.69485000	2.74776400	-1.38177900
H	-3.18807900	2.01227400	-1.49458700
H	-1.37374400	6.01166700	0.72220600
B	-0.03582500	4.19899200	-0.57089700
H	-2.14283900	4.82612000	-1.96975700
H	0.89720100	4.31396000	1.86248600
H	-0.34935000	2.42569000	-2.47475800
H	0.78364100	4.87281600	-1.10783400
B	-2.30077300	2.19830000	0.96237700
I	-1.49858000	-0.83327500	-0.24218200
C	0.30854900	-1.60498600	0.62141700
C	0.59481400	-1.30476000	1.94577400
C	1.15058800	-2.37935500	-0.16634800
C	1.78870900	-1.78024800	2.49045800
H	-0.08499800	-0.71240100	2.54116600
C	2.33612500	-2.85137100	0.39649400
H	0.90598400	-2.59577300	-1.19731800
C	2.65882300	-2.54669700	1.71785000
H	2.03224100	-1.54473400	3.52022300
H	3.01186600	-3.44402700	-0.20882800
H	3.58899700	-2.90454900	2.14344000
O	-2.09800800	-3.36397500	0.11906000
C	-3.28833700	-3.56747400	-0.26803300
O	-4.04613400	-2.70325200	-0.78935000
C	-3.80393900	-4.97532300	-0.03784600
H	-4.13399600	-5.05571600	1.00362900
H	-4.64975500	-5.21247300	-0.68552600
H	-3.00252000	-5.70106700	-0.18836800
H	0.50364400	0.89968600	-1.69313100
H	-3.08423700	1.47728600	1.48770900
N	1.79747100	2.03238100	-0.07850800
C	2.15254800	0.97101500	-0.74532300
H	2.52480700	2.47122200	0.47617000
C	3.46845300	0.34190400	-0.63298900
O	1.31378800	0.37485800	-1.55658600
C	3.95777100	-0.44848500	-1.68206000

C	4.20633000	0.47499400	0.54825400
C	5.18683300	-1.08340400	-1.54907600
H	3.38025100	-0.55759200	-2.59072400
C	5.42736300	-0.17382600	0.67852000
H	3.81341900	1.04487000	1.38129300
C	5.91963800	-0.95164800	-0.36888700
H	5.56969800	-1.68868200	-2.36214000
H	5.98635200	-0.08489800	1.60220500
H	6.87096300	-1.46047000	-0.26334300

IRC_TS1_point185

B	-2.72842400	3.80719600	0.36482500
B	-1.63381100	3.63193000	1.75946700
B	-0.59374000	2.21970500	1.46744100
B	-2.36138500	2.50689800	-0.79959300
B	-1.07478800	1.54355900	-0.09044400
B	-1.29192700	4.84357200	0.50585900
B	-1.74048400	4.15545600	-1.07277300
H	-3.83144000	4.23733700	0.48312700
B	0.02917700	3.86653500	1.18119100
H	-1.95939100	3.93644000	2.86284800
B	0.38520600	2.57826000	0.02507600
H	-0.16282800	1.53610700	2.33405200
B	-0.69623700	2.74423000	-1.38017500
H	-3.19034400	2.01197800	-1.49284300
H	-1.37166300	6.01146500	0.72037900
B	-0.03585300	4.19622000	-0.57128400
H	-2.14186800	4.82389700	-1.97095000
H	0.89777200	4.31183100	1.86163100
H	-0.35102700	2.42009000	-2.47273200
H	0.78453900	4.86839200	-1.10893500
B	-2.30288900	2.19928900	0.96400600
I	-1.49778600	-0.83046000	-0.24221600
C	0.30887700	-1.60398400	0.62126900
C	0.59509600	-1.30440000	1.94579600
C	1.15048700	-2.37894500	-0.16638800
C	1.78880900	-1.78034700	2.49047300
H	-0.08454000	-0.71194000	2.54129500
C	2.33590700	-2.85138200	0.39647800
H	0.90585500	-2.59539600	-1.19734300
C	2.65887800	-2.54674400	1.71776400
H	2.03227900	-1.54505800	3.52030700
H	3.01139300	-3.44427200	-0.20889600
H	3.58904300	-2.90471000	2.14326200

O	-2.09819300	-3.36940100	0.11892000
C	-3.28889800	-3.57093200	-0.26782000
O	-4.04537600	-2.70520900	-0.78878200
C	-3.80778400	-4.97792500	-0.03820700
H	-4.13748300	-5.05820200	1.00337400
H	-4.65437900	-5.21258600	-0.68565800
H	-3.00813600	-5.70546800	-0.18957500
H	0.51206100	0.90970800	-1.71448600
H	-3.08702400	1.47954900	1.49004200
N	1.79594900	2.03044000	-0.07822400
C	2.15338400	0.97050600	-0.74607400
H	2.52214800	2.46892000	0.47827000
C	3.46879600	0.34158900	-0.63198900
O	1.31810700	0.37487000	-1.56100000
C	3.95764600	-0.44840500	-1.68157200
C	4.20669200	0.47480300	0.54912100
C	5.18652200	-1.08344700	-1.54916100
H	3.37979800	-0.55699700	-2.59001700
C	5.42784600	-0.17382100	0.67863800
H	3.81391100	1.04462700	1.38227200
C	5.91955100	-0.95158800	-0.36913400
H	5.56925500	-1.68866400	-2.36232600
H	5.98745300	-0.08499300	1.60196800
H	6.87096300	-1.46035000	-0.26390500

IRC_TS1_point186

B	-2.72852900	3.80821000	0.36481900
B	-1.63400400	3.63287400	1.75959800
B	-0.59570300	2.21898200	1.46874700
B	-2.36313500	2.50612100	-0.79818900
B	-1.07726100	1.54220900	-0.08830200
B	-1.29097100	4.84306900	0.50487200
B	-1.74009100	4.15371000	-1.07329900
H	-3.83109900	4.23962000	0.48267000
B	0.02906200	3.86488600	1.18081900
H	-1.95903000	3.93878300	2.86275500
B	0.38339300	2.57532500	0.02563100
H	-0.16550500	1.53588500	2.33609000
B	-0.69761900	2.74059000	-1.37855900
H	-3.19265900	2.01160700	-1.49102600
H	-1.36950200	6.01121600	0.71845400
B	-0.03585800	4.19332100	-0.57172000
H	-2.14086800	4.82157400	-1.97216100
H	0.89835900	4.30964800	1.86072200

H	-0.35280400	2.41461600	-2.47108600
H	0.78544100	4.86383100	-1.11006300
B	-2.30499900	2.20029900	0.96569300
I	-1.49696400	-0.82760800	-0.24223300
C	0.30922400	-1.60296600	0.62115600
C	0.59539400	-1.30400700	1.94584400
C	1.15038800	-2.37849900	-0.16640800
C	1.78889900	-1.78044500	2.49052500
H	-0.08406100	-0.71144900	2.54144300
C	2.33567200	-2.85140300	0.39649500
H	0.90572300	-2.59498700	-1.19735100
C	2.65890200	-2.54682000	1.71771100
H	2.03232100	-1.54539900	3.52042200
H	3.01088900	-3.44453500	-0.20894700
H	3.58905800	-2.90493300	2.14310800
O	-2.09840700	-3.37493200	0.11875300
C	-3.28940200	-3.57448500	-0.26757200
O	-4.04463900	-2.70723200	-0.78821800
C	-3.81173100	-4.98057300	-0.03856400
H	-4.14110300	-5.06075900	1.00313400
H	-4.65918200	-5.21277600	-0.68580300
H	-3.01391600	-5.70998700	-0.19078100
H	0.52342500	0.91310500	-1.72857200
H	-3.08986700	1.48184000	1.49243100
N	1.79442300	2.02833200	-0.07784900
C	2.15427500	0.97004900	-0.74685600
H	2.51940200	2.46645800	0.48055800
C	3.46914300	0.34122300	-0.63094700
O	1.32188100	0.37595600	-1.56662700
C	3.95759200	-0.44837600	-1.68101800
C	4.20708200	0.47455100	0.55005400
C	5.18628300	-1.08354000	-1.54915800
H	3.37941700	-0.55643900	-2.58928200
C	5.42836600	-0.17386400	0.67882200
H	3.81440300	1.04431400	1.38329800
C	5.91953100	-0.95157800	-0.36929900
H	5.56885000	-1.68867600	-2.36245800
H	5.98856200	-0.08510900	1.60178400
H	6.87101400	-1.46025700	-0.26441600

IRC_TS1_point187

B	-2.72866500	3.80920700	0.36480900
B	-1.63421800	3.63382900	1.75972500
B	-0.59766300	2.21830200	1.47011900

B	-2.36493300	2.50535800	-0.79674100
B	-1.07970200	1.54100900	-0.08616900
B	-1.29000800	4.84252200	0.50383800
B	-1.73979200	4.15193100	-1.07380800
H	-3.83077700	4.24188200	0.48223800
B	0.02893600	3.86322600	1.18045100
H	-1.95869100	3.94116800	2.86264800
B	0.38162900	2.57238200	0.02625400
H	-0.16820500	1.53566900	2.33817900
B	-0.69912000	2.73705200	-1.37711100
H	-3.19497300	2.01112200	-1.48914900
H	-1.36729200	6.01093100	0.71646100
B	-0.03588400	4.19032100	-0.57220000
H	-2.13992900	4.81925100	-1.97337000
H	0.89892400	4.30753300	1.85980600
H	-0.35474500	2.40949600	-2.46951700
H	0.78630700	4.85920200	-1.11124000
B	-2.30712200	2.20130100	0.96739200
I	-1.49613500	-0.82471700	-0.24225100
C	0.30960000	-1.60186100	0.62101000
C	0.59571000	-1.30356300	1.94587700
C	1.15029200	-2.37798700	-0.16648100
C	1.78900100	-1.78052900	2.49054900
H	-0.08356200	-0.71090600	2.54158500
C	2.33541200	-2.85141000	0.39645900
H	0.90558100	-2.59447000	-1.19741100
C	2.65890300	-2.54690400	1.71761500
H	2.03237900	-1.54575300	3.52052000
H	3.01035000	-3.44480900	-0.20903000
H	3.58902500	-2.90520500	2.14292400
O	-2.09858700	-3.38041400	0.11853000
C	-3.28996000	-3.57806000	-0.26736000
O	-4.04390600	-2.70933500	-0.78764300
C	-3.81567600	-4.98322900	-0.03891400
H	-4.14475900	-5.06330200	1.00287600
H	-4.66393900	-5.21289200	-0.68594300
H	-3.01973500	-5.71454200	-0.19196500
H	0.53121200	0.91977700	-1.74546400
H	-3.09265800	1.48406100	1.49481100
N	1.79285400	2.02612200	-0.07742000
C	2.15505600	0.96954300	-0.74778300
H	2.51658800	2.46364900	0.48310900
C	3.46949600	0.34086200	-0.62997400
O	1.32597000	0.37651400	-1.57160400

C	3.95759300	-0.44834200	-1.68047000
C	4.20747300	0.47427100	0.55095800
C	5.18610100	-1.08363300	-1.54916300
H	3.37914000	-0.55591000	-2.58855800
C	5.42891600	-0.17392000	0.67897800
H	3.81494600	1.04393500	1.38435500
C	5.91957900	-0.95157200	-0.36948500
H	5.56850200	-1.68869600	-2.36258800
H	5.98969000	-0.08523600	1.60160000
H	6.87115000	-1.46016700	-0.26491900

IRC_TS1_point188

B	-2.72880500	3.81019400	0.36480200
B	-1.63444500	3.63482400	1.75984700
B	-0.59965100	2.21764900	1.47156700
B	-2.36674700	2.50455400	-0.79528400
B	-1.08210500	1.53981600	-0.08399700
B	-1.28900500	4.84193600	0.50274900
B	-1.73950700	4.15010500	-1.07433500
H	-3.83045200	4.24415200	0.48180200
B	0.02881600	3.86153500	1.18008200
H	-1.95836500	3.94363500	2.86251900
B	0.37985900	2.56937300	0.02688000
H	-0.17095500	1.53545800	2.34032800
B	-0.70063700	2.73349600	-1.37572300
H	-3.19731700	2.01055000	-1.48719400
H	-1.36500600	6.01060800	0.71436900
B	-0.03590000	4.18722400	-0.57272300
H	-2.13900500	4.81686700	-1.97458900
H	0.89949600	4.30541100	1.85884400
H	-0.35681800	2.40451900	-2.46821600
H	0.78717800	4.85444300	-1.11247000
B	-2.30924100	2.20231600	0.96913300
I	-1.49527900	-0.82179400	-0.24225900
C	0.30999800	-1.60072100	0.62088500
C	0.59604300	-1.30307900	1.94592400
C	1.15019700	-2.37742900	-0.16655200
C	1.78909700	-1.78061000	2.49059200
H	-0.08303900	-0.71031500	2.54173500
C	2.33513300	-2.85141800	0.39643300
H	0.90543300	-2.59387600	-1.19748000
C	2.65887300	-2.54701300	1.71753500
H	2.03244200	-1.54612300	3.52063400
H	3.00977100	-3.44509900	-0.20911500

H	3.58894900	-2.90554300	2.14274800
O	-2.09878200	-3.38594000	0.11826900
C	-3.29048100	-3.58169400	-0.26713000
O	-4.04319900	-2.71149600	-0.78707500
C	-3.81967800	-4.98591700	-0.03925300
H	-4.14850100	-5.06586900	1.00263200
H	-4.66877700	-5.21301400	-0.68609600
H	-3.02566200	-5.71918400	-0.19312700
H	0.53942200	0.92211600	-1.75675600
H	-3.09544300	1.48627100	1.49720300
N	1.79126400	2.02377200	-0.07688900
C	2.15584800	0.96904800	-0.74875300
H	2.51369600	2.46053500	0.48593100
C	3.46985600	0.34047500	-0.62901000
O	1.32972600	0.37771200	-1.57727000
C	3.95766600	-0.44835200	-1.67989000
C	4.20787200	0.47393700	0.55188100
C	5.18599400	-1.08376700	-1.54910600
H	3.37895700	-0.55543100	-2.58782800
C	5.42949000	-0.17401700	0.67917400
H	3.81550500	1.04348500	1.38544200
C	5.91969600	-0.95160300	-0.36961000
H	5.56821700	-1.68874700	-2.36267300
H	5.99082000	-0.08538300	1.60145500
H	6.87135700	-1.46009100	-0.26537200

IRC_TS1_point189

B	-2.72896700	3.81116800	0.36479700
B	-1.63468600	3.63583700	1.75996600
B	-0.60163900	2.21703700	1.47306100
B	-2.36859600	2.50375600	-0.79379100
B	-1.08449000	1.53869400	-0.08184600
B	-1.28799100	4.84131600	0.50161600
B	-1.73929400	4.14825100	-1.07485000
H	-3.83012000	4.24648100	0.48137600
B	0.02868900	3.85983800	1.17971200
H	-1.95803400	3.94620100	2.86237100
B	0.37811100	2.56636300	0.02755500
H	-0.17377500	1.53526800	2.34255000
B	-0.70224500	2.73001200	-1.37445000
H	-3.19972300	2.00991400	-1.48514300
H	-1.36263600	6.01026500	0.71217200
B	-0.03592600	4.18404600	-0.57328400
H	-2.13810300	4.81441900	-1.97584400

H	0.90009500	4.30327600	1.85784500
H	-0.35903600	2.39953400	-2.46684400
H	0.78805300	4.84955800	-1.11376500
B	-2.31135900	2.20333100	0.97088500
I	-1.49440600	-0.81884200	-0.24226800
C	0.31042200	-1.59950800	0.62074300
C	0.59639600	-1.30254300	1.94596400
C	1.15010500	-2.37680600	-0.16665900
C	1.78920400	-1.78067800	2.49061900
H	-0.08247700	-0.70965600	2.54188500
C	2.33483100	-2.85141100	0.39637000
H	0.90528400	-2.59317600	-1.19758700
C	2.65882000	-2.54713600	1.71742700
H	2.03251900	-1.54651000	3.52074100
H	3.00915400	-3.44539800	-0.20922600
H	3.58883100	-2.90593900	2.14255300
O	-2.09895000	-3.39142900	0.11795400
C	-3.29103900	-3.58535100	-0.26693000
O	-4.04250200	-2.71372300	-0.78650500
C	-3.82368800	-4.98861400	-0.03958200
H	-4.15233400	-5.06846600	1.00236900
H	-4.67364500	-5.21307400	-0.68621600
H	-3.03172700	-5.72394500	-0.19428800
H	0.54511600	0.92601700	-1.76876900
H	-3.09825300	1.48853500	1.49965500
N	1.78962900	2.02131100	-0.07627800
C	2.15653500	0.96851800	-0.74980600
H	2.51069900	2.45713400	0.48903700
C	3.47022400	0.34009300	-0.62812800
O	1.33361900	0.37865600	-1.58259200
C	3.95780400	-0.44837300	-1.67932400
C	4.20826300	0.47357100	0.55276800
C	5.18595700	-1.08391300	-1.54903700
H	3.37889400	-0.55500200	-2.58713800
C	5.43007900	-0.17413200	0.67935800
H	3.81607400	1.04296500	1.38653300
C	5.91988100	-0.95164200	-0.36972900
H	5.56799600	-1.68881700	-2.36273900
H	5.99193800	-0.08552800	1.60132100
H	6.87164300	-1.46000500	-0.26580000
IRC_TS1_point190			
B	-2.72913400	3.81212800	0.36479600
B	-1.63493400	3.63688100	1.76007600

B	-0.60363900	2.21645600	1.47460000
B	-2.37045700	2.50293300	-0.79229400
B	-1.08684800	1.53758100	-0.07968900
B	-1.28695300	4.84067000	0.50043700
B	-1.73910900	4.14637100	-1.07537700
H	-3.82979400	4.24877400	0.48095600
B	0.02856600	3.85813400	1.17933900
H	-1.95771400	3.94880000	2.86220400
B	0.37636800	2.56332500	0.02824100
H	-0.17658700	1.53509700	2.34478500
B	-0.70387500	2.72653500	-1.37323400
H	-3.20212500	2.00921400	-1.48305500
H	-1.36023400	6.00989500	0.70990900
B	-0.03594600	4.18080700	-0.57388700
H	-2.13724500	4.81195900	-1.97708600
H	0.90069200	4.30117500	1.85681100
H	-0.36136100	2.39457300	-2.46560600
H	0.78891200	4.84463100	-1.11509400
B	-2.31346100	2.20435400	0.97266100
I	-1.49351000	-0.81587700	-0.24227100
C	0.31086800	-1.59826000	0.62061900
C	0.59676500	-1.30196500	1.94601300
C	1.15001400	-2.37613600	-0.16677300
C	1.78930900	-1.78074200	2.49065400
H	-0.08189600	-0.70894600	2.54203600
C	2.33450900	-2.85140000	0.39630600
H	0.90513000	-2.59239200	-1.19771100
C	2.65873800	-2.54728300	1.71732600
H	2.03260200	-1.54690700	3.52085500
H	3.00850300	-3.44570400	-0.20934600
H	3.58866500	-2.90640200	2.14236200
O	-2.09912600	-3.39691000	0.11759500
C	-3.29157000	-3.58903200	-0.26672400
O	-4.04183700	-2.71599300	-0.78594500
C	-3.82771800	-4.99132100	-0.03989500
H	-4.15617100	-5.07102700	1.00213100
H	-4.67850700	-5.21312400	-0.68635100
H	-3.03779200	-5.72869700	-0.19540700
H	0.55055700	0.92722200	-1.77660600
H	-3.10100500	1.49075200	1.50208400
N	1.78796900	2.01872900	-0.07555300
C	2.15721200	0.96797300	-0.75088100
H	2.50765700	2.45344500	0.49237500
C	3.47059800	0.33970100	-0.62729600

O	1.33726800	0.38001200	-1.58830300
C	3.95801300	-0.44843500	-1.67875700
C	4.20864500	0.47315800	0.55363700
C	5.18599700	-1.08409500	-1.54891900
H	3.37894400	-0.55464600	-2.58647700
C	5.43067100	-0.17428000	0.67956700
H	3.81663500	1.04238000	1.38761200
C	5.92013200	-0.95170800	-0.36979400
H	5.56786000	-1.68892200	-2.36275800
H	5.99301600	-0.08568400	1.60123100
H	6.87200200	-1.45992500	-0.26616300

IRC_TS1_point191

B	-2.72931700	3.81307700	0.36480000
B	-1.63518600	3.63794500	1.76018000
B	-0.60563400	2.21591400	1.47616300
B	-2.37234400	2.50211500	-0.79076800
B	-1.08920500	1.53652600	-0.07754300
B	-1.28590600	4.84000400	0.49921900
B	-1.73898000	4.14447300	-1.07589700
H	-3.82945400	4.25114000	0.48054300
B	0.02844000	3.85643500	1.17895800
H	-1.95737800	3.95150000	2.86201600
B	0.37463300	2.56029700	0.02896600
H	-0.17945800	1.53495900	2.34708100
B	-0.70557500	2.72310400	-1.37207900
H	-3.20459600	2.00848200	-1.48088100
H	-1.35776400	6.00951500	0.70754700
B	-0.03596900	4.17751800	-0.57452300
H	-2.13640600	4.80943300	-1.97837000
H	0.90132600	4.29904900	1.85573600
H	-0.36381000	2.38944800	-2.46426200
H	0.78978300	4.83960300	-1.11648200
B	-2.31555300	2.20537800	0.97444200
I	-1.49260000	-0.81290400	-0.24227200
C	0.31133900	-1.59694900	0.62048800
C	0.59715600	-1.30133700	1.94605900
C	1.14992900	-2.37540400	-0.16691400
C	1.78942200	-1.78079500	2.49068000
H	-0.08127000	-0.70816500	2.54219000
C	2.33416900	-2.85137500	0.39621300
H	0.90497800	-2.59150800	-1.19786600
C	2.65863300	-2.54744700	1.71720600
H	2.03270000	-1.54732100	3.52096600

H	3.00781800	-3.44601300	-0.20948900
H	3.58845800	-2.90692800	2.14216100
O	-2.09928200	-3.40233900	0.11718400
C	-3.29212900	-3.59272000	-0.26654700
O	-4.04118600	-2.71831100	-0.78539000
C	-3.83174200	-4.99402200	-0.04019500
H	-4.16008400	-5.07361100	1.00188100
H	-4.68339900	-5.21312500	-0.68644100
H	-3.04398000	-5.73355600	-0.19652200
H	0.55439300	0.92958300	-1.78495300
H	-3.10379800	1.49305800	1.50459000
N	1.78626900	2.01603500	-0.07473400
C	2.15780300	0.96738900	-0.75199000
H	2.50451200	2.44952400	0.49596100
C	3.47098100	0.33931200	-0.62655700
O	1.34097200	0.38125700	-1.59378600
C	3.95828900	-0.44851700	-1.67821900
C	4.20901000	0.47271300	0.55445500
C	5.18611200	-1.08429400	-1.54878400
H	3.37912100	-0.55435800	-2.58587800
C	5.43126100	-0.17444400	0.67977100
H	3.81717200	1.04172800	1.38866400
C	5.92044500	-0.95178100	-0.36984000
H	5.56780200	-1.68905500	-2.36274600
H	5.99404800	-0.08583500	1.60116500
H	6.87243100	-1.45983100	-0.26648100
IRC_TS1_point192			
B	-2.72950500	3.81401000	0.36480700
B	-1.63543900	3.63903200	1.76027400
B	-0.60763100	2.21540400	1.47775100
B	-2.37423900	2.50128200	-0.78924100
B	-1.09154800	1.53548800	-0.07538700
B	-1.28484700	4.83932100	0.49796400
B	-1.73888000	4.14256200	-1.07642800
H	-3.82913200	4.25342400	0.48014400
B	0.02831800	3.85474400	1.17857000
H	-1.95705600	3.95418200	2.86181500
B	0.37290600	2.55726000	0.02970500
H	-0.18226100	1.53484500	2.34934300
B	-0.70729900	2.71967600	-1.37095600
H	-3.20702200	2.00770500	-1.47872000
H	-1.35531600	6.00911200	0.70516200
B	-0.03598700	4.17419600	-0.57519800
H	-2.13563200	4.80694000	-1.97961300

H	0.90193700	4.29699700	1.85464200
H	-0.36631400	2.38430700	-2.46298300
H	0.79061100	4.83462300	-1.11788000
B	-2.31762400	2.20640800	0.97623800
I	-1.49167600	-0.80993400	-0.24226800
C	0.31182600	-1.59560400	0.62037100
C	0.59756300	-1.30066900	1.94611400
C	1.14984500	-2.37462500	-0.16706300
C	1.78953600	-1.78084300	2.49071200
H	-0.08063200	-0.70734200	2.54234400
C	2.33381100	-2.85134300	0.39611500
H	0.90482200	-2.59055000	-1.19803500
C	2.65850000	-2.54763600	1.71709100
H	2.03280700	-1.54773800	3.52108000
H	3.00711000	-3.44632100	-0.20964200
H	3.58820500	-2.90751600	2.14196600
O	-2.09944600	-3.40773600	0.11673000
C	-3.29266700	-3.59641100	-0.26637000
O	-4.04057300	-2.72065700	-0.78485100
C	-3.83575500	-4.99671600	-0.04047300
H	-4.16392700	-5.07611000	1.00167200
H	-4.68821300	-5.21314000	-0.68655300
H	-3.05005400	-5.73830000	-0.19756800
H	0.55822700	0.93035000	-1.79056700
H	-3.10649100	1.49526900	1.50703800
N	1.78454500	2.01323000	-0.07379600
C	2.15838000	0.96678200	-0.75310300
H	2.50136400	2.44539000	0.49969000
C	3.47136700	0.33891100	-0.62588300
O	1.34447400	0.38281000	-1.59950800
C	3.95863500	-0.44864100	-1.67770300
C	4.20935700	0.47222400	0.55523200
C	5.18630400	-1.08452800	-1.54860900
H	3.37941200	-0.55415400	-2.58532800
C	5.43183800	-0.17463800	0.67999300
H	3.81767600	1.04102400	1.38966900
C	5.92081400	-0.95187800	-0.36983400
H	5.56784200	-1.68922600	-2.36268400
H	5.99500700	-0.08599700	1.60114900
H	6.87292200	-1.45974600	-0.26671800
IRC_TS1_point193			
B	-2.72970400	3.81493400	0.36481900
B	-1.63569100	3.64013700	1.76036000

B	-0.60962200	2.21493200	1.47935100
B	-2.37615600	2.50045400	-0.78769100
B	-1.09389500	1.53450500	-0.07323000
B	-1.28378500	4.83862800	0.49667500
B	-1.73882400	4.14063900	-1.07695800
H	-3.82879700	4.25577700	0.47975100
B	0.02819500	3.85306900	1.17816900
H	-1.95671500	3.95696100	2.86159500
B	0.37118000	2.55423600	0.03047600
H	-0.18511200	1.53476900	2.35166000
B	-0.70907400	2.71626900	-1.36985600
H	-3.20951600	2.00690600	-1.47648400
H	-1.35281600	6.00870700	0.70268600
B	-0.03601000	4.17084500	-0.57590300
H	-2.13488000	4.80438500	-1.98089900
H	0.90258100	4.29492900	1.85351200
H	-0.36892700	2.37896900	-2.46160500
H	0.79144900	4.82956100	-1.11933800
B	-2.31968400	2.20744000	0.97804000
I	-1.49074100	-0.80696700	-0.24226100
C	0.31233500	-1.59420100	0.62025200
C	0.59799200	-1.29995200	1.94616700
C	1.14976700	-2.37378700	-0.16723300
C	1.78965800	-1.78088200	2.49073700
H	-0.07994700	-0.70644900	2.54250300
C	2.33343700	-2.85129700	0.39599300
H	0.90466900	-2.58949600	-1.19823000
C	2.65834500	-2.54784400	1.71696100
H	2.03293100	-1.54817200	3.52119300
H	3.00637000	-3.44662800	-0.20981900
H	3.58791000	-2.90817200	2.14176300
O	-2.09959700	-3.41307900	0.11622400
C	-3.29323100	-3.60009800	-0.26622300
O	-4.03998100	-2.72303900	-0.78432300
C	-3.83974700	-4.99939500	-0.04073400
H	-4.16783300	-5.07862500	1.00145600
H	-4.69304500	-5.21312800	-0.68661200
H	-3.05622200	-5.74313700	-0.19859900
H	0.56114500	0.93219300	-1.79702900
H	-3.10923300	1.49757300	1.50957300
N	1.78278500	2.01031700	-0.07276000
C	2.15889500	0.96613700	-0.75422500
H	2.49812000	2.44105700	0.50363700
C	3.47176000	0.33850400	-0.62529900

O	1.34799100	0.38432000	-1.60504000
C	3.95904700	-0.44878900	-1.67722900
C	4.20968200	0.47170400	0.55595100
C	5.18657200	-1.08477800	-1.54841800
H	3.37982100	-0.55402000	-2.58484900
C	5.43240200	-0.17484600	0.68021400
H	3.81814100	1.04025600	1.39063200
C	5.92123700	-0.95198100	-0.36980300
H	5.56797100	-1.68942600	-2.36258900
H	5.99590400	-0.08615300	1.60116200
H	6.87347300	-1.45964900	-0.26689900

IRC_TS1_point194

B	-2.72990800	3.81584500	0.36483500
B	-1.63594200	3.64126300	1.76043700
B	-0.61160900	2.21449300	1.48096700
B	-2.37808100	2.49961800	-0.78613900
B	-1.09623900	1.53353600	-0.07105300
B	-1.28272000	4.83792600	0.49535400
B	-1.73879400	4.13870800	-1.07750000
H	-3.82848500	4.25803800	0.47937300
B	0.02807500	3.85141200	1.17776000
H	-1.95638600	3.95971000	2.86136300
B	0.36946500	2.55120800	0.03126200
H	-0.18787500	1.53472300	2.35392900
B	-0.71086900	2.71285900	-1.36876700
H	-3.21195400	2.00606900	-1.47427600
H	-1.35036100	6.00828500	0.70020500
B	-0.03603100	4.16748000	-0.57664400
H	-2.13419600	4.80187600	-1.98213900
H	0.90319200	4.29295300	1.85236800
H	-0.37157500	2.37358400	-2.46024800
H	0.79223500	4.82457400	-1.12080000
B	-2.32172600	2.20847800	0.97985800
I	-1.48979500	-0.80401000	-0.24224800
C	0.31285700	-1.59276300	0.62014500
C	0.59843900	-1.29919500	1.94622800
C	1.14969100	-2.37290200	-0.16741000
C	1.78978100	-1.78091600	2.49076600
H	-0.07925100	-0.70551700	2.54266500
C	2.33304600	-2.85124400	0.39586400
H	0.90451200	-2.58837300	-1.19843800
C	2.65816300	-2.54807700	1.71683300
H	2.03306400	-1.54860900	3.52130800

H	3.00561100	-3.44693100	-0.21000700
H	3.58757100	-2.90888900	2.14156500
O	-2.09975900	-3.41838600	0.11567300
C	-3.29377800	-3.60377400	-0.26608100
O	-4.03942900	-2.72543900	-0.78381600
C	-3.84370600	-5.00205800	-0.04096900
H	-4.17164000	-5.08103800	1.00128900
H	-4.69776600	-5.21315100	-0.68668700
H	-3.06222800	-5.74782000	-0.19954500
H	0.56435200	0.93313200	-1.80184600
H	-3.11186400	1.49977200	1.51204500
N	1.78100600	2.00729900	-0.07160500
C	2.15939500	0.96547400	-0.75534300
H	2.49489000	2.43655900	0.50768000
C	3.47215200	0.33807300	-0.62478100
O	1.35133200	0.38607400	-1.61073000
C	3.95952300	-0.44897800	-1.67678800
C	4.20998500	0.47114400	0.55662200
C	5.18691400	-1.08505900	-1.54819800
H	3.38033400	-0.55396600	-2.58442600
C	5.43294600	-0.17507900	0.68045100
H	3.81856300	1.03944600	1.39153300
C	5.92170700	-0.95210400	-0.36972300
H	5.56820400	-1.68966200	-2.36244900
H	5.99671700	-0.08631900	1.60122500
H	6.87407100	-1.45956200	-0.26699500
IRC_TS1_point195			
B	-2.73012300	3.81674800	0.36485600
B	-1.63619000	3.64240600	1.76050700
B	-0.61358700	2.21409000	1.48259100
B	-2.38002400	2.49878500	-0.78456400
B	-1.09858300	1.53261400	-0.06886700
B	-1.28165700	4.83721900	0.49400400
B	-1.73879800	4.13676600	-1.07804500
H	-3.82816200	4.26036800	0.47899700
B	0.02795600	3.84977900	1.17733300
H	-1.95603600	3.96256000	2.86111300
B	0.36774700	2.54819300	0.03207700
H	-0.19068400	1.53472100	2.35625500
B	-0.71270200	2.70945600	-1.36767600
H	-3.21445800	2.00521300	-1.47199400
H	-1.34786500	6.00786600	0.69763600
B	-0.03605900	4.16410000	-0.57741300
H	-2.13353300	4.79930200	-1.98342300

H	0.90383000	4.29097100	1.85119000
H	-0.37432300	2.36800500	-2.45880000
H	0.79303200	4.81951000	-1.12232800
B	-2.32375900	2.20951900	0.98168300
I	-1.48884000	-0.80106500	-0.24223300
C	0.31340000	-1.59126700	0.62003700
C	0.59890800	-1.29839300	1.94628900
C	1.14962100	-2.37195900	-0.16760500
C	1.78991400	-1.78094200	2.49078900
H	-0.07850600	-0.70451500	2.54283300
C	2.33264200	-2.85117500	0.39571200
H	0.90435800	-2.58715600	-1.19866800
C	2.65796100	-2.54833000	1.71669300
H	2.03321600	-1.54906400	3.52142200
H	3.00481900	-3.44723200	-0.21021900
H	3.58719200	-2.90967500	2.14136000
O	-2.09991400	-3.42364200	0.11507400
C	-3.29435000	-3.60743900	-0.26596800
O	-4.03890300	-2.72786400	-0.78332400
C	-3.84763100	-5.00470300	-0.04118200
H	-4.17550000	-5.08346000	1.00111800
H	-4.70249400	-5.21316500	-0.68670500
H	-3.06830600	-5.75258900	-0.20046500
H	0.56706300	0.93506200	-1.80771600
H	-3.11455100	1.50206600	1.51461200
N	1.77919900	2.00418200	-0.07035400
C	2.15985000	0.96477700	-0.75645800
H	2.49157200	2.43187600	0.51193000
C	3.47254500	0.33762600	-0.62434400
O	1.35466600	0.38781600	-1.61625300
C	3.96006100	-0.44919100	-1.67639300
C	4.21026400	0.47055300	0.55723300
C	5.18732800	-1.08535500	-1.54796500
H	3.38095300	-0.55397600	-2.58407500
C	5.43347000	-0.17532400	0.68068800
H	3.81894300	1.03857700	1.39238700
C	5.92222100	-0.95223200	-0.36961600
H	5.56853000	-1.68992300	-2.36227800
H	5.99746800	-0.08648100	1.60131700
H	6.87471800	-1.45946500	-0.26703100
IRC_TS1_point196			
B	-2.73034400	3.81764100	0.36487900
B	-1.63643500	3.64357000	1.76056800

B	-0.61555900	2.21372400	1.48423000
B	-2.38197300	2.49794700	-0.78298600
B	-1.10092800	1.53170400	-0.06665400
B	-1.28059800	4.83651000	0.49262500
B	-1.73882400	4.13481800	-1.07860200
H	-3.82786000	4.26261400	0.47863600
B	0.02783800	3.84817200	1.17689500
H	-1.95569500	3.96538800	2.86085000
B	0.36604200	2.54518000	0.03290900
H	-0.19341100	1.53475500	2.35854200
B	-0.71454900	2.70604800	-1.36658100
H	-3.21690900	2.00432200	-1.46973700
H	-1.34541900	6.00743500	0.69506400
B	-0.03608800	4.16071500	-0.57821300
H	-2.13293300	4.79676600	-1.98467100
H	0.90443500	4.28908300	1.85000100
H	-0.37709900	2.36235800	-2.45734200
H	0.79377900	4.81451700	-1.12386400
B	-2.32577600	2.21056700	0.98352600
I	-1.48787800	-0.79813500	-0.24221300
C	0.31395400	-1.58973600	0.61993900
C	0.59939500	-1.29755100	1.94635700
C	1.14955500	-2.37096800	-0.16780700
C	1.79005000	-1.78096400	2.49081500
H	-0.07774500	-0.70347400	2.54300300
C	2.33222400	-2.85109800	0.39555300
H	0.90420200	-2.58587300	-1.19891000
C	2.65773600	-2.54860800	1.71655400
H	2.03337900	-1.54952200	3.52153700
H	3.00401000	-3.44752800	-0.21044400
H	3.58677100	-2.91052300	2.14116100
O	-2.10008200	-3.42886100	0.11443100
C	-3.29491000	-3.61108800	-0.26586500
O	-4.03842000	-2.73030100	-0.78285600
C	-3.85151300	-5.00732800	-0.04136600
H	-4.17925700	-5.08578200	1.00099600
H	-4.70710200	-5.21322600	-0.68673000
H	-3.07421600	-5.75720200	-0.20129400
H	0.57017800	0.93650400	-1.81259200
H	-3.11713600	1.50427100	1.51712800
N	1.77737700	2.00097200	-0.06899200
C	2.16028500	0.96406800	-0.75756600
H	2.48827100	2.42704600	0.51626500
C	3.47293000	0.33714700	-0.62396700

O	1.35784700	0.38975500	-1.62188900
C	3.96065700	-0.44944300	-1.67603500
C	4.21051800	0.46992400	0.55779700
C	5.18781300	-1.08567600	-1.54771100
H	3.38166300	-0.55405600	-2.58378100
C	5.43397200	-0.17559000	0.68093900
H	3.81927900	1.03767100	1.39317800
C	5.92277300	-0.95237700	-0.36946500
H	5.56896000	-1.69021100	-2.36207100
H	5.99813600	-0.08664800	1.60145500
H	6.87540300	-1.45937900	-0.26698400
IRC_TS1_point197			
B	-2.73057400	3.81852900	0.36490700
B	-1.63667600	3.64475500	1.76062300
B	-0.61752200	2.21339400	1.48587700
B	-2.38393700	2.49711000	-0.78138500
B	-1.10327100	1.53083300	-0.06442700
B	-1.27954600	4.83580200	0.49121900
B	-1.73887800	4.13286000	-1.07916300
H	-3.82755000	4.26492000	0.47827200
B	0.02772200	3.84659400	1.17643900
H	-1.95533300	3.96831400	2.86056900
B	0.36433500	2.54217900	0.03376800
H	-0.19617700	1.53484100	2.36088700
B	-0.71642200	2.70263900	-1.36547100
H	-3.21941800	2.00341200	-1.46741000
H	-1.34294300	6.00701300	0.69241300
B	-0.03612600	4.15732400	-0.57903800
H	-2.13235200	4.79416500	-1.98596400
H	0.90506200	4.28720000	1.84878000
H	-0.37996600	2.35659000	-2.45582400
H	0.79453300	4.80945600	-1.12546600
B	-2.32778500	2.21162000	0.98538100
I	-1.48690800	-0.79522000	-0.24219200
C	0.31452700	-1.58815100	0.61983900
C	0.59990600	-1.29666400	1.94642400
C	1.14949700	-2.36992000	-0.16802500
C	1.79019600	-1.78097800	2.49083500
H	-0.07693600	-0.70236600	2.54318000
C	2.33179300	-2.85100500	0.39537200
H	0.90405000	-2.58449800	-1.19917300
C	2.65749300	-2.54890400	1.71640400
H	2.03356100	-1.54999800	3.52165200
H	3.00317000	-3.44782100	-0.21069300

H	3.58631100	-2.91143900	2.14095500
O	-2.10024600	-3.43403200	0.11374200
C	-3.29549500	-3.61472100	-0.26579100
O	-4.03796500	-2.73275600	-0.78240700
C	-3.85535400	-5.00993500	-0.04152600
H	-4.18305000	-5.08810300	1.00087800
H	-4.71170500	-5.21329100	-0.68669700
H	-3.08016800	-5.76188400	-0.20208800
H	0.57299100	0.93877500	-1.81845100
H	-3.11977300	1.50656700	1.51973900
N	1.77553300	1.99767100	-0.06754000
C	2.16068600	0.96332700	-0.75866500
H	2.48489200	2.42203700	0.52079500
C	3.47331000	0.33664100	-0.62365900
O	1.36100900	0.39170400	-1.62738200
C	3.96130600	-0.44971900	-1.67572400
C	4.21074700	0.46926300	0.55830700
C	5.18836400	-1.08600700	-1.54745000
H	3.38246800	-0.55419100	-2.58355600
C	5.43445100	-0.17586700	0.68119100
H	3.81957200	1.03671600	1.39392000
C	5.92336100	-0.95252800	-0.36928900
H	5.56948400	-1.69051400	-2.36183900
H	5.99874400	-0.08681000	1.60161900
H	6.87612800	-1.45928500	-0.26688000

IRC_TS1_point198

B	-2.73080900	3.81941000	0.36493500
B	-1.63691400	3.64596300	1.76067000
B	-0.61947700	2.21310300	1.48754100
B	-2.38590600	2.49626800	-0.77977600
B	-1.10562300	1.52997400	-0.06217200
B	-1.27850100	4.83509600	0.48978600
B	-1.73895200	4.13089400	-1.07973400
H	-3.82725800	4.26715700	0.47791900
B	0.02760700	3.84504700	1.17597200
H	-1.95497600	3.97123200	2.86027600
B	0.36264200	2.53918100	0.03464600
H	-0.19887200	1.53496900	2.36320500
B	-0.71830500	2.69922800	-1.36435700
H	-3.22188100	2.00247100	-1.46509700
H	-1.34051300	6.00658400	0.68975100
B	-0.03616700	4.15393200	-0.57989000
H	-2.13182300	4.79158500	-1.98723200

H	0.90565800	4.28540800	1.84754600
H	-0.38286400	2.35091900	-2.45435200
H	0.79524100	4.80445000	-1.12708300
B	-2.32978100	2.21268400	0.98725600
I	-1.48593100	-0.79232200	-0.24216600
C	0.31511300	-1.58652900	0.61974600
C	0.60043700	-1.29573900	1.94649600
C	1.14944400	-2.36882400	-0.16825000
C	1.79034800	-1.78098700	2.49085700
H	-0.07610700	-0.70121700	2.54335900
C	2.33135100	-2.85090200	0.39518200
H	0.90389900	-2.58305600	-1.19944700
C	2.65722900	-2.54922500	1.71625300
H	2.03375600	-1.55047800	3.52176600
H	3.00231300	-3.44810800	-0.21095700
H	3.58581200	-2.91241800	2.14075300
O	-2.10042300	-3.43917100	0.11300900
C	-3.29607200	-3.61833600	-0.26572900
O	-4.03755200	-2.73521900	-0.78198300
C	-3.85915000	-5.01252500	-0.04165700
H	-4.18674800	-5.09033100	1.00080700
H	-4.71619600	-5.21341100	-0.68666200
H	-3.08596400	-5.76642400	-0.20279100
H	0.57611700	0.94067900	-1.82349200
H	-3.12232300	1.50879500	1.52231600
N	1.77367500	1.99428300	-0.06598500
C	2.16106500	0.96257600	-0.75975700
H	2.48152100	2.41687600	0.52542200
C	3.47367800	0.33609600	-0.62340200
O	1.36405300	0.39380600	-1.63296100
C	3.96200600	-0.45002900	-1.67545000
C	4.21095000	0.46856500	0.55877200
C	5.18897900	-1.08635500	-1.54717300
H	3.38335400	-0.55438500	-2.58338700
C	5.43490700	-0.17616200	0.68145500
H	3.81982600	1.03572800	1.39460500
C	5.92397900	-0.95269300	-0.36907400
H	5.57010700	-1.69083200	-2.36157900
H	5.99927800	-0.08697500	1.60182200
H	6.87688300	-1.45919900	-0.26670200
IRC_TS1_point199			
B	-2.73105300	3.82029100	0.36496800
B	-1.63714800	3.64719600	1.76071000
B	-0.62142400	2.21284900	1.48921200

B	-2.38788900	2.49542700	-0.77814500
B	-1.10798600	1.52914600	-0.05990000
B	-1.27746500	4.83439500	0.48832900
B	-1.73904800	4.12891700	-1.08030600
H	-3.82696100	4.26944700	0.47756400
B	0.02749200	3.84353300	1.17548500
H	-1.95459800	3.97423600	2.85996800
B	0.36094600	2.53619500	0.03554600
H	-0.20159400	1.53515200	2.36557400
B	-0.72020500	2.69582500	-1.36323700
H	-3.22439700	2.00151800	-1.46272200
H	-1.33806700	6.00616700	0.68702000
B	-0.03621800	4.15053700	-0.58075900
H	-2.13130900	4.78894100	-1.98854200
H	0.90627100	4.28362800	1.84628600
H	-0.38583800	2.34540200	-2.45293500
H	0.79594800	4.79939200	-1.12876000
B	-2.33177300	2.21375700	0.98914600
I	-1.48494700	-0.78944100	-0.24213800
C	0.31571900	-1.58485300	0.61965200
C	0.60099300	-1.29477100	1.94656700
C	1.14939900	-2.36767300	-0.16849100
C	1.79051100	-1.78099000	2.49087200
H	-0.07523000	-0.70000400	2.54354400
C	2.33089900	-2.85078300	0.39497200
H	0.90375300	-2.58152800	-1.19974100
C	2.65695000	-2.54956500	1.71609200
H	2.03397000	-1.55097500	3.52187900
H	3.00142800	-3.44839100	-0.21124500
H	3.58527700	-2.91346300	2.14054500
O	-2.10060000	-3.44427100	0.11222900
C	-3.29667400	-3.62193800	-0.26569700
O	-4.03716900	-2.73769900	-0.78157900
C	-3.86290400	-5.01509800	-0.04176100
H	-4.19046500	-5.09255000	1.00074700
H	-4.72067200	-5.21355000	-0.68657100
H	-3.09177600	-5.77101200	-0.20345100
H	0.57895400	0.94314500	-1.82918600
H	-3.12491700	1.51110600	1.52498100
N	1.77179600	1.99080800	-0.06434800
C	2.16141900	0.96179200	-0.76083500
H	2.47807700	2.41154000	0.53022700
C	3.47403800	0.33552000	-0.62320400
O	1.36709100	0.39592100	-1.63842300

C	3.96275200	-0.45036300	-1.67521900
C	4.21112700	0.46783600	0.55919000
C	5.18965500	-1.08671100	-1.54689400
H	3.38432400	-0.55462700	-2.58328400
C	5.43534100	-0.17646900	0.68172100
H	3.82004100	1.03470000	1.39524100
C	5.92462600	-0.95286200	-0.36883500
H	5.57081900	-1.69115500	-2.36130300
H	5.99975300	-0.08713300	1.60205000
H	6.87767000	-1.45910500	-0.26647200

IRC_TS1_point200

B	-2.73130300	3.82117000	0.36500300
B	-1.63737700	3.64845600	1.76074400
B	-0.62336300	2.21263600	1.49089600
B	-2.38987500	2.49458300	-0.77650600
B	-1.11037700	1.52832200	-0.05759200
B	-1.27644000	4.83370200	0.48684900
B	-1.73916200	4.12693400	-1.08088100
H	-3.82667700	4.27168700	0.47721900
B	0.02737800	3.84205400	1.17498700
H	-1.95422100	3.97723800	2.85965000
B	0.35926200	2.53321600	0.03646100
H	-0.20425200	1.53538000	2.36791900
B	-0.72211000	2.69243900	-1.36212400
H	-3.22687900	2.00054700	-1.46035800
H	-1.33566600	6.00575000	0.68428200
B	-0.03627400	4.14714800	-0.58164700
H	-2.13083300	4.78630700	-1.98983200
H	0.90686000	4.28193000	1.84501500
H	-0.38885400	2.34005700	-2.45160000
H	0.79660800	4.79438800	-1.13045100
B	-2.33375600	2.21484500	0.99105600
I	-1.48395700	-0.78658100	-0.24210800
C	0.31634000	-1.58313600	0.61956400
C	0.60157000	-1.29376400	1.94664300
C	1.14936200	-2.36647400	-0.16873800
C	1.79068200	-1.78098800	2.49088900
H	-0.07432900	-0.69875100	2.54373200
C	2.33043700	-2.85065400	0.39475200
H	0.90361000	-2.57993500	-1.20004500
C	2.65665300	-2.54992900	1.71592900
H	2.03419800	-1.55147800	3.52199200
H	3.00052800	-3.44866700	-0.21154700

H	3.58470700	-2.91456800	2.14034000
O	-2.10079300	-3.44934000	0.11140500
C	-3.29727600	-3.62552100	-0.26568100
O	-4.03682600	-2.74018500	-0.78120100
C	-3.86661200	-5.01765500	-0.04183300
H	-4.19409200	-5.09468500	1.00073300
H	-4.72504200	-5.21375200	-0.68647000
H	-3.09744200	-5.77546700	-0.20402100
H	0.58202800	0.94538800	-1.83419500
H	-3.12744000	1.51337300	1.52762600
N	1.76990300	1.98724800	-0.06261700
C	2.16175100	0.96099600	-0.76190100
H	2.47463300	2.40606200	0.53512000
C	3.47438700	0.33490400	-0.62305100
O	1.37004900	0.39815800	-1.64395400
C	3.96354100	-0.45073000	-1.67502300
C	4.21127700	0.46707000	0.55956800
C	5.19038900	-1.08707900	-1.54660300
H	3.38536900	-0.55491900	-2.58323600
C	5.43574900	-0.17679400	0.68199900
H	3.82021600	1.03364500	1.39582200
C	5.92529700	-0.95304500	-0.36856300
H	5.57162400	-1.69148200	-2.36100700
H	6.00015900	-0.08729400	1.60231200
H	6.87848200	-1.45901800	-0.26617600

IRC_TS1_point201

B	-2.73156000	3.82205200	0.36504100
B	-1.63760100	3.64974400	1.76077100
B	-0.62529300	2.21246000	1.49258500
B	-2.39187200	2.49374200	-0.77484600
B	-1.11277700	1.52752200	-0.05526700
B	-1.27542600	4.83301800	0.48534800
B	-1.73929500	4.12494300	-1.08145400
H	-3.82639000	4.27397500	0.47687200
B	0.02726600	3.84061000	1.17447100
H	-1.95382300	3.98031500	2.85931900
B	0.35757400	2.53025000	0.03739100
H	-0.20692400	1.53566400	2.37030500
B	-0.72402700	2.68907400	-1.36101100
H	-3.22940500	1.99957700	-1.45794400
H	-1.33326100	6.00534700	0.68148800
B	-0.03633900	4.14376500	-0.58254700
H	-2.13037300	4.78362100	-1.99115300

H	0.90746000	4.28025000	1.84372100
H	-0.39195900	2.33479700	-2.45030400
H	0.79726100	4.78935600	-1.13218700
B	-2.33573500	2.21594700	0.99298100
I	-1.48296100	-0.78374100	-0.24207600
C	0.31698400	-1.58136700	0.61947500
C	0.60217300	-1.29271500	1.94671900
C	1.14933600	-2.36522100	-0.16899800
C	1.79086400	-1.78097900	2.49090000
H	-0.07338100	-0.69743700	2.54392600
C	2.32996700	-2.85051000	0.39451500
H	0.90347400	-2.57826400	-1.20036500
C	2.65634200	-2.55031200	1.71575800
H	2.03444300	-1.55199600	3.52210500
H	2.99960500	-3.44893700	-0.21187200
H	3.58410300	-2.91573700	2.14013100
O	-2.10098900	-3.45437600	0.11053600
C	-3.29790200	-3.62909200	-0.26569200
O	-4.03651200	-2.74268400	-0.78084400
C	-3.87027600	-5.02019800	-0.04187700
H	-4.19772200	-5.09680200	1.00073600
H	-4.72938600	-5.21398700	-0.68631500
H	-3.10309800	-5.77995000	-0.20454100
H	0.58487700	0.94809000	-1.83967600
H	-3.13000300	1.51571900	1.53035000
N	1.76798900	1.98360400	-0.06081200
C	2.16206500	0.96016400	-0.76295000
H	2.47112100	2.40042300	0.54016900
C	3.47472800	0.33425300	-0.62294700
O	1.37300000	0.40042700	-1.64939200
C	3.96437000	-0.45111900	-1.67486600
C	4.21140300	0.46627400	0.55990500
C	5.19117600	-1.08745000	-1.54631200
H	3.38648800	-0.55525300	-2.58324800
C	5.43613600	-0.17713200	0.68228000
H	3.82035600	1.03255000	1.39636100
C	5.92599200	-0.95323200	-0.36826900
H	5.57251400	-1.69180600	-2.36069900
H	6.00050900	-0.08745200	1.60259900
H	6.87932000	-1.45892300	-0.26583300
IRC_TS1_point202			
B	-2.73182400	3.82293600	0.36508200
B	-1.63782000	3.65106100	1.76079200
B	-0.62721600	2.21232500	1.49428300

B	-2.39387300	2.49290000	-0.77317700
B	-1.11518700	1.52673100	-0.05292000
B	-1.27442300	4.83234600	0.48382900
B	-1.73944500	4.12295000	-1.08202700
H	-3.82611600	4.27622500	0.47653200
B	0.02715400	3.83920100	1.17394400
H	-1.95342200	3.98339800	2.85898000
B	0.35589700	2.52729100	0.03833300
H	-0.20954100	1.53599600	2.37267200
B	-0.72595100	2.68573000	-1.35990500
H	-3.23190400	1.99859500	-1.45553500
H	-1.33089600	6.00494900	0.67868200
B	-0.03640900	4.14039200	-0.58346200
H	-2.12995000	4.78094400	-1.99245700
H	0.90804000	4.27864400	1.84241600
H	-0.39510300	2.32964000	-2.44904600
H	0.79787300	4.78437400	-1.13393600
B	-2.33770800	2.21706700	0.99492700
I	-1.48195900	-0.78092400	-0.24204200
C	0.31764500	-1.57955700	0.61938900
C	0.60280000	-1.29162800	1.94679900
C	1.14932000	-2.36392100	-0.16926600
C	1.79105600	-1.78096700	2.49091200
H	-0.07240700	-0.69608100	2.54412300
C	2.32949100	-2.85035500	0.39426800
H	0.90334400	-2.57652700	-1.20069600
C	2.65601600	-2.55071600	1.71558500
H	2.03470400	-1.55252300	3.52221700
H	2.99866800	-3.44920100	-0.21221100
H	3.58346600	-2.91696400	2.13992500
O	-2.10120200	-3.45938400	0.10962300
C	-3.29853200	-3.63264700	-0.26572100
O	-4.03623700	-2.74519000	-0.78051400
C	-3.87389500	-5.02272900	-0.04189000
H	-4.20127200	-5.09884500	1.00078400
H	-4.73363600	-5.21428900	-0.68614300
H	-3.10862100	-5.78432000	-0.20497300
H	0.58785000	0.95060500	-1.84451800
H	-3.13250600	1.51803500	1.53306300
N	1.76606100	1.97987900	-0.05892100
C	2.16235700	0.95931600	-0.76398400
H	2.46759500	2.39462300	0.54532400
C	3.47505900	0.33356100	-0.62288100
O	1.37588200	0.40280700	-1.65488100

C	3.96523500	-0.45153800	-1.67474100
C	4.21150400	0.46544400	0.56020900
C	5.19201500	-1.08783000	-1.54601300
H	3.38766900	-0.55563000	-2.58330800
C	5.43649800	-0.17748900	0.68257100
H	3.82046300	1.03142800	1.39685400
C	5.92670600	-0.95343100	-0.36794500
H	5.57349000	-1.69212700	-2.36037900
H	6.00079800	-0.08761600	1.60291600
H	6.88017900	-1.45883300	-0.26543300
IRC_TS1_point203			
B	-2.73209500	3.82382500	0.36512600
B	-1.63803500	3.65240700	1.76080800
B	-0.62913100	2.21222800	1.49598400
B	-2.39588100	2.49206200	-0.77148800
B	-1.11758100	1.52597700	-0.05057000
B	-1.27343200	4.83168700	0.48229100
B	-1.73961300	4.12095300	-1.08259900
H	-3.82583800	4.27851900	0.47618900
B	0.02704400	3.83782700	1.17340000
H	-1.95300000	3.98655200	2.85862900
B	0.35421700	2.52434600	0.03928800
H	-0.21216600	1.53638300	2.37507300
B	-0.72788300	2.68240500	-1.35878900
H	-3.23443800	1.99761500	-1.45308400
H	-1.32853100	6.00456700	0.67582700
B	-0.03648700	4.13703000	-0.58438700
H	-2.12954200	4.77822400	-1.99378700
H	0.90863000	4.27706000	1.84108900
H	-0.39828800	2.32445600	-2.44775300
H	0.79847600	4.77937800	-1.13572200
B	-2.33967700	2.21820300	0.99688600
I	-1.48095200	-0.77812900	-0.24200800
C	0.31833100	-1.57769800	0.61930400
C	0.60345400	-1.29050000	1.94687800
C	1.14931600	-2.36257000	-0.16954600
C	1.79126100	-1.78094900	2.49092000
H	-0.07138600	-0.69466700	2.54432500
C	2.32900900	-2.85018500	0.39400400
H	0.90322200	-2.57471700	-1.20104100
C	2.65567900	-2.55114000	1.71540500
H	2.03498200	-1.55306400	3.52233000
H	2.99771100	-3.44946000	-0.21257000
H	3.58279900	-2.91825300	2.13971600

O	-2.10142200	-3.46436300	0.10866400
C	-3.29918900	-3.63619200	-0.26577700
O	-4.03599200	-2.74770700	-0.78020700
C	-3.87747400	-5.02524900	-0.04187200
H	-4.20481700	-5.10086800	1.00085200
H	-4.73785700	-5.21463300	-0.68591800
H	-3.11412400	-5.78870800	-0.20535100
H	0.59054700	0.95341800	-1.84968000
H	-3.13503900	1.52042400	1.53584600
N	1.76411200	1.97607500	-0.05696100
C	2.16262600	0.95843400	-0.76499800
H	2.46400000	2.38864600	0.55064200
C	3.47537800	0.33283400	-0.62285700
O	1.37874500	0.40523500	-1.66029400
C	3.96613400	-0.45197800	-1.67465000
C	4.21158100	0.46458400	0.56047800
C	5.19290200	-1.08821100	-1.54571600
H	3.38891500	-0.55604400	-2.58342200
C	5.43683900	-0.17786000	0.68286800
H	3.82053900	1.03028000	1.39730500
C	5.92743800	-0.95363400	-0.36760300
H	5.57454300	-1.69244000	-2.36005200
H	6.00103600	-0.08778100	1.60325600
H	6.88105900	-1.45873700	-0.26499300

IRC_TS1_point204

B	-2.73237100	3.82471900	0.36517300
B	-1.63824500	3.65378300	1.76081800
B	-0.63103800	2.21217300	1.49769500
B	-2.39789100	2.49122700	-0.76978800
B	-1.11996500	1.52524800	-0.04821000
B	-1.27245100	4.83104200	0.48073500
B	-1.73979800	4.11895600	-1.08317200
H	-3.82557300	4.28077900	0.47584900
B	0.02693500	3.83648900	1.17284700
H	-1.95257400	3.98971700	2.85826900
B	0.35255200	2.52141400	0.04025800
H	-0.21474100	1.53681800	2.37745700
B	-0.72981800	2.67909600	-1.35767900
H	-3.23694300	1.99662000	-1.45063300
H	-1.32619900	6.00419300	0.67295600
B	-0.03656800	4.13368000	-0.58532700
H	-2.12916800	4.77551500	-1.99510200
H	0.90920200	4.27554800	1.83975100

H	-0.40151200	2.31934200	-2.44648900
H	0.79904300	4.77442800	-1.13751900
B	-2.34163500	2.21935900	0.99886300
I	-1.47994000	-0.77535600	-0.24197300
C	0.31903500	-1.57579800	0.61922200
C	0.60413300	-1.28933500	1.94696000
C	1.14932500	-2.36117200	-0.16983300
C	1.79147700	-1.78092700	2.49092700
H	-0.07033500	-0.69321000	2.54452900
C	2.32852300	-2.85000400	0.39373100
H	0.90310800	-2.57284200	-1.20139800
C	2.65532900	-2.55158500	1.71522300
H	2.03527800	-1.55361400	3.52244200
H	2.99674100	-3.44971300	-0.21294400
H	3.58210000	-2.91960100	2.13951000
O	-2.10165900	-3.46932300	0.10766100
C	-3.29985100	-3.63972500	-0.26585200
O	-4.03578500	-2.75023300	-0.77992500
C	-3.88101100	-5.02776100	-0.04182200
H	-4.20828900	-5.10282500	1.00096500
H	-4.74199300	-5.21504800	-0.68567200
H	-3.11950400	-5.79299700	-0.20564300
H	0.59325400	0.95601100	-1.85415300
H	-3.13751200	1.52278300	1.53861500
N	1.76214500	1.97219500	-0.05492100
C	2.16286300	0.95753900	-0.76599900
H	2.46037700	2.38247700	0.55609500
C	3.47568300	0.33206800	-0.62286700
O	1.38154500	0.40775800	-1.66574600
C	3.96706300	-0.45244500	-1.67458800
C	4.21163400	0.46369300	0.56071500
C	5.19383400	-1.08859600	-1.54541400
H	3.39021300	-0.55649600	-2.58357900
C	5.43715600	-0.17825000	0.68317400
H	3.82059400	1.02911800	1.39771100
C	5.92818700	-0.95384800	-0.36723500
H	5.57567500	-1.69274100	-2.35971700
H	6.00121800	-0.08795300	1.60362400
H	6.88195700	-1.45864400	-0.26450400
IRC_TS1_point205			
B	-2.73265200	3.82562000	0.36522200
B	-1.63845000	3.65519000	1.76082100
B	-0.63293600	2.21215800	1.49940900
B	-2.39990500	2.49039700	-0.76806800

B	-1.12231400	1.52457200	-0.04585700
B	-1.27147900	4.83041000	0.47916000
B	-1.73999900	4.11695700	-1.08374500
H	-3.82530400	4.28308100	0.47550300
B	0.02682800	3.83518600	1.17227900
H	-1.95212700	3.99294900	2.85789800
B	0.35088700	2.51850200	0.04124200
H	-0.21732100	1.53730700	2.37987000
B	-0.73175600	2.67580200	-1.35655800
H	-3.23947400	1.99562700	-1.44814300
H	-1.32386800	6.00383600	0.67003900
B	-0.03665400	4.13034400	-0.58627600
H	-2.12880700	4.77276800	-1.99644200
H	0.90978500	4.27406100	1.83839500
H	-0.40475000	2.31417900	-2.44517800
H	0.79960300	4.76947400	-1.13934800
B	-2.34358300	2.22053200	1.00085000
I	-1.47892300	-0.77260700	-0.24193800
C	0.31976500	-1.57385200	0.61914100
C	0.60484000	-1.28812900	1.94704300
C	1.14934900	-2.35972500	-0.17013100
C	1.79170700	-1.78090000	2.49093100
H	-0.06923800	-0.69169600	2.54473700
C	2.32803500	-2.84980900	0.39344200
H	0.90300700	-2.57089700	-1.20176700
C	2.65496900	-2.55204800	1.71503400
H	2.03559100	-1.55417900	3.52255500
H	2.99575600	-3.44995900	-0.21333800
H	3.58137300	-2.92100700	2.13930300
O	-2.10190400	-3.47426200	0.10661200
C	-3.30054200	-3.64325200	-0.26595300
O	-4.03560700	-2.75277200	-0.77966600
C	-3.88451000	-5.03026700	-0.04174200
H	-4.21175400	-5.10476300	1.00110200
H	-4.74610300	-5.21551100	-0.68537400
H	-3.12486100	-5.79730100	-0.20587900
H	0.59562400	0.95876600	-1.85880900
H	-3.14000500	1.52520900	1.54144500
N	1.76015400	1.96823800	-0.05281500
C	2.16307400	0.95661000	-0.76697900
H	2.45667600	2.37610500	0.56172500
C	3.47597300	0.33127000	-0.62291300
O	1.38431900	0.41033600	-1.67113000
C	3.96801700	-0.45293200	-1.67455600

C	4.21166400	0.46277700	0.56091900
C	5.19480800	-1.08897800	-1.54511500
H	3.39156500	-0.55698300	-2.58378400
C	5.43745000	-0.17865700	0.68348400
H	3.82063000	1.02794600	1.39807200
C	5.92894900	-0.95406800	-0.36685100
H	5.57687600	-1.69302700	-2.35938200
H	6.00135000	-0.08812700	1.60401100
H	6.88287100	-1.45854600	-0.26398000
IRC_TS1_point206			
B	-2.73293700	3.82652600	0.36527200
B	-1.63864900	3.65662700	1.76082000
B	-0.63482400	2.21218900	1.50113200
B	-2.40191400	2.48957200	-0.76634000
B	-1.12464500	1.52393100	-0.04349600
B	-1.27051500	4.82979500	0.47756800
B	-1.74021300	4.11496000	-1.08432000
H	-3.82504400	4.28535100	0.47515800
B	0.02672300	3.83392300	1.17170600
H	-1.95167500	3.99619300	2.85751900
B	0.34924200	2.51561100	0.04224400
H	-0.21985000	1.53784200	2.38226300
B	-0.73368800	2.67252300	-1.35544400
H	-3.24196900	1.99461700	-1.44565400
H	-1.32156700	6.00349000	0.66710400
B	-0.03674100	4.12702400	-0.58723900
H	-2.12847600	4.77003300	-1.99776800
H	0.91035100	4.27264800	1.83702900
H	-0.40800800	2.30906100	-2.44388500
H	0.80013000	4.76457200	-1.14118600
B	-2.34551700	2.22172700	1.00285000
I	-1.47790200	-0.76988200	-0.24190200
C	0.32051300	-1.57186800	0.61906200
C	0.60557400	-1.28688800	1.94712800
C	1.14938900	-2.35823300	-0.17043600
C	1.79194900	-1.78086900	2.49093400
H	-0.06810800	-0.69014000	2.54494700
C	2.32754600	-2.84960200	0.39314400
H	0.90291700	-2.56888800	-1.20214700
C	2.65460000	-2.55253200	1.71484400
H	2.03592300	-1.55475100	3.52266800
H	2.99476300	-3.45019800	-0.21374500
H	3.58061800	-2.92247000	2.13909900
O	-2.10216900	-3.47919000	0.10551700

C	-3.30124100	-3.64677300	-0.26607300
O	-4.03546600	-2.75532000	-0.77943200
C	-3.88797100	-5.03276900	-0.04162800
H	-4.21514900	-5.10664100	1.00128300
H	-4.75013400	-5.21605100	-0.68505200
H	-3.13010000	-5.80151200	-0.20602900
H	0.59795300	0.96130900	-1.86278100
H	-3.14243000	1.52760300	1.54425600
N	1.75814200	1.96420900	-0.05063200
C	2.16324500	0.95567100	-0.76794700
H	2.45293200	2.36950900	0.56751900
C	3.47624400	0.33043600	-0.62299000
O	1.38703700	0.41299700	-1.67654500
C	3.96899300	-0.45344300	-1.67455000
C	4.21167200	0.46183900	0.56109200
C	5.19581900	-1.08936200	-1.54481400
H	3.39296000	-0.55750800	-2.58402700
C	5.43771900	-0.17908200	0.68380200
H	3.82065500	1.02678000	1.39838400
C	5.92972300	-0.95429700	-0.36644500
H	5.57814600	-1.69329700	-2.35904300
H	6.00142800	-0.08830900	1.60442200
H	6.88379800	-1.45845200	-0.26341500

IRC_TS1_point207

B	-2.73322300	3.82744100	0.36532400
B	-1.63884300	3.65809500	1.76081200
B	-0.63669700	2.21226200	1.50285700
B	-2.40392200	2.48875500	-0.76459400
B	-1.12694000	1.52334800	-0.04113700
B	-1.26955900	4.82919600	0.47595800
B	-1.74043800	4.11296300	-1.08489700
H	-3.82478000	4.28766000	0.47480400
B	0.02662200	3.83269900	1.17112000
H	-1.95120400	3.99949900	2.85712800
B	0.34759900	2.51274800	0.04326100
H	-0.22237500	1.53843100	2.38468000
B	-0.73561200	2.66925600	-1.35431700
H	-3.24448000	1.99360900	-1.44313100
H	-1.31927100	6.00316200	0.66412600
B	-0.03683000	4.12372400	-0.58821000
H	-2.12815300	4.76726600	-1.99911900
H	0.91092600	4.27126500	1.83565000
H	-0.41125100	2.30388000	-2.44253800

H	0.80065100	4.75967900	-1.14304800
B	-2.34743500	2.22293900	1.00485600
I	-1.47687900	-0.76718400	-0.24186500
C	0.32128700	-1.56984100	0.61898400
C	0.60633700	-1.28560900	1.94721300
C	1.14944600	-2.35669400	-0.17075000
C	1.79220700	-1.78083300	2.49093500
H	-0.06693300	-0.68853200	2.54516200
C	2.32705800	-2.84938200	0.39283400
H	0.90284200	-2.56681500	-1.20253800
C	2.65422400	-2.55303400	1.71464900
H	2.03627200	-1.55533600	3.52278100
H	2.99376000	-3.45043000	-0.21416900
H	3.57983800	-2.92398800	2.13889600
O	-2.10244200	-3.48410400	0.10437500
C	-3.30197100	-3.65029000	-0.26622000
O	-4.03535300	-2.75788100	-0.77922000
C	-3.89139700	-5.03526800	-0.04148300
H	-4.21853400	-5.10849800	1.00149100
H	-4.75413900	-5.21664500	-0.68467600
H	-3.13531100	-5.80573700	-0.20612000
H	0.59995900	0.96396200	-1.86692500
H	-3.14486800	1.53006000	1.54711900
N	1.75610400	1.96010500	-0.04838800
C	2.16338800	0.95470000	-0.76889000
H	2.44909300	2.36267500	0.57352000
C	3.47649700	0.32957300	-0.62310100
O	1.38972800	0.41572300	-1.68189900
C	3.96998500	-0.45397200	-1.67457000
C	4.21165900	0.46088400	0.56123000
C	5.19686400	-1.08974000	-1.54451700
H	3.39439700	-0.55806900	-2.58431400
C	5.43796300	-0.17952300	0.68412300
H	3.82067400	1.02563000	1.39864100
C	5.93050400	-0.95453300	-0.36602600
H	5.57947500	-1.69354700	-2.35870700
H	6.00145600	-0.08849200	1.60485000
H	6.88473600	-1.45835400	-0.26282000
IRC_TS1_point208			
B	-2.73351000	3.82836200	0.36537200
B	-1.63903000	3.65959300	1.76079900
B	-0.63855500	2.21238400	1.50459000
B	-2.40591800	2.48794800	-0.76284500
B	-1.12922300	1.52280100	-0.03876300

B	-1.26861200	4.82861400	0.47433100
B	-1.74067200	4.11097200	-1.08547900
H	-3.82452300	4.28993600	0.47444700
B	0.02652500	3.83152000	1.17053200
H	-1.95073100	4.00281700	2.85672700
B	0.34598000	2.50991400	0.04429600
H	-0.22484600	1.53906900	2.38707700
B	-0.73752400	2.66600600	-1.35319700
H	-3.24694700	1.99258500	-1.44061300
H	-1.31700500	6.00284600	0.66113100
B	-0.03691500	4.12044700	-0.58919500
H	-2.12785400	4.76451500	-2.00045700
H	0.91148500	4.26996100	1.83426700
H	-0.41450000	2.29872600	-2.44119900
H	0.80114500	4.75484300	-1.14491700
B	-2.34933400	2.22417400	1.00687300
I	-1.47585400	-0.76451300	-0.24182700
C	0.32207900	-1.56777900	0.61890900
C	0.60712500	-1.28429800	1.94730100
C	1.14952100	-2.35511200	-0.17107000
C	1.79247900	-1.78079300	2.49093500
H	-0.06572700	-0.68688500	2.54537900
C	2.32657200	-2.84915100	0.39251500
H	0.90278200	-2.56468200	-1.20293900
C	2.65384100	-2.55355500	1.71445400
H	2.03664000	-1.55592800	3.52289400
H	2.99275200	-3.45065500	-0.21460600
H	3.57903400	-2.92555900	2.13869700
O	-2.10273500	-3.48901400	0.10318600
C	-3.30271000	-3.65380200	-0.26638600
O	-4.03527300	-2.76044900	-0.77903200
C	-3.89478500	-5.03776500	-0.04130400
H	-4.22185200	-5.11030000	1.00174300
H	-4.75806800	-5.21731900	-0.68427500
H	-3.14040700	-5.80987200	-0.20612700
H	0.60196400	0.96647300	-1.87047400
H	-3.14723400	1.53248500	1.54995700
N	1.75404100	1.95593300	-0.04607100
C	2.16348700	0.95372200	-0.76982200
H	2.44518900	2.35556900	0.57973100
C	3.47672700	0.32867900	-0.62323900
O	1.39237300	0.41852200	-1.68728000
C	3.97098900	-0.45452400	-1.67461200
C	4.21162700	0.45991800	0.56133500

C	5.19793700	-1.09011600	-1.54422100
H	3.39586000	-0.55866600	-2.58463100
C	5.43818100	-0.17998000	0.68444900
H	3.82069800	1.02451200	1.39884300
C	5.93129000	-0.95477800	-0.36558900
H	5.58086000	-1.69377500	-2.35837300
H	6.00143300	-0.08868200	1.60529600
H	6.88567800	-1.45826300	-0.26219000

IRC_TS1_point209

B	-2.73379500	3.82929200	0.36541900
B	-1.63921000	3.66112200	1.76077800
B	-0.64039500	2.21255000	1.50632300
B	-2.40790600	2.48714900	-0.76108400
B	-1.13147600	1.52231000	-0.03638700
B	-1.26767100	4.82805200	0.47268700
B	-1.74090900	4.10898300	-1.08606500
H	-3.82425800	4.29224900	0.47407600
B	0.02643400	3.83038500	1.16993200
H	-1.95024100	4.00619300	2.85631500
B	0.34436400	2.50711400	0.04534400
H	-0.22730900	1.53976300	2.38949700
B	-0.73941700	2.66276800	-1.35206100
H	-3.24942300	1.99156700	-1.43806900
H	-1.31474700	6.00255100	0.65809600
B	-0.03699800	4.11719700	-0.59018500
H	-2.12756000	4.76173800	-2.00182100
H	0.91205200	4.26869300	1.83287600
H	-0.41771800	2.29352100	-2.43980400
H	0.80163700	4.75002600	-1.14680600
B	-2.35121600	2.22542900	1.00889200
I	-1.47482900	-0.76187300	-0.24178700
C	0.32289500	-1.56567900	0.61883500
C	0.60794100	-1.28295400	1.94738800
C	1.14961500	-2.35348700	-0.17139700
C	1.79276600	-1.78074800	2.49093300
H	-0.06447600	-0.68519200	2.54560000
C	2.32609000	-2.84890600	0.39218500
H	0.90274100	-2.56249000	-1.20334900
C	2.65345500	-2.55409200	1.71425600
H	2.03702500	-1.55653000	3.52300800
H	2.99173800	-3.45087000	-0.21505700
H	3.57820900	-2.92717900	2.13850100
O	-2.10303500	-3.49391700	0.10195000

C	-3.30347900	-3.65731200	-0.26657700
O	-4.03521700	-2.76302600	-0.77886400
C	-3.89814000	-5.04026000	-0.04109300
H	-4.22515700	-5.11208100	1.00202200
H	-4.76197400	-5.21804900	-0.68382100
H	-3.14547500	-5.81402200	-0.20607400
H	0.60370500	0.96907500	-1.87426100
H	-3.14961200	1.53497400	1.55284400
N	1.75195100	1.95168800	-0.04369700
C	2.16356200	0.95271300	-0.77072500
H	2.44117200	2.34818300	0.58617800
C	3.47693600	0.32775900	-0.62340300
O	1.39499500	0.42139600	-1.69260600
C	3.97199900	-0.45509400	-1.67467600
C	4.21158000	0.45895100	0.56140200
C	5.19903400	-1.09048500	-1.54393100
H	3.39734900	-0.55930000	-2.58498200
C	5.43837300	-0.18044900	0.68477500
H	3.82073300	1.02344100	1.39898300
C	5.93207600	-0.95502900	-0.36514200
H	5.58229100	-1.69398200	-2.35804600
H	6.00136400	-0.08886800	1.60575300
H	6.88662100	-1.45817200	-0.26153600

IRC_TS1_point210

B	-2.73407800	3.83023000	0.36546000
B	-1.63938100	3.66268100	1.76075200
B	-0.64221500	2.21276700	1.50806500
B	-2.40987900	2.48636400	-0.75932400
B	-1.13372800	1.52184900	-0.03399400
B	-1.26673700	4.82750900	0.47102900
B	-1.74115000	4.10700400	-1.08665500
H	-3.82399900	4.29453100	0.47369900
B	0.02634900	3.82929900	1.16933200
H	-1.94975200	4.00958400	2.85589100
B	0.34277300	2.50434700	0.04641200
H	-0.22971700	1.54050700	2.39189800
B	-0.74129300	2.65955300	-1.35093100
H	-3.25185300	1.99053600	-1.43553300
H	-1.31251700	6.00227200	0.65504500
B	-0.03707600	4.11397500	-0.59118500
H	-2.12728300	4.75897800	-2.00317400
H	0.91260400	4.26750700	1.83148500
H	-0.42093500	2.28839100	-2.43842600

H	0.80210700	4.74526700	-1.14870200
B	-2.35307700	2.22670700	1.01092000
I	-1.47380700	-0.75926500	-0.24174500
C	0.32372700	-1.56354900	0.61876400
C	0.60878300	-1.28158100	1.94747900
C	1.14972800	-2.35182300	-0.17173000
C	1.79306700	-1.78069800	2.49093000
H	-0.06319600	-0.68346400	2.54582300
C	2.32561400	-2.84865000	0.39184800
H	0.90271700	-2.56024200	-1.20376800
C	2.65306500	-2.55464500	1.71405700
H	2.03742900	-1.55713800	3.52312100
H	2.99072300	-3.45107700	-0.21552100
H	3.57736400	-2.92884700	2.13830900
O	-2.10335000	-3.49882300	0.10066500
C	-3.30425600	-3.66081800	-0.26678800
O	-4.03519000	-2.76560800	-0.77871700
C	-3.90146000	-5.04275400	-0.04084900
H	-4.22840100	-5.11381000	1.00234500
H	-4.76581000	-5.21885700	-0.68334000
H	-3.15043500	-5.81808800	-0.20593800
H	0.60549600	0.97158400	-1.87753800
H	-3.15191800	1.53743300	1.55570400
N	1.74983300	1.94737700	-0.04125200
C	2.16359100	0.95170600	-0.77161800
H	2.43706800	2.34047300	0.59287300
C	3.47712100	0.32681500	-0.62359000
O	1.39759200	0.42432900	-1.69795700
C	3.97301000	-0.45568400	-1.67475800
C	4.21152000	0.45798900	0.56143500
C	5.20014900	-1.09084900	-1.54364500
H	3.39884500	-0.55997000	-2.58535200
C	5.43853900	-0.18093000	0.68510100
H	3.82079600	1.02242600	1.39906700
C	5.93285900	-0.95529000	-0.36468300
H	5.58376500	-1.69416400	-2.35772400
H	6.00125200	-0.08905600	1.60621900
H	6.88756000	-1.45809000	-0.26085500

IRC_TS1_point211

B	-2.73435600	3.83117900	0.36549500
B	-1.63954400	3.66427200	1.76071800
B	-0.64401500	2.21302700	1.50980400
B	-2.41183900	2.48558900	-0.75755500

B	-1.13596700	1.52143700	-0.03159600
B	-1.26581100	4.82698900	0.46935700
B	-1.74138700	4.10503100	-1.08725100
H	-3.82372900	4.29685200	0.47330400
B	0.02627200	3.82826000	1.16872100
H	-1.94924700	4.01303000	2.85545400
B	0.34118200	2.50161500	0.04749000
H	-0.23211200	1.54131000	2.39432000
B	-0.74314200	2.65635700	-1.34978100
H	-3.25428600	1.98952100	-1.43298100
H	-1.31030200	6.00201500	0.65196000
B	-0.03714800	4.11078600	-0.59218700
H	-2.12700500	4.75619700	-2.00455100
H	0.91316200	4.26635900	1.83009200
H	-0.42410700	2.28323500	-2.43699600
H	0.80257700	4.74053500	-1.15061200
B	-2.35492100	2.22800500	1.01294800
I	-1.47278800	-0.75669300	-0.24170100
C	0.32458100	-1.56138700	0.61869500
C	0.60965000	-1.28018000	1.94757000
C	1.14986000	-2.35011900	-0.17206900
C	1.79338500	-1.78064400	2.49092500
H	-0.06187500	-0.68169600	2.54605100
C	2.32514400	-2.84838000	0.39150100
H	0.90271300	-2.55794200	-1.20419400
C	2.65267400	-2.55521200	1.71385600
H	2.03785000	-1.55775300	3.52323500
H	2.98970700	-3.45127200	-0.21599700
H	3.57650300	-2.93055800	2.13812000
O	-2.10366900	-3.50372900	0.09933000
C	-3.30506000	-3.66432200	-0.26702300
O	-4.03518200	-2.76819500	-0.77858900
C	-3.90474900	-5.04524500	-0.04057300
H	-4.23163200	-5.11551600	1.00269700
H	-4.76962600	-5.21971800	-0.68280700
H	-3.15536800	-5.82216900	-0.20574400
H	0.60709400	0.97417700	-1.88114400
H	-3.15424000	1.53996200	1.55861200
N	1.74768300	1.94299200	-0.03875200
C	2.16360200	0.95066800	-0.77247900
H	2.43284300	2.33246000	0.59979700
C	3.47728500	0.32585100	-0.62379500
O	1.40018000	0.42734500	-1.70326200
C	3.97401700	-0.45628900	-1.67485700

C	4.21145300	0.45704300	0.56143200
C	5.20127500	-1.09120400	-1.54336600
H	3.40034800	-0.56067800	-2.58574600
C	5.43868200	-0.18141700	0.68542200
H	3.82088700	1.02148400	1.39909000
C	5.93363400	-0.95555700	-0.36421800
H	5.58526800	-1.69432400	-2.35741300
H	6.00110200	-0.08923600	1.60668900
H	6.88849000	-1.45801300	-0.26015600
IRC_TS1_point212			
B	-2.73462900	3.83213700	0.36552200
B	-1.63969800	3.66589200	1.76067800
B	-0.64579600	2.21333900	1.51154900
B	-2.41378100	2.48483400	-0.75579400
B	-1.13823100	1.52104300	-0.02917400
B	-1.26489200	4.82649200	0.46767400
B	-1.74162300	4.10307300	-1.08785000
H	-3.82346100	4.29914500	0.47290100
B	0.02620100	3.82727100	1.16811300
H	-1.94874600	4.01648900	2.85500500
B	0.33961600	2.49891900	0.04858800
H	-0.23445100	1.54216400	2.39672100
B	-0.74497100	2.65319300	-1.34863900
H	-3.25667200	1.98850400	-1.43044500
H	-1.30811400	6.00177700	0.64886400
B	-0.03721000	4.10763200	-0.59319600
H	-2.12674000	4.75344000	-2.00591700
H	0.91370500	4.26529300	1.82870400
H	-0.42729200	2.27813800	-2.43558400
H	0.80303200	4.73586500	-1.15252300
B	-2.35674700	2.22932900	1.01498300
I	-1.47177400	-0.75415700	-0.24165300
C	0.32544700	-1.55920100	0.61862700
C	0.61054100	-1.27875600	1.94766400
C	1.15001200	-2.34838000	-0.17241100
C	1.79371700	-1.78058600	2.49092000
H	-0.06052700	-0.67990100	2.54628300
C	2.32468300	-2.84809900	0.39114900
H	0.90272900	-2.55559100	-1.20462800
C	2.65228200	-2.55579200	1.71365500
H	2.03828900	-1.55837100	3.52334800
H	2.98869500	-3.45145700	-0.21648400
H	3.57562600	-2.93230800	2.13793500
O	-2.10399700	-3.50864500	0.09794300

C	-3.30586800	-3.66782000	-0.26727700
O	-4.03519600	-2.77078200	-0.77848100
C	-3.90800400	-5.04773200	-0.04026400
H	-4.23480200	-5.11716900	1.00309100
H	-4.77337400	-5.22065300	-0.68224700
H	-3.16019800	-5.82616700	-0.20546800
H	0.60885800	0.97680500	-1.88435300
H	-3.15649500	1.54246700	1.56149000
N	1.74550100	1.93854000	-0.03618700
C	2.16357300	0.94964000	-0.77333400
H	2.42853200	2.32412300	0.60694200
C	3.47742600	0.32487000	-0.62401500
O	1.40277100	0.43040600	-1.70859400
C	3.97501400	-0.45691200	-1.67496600
C	4.21138100	0.45611900	0.56139900
C	5.20240800	-1.09155300	-1.54309400
H	3.40183900	-0.56141900	-2.58614500
C	5.43880300	-0.18190800	0.68574000
H	3.82102200	1.02061400	1.39907100
C	5.93440000	-0.95583300	-0.36374600
H	5.58679600	-1.69446300	-2.35711000
H	6.00092000	-0.08941300	1.60715900
H	6.88940700	-1.45795000	-0.25943700

IRC_TS1_point213

B	-2.73489700	3.83311100	0.36554200
B	-1.63984400	3.66754500	1.76063000
B	-0.64755800	2.21369100	1.51328800
B	-2.41571100	2.48409400	-0.75402700
B	-1.14048600	1.52069700	-0.02675600
B	-1.26397900	4.82602100	0.46598000
B	-1.74184800	4.10112600	-1.08845500
H	-3.82318200	4.30148300	0.47247600
B	0.02614100	3.82632800	1.16749400
H	-1.94823200	4.02000100	2.85454300
B	0.33804200	2.49625200	0.04969300
H	-0.23678300	1.54307600	2.39914600
B	-0.74676800	2.65005300	-1.34747300
H	-3.25906500	1.98751600	-1.42790000
H	-1.30594100	6.00156400	0.64574000
B	-0.03726400	4.10451500	-0.59420100
H	-2.12646800	4.75066700	-2.00730600
H	0.91425400	4.26426200	1.82731900
H	-0.43045000	2.27301300	-2.43412500

H	0.80349400	4.73122300	-1.15444400
B	-2.35856000	2.23067600	1.01701700
I	-1.47076700	-0.75166200	-0.24160200
C	0.32633300	-1.55699000	0.61856400
C	0.61145400	-1.27730800	1.94775900
C	1.15018400	-2.34660500	-0.17275900
C	1.79406400	-1.78052300	2.49091200
H	-0.05914200	-0.67807300	2.54652000
C	2.32423000	-2.84780300	0.39078900
H	0.90276700	-2.55319300	-1.20506900
C	2.65189300	-2.55638200	1.71345300
H	2.03874400	-1.55899400	3.52346100
H	2.98768500	-3.45162700	-0.21698400
H	3.57473800	-2.93409400	2.13775300
O	-2.10432300	-3.51356500	0.09650500
C	-3.30669800	-3.67131800	-0.26755500
O	-4.03522300	-2.77337200	-0.77838900
C	-3.91123200	-5.05021700	-0.03992300
H	-4.23796300	-5.11879900	1.00351200
H	-4.77710900	-5.22163200	-0.68163400
H	-3.16501100	-5.83018600	-0.20513700
H	0.61048000	0.97949500	-1.88797700
H	-3.15877800	1.54505300	1.56441900
N	1.74328700	1.93401200	-0.03357300
C	2.16354000	0.94857900	-0.77415300
H	2.42411600	2.31551200	0.61424800
C	3.47755100	0.32387500	-0.62424200
O	1.40535800	0.43356800	-1.71388400
C	3.97599900	-0.45754800	-1.67508300
C	4.21130700	0.45522400	0.56133900
C	5.20354200	-1.09189500	-1.54283000
H	3.40331900	-0.56219400	-2.58655200
C	5.43890500	-0.18239700	0.68605000
H	3.82119300	1.01982200	1.39901100
C	5.93515200	-0.95611400	-0.36327200
H	5.58833500	-1.69458300	-2.35681900
H	6.00071500	-0.08957600	1.60762400
H	6.89030700	-1.45789500	-0.25870800

IRC_TS1_point214

B	-2.73516000	3.83409800	0.36555300
B	-1.63998000	3.66923000	1.76057600
B	-0.64930600	2.21409400	1.51503500
B	-2.41762600	2.48338400	-0.75227000

B	-1.14276500	1.52036900	-0.02432300
B	-1.26307100	4.82557300	0.46427500
B	-1.74207100	4.09920100	-1.08906300
H	-3.82290300	4.30380300	0.47204000
B	0.02608600	3.82543200	1.16687900
H	-1.94772100	4.02353500	2.85406800
B	0.33649400	2.49361500	0.05081800
H	-0.23907300	1.54403600	2.40155200
B	-0.74855000	2.64695900	-1.34632300
H	-3.26141600	1.98653300	-1.42536800
H	-1.30378200	6.00137200	0.64260000
B	-0.03730600	4.10142900	-0.59521200
H	-2.12620400	4.74792300	-2.00868600
H	0.91478800	4.26330800	1.82593800
H	-0.43364100	2.26794300	-2.43268900
H	0.80394900	4.72662600	-1.15636900
B	-2.36036000	2.23205300	1.01906000
I	-1.46976700	-0.74920500	-0.24154700
C	0.32723100	-1.55475600	0.61850200
C	0.61239000	-1.27584100	1.94785600
C	1.15037700	-2.34479500	-0.17311100
C	1.79442700	-1.78045600	2.49090400
H	-0.05773100	-0.67621900	2.54676000
C	2.32378800	-2.84749300	0.39042100
H	0.90282500	-2.55074200	-1.20551800
C	2.65150500	-2.55698300	1.71324900
H	2.03921900	-1.55962000	3.52357300
H	2.98668000	-3.45178600	-0.21749500
H	3.57383600	-2.93591600	2.13757400
O	-2.10465200	-3.51850600	0.09501000
C	-3.30752600	-3.67481300	-0.26785100
O	-4.03526600	-2.77596500	-0.77831800
C	-3.91443400	-5.05269900	-0.03955100
H	-4.24107800	-5.12037700	1.00397400
H	-4.78079000	-5.22267200	-0.68099600
H	-3.16974300	-5.83413700	-0.20472800
H	0.61225700	0.98220200	-1.89114100
H	-3.16099900	1.54762000	1.56731600
N	1.74103700	1.92941400	-0.03090100
C	2.16346700	0.94753500	-0.77497600
H	2.41962800	2.30661300	0.62171100
C	3.47765600	0.32287300	-0.62447500
O	1.40796900	0.43674800	-1.71919200
C	3.97697000	-0.45819800	-1.67520300

C	4.21123200	0.45435800	0.56126300
C	5.20467400	-1.09223000	-1.54257300
H	3.40477200	-0.56299800	-2.58695000
C	5.43899200	-0.18288200	0.68635300
H	3.82140800	1.01909300	1.39894000
C	5.93589100	-0.95640100	-0.36279700
H	5.58988500	-1.69468600	-2.35653700
H	6.00049500	-0.08973300	1.60808100
H	6.89118900	-1.45785200	-0.25796600

IRC_TS1_point215

B	-2.73541600	3.83510800	0.36555700
B	-1.64011000	3.67095100	1.76051200
B	-0.65104300	2.21453300	1.51677400
B	-2.41953200	2.48269500	-0.75050700
B	-1.14502500	1.52009700	-0.02190700
B	-1.26216400	4.82515300	0.46255800
B	-1.74228000	4.09728900	-1.08967800
H	-3.82261000	4.30617900	0.47158100
B	0.02604300	3.82457700	1.16625100
H	-1.94719700	4.02712100	2.85358000
B	0.33493300	2.49100100	0.05194600
H	-0.24136400	1.54505200	2.40398200
B	-0.75030000	2.64389600	-1.34515100
H	-3.26377700	1.98559200	-1.42283300
H	-1.30163300	6.00120500	0.63943600
B	-0.03733400	4.09837800	-0.59621800
H	-2.12592800	4.74516900	-2.01008800
H	0.91533100	4.26238200	1.82456100
H	-0.43680100	2.26285600	-2.43121100
H	0.80441600	4.72205900	-1.15829800
B	-2.36215100	2.23345600	1.02109900
I	-1.46877500	-0.74678800	-0.24148800
C	0.32814800	-1.55250500	0.61844400
C	0.61334700	-1.27435200	1.94795400
C	1.15059100	-2.34294900	-0.17346900
C	1.79480600	-1.78038300	2.49089300
H	-0.05628500	-0.67433700	2.54700600
C	2.32335700	-2.84716700	0.39004600
H	0.90290700	-2.54824700	-1.20597500
C	2.65112100	-2.55759100	1.71304300
H	2.03970900	-1.56024800	3.52368300
H	2.98568100	-3.45192500	-0.21802000
H	3.57292700	-2.93776700	2.13739600

O	-2.10497200	-3.52345900	0.09346300
C	-3.30837500	-3.67831600	-0.26817100
O	-4.03531600	-2.77856700	-0.77826100
C	-3.91762000	-5.05518100	-0.03914700
H	-4.24419100	-5.12193200	1.00446500
H	-4.78447100	-5.22374900	-0.68030500
H	-3.17447500	-5.83811800	-0.20426400
H	0.61379300	0.98479500	-1.89468800
H	-3.16325900	1.55027700	1.57026300
N	1.73875300	1.92473600	-0.02818600
C	2.16340100	0.94645400	-0.77576000
H	2.41508200	2.29755600	0.62918300
C	3.47775100	0.32186300	-0.62470400
O	1.41057400	0.44003700	-1.72446000
C	3.97792300	-0.45885700	-1.67532200
C	4.21115500	0.45351900	0.56117600
C	5.20579800	-1.09256000	-1.54232300
H	3.40620500	-0.56382900	-2.58734500
C	5.43906600	-0.18336000	0.68664900
H	3.82164200	1.01843100	1.39884800
C	5.93661300	-0.95669000	-0.36232300
H	5.59142900	-1.69477900	-2.35626400
H	6.00026400	-0.08987300	1.60852700
H	6.89205200	-1.45781600	-0.25722100

IRC_TS1_point216

B	-2.73566600	3.83613800	0.36554900
B	-1.64023100	3.67270800	1.76044200
B	-0.65277300	2.21502700	1.51852200
B	-2.42142600	2.48204400	-0.74875600
B	-1.14732000	1.51984300	-0.01947400
B	-1.26125600	4.82475700	0.46082900
B	-1.74248700	4.09540500	-1.09029500
H	-3.82231300	4.30854600	0.47111000
B	0.02600400	3.82376600	1.16563100
H	-1.94667500	4.03073700	2.85307800
B	0.33340100	2.48841500	0.05309900
H	-0.24362300	1.54611300	2.40639100
B	-0.75204800	2.64088400	-1.34400500
H	-3.26609900	1.98466400	-1.42031000
H	-1.29948400	6.00106200	0.63625300
B	-0.03734800	4.09535300	-0.59723100
H	-2.12565500	4.74245300	-2.01148100
H	0.91586100	4.26152800	1.82318700

H	-0.44000100	2.25783200	-2.42976400
H	0.80488300	4.71752900	-1.16022800
B	-2.36393200	2.23489800	1.02314500
I	-1.46779000	-0.74440600	-0.24142400
C	0.32907000	-1.55023700	0.61838600
C	0.61432700	-1.27284500	1.94805300
C	1.15082700	-2.34106900	-0.17383300
C	1.79520000	-1.78030400	2.49088000
H	-0.05481400	-0.67243300	2.54725400
C	2.32293800	-2.84682600	0.38966200
H	0.90301200	-2.54569600	-1.20644200
C	2.65074000	-2.55820800	1.71283400
H	2.04021900	-1.56087800	3.52379200
H	2.98469000	-3.45205000	-0.21855800
H	3.57200700	-2.93965000	2.13721900
O	-2.10529200	-3.52844200	0.09185300
C	-3.30921500	-3.68182400	-0.26850800
O	-4.03538000	-2.78118200	-0.77822500
C	-3.92078900	-5.05766400	-0.03871000
H	-4.24726600	-5.12343600	1.00499600
H	-4.78810700	-5.22487900	-0.67958800
H	-3.17914400	-5.84204400	-0.20372300
H	0.61544900	0.98739200	-1.89760600
H	-3.16545700	1.55291800	1.57317000
N	1.73643000	1.91999200	-0.02542700
C	2.16329300	0.94540500	-0.77656500
H	2.41050400	2.28830700	0.63672800
C	3.47783100	0.32085800	-0.62494000
O	1.41322700	0.44329700	-1.72973700
C	3.97886000	-0.45952500	-1.67543800
C	4.21107000	0.45270200	0.56108700
C	5.20691400	-1.09288600	-1.54207700
H	3.40760400	-0.56468300	-2.58772200
C	5.43912900	-0.18383000	0.68693900
H	3.82189100	1.01780500	1.39876700
C	5.93732200	-0.95697900	-0.36184900
H	5.59297100	-1.69486300	-2.35599600
H	6.00002700	-0.09000700	1.60896600
H	6.89289900	-1.45778500	-0.25646900

IRC_TS1_point217

B	-2.73590800	3.83720000	0.36553300
B	-1.64034600	3.67450400	1.76036000
B	-0.65449500	2.21555100	1.52025900

B	-2.42331500	2.48141900	-0.74700000
B	-1.14958900	1.51965600	-0.01706200
B	-1.26034100	4.82439100	0.45908600
B	-1.74267400	4.09353800	-1.09092300
H	-3.82199900	4.31098400	0.47061400
B	0.02598000	3.82298900	1.16499400
H	-1.94613800	4.03440200	2.85256100
B	0.33184500	2.48584700	0.05424700
H	-0.24588800	1.54722500	2.40882300
B	-0.75376500	2.63788800	-1.34282800
H	-3.26843800	1.98379700	-1.41779200
H	-1.29734500	6.00094400	0.63305300
B	-0.03734600	4.09236100	-0.59823700
H	-2.12536100	4.73973500	-2.01289700
H	0.91640100	4.26069200	1.82181800
H	-0.44314500	2.25279100	-2.42827000
H	0.80536300	4.71303700	-1.16215300
B	-2.36570900	2.23636900	1.02518100
I	-1.46681100	-0.74206400	-0.24135500
C	0.33001300	-1.54795800	0.61833300
C	0.61532700	-1.27132100	1.94815200
C	1.15108400	-2.33915700	-0.17420200
C	1.79561000	-1.78022100	2.49086400
H	-0.05331300	-0.67050700	2.54750600
C	2.32253100	-2.84646700	0.38927100
H	0.90314400	-2.54311000	-1.20691500
C	2.65036500	-2.55883000	1.71262400
H	2.04074400	-1.56150700	3.52389800
H	2.98371200	-3.45214800	-0.21910800
H	3.57108300	-2.94155500	2.13704300
O	-2.10559700	-3.53344500	0.09018800
C	-3.31007700	-3.68535100	-0.26886900
O	-4.03545100	-2.78381800	-0.77820400
C	-3.92394700	-5.06015000	-0.03823800
H	-4.25034400	-5.12491700	1.00556000
H	-4.79174800	-5.22604300	-0.67881500
H	-3.18382300	-5.84600500	-0.20312300
H	0.61680400	0.98978000	-1.90098500
H	-3.16770900	1.55566600	1.57612600
N	1.73407400	1.91517500	-0.02263500
C	2.16321100	0.94431200	-0.77732300
H	2.40592900	2.27911700	0.64405700
C	3.47790900	0.31984900	-0.62516500
O	1.41585600	0.44669300	-1.73497500

C	3.97978000	-0.46020000	-1.67554900
C	4.21098100	0.45189600	0.56100100
C	5.20801700	-1.09321100	-1.54183300
H	3.40898300	-0.56556000	-2.58809300
C	5.43918000	-0.18429200	0.68722700
H	3.82211100	1.01720000	1.39868000
C	5.93801500	-0.95726800	-0.36137700
H	5.59449400	-1.69494800	-2.35573000
H	5.99978000	-0.09012800	1.60939900
H	6.89372700	-1.45775400	-0.25571700

IRC_TS1_point218

B	-2.73614300	3.83829000	0.36550300
B	-1.64045100	3.67633900	1.76027100
B	-0.65621500	2.21613400	1.52201000
B	-2.42519700	2.48084400	-0.74526000
B	-1.15190900	1.51948300	-0.01462100
B	-1.25942000	4.82405100	0.45733100
B	-1.74286100	4.09170500	-1.09155100
H	-3.82168000	4.31342000	0.47010600
B	0.02595800	3.82225300	1.16437000
H	-1.94560200	4.03810500	2.85202800
B	0.33032200	2.48330400	0.05542100
H	-0.24813200	1.54838000	2.41123300
B	-0.75549500	2.63495000	-1.34168900
H	-3.27074200	1.98294300	-1.41528300
H	-1.29518400	6.00085300	0.62982700
B	-0.03732900	4.08938700	-0.59925300
H	-2.12506400	4.73706300	-2.01430300
H	0.91693300	4.25992700	1.82044900
H	-0.44634700	2.24783400	-2.42682400
H	0.80585300	4.70856300	-1.16408500
B	-2.36748100	2.23788900	1.02722700
I	-1.46584000	-0.73974900	-0.24127900
C	0.33095800	-1.54566300	0.61827800
C	0.61634900	-1.26978100	1.94825100
C	1.15136300	-2.33721200	-0.17457700
C	1.79603600	-1.78013100	2.49084500
H	-0.05178700	-0.66856100	2.54776000
C	2.32213900	-2.84609100	0.38887100
H	0.90330000	-2.54046500	-1.20740000
C	2.64999500	-2.55945700	1.71241000
H	2.04128900	-1.56213700	3.52400200
H	2.98274400	-3.45223100	-0.21967300

H	3.57015000	-2.94348800	2.13686700
O	-2.10590200	-3.53849200	0.08845500
C	-3.31092500	-3.68889500	-0.26924900
O	-4.03553500	-2.78648100	-0.77820700
C	-3.92709500	-5.06264500	-0.03773000
H	-4.25339200	-5.12634600	1.00616700
H	-4.79535400	-5.22725800	-0.67801400
H	-3.18845300	-5.84992800	-0.20244100
H	0.61832900	0.99222400	-1.90356200
H	-3.16989500	1.55839500	1.57903200
N	1.73167700	1.91031300	-0.01982800
C	2.16308500	0.94327300	-0.77812000
H	2.40130600	2.26988800	0.65145200
C	3.47797700	0.31885600	-0.62540100
O	1.41856100	0.45000300	-1.74020500
C	3.98068500	-0.46087800	-1.67565600
C	4.21087700	0.45108600	0.56092300
C	5.20910700	-1.09353500	-1.54159000
H	3.41032800	-0.56644700	-2.58844300
C	5.43922300	-0.18475100	0.68751300
H	3.82229500	1.01650000	1.39865800
C	5.93869700	-0.95755200	-0.36090600
H	5.59600800	-1.69503600	-2.35546100
H	5.99952800	-0.09025700	1.60983200
H	6.89454500	-1.45772200	-0.25496200

IRC_TS1_point219

B	-2.73636600	3.83942200	0.36546300
B	-1.64055000	3.67821900	1.76016600
B	-0.65793300	2.21674100	1.52374400
B	-2.42707900	2.48029500	-0.74351300
B	-1.15419200	1.51939100	-0.01221300
B	-1.25848500	4.82374300	0.45556200
B	-1.74301900	4.08989000	-1.09219400
H	-3.82133600	4.31595000	0.46957100
B	0.02595800	3.82154600	1.16372000
H	-1.94504800	4.04186200	2.85148000
B	0.32875400	2.48077400	0.05657400
H	-0.25039300	1.54958700	2.41367100
B	-0.75719000	2.63201900	-1.34050500
H	-3.27307700	1.98216900	-1.41278100
H	-1.29303200	6.00078900	0.62658900
B	-0.03729500	4.08644700	-0.60026000
H	-2.12473800	4.73439100	-2.01573700

H	0.91748200	4.25916300	1.81908300
H	-0.44946500	2.24286500	-2.42532000
H	0.80635700	4.70412700	-1.16600700
B	-2.36925400	2.23944300	1.02925700
I	-1.46487400	-0.73747500	-0.24119700
C	0.33193000	-1.54335800	0.61823100
C	0.61739000	-1.26822500	1.94835100
C	1.15166400	-2.33523800	-0.17495700
C	1.79647700	-1.78003700	2.49082500
H	-0.05023300	-0.66659600	2.54801800
C	2.32176200	-2.84569700	0.38846500
H	0.90348200	-2.53779400	-1.20789000
C	2.64963200	-2.56008800	1.71219600
H	2.04184700	-1.56276300	3.52410300
H	2.98179400	-3.45228100	-0.22025000
H	3.56921800	-2.94543400	2.13669100
O	-2.10619000	-3.54356500	0.08666300
C	-3.31180100	-3.69247300	-0.26965400
O	-4.03562700	-2.78918100	-0.77822700
C	-3.93024200	-5.06515100	-0.03718100
H	-4.25645100	-5.12775600	1.00681300
H	-4.79897700	-5.22851600	-0.67714600
H	-3.19311000	-5.85390300	-0.20169200
H	0.61949300	0.99433600	-1.90687000
H	-3.17216100	1.56126200	1.58199900
N	1.72924800	1.90539900	-0.01699600
C	2.16300700	0.94218100	-0.77885100
H	2.39674600	2.26098200	0.65835600
C	3.47805100	0.31786000	-0.62562100
O	1.42120700	0.45349200	-1.74538500
C	3.98157700	-0.46155800	-1.67575900
C	4.21076100	0.45025300	0.56086000
C	5.21018200	-1.09386400	-1.54134400
H	3.41166600	-0.56734400	-2.58879700
C	5.43925900	-0.18521000	0.68780300
H	3.82236900	1.01570700	1.39865500
C	5.93936800	-0.95783200	-0.36043700
H	5.59749400	-1.69513900	-2.35518700
H	5.99925900	-0.09039500	1.61027200
H	6.89534900	-1.45768300	-0.25421600
IRC_TS1_point220			
B	-2.73658200	3.84059100	0.36540600
B	-1.64063700	3.68014300	1.76005700
B	-0.65965400	2.21741700	1.52550000

B	-2.42895700	2.47981100	-0.74178800
B	-1.15655100	1.51929600	-0.00975900
B	-1.25753900	4.82346300	0.45377900
B	-1.74318600	4.08812100	-1.09283300
H	-3.82098700	4.31847800	0.46902400
B	0.02595300	3.82087800	1.16309100
H	-1.94449500	4.04566900	2.85091200
B	0.32723200	2.47827200	0.05776100
H	-0.25264200	1.55083400	2.41608500
B	-0.75892200	2.62916300	-1.33938600
H	-3.27537800	1.98140300	-1.41028000
H	-1.29082900	6.00075600	0.62331400
B	-0.03724800	4.08351600	-0.60128200
H	-2.12441100	4.73177800	-2.01715900
H	0.91802400	4.25847500	1.81770800
H	-0.45268200	2.23805100	-2.42390000
H	0.80687900	4.69967900	-1.16794900
B	-2.37102700	2.24105800	1.03130100
I	-1.46391400	-0.73522100	-0.24110700
C	0.33290200	-1.54103400	0.61817600
C	0.61845500	-1.26665300	1.94844900
C	1.15198800	-2.33323100	-0.17534500
C	1.79693500	-1.77993600	2.49080000
H	-0.04865300	-0.66461200	2.54827600
C	2.32140100	-2.84528300	0.38804500
H	0.90369100	-2.53505400	-1.20839500
C	2.64927600	-2.56072100	1.71197400
H	2.04242800	-1.56339300	3.52420200
H	2.98085300	-3.45231900	-0.22084200
H	3.56827700	-2.94741000	2.13651100
O	-2.10648400	-3.54870200	0.08479200
C	-3.31265600	-3.69608100	-0.27008000
O	-4.03573800	-2.79192400	-0.77827500
C	-3.93338400	-5.06767600	-0.03659300
H	-4.25948800	-5.12911500	1.00750600
H	-4.80257300	-5.22982400	-0.67625000
H	-3.19773000	-5.85785700	-0.20085000
H	0.62093400	0.99659100	-1.90899900
H	-3.17434200	1.56409300	1.58489400
N	1.72678000	1.90047500	-0.01419500
C	2.16287400	0.94118200	-0.77965100
H	2.39208600	2.25196600	0.66557000
C	3.47811800	0.31689500	-0.62586100
O	1.42397400	0.45678200	-1.75052200

C	3.98246100	-0.46222900	-1.67586300
C	4.21061800	0.44938400	0.56081400
C	5.21124400	-1.09419100	-1.54109800
H	3.41297500	-0.56822900	-2.58913200
C	5.43928600	-0.18567800	0.68809500
H	3.82237300	1.01473900	1.39875200
C	5.94003500	-0.95810200	-0.35997300
H	5.59896900	-1.69524800	-2.35490600
H	5.99897900	-0.09057100	1.61072300
H	6.89615600	-1.45763300	-0.25347600
IRC_TS1_point221			
B	-2.73678300	3.84181700	0.36534000
B	-1.64072000	3.68211800	1.75992500
B	-0.66137600	2.21810300	1.52722500
B	-2.43084200	2.47934900	-0.74004800
B	-1.15883300	1.51930500	-0.00736900
B	-1.25657000	4.82322300	0.45197900
B	-1.74331100	4.08636900	-1.09349400
H	-3.82060500	4.32113900	0.46844800
B	0.02597900	3.82023300	1.16242100
H	-1.94391600	4.04953400	2.85032900
B	0.32563600	2.47577700	0.05890200
H	-0.25492500	1.55213700	2.41853700
B	-0.76060200	2.62630100	-1.33819100
H	-3.27773300	1.98074800	-1.40778900
H	-1.28864100	6.00075400	0.62003200
B	-0.03718200	4.08062600	-0.60228700
H	-2.12404200	4.72915900	-2.01862000
H	0.91859500	4.25776100	1.81633400
H	-0.45576200	2.23324100	-2.42240500
H	0.80741400	4.69527800	-1.16987400
B	-2.37280300	2.24270900	1.03331800
I	-1.46295700	-0.73300900	-0.24100900
C	0.33391100	-1.53870300	0.61813300
C	0.61954000	-1.26506200	1.94854600
C	1.15233500	-2.33119500	-0.17573900
C	1.79741000	-1.77983100	2.49077400
H	-0.04704400	-0.66260700	2.54853800
C	2.32105600	-2.84485000	0.38762200
H	0.90392800	-2.53229600	-1.20890300
C	2.64892900	-2.56135400	1.71175300
H	2.04301900	-1.56401700	3.52429900
H	2.97993600	-3.45231500	-0.22144800
H	3.56734300	-2.94939100	2.13633300

O	-2.10675700	-3.55386400	0.08286200
C	-3.31355200	-3.69974100	-0.27053400
O	-4.03585700	-2.79472000	-0.77834000
C	-3.93653600	-5.07022500	-0.03595500
H	-4.26255200	-5.13046300	1.00824600
H	-4.80620500	-5.23118900	-0.67527000
H	-3.20240500	-5.86189000	-0.19993400
H	0.62185300	0.99829500	-1.91238300
H	-3.17665100	1.56711800	1.58788000
N	1.72428700	1.89550100	-0.01134300
C	2.16281900	0.94009700	-0.78033900
H	2.38763500	2.24357700	0.67175700
C	3.47820100	0.31591500	-0.62607300
O	1.42660300	0.46034900	-1.75559700
C	3.98333900	-0.46289400	-1.67596600
C	4.21045700	0.44846400	0.56079600
C	5.21229200	-1.09452500	-1.54084800
H	3.41429900	-0.56910700	-2.58948800
C	5.43930400	-0.18616200	0.68840100
H	3.82221700	1.01365100	1.39885200
C	5.94069600	-0.95836800	-0.35951100
H	5.60041300	-1.69537700	-2.35461800
H	5.99867200	-0.09077800	1.61119400
H	6.89695500	-1.45757000	-0.25275100

IRC_TS1_point222

B	-2.73697900	3.84308400	0.36525300
B	-1.64078600	3.68414100	1.75979400
B	-0.66310300	2.21888000	1.52898700
B	-2.43272300	2.47897700	-0.73834600
B	-1.16124700	1.51927900	-0.00490000
B	-1.25558900	4.82301200	0.45017000
B	-1.74346500	4.08468500	-1.09413800
H	-3.82022200	4.32377100	0.46786600
B	0.02599100	3.81963400	1.16179100
H	-1.94334000	4.05345300	2.84972400
B	0.32412200	2.47332300	0.06009600
H	-0.25719400	1.55347600	2.42094800
B	-0.76235700	2.62355600	-1.33711600
H	-3.28003900	1.98008600	-1.40529200
H	-1.28636600	6.00078900	0.61670400
B	-0.03711100	4.07773800	-0.60331800
H	-2.12368200	4.72662800	-2.02005100
H	0.91915600	4.25714800	1.81494500

H	-0.45901700	2.22872200	-2.42107100
H	0.80797300	4.69083700	-1.17183300
B	-2.37458200	2.24443900	1.03535800
I	-1.46200700	-0.73080600	-0.24090000
C	0.33491200	-1.53634500	0.61807500
C	0.62065200	-1.26345600	1.94864000
C	1.15270800	-2.32912500	-0.17614200
C	1.79790200	-1.77971600	2.49074100
H	-0.04540700	-0.66058200	2.54879700
C	2.32073100	-2.84439500	0.38718000
H	0.90419300	-2.52945500	-1.20943300
C	2.64859200	-2.56198700	1.71152000
H	2.04363900	-1.56464800	3.52439100
H	2.97902700	-3.45230500	-0.22207200
H	3.56639800	-2.95140200	2.13614500
O	-2.10704800	-3.55911100	0.08083900
C	-3.31441300	-3.70344000	-0.27100900
O	-4.03600400	-2.79757400	-0.77844200
C	-3.93968700	-5.07280100	-0.03527300
H	-4.26559100	-5.13175300	1.00903900
H	-4.80980400	-5.23260500	-0.67426500
H	-3.20704000	-5.86590400	-0.19890900
H	0.62321600	1.00028500	-1.91372800
H	-3.17881700	1.57005400	1.59074200
N	1.72176600	1.89057000	-0.00862200
C	2.16267400	0.93915800	-0.78115700
H	2.38284900	2.23455500	0.67921200
C	3.47827100	0.31499100	-0.62632500
O	1.42945200	0.46350100	-1.76058100
C	3.98421400	-0.46353600	-1.67607700
C	4.21025700	0.44749800	0.56079600
C	5.21332800	-1.09484800	-1.54060300
H	3.41559300	-0.56994600	-2.58982400
C	5.43930800	-0.18666900	0.68871100
H	3.82203200	1.01234300	1.39910200
C	5.94135800	-0.95862000	-0.35905800
H	5.60185200	-1.69550200	-2.35432900
H	5.99834700	-0.09105100	1.61168300
H	6.89776700	-1.45748700	-0.25203800

IRC_TS1_point223

B	-2.73715000	3.84442500	0.36516100
B	-1.64084800	3.68622000	1.75962900
B	-0.66483100	2.21963700	1.53068500

B	-2.43461300	2.47861200	-0.73661400
B	-1.16350500	1.51941300	-0.00254900
B	-1.25457300	4.82285500	0.44834500
B	-1.74354700	4.08301200	-1.09482100
H	-3.81978900	4.32661400	0.46724800
B	0.02605300	3.81904800	1.16109000
H	-1.94272300	4.05744500	2.84910300
B	0.32248500	2.47087600	0.06120200
H	-0.25951800	1.55488100	2.42342200
B	-0.76401000	2.62076900	-1.33589800
H	-3.28243700	1.97958500	-1.40281200
H	-1.28412800	6.00086500	0.61338300
B	-0.03701100	4.07491300	-0.60431900
H	-2.12325700	4.72407200	-2.02154900
H	0.91976700	4.25646100	1.81355600
H	-0.46202700	2.22398200	-2.41955600
H	0.80854600	4.68647900	-1.17376400
B	-2.37636200	2.24619600	1.03734400
I	-1.46106000	-0.72866200	-0.24078200
C	0.33596700	-1.53399000	0.61803400
C	0.62178300	-1.26182900	1.94873300
C	1.15310400	-2.32703100	-0.17654900
C	1.79841300	-1.77959800	2.49070900
H	-0.04373600	-0.65853100	2.54905900
C	2.32042500	-2.84391900	0.38674100
H	0.90449100	-2.52661000	-1.20996000
C	2.64826800	-2.56261900	1.71129300
H	2.04426400	-1.56526900	3.52448300
H	2.97815200	-3.45223800	-0.22270900
H	3.56546800	-2.95341300	2.13596400
O	-2.10730600	-3.56435900	0.07876300
C	-3.31534400	-3.70720000	-0.27151900
O	-4.03615700	-2.80049100	-0.77856200
C	-3.94285700	-5.07541000	-0.03453200
H	-4.26868000	-5.13304400	1.00988500
H	-4.81347000	-5.23409700	-0.67314300
H	-3.21177200	-5.87004400	-0.19780100
H	0.62378700	1.00142900	-1.91759800
H	-3.18120700	1.57329900	1.59377000
N	1.71922300	1.88554100	-0.00571500
C	2.16265400	0.93805500	-0.78177100
H	2.37870300	2.22684200	0.68406900
C	3.47837100	0.31402100	-0.62651900
O	1.43199000	0.46717200	-1.76552500

C	3.98509000	-0.46416900	-1.67618700
C	4.21004300	0.44647600	0.56083500
C	5.21435600	-1.09517800	-1.54035200
H	3.41693600	-0.57077000	-2.59020600
C	5.43929800	-0.18720600	0.68904800
H	3.82161900	1.01097200	1.39928500
C	5.94201000	-0.95887200	-0.35860200
H	5.60326800	-1.69563800	-2.35403500
H	5.99797900	-0.09137200	1.61220900
H	6.89856700	-1.45739300	-0.25133800

IRC_TS1_point224

B	-2.73731800	3.84580100	0.36504100
B	-1.64088100	3.68833900	1.75947900
B	-0.66655200	2.22052900	1.53244900
B	-2.43648600	2.47838600	-0.73495300
B	-1.16601300	1.51944600	-0.00003900
B	-1.25355500	4.82272200	0.44652000
B	-1.74369600	4.08144800	-1.09546100
H	-3.81936100	4.32935200	0.46663700
B	0.02608400	3.81852500	1.16047200
H	-1.94211200	4.06148100	2.84845300
B	0.32101500	2.46849300	0.06240700
H	-0.26180300	1.55631600	2.42581500
B	-0.76579900	2.61816800	-1.33490600
H	-3.28473700	1.97904700	-1.40032200
H	-1.28175300	6.00097500	0.61000600
B	-0.03691500	4.07208600	-0.60536600
H	-2.12287000	4.72166200	-2.02297600
H	0.92035000	4.25594100	1.81215300
H	-0.46538400	2.21963300	-2.41829100
H	0.80914600	4.68204800	-1.17573900
B	-2.37814100	2.24805600	1.03937400
I	-1.46012600	-0.72651600	-0.24065100
C	0.33698600	-1.53160600	0.61796500
C	0.62294500	-1.26019600	1.94881600
C	1.15352600	-2.32490800	-0.17696800
C	1.79894200	-1.77946600	2.49066300
H	-0.04203600	-0.65646500	2.54931100
C	2.32014100	-2.84342100	0.38627300
H	0.90482000	-2.52366600	-1.21051900
C	2.64795600	-2.56324200	1.71104200
H	2.04492600	-1.56589700	3.52456200
H	2.97728100	-3.45217800	-0.22336800

H	3.56452200	-2.95545200	2.13576200
O	-2.10760800	-3.56971500	0.07658000
C	-3.31620100	-3.71099000	-0.27204600
O	-4.03634800	-2.80346400	-0.77873000
C	-3.94600600	-5.07803800	-0.03374600
H	-4.27171000	-5.13424800	1.01079000
H	-4.81706000	-5.23563700	-0.67201900
H	-3.21641200	-5.87411400	-0.19655900
H	0.62519000	1.00329200	-1.91760900
H	-3.18332600	1.57633500	1.59656400
N	1.71668300	1.88069100	-0.00324000
C	2.16247100	0.93720000	-0.78264500
H	2.37338800	2.21702700	0.69321200
C	3.47843700	0.31316300	-0.62679100
O	1.43497500	0.47001500	-1.77028600
C	3.98596100	-0.46475300	-1.67631300
C	4.20977900	0.44541700	0.56088200
C	5.21537000	-1.09547700	-1.54011600
H	3.41822100	-0.57152200	-2.59055000
C	5.43926100	-0.18777200	0.68938200
H	3.82132700	1.00932400	1.39973100
C	5.94266400	-0.95910600	-0.35816500
H	5.60468400	-1.69574100	-2.35375400
H	5.99758100	-0.09178500	1.61275100
H	6.89938400	-1.45727400	-0.25065400
IRC_TS1_point225			
B	-2.73744800	3.84727900	0.36492500
B	-1.64091600	3.69053000	1.75927400
B	-0.66827600	2.22134900	1.53409900
B	-2.43837200	2.47812400	-0.73322900
B	-1.16819400	1.51973800	0.00224300
B	-1.25247800	4.82266800	0.44467500
B	-1.74371300	4.07987300	-1.09618000
H	-3.81885200	4.33245900	0.46596800
B	0.02619600	3.81800500	1.15972300
H	-1.94143500	4.06568700	2.84778500
B	0.31933000	2.46612000	0.06344800
H	-0.26420700	1.55785900	2.42835300
B	-0.76740500	2.61544100	-1.33363800
H	-3.28721600	1.97871900	-1.39781100
H	-1.27941300	6.00116500	0.60659700
B	-0.03676900	4.06935500	-0.60636400
H	-2.12237700	4.71915900	-2.02454700
H	0.92103300	4.25527100	1.81072100

H	-0.46836900	2.21471300	-2.41668800
H	0.80979900	4.67769300	-1.17772900
B	-2.37991300	2.24992000	1.04131300
I	-1.45919800	-0.72446900	-0.24051500
C	0.33808800	-1.52924900	0.61792700
C	0.62412200	-1.25853400	1.94889600
C	1.15397200	-2.32276800	-0.17739300
C	1.79949500	-1.77933400	2.49062000
H	-0.04027200	-0.65432800	2.54956000
C	2.31988300	-2.84290200	0.38581400
H	0.90519800	-2.52069300	-1.21108400
C	2.64766400	-2.56386700	1.71080700
H	2.04559900	-1.56651300	3.52464300
H	2.97645700	-3.45203700	-0.22405100
H	3.56359700	-2.95751900	2.13557800
O	-2.10784400	-3.57499400	0.07437100
C	-3.31716900	-3.71483600	-0.27261900
O	-4.03653500	-2.80649400	-0.77891500
C	-3.94919900	-5.08070200	-0.03289400
H	-4.27487100	-5.13546400	1.01174600
H	-4.82080800	-5.23725800	-0.67071000
H	-3.22127600	-5.87844900	-0.19522500
H	0.62548800	1.00395800	-1.92265700
H	-3.18584900	1.57989600	1.59969200
N	1.71408300	1.87555300	-0.00008200
C	2.16250400	0.93604200	-0.78313400
H	2.36999400	2.21062600	0.69501200
C	3.47856300	0.31219000	-0.62694700
O	1.43728700	0.47385700	-1.77508200
C	3.98684700	-0.46533000	-1.67643300
C	4.20951900	0.44430400	0.56098700
C	5.21639200	-1.09577700	-1.53987300
H	3.41962100	-0.57225500	-2.59098200
C	5.43921600	-0.18837300	0.68976200
H	3.82061400	1.00772700	1.39995000
C	5.94330600	-0.95934200	-0.35771300
H	5.60611100	-1.69583300	-2.35347200
H	5.99713200	-0.09226100	1.61335400
H	6.90018400	-1.45714700	-0.24997200

IRC_TS1_point226

B	-2.73756500	3.84878100	0.36477400
B	-1.64089300	3.69274500	1.75910800
B	-0.66996700	2.22235100	1.53585800

B	-2.44022000	2.47806200	-0.73160400
B	-1.17077000	1.51983600	0.00479000
B	-1.25140900	4.82262400	0.44285000
B	-1.74383300	4.07844500	-1.09680700
H	-3.81830700	4.33543800	0.46530600
B	0.02626600	3.81756500	1.15912000
H	-1.94073500	4.06993800	2.84705600
B	0.31792100	2.46382300	0.06466200
H	-0.26657100	1.55944900	2.43081000
B	-0.76919300	2.61298500	-1.33270100
H	-3.28957300	1.97837700	-1.39526700
H	-1.27689800	6.00135800	0.60312000
B	-0.03664100	4.06661900	-0.60741200
H	-2.12191600	4.71680500	-2.02602300
H	0.92169200	4.25480600	1.80928700
H	-0.47181700	2.21041100	-2.41539600
H	0.81046800	4.67321600	-1.17973400
B	-2.38168000	2.25192300	1.04332300
I	-1.45829900	-0.72242600	-0.24036100
C	0.33911500	-1.52687600	0.61785000
C	0.62533200	-1.25689200	1.94896500
C	1.15444800	-2.32061100	-0.17782600
C	1.80006400	-1.77919100	2.49055400
H	-0.03845200	-0.65216800	2.54979400
C	2.31965300	-2.84236000	0.38531700
H	0.90563000	-2.51759600	-1.21169000
C	2.64738500	-2.56448400	1.71053400
H	2.04631800	-1.56714000	3.52470000
H	2.97564500	-3.45189300	-0.22476700
H	3.56263800	-2.95962000	2.13535900
O	-2.10816800	-3.58039200	0.07205300
C	-3.31801600	-3.71868300	-0.27320300
O	-4.03676100	-2.80955600	-0.77916300
C	-3.95234000	-5.08335600	-0.03199900
H	-4.27792900	-5.13654000	1.01276100
H	-4.82442300	-5.23892000	-0.66940500
H	-3.22602400	-5.88263600	-0.19369900
H	0.62685700	1.00567200	-1.92181800
H	-3.18801400	1.58324700	1.60252700
N	1.71160100	1.87095100	0.00181800
C	2.16224100	0.93527100	-0.78404100
H	2.36365300	2.19922300	0.70785300
C	3.47860200	0.31140800	-0.62722000
O	1.44037800	0.47637300	-1.77954800

C	3.98771800	-0.46581800	-1.67657300
C	4.20919000	0.44316400	0.56109200
C	5.21739500	-1.09600600	-1.53964900
H	3.42093400	-0.57287400	-2.59135400
C	5.43912700	-0.18899800	0.69013500
H	3.82026200	1.00573200	1.40063600
C	5.94394500	-0.95954500	-0.35727900
H	5.60754800	-1.69583800	-2.35320900
H	5.99662100	-0.09284500	1.61398700
H	6.90099800	-1.45698300	-0.24929300

IRC_TS1_point227

B	-2.73765500	3.85040000	0.36461500
B	-1.64088600	3.69506700	1.75887000
B	-0.67168100	2.22329800	1.53749500
B	-2.44209200	2.47794400	-0.72993300
B	-1.17298500	1.52018900	0.00707600
B	-1.25026600	4.82268300	0.44096700
B	-1.74383300	4.07701500	-1.09756200
H	-3.81778900	4.33854900	0.46463200
B	0.02641200	3.81714600	1.15835000
H	-1.94003900	4.07421100	2.84635900
B	0.31627000	2.46156000	0.06566700
H	-0.26890900	1.56106300	2.43324600
B	-0.77084100	2.61039000	-1.33153700
H	-3.29196900	1.97812700	-1.39282000
H	-1.27443600	6.00166200	0.59969500
B	-0.03645400	4.06395800	-0.60847300
H	-2.12142900	4.71455100	-2.02753800
H	0.92238300	4.25430700	1.80781800
H	-0.47491900	2.20581200	-2.41398300
H	0.81117300	4.66892200	-1.18178300
B	-2.38343200	2.25393300	1.04524400
I	-1.45740200	-0.72046500	-0.24020700
C	0.34022600	-1.52452600	0.61779700
C	0.62655900	-1.25519300	1.94901600
C	1.15493500	-2.31843100	-0.17828300
C	1.80066700	-1.77903200	2.49048000
H	-0.03666900	-0.65003400	2.55001400
C	2.31944600	-2.84179400	0.38481500
H	0.90605100	-2.51458400	-1.21228700
C	2.64713100	-2.56509300	1.71026700
H	2.04704800	-1.56771700	3.52474500
H	2.97487900	-3.45170500	-0.22549100

H	3.56174900	-2.96167000	2.13514300
O	-2.10839000	-3.58569600	0.06970500
C	-3.31898100	-3.72257800	-0.27382000
O	-4.03700200	-2.81268300	-0.77943300
C	-3.95553500	-5.08604400	-0.03101900
H	-4.28106100	-5.13759600	1.01385500
H	-4.82810900	-5.24063000	-0.66802500
H	-3.23079800	-5.88691500	-0.19213100
H	0.62761400	1.00642500	-1.92588300
H	-3.19035900	1.58673000	1.60546300
N	1.70889500	1.86566700	0.00544400
C	2.16231700	0.93413300	-0.78453100
H	2.36078200	2.19351800	0.70700900
C	3.47875200	0.31047800	-0.62737200
O	1.44264600	0.47989400	-1.78413900
C	3.98861500	-0.46630200	-1.67671600
C	4.20887900	0.44198100	0.56124500
C	5.21841300	-1.09623200	-1.53944800
H	3.42231600	-0.57342300	-2.59179800
C	5.43903900	-0.18967200	0.69053500
H	3.81940300	1.00393200	1.40094900
C	5.94457700	-0.95975700	-0.35685800
H	5.60896800	-1.69581500	-2.35299900
H	5.99611700	-0.09349500	1.61462900
H	6.90179400	-1.45682700	-0.24867300

IRC_TS1_point228

B	-2.73770200	3.85208200	0.36445000
B	-1.64081800	3.69741600	1.75865000
B	-0.67337100	2.22432600	1.53918300
B	-2.44395400	2.47796900	-0.72825200
B	-1.17542200	1.52052100	0.00952600
B	-1.24909900	4.82275000	0.43911000
B	-1.74382300	4.07563900	-1.09823400
H	-3.81713800	4.34189100	0.46391400
B	0.02658400	3.81674400	1.15765100
H	-1.93924200	4.07855000	2.84561300
B	0.31473900	2.45924900	0.06680500
H	-0.27129900	1.56275000	2.43574000
B	-0.77248700	2.60789100	-1.33039400
H	-3.29440600	1.97811700	-1.39035700
H	-1.27195200	6.00193100	0.59628400
B	-0.03625600	4.06131300	-0.60948000
H	-2.12081700	4.71225000	-2.02908700

H	0.92313000	4.25376200	1.80640400
H	-0.47789700	2.20127200	-2.41237800
H	0.81186000	4.66465300	-1.18369100
B	-2.38521000	2.25605800	1.04718900
I	-1.45651500	-0.71851600	-0.24002100
C	0.34132100	-1.52215100	0.61773600
C	0.62782100	-1.25352000	1.94907800
C	1.15546100	-2.31623500	-0.17872400
C	1.80127800	-1.77887900	2.49040700
H	-0.03481400	-0.64788300	2.55025400
C	2.31926300	-2.84120700	0.38430800
H	0.90652300	-2.51154800	-1.21287200
C	2.64688300	-2.56570600	1.70999300
H	2.04779200	-1.56830800	3.52478900
H	2.97415600	-3.45144700	-0.22623400
H	3.56084800	-2.96370900	2.13491100
O	-2.10871600	-3.59119100	0.06722800
C	-3.31993200	-3.72657900	-0.27447600
O	-4.03725800	-2.81591800	-0.77976200
C	-3.95872300	-5.08877000	-0.02997600
H	-4.28417700	-5.13860800	1.01501100
H	-4.83178800	-5.24246400	-0.66652000
H	-3.23562700	-5.89123400	-0.19035400
H	0.62807100	1.00732800	-1.92833100
H	-3.19282600	1.59055600	1.60848900
N	1.70646900	1.86106700	0.00696400
C	2.16207000	0.93316900	-0.78512300
H	2.35479300	2.18317500	0.71884700
C	3.47878400	0.30961300	-0.62752500
O	1.44533900	0.48298300	-1.78846000
C	3.98950300	-0.46672100	-1.67685000
C	4.20851000	0.44071900	0.56146200
C	5.21942900	-1.09640300	-1.53922600
H	3.42370500	-0.57389500	-2.59222900
C	5.43890100	-0.19039700	0.69100200
H	3.81881300	1.00186400	1.40161500
C	5.94519100	-0.95996900	-0.35639700
H	5.61040900	-1.69571000	-2.35277900
H	5.99552800	-0.09423300	1.61537100
H	6.90257100	-1.45667500	-0.24800200

IRC_TS1_point229

B	-2.73775800	3.85381600	0.36423200
B	-1.64075500	3.69984200	1.75841200

B	-0.67507900	2.22547900	1.54088300
B	-2.44579400	2.47807400	-0.72670400
B	-1.17791600	1.52077400	0.01199100
B	-1.24790500	4.82288400	0.43721000
B	-1.74387200	4.07439300	-1.09896700
H	-3.81665100	4.34478700	0.46326400
B	0.02671800	3.81642700	1.15696400
H	-1.93857900	4.08265800	2.84493600
B	0.31326500	2.45710000	0.06791400
H	-0.27345700	1.56432900	2.43791800
B	-0.77428800	2.60554800	-1.32953100
H	-3.29656900	1.97791000	-1.38809200
H	-1.26943400	6.00229100	0.59299800
B	-0.03604300	4.05867200	-0.61062300
H	-2.12036200	4.71036000	-2.03043900
H	0.92376800	4.25347000	1.80499000
H	-0.48114200	2.19751600	-2.41137400
H	0.81256000	4.66055300	-1.18566700
B	-2.38695700	2.25826400	1.04914900
I	-1.45563400	-0.71654400	-0.23982600
C	0.34239800	-1.51976800	0.61764700
C	0.62909400	-1.25179700	1.94910400
C	1.15598000	-2.31402800	-0.17919800
C	1.80192000	-1.77867800	2.49030400
H	-0.03311100	-0.64587800	2.55047400
C	2.31910000	-2.84059800	0.38376900
H	0.90690600	-2.50865400	-1.21344900
C	2.64666700	-2.56627100	1.70968800
H	2.04854200	-1.56884800	3.52481400
H	2.97343500	-3.45126800	-0.22695000
H	3.56002900	-2.96562000	2.13465300
O	-2.10899300	-3.59672300	0.06465500
C	-3.32085900	-3.73058400	-0.27512600
O	-4.03759200	-2.81921300	-0.78014100
C	-3.96189000	-5.09152600	-0.02885300
H	-4.28713700	-5.13956300	1.01627100
H	-4.83527600	-5.24433300	-0.66514200
H	-3.24005400	-5.89524800	-0.18857300
H	0.63004200	1.00887600	-1.92849600
H	-3.19476500	1.59365400	1.61097300
N	1.70362500	1.85582900	0.01062200
C	2.16199900	0.93225500	-0.78603900
H	2.35151900	2.17666000	0.71978000
C	3.47888200	0.30878500	-0.62776400

O	1.44809000	0.48542400	-1.79288300
C	3.99039900	-0.46711900	-1.67701500
C	4.20809400	0.43946100	0.56164400
C	5.22043900	-1.09655100	-1.53906600
H	3.42499600	-0.57426500	-2.59262200
C	5.43873600	-0.19117600	0.69142300
H	3.81809600	0.99997800	1.40208900
C	5.94579800	-0.96019200	-0.35599100
H	5.61180600	-1.69557100	-2.35264100
H	5.99498500	-0.09501500	1.61602400
H	6.90334500	-1.45654900	-0.24741200
IRC_TS1_point230			
B	-2.73773400	3.85565000	0.36403900
B	-1.64064700	3.70228300	1.75811300
B	-0.67673500	2.22649000	1.54240900
B	-2.44763600	2.47816600	-0.72500800
B	-1.18009100	1.52148100	0.01421500
B	-1.24665700	4.82306600	0.43533800
B	-1.74370100	4.07309300	-1.09970900
H	-3.81590900	4.34848700	0.46246600
B	0.02700800	3.81606500	1.15612300
H	-1.93767500	4.08717500	2.84415800
B	0.31156200	2.45482500	0.06885300
H	-0.27589400	1.56612200	2.44045800
B	-0.77570300	2.60304400	-1.32814100
H	-3.29910500	1.97817800	-1.38568400
H	-1.26689000	6.00268800	0.58957100
B	-0.03577700	4.05619400	-0.61156800
H	-2.11962600	4.70811100	-2.03208300
H	0.92460800	4.25287800	1.80354500
H	-0.48380000	2.19271100	-2.40953300
H	0.81334600	4.65639400	-1.18760400
B	-2.38870500	2.26045300	1.05093400
I	-1.45476500	-0.71470200	-0.23961100
C	0.34357100	-1.51742900	0.61760500
C	0.63038100	-1.25010400	1.94915000
C	1.15653100	-2.31184400	-0.17963900
C	1.80257400	-1.77848900	2.49021200
H	-0.03120100	-0.64368700	2.55070400
C	2.31896100	-2.83997300	0.38326300
H	0.90740300	-2.50563000	-1.21403100
C	2.64647400	-2.56682600	1.70940500
H	2.04932200	-1.56938200	3.52483100
H	2.97276300	-3.45092200	-0.22772500

H	3.55920400	-2.96758500	2.13439200
O	-2.10928900	-3.60227500	0.06203300
C	-3.32194800	-3.73472300	-0.27585000
O	-4.03787000	-2.82260000	-0.78053400
C	-3.96508100	-5.09433300	-0.02763800
H	-4.29032600	-5.14055100	1.01758500
H	-4.83904600	-5.24640800	-0.66335600
H	-3.24496800	-5.89983000	-0.18650300
H	0.62917700	1.00856900	-1.93395100
H	-3.19751600	1.59789400	1.61416800
N	1.70123700	1.85104900	0.01211100
C	2.16186100	0.93093100	-0.78607700
H	2.34612800	2.16723900	0.72899700
C	3.47892600	0.30780500	-0.62776900
O	1.45016100	0.48940900	-1.79701800
C	3.99128800	-0.46747500	-1.67716000
C	4.20771700	0.43811200	0.56193600
C	5.22145100	-1.09667200	-1.53887600
H	3.42647300	-0.57463400	-2.59315000
C	5.43854600	-0.19199800	0.69194400
H	3.81726200	0.99777900	1.40274200
C	5.94636200	-0.96043100	-0.35552800
H	5.61327000	-1.69534200	-2.35249300
H	5.99428800	-0.09592500	1.61684400
H	6.90406300	-1.45642100	-0.24675800

IRC_TS1_point231

B	-2.73773000	3.85749600	0.36377500
B	-1.64051600	3.70477700	1.75788000
B	-0.67840500	2.22780000	1.54413300
B	-2.44940600	2.47849400	-0.72358100
B	-1.18277000	1.52159600	0.01679000
B	-1.24540800	4.82329100	0.43347200
B	-1.74374300	4.07204400	-1.10040500
H	-3.81529800	4.35155300	0.46177400
B	0.02715600	3.81584600	1.15552700
H	-1.93695300	4.09138800	2.84342100
B	0.31027800	2.45282900	0.07007500
H	-0.27807600	1.56781400	2.44260300
B	-0.77758800	2.60094700	-1.32750400
H	-3.30124000	1.97817200	-1.38343500
H	-1.26425100	6.00312500	0.58626600
B	-0.03550300	4.05364000	-0.61274100
H	-2.11907400	4.70636500	-2.03345800

H	0.92532600	4.25264500	1.80214500
H	-0.48705900	2.18909200	-2.40858600
H	0.81410500	4.65235500	-1.18954200
B	-2.39042700	2.26281900	1.05289600
I	-1.45392100	-0.71277700	-0.23937400
C	0.34458800	-1.51508000	0.61749900
C	0.63168000	-1.24839300	1.94916100
C	1.15707100	-2.30965200	-0.18011400
C	1.80325300	-1.77825100	2.49008700
H	-0.02943300	-0.64163900	2.55090500
C	2.31884900	-2.83932700	0.38269800
H	0.90783700	-2.50269100	-1.21462500
C	2.64631100	-2.56733500	1.70906800
H	2.05013400	-1.56987400	3.52482700
H	2.97211100	-3.45067900	-0.22847400
H	3.55842500	-2.96944600	2.13410400
O	-2.10961200	-3.60792200	0.05926500
C	-3.32281900	-3.73879600	-0.27656200
O	-4.03825500	-2.82600800	-0.78101600
C	-3.96821300	-5.09714500	-0.02638300
H	-4.29324500	-5.14136400	1.01898700
H	-4.84249700	-5.24847800	-0.66179300
H	-3.24936400	-5.90387000	-0.18439800
H	0.63176100	1.01055600	-1.93215100
H	-3.19938700	1.60119300	1.61655600
N	1.69832300	1.84597400	0.01562000
C	2.16158100	0.93024200	-0.78738000
H	2.34229300	2.15981200	0.73200000
C	3.47896100	0.30706500	-0.62806900
O	1.45330300	0.49100100	-1.80128800
C	3.99217300	-0.46777700	-1.67734000
C	4.20720200	0.43680100	0.56216200
C	5.22245100	-1.09671700	-1.53874500
H	3.42775600	-0.57483800	-2.59355100
C	5.43830200	-0.19286100	0.69240800
H	3.81653500	0.99577100	1.40334600
C	5.94693100	-0.96065500	-0.35512000
H	5.61471400	-1.69502800	-2.35241400
H	5.99363400	-0.09689400	1.61758400
H	6.90479700	-1.45631400	-0.24615700
IRC_TS1_point232			
B	-2.73763900	3.85947900	0.36353800
B	-1.64036400	3.70733400	1.75754000
B	-0.68004300	2.22888500	1.54560400

B	-2.45121100	2.47871300	-0.72193600
B	-1.18491100	1.52250600	0.01897000
B	-1.24407300	4.82358800	0.43158300
B	-1.74348100	4.07088800	-1.10119800
H	-3.81451900	4.35525600	0.46096300
B	0.02752500	3.81556600	1.15464200
H	-1.93604000	4.09594300	2.84260700
B	0.30855000	2.45061600	0.07092200
H	-0.28044300	1.56965000	2.44502800
B	-0.77892100	2.59852900	-1.32609900
H	-3.30365300	1.97855500	-1.38115200
H	-1.26158500	6.00362800	0.58286100
B	-0.03516500	4.05127200	-0.61369400
H	-2.11828500	4.70439200	-2.03502300
H	0.92616900	4.25220300	1.80069600
H	-0.48981600	2.18468800	-2.40690700
H	0.81497900	4.64828100	-1.19151100
B	-2.39214500	2.26513500	1.05460200
I	-1.45308300	-0.71100700	-0.23912100
C	0.34577100	-1.51278300	0.61747000
C	0.63299100	-1.24668400	1.94919200
C	1.15763000	-2.30748100	-0.18056100
C	1.80395700	-1.77801500	2.48996700
H	-0.02752700	-0.63947500	2.55112100
C	2.31875100	-2.83866400	0.38217100
H	0.90832700	-2.49970800	-1.21520300
C	2.64617200	-2.56783300	1.70875800
H	2.05098000	-1.57032200	3.52480300
H	2.97148800	-3.45029300	-0.22927100
H	3.55767700	-2.97130700	2.13379800
O	-2.10987500	-3.61357700	0.05644600
C	-3.32395700	-3.74304200	-0.27734300
O	-4.03858900	-2.82953400	-0.78150100
C	-3.97139300	-5.10002300	-0.02499100
H	-4.29638500	-5.14222900	1.02048900
H	-4.84618400	-5.25080100	-0.65987200
H	-3.25415400	-5.90841100	-0.18199800
H	0.63101500	1.01008500	-1.93758800
H	-3.20197500	1.60537900	1.61952700
N	1.69592000	1.84104900	0.01726700
C	2.16150700	0.92874800	-0.78718300
H	2.33745100	2.15104300	0.73903000
C	3.47898700	0.30604400	-0.62800900
O	1.45512700	0.49510100	-1.80533500

C	3.99306100	-0.46805900	-1.67750500
C	4.20677700	0.43538500	0.56249600
C	5.22346400	-1.09676200	-1.53859700
H	3.42924400	-0.57505400	-2.59411500
C	5.43803300	-0.19378600	0.69296700
H	3.81560800	0.99351000	1.40401400
C	5.94744500	-0.96091800	-0.35465700
H	5.61620500	-1.69464200	-2.35235100
H	5.99283600	-0.09798100	1.61845700
H	6.90546000	-1.45622000	-0.24551300

IRC_TS1_point233

B	-2.73755300	3.86147800	0.36323300
B	-1.64016700	3.70991600	1.75726300
B	-0.68167700	2.23025300	1.54726000
B	-2.45294100	2.47918800	-0.72054000
B	-1.18754600	1.52274300	0.02149600
B	-1.24273200	4.82391700	0.42972500
B	-1.74340300	4.06996100	-1.10190300
H	-3.81380700	4.35859300	0.46021000
B	0.02775800	3.81539800	1.15400900
H	-1.93522700	4.10015000	2.84186200
B	0.30724100	2.44867100	0.07211200
H	-0.28261900	1.57138800	2.44714300
B	-0.78070800	2.59651900	-1.32539000
H	-3.30579500	1.97887000	-1.37903900
H	-1.25898200	6.00412400	0.57969300
B	-0.03481300	4.04883600	-0.61482900
H	-2.11758900	4.70275200	-2.03645100
H	0.92697300	4.25189500	1.79936200
H	-0.49263100	2.18096700	-2.40572200
H	0.81577400	4.64447600	-1.19330400
B	-2.39385600	2.26762700	1.05648300
I	-1.45227000	-0.70913500	-0.23883100
C	0.34679800	-1.51046800	0.61738500
C	0.63431000	-1.24497400	1.94920400
C	1.15817700	-2.30531500	-0.18102100
C	1.80467800	-1.77772600	2.48982400
H	-0.02578200	-0.63750000	2.55134200
C	2.31867600	-2.83798000	0.38160300
H	0.90872300	-2.49695200	-1.21573700
C	2.64606200	-2.56826900	1.70840300
H	2.05181800	-1.57072500	3.52477500
H	2.97090100	-3.44997600	-0.23001800

H	3.55700300	-2.97297900	2.13347000
O	-2.11021500	-3.61938400	0.05345400
C	-3.32488600	-3.74727300	-0.27812900
O	-4.03900900	-2.83312500	-0.78206600
C	-3.97451700	-5.10291200	-0.02356200
H	-4.29928400	-5.14298800	1.02205200
H	-4.84964900	-5.25302800	-0.65810200
H	-3.25854800	-5.91256800	-0.17966000
H	0.63309700	1.01167000	-1.93753600
H	-3.20406800	1.60905300	1.62201000
N	1.69302600	1.83605700	0.02039400
C	2.16117200	0.92798400	-0.78844900
H	2.33318500	2.14327500	0.74348600
C	3.47898900	0.30525700	-0.62825900
O	1.45821200	0.49678200	-1.80946500
C	3.99393900	-0.46829600	-1.67769800
C	4.20619900	0.43398100	0.56279500
C	5.22445800	-1.09673600	-1.53849500
H	3.43053000	-0.57513700	-2.59454900
C	5.43771000	-0.19475500	0.69349700
H	3.81483400	0.99144600	1.40467200
C	5.94795400	-0.96117200	-0.35423400
H	5.61763100	-1.69421200	-2.35233500
H	5.99210300	-0.09906800	1.61926000
H	6.90611600	-1.45616500	-0.24491800

IRC_TS1_point234

B	-2.73739900	3.86359500	0.36294300
B	-1.63995700	3.71256600	1.75691800
B	-0.68329600	2.23148700	1.54874900
B	-2.45468700	2.47961200	-0.71900900
B	-1.18986300	1.52365700	0.02379200
B	-1.24131900	4.82431000	0.42784900
B	-1.74310400	4.06899200	-1.10269800
H	-3.81300300	4.36224300	0.45940000
B	0.02816200	3.81520400	1.15318200
H	-1.93432000	4.10466400	2.84106700
B	0.30564600	2.44658400	0.07299100
H	-0.28488900	1.57322600	2.44941000
B	-0.78208500	2.59429700	-1.32416200
H	-3.30804700	1.97935500	-1.37689000
H	-1.25620900	6.00474000	0.57637900
B	-0.03440400	4.04653800	-0.61581600
H	-2.11675800	4.70107400	-2.03793000

H	0.92782200	4.25158400	1.79796900
H	-0.49547100	2.17704300	-2.40432700
H	0.81673600	4.64054100	-1.19525500
B	-2.39555700	2.27011200	1.05818000
I	-1.45146200	-0.70736900	-0.23852200
C	0.34794200	-1.50819100	0.61735800
C	0.63563700	-1.24326200	1.94923200
C	1.15872700	-2.30317200	-0.18145700
C	1.80542900	-1.77742700	2.48968400
H	-0.02393100	-0.63541100	2.55156900
C	2.31861200	-2.83728300	0.38105900
H	0.90914900	-2.49407000	-1.21628400
C	2.64598500	-2.56867900	1.70805900
H	2.05271700	-1.57109500	3.52472800
H	2.97031100	-3.44958300	-0.23081100
H	3.55635800	-2.97467900	2.13312000
O	-2.11047300	-3.62526300	0.05035800
C	-3.32600900	-3.75165500	-0.27897400
O	-4.03941400	-2.83682600	-0.78265700
C	-3.97768300	-5.10588300	-0.02200700
H	-4.30230500	-5.14376400	1.02373900
H	-4.85324200	-5.25554600	-0.65606000
H	-3.26313000	-5.91700700	-0.17702200
H	0.63338800	1.01170400	-1.94142800
H	-3.20640000	1.61306900	1.62466000
N	1.69052700	1.83105800	0.02220500
C	2.16095600	0.92656500	-0.78841700
H	2.32884900	2.13496400	0.74887300
C	3.47894100	0.30425400	-0.62820900
O	1.46026500	0.50025200	-1.81351100
C	3.99481700	-0.46850800	-1.67787200
C	4.20568000	0.43249800	0.56316700
C	5.22546000	-1.09670600	-1.53838100
H	3.43198500	-0.57521600	-2.59510300
C	5.43735600	-0.19579000	0.69408600
H	3.81389900	0.98914100	1.40540600
C	5.94842000	-0.96147100	-0.35376800
H	5.61913400	-1.69369300	-2.35234100
H	5.99123700	-0.10030300	1.62016300
H	6.90672800	-1.45612700	-0.24427400

IRC_TS1_point235

B	-2.73722200	3.86575000	0.36260600
B	-1.63969800	3.71523700	1.75659700

B	-0.68489100	2.23287900	1.55031100
B	-2.45637300	2.48021700	-0.71763300
B	-1.19238000	1.52412800	0.02619900
B	-1.23988000	4.82475100	0.42600900
B	-1.74288100	4.06819300	-1.10342600
H	-3.81216400	4.36590200	0.45857800
B	0.02850200	3.81508400	1.15249100
H	-1.93341200	4.10904000	2.84026900
B	0.30424600	2.44468300	0.07407300
H	-0.28713200	1.57507300	2.45158200
B	-0.78372300	2.59235400	-1.32331600
H	-3.31025400	1.97995200	-1.37480700
H	-1.25349100	6.00533100	0.57320900
B	-0.03397500	4.04424600	-0.61689200
H	-2.11591500	4.69953300	-2.03941000
H	0.92872900	4.25126200	1.79663000
H	-0.49812500	2.17325000	-2.40297000
H	0.81763800	4.63677700	-1.19703600
B	-2.39724400	2.27271200	1.05995000
I	-1.45069200	-0.70557000	-0.23818200
C	0.34899000	-1.50592700	0.61731500
C	0.63696500	-1.24155700	1.94925500
C	1.15925900	-2.30104800	-0.18189300
C	1.80619800	-1.77708100	2.48952400
H	-0.02213300	-0.63340100	2.55180600
C	2.31856300	-2.83656300	0.38049200
H	0.90953100	-2.49133800	-1.21679300
C	2.64593800	-2.56902300	1.70768000
H	2.05363000	-1.57140300	3.52466500
H	2.96975200	-3.44919100	-0.23158700
H	3.55577200	-2.97622100	2.13273600
O	-2.11079200	-3.63119100	0.04713000
C	-3.32701100	-3.75604300	-0.27985000
O	-4.03985700	-2.84058800	-0.78329900
C	-3.98080900	-5.10885900	-0.02039700
H	-4.30522900	-5.14445400	1.02547900
H	-4.85680900	-5.25799100	-0.65398000
H	-3.26764900	-5.92142300	-0.17436100
H	0.63486800	1.01272300	-1.94296300
H	-3.20870000	1.61713500	1.62725600
N	1.68766800	1.82611400	0.02495700
C	2.16070900	0.92557100	-0.78951900
H	2.32440700	2.12705600	0.75388400
C	3.47893800	0.30339700	-0.62838200

O	1.46313200	0.50226700	-1.81746300
C	3.99569100	-0.46869000	-1.67807800
C	4.20505100	0.43101100	0.56352900
C	5.22644600	-1.09662400	-1.53830800
H	3.43333400	-0.57517700	-2.59560700
C	5.43694900	-0.19685800	0.69466800
H	3.81300000	0.98693500	1.40612500
C	5.94886300	-0.96176000	-0.35333300
H	5.62060100	-1.69312100	-2.35239000
H	5.99036800	-0.10157400	1.62105000
H	6.90731400	-1.45610500	-0.24366700

IRC_TS1_point236

B	-2.73698700	3.86800800	0.36227400
B	-1.63941100	3.71796800	1.75624900
B	-0.68646300	2.23422700	1.55179500
B	-2.45805500	2.48084100	-0.71619500
B	-1.19482800	1.52498800	0.02856500
B	-1.23837600	4.82524600	0.42416400
B	-1.74251700	4.06741100	-1.10421100
H	-3.81124400	4.36970000	0.45774500
B	0.02896300	3.81496600	1.15171200
H	-1.93243400	4.11363900	2.83944400
B	0.30279300	2.44273100	0.07497400
H	-0.28939800	1.57697700	2.45379400
B	-0.78512100	2.59031400	-1.32222100
H	-3.31244900	1.98064200	-1.37272000
H	-1.25056100	6.00604800	0.56990900
B	-0.03348300	4.04203800	-0.61788900
H	-2.11497200	4.69805400	-2.04088000
H	0.92965900	4.25100000	1.79526000
H	-0.50095300	2.16943400	-2.40163400
H	0.81870100	4.63289300	-1.19897000
B	-2.39891500	2.27535100	1.06162200
I	-1.44993300	-0.70385000	-0.23782400
C	0.35009100	-1.50368800	0.61730800
C	0.63830200	-1.23985800	1.94929600
C	1.15979100	-2.29894600	-0.18230700
C	1.80700300	-1.77672100	2.48936600
H	-0.02026400	-0.63132100	2.55205000
C	2.31853100	-2.83583400	0.37993400
H	0.90992300	-2.48850200	-1.21731200
C	2.64592900	-2.56934100	1.70730300
H	2.05461900	-1.57167700	3.52458700

H	2.96920200	-3.44875500	-0.23239900
H	3.55522300	-2.97778100	2.13233000
O	-2.11104700	-3.63718500	0.04379200
C	-3.32810100	-3.76052700	-0.28077500
O	-4.04031000	-2.84443100	-0.78399200
C	-3.98395200	-5.11189500	-0.01868200
H	-4.30817900	-5.14509000	1.02734200
H	-4.86037300	-5.26070800	-0.65173000
H	-3.27219700	-5.92588200	-0.17140900
H	0.63578700	1.01316800	-1.94613200
H	-3.21095000	1.62128700	1.62977600
N	1.68518100	1.82118000	0.02672600
C	2.16031000	0.92422300	-0.78957600
H	2.32026500	2.11873400	0.75867100
C	3.47881300	0.30239500	-0.62832100
O	1.46534300	0.50524300	-1.82150400
C	3.99655800	-0.46883000	-1.67826100
C	4.20444700	0.42946100	0.56395000
C	5.22744500	-1.09651000	-1.53822500
H	3.43479700	-0.57511200	-2.59618100
C	5.43651800	-0.19798400	0.69530100
H	3.81201200	0.98453100	1.40694300
C	5.94928200	-0.96207800	-0.35285800
H	5.62214900	-1.69243700	-2.35246300
H	5.98940500	-0.10298100	1.62202300
H	6.90787300	-1.45610600	-0.24300700
IRC_TS1_point237			
B	-2.73670400	3.87032300	0.36190700
B	-1.63907000	3.72072700	1.75589200
B	-0.68801400	2.23565300	1.55328400
B	-2.45968500	2.48158600	-0.71485000
B	-1.19727700	1.52562500	0.03089200
B	-1.23682000	4.82579800	0.42234000
B	-1.74215800	4.06674900	-1.10495800
H	-3.81026500	4.37360500	0.45687500
B	0.02940900	3.81489500	1.15098600
H	-1.93141600	4.11815100	2.83859900
B	0.30135400	2.44088800	0.07596900
H	-0.29165400	1.57891100	2.45597200
B	-0.78664500	2.58844800	-1.32129600
H	-3.31466100	1.98149900	-1.37068700
H	-1.24768800	6.00674100	0.56674200
B	-0.03297100	4.03987300	-0.61893200
H	-2.11398400	4.69665600	-2.04237700

H	0.93067300	4.25068300	1.79391400
H	-0.50357400	2.16572400	-2.40022100
H	0.81973400	4.62915400	-1.20075700
B	-2.40056300	2.27807000	1.06330900
I	-1.44922000	-0.70214400	-0.23744300
C	0.35113100	-1.50149400	0.61731100
C	0.63963500	-1.23816400	1.94933900
C	1.16030000	-2.29687200	-0.18271500
C	1.80782800	-1.77631500	2.48919000
H	-0.01843300	-0.62930300	2.55231300
C	2.31850700	-2.83508400	0.37936500
H	0.91026700	-2.48581900	-1.21778700
C	2.64594900	-2.56959600	1.70689700
H	2.05562800	-1.57187700	3.52448600
H	2.96867600	-3.44829600	-0.23320300
H	3.55473900	-2.97917800	2.13188300
O	-2.11133100	-3.64316300	0.04036700
C	-3.32913500	-3.76501800	-0.28172700
O	-4.04078700	-2.84833200	-0.78472400
C	-3.98706000	-5.11491800	-0.01688800
H	-4.31107400	-5.14562700	1.02927200
H	-4.86399100	-5.26331700	-0.64937200
H	-3.27678800	-5.93046900	-0.16841000
H	0.63706100	1.01399700	-1.94845900
H	-3.21333300	1.62565700	1.63239300
N	1.68235600	1.81633700	0.02928500
C	2.16014900	0.92310100	-0.79065200
H	2.31564600	2.11064500	0.76394800
C	3.47878500	0.30147000	-0.62844400
O	1.46802300	0.50744300	-1.82533000
C	3.99743000	-0.46896400	-1.67847800
C	4.20375000	0.42789700	0.56436400
C	5.22843300	-1.09636200	-1.53817700
H	3.43619300	-0.57494700	-2.59673800
C	5.43602300	-0.19914600	0.69593300
H	3.81101100	0.98223000	1.40770700
C	5.94966800	-0.96239000	-0.35240700
H	5.62367500	-1.69170400	-2.35257800
H	5.98840700	-0.10441700	1.62298700
H	6.90840000	-1.45610300	-0.24238200
IRC_TS1_point238			
B	-2.73636800	3.87273500	0.36154600
B	-1.63868600	3.72355000	1.75553600

B	-0.68952900	2.23708700	1.55475200
B	-2.46131600	2.48239100	-0.71346700
B	-1.19981400	1.52644800	0.03329900
B	-1.23519800	4.82639400	0.42051400
B	-1.74170600	4.06613000	-1.10573500
H	-3.80921400	4.37760900	0.45602200
B	0.02995100	3.81483600	1.15022900
H	-1.93033100	4.12287300	2.83774900
B	0.30002000	2.43904500	0.07686600
H	-0.29393600	1.58088400	2.45817900
B	-0.78804800	2.58654200	-1.32027100
H	-3.31685000	1.98240500	-1.36861700
H	-1.24456500	6.00756000	0.56344100
B	-0.03238900	4.03773500	-0.61993100
H	-2.11291600	4.69533300	-2.04385900
H	0.93171100	4.25043800	1.79255400
H	-0.50638500	2.16189000	-2.39888300
H	0.82091500	4.62526800	-1.20269600
B	-2.40220100	2.28085800	1.06495900
I	-1.44852500	-0.70049400	-0.23704800
C	0.35218800	-1.49931700	0.61733200
C	0.64098000	-1.23648400	1.94939300
C	1.16080700	-2.29481500	-0.18310600
C	1.80869300	-1.77589300	2.48901000
H	-0.01654400	-0.62723500	2.55258100
C	2.31850200	-2.83432100	0.37878900
H	0.91061600	-2.48303000	-1.21827900
C	2.64601000	-2.56982300	1.70647900
H	2.05671800	-1.57204900	3.52436900
H	2.96815800	-3.44780800	-0.23404500
H	3.55429500	-2.98059500	2.13140700
O	-2.11157400	-3.64922100	0.03683400
C	-3.33019500	-3.76958700	-0.28272500
O	-4.04127700	-2.85231400	-0.78552800
C	-3.99017900	-5.11799000	-0.01500300
H	-4.31398900	-5.14610100	1.03130500
H	-4.86754200	-5.26618100	-0.64689900
H	-3.28133900	-5.93498000	-0.16513000
H	0.63837200	1.01487800	-1.95131500
H	-3.21557100	1.63002200	1.63487900
N	1.67996300	1.81152900	0.03081400
C	2.15960400	0.92177900	-0.79065500
H	2.31161000	2.10213400	0.76840300
C	3.47857900	0.30044600	-0.62834300

O	1.47029500	0.51013700	-1.82930300
C	3.99828200	-0.46903200	-1.67866600
C	4.20306600	0.42627200	0.56484000
C	5.22943300	-1.09615100	-1.53812300
H	3.43766800	-0.57474400	-2.59733600
C	5.43551200	-0.20035600	0.69661500
H	3.80996900	0.97972800	1.40860800
C	5.95004300	-0.96271500	-0.35191900
H	5.62528000	-1.69083300	-2.35271800
H	5.98734200	-0.10598000	1.62403200
H	6.90891600	-1.45611700	-0.24170900

IRC_TS1_point239

B	-2.73596500	3.87519900	0.36115000
B	-1.63824200	3.72638600	1.75514600
B	-0.69102500	2.23854700	1.55616800
B	-2.46288000	2.48327300	-0.71215600
B	-1.20219600	1.52718600	0.03554000
B	-1.23351200	4.82704700	0.41870300
B	-1.74121800	4.06560100	-1.10650000
H	-3.80809700	4.38167800	0.45512900
B	0.03050500	3.81480900	1.14947400
H	-1.92919700	4.12742200	2.83687500
B	0.29856200	2.43726600	0.07779100
H	-0.29612000	1.58286500	2.46028100
B	-0.78948300	2.58476000	-1.31930500
H	-3.31901200	1.98351300	-1.36667800
H	-1.24156600	6.00833300	0.56032900
B	-0.03179100	4.03568200	-0.62096200
H	-2.11179600	4.69411100	-2.04533600
H	0.93283200	4.25012700	1.79120300
H	-0.50892100	2.15836200	-2.39744700
H	0.82204900	4.62161600	-1.20445800
B	-2.40378900	2.28369300	1.06657300
I	-1.44788000	-0.69888900	-0.23663300
C	0.35320000	-1.49721000	0.61737900
C	0.64231000	-1.23481700	1.94945500
C	1.16128600	-2.29281000	-0.18348400
C	1.80957100	-1.77542500	2.48881700
H	-0.01472200	-0.62526200	2.55287100
C	2.31850300	-2.83354600	0.37821900
H	0.91090100	-2.48047000	-1.21870500
C	2.64609900	-2.56998300	1.70604500
H	2.05781900	-1.57212300	3.52422600

H	2.96767500	-3.44728900	-0.23486400
H	3.55393600	-2.98180000	2.13089400
O	-2.11183300	-3.65522500	0.03326400
C	-3.33124400	-3.77414600	-0.28372700
O	-4.04178800	-2.85634100	-0.78636000
C	-3.99323300	-5.12102400	-0.01300900
H	-4.31679400	-5.14644300	1.03344200
H	-4.87111000	-5.26895400	-0.64429200
H	-3.28585900	-5.93957300	-0.16177000
H	0.63961700	1.01579500	-1.95415500
H	-3.21793900	1.63458100	1.63743400
N	1.67715300	1.80681100	0.03337600
C	2.15952600	0.92061200	-0.79183900
H	2.30682400	2.09399000	0.77390400
C	3.47852300	0.29944900	-0.62843500
O	1.47280900	0.51250600	-1.83306700
C	3.99914600	-0.46913700	-1.67889200
C	4.20228600	0.42462700	0.56530600
C	5.23042500	-1.09594200	-1.53809800
H	3.43908800	-0.57446900	-2.59793200
C	5.43492700	-0.20160800	0.69729700
H	3.80886900	0.97735800	1.40940400
C	5.95037400	-0.96304400	-0.35145300
H	5.62686000	-1.68994400	-2.35289800
H	5.98622500	-0.10755900	1.62506500
H	6.90939100	-1.45612400	-0.24107200
IRC_TS1_point240			
B	-2.73551800	3.87775700	0.36077700
B	-1.63774600	3.72929300	1.75478300
B	-0.69246800	2.24004900	1.55761400
B	-2.46446300	2.48424200	-0.71080400
B	-1.20478500	1.52798900	0.03796700
B	-1.23176000	4.82773300	0.41689300
B	-1.74067500	4.06512400	-1.10726600
H	-3.80690000	4.38592000	0.45426400
B	0.03114400	3.81479600	1.14872900
H	-1.92796800	4.13231300	2.83600800
B	0.29736000	2.43552200	0.07867300
H	-0.29843800	1.58490700	2.46253000
B	-0.79089500	2.58296100	-1.31832500
H	-3.32123800	1.98462000	-1.36457300
H	-1.23819800	6.00926000	0.55698900
B	-0.03112000	4.03359600	-0.62196400
H	-2.11060000	4.69289800	-2.04685000

H	0.93400800	4.24986900	1.78983400
H	-0.51179000	2.15441000	-2.39610100
H	0.82338100	4.61765000	-1.20645700
B	-2.40537600	2.28661300	1.06820200
I	-1.44725500	-0.69731500	-0.23621000
C	0.35421700	-1.49510000	0.61742500
C	0.64365600	-1.23316500	1.94952000
C	1.16176400	-2.29080300	-0.18385800
C	1.81049700	-1.77494200	2.48860800
H	-0.01281200	-0.62320600	2.55316100
C	2.31852300	-2.83275300	0.37762100
H	0.91119800	-2.47772200	-1.21917600
C	2.64623300	-2.57011500	1.70558100
H	2.05901300	-1.57219600	3.52406400
H	2.96718100	-3.44675600	-0.23574500
H	3.55360300	-2.98307300	2.13034000
O	-2.11206500	-3.66136200	0.02956800
C	-3.33227500	-3.77879800	-0.28479300
O	-4.04229400	-2.86045600	-0.78728800
C	-3.99634000	-5.12412000	-0.01094800
H	-4.31971000	-5.14673700	1.03564100
H	-4.87472200	-5.27190600	-0.64156500
H	-3.29049500	-5.94424700	-0.15816700
H	0.64119400	1.01717500	-1.95664300
H	-3.22019900	1.63920200	1.63996200
N	1.67492400	1.80218000	0.03447200
C	2.15882300	0.91930200	-0.79164000
H	2.30299800	2.08530900	0.77791900
C	3.47821200	0.29840400	-0.62827700
O	1.47509700	0.51503500	-1.83687600
C	3.99996900	-0.46912800	-1.67907800
C	4.20151800	0.42292500	0.56583800
C	5.23142100	-1.09562400	-1.53806800
H	3.44056900	-0.57413600	-2.59855300
C	5.43433500	-0.20289500	0.69802700
H	3.80776100	0.97473900	1.41039600
C	5.95070900	-0.96336100	-0.35095300
H	5.62852200	-1.68887200	-2.35310100
H	5.98505500	-0.10926600	1.62618100
H	6.90987400	-1.45611900	-0.24039100
IRC_TS1_point241			
B	-2.73498400	3.88033700	0.36035600
B	-1.63718400	3.73217100	1.75435900

B	-0.69388200	2.24152200	1.55893600
B	-2.46593800	2.48524000	-0.70954200
B	-1.20705200	1.52877500	0.04007900
B	-1.22994700	4.82847400	0.41510000
B	-1.74006500	4.06472400	-1.10804800
H	-3.80564600	4.39006000	0.45337200
B	0.03180500	3.81481200	1.14794300
H	-1.92671900	4.13677700	2.83510900
B	0.29588200	2.43381800	0.07953800
H	-0.30044700	1.58689800	2.46446500
B	-0.79223900	2.58127300	-1.31734400
H	-3.32328100	1.98596500	-1.36278200
H	-1.23513900	6.01007800	0.55399300
B	-0.03043600	4.03166400	-0.62299200
H	-2.10936600	4.69189200	-2.04826500
H	0.93522900	4.24957900	1.78847700
H	-0.51414200	2.15114100	-2.39463600
H	0.82455900	4.61418700	-1.20813800
B	-2.40686600	2.28953100	1.06973100
I	-1.44668700	-0.69581800	-0.23576600
C	0.35518700	-1.49310000	0.61750400
C	0.64496400	-1.23154400	1.94959800
C	1.16220500	-2.28889400	-0.18420300
C	1.81141700	-1.77441400	2.48839900
H	-0.01103900	-0.62132500	2.55347200
C	2.31854900	-2.83196600	0.37705900
H	0.91141700	-2.47535000	-1.21954200
C	2.64639200	-2.57017500	1.70512400
H	2.06019200	-1.57212500	3.52387700
H	2.96675600	-3.44618000	-0.23656100
H	3.55338600	-2.98404000	2.12976200
O	-2.11231300	-3.66738600	0.02590800
C	-3.33334800	-3.78338800	-0.28582000
O	-4.04283000	-2.86458000	-0.78822400
C	-3.99929800	-5.12713300	-0.00873700
H	-4.32236800	-5.14686200	1.03800000
H	-4.87807800	-5.27494500	-0.63874900
H	-3.29475000	-5.94859200	-0.15435900
H	0.64249300	1.01838500	-1.96008100
H	-3.22244100	1.64383100	1.64235800
N	1.67210100	1.79761000	0.03729800
C	2.15886400	0.91815800	-0.79307700
H	2.29806800	2.07729700	0.78372600
C	3.47813500	0.29732800	-0.62835500

O	1.47741600	0.51767100	-1.84066600
C	4.00081200	-0.46922900	-1.67931000
C	4.20064600	0.42120400	0.56635200
C	5.23240400	-1.09536900	-1.53806200
H	3.44199000	-0.57376500	-2.59918100
C	5.43365400	-0.20423100	0.69876000
H	3.80654100	0.97234400	1.41119100
C	5.95097700	-0.96370400	-0.35047100
H	5.63014100	-1.68784100	-2.35334100
H	5.98381200	-0.11097600	1.62728300
H	6.91028800	-1.45613000	-0.23974400

IRC_TS1_point242

B	-2.73442400	3.88300500	0.35998900
B	-1.63657000	3.73513200	1.75400200
B	-0.69523400	2.24307100	1.56036800
B	-2.46746800	2.48634700	-0.70820700
B	-1.20970800	1.52954600	0.04256900
B	-1.22807800	4.82922700	0.41332100
B	-1.73943300	4.06436600	-1.10878500
H	-3.80428100	4.39458200	0.45249900
B	0.03254300	3.81483300	1.14721700
H	-1.92531400	4.14190400	2.83423300
B	0.29483600	2.43217700	0.08042000
H	-0.30283000	1.58902100	2.46683000
B	-0.79365100	2.57957000	-1.31637800
H	-3.32559400	1.98726400	-1.36058600
H	-1.23148400	6.01111500	0.55057800
B	-0.02968800	4.02962100	-0.62398000
H	-2.10803400	4.69071900	-2.04984600
H	0.93657500	4.24926800	1.78708500
H	-0.51716200	2.14694600	-2.39326800
H	0.82608800	4.61004300	-1.21024700
B	-2.40838700	2.29254100	1.07134500
I	-1.44613600	-0.69433000	-0.23532900
C	0.35616200	-1.49107500	0.61756600
C	0.64629800	-1.22994000	1.94966100
C	1.16265300	-2.28695300	-0.18456700
C	1.81239400	-1.77388000	2.48815300
H	-0.00910100	-0.61927300	2.55377000
C	2.31859300	-2.83114800	0.37643300
H	0.91166500	-2.47263700	-1.22000700
C	2.64660000	-2.57021000	1.70460600
H	2.06148600	-1.57210400	3.52366100

H	2.96628300	-3.44560500	-0.23749200
H	3.55316700	-2.98517300	2.12912300
O	-2.11253800	-3.67360500	0.02208400
C	-3.33432900	-3.78811300	-0.28696000
O	-4.04331900	-2.86880600	-0.78928100
C	-4.00241800	-5.13023200	-0.00650600
H	-4.32535200	-5.14690200	1.04035400
H	-4.88193100	-5.27785700	-0.63569600
H	-3.29966800	-5.95370700	-0.15044400
H	0.64443900	1.02051500	-1.96233500
H	-3.22480500	1.64880200	1.64505300
N	1.67011300	1.79324400	0.03769200
C	2.15796400	0.91690400	-0.79252000
H	2.29451400	2.06840700	0.78719200
C	3.47769500	0.29629900	-0.62813600
O	1.47977300	0.52005400	-1.84421100
C	4.00158400	-0.46912500	-1.67949000
C	4.19978600	0.41944400	0.56693300
C	5.23337800	-1.09493000	-1.53804900
H	3.44346700	-0.57329900	-2.59982500
C	5.43297200	-0.20557000	0.69953400
H	3.80534000	0.96960000	1.41227800
C	5.95126500	-0.96398900	-0.34996000
H	5.63185100	-1.68655500	-2.35359600
H	5.98251300	-0.11281900	1.62847600
H	6.91073900	-1.45607500	-0.23905500

IRC_TS1_point243

B	-2.73376800	3.88564600	0.35955300
B	-1.63589000	3.73800200	1.75356000
B	-0.69654000	2.24452800	1.56160300
B	-2.46883000	2.48741800	-0.70699800
B	-1.21186800	1.53031300	0.04459600
B	-1.22616400	4.83003400	0.41156900
B	-1.73871100	4.06407700	-1.10958000
H	-3.80290100	4.39868700	0.45165000
B	0.03330200	3.81488800	1.14640900
H	-1.92396500	4.14620000	2.83331500
B	0.29333200	2.43056000	0.08122600
H	-0.30459600	1.59100000	2.46857400
B	-0.79489100	2.57796100	-1.31538500
H	-3.32746500	1.98878900	-1.35895900
H	-1.22842000	6.01194200	0.54774900
B	-0.02893000	4.02782100	-0.62500400

H	-2.10671900	4.68994100	-2.05114900
H	0.93786100	4.24902800	1.78574000
H	-0.51927800	2.14390800	-2.39175200
H	0.82726600	4.60682500	-1.21180400
B	-2.40976300	2.29549300	1.07280100
I	-1.44564800	-0.69296500	-0.23486600
C	0.35707000	-1.48921600	0.61766200
C	0.64755900	-1.22840000	1.94974600
C	1.16305300	-2.28517900	-0.18487900
C	1.81333200	-1.77330900	2.48793200
H	-0.00741700	-0.61752600	2.55408300
C	2.31864600	-2.83037200	0.37589300
H	0.91183400	-2.47049700	-1.22031500
C	2.64682400	-2.57017800	1.70413700
H	2.06271800	-1.57189100	3.52343000
H	2.96593800	-3.44498000	-0.23828900
H	3.55309700	-2.98588600	2.12849500
O	-2.11277800	-3.67959700	0.01840500
C	-3.33544100	-3.79266300	-0.28797900
O	-4.04386700	-2.87295400	-0.79031600
C	-4.00523800	-5.13316900	-0.00408400
H	-4.32782700	-5.14680100	1.04291500
H	-4.88485000	-5.28126200	-0.63276300
H	-3.30343700	-5.95741400	-0.14611300
H	0.64617500	1.02244100	-1.96697400
H	-3.22681200	1.65337000	1.64721700
N	1.66727500	1.78887700	0.04098500
C	2.15817800	0.91585400	-0.79436000
H	2.28955100	2.06073100	0.79320600
C	3.47759900	0.29514800	-0.62819000
O	1.48189400	0.52307100	-1.84819000
C	4.00238800	-0.46922700	-1.67971300
C	4.19881800	0.41767300	0.56750500
C	5.23432800	-1.09463500	-1.53804800
H	3.44486800	-0.57281600	-2.60047000
C	5.43219300	-0.20696200	0.70032100
H	3.80398300	0.96721100	1.41307300
C	5.95145500	-0.96433300	-0.34945700
H	5.63348200	-1.68537700	-2.35389000
H	5.98114500	-0.11463300	1.62964700
H	6.91107600	-1.45607400	-0.23839500

IRC_TS1_point244

B	-2.73310400	3.88837200	0.35921300
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B	-1.63517000	3.74097300	1.75322500
B	-0.69779300	2.24609300	1.56303200
B	-2.47030200	2.48861700	-0.70566400
B	-1.21456700	1.53104100	0.04716300
B	-1.22421400	4.83082200	0.40985000
B	-1.73800700	4.06380300	-1.11026400
H	-3.80138600	4.40343900	0.45077200
B	0.03412000	3.81492700	1.14571200
H	-1.92240000	4.15148300	2.83245000
B	0.29240200	2.42900600	0.08212200
H	-0.30697000	1.59318300	2.47104200
B	-0.79629500	2.57633900	-1.31437700
H	-3.32984800	1.99027100	-1.35670200
H	-1.22457500	6.01304300	0.54431800
B	-0.02814000	4.02582500	-0.62594600
H	-2.10527000	4.68877900	-2.05277300
H	0.93938000	4.24863800	1.78431900
H	-0.52239800	2.13953300	-2.39029800
H	0.82894600	4.60253700	-1.21397200
B	-2.41121200	2.29854000	1.07441400
I	-1.44517300	-0.69157700	-0.23443200
C	0.35799200	-1.48731400	0.61772700
C	0.64885900	-1.22686700	1.94979400
C	1.16346700	-2.28333200	-0.18524300
C	1.81434100	-1.77273500	2.48764200
H	-0.00548600	-0.61551400	2.55437500
C	2.31871300	-2.82954300	0.37523700
H	0.91201600	-2.46790900	-1.22076800
C	2.64709800	-2.57011800	1.70356300
H	2.06409000	-1.57176200	3.52314900
H	2.96549600	-3.44437100	-0.23926100
H	3.55300400	-2.98683400	2.12776400
O	-2.11299900	-3.68582800	0.01450700
C	-3.33634200	-3.79740900	-0.28918300
O	-4.04431800	-2.87724500	-0.79148800
C	-4.00834900	-5.13621600	-0.00167200
H	-4.33096400	-5.14644600	1.04541600
H	-4.88897800	-5.28409400	-0.62939100
H	-3.30866700	-5.96314400	-0.14175700
H	0.64881500	1.02574800	-1.96961400
H	-3.22934000	1.65868900	1.65013800
N	1.66552600	1.78485800	0.04060100
C	2.15711800	0.91475300	-0.79345100
H	2.28598600	2.05149000	0.79661400

C	3.47703400	0.29417600	-0.62793900
O	1.48445400	0.52534500	-1.85145700
C	4.00310100	-0.46902100	-1.67989500
C	4.19785000	0.41587200	0.56811800
C	5.23526400	-1.09408400	-1.53804700
H	3.44633900	-0.57221100	-2.60114500
C	5.43140700	-0.20833200	0.70113100
H	3.80264900	0.96436500	1.41422000
C	5.95168500	-0.96457100	-0.34893500
H	5.63522100	-1.68391500	-2.35417100
H	5.97969800	-0.11659200	1.63091500
H	6.91148300	-1.45595700	-0.23769100

IRC_TS1_point245

B	-2.73236100	3.89104700	0.35879000
B	-1.63439000	3.74384000	1.75279400
B	-0.69899300	2.24753300	1.56424400
B	-2.47158900	2.48972100	-0.70445700
B	-1.21665700	1.53174400	0.04918100
B	-1.22222100	4.83167400	0.40812900
B	-1.73722100	4.06357800	-1.11106400
H	-3.79994400	4.40742300	0.45002000
B	0.03496200	3.81500700	1.14490400
H	-1.92096700	4.15569000	2.83155100
B	0.29094400	2.42747100	0.08288100
H	-0.30862900	1.59514400	2.47275000
B	-0.79749300	2.57475500	-1.31339400
H	-3.33161200	1.99178300	-1.35505800
H	-1.22144200	6.01389900	0.54158200
B	-0.02732800	4.02408600	-0.62698600
H	-2.10396600	4.68810100	-2.05400000
H	0.94069200	4.24844400	1.78302100
H	-0.52451100	2.13634300	-2.38875200
H	0.83018000	4.59934000	-1.21554300
B	-2.41249700	2.30151000	1.07586500
I	-1.44475300	-0.69032300	-0.23396300
C	0.35884100	-1.48559000	0.61781800
C	0.65007300	-1.22540900	1.94986700
C	1.16383500	-2.28168300	-0.18554300
C	1.81529300	-1.77212600	2.48739600
H	-0.00390700	-0.61391100	2.55466300
C	2.31879600	-2.82877900	0.37470100
H	0.91214400	-2.46595500	-1.22105400
C	2.64738400	-2.57000200	1.70307200

H	2.06533500	-1.57147200	3.52288400
H	2.96520400	-3.44374800	-0.24004400
H	3.55304600	-2.98737300	2.12709900
O	-2.11320400	-3.69180200	0.01080700
C	-3.33747300	-3.80192600	-0.29017500
O	-4.04486000	-2.88142300	-0.79263000
C	-4.01113500	-5.13907900	0.00091200
H	-4.33335900	-5.14619100	1.04810000
H	-4.89164600	-5.28753800	-0.62641400
H	-3.31221500	-5.96629800	-0.13719100
H	0.65122600	1.02869900	-1.97493300
H	-3.23108200	1.66313000	1.65216100
N	1.66277900	1.78072500	0.04410900
C	2.15745900	0.91380700	-0.79553900
H	2.28148500	2.04440000	0.80175200
C	3.47689700	0.29296900	-0.62791000
O	1.48641400	0.52871000	-1.85557000
C	4.00385800	-0.46908500	-1.68008400
C	4.19680200	0.41407600	0.56877300
C	5.23616700	-1.09372500	-1.53803900
H	3.44768000	-0.57159400	-2.60175800
C	5.43055200	-0.20975000	0.70197200
H	3.80124900	0.96204600	1.41505200
C	5.95180300	-0.96489200	-0.34841000
H	5.63681000	-1.68260100	-2.35449800
H	5.97830200	-0.11840400	1.63210300
H	6.91176900	-1.45589200	-0.23704500
IRC_TS1_point246			
B	-2.73160000	3.89378300	0.35847800
B	-1.63356400	3.74679200	1.75246800
B	-0.70014100	2.24908500	1.56563200
B	-2.47298700	2.49094400	-0.70311200
B	-1.21923500	1.53242500	0.05169100
B	-1.22020600	4.83247900	0.40645100
B	-1.73646300	4.06334700	-1.11171300
H	-3.79839400	4.41204400	0.44919400
B	0.03585000	3.81506300	1.14419600
H	-1.91933900	4.16069800	2.83073100
B	0.29000400	2.42595200	0.08376400
H	-0.31068000	1.59726400	2.47500400
B	-0.79886800	2.57318000	-1.31231500
H	-3.33382900	1.99334700	-1.35294100
H	-1.21773800	6.01494600	0.53836100
B	-0.02652500	4.02214900	-0.62790000

H	-2.10251800	4.68707800	-2.05550100
H	0.94229000	4.24807700	1.78158200
H	-0.52735500	2.13223600	-2.38713000
H	0.83174300	4.59532000	-1.21754300
B	-2.41382600	2.30455200	1.07745600
I	-1.44435200	-0.68901800	-0.23351000
C	0.35972800	-1.48378300	0.61787600
C	0.65132900	-1.22393200	1.94989800
C	1.16420800	-2.27994200	-0.18590300
C	1.81631200	-1.77150200	2.48707500
H	-0.00211300	-0.61207200	2.55495400
C	2.31887400	-2.82795200	0.37404200
H	0.91221300	-2.46369900	-1.22143700
C	2.64770800	-2.56984300	1.70246300
H	2.06671500	-1.57122300	3.52255700
H	2.96480200	-3.44314300	-0.24098300
H	3.55308100	-2.98804400	2.12630900
O	-2.11346700	-3.69807400	0.00685300
C	-3.33837900	-3.80670400	-0.29139100
O	-4.04532700	-2.88581900	-0.79391700
C	-4.01415200	-5.14205900	0.00354700
H	-4.33649200	-5.14562200	1.05078500
H	-4.89548800	-5.29064900	-0.62295800
H	-3.31711400	-5.97187500	-0.13230400
H	0.65443600	1.03306600	-1.97863700
H	-3.23346700	1.66832400	1.65498700
N	1.66114700	1.77707200	0.04352000
C	2.15646000	0.91291800	-0.79467800
H	2.27754900	2.03508800	0.80622200
C	3.47627100	0.29198900	-0.62765800
O	1.48915200	0.53124000	-1.85889400
C	4.00451500	-0.46886000	-1.68026100
C	4.19571500	0.41220100	0.56943000
C	5.23705100	-1.09314600	-1.53803800
H	3.44909300	-0.57091800	-2.60242800
C	5.42965400	-0.21117800	0.70282900
H	3.79978500	0.95924400	1.41616600
C	5.95195200	-0.96513400	-0.34786900
H	5.63850700	-1.68110300	-2.35477800
H	5.97676500	-0.12040300	1.63340200
H	6.91210000	-1.45577000	-0.23632900

IRC_TS1_point247

B	-2.73079000	3.89646600	0.35809000
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B	-1.63269400	3.74966400	1.75205600
B	-0.70123200	2.25054400	1.56684900
B	-2.47422700	2.49207300	-0.70187300
B	-1.22129600	1.53309500	0.05375900
B	-1.21816100	4.83334700	0.40474500
B	-1.73566000	4.06314300	-1.11249200
H	-3.79692300	4.41600200	0.44850600
B	0.03676000	3.81515800	1.14339200
H	-1.91779400	4.16499800	2.82989800
B	0.28870200	2.42451100	0.08450100
H	-0.31234900	1.59922800	2.47683600
B	-0.80006600	2.57163000	-1.31137100
H	-3.33562500	1.99478600	-1.35113700
H	-1.21445700	6.01588400	0.53558100
B	-0.02568500	4.02041400	-0.62896400
H	-2.10125300	4.68630800	-2.05678300
H	0.94368400	4.24783200	1.78030200
H	-0.52968100	2.12861600	-2.38562900
H	0.83314600	4.59193300	-1.21930800
B	-2.41501800	2.30751900	1.07893500
I	-1.44398600	-0.68781800	-0.23302500
C	0.36057300	-1.48208900	0.61794100
C	0.65253000	-1.22249800	1.94994200
C	1.16455900	-2.27835400	-0.18621400
C	1.81729500	-1.77083300	2.48678500
H	-0.00058600	-0.61052400	2.55521200
C	2.31897700	-2.82717600	0.37348300
H	0.91227400	-2.46184300	-1.22172500
C	2.64805600	-2.56962300	1.70192400
H	2.06795700	-1.57090300	3.52226500
H	2.96449600	-3.44256600	-0.24177100
H	3.55319700	-2.98848100	2.12560300
O	-2.11364700	-3.70417800	0.00304700
C	-3.33948300	-3.81133000	-0.29240800
O	-4.04585400	-2.89015800	-0.79519000
C	-4.01705100	-5.14496200	0.00627000
H	-4.33901600	-5.14521500	1.05357000
H	-4.89859000	-5.29370800	-0.61974500
H	-3.32111800	-5.97553300	-0.12778700
H	0.65720500	1.03682200	-1.98340100
H	-3.23517100	1.67281400	1.65716300
N	1.65860400	1.77310900	0.04672300
C	2.15675300	0.91214300	-0.79661600
H	2.27386400	2.02875500	0.80931800

C	3.47605000	0.29081800	-0.62758500
O	1.49115400	0.53482200	-1.86286600
C	4.00521600	-0.46886400	-1.68042900
C	4.19458500	0.41038100	0.57012800
C	5.23789500	-1.09273900	-1.53801300
H	3.45037300	-0.57025300	-2.60301300
C	5.42871700	-0.21263000	0.70370900
H	3.79837600	0.95701500	1.41699700
C	5.95200700	-0.96544100	-0.34731900
H	5.64001100	-1.67976800	-2.35507700
H	5.97534500	-0.12219600	1.63459000
H	6.91234500	-1.45565800	-0.23568600

IRC_TS1_point248

B	-2.72995000	3.89915900	0.35780900
B	-1.63175900	3.75256400	1.75173300
B	-0.70223400	2.25205600	1.56815400
B	-2.47552300	2.49326600	-0.70053200
B	-1.22360600	1.53372900	0.05605500
B	-1.21610500	4.83416300	0.40309300
B	-1.73488500	4.06294100	-1.11312900
H	-3.79538000	4.42027500	0.44779800
B	0.03771800	3.81524100	1.14265000
H	-1.91612500	4.16958800	2.82910800
B	0.28775200	2.42304300	0.08529900
H	-0.31400800	1.60126100	2.47878300
B	-0.80138200	2.57010700	-1.31031000
H	-3.33758700	1.99630800	-1.34915500
H	-1.21095100	6.01684700	0.53259400
B	-0.02487200	4.01856400	-0.62989300
H	-2.09989800	4.68546600	-2.05808400
H	0.94528800	4.24758600	1.77885300
H	-0.53222500	2.12510100	-2.38399500
H	0.83449100	4.58829700	-1.22112300
B	-2.41617900	2.31052100	1.08048700
I	-1.44365700	-0.68659100	-0.23252100
C	0.36144500	-1.48032200	0.61799300
C	0.65375800	-1.22103700	1.94996500
C	1.16490200	-2.27669100	-0.18656000
C	1.81832300	-1.77014900	2.48645100
H	0.00108900	-0.60881500	2.55549500
C	2.31906600	-2.82635400	0.37284400
H	0.91227400	-2.45982700	-1.22205000
C	2.64842300	-2.56937500	1.70130400

H	2.06933600	-1.57054200	3.52191100
H	2.96412800	-3.44196800	-0.24265600
H	3.55332800	-2.98892600	2.12479000
O	-2.11398200	-3.71059200	-0.00096300
C	-3.34051200	-3.81618900	-0.29359900
O	-4.04638100	-2.89469700	-0.79660600
C	-4.01999200	-5.14793800	0.00911200
H	-4.34185200	-5.14474900	1.05647000
H	-4.90185600	-5.29734300	-0.61624500
H	-3.32536800	-5.98012100	-0.12256800
H	0.66028900	1.04139400	-1.98726700
H	-3.23707800	1.67756600	1.65963300
N	1.65706000	1.76988700	0.04632700
C	2.15599400	0.91144700	-0.79613700
H	2.26972600	2.01946700	0.81539000
C	3.47542800	0.28979200	-0.62731000
O	1.49386900	0.53800000	-1.86650300
C	4.00581200	-0.46867300	-1.68057400
C	4.19340900	0.40844700	0.57084900
C	5.23870100	-1.09220300	-1.53798000
H	3.45169800	-0.56953400	-2.60364600
C	5.42772000	-0.21413400	0.70462600
H	3.79682000	0.95423200	1.41813400
C	5.95205400	-0.96573400	-0.34673800
H	5.64161400	-1.67830400	-2.35533700
H	5.97373500	-0.12424200	1.63592600
H	6.91257300	-1.45557900	-0.23494500

IRC_TS1_point249

B	-2.72907000	3.90181500	0.35747600
B	-1.63079000	3.75540600	1.75131900
B	-0.70319200	2.25353200	1.56929800
B	-2.47669900	2.49442200	-0.69927500
B	-1.22552500	1.53446000	0.05802000
B	-1.21403200	4.83503100	0.40141300
B	-1.73408900	4.06276600	-1.11385400
H	-3.79380300	4.42444800	0.44712500
B	0.03868800	3.81536200	1.14182500
H	-1.91436600	4.17410300	2.82830300
B	0.28664200	2.42172400	0.08598300
H	-0.31564600	1.60327900	2.48068300
B	-0.80255600	2.56870400	-1.30944900
H	-3.33950200	1.99782400	-1.34719800
H	-1.20747500	6.01786000	0.52968700
B	-0.02402500	4.01688300	-0.63095700

H	-2.09858900	4.68459500	-2.05946900
H	0.94687600	4.24724700	1.77746100
H	-0.53471100	2.12153600	-2.38267700
H	0.83604300	4.58474700	-1.22308800
B	-2.41721200	2.31343000	1.08193200
I	-1.44335600	-0.68545500	-0.23201100
C	0.36231700	-1.47859300	0.61803300
C	0.65498000	-1.21957500	1.94997400
C	1.16524900	-2.27509900	-0.18689800
C	1.81935900	-1.76940600	2.48610200
H	0.00270000	-0.60716800	2.55573000
C	2.31918500	-2.82553500	0.37223100
H	0.91229500	-2.45792800	-1.22236600
C	2.64882900	-2.56905600	1.70069400
H	2.07067100	-1.57013000	3.52154900
H	2.96381400	-3.44135500	-0.24351500
H	3.55351900	-2.98926400	2.12399000
O	-2.11418700	-3.71688600	-0.00489200
C	-3.34154600	-3.82100500	-0.29472900
O	-4.04687600	-2.89925300	-0.79801900
C	-4.02304200	-5.15091600	0.01200800
H	-4.34465700	-5.14396000	1.05943900
H	-4.90575000	-5.30010600	-0.61249000
H	-3.33023200	-5.98515700	-0.11776900
H	0.66259200	1.04517500	-1.99065500
H	-3.23894100	1.68236600	1.66215200
N	1.65474900	1.76602500	0.04921600
C	2.15616800	0.91090500	-0.79769300
H	2.26663000	2.01388800	0.81648400
C	3.47514300	0.28878000	-0.62731000
O	1.49598100	0.54169200	-1.87005200
C	4.00645900	-0.46859400	-1.68077500
C	4.19219000	0.40664300	0.57151900
C	5.23947800	-1.09175400	-1.53795000
H	3.45298800	-0.56879600	-2.60430100
C	5.42666400	-0.21561800	0.70553400
H	3.79524100	0.95201700	1.41888900
C	5.95203000	-0.96603000	-0.34616600
H	5.64310000	-1.67691600	-2.35561400
H	5.97211300	-0.12619500	1.63720900
H	6.91273100	-1.45547500	-0.23424800
IRC_TS1_point250			
B	-2.72816300	3.90442800	0.35722800

B	-1.62973900	3.75820100	1.75100400
B	-0.70400000	2.25498500	1.57045500
B	-2.47785400	2.49560300	-0.69800800
B	-1.22756700	1.53500700	0.06001400
B	-1.21196400	4.83586400	0.39982500
B	-1.73331100	4.06265200	-1.11446400
H	-3.79222200	4.42834900	0.44656400
B	0.03971900	3.81548900	1.14105900
H	-1.91261400	4.17829400	2.82752600
B	0.28578000	2.42037700	0.08664700
H	-0.31693400	1.60521700	2.48231500
B	-0.80375600	2.56734700	-1.30856700
H	-3.34121800	1.99933700	-1.34535700
H	-1.20410200	6.01876800	0.52691500
B	-0.02318400	4.01518600	-0.63190800
H	-2.09732500	4.68397100	-2.06056300
H	0.94847600	4.24710700	1.77602000
H	-0.53707600	2.11895700	-2.38143900
H	0.83725200	4.58147500	-1.22479900
B	-2.41817700	2.31635700	1.08340400
I	-1.44310000	-0.68435000	-0.23144900
C	0.36317400	-1.47684300	0.61809000
C	0.65620700	-1.21811800	1.95000300
C	1.16557900	-2.27348200	-0.18721800
C	1.82041300	-1.76867200	2.48576300
H	0.00433700	-0.60551600	2.55601100
C	2.31929700	-2.82470800	0.37160900
H	0.91227400	-2.45600700	-1.22265400
C	2.64924100	-2.56874400	1.70007400
H	2.07209900	-1.56966400	3.52117200
H	2.96349600	-3.44072900	-0.24438100
H	3.55373800	-2.98956200	2.12315700
O	-2.11457100	-3.72346500	-0.00894700
C	-3.34274400	-3.82594000	-0.29587200
O	-4.04745900	-2.90390400	-0.79957500
C	-4.02596900	-5.15392000	0.01506700
H	-4.34714000	-5.14357200	1.06256100
H	-4.90857100	-5.30422000	-0.60886600
H	-3.33391300	-5.98848300	-0.11223800
H	0.66490400	1.04904600	-1.99359600
H	-3.24025400	1.68666100	1.66417800
N	1.65332100	1.76325900	0.04908900
C	2.15565300	0.91042700	-0.79762800
H	2.26237500	2.00436900	0.82422400

C	3.47456200	0.28777200	-0.62701100
O	1.49844000	0.54558000	-1.87396500
C	4.00701400	-0.46839700	-1.68089600
C	4.19096300	0.40470800	0.57228900
C	5.24020700	-1.09125300	-1.53786400
H	3.45427300	-0.56798500	-2.60492100
C	5.42556900	-0.21719700	0.70652800
H	3.79363400	0.94920600	1.42009400
C	5.95196300	-0.96638800	-0.34551200
H	5.64461700	-1.67546800	-2.35582900
H	5.97036400	-0.12836600	1.63864000
H	6.91282600	-1.45548800	-0.23343200

IRC_TS1_point251

B	-2.72720600	3.90705100	0.35696600
B	-1.62866000	3.76097700	1.75058400
B	-0.70480200	2.25645900	1.57144700
B	-2.47894900	2.49681800	-0.69677300
B	-1.22929200	1.53588400	0.06177600
B	-1.20987000	4.83675100	0.39821000
B	-1.73251200	4.06257300	-1.11511800
H	-3.79054400	4.43270700	0.44594400
B	0.04075700	3.81565000	1.14019900
H	-1.91065100	4.18284800	2.82675400
B	0.28483700	2.41920400	0.08721900
H	-0.31840800	1.60722000	2.48407700
B	-0.80488700	2.56614500	-1.30778000
H	-3.34316800	2.00099600	-1.34337400
H	-1.20053800	6.01982600	0.52402400
B	-0.02232500	4.01364800	-0.63295200
H	-2.09597600	4.68316300	-2.06194900
H	0.95025700	4.24670500	1.77451500
H	-0.53954800	2.11571900	-2.38028000
H	0.83881500	4.57804500	-1.22680700
B	-2.41900700	2.31918200	1.08474100
I	-1.44287400	-0.68330400	-0.23091200
C	0.36406500	-1.47505700	0.61813200
C	0.65746900	-1.21659900	1.94999300
C	1.16591500	-2.27184400	-0.18757800
C	1.82151900	-1.76785400	2.48535400
H	0.00605200	-0.60376100	2.55625900
C	2.31942600	-2.82382200	0.37092900
H	0.91224200	-2.45404200	-1.22298200
C	2.64970000	-2.56833700	1.69938200

H	2.07356000	-1.56915500	3.52073600
H	2.96317200	-3.44004400	-0.24533000
H	3.55400100	-2.98980300	2.12224800
O	-2.11485900	-3.72994200	-0.01300100
C	-3.34372000	-3.83094800	-0.29714300
O	-4.04794000	-2.90869600	-0.80114500
C	-4.02910600	-5.15692500	0.01820700
H	-4.35032400	-5.14231000	1.06573900
H	-4.91285700	-5.30709800	-0.60466300
H	-3.33935000	-5.99474000	-0.10669900
H	0.66641200	1.05229300	-1.99580200
H	-3.24219300	1.69166300	1.66691000
N	1.65124600	1.75954300	0.05163200
C	2.15571100	0.91011900	-0.79869700
H	2.25945000	1.99910200	0.82418200
C	3.47423800	0.28699600	-0.62712500
O	1.50070800	0.54916400	-1.87700000
C	4.00760700	-0.46817900	-1.68116200
C	4.18965500	0.40296000	0.57290700
C	5.24090400	-1.09073700	-1.53784500
H	3.45556000	-0.56711100	-2.60566900
C	5.42436300	-0.21872600	0.70747000
H	3.79185300	0.94702400	1.42075200
C	5.95182400	-0.96669300	-0.34491400
H	5.64607100	-1.67401500	-2.35609100
H	5.96847500	-0.13054900	1.64004900
H	6.91282500	-1.45547400	-0.23264800
IRC_TS1_point252			
B	-2.72622600	3.90959500	0.35673200
B	-1.62749600	3.76363800	1.75027200
B	-0.70540600	2.25787000	1.57242900
B	-2.47993700	2.49805000	-0.69564100
B	-1.23116500	1.53638800	0.06353800
B	-1.20779900	4.83761800	0.39671500
B	-1.73170500	4.06259700	-1.11571500
H	-3.78894600	4.43625600	0.44551800
B	0.04186000	3.81583500	1.13942500
H	-1.90884900	4.18661000	2.82603300
B	0.28410000	2.41803800	0.08776800
H	-0.31935500	1.60901000	2.48538400
B	-0.80592600	2.56498800	-1.30711000
H	-3.34462300	2.00255300	-1.34175500
H	-1.19734200	6.02072500	0.52155400
B	-0.02143100	4.01215600	-0.63392800

H	-2.09479200	4.68278600	-2.06289100
H	0.95183800	4.24661800	1.77316400
H	-0.54164700	2.11347800	-2.37930900
H	0.84001800	4.57518900	-1.22843700
B	-2.41978700	2.32202800	1.08610100
I	-1.44267900	-0.68231700	-0.23028600
C	0.36489600	-1.47331400	0.61821200
C	0.65870700	-1.21513700	1.95004200
C	1.16623500	-2.27025600	-0.18785600
C	1.82261100	-1.76705900	2.48501800
H	0.00763500	-0.60219700	2.55656400
C	2.31956800	-2.82296800	0.37033000
H	0.91218400	-2.45224300	-1.22320500
C	2.65016800	-2.56794900	1.69876800
H	2.07501000	-1.56861700	3.52036000
H	2.96289400	-3.43939000	-0.24616900
H	3.55430800	-2.98996100	2.12141200
O	-2.11521500	-3.73671500	-0.01717400
C	-3.34502800	-3.83599700	-0.29824700
O	-4.04855600	-2.91352200	-0.80285600
C	-4.03212400	-5.15997700	0.02148700
H	-4.35261500	-5.14180400	1.06907800
H	-4.91579100	-5.31111200	-0.60082400
H	-3.34297800	-5.99749800	-0.10112200
H	0.66805300	1.05549100	-1.99802600
H	-3.24305900	1.69558400	1.66858100
N	1.64987400	1.75712100	0.05184700
C	2.15541100	0.90988000	-0.79912300
H	2.25542500	1.99025000	0.83181600
C	3.47372800	0.28607800	-0.62685800
O	1.50278700	0.55351000	-1.88097000
C	4.00814700	-0.46794500	-1.68128000
C	4.18840200	0.40111800	0.57368200
C	5.24155400	-1.09027700	-1.53769900
H	3.45681800	-0.56622000	-2.60628900
C	5.42315400	-0.22037300	0.70854500
H	3.79031200	0.94456300	1.42182200
C	5.95161500	-0.96715200	-0.34416200
H	5.64745100	-1.67265400	-2.35623200
H	5.96662000	-0.13275900	1.64154100
H	6.91273500	-1.45565400	-0.23172700

IRC_TS1_point253

B	-2.72520000	3.91217300	0.35653000
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B	-1.62631600	3.76632800	1.74986400
B	-0.70603200	2.25933600	1.57326100
B	-2.48091500	2.49933300	-0.69448400
B	-1.23269900	1.53737400	0.06507800
B	-1.20570000	4.83854300	0.39519300
B	-1.73089400	4.06266000	-1.11630900
H	-3.78728700	4.44041100	0.44500300
B	0.04296900	3.81605900	1.13854200
H	-1.90683100	4.19085200	2.82534100
B	0.28329500	2.41701600	0.08819800
H	-0.32051500	1.61090100	2.48684000
B	-0.80698500	2.56399000	-1.30640900
H	-3.34638700	2.00426100	-1.33993100
H	-1.19390000	6.02180100	0.51889200
B	-0.02055100	4.01080600	-0.63495400
H	-2.09350300	4.68222800	-2.06411900
H	0.95367000	4.24629400	1.77165900
H	-0.54406700	2.11094900	-2.37835300
H	0.84145900	4.57218000	-1.23032700
B	-2.42041800	2.32478400	1.08731300
I	-1.44253000	-0.68133500	-0.22967400
C	0.36576800	-1.47150000	0.61829400
C	0.65999600	-1.21355300	1.95004800
C	1.16653800	-2.26858400	-0.18819400
C	1.82378100	-1.76614600	2.48458900
H	0.00934900	-0.60044200	2.55686800
C	2.31970000	-2.82201000	0.36962800
H	0.91205500	-2.45032300	-1.22347900
C	2.65067800	-2.56743800	1.69803800
H	2.07653900	-1.56802800	3.51990800
H	2.96254600	-3.43867200	-0.24712400
H	3.55462700	-2.99009100	2.12046200
O	-2.11560900	-3.74346600	-0.02144600
C	-3.34605800	-3.84122900	-0.29960100
O	-4.04910300	-2.91861900	-0.80462500
C	-4.03524400	-5.16302500	0.02489900
H	-4.35574900	-5.14059100	1.07248600
H	-4.91974600	-5.31452300	-0.59643400
H	-3.34814600	-6.00361500	-0.09505000
H	0.66925600	1.05841500	-1.99976200
H	-3.24470400	1.70026700	1.67107000
N	1.64807900	1.75376500	0.05383400
C	2.15538800	0.90977100	-0.79978700
H	2.25244100	1.98470000	0.83250500

C	3.47335900	0.28549600	-0.62702900
O	1.50523000	0.55700000	-1.88384800
C	4.00867000	-0.46761900	-1.68158400
C	4.18704300	0.39944000	0.57425200
C	5.24213100	-1.08977500	-1.53765800
H	3.45802900	-0.56526800	-2.60706200
C	5.42180500	-0.22197400	0.70952100
H	3.78850300	0.94250900	1.42242700
C	5.95131200	-0.96756900	-0.34350400
H	5.64876500	-1.67131000	-2.35641700
H	5.96457000	-0.13504900	1.64300200
H	6.91250700	-1.45587200	-0.23082000

IRC_TS1_point254

B	-2.72414900	3.91466900	0.35630200
B	-1.62505700	3.76887300	1.74953200
B	-0.70644800	2.26073700	1.57405300
B	-2.48174100	2.50065200	-0.69349200
B	-1.23439000	1.53795500	0.06662000
B	-1.20363500	4.83945700	0.39379100
B	-1.73004800	4.06283600	-1.11689000
H	-3.78567700	4.44383700	0.44465000
B	0.04413800	3.81631100	1.13774300
H	-1.90497200	4.19435000	2.82468200
B	0.28269200	2.41605600	0.08861600
H	-0.32123500	1.61258500	2.48790200
B	-0.80786200	2.56308600	-1.30592500
H	-3.34768900	2.00591200	-1.33847200
H	-1.19082000	6.02274500	0.51665200
B	-0.01961600	4.00954500	-0.63593800
H	-2.09234500	4.68203400	-2.06501500
H	0.95530600	4.24620800	1.77035100
H	-0.54586200	2.10891400	-2.37758500
H	0.84271600	4.56966500	-1.23193200
B	-2.42100500	2.32753900	1.08851400
I	-1.44239800	-0.68042200	-0.22896400
C	0.36655300	-1.46977800	0.61842500
C	0.66124300	-1.21205800	1.95012500
C	1.16682600	-2.26701000	-0.18842100
C	1.82492500	-1.76525000	2.48425100
H	0.01091800	-0.59887800	2.55720800
C	2.31985700	-2.82109800	0.36904600
H	0.91192100	-2.44861000	-1.22363100
C	2.65120400	-2.56693200	1.69741800

H	2.07803700	-1.56737100	3.51952300
H	2.96227300	-3.43796100	-0.24794900
H	3.55501700	-2.99008300	2.11960400
O	-2.11591100	-3.75045300	-0.02587000
C	-3.34735400	-3.84649700	-0.30077800
O	-4.04974700	-2.92375600	-0.80651000
C	-4.03833300	-5.16619400	0.02841000
H	-4.35802200	-5.13984400	1.07608700
H	-4.92320800	-5.31826900	-0.59214300
H	-3.35216800	-6.00706000	-0.08940700
H	0.67053300	1.06143400	-2.00167800
H	-3.24542400	1.70404400	1.67263500
N	1.64674100	1.75150700	0.05434500
C	2.15524200	0.90976000	-0.80057200
H	2.24895300	1.97721500	0.83830100
C	3.47291700	0.28472000	-0.62687400
O	1.50702900	0.56148100	-1.88751700
C	4.00918700	-0.46735500	-1.68173300
C	4.18577000	0.39773700	0.57496900
C	5.24266800	-1.08940700	-1.53746700
H	3.45925800	-0.56433300	-2.60771400
C	5.42047900	-0.22367100	0.71063300
H	3.78698900	0.94047300	1.42325900
C	5.95093300	-0.96817500	-0.34267100
H	5.64997500	-1.67012200	-2.35647800
H	5.96261100	-0.13729600	1.64451700
H	6.91218700	-1.45630600	-0.22978600

IRC_TS1_point255

B	-2.72307300	3.91719300	0.35613800
B	-1.62380200	3.77145500	1.74914400
B	-0.70690200	2.26217200	1.57473400
B	-2.48257200	2.50199000	-0.69245100
B	-1.23570500	1.53896400	0.06792100
B	-1.20155700	4.84043400	0.39238300
B	-1.72921800	4.06306300	-1.11744200
H	-3.78401200	4.44776700	0.44422900
B	0.04529800	3.81660400	1.13686600
H	-1.90291100	4.19830700	2.82404600
B	0.28201000	2.41521600	0.08891200
H	-0.32213400	1.61440200	2.48911300
B	-0.80880100	2.56229700	-1.30532700
H	-3.34925400	2.00769200	-1.33682200
H	-1.18747800	6.02385400	0.51421600

B	-0.01871300	4.00842200	-0.63693700
H	-2.09109600	4.68174100	-2.06609700
H	0.95715300	4.24597200	1.76887900
H	-0.54812400	2.10687400	-2.37679400
H	0.84409700	4.56702500	-1.23372300
B	-2.42146500	2.33022100	1.08960300
I	-1.44232800	-0.67951500	-0.22825600
C	0.36734700	-1.46803000	0.61858300
C	0.66252400	-1.21045300	1.95017500
C	1.16706900	-2.26536500	-0.18870000
C	1.82614200	-1.76423800	2.48383100
H	0.01262200	-0.59710800	2.55756000
C	2.31999200	-2.82007800	0.36836100
H	0.91169500	-2.44676300	-1.22382900
C	2.65176500	-2.56630300	1.69668300
H	2.07966600	-1.56661900	3.51905700
H	2.96194000	-3.43715800	-0.24889800
H	3.55543400	-2.99002600	2.11861600
O	-2.11634500	-3.75740400	-0.03041100
C	-3.34846400	-3.85193300	-0.30219800
O	-4.05037900	-2.92914900	-0.80849200
C	-4.04141800	-5.16933000	0.03208800
H	-4.36086300	-5.13872200	1.07974800
H	-4.92684900	-5.32215000	-0.58746200
H	-3.35699900	-6.01254500	-0.08293400
H	0.67186600	1.06433600	-2.00335100
H	-3.24670900	1.70841000	1.67479700
N	1.64519900	1.74865200	0.05583900
C	2.15522500	0.90982600	-0.80107700
H	2.24606000	1.97158500	0.84004000
C	3.47254700	0.28430600	-0.62706500
O	1.50955000	0.56495500	-1.89042900
C	4.00964500	-0.46695100	-1.68204900
C	4.18441400	0.39619600	0.57549000
C	5.24310200	-1.08898300	-1.53737400
H	3.46040900	-0.56327000	-2.60850100
C	5.41902200	-0.22531200	0.71164000
H	3.78521200	0.93861300	1.42380500
C	5.95044600	-0.96875000	-0.34192800
H	5.65111800	-1.66893200	-2.35657200
H	5.96041800	-0.13968500	1.64603400
H	6.91169600	-1.45682200	-0.22873100
IRC_TS1_point256			
B	-2.72196200	3.91963700	0.35590900

B	-1.62247400	3.77389100	1.74878900
B	-0.70714900	2.26356200	1.57535900
B	-2.48325300	2.50338100	-0.69159500
B	-1.23722400	1.53961400	0.06926500
B	-1.19950600	4.84138600	0.39106500
B	-1.72833800	4.06337900	-1.11800600
H	-3.78235200	4.45116600	0.44391600
B	0.04651400	3.81692600	1.13605200
H	-1.90098500	4.20164300	2.82339500
B	0.28156300	2.41445100	0.08921800
H	-0.32267000	1.61603300	2.48997800
B	-0.80953200	2.56161200	-1.30499100
H	-3.35044100	2.00944000	-1.33548600
H	-1.18443300	6.02483000	0.51210400
B	-0.01774900	4.00736800	-0.63791600
H	-2.08991500	4.68171300	-2.06696300
H	0.95886100	4.24590800	1.76755900
H	-0.54969600	2.10506400	-2.37614800
H	0.84537600	4.56475300	-1.23530000
B	-2.42186400	2.33287800	1.09063300
I	-1.44226600	-0.67868000	-0.22747800
C	0.36804900	-1.46639300	0.61877600
C	0.66376100	-1.20895100	1.95028300
C	1.16729900	-2.26384300	-0.18887300
C	1.82734000	-1.76323500	2.48348600
H	0.01421800	-0.59550400	2.55793500
C	2.32016000	-2.81910700	0.36779000
H	0.91147600	-2.44511900	-1.22391500
C	2.65235500	-2.56566700	1.69604700
H	2.08127700	-1.56578000	3.51863500
H	2.96169200	-3.43635200	-0.24973400
H	3.55594100	-2.98981100	2.11770400
O	-2.11660400	-3.76446700	-0.03508900
C	-3.34968000	-3.85737800	-0.30351200
O	-4.05106400	-2.93458300	-0.81057000
C	-4.04446000	-5.17255000	0.03586200
H	-4.36301700	-5.13758400	1.08365900
H	-4.93067400	-5.32588000	-0.58256900
H	-3.36136600	-6.01681100	-0.07688300
H	0.67302500	1.06766500	-2.00531900
H	-3.24731600	1.71213000	1.67628000
N	1.64399600	1.74658800	0.05648500
C	2.15514100	0.91002700	-0.80199300
H	2.24304900	1.96516000	0.84444200

C	3.47214000	0.28368700	-0.62702400
O	1.51108700	0.56946000	-1.89371700
C	4.01013800	-0.46664000	-1.68223700
C	4.18313600	0.39464700	0.57612900
C	5.24352800	-1.08871100	-1.53713900
H	3.46165400	-0.56225400	-2.60922000
C	5.41760300	-0.22702200	0.71276500
H	3.78365700	0.93682600	1.42446900
C	5.94990700	-0.96950400	-0.34102200
H	5.65220000	-1.66790100	-2.35654800
H	5.95831200	-0.14202400	1.64759800
H	6.91112900	-1.45755600	-0.22754400
IRC_TS1_point257			
B	-2.72084500	3.92210500	0.35576800
B	-1.62116900	3.77638200	1.74841400
B	-0.70746700	2.26496500	1.57591800
B	-2.48393800	2.50474300	-0.69065200
B	-1.23829100	1.54062900	0.07034500
B	-1.19745400	4.84241300	0.38975000
B	-1.72748800	4.06373700	-1.11852800
H	-3.78066300	4.45495600	0.44354100
B	0.04770600	3.81728100	1.13518700
H	-1.89886800	4.20546400	2.82278600
B	0.28097800	2.41377300	0.08941100
H	-0.32340100	1.61782100	2.49105500
B	-0.81034500	2.56101500	-1.30447300
H	-3.35185800	2.01127200	-1.33395000
H	-1.18113900	6.02598200	0.50980900
B	-0.01683000	4.00645500	-0.63888900
H	-2.08868800	4.68159600	-2.06796400
H	0.96072700	4.24573800	1.76610800
H	-0.55190400	2.10330600	-2.37551000
H	0.84677500	4.56233400	-1.23706500
B	-2.42217900	2.33547700	1.09161900
I	-1.44228200	-0.67786700	-0.22669800
C	0.36873700	-1.46478300	0.61901000
C	0.66501000	-1.20736200	1.95037100
C	1.16746200	-2.26227600	-0.18909600
C	1.82860000	-1.76212300	2.48306200
H	0.01591200	-0.59371800	2.55831300
C	2.32029900	-2.81803700	0.36711500
H	0.91114100	-2.44337900	-1.22404400
C	2.65297300	-2.56490900	1.69529400
H	2.08302500	-1.56482900	3.51812700

H	2.96138700	-3.43545000	-0.25069800
H	3.55648400	-2.98952500	2.11664800
O	-2.11702200	-3.77143400	-0.03988600
C	-3.35084500	-3.86293100	-0.30498700
O	-4.05178900	-2.94022100	-0.81277800
C	-4.04745000	-5.17574000	0.03983500
H	-4.36557800	-5.13642600	1.08757000
H	-4.93408400	-5.33009200	-0.57754600
H	-3.36589000	-6.02174800	-0.06994500
H	0.67468400	1.07078300	-2.00696800
H	-3.24838200	1.71633800	1.67826300
N	1.64264500	1.74418500	0.05769400
C	2.15521200	0.91027800	-0.80245700
H	2.24028200	1.95968300	0.84669800
C	3.47181400	0.28345500	-0.62723900
O	1.51365100	0.57284800	-1.89658200
C	4.01055100	-0.46613800	-1.68256700
C	4.18180900	0.39326500	0.57660600
C	5.24382500	-1.08835300	-1.53699800
H	3.46275900	-0.56102300	-2.61002200
C	5.41606900	-0.22867300	0.71379500
H	3.78192400	0.93516900	1.42494800
C	5.94925000	-0.97021800	-0.34020300
H	5.65317300	-1.66684800	-2.35655800
H	5.95600900	-0.14449700	1.64916000
H	6.91038500	-1.45836500	-0.22635700
IRC_TS1_point258			
B	-2.71968700	3.92448400	0.35552500
B	-1.61978900	3.77871300	1.74803900
B	-0.70755500	2.26633900	1.57641100
B	-2.48448100	2.50617500	-0.68992500
B	-1.23967400	1.54129400	0.07153700
B	-1.19542500	4.84338400	0.38849900
B	-1.72657300	4.06415500	-1.11908500
H	-3.77897800	4.45823900	0.44325600
B	0.04895800	3.81766300	1.13436900
H	-1.89693100	4.20856400	2.82213000
B	0.28070500	2.41317500	0.08963300
H	-0.32373800	1.61938000	2.49171200
B	-0.81093200	2.56049000	-1.30427700
H	-3.35288500	2.01305400	-1.33275700
H	-1.17816300	6.02695900	0.50781900
B	-0.01583400	4.00555800	-0.63985500
H	-2.08748500	4.68171600	-2.06878500

H	0.96246500	4.24572200	1.76479700
H	-0.55314300	2.10182700	-2.37495900
H	0.84801900	4.56032300	-1.23855600
B	-2.42241200	2.33804100	1.09249400
I	-1.44229300	-0.67711400	-0.22586700
C	0.36934700	-1.46327600	0.61924800
C	0.66621700	-1.20589200	1.95049500
C	1.16762500	-2.26085800	-0.18922000
C	1.82984700	-1.76102400	2.48270000
H	0.01749100	-0.59213600	2.55870600
C	2.32048300	-2.81703200	0.36655400
H	0.91082100	-2.44189200	-1.22406100
C	2.65363500	-2.56414200	1.69463600
H	2.08474400	-1.56380300	3.51765700
H	2.96118100	-3.43457200	-0.25153400
H	3.55713400	-2.98906600	2.11567500
O	-2.11725400	-3.77845400	-0.04477300
C	-3.35194000	-3.86848600	-0.30644700
O	-4.05253000	-2.94592500	-0.81507700
C	-4.05037500	-5.17894100	0.04389800
H	-4.36755900	-5.13474700	1.09181800
H	-4.93807600	-5.33390000	-0.57205800
H	-3.37044500	-6.02664700	-0.06334400
H	0.67575200	1.07457900	-2.00904100
H	-3.24878200	1.71988800	1.67955400
N	1.64166900	1.74241000	0.05833000
C	2.15515900	0.91067900	-0.80339200
H	2.23765000	1.95404500	0.85028900
C	3.47142600	0.28296100	-0.62726200
O	1.51482500	0.57743200	-1.89949600
C	4.01102600	-0.46577900	-1.68277800
C	4.18055900	0.39186600	0.57718400
C	5.24415700	-1.08817000	-1.53671600
H	3.46402400	-0.55992600	-2.61079000
C	5.41459400	-0.23038200	0.71493300
H	3.78039600	0.93365800	1.42546100
C	5.94857600	-0.97111600	-0.33922700
H	5.65413400	-1.66597600	-2.35645000
H	5.95381900	-0.14688100	1.65075500
H	6.90959600	-1.45939700	-0.22502700

IRC_TS1_point259

B	-2.71854300	3.92688200	0.35539700
B	-1.61846300	3.78112600	1.74766200

B	-0.70777400	2.26771300	1.57686800
B	-2.48502700	2.50752600	-0.68905300
B	-1.24046200	1.54233200	0.07241000
B	-1.19341500	4.84445300	0.38725600
B	-1.72571100	4.06460400	-1.11958000
H	-3.77728800	4.46191800	0.44289100
B	0.05015500	3.81807900	1.13351400
H	-1.89477000	4.21233900	2.82155300
B	0.28017800	2.41264600	0.08974600
H	-0.32435600	1.62117200	2.49273300
B	-0.81163000	2.56006800	-1.30379000
H	-3.35418100	2.01490200	-1.33130300
H	-1.17493000	6.02815900	0.50562700
B	-0.01491800	4.00484200	-0.64079900
H	-2.08628500	4.68169300	-2.06975200
H	0.96433500	4.24560400	1.76336800
H	-0.55538800	2.10022500	-2.37447100
H	0.84948100	4.55805200	-1.24034000
B	-2.42259500	2.34053800	1.09338800
I	-1.44240400	-0.67639000	-0.22503400
C	0.36993600	-1.46181700	0.61953300
C	0.66742500	-1.20433200	1.95059600
C	1.16770200	-2.25939900	-0.18940800
C	1.83114500	-1.75981200	2.48225100
H	0.01915700	-0.59035000	2.55908200
C	2.32062300	-2.81592700	0.36587300
H	0.91036300	-2.44030500	-1.22413800
C	2.65431300	-2.56324700	1.69384300
H	2.08659600	-1.56265200	3.51708700
H	2.96089800	-3.43359800	-0.25251800
H	3.55781200	-2.98853000	2.11453300
O	-2.11765300	-3.78537000	-0.04980500
C	-3.35320200	-3.87407900	-0.30792900
O	-4.05336000	-2.95174800	-0.81751700
C	-4.05320600	-5.18212600	0.04817600
H	-4.36976200	-5.13366300	1.09594700
H	-4.94121800	-5.33838200	-0.56670900
H	-3.37452400	-6.03090200	-0.05603200
H	0.67773500	1.07779500	-2.01052500
H	-3.24975700	1.72402000	1.68149200
N	1.64044300	1.74036000	0.05943900
C	2.15537100	0.91111800	-0.80383600
H	2.23494100	1.94867800	0.85288700
C	3.47118700	0.28295100	-0.62751600

O	1.51755800	0.58059800	-1.90225100
C	4.01139900	-0.46516300	-1.68312100
C	4.17929100	0.39066600	0.57761300
C	5.24432200	-1.08786200	-1.53654200
H	3.46506300	-0.55852000	-2.61158800
C	5.41301800	-0.23201800	0.71596400
H	3.77875500	0.93221900	1.42588900
C	5.94777300	-0.97194100	-0.33836300
H	5.65492200	-1.66506000	-2.35638800
H	5.95145400	-0.14941400	1.65233500
H	6.90862200	-1.46047300	-0.22374700
IRC_TS1_point260			
B	-2.71735900	3.92916400	0.35512400
B	-1.61705800	3.78332800	1.74727800
B	-0.70770100	2.26905900	1.57725200
B	-2.48543000	2.50897200	-0.68847100
B	-1.24176800	1.54296600	0.07350200
B	-1.19143300	4.84541500	0.38607800
B	-1.72476000	4.06509300	-1.12013700
H	-3.77561800	4.46496900	0.44263100
B	0.05142800	3.81851500	1.13272000
H	-1.89290500	4.21507200	2.82089300
B	0.28011300	2.41219700	0.08992000
H	-0.32446300	1.62262000	2.49314800
B	-0.81205000	2.55965900	-1.30374200
H	-3.35499000	2.01666000	-1.33030300
H	-1.17210100	6.02910300	0.50379700
B	-0.01388400	4.00407100	-0.64173400
H	-2.08506100	4.68196200	-2.07049900
H	0.96604600	4.24567400	1.76211700
H	-0.55611100	2.09921600	-2.37399500
H	0.85061100	4.55639400	-1.24164800
B	-2.42268500	2.34300100	1.09411800
I	-1.44248300	-0.67570300	-0.22416400
C	0.37045400	-1.46046200	0.61978200
C	0.66858800	-1.20292900	1.95071100
C	1.16780200	-2.25813100	-0.18949200
C	1.83242300	-1.75863900	2.48186200
H	0.02067800	-0.58884500	2.55946000
C	2.32082800	-2.81492500	0.36532700
H	0.90994900	-2.43905800	-1.22409000
C	2.65504800	-2.56236400	1.69316700
H	2.08838900	-1.56144600	3.51656000
H	2.96074700	-3.43269000	-0.25333500

H	3.55861700	-2.98781100	2.11350600
O	-2.11788900	-3.79229800	-0.05481400
C	-3.35411400	-3.87969200	-0.30957000
O	-4.05413200	-2.95767000	-0.82004200
C	-4.05597400	-5.18525300	0.05252600
H	-4.37165900	-5.13116000	1.10055000
H	-4.94525200	-5.34231000	-0.56066700
H	-3.37918200	-6.03645000	-0.04867400
H	0.67856000	1.08195000	-2.01271400
H	-3.24984000	1.72723400	1.68244400
N	1.63974600	1.73890900	0.05995400
C	2.15529600	0.91167800	-0.80472300
H	2.23267800	1.94378400	0.85579700
C	3.47079800	0.28252000	-0.62754400
O	1.51822800	0.58538500	-1.90482100
C	4.01185400	-0.46479000	-1.68332000
C	4.17811100	0.38942000	0.57814500
C	5.24457400	-1.08778100	-1.53620700
H	3.46633300	-0.55739200	-2.61236600
C	5.41154200	-0.23371000	0.71710900
H	3.77734600	0.93108100	1.42622400
C	5.94699700	-0.97298700	-0.33732100
H	5.65575800	-1.66435800	-2.35620200
H	5.94926700	-0.15177900	1.65392700
H	6.90764800	-1.46180000	-0.22230100
IRC_TS1_point261			
B	-2.71621200	3.93146300	0.35501000
B	-1.61575300	3.78565000	1.74690200
B	-0.70786400	2.27039700	1.57762600
B	-2.48584300	2.51028400	-0.68765500
B	-1.24225700	1.54405700	0.07417200
B	-1.18949900	4.84651400	0.38491400
B	-1.72390000	4.06560800	-1.12059500
H	-3.77394800	4.46856800	0.44224900
B	0.05259200	3.81898200	1.13189500
H	-1.89072800	4.21886000	2.82035900
B	0.27958300	2.41181300	0.08997100
H	-0.32501600	1.62442700	2.49416700
B	-0.81264100	2.55941700	-1.30323800
H	-3.35618500	2.01851000	-1.32892400
H	-1.16895700	6.03034400	0.50170400
B	-0.01299800	4.00355900	-0.64262300
H	-2.08388400	4.68198400	-2.07145600
H	0.96789800	4.24558400	1.76073100

H	-0.55846300	2.09762800	-2.37363500
H	0.85218600	4.55421500	-1.24347100
B	-2.42275600	2.34536300	1.09492000
I	-1.44268800	-0.67506300	-0.22330300
C	0.37096800	-1.45913900	0.62008600
C	0.66975100	-1.20140300	1.95079700
C	1.16780000	-2.25679300	-0.18966800
C	1.83374900	-1.75733800	2.48136900
H	0.02231200	-0.58706200	2.55980600
C	2.32096500	-2.81380600	0.36463000
H	0.90937400	-2.43764600	-1.22413700
C	2.65578100	-2.56133900	1.69232200
H	2.09032700	-1.56011100	3.51591400
H	2.96047800	-3.43167800	-0.25433900
H	3.55942500	-2.98703000	2.11227200
O	-2.11825600	-3.79914600	-0.06005500
C	-3.35556100	-3.88525400	-0.31096700
O	-4.05505000	-2.96357700	-0.82268400
C	-4.05866300	-5.18837100	0.05710000
H	-4.37333800	-5.13036200	1.10484900
H	-4.94825500	-5.34693800	-0.55493000
H	-3.38279200	-6.03978200	-0.04125600
H	0.68081100	1.08498400	-2.01381200
H	-3.25086500	1.73136000	1.68445300
N	1.63854900	1.73710900	0.06111200
C	2.15569600	0.91230600	-0.80520800
H	2.22990600	1.93831500	0.85890300
C	3.47069100	0.28278700	-0.62787400
O	1.52132300	0.58817300	-1.90743700
C	4.01219400	-0.46406300	-1.68367600
C	4.17693300	0.38843600	0.57851100
C	5.24461400	-1.08751900	-1.53600400
H	3.46729700	-0.55585300	-2.61314100
C	5.40995500	-0.23529700	0.71811800
H	3.77584100	0.92985000	1.42663100
C	5.94607800	-0.97388900	-0.33643300
H	5.65635300	-1.66360500	-2.35605500
H	5.94686700	-0.15434200	1.65550700
H	6.90647000	-1.46311700	-0.22094300

IRC_TS1_point262

B	-2.71503100	3.93364200	0.35471100
B	-1.61435500	3.78772500	1.74652800
B	-0.70766100	2.27170700	1.57793700

B	-2.48613000	2.51172600	-0.68721000
B	-1.24354400	1.54462700	0.07520900
B	-1.18758300	4.84745200	0.38381600
B	-1.72291700	4.06614800	-1.12114600
H	-3.77231700	4.47136500	0.44200800
B	0.05387000	3.81945800	1.13114500
H	-1.88896400	4.22124300	2.81970100
B	0.27973400	2.41146600	0.09013200
H	-0.32494100	1.62577200	2.49439300
B	-0.81291200	2.55907800	-1.30332900
H	-3.35678900	2.02022300	-1.32811200
H	-1.16629100	6.03124800	0.50004200
B	-0.01191900	4.00287800	-0.64351100
H	-2.08264300	4.68239200	-2.07211300
H	0.96953500	4.24575200	1.75957300
H	-0.55871600	2.09711000	-2.37323200
H	0.85316100	4.55293100	-1.24454000
B	-2.42275300	2.34773000	1.09553800
I	-1.44281900	-0.67442600	-0.22241700
C	0.37141100	-1.45792300	0.62031600
C	0.67087100	-1.20007400	1.95088200
C	1.16784000	-2.25568600	-0.18973300
C	1.83504800	-1.75611200	2.48094200
H	0.02378200	-0.58562500	2.56013500
C	2.32118400	-2.81283500	0.36408800
H	0.90886800	-2.43664500	-1.22404500
C	2.65657800	-2.56037100	1.69161700
H	2.09218800	-1.55873300	3.51531000
H	2.96037600	-3.43076400	-0.25515400
H	3.56037800	-2.98607400	2.11117800
O	-2.11859100	-3.80591600	-0.06505800
C	-3.35624900	-3.89086100	-0.31283200
O	-4.05583600	-2.96964700	-0.82542400
C	-4.06119800	-5.19137000	0.06170500
H	-4.37536100	-5.12683600	1.10975900
H	-4.95194600	-5.35116900	-0.54857100
H	-3.38731300	-6.04587700	-0.03278400
H	0.68139400	1.08932700	-2.01624500
H	-3.25062700	1.73420900	1.68503800
N	1.63813400	1.73590200	0.06145800
C	2.15554900	0.91292500	-0.80589400
H	2.22802500	1.93422700	0.86094700
C	3.47028400	0.28236200	-0.62782500
O	1.52149200	0.59321000	-1.90977900

C	4.01261600	-0.46369400	-1.68383200
C	4.17587200	0.38735400	0.57901600
C	5.24478800	-1.08753700	-1.53562200
H	3.46852700	-0.55469900	-2.61388300
C	5.40853100	-0.23695000	0.71925700
H	3.77461800	0.92916000	1.42676400
C	5.94522300	-0.97507700	-0.33534300
H	5.65704600	-1.66306200	-2.35581800
H	5.94475900	-0.15665800	1.65706800
H	6.90533400	-1.46473300	-0.21942400

IRC_TS1_point263

B	-2.71390000	3.93580200	0.35458900
B	-1.61310700	3.78989100	1.74615900
B	-0.70777400	2.27298300	1.57823500
B	-2.48640900	2.51300200	-0.68649000
B	-1.24381000	1.54576600	0.07571500
B	-1.18575500	4.84853500	0.38276000
B	-1.72205700	4.06671200	-1.12156400
H	-3.77070400	4.47476600	0.44161300
B	0.05497200	3.81995000	1.13039900
H	-1.88691700	4.22479300	2.81921000
B	0.27919600	2.41123000	0.09014800
H	-0.32539800	1.62747300	2.49530300
B	-0.81336400	2.55901200	-1.30282500
H	-3.35780800	2.02203100	-1.32689600
H	-1.16334200	6.03245500	0.49813400
B	-0.01107900	4.00255000	-0.64430000
H	-2.08146900	4.68248700	-2.07302600
H	0.97130600	4.24567900	1.75831400
H	-0.56082700	2.09557600	-2.37290200
H	0.85480100	4.55091700	-1.24627800
B	-2.42272300	2.34992500	1.09621100
I	-1.44309300	-0.67384700	-0.22154900
C	0.37188500	-1.45669600	0.62060900
C	0.67199900	-1.19858500	1.95093700
C	1.16778700	-2.25447400	-0.18990200
C	1.83638800	-1.75474800	2.48040900
H	0.02535600	-0.58390900	2.56044700
C	2.32132500	-2.81173400	0.36339200
H	0.90821200	-2.43546100	-1.22405600
C	2.65736100	-2.55924700	1.69074000
H	2.09415000	-1.55729100	3.51461600
H	2.96011800	-3.42979700	-0.25612500

H	3.56128700	-2.98510600	2.10990300
O	-2.11881100	-3.81277700	-0.07052200
C	-3.35785800	-3.89637300	-0.31409900
O	-4.05677800	-2.97556500	-0.82821600
C	-4.06393200	-5.19435600	0.06657400
H	-4.37667400	-5.12601500	1.11422600
H	-4.95536800	-5.35554500	-0.54227900
H	-3.39096800	-6.04867000	-0.02540900
H	0.68360200	1.09217300	-2.01674200
H	-3.25163500	1.73814700	1.68695300
N	1.63694800	1.73439900	0.06265000
C	2.15613400	0.91380000	-0.80663400
H	2.22518100	1.92864100	0.86472600
C	3.47031800	0.28288800	-0.62828500
O	1.52474600	0.59569600	-1.91207700
C	4.01295000	-0.46294100	-1.68418100
C	4.17479200	0.38658000	0.57930300
C	5.24474200	-1.08737900	-1.53535400
H	3.46946400	-0.55321300	-2.61461800
C	5.40696800	-0.23846300	0.72023500
H	3.77332100	0.92815500	1.42715200
C	5.94424400	-0.97605400	-0.33441800
H	5.65748100	-1.66256500	-2.35552900
H	5.94240500	-0.15911400	1.65860600
H	6.90403200	-1.46624500	-0.21797700

IRC_TS1_point264

B	-2.71274700	3.93790400	0.35428700
B	-1.61175900	3.79190600	1.74579500
B	-0.70753900	2.27426900	1.57850100
B	-2.48661400	2.51440500	-0.68611000
B	-1.24497700	1.54632400	0.07665700
B	-1.18391200	4.84949000	0.38172200
B	-1.72106400	4.06729700	-1.12210300
H	-3.76914500	4.47743400	0.44134200
B	0.05622200	3.82047100	1.12967400
H	-1.88519000	4.22717800	2.81859400
B	0.27946300	2.41094500	0.09029300
H	-0.32531500	1.62883000	2.49554500
B	-0.81356500	2.55873100	-1.30296200
H	-3.35831000	2.02370200	-1.32618300
H	-1.16079500	6.03339600	0.49658000
B	-0.00996400	4.00197500	-0.64515800
H	-2.08026200	4.68295300	-2.07364800

H	0.97285400	4.24592000	1.75724400
H	-0.56122400	2.09530800	-2.37269600
H	0.85574400	4.54985400	-1.24725800
B	-2.42268800	2.35220300	1.09677300
I	-1.44328100	-0.67323000	-0.22064300
C	0.37226300	-1.45557800	0.62082100
C	0.67309600	-1.19727100	1.95097900
C	1.16775700	-2.25347700	-0.18997400
C	1.83771500	-1.75344700	2.47992100
H	0.02681100	-0.58244600	2.56071000
C	2.32153100	-2.81077700	0.36282100
H	0.90759400	-2.43461800	-1.22395700
C	2.65819900	-2.55819500	1.68997600
H	2.09607700	-1.55575000	3.51392200
H	2.96000400	-3.42888400	-0.25697600
H	3.56233200	-2.98397800	2.10871800
O	-2.11937700	-3.81948400	-0.07549400
C	-3.35849800	-3.90196200	-0.31608000
O	-4.05760900	-2.98175000	-0.83113900
C	-4.06611500	-5.19724000	0.07135000
H	-4.37841800	-5.12242100	1.11926200
H	-4.95813100	-5.36029000	-0.53598300
H	-3.39464700	-6.05414600	-0.01637200
H	0.68444800	1.09642900	-2.01958300
H	-3.25137100	1.74089000	1.68747900
N	1.63669200	1.73319000	0.06303400
C	2.15595700	0.91434000	-0.80682800
H	2.22358400	1.92527800	0.86585700
C	3.46991800	0.28250500	-0.62809300
O	1.52499500	0.60073100	-1.91458600
C	4.01328900	-0.46252900	-1.68429000
C	4.17388900	0.38566600	0.57979300
C	5.24478100	-1.08746800	-1.53497100
H	3.47050600	-0.55197000	-2.61525800
C	5.40563900	-0.24005200	0.72132300
H	3.77229500	0.92776300	1.42718900
C	5.94330900	-0.97734000	-0.33335000
H	5.65793300	-1.66218400	-2.35528400
H	5.94044400	-0.16137700	1.66007700
H	6.90275300	-1.46807700	-0.21650000

IRC_TS1_point265

B	-2.71164500	3.93991300	0.35412000
B	-1.61057100	3.79387500	1.74544100

B	-0.70756200	2.27546900	1.57874100
B	-2.48677500	2.51567600	-0.68555200
B	-1.24522100	1.54743300	0.07710100
B	-1.18219700	4.85050400	0.38078800
B	-1.72019200	4.06788100	-1.12249400
H	-3.76762800	4.48045100	0.44096400
B	0.05727200	3.82094700	1.12904200
H	-1.88343200	4.23008700	2.81810300
B	0.27900600	2.41082400	0.09029000
H	-0.32563700	1.63028900	2.49619500
B	-0.81383900	2.55876700	-1.30254800
H	-3.35908600	2.02540600	-1.32519500
H	-1.15813800	6.03448100	0.49492300
B	-0.00917100	4.00174500	-0.64582100
H	-2.07907000	4.68313300	-2.07447500
H	0.97450300	4.24585300	1.75617100
H	-0.56248900	2.09415100	-2.37223900
H	0.85725400	4.54815200	-1.24870100
B	-2.42257700	2.35426200	1.09729100
I	-1.44360100	-0.67265300	-0.21975400
C	0.37269200	-1.45443000	0.62109600
C	0.67418500	-1.19582800	1.95100600
C	1.16765900	-2.25240000	-0.19011100
C	1.83904700	-1.75205200	2.47937500
H	0.02829500	-0.58084700	2.56099400
C	2.32166600	-2.80973100	0.36216600
H	0.90687500	-2.43370600	-1.22390200
C	2.65900700	-2.55702500	1.68911300
H	2.09799200	-1.55427100	3.51322600
H	2.95974300	-3.42802200	-0.25785500
H	3.56327900	-2.98291800	2.10748400
O	-2.11932200	-3.82656100	-0.08121000
C	-3.35997200	-3.90752500	-0.31742600
O	-4.05843800	-2.98769300	-0.83402600
C	-4.06910500	-5.20007700	0.07642200
H	-4.38030200	-5.12042900	1.12390600
H	-4.96242800	-5.36404400	-0.52920000
H	-3.39926700	-6.05809200	-0.00842500
H	0.68600000	1.09921700	-2.01921000
H	-3.25206400	1.74431600	1.68891000
N	1.63564700	1.73224000	0.06386700
C	2.15672200	0.91557600	-0.80814800
H	2.22081500	1.91996600	0.87008900
C	3.47010300	0.28319000	-0.62871700

O	1.52780100	0.60319100	-1.91604800
C	4.01365500	-0.46190200	-1.68459800
C	4.17293600	0.38505700	0.58000400
C	5.24470300	-1.08753200	-1.53460200
H	3.47147000	-0.55076400	-2.61593100
C	5.40416100	-0.24150900	0.72227300
H	3.77129900	0.92711600	1.42745400
C	5.94234200	-0.97843200	-0.33238100
H	5.65823700	-1.66206400	-2.35483000
H	5.93828400	-0.16359300	1.66150600
H	6.90145200	-1.46973100	-0.21501200

IRC_TS1_point266

B	-2.71056100	3.94188900	0.35383100
B	-1.60934400	3.79577800	1.74508300
B	-0.70736300	2.27671700	1.57892200
B	-2.48688700	2.51700100	-0.68522500
B	-1.24609800	1.54809500	0.07784000
B	-1.18049900	4.85148100	0.37984000
B	-1.71923200	4.06853400	-1.12300000
H	-3.76617100	4.48307100	0.44062700
B	0.05841500	3.82153100	1.12835200
H	-1.88173500	4.23263600	2.81758500
B	0.27928000	2.41066900	0.09042700
H	-0.32553400	1.63168600	2.49645600
B	-0.81397200	2.55866600	-1.30264600
H	-3.35947400	2.02707500	-1.32465100
H	-1.15574800	6.03548400	0.49351500
B	-0.00806900	4.00138400	-0.64661500
H	-2.07791900	4.68371900	-2.07504400
H	0.97590900	4.24618800	1.75519900
H	-0.56330400	2.09392100	-2.37234000
H	0.85828300	4.54729200	-1.24967200
B	-2.42250500	2.35635700	1.09775200
I	-1.44384200	-0.67205800	-0.21885400
C	0.37300800	-1.45338400	0.62128300
C	0.67525600	-1.19451300	1.95100400
C	1.16755300	-2.25148700	-0.19020500
C	1.84038800	-1.75067200	2.47882100
H	0.02975300	-0.57931500	2.56119700
C	2.32184000	-2.80877900	0.36155500
H	0.90614400	-2.43297500	-1.22381500
C	2.65986500	-2.55588100	1.68827600
H	2.10000700	-1.55253100	3.51241800

H	2.95959400	-3.42710300	-0.25875600
H	3.56441300	-2.98158000	2.10617100
O	-2.12006000	-3.83332300	-0.08620200
C	-3.36086500	-3.91301500	-0.31921700
O	-4.05926200	-2.99380300	-0.83700700
C	-4.07100400	-5.20283400	0.08136600
H	-4.38094500	-5.11796500	1.12896900
H	-4.96441200	-5.36924300	-0.52284000
H	-3.40167400	-6.06120300	0.00008900
H	0.68769100	1.10325600	-2.02290300
H	-3.25203000	1.74707000	1.68959500
N	1.63539900	1.73070400	0.06484400
C	2.15645300	0.91587200	-0.80749700
H	2.21949500	1.91712000	0.87051200
C	3.46967600	0.28287500	-0.62831300
O	1.52866900	0.60803400	-1.91940600
C	4.01385900	-0.46139600	-1.68465600
C	4.17222400	0.38434000	0.58047100
C	5.24457100	-1.08763700	-1.53424700
H	3.47225900	-0.54940700	-2.61644900
C	5.40297500	-0.24295500	0.72324700
H	3.77047400	0.92682500	1.42754600
C	5.94134800	-0.97974600	-0.33139000
H	5.65840100	-1.66183600	-2.35457700
H	5.93646200	-0.16582200	1.66288300
H	6.90000400	-1.47178500	-0.21357700

IRC_TS1_point267

B	-2.70952100	3.94379600	0.35368200
B	-1.60823800	3.79757900	1.74482500
B	-0.70734300	2.27777700	1.57921700
B	-2.48701100	2.51827900	-0.68478200
B	-1.24652700	1.54897700	0.07833900
B	-1.17886100	4.85239900	0.37908000
B	-1.71833300	4.06911700	-1.12329300
H	-3.76466000	4.48599200	0.44031600
B	0.05942200	3.82190900	1.12789600
H	-1.88011900	4.23517300	2.81711700
B	0.27895000	2.41051600	0.09045400
H	-0.32590200	1.63297400	2.49712300
B	-0.81415500	2.55865300	-1.30232900
H	-3.36023100	2.02882200	-1.32376100
H	-1.15308400	6.03648200	0.49200800
B	-0.00729700	4.00110400	-0.64710700

H	-2.07655500	4.68393900	-2.07580000
H	0.97752600	4.24603100	1.75426900
H	-0.56399400	2.09316800	-2.37174400
H	0.85966200	4.54570900	-1.25077600
B	-2.42245300	2.35833200	1.09824300
I	-1.44417300	-0.67146100	-0.21804100
C	0.37332100	-1.45241000	0.62154500
C	0.67626000	-1.19320000	1.95099500
C	1.16736400	-2.25059100	-0.19032800
C	1.84167300	-1.74935400	2.47824500
H	0.03128700	-0.57766100	2.56139600
C	2.32192400	-2.80785000	0.36090500
H	0.90532800	-2.43222400	-1.22374500
C	2.66064800	-2.55478200	1.68740700
H	2.10203900	-1.55086700	3.51159700
H	2.95934700	-3.42621700	-0.25969800
H	3.56548100	-2.98037700	2.10483800
O	-2.11991900	-3.84047700	-0.09182800
C	-3.36178200	-3.91856000	-0.32104800
O	-4.05980600	-2.99961300	-0.83995400
C	-4.07393400	-5.20533800	0.08656100
H	-4.38405400	-5.11304700	1.13383400
H	-4.96888600	-5.37306300	-0.51563000
H	-3.40732500	-6.06783200	0.01067100
H	0.68826500	1.10633600	-2.02143900
H	-3.25250400	1.75016300	1.69065800
N	1.63457500	1.73058700	0.06467700
C	2.15745700	0.91753900	-0.80971700
H	2.21680000	1.91218800	0.87500000
C	3.47002900	0.28365400	-0.62910800
O	1.53062800	0.61043400	-1.91925700
C	4.01429300	-0.46093100	-1.68489300
C	4.17136100	0.38383300	0.58067200
C	5.24451000	-1.08790300	-1.53376500
H	3.47333000	-0.54832400	-2.61708500
C	5.40157100	-0.24440300	0.72423600
H	3.76963100	0.92649500	1.42767500
C	5.94040900	-0.98095500	-0.33034600
H	5.65864900	-1.66197300	-2.35401100
H	5.93433600	-0.16807700	1.66436500
H	6.89862200	-1.47375100	-0.21196200

IRC_TS1_point268

B	-2.70855800	3.94552000	0.35340300
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B	-1.60721800	3.79920000	1.74448200
B	-0.70725500	2.27889400	1.57929600
B	-2.48705400	2.51946300	-0.68452100
B	-1.24702700	1.54985400	0.07882000
B	-1.17741900	4.85330400	0.37830100
B	-1.71748700	4.06977700	-1.12375900
H	-3.76337400	4.48825200	0.43995100
B	0.06034400	3.82246400	1.12732400
H	-1.87874700	4.23728800	2.81666300
B	0.27907000	2.41054400	0.09058700
H	-0.32587000	1.63417400	2.49723600
B	-0.81419300	2.55878600	-1.30231300
H	-3.36048500	2.03034300	-1.32336700
H	-1.15112700	6.03732600	0.49096000
B	-0.00635700	4.00098800	-0.64773500
H	-2.07557500	4.68460500	-2.07624300
H	0.97867400	4.24626400	1.75353500
H	-0.56458500	2.09283300	-2.37178500
H	0.86070200	4.54500100	-1.25157600
B	-2.42232500	2.36010700	1.09851400
I	-1.44442100	-0.67095900	-0.21728200
C	0.37362100	-1.45143300	0.62165400
C	0.67729200	-1.19192000	1.95091300
C	1.16721800	-2.24978300	-0.19048500
C	1.84299300	-1.74795200	2.47760400
H	0.03265300	-0.57624400	2.56151900
C	2.32208000	-2.80693300	0.36022800
H	0.90453200	-2.43170300	-1.22369200
C	2.66150800	-2.55358800	1.68648000
H	2.10400000	-1.54918000	3.51073800
H	2.95915800	-3.42543500	-0.26060400
H	3.56660500	-2.97901900	2.10347000
O	-2.12015700	-3.84720800	-0.09704300
C	-3.36303300	-3.92368500	-0.32219600
O	-4.06039100	-3.00522100	-0.84273000
C	-4.07643600	-5.20764900	0.09192700
H	-4.38560500	-5.11093300	1.13852300
H	-4.97125800	-5.37729400	-0.50948100
H	-3.40992800	-6.06832000	0.01933000
H	0.69067500	1.10976300	-2.02484400
H	-3.25263900	1.75268900	1.69127300
N	1.63424000	1.72867300	0.06673400
C	2.15710000	0.91761000	-0.80810000
H	2.21549000	1.90955100	0.87545700

C	3.46967800	0.28360200	-0.62864000
O	1.53211600	0.61480100	-1.92336800
C	4.01447400	-0.46023700	-1.68498400
C	4.17086800	0.38341400	0.58101200
C	5.24431700	-1.08795100	-1.53343900
H	3.47403300	-0.54695800	-2.61755800
C	5.40054000	-0.24560000	0.72506100
H	3.76903200	0.92626500	1.42781600
C	5.93945400	-0.98215600	-0.32943600
H	5.65864900	-1.66196300	-2.35363000
H	5.93264700	-0.17009900	1.66561500
H	6.89717600	-1.47576700	-0.21054500
IRC_TS1_point269			
B	-2.70756200	3.94741100	0.35326200
B	-1.60618700	3.80097200	1.74430600
B	-0.70722600	2.27990000	1.57967900
B	-2.48715400	2.52075200	-0.68413700
B	-1.24774700	1.55038900	0.07947300
B	-1.17579500	4.85420200	0.37762100
B	-1.71651600	4.07039400	-1.12399300
H	-3.76192300	4.49120400	0.43959800
B	0.06134900	3.82284900	1.12697400
H	-1.87717300	4.24007200	2.81629000
B	0.27901600	2.41028100	0.09078500
H	-0.32621600	1.63541700	2.49796700
B	-0.81435100	2.55864300	-1.30211100
H	-3.36107900	2.03209800	-1.32268800
H	-1.14847300	6.03839700	0.48951500
B	-0.00543300	4.00062400	-0.64818100
H	-2.07413700	4.68494000	-2.07690700
H	0.98011400	4.24628900	1.75278800
H	-0.56561000	2.09227500	-2.37149200
H	0.86200700	4.54367800	-1.25246700
B	-2.42240600	2.36207600	1.09905700
I	-1.44475200	-0.67031600	-0.21649600
C	0.37381600	-1.45056100	0.62186900
C	0.67827300	-1.19066900	1.95084900
C	1.16694100	-2.24900300	-0.19062400
C	1.84429600	-1.74663500	2.47695100
H	0.03424400	-0.57453000	2.56165000
C	2.32211900	-2.80608600	0.35953800
H	0.90361400	-2.43105300	-1.22364600
C	2.66230500	-2.55251300	1.68554400
H	2.10616400	-1.54730900	3.50975300

H	2.95887100	-3.42455500	-0.26164500
H	3.56779600	-2.97764700	2.10196600
O	-2.12070700	-3.85445200	-0.10222600
C	-3.36356400	-3.92925100	-0.32438800
O	-4.06084600	-3.01120100	-0.84587200
C	-4.07855300	-5.20978400	0.09711400
H	-4.38817900	-5.10519100	1.14349500
H	-4.97371300	-5.38255800	-0.50288200
H	-3.41393500	-6.07434800	0.03114400
H	0.69131200	1.11382300	-2.02541100
H	-3.25315700	1.75571900	1.69228600
N	1.63370800	1.72885900	0.06589700
C	2.15808600	0.91929600	-0.81049800
H	2.21332400	1.90547000	0.87894800
C	3.46995100	0.28410800	-0.62911600
O	1.53343900	0.61769000	-1.92300900
C	4.01484000	-0.45985100	-1.68503700
C	4.17011200	0.38283900	0.58143100
C	5.24417600	-1.08830000	-1.53289500
H	3.47497900	-0.54565200	-2.61803800
C	5.39927600	-0.24710100	0.72613300
H	3.76837600	0.92611800	1.42799700
C	5.93847200	-0.98353400	-0.32834300
H	5.65876300	-1.66201800	-2.35317600
H	5.93081400	-0.17232900	1.66706200
H	6.89568100	-1.47801500	-0.20898200

IRC_TS1_point270

B	-2.70665000	3.94900400	0.35294300
B	-1.60525200	3.80249300	1.74393900
B	-0.70713500	2.28100200	1.57970600
B	-2.48710200	2.52188900	-0.68395800
B	-1.24788100	1.55157700	0.07972900
B	-1.17448800	4.85508300	0.37690600
B	-1.71573700	4.07103700	-1.12445300
H	-3.76087300	4.49276900	0.43926900
B	0.06217600	3.82339600	1.12648000
H	-1.87624700	4.24135400	2.81578800
B	0.27898000	2.41046800	0.09075400
H	-0.32631500	1.63642300	2.49799900
B	-0.81429200	2.55897100	-1.30205500
H	-3.36117200	2.03324900	-1.32229600
H	-1.14700600	6.03908800	0.48872500
B	-0.00466900	4.00066700	-0.64869800

H	-2.07336200	4.68546900	-2.07735100
H	0.98109400	4.24650300	1.75226800
H	-0.56566700	2.09227800	-2.37130500
H	0.86292600	4.54313900	-1.25312800
B	-2.42215600	2.36373800	1.09918300
I	-1.44509400	-0.66975200	-0.21566100
C	0.37413000	-1.44953100	0.62197200
C	0.67926100	-1.18929600	1.95073100
C	1.16673100	-2.24823200	-0.19077200
C	1.84555300	-1.74515200	2.47631200
H	0.03529800	-0.57338100	2.56177000
C	2.32218800	-2.80519900	0.35891300
H	0.90276900	-2.43076000	-1.22353900
C	2.66308800	-2.55127200	1.68465600
H	2.10766700	-1.54604200	3.50911300
H	2.95848900	-3.42413200	-0.26229300
H	3.56854800	-2.97671700	2.10092000
O	-2.12000900	-3.86171600	-0.10809600
C	-3.36480000	-3.93448300	-0.32533700
O	-4.06121600	-3.01680300	-0.84855900
C	-4.08165100	-5.21211600	0.10252000
H	-4.39166200	-5.10238700	1.14766200
H	-4.97700800	-5.38537400	-0.49747400
H	-3.41806600	-6.07658800	0.03983400
H	0.69351700	1.11669700	-2.02652400
H	-3.25294300	1.75762400	1.69241100
N	1.63331700	1.72735100	0.06793300
C	2.15801900	0.91978100	-0.80932700
H	2.21195000	1.90300200	0.88009000
C	3.46979200	0.28437500	-0.62897700
O	1.53528800	0.62133500	-1.92631800
C	4.01496400	-0.45934200	-1.68511600
C	4.16968800	0.38253100	0.58160500
C	5.24388300	-1.08860500	-1.53253700
H	3.47543800	-0.54493000	-2.61828900
C	5.39831600	-0.24823900	0.72679600
H	3.76811600	0.92609900	1.42806400
C	5.93757800	-0.98474700	-0.32755000
H	5.65857100	-1.66239000	-2.35270200
H	5.92963000	-0.17370500	1.66786200
H	6.89463900	-1.47950600	-0.20797600
IRC_TS1_point271			
B	-2.70567900	3.95082100	0.35268900
B	-1.60426400	3.80421800	1.74366700

B	-0.70702500	2.28207800	1.57998300
B	-2.48710900	2.52313900	-0.68368800
B	-1.24860700	1.55209500	0.08040500
B	-1.17295100	4.85602700	0.37614300
B	-1.71475600	4.07168900	-1.12481300
H	-3.75963200	4.49552000	0.43879400
B	0.06316100	3.82392300	1.12604500
H	-1.87480400	4.24417000	2.81548500
B	0.27917200	2.41034500	0.09098800
H	-0.32651800	1.63765500	2.49851100
B	-0.81430500	2.55886000	-1.30197900
H	-3.36153300	2.03479100	-1.32176800
H	-1.14459300	6.04027500	0.48726200
B	-0.00366300	4.00041400	-0.64925300
H	-2.07207000	4.68578800	-2.07811200
H	0.98244700	4.24667000	1.75153800
H	-0.56638600	2.09145800	-2.37115300
H	0.86424900	4.54203900	-1.25412600
B	-2.42216200	2.36563300	1.09958900
I	-1.44546300	-0.66900300	-0.21473700
C	0.37432300	-1.44857200	0.62215100
C	0.68027400	-1.18793800	1.95064700
C	1.16645300	-2.24742400	-0.19089300
C	1.84685800	-1.74372200	2.47566900
H	0.03676400	-0.57171400	2.56192000
C	2.32221000	-2.80433900	0.35827600
H	0.90182900	-2.43017100	-1.22346200
C	2.66387100	-2.55013700	1.68376100
H	2.10958600	-1.54429500	3.50822700
H	2.95807800	-3.42343700	-0.26317700
H	3.56951100	-2.97548500	2.09958700
O	-2.12100900	-3.86954900	-0.11316600
C	-3.36530800	-3.94046400	-0.32743000
O	-4.06144900	-3.02319200	-0.85186900
C	-4.08391300	-5.21452800	0.10738100
H	-4.39330000	-5.09916000	1.15222100
H	-4.97934000	-5.39009500	-0.49156300
H	-3.42147900	-6.08016200	0.04871100
H	0.69420000	1.12053900	-2.02771900
H	-3.25347200	1.76043100	1.69340600
N	1.63307600	1.72737100	0.06749400
C	2.15885000	0.92117000	-0.81074900
H	2.21040200	1.90012700	0.88235400
C	3.46999800	0.28469800	-0.62918200

O	1.53640000	0.62486200	-1.92666500
C	4.01516600	-0.45913400	-1.68512000
C	4.16921200	0.38208600	0.58194400
C	5.24360400	-1.08914500	-1.53204900
H	3.47604200	-0.54410700	-2.61863400
C	5.39733200	-0.24955900	0.72766000
H	3.76779400	0.92621500	1.42808900
C	5.93667900	-0.98609200	-0.32663700
H	5.65838000	-1.66289100	-2.35220800
H	5.92825600	-0.17547400	1.66899300
H	6.89336900	-1.48144400	-0.20673500
IRC_TS1_point272			
B	-2.70484900	3.95229400	0.35235600
B	-1.60344000	3.80567400	1.74332100
B	-0.70690200	2.28317100	1.57994000
B	-2.48692100	2.52423200	-0.68360900
B	-1.24845300	1.55330600	0.08043200
B	-1.17181900	4.85692000	0.37552700
B	-1.71399800	4.07236500	-1.12520300
H	-3.75864800	4.49697200	0.43840500
B	0.06390000	3.82455300	1.12562400
H	-1.87395200	4.24530700	2.81498100
B	0.27910900	2.41068100	0.09093100
H	-0.32642100	1.63877000	2.49851000
B	-0.81415500	2.55932300	-1.30186500
H	-3.36144600	2.03607800	-1.32167700
H	-1.14339300	6.04095800	0.48663100
B	-0.00297600	4.00067900	-0.64963800
H	-2.07119900	4.68646800	-2.07845600
H	0.98326800	4.24710300	1.75108800
H	-0.56661800	2.09208300	-2.37108100
H	0.86493200	4.54204100	-1.25448100
B	-2.42188300	2.36720400	1.09963000
I	-1.44591200	-0.66842600	-0.21379600
C	0.37454400	-1.44755000	0.62230500
C	0.68117200	-1.18653700	1.95055600
C	1.16610900	-2.24670900	-0.19097100
C	1.84802800	-1.74220600	2.47507200
H	0.03789600	-0.57027000	2.56198500
C	2.32215100	-2.80349200	0.35773000
H	0.90083500	-2.42991800	-1.22328400
C	2.66455700	-2.54887800	1.68293100
H	2.11129100	-1.54255500	3.50745900
H	2.95765500	-3.42284800	-0.26383900

H	3.57039100	-2.97418100	2.09841200
O	-2.12004800	-3.87738600	-0.11930600
C	-3.36642500	-3.94583500	-0.32879300
O	-4.06163500	-3.02872400	-0.85454300
C	-4.08678700	-5.21662500	0.11264100
H	-4.39614700	-5.09467300	1.15695900
H	-4.98295500	-5.39316200	-0.48518600
H	-3.42637100	-6.08500000	0.05850100
H	0.69630000	1.12321800	-2.02884300
H	-3.25307600	1.76208900	1.69325600
N	1.63264300	1.72628300	0.06917300
C	2.15909100	0.92201300	-0.81035900
H	2.20904200	1.89747900	0.88427200
C	3.46997900	0.28509700	-0.62910500
O	1.53870100	0.62813100	-1.92956800
C	4.01513200	-0.45881000	-1.68507600
C	4.16894000	0.38189400	0.58213000
C	5.24310200	-1.08968400	-1.53166400
H	3.47619900	-0.54344400	-2.61868900
C	5.39653400	-0.25063300	0.72823100
H	3.76783500	0.92636100	1.42822000
C	5.93575600	-0.98740300	-0.32593900
H	5.65779900	-1.66359600	-2.35174100
H	5.92724600	-0.17695300	1.66971400
H	6.89206800	-1.48343900	-0.20575200
IRC_TS1_point273			
B	-2.70390900	3.95411000	0.35203200
B	-1.60253200	3.80736800	1.74302600
B	-0.70679200	2.28427400	1.58024200
B	-2.48690400	2.52552800	-0.68344800
B	-1.24932200	1.55387400	0.08121700
B	-1.17033100	4.85788800	0.37478800
B	-1.71298500	4.07308200	-1.12562100
H	-3.75738200	4.49974500	0.43789800
B	0.06484000	3.82511700	1.12524500
H	-1.87269200	4.24801700	2.81459700
B	0.27943000	2.41061600	0.09114500
H	-0.32677600	1.63998600	2.49907800
B	-0.81405700	2.55928300	-1.30192300
H	-3.36183200	2.03761200	-1.32116700
H	-1.14094600	6.04217400	0.48518600
B	-0.00194500	4.00045700	-0.65016900
H	-2.06980100	4.68686300	-2.07930000
H	0.98462100	4.24727200	1.75040700

H	-0.56679800	2.09101100	-2.37084400
H	0.86651900	4.54079000	-1.25553300
B	-2.42188600	2.36906900	1.09994400
I	-1.44628100	-0.66770900	-0.21290500
C	0.37469000	-1.44662600	0.62247300
C	0.68219100	-1.18513700	1.95044100
C	1.16579700	-2.24593500	-0.19109000
C	1.84935400	-1.74070000	2.47438900
H	0.03945000	-0.56849100	2.56208400
C	2.32215100	-2.80263100	0.35707900
H	0.89985700	-2.42936500	-1.22319700
C	2.66533600	-2.54772000	1.68201500
H	2.11332100	-1.54069000	3.50652900
H	2.95723900	-3.42216700	-0.26474000
H	3.57139200	-2.97297800	2.09707200
O	-2.12089800	-3.88522300	-0.12449500
C	-3.36697900	-3.95187200	-0.33067300
O	-4.06157100	-3.03509700	-0.85802400
C	-4.08928400	-5.21930700	0.11773800
H	-4.39677100	-5.09335600	1.16155000
H	-4.98626300	-5.39728800	-0.47838500
H	-3.42956300	-6.08661100	0.06579400
H	0.69682200	1.12709600	-2.02939500
H	-3.25370400	1.76495700	1.69420600
N	1.63260500	1.72633100	0.06878300
C	2.15972300	0.92331700	-0.81120800
H	2.20794500	1.89574900	0.88521900
C	3.47016700	0.28545300	-0.62933800
O	1.53932700	0.63181600	-1.92965600
C	4.01534300	-0.45868700	-1.68507900
C	4.16860800	0.38162600	0.58233800
C	5.24282400	-1.09037300	-1.53113800
H	3.47686800	-0.54287100	-2.61904000
C	5.39565300	-0.25184900	0.72901400
H	3.76762300	0.92669900	1.42806300
C	5.93490000	-0.98882500	-0.32501700
H	5.65753900	-1.66440500	-2.35112900
H	5.92590000	-0.17867100	1.67079800
H	6.89079100	-1.48556500	-0.20443500
IRC_TS1_point274			
B	-2.70310600	3.95555200	0.35170800
B	-1.60177800	3.80877500	1.74270300
B	-0.70673200	2.28532100	1.58015700
B	-2.48666900	2.52661000	-0.68338300

B	-1.24899200	1.55503800	0.08106400
B	-1.16925500	4.85879000	0.37424200
B	-1.71221600	4.07380900	-1.12594900
H	-3.75634700	4.50144900	0.43738300
B	0.06550400	3.82577000	1.12488000
H	-1.87170100	4.24960000	2.81413000
B	0.27927600	2.41104600	0.09118100
H	-0.32668300	1.64116100	2.49907000
B	-0.81389300	2.55981300	-1.30169000
H	-3.36166500	2.03905200	-1.32121200
H	-1.13965500	6.04289900	0.48455600
B	-0.00126200	4.00085100	-0.65046700
H	-2.06885800	4.68763500	-2.07958900
H	0.98533800	4.24773300	1.75004300
H	-0.56741200	2.09178200	-2.37084800
H	0.86708300	4.54102900	-1.25565900
B	-2.42166100	2.37059600	1.09995100
I	-1.44681100	-0.66724900	-0.21195500
C	0.37480600	-1.44570000	0.62264800
C	0.68305500	-1.18374300	1.95033800
C	1.16531500	-2.24532900	-0.19115800
C	1.85053600	-1.73913000	2.47373100
H	0.04068300	-0.56688000	2.56211200
C	2.32200700	-2.80183200	0.35650300
H	0.89864700	-2.42925100	-1.22298700
C	2.66601100	-2.54641200	1.68111100
H	2.11523200	-1.53863400	3.50558100
H	2.95673200	-3.42156100	-0.26548300
H	3.57241000	-2.97133500	2.09568900
O	-2.12038500	-3.89249800	-0.13008000
C	-3.36765300	-3.95718800	-0.33255100
O	-4.06176200	-3.04089700	-0.86093900
C	-4.09138500	-5.22093500	0.12301100
H	-4.39883800	-5.08648400	1.16678100
H	-4.98924300	-5.40041100	-0.47120400
H	-3.43452300	-6.09321300	0.07728200
H	0.69930200	1.12989800	-2.03119200
H	-3.25349600	1.76684100	1.69415200
N	1.63203600	1.72530300	0.07070500
C	2.16020200	0.92427000	-0.81111600
H	2.20621500	1.89197100	0.88891800
C	3.47022900	0.28591100	-0.62914600
O	1.54219600	0.63515800	-1.93300800
C	4.01519100	-0.45836500	-1.68495700

C	4.16846700	0.38153200	0.58256300
C	5.24212500	-1.09103700	-1.53072800
H	3.47683400	-0.54206800	-2.61898700
C	5.39494600	-0.25289100	0.72953100
H	3.76792100	0.92689600	1.42832900
C	5.93387400	-0.99024800	-0.32435500
H	5.65662700	-1.66538700	-2.35059300
H	5.92498100	-0.18020500	1.67146700
H	6.88924400	-1.48791700	-0.20344500
IRC_TS1_point275			
B	-2.70223900	3.95732400	0.35133900
B	-1.60099400	3.81042500	1.74242800
B	-0.70669200	2.28639700	1.58050300
B	-2.48665700	2.52789000	-0.68330200
B	-1.24995100	1.55555500	0.08190000
B	-1.16786500	4.85972800	0.37357800
B	-1.71121900	4.07450800	-1.12635900
H	-3.75519300	4.50385700	0.43687500
B	0.06635900	3.82630400	1.12461400
H	-1.87083500	4.25161900	2.81367600
B	0.27964000	2.41091400	0.09140400
H	-0.32717100	1.64228600	2.49965600
B	-0.81377500	2.55976500	-1.30177100
H	-3.36201400	2.04051500	-1.32080800
H	-1.13756000	6.04397300	0.48332100
B	-0.00028800	4.00060600	-0.65087600
H	-2.06746200	4.68804500	-2.08038100
H	0.98652700	4.24791500	1.74953300
H	-0.56732600	2.09104000	-2.37056000
H	0.86857800	4.53986700	-1.25653100
B	-2.42171100	2.37242100	1.10019800
I	-1.44718100	-0.66668300	-0.21116600
C	0.37493500	-1.44479700	0.62276000
C	0.68406300	-1.18231300	1.95014800
C	1.16498000	-2.24462400	-0.19129300
C	1.85187500	-1.73755500	2.47298700
H	0.04218800	-0.56510200	2.56211400
C	2.32199100	-2.80100000	0.35583400
H	0.89762500	-2.42885300	-1.22288800
C	2.66680000	-2.54521000	1.68016200
H	2.11725000	-1.53669400	3.50460300
H	2.95628800	-3.42096700	-0.26635800
H	3.57342100	-2.97012400	2.09434400
O	-2.12011200	-3.90003900	-0.13608500

C	-3.36855900	-3.96276900	-0.33388800
O	-4.06176400	-3.04684100	-0.86448600
C	-4.09428300	-5.22333900	0.12881800
H	-4.39983600	-5.08533500	1.17161100
H	-4.99288900	-5.40426000	-0.46388600
H	-3.43780200	-6.09338500	0.08511200
H	0.69986000	1.13405000	-2.03134000
H	-3.25392500	1.76936000	1.69468700
N	1.63216900	1.72548300	0.07005900
C	2.16078900	0.92565500	-0.81167900
H	2.20544400	1.89162400	0.88808800
C	3.47049100	0.28640000	-0.62940800
O	1.54249100	0.63858300	-1.93239000
C	4.01542000	-0.45826500	-1.68490100
C	4.16826700	0.38141700	0.58275500
C	5.24182700	-1.09182500	-1.53013500
H	3.47744200	-0.54161300	-2.61921200
C	5.39416400	-0.25404000	0.73032500
H	3.76790200	0.92763000	1.42801000
C	5.93304000	-0.99173000	-0.32339100
H	5.65625900	-1.66636900	-2.34991300
H	5.92385300	-0.18176100	1.67248500
H	6.88797500	-1.49013700	-0.20212300

IRC_TS1_point276

B	-2.70137100	3.95885100	0.35099200
B	-1.60023500	3.81184200	1.74209700
B	-0.70669700	2.28740400	1.58049800
B	-2.48644800	2.52902400	-0.68321300
B	-1.24982100	1.55665500	0.08187300
B	-1.16666200	4.86063000	0.37300000
B	-1.71034100	4.07524600	-1.12670500
H	-3.75402400	4.50608500	0.43625100
B	0.06703400	3.82689600	1.12428400
H	-1.86968800	4.25389100	2.81327200
B	0.27948600	2.41131400	0.09154000
H	-0.32732700	1.64352200	2.49990000
B	-0.81357200	2.56020900	-1.30155100
H	-3.36200000	2.04207100	-1.32072800
H	-1.13564800	6.04490100	0.48236900
B	0.00049900	4.00087700	-0.65119700
H	-2.06628300	4.68873700	-2.08084700
H	0.98742900	4.24818700	1.74912100
H	-0.56780900	2.09100600	-2.37044000

H	0.86968000	4.53939000	-1.25696900
B	-2.42155400	2.37397900	1.10022800
I	-1.44774400	-0.66628000	-0.21022000
C	0.37499700	-1.44400300	0.62291100
C	0.68501000	-1.18090100	1.94997300
C	1.16444800	-2.24410400	-0.19142400
C	1.85319200	-1.73589700	2.47218700
H	0.04363400	-0.56330700	2.56206100
C	2.32185300	-2.80023000	0.35514600
H	0.89632800	-2.42877400	-1.22274800
C	2.66755100	-2.54388100	1.67911200
H	2.11945600	-1.53439800	3.50343700
H	2.95575100	-3.42036800	-0.26727000
H	3.57454400	-2.96844900	2.09275400
O	-2.12102400	-3.90643000	-0.14049700
C	-3.36854400	-3.96819900	-0.33630100
O	-4.06194300	-3.05337600	-0.86815900
C	-4.09537500	-5.22478100	0.13413000
H	-4.39988700	-5.07841700	1.17703600
H	-4.99556800	-5.40745600	-0.45582300
H	-3.44159700	-6.09917600	0.09593800
H	0.70244300	1.13761800	-2.03317500
H	-3.25426300	1.77182000	1.69513000
N	1.63157900	1.72452300	0.07218000
C	2.16132200	0.92671100	-0.81171200
H	2.20344200	1.88681600	0.89324600
C	3.47055700	0.28683300	-0.62918100
O	1.54518500	0.64246000	-1.93581100
C	4.01526900	-0.45799700	-1.68474300
C	4.16820700	0.38139000	0.58295000
C	5.24109600	-1.09261600	-1.52965800
H	3.47752300	-0.54085700	-2.61921100
C	5.39348200	-0.25510600	0.73084100
H	3.76837800	0.92792900	1.42828800
C	5.93197800	-0.99329700	-0.32266800
H	5.65530200	-1.66756100	-2.34925500
H	5.92283600	-0.18340500	1.67324200
H	6.88631000	-1.49276500	-0.20095500

IRC_TS1_point277

B	-2.70059400	3.96049700	0.35057000
B	-1.59956200	3.81344200	1.74180400
B	-0.70675300	2.28843100	1.58077100
B	-2.48640500	2.53016000	-0.68317400

B	-1.25048300	1.55712500	0.08248100
B	-1.16540800	4.86150800	0.37233400
B	-1.70941100	4.07585100	-1.12712300
H	-3.75302500	4.50801200	0.43567500
B	0.06777200	3.82742000	1.12403100
H	-1.86899600	4.25551100	2.81275400
B	0.27974700	2.41117000	0.09181700
H	-0.32774600	1.64454100	2.50026700
B	-0.81349600	2.56013700	-1.30151100
H	-3.36214000	2.04335900	-1.32054300
H	-1.13411200	6.04569100	0.48141300
B	0.00138700	4.00068500	-0.65154200
H	-2.06505300	4.68911700	-2.08150800
H	0.98827100	4.24845000	1.74878500
H	-0.56814100	2.09086800	-2.37027100
H	0.87055400	4.53890500	-1.25730200
B	-2.42165400	2.37571700	1.10041300
I	-1.44821100	-0.66586300	-0.20941500
C	0.37511700	-1.44308100	0.62296800
C	0.68597400	-1.17943600	1.94971500
C	1.16404200	-2.24349600	-0.19155400
C	1.85450000	-1.73424900	2.47140200
H	0.04498000	-0.56163700	2.56198600
C	2.32177400	-2.79945400	0.35450000
H	0.89521600	-2.42865500	-1.22259800
C	2.66831800	-2.54260300	1.67814800
H	2.12135700	-1.53243800	3.50244800
H	2.95523500	-3.41992600	-0.26803500
H	3.57552900	-2.96709700	2.09142900
O	-2.11933000	-3.91364100	-0.14741200
C	-3.36988500	-3.97310100	-0.33730300
O	-4.06226900	-3.05883900	-0.87168300
C	-4.09809800	-5.22653500	0.14037900
H	-4.40157000	-5.07526800	1.18223600
H	-4.99817100	-5.41114200	-0.44862100
H	-3.44485700	-6.10020300	0.10588400
H	0.70358400	1.14183000	-2.03373400
H	-3.25436700	1.77385600	1.69518500
N	1.63164700	1.72451800	0.07187500
C	2.16202200	0.92810400	-0.81199900
H	2.20245900	1.88634300	0.89249600
C	3.47087100	0.28741700	-0.62930600
O	1.54608000	0.64565400	-1.93544400
C	4.01532300	-0.45790800	-1.68458100

C	4.16816000	0.38139400	0.58319000
C	5.24057300	-1.09350200	-1.52906500
H	3.47770700	-0.54042300	-2.61915700
C	5.39284100	-0.25615500	0.73154900
H	3.76866300	0.92886000	1.42803200
C	5.93107800	-0.99480600	-0.32180100
H	5.65456800	-1.66870700	-2.34860000
H	5.92213500	-0.18465100	1.67397300
H	6.88501800	-1.49496000	-0.19990800
IRC_TS1_point278			
B	-2.69971900	3.96198900	0.35017600
B	-1.59885700	3.81480400	1.74146900
B	-0.70676800	2.28940900	1.58088000
B	-2.48620100	2.53129300	-0.68312500
B	-1.25067100	1.55812600	0.08269800
B	-1.16420700	4.86234700	0.37177900
B	-1.70847700	4.07652600	-1.12747900
H	-3.75190600	4.51016100	0.43498900
B	0.06844200	3.82794400	1.12379000
H	-1.86811900	4.25748100	2.81233000
B	0.27972100	2.41143800	0.09198200
H	-0.32808600	1.64572900	2.50071000
B	-0.81322200	2.56046900	-1.30137900
H	-3.36218200	2.04479900	-1.32039200
H	-1.13212600	6.04669000	0.48031700
B	0.00219400	4.00080200	-0.65180400
H	-2.06378100	4.68963100	-2.08211100
H	0.98925400	4.24864200	1.74840700
H	-0.56819900	2.09049100	-2.37002200
H	0.87210100	4.53786800	-1.25809800
B	-2.42148900	2.37724100	1.10040400
I	-1.44877000	-0.66543500	-0.20849400
C	0.37515400	-1.44237500	0.62306000
C	0.68698500	-1.17800300	1.94945000
C	1.16352200	-2.24302300	-0.19175200
C	1.85590100	-1.73252800	2.47049500
H	0.04650700	-0.55978100	2.56185000
C	2.32166600	-2.79870500	0.35373500
H	0.89391300	-2.42860700	-1.22252500
C	2.66912500	-2.54127900	1.67701400
H	2.12361100	-1.53011000	3.50119300
H	2.95468000	-3.41941100	-0.26900800
H	3.57664900	-2.96555600	2.08980000
O	-2.12101500	-3.91953400	-0.15139700

C	-3.36939200	-3.97861500	-0.33989900
O	-4.06226700	-3.06580600	-0.87607500
C	-4.09908300	-5.22802800	0.14613500
H	-4.40194000	-5.06934800	1.18743800
H	-5.00073200	-5.41457500	-0.44050100
H	-3.44756300	-6.10354800	0.11657900
H	0.70590900	1.14606700	-2.03496400
H	-3.25481400	1.77626800	1.69564500
N	1.63122200	1.72381000	0.07358000
C	2.16258300	0.92933700	-0.81209900
H	2.20062100	1.88228700	0.89671400
C	3.47100600	0.28784900	-0.62912000
O	1.54815800	0.64986000	-1.93801200
C	4.01520800	-0.45779300	-1.68436500
C	4.16823200	0.38143400	0.58336300
C	5.23987400	-1.09446000	-1.52852400
H	3.47782300	-0.53993900	-2.61910700
C	5.39227800	-0.25721700	0.73207000
H	3.76935100	0.92952800	1.42811500
C	5.93010000	-0.99645600	-0.32105100
H	5.65359100	-1.67010600	-2.34787700
H	5.92131000	-0.18617000	1.67470500
H	6.88349100	-1.49757500	-0.19875600

IRC_TS1_point279

B	-2.69899400	3.96353100	0.34968100
B	-1.59826900	3.81632200	1.74112500
B	-0.70689900	2.29037500	1.58106200
B	-2.48611100	2.53230300	-0.68313400
B	-1.25108300	1.55859900	0.08310900
B	-1.16301100	4.86317900	0.37104600
B	-1.70754600	4.07706500	-1.12795800
H	-3.75093500	4.51216300	0.43427000
B	0.06907800	3.82846100	1.12349700
H	-1.86732100	4.25955100	2.81183400
B	0.27985700	2.41140000	0.09232800
H	-0.32847400	1.64676500	2.50100200
B	-0.81308800	2.56038300	-1.30127100
H	-3.36221200	2.04603900	-1.32037900
H	-1.13055300	6.04742200	0.47933400
B	0.00309800	4.00065100	-0.65219700
H	-2.06252700	4.69001800	-2.08277600
H	0.98994800	4.24888800	1.74810400
H	-0.56857600	2.09013000	-2.36984600

H	0.87280700	4.53759100	-1.25817100
B	-2.42165800	2.37885800	1.10053900
I	-1.44934700	-0.66512700	-0.20762100
C	0.37524600	-1.44147400	0.62309700
C	0.68793900	-1.17652000	1.94915000
C	1.16303100	-2.24251900	-0.19187400
C	1.85722400	-1.73081000	2.46965800
H	0.04786800	-0.55804600	2.56169900
C	2.32153200	-2.79798200	0.35309100
H	0.89269700	-2.42866700	-1.22234900
C	2.66989400	-2.53993800	1.67600700
H	2.12563900	-1.52790600	3.50007700
H	2.95413200	-3.41897800	-0.26978700
H	3.57771400	-2.96398000	2.08835800
O	-2.11888800	-3.92648000	-0.15851400
C	-3.37090500	-3.98309400	-0.34083900
O	-4.06286600	-3.07117400	-0.87962000
C	-4.10096200	-5.22908500	0.15231700
H	-4.40206500	-5.06462900	1.19296000
H	-5.00278700	-5.41834700	-0.43268800
H	-3.45031000	-6.10540700	0.12686900
H	0.70758200	1.15051200	-2.03607100
H	-3.25510700	1.77835200	1.69579100
N	1.63109200	1.72345500	0.07408800
C	2.16330700	0.93069300	-0.81218500
H	2.19906300	1.87998600	0.89817100
C	3.47126100	0.28840400	-0.62905700
O	1.54974300	0.65347900	-1.93856100
C	4.01506100	-0.45777400	-1.68409000
C	4.16832700	0.38154800	0.58360000
C	5.23913600	-1.09546700	-1.52791700
H	3.47772500	-0.53960300	-2.61888400
C	5.39176700	-0.25816400	0.73265300
H	3.76999700	0.93049100	1.42803300
C	5.92913800	-0.99801800	-0.32026900
H	5.65252300	-1.67150300	-2.34717200
H	5.92078200	-0.18732700	1.67528800
H	6.88205600	-1.49997400	-0.19777500

IRC_TS1_point280

B	-2.69819000	3.96494500	0.34924700
B	-1.59767600	3.81767900	1.74080500
B	-0.70699400	2.29131000	1.58128200
B	-2.48593700	2.53333600	-0.68311700

B	-1.25140400	1.55944200	0.08344700
B	-1.16189200	4.86393700	0.37051300
B	-1.70662800	4.07762200	-1.12831700
H	-3.74993600	4.51391100	0.43355000
B	0.06969900	3.82892500	1.12335000
H	-1.86682200	4.26092000	2.81129400
B	0.27991000	2.41143500	0.09257100
H	-0.32896600	1.64782100	2.50149300
B	-0.81285500	2.56054400	-1.30112100
H	-3.36223100	2.04726200	-1.32024900
H	-1.12894600	6.04824400	0.47834800
B	0.00386000	4.00063000	-0.65235600
H	-2.06125500	4.69035900	-2.08342600
H	0.99077600	4.24911300	1.74785400
H	-0.56879100	2.08993000	-2.36962000
H	0.87423900	4.53660700	-1.25885200
B	-2.42155400	2.38036100	1.10052900
I	-1.44992700	-0.66466000	-0.20672500
C	0.37524300	-1.44082200	0.62313800
C	0.68895300	-1.17506800	1.94880600
C	1.16248100	-2.24208700	-0.19211900
C	1.85864500	-1.72904700	2.46867400
H	0.04937000	-0.55621700	2.56150100
C	2.32140600	-2.79725600	0.35227600
H	0.89135400	-2.42871300	-1.22230300
C	2.67070600	-2.53861100	1.67481500
H	2.12783600	-1.52563200	3.49879500
H	2.95352800	-3.41857900	-0.27075600
H	3.57879700	-2.96252200	2.08673800
O	-2.12051800	-3.93204700	-0.16265600
C	-3.37011700	-3.98846800	-0.34363000
O	-4.06266900	-3.07811400	-0.88448600
C	-4.10211700	-5.23055700	0.15867300
H	-4.40359300	-5.05845000	1.19831600
H	-5.00470300	-5.42183200	-0.42474500
H	-3.45258100	-6.10769400	0.13883300
H	0.70979000	1.15491700	-2.03663200
H	-3.25533500	1.78036800	1.69585900
N	1.63079500	1.72290000	0.07530300
C	2.16402500	0.93203700	-0.81219500
H	2.19741700	1.87753000	0.90032400
C	3.47154800	0.28892700	-0.62893800
O	1.55166900	0.65752900	-1.94014100
C	4.01491000	-0.45779800	-1.68383400

C	4.16856000	0.38170200	0.58374900
C	5.23837500	-1.09659000	-1.52736600
H	3.47762400	-0.53938400	-2.61867100
C	5.39135000	-0.25916500	0.73313300
H	3.77085500	0.93161200	1.42784900
C	5.92820500	-0.99969800	-0.31957200
H	5.65138000	-1.67314800	-2.34643800
H	5.92031200	-0.18857300	1.67582900
H	6.88064800	-1.50249900	-0.19681700
IRC_TS1_point281			
B	-2.69749200	3.96631800	0.34866600
B	-1.59719300	3.81896900	1.74040600
B	-0.70714400	2.29220500	1.58138000
B	-2.48576500	2.53428600	-0.68321400
B	-1.25175000	1.55997500	0.08377000
B	-1.16080300	4.86467900	0.36981600
B	-1.70567300	4.07812300	-1.12880500
H	-3.74898700	4.51599700	0.43265700
B	0.07021800	3.82940900	1.12309900
H	-1.86605100	4.26317400	2.81084900
B	0.27997700	2.41159400	0.09292900
H	-0.32937900	1.64887600	2.50181100
B	-0.81257200	2.56056200	-1.30101700
H	-3.36215800	2.04849400	-1.32039400
H	-1.12723900	6.04903600	0.47726500
B	0.00475300	4.00055200	-0.65270100
H	-2.05996200	4.69072600	-2.08409800
H	0.99140500	4.24927700	1.74763800
H	-0.56875400	2.08942000	-2.36935100
H	0.87520600	4.53610000	-1.25902800
B	-2.42169800	2.38177200	1.10050100
I	-1.45054600	-0.66443900	-0.20582800
C	0.37530600	-1.43997000	0.62315400
C	0.68990200	-1.17362000	1.94848200
C	1.16193800	-2.24169000	-0.19223600
C	1.85997600	-1.72731800	2.46779500
H	0.05078300	-0.55442000	2.56129200
C	2.32124000	-2.79660800	0.35163200
H	0.89005400	-2.42888700	-1.22212200
C	2.67147900	-2.53726900	1.67377600
H	2.12998200	-1.52324900	3.49756100
H	2.95294600	-3.41817700	-0.27157200
H	3.57993300	-2.96082700	2.08518400
O	-2.11846600	-3.93868300	-0.16952400

C	-3.37167000	-3.99270200	-0.34429800
O	-4.06336400	-3.08356500	-0.88805100
C	-4.10330300	-5.23109300	0.16468900
H	-4.40298500	-5.05391500	1.20333100
H	-5.00647700	-5.42536900	-0.41684700
H	-3.45451400	-6.10887400	0.14886700
H	0.71165200	1.15973000	-2.03831200
H	-3.25596700	1.78261300	1.69622800
N	1.63053100	1.72235800	0.07646500
C	2.16465100	0.93345000	-0.81234600
H	2.19541100	1.87305400	0.90450200
C	3.47168900	0.28934100	-0.62865100
O	1.55348200	0.66207300	-1.94172800
C	4.01463000	-0.45792900	-1.68338500
C	4.16879800	0.38186800	0.58401400
C	5.23751700	-1.09776400	-1.52667200
H	3.47739900	-0.53924400	-2.61829200
C	5.39100300	-0.26003900	0.73364200
H	3.77191600	0.93259800	1.42796200
C	5.92726400	-1.00134400	-0.31880500
H	5.65006900	-1.67482500	-2.34562400
H	5.91996400	-0.18964700	1.67634600
H	6.87917500	-1.50509100	-0.19582400

IRC_TS1_point282

B	-2.69682400	3.96770700	0.34821800
B	-1.59677500	3.82039000	1.74014800
B	-0.70745300	2.29303900	1.58173900
B	-2.48567400	2.53517400	-0.68321000
B	-1.25214500	1.56058500	0.08417800
B	-1.15972700	4.86538500	0.36925200
B	-1.70477200	4.07856300	-1.12919600
H	-3.74810300	4.51762900	0.43186200
B	0.07074200	3.82978200	1.12303000
H	-1.86577200	4.26455700	2.81027700
B	0.28001200	2.41129700	0.09334000
H	-0.33008300	1.64979000	2.50235900
B	-0.81241100	2.56046400	-1.30079300
H	-3.36219000	2.04957700	-1.32036600
H	-1.12585400	6.04966100	0.47639400
B	0.00552700	4.00034200	-0.65281800
H	-2.05858500	4.69098700	-2.08479400
H	0.99201500	4.24947400	1.74752000
H	-0.56913700	2.08888000	-2.36907000

H	0.87629700	4.53540400	-1.25922000
B	-2.42184900	2.38328100	1.10061800
I	-1.45115300	-0.66395900	-0.20501000
C	0.37525300	-1.43940200	0.62315000
C	0.69088700	-1.17218100	1.94805600
C	1.16132300	-2.24133500	-0.19252900
C	1.86139900	-1.72554400	2.46672700
H	0.05228300	-0.55257500	2.56100100
C	2.32106800	-2.79592200	0.35075200
H	0.88862900	-2.42908900	-1.22209000
C	2.67228300	-2.53594000	1.67250600
H	2.13222800	-1.52088000	3.49617200
H	2.95230400	-3.41783300	-0.27258100
H	3.58105900	-2.95928300	2.08347500
O	-2.11971000	-3.94395700	-0.17402800
C	-3.37062600	-3.99770100	-0.34749100
O	-4.06315700	-3.09011200	-0.89300700
C	-4.10434900	-5.23217800	0.17151700
H	-4.40352600	-5.04506300	1.20996500
H	-5.00847600	-5.42933200	-0.40757000
H	-3.45681900	-6.11120100	0.16182300
H	0.71400900	1.16416600	-2.03818600
H	-3.25616400	1.78432100	1.69597200
N	1.63022300	1.72165400	0.07748100
C	2.16556600	0.93476500	-0.81198900
H	2.19380100	1.87219100	0.90435700
C	3.47213900	0.29007800	-0.62867600
O	1.55569400	0.66555900	-1.94227400
C	4.01439900	-0.45800100	-1.68316800
C	4.16916200	0.38223200	0.58406700
C	5.23663500	-1.09898600	-1.52615900
H	3.47702700	-0.53923700	-2.61796700
C	5.39067600	-0.26089500	0.73402800
H	3.77287200	0.93416700	1.42750000
C	5.92630600	-1.00299200	-0.31819600
H	5.64866400	-1.67679800	-2.34483500
H	5.91968500	-0.19067800	1.67672500
H	6.87768700	-1.50768300	-0.19494900
IRC_TS1_point283			
B	-2.69615200	3.96885700	0.34761400
B	-1.59641600	3.82136000	1.73975500
B	-0.70761500	2.29380800	1.58181400
B	-2.48543700	2.53608500	-0.68336900
B	-1.25248200	1.56118900	0.08444600

B	-1.15881500	4.86596600	0.36878000
B	-1.70382900	4.07902700	-1.12956500
H	-3.74721800	4.51939600	0.43094900
B	0.07113900	3.83015700	1.12297700
H	-1.86536100	4.26609900	2.80982500
B	0.28003900	2.41161400	0.09371600
H	-0.33067100	1.65071600	2.50276700
B	-0.81204800	2.56063700	-1.30063800
H	-3.36205300	2.05075000	-1.32057700
H	-1.12431300	6.05037400	0.47550400
B	0.00630900	4.00033900	-0.65289600
H	-2.05728500	4.69130500	-2.08537700
H	0.99252100	4.24953400	1.74755600
H	-0.56903900	2.08887300	-2.36880300
H	0.87759900	4.53456300	-1.25952500
B	-2.42188700	2.38444300	1.10035300
I	-1.45173800	-0.66380600	-0.20421100
C	0.37526900	-1.43865900	0.62310200
C	0.69182400	-1.17083700	1.94767700
C	1.16074200	-2.24105600	-0.19270600
C	1.86272600	-1.72388500	2.46576700
H	0.05372600	-0.55081300	2.56071600
C	2.32087800	-2.79538300	0.35004100
H	0.88726600	-2.42933600	-1.22198300
C	2.67304900	-2.53468400	1.67138200
H	2.13442500	-1.51853000	3.49483000
H	2.95167300	-3.41753700	-0.27350300
H	3.58220800	-2.95768700	2.08180100
O	-2.11819300	-3.94981600	-0.18002900
C	-3.37201500	-4.00172900	-0.34774300
O	-4.06355000	-3.09575800	-0.89705900
C	-4.10527100	-5.23229100	0.17793200
H	-4.40529400	-5.04220800	1.21340800
H	-5.00857000	-5.43207900	-0.40114300
H	-3.45787900	-6.11119700	0.17398000
H	0.71588400	1.16914900	-2.04026600
H	-3.25691800	1.78645000	1.69628000
N	1.62993000	1.72124800	0.07882400
C	2.16612300	0.93630600	-0.81241000
H	2.19160500	1.86632300	0.91064400
C	3.47223600	0.29031700	-0.62812700
O	1.55738900	0.67096000	-1.94467900
C	4.01407800	-0.45827800	-1.68251900
C	4.16956400	0.38242400	0.58442300

C	5.23573700	-1.10032000	-1.52534300
H	3.47674300	-0.53922600	-2.61740500
C	5.39050600	-0.26174700	0.73455200
H	3.77430100	0.93531600	1.42770800
C	5.92541700	-1.00475000	-0.31737400
H	5.64722100	-1.67866500	-2.34393100
H	5.91960200	-0.19164100	1.67719200
H	6.87626600	-1.51038500	-0.19396400
IRC_TS1_point284			
B	-2.69560700	3.97020500	0.34708100
B	-1.59618700	3.82273500	1.73948900
B	-0.70812100	2.29455200	1.58218000
B	-2.48537300	2.53688300	-0.68346700
B	-1.25294700	1.56161300	0.08483900
B	-1.15776900	4.86664200	0.36813800
B	-1.70289900	4.07941900	-1.13003400
H	-3.74642800	4.52124500	0.42994600
B	0.07152100	3.83048300	1.12292200
H	-1.86506900	4.26806500	2.80936000
B	0.28004600	2.41118600	0.09427500
H	-0.33150400	1.65153500	2.50325400
B	-0.81182900	2.56044200	-1.30044100
H	-3.36200500	2.05179700	-1.32080600
H	-1.12282100	6.05098600	0.47456400
B	0.00717900	4.00002500	-0.65307900
H	-2.05585000	4.69156500	-2.08610000
H	0.99292200	4.24960100	1.74759200
H	-0.56907300	2.08792100	-2.36843500
H	0.87852500	4.53401200	-1.25936800
B	-2.42231200	2.38588300	1.10050700
I	-1.45237200	-0.66338900	-0.20345000
C	0.37523300	-1.43807100	0.62304000
C	0.69280900	-1.16937400	1.94717200
C	1.16009800	-2.24076600	-0.19301100
C	1.86415700	-1.72208300	2.46463700
H	0.05522700	-0.54895300	2.56034000
C	2.32067000	-2.79475800	0.34915100
H	0.88581300	-2.42968000	-1.22193800
C	2.67385300	-2.53333800	1.67007800
H	2.13669500	-1.51607000	3.49335600
H	2.95099000	-3.41728300	-0.27448800
H	3.58336200	-2.95604600	2.08004200
O	-2.11834500	-3.95517800	-0.18528300
C	-3.37123300	-4.00616800	-0.35074100

O	-4.06382100	-3.10179000	-0.90136400
C	-4.10591000	-5.23277300	0.18461200
H	-4.40483600	-5.02961200	1.22099000
H	-5.01065400	-5.43713700	-0.39135400
H	-3.45948800	-6.11235900	0.18708800
H	0.71830200	1.17385500	-2.04025200
H	-3.25746200	1.78821100	1.69609000
N	1.62951300	1.72005400	0.08035200
C	2.16704300	0.93758800	-0.81174600
H	2.18973800	1.86492900	0.91041900
C	3.47267400	0.29117000	-0.62823400
O	1.55988000	0.67440600	-1.94490300
C	4.01371100	-0.45844100	-1.68226500
C	4.17000400	0.38293000	0.58439500
C	5.23470900	-1.10166600	-1.52480000
H	3.47615900	-0.53947600	-2.61696400
C	5.39026700	-0.26243400	0.73481600
H	3.77546600	0.93695900	1.42728300
C	5.92444800	-1.00637400	-0.31683300
H	5.64555500	-1.68093800	-2.34303400
H	5.91948600	-0.19242300	1.67742000
H	6.87472600	-1.51303700	-0.19312500
IRC_TS1_point285			
B	-2.69496900	3.97134400	0.34647900
B	-1.59591100	3.82377100	1.73914900
B	-0.70841300	2.29527200	1.58241000
B	-2.48516800	2.53773400	-0.68359300
B	-1.25327900	1.56224800	0.08515500
B	-1.15688700	4.86716700	0.36772500
B	-1.70195400	4.07980300	-1.13038000
H	-3.74561500	4.52263500	0.42907100
B	0.07189100	3.83075600	1.12300500
H	-1.86501300	4.26906100	2.80878200
B	0.28001200	2.41129000	0.09472800
H	-0.33230700	1.65235000	2.50380800
B	-0.81150900	2.56050700	-1.30014900
H	-3.36189400	2.05279100	-1.32093500
H	-1.12161500	6.05151100	0.47385100
B	0.00789200	3.99993200	-0.65297900
H	-2.05452600	4.69178200	-2.08670500
H	0.99333900	4.24971700	1.74771500
H	-0.56926200	2.08780400	-2.36811000
H	0.87973600	4.53321600	-1.25952000
B	-2.42239000	2.38707900	1.10026000

I	-1.45300700	-0.66316000	-0.20264700
C	0.37519900	-1.43742000	0.62294900
C	0.69376600	-1.16800900	1.94671800
C	1.15948300	-2.24050200	-0.19328300
C	1.86551800	-1.72037700	2.46357100
H	0.05660700	-0.54729500	2.56002200
C	2.32046400	-2.79421200	0.34833500
H	0.88446100	-2.42990500	-1.22193900
C	2.67461800	-2.53208500	1.66884500
H	2.13876400	-1.51391200	3.49200900
H	2.95032400	-3.41705600	-0.27545700
H	3.58437500	-2.95467200	2.07838700
O	-2.11782200	-3.96039200	-0.19044500
C	-3.37173600	-4.01040500	-0.35150200
O	-4.06361800	-3.10796600	-0.90635400
C	-4.10689500	-5.23276800	0.19159900
H	-4.40707000	-5.02812100	1.22393700
H	-5.01048300	-5.43939300	-0.38476400
H	-3.46103500	-6.11312400	0.19981100
H	0.72037400	1.17830800	-2.04170200
H	-3.25794100	1.78993900	1.69594700
N	1.62920700	1.71985900	0.08118700
C	2.16781900	0.93919100	-0.81204700
H	2.18760800	1.86053600	0.91515800
C	3.47294800	0.29148500	-0.62765900
O	1.56189700	0.67958800	-1.94701900
C	4.01334900	-0.45879300	-1.68160300
C	4.17055300	0.38322600	0.58473100
C	5.23372700	-1.10312900	-1.52400600
H	3.47573700	-0.53952700	-2.61633900
C	5.39019700	-0.26327400	0.73531100
H	3.77687100	0.93846100	1.42720400
C	5.92355300	-1.00816700	-0.31606300
H	5.64407400	-1.68284400	-2.34220500
H	5.91962900	-0.19322800	1.67775900
H	6.87345900	-1.51549200	-0.19235300

IRC_TS1_point286

B	-2.69443800	3.97248500	0.34581100
B	-1.59574900	3.82485300	1.73875300
B	-0.70879900	2.29601100	1.58257200
B	-2.48498400	2.53851300	-0.68386200
B	-1.25370700	1.56267800	0.08542700
B	-1.15599900	4.86776700	0.36712100

B	-1.70104200	4.08020600	-1.13086500
H	-3.74494500	4.52427400	0.42798700
B	0.07217500	3.83113600	1.12294600
H	-1.86481800	4.27078900	2.80835400
B	0.28011100	2.41122600	0.09520000
H	-0.33305600	1.65315300	2.50414700
B	-0.81116500	2.56050600	-1.30010300
H	-3.36168400	2.05371400	-1.32132100
H	-1.12018800	6.05220300	0.47289500
B	0.00874500	3.99976100	-0.65316800
H	-2.05322300	4.69200900	-2.08742400
H	0.99363700	4.24978800	1.74784400
H	-0.56904600	2.08741400	-2.36787800
H	0.88090600	4.53250400	-1.25965500
B	-2.42267900	2.38828700	1.10010900
I	-1.45370800	-0.66282500	-0.20176300
C	0.37517800	-1.43670200	0.62285600
C	0.69470300	-1.16654100	1.94622900
C	1.15885100	-2.24020100	-0.19353000
C	1.86685800	-1.71859700	2.46251700
H	0.05794400	-0.54555900	2.55967600
C	2.32022600	-2.79362900	0.34756400
H	0.88306200	-2.43022400	-1.22186100
C	2.67535800	-2.53076300	1.66766000
H	2.14079900	-1.51162000	3.49066400
H	2.94959700	-3.41688500	-0.27630500
H	3.58536500	-2.95317800	2.07679800
O	-2.11699800	-3.96610800	-0.19625000
C	-3.37173300	-4.01458500	-0.35370500
O	-4.06418100	-3.11391000	-0.91051400
C	-4.10720000	-5.23310100	0.19800200
H	-4.40635900	-5.01600700	1.23126400
H	-5.01189400	-5.44362500	-0.37583600
H	-3.46163200	-6.11262900	0.21163500
H	0.72240300	1.18291300	-2.04238800
H	-3.25870800	1.79174600	1.69597800
N	1.62888800	1.71874300	0.08315100
C	2.16868000	0.94068500	-0.81181500
H	2.18574500	1.85724700	0.91758000
C	3.47329200	0.29213900	-0.62758400
O	1.56423400	0.68402000	-1.94806400
C	4.01290100	-0.45922700	-1.68113100
C	4.17112900	0.38371300	0.58475900
C	5.23263900	-1.10472600	-1.52331100

H	3.47508700	-0.54007500	-2.61570000
C	5.39016000	-0.26389200	0.73553200
H	3.77843900	0.93999800	1.42702100
C	5.92268800	-1.00986100	-0.31550500
H	5.64229200	-1.68531600	-2.34121100
H	5.91986100	-0.19374500	1.67784600
H	6.87213200	-1.51803600	-0.19161900

IRC_TS1_point287

B	-2.69388600	3.97377000	0.34521700
B	-1.59556800	3.82610700	1.73847400
B	-0.70930100	2.29671500	1.58292800
B	-2.48486600	2.53934700	-0.68396400
B	-1.25411200	1.56329700	0.08580700
B	-1.15503900	4.86835400	0.36659700
B	-1.70005800	4.08057000	-1.13128400
H	-3.74414400	4.52601700	0.42698300
B	0.07252700	3.83137700	1.12301400
H	-1.86471400	4.27233200	2.80779700
B	0.28000800	2.41100100	0.09575700
H	-0.33396100	1.65397700	2.50473100
B	-0.81086000	2.56040600	-1.29973600
H	-3.36161700	2.05482200	-1.32155500
H	-1.11888900	6.05271100	0.47210000
B	0.00952900	3.99953900	-0.65311600
H	-2.05171500	4.69227700	-2.08809900
H	0.99402300	4.24987700	1.74793500
H	-0.56908300	2.08663600	-2.36738400
H	0.88182400	4.53201500	-1.25937600
B	-2.42302900	2.38965100	1.10007800
I	-1.45440900	-0.66249000	-0.20092600
C	0.37511700	-1.43607800	0.62277200
C	0.69568400	-1.16511800	1.94573200
C	1.15817900	-2.23989500	-0.19386200
C	1.86827400	-1.71682400	2.46136200
H	0.05946000	-0.54370100	2.55931200
C	2.31998800	-2.79301800	0.34663500
H	0.88160500	-2.43043500	-1.22188600
C	2.67613800	-2.52944800	1.66630500
H	2.14308100	-1.50917300	3.48914400
H	2.94890300	-3.41654900	-0.27740100
H	3.58649300	-2.95155500	2.07494000
O	-2.11690100	-3.97133600	-0.20118600
C	-3.37145800	-4.01902000	-0.35526500

O	-4.06377300	-3.12041400	-0.91582000
C	-4.10795400	-5.23285900	0.20498000
H	-4.40793000	-5.01324900	1.23451700
H	-5.01201200	-5.44629100	-0.36834900
H	-3.46347100	-6.11451300	0.22523500
H	0.72459700	1.18695600	-2.04307400
H	-3.25915800	1.79335900	1.69557300
N	1.62847800	1.71823900	0.08383200
C	2.16956800	0.94211400	-0.81153700
H	2.18369500	1.85452000	0.91969900
C	3.47371300	0.29273300	-0.62724200
O	1.56677500	0.68842900	-1.94937900
C	4.01248600	-0.45955100	-1.68060400
C	4.17175400	0.38421500	0.58492000
C	5.23154500	-1.10625600	-1.52259400
H	3.47448900	-0.54031300	-2.61509200
C	5.39009900	-0.26462200	0.73590800
H	3.77981000	0.94177000	1.42667600
C	5.92173000	-1.01164600	-0.31482100
H	5.64053600	-1.68765300	-2.34026100
H	5.91994300	-0.19455700	1.67814300
H	6.87061800	-1.52080000	-0.19074400
IRC_TS1_point288			
B	-2.69336900	3.97470300	0.34451100
B	-1.59547400	3.82691200	1.73806500
B	-0.70960700	2.29737700	1.58300800
B	-2.48459200	2.54011700	-0.68434500
B	-1.25446700	1.56376300	0.08597000
B	-1.15436200	4.86884300	0.36623100
B	-1.69919100	4.08100200	-1.13165800
H	-3.74352400	4.52710900	0.42595300
B	0.07272000	3.83171300	1.12312400
H	-1.86488500	4.27314600	2.80726600
B	0.28011200	2.41118300	0.09619300
H	-0.33478300	1.65466400	2.50508900
B	-0.81047500	2.56056600	-1.29968200
H	-3.36131200	2.05570900	-1.32207000
H	-1.11787700	6.05325100	0.47151400
B	0.01023500	3.99954800	-0.65305200
H	-2.05045700	4.69256600	-2.08870600
H	0.99413700	4.24997200	1.74831400
H	-0.56895700	2.08689500	-2.36728000
H	0.88316800	4.53128800	-1.25954300
B	-2.42314400	2.39063600	1.09964200

I	-1.45510100	-0.66220800	-0.20004400
C	0.37503200	-1.43541000	0.62267800
C	0.69653000	-1.16377300	1.94528100
C	1.15751600	-2.23966300	-0.19407500
C	1.86951000	-1.71514800	2.46036000
H	0.06069700	-0.54209300	2.55896500
C	2.31971200	-2.79251100	0.34592300
H	0.88019500	-2.43079500	-1.22179600
C	2.67681200	-2.52821000	1.66517900
H	2.14503800	-1.50698100	3.48784100
H	2.94816100	-3.41641700	-0.27822600
H	3.58746000	-2.95015500	2.07338300
O	-2.11588900	-3.97686800	-0.20683900
C	-3.37166600	-4.02301100	-0.35707200
O	-4.06394100	-3.12617100	-0.92037900
C	-4.10827100	-5.23310300	0.21178300
H	-4.40525700	-5.00286000	1.24231400
H	-5.01441700	-5.44950700	-0.35786900
H	-3.46413700	-6.11288800	0.23475700
H	0.72647600	1.19133000	-2.04423700
H	-3.25993700	1.79503300	1.69547400
N	1.62818600	1.71751200	0.08554500
C	2.17040400	0.94377300	-0.81190800
H	2.18176800	1.85019500	0.92394500
C	3.47402300	0.29318000	-0.62692300
O	1.56888300	0.69345500	-1.95116600
C	4.01202400	-0.46016200	-1.67991900
C	4.17241900	0.38470300	0.58506900
C	5.23044000	-1.10801900	-1.52173100
H	3.47379900	-0.54097100	-2.61426800
C	5.39017500	-0.26522200	0.73621000
H	3.78158200	0.94346900	1.42654200
C	5.92089000	-1.01344400	-0.31413500
H	5.63867200	-1.69027000	-2.33917500
H	5.92038000	-0.19491200	1.67820600
H	6.86932600	-1.52341000	-0.18997800

IRC_TS1_point289

B	-2.69290400	3.97601700	0.34392200
B	-1.59542300	3.82813400	1.73781900
B	-0.71026200	2.29801200	1.58338100
B	-2.48454400	2.54094000	-0.68450000
B	-1.25503900	1.56426200	0.08638000
B	-1.15335800	4.86943700	0.36566600

B	-1.69818500	4.08137900	-1.13211200
H	-3.74277800	4.52928000	0.42483400
B	0.07299400	3.83191200	1.12318800
H	-1.86469300	4.27531500	2.80688800
B	0.28001900	2.41080800	0.09678900
H	-0.33581400	1.65538500	2.50560300
B	-0.81018200	2.56040300	-1.29942400
H	-3.36128500	2.05685200	-1.32241000
H	-1.11619700	6.05390900	0.47053900
B	0.01113000	3.99919200	-0.65310400
H	-2.04885800	4.69288100	-2.08940400
H	0.99450100	4.24991200	1.74844600
H	-0.56873300	2.08587700	-2.36679700
H	0.88415300	4.53066400	-1.25920100
B	-2.42373100	2.39199300	1.09969600
I	-1.45581200	-0.66185300	-0.19927300
C	0.37496800	-1.43479500	0.62255900
C	0.69749100	-1.16238700	1.94473800
C	1.15682800	-2.23936700	-0.19444800
C	1.87091300	-1.71344100	2.45915700
H	0.06222600	-0.54026100	2.55858700
C	2.31945400	-2.79192100	0.34493600
H	0.87870200	-2.43102700	-1.22184500
C	2.67758100	-2.52693500	1.66377200
H	2.14731900	-1.50458700	3.48626800
H	2.94743100	-3.41612200	-0.27936800
H	3.58858900	-2.94853100	2.07146600
O	-2.11549400	-3.98208300	-0.21190700
C	-3.37116800	-4.02723000	-0.35892400
O	-4.06376100	-3.13263900	-0.92542200
C	-4.10842300	-5.23225400	0.21861200
H	-4.40734300	-4.99701400	1.24567900
H	-5.01318000	-5.45192400	-0.35075700
H	-3.46521800	-6.11509300	0.25118600
H	0.72850600	1.19550100	-2.04440400
H	-3.26068300	1.79673000	1.69516400
N	1.62776000	1.71656900	0.08668500
C	2.17125600	0.94505000	-0.81117400
H	2.17988800	1.84825600	0.92468900
C	3.47445300	0.29392900	-0.62682100
O	1.57140200	0.69752000	-1.95182800
C	4.01158200	-0.46052200	-1.67948800
C	4.17304500	0.38535200	0.58505700
C	5.22930900	-1.10961400	-1.52101300

H	3.47315800	-0.54148700	-2.61369700
C	5.39009700	-0.26580400	0.73648700
H	3.78297100	0.94532500	1.42608700
C	5.91992000	-1.01518100	-0.31347800
H	5.63680500	-1.69292900	-2.33805600
H	5.92039600	-0.19558200	1.67846800
H	6.86773000	-1.52625200	-0.18898300
IRC_TS1_point290			
B	-2.69241200	3.97697500	0.34325300
B	-1.59537600	3.82898100	1.73748600
B	-0.71067700	2.29860400	1.58354400
B	-2.48429000	2.54170600	-0.68481800
B	-1.25527300	1.56483900	0.08649900
B	-1.15272400	4.86989000	0.36540500
B	-1.69731600	4.08178800	-1.13242400
H	-3.74213300	4.53024800	0.42385200
B	0.07315700	3.83214800	1.12341900
H	-1.86502900	4.27578800	2.80627900
B	0.27998700	2.41093900	0.09728400
H	-0.33679100	1.65601500	2.50608000
B	-0.80980200	2.56055800	-1.29915100
H	-3.36100600	2.05779500	-1.32290100
H	-1.11552200	6.05420700	0.47024600
B	0.01172500	3.99925700	-0.65282400
H	-2.04755500	4.69319800	-2.08993700
H	0.99452600	4.24998300	1.74892000
H	-0.56869000	2.08605400	-2.36652000
H	0.88511200	4.53037000	-1.25886300
B	-2.42388700	2.39300100	1.09927700
I	-1.45652100	-0.66155700	-0.19844500
C	0.37482200	-1.43420300	0.62246500
C	0.69829800	-1.16110000	1.94428200
C	1.15610400	-2.23915000	-0.19471900
C	1.87212000	-1.71181000	2.45810400
H	0.06345600	-0.53866300	2.55822700
C	2.31912900	-2.79142100	0.34413400
H	0.87725100	-2.43132900	-1.22183100
C	2.67821400	-2.52572900	1.66255300
H	2.14929100	-1.50240800	3.48489100
H	2.94665900	-3.41592200	-0.28032800
H	3.58954600	-2.94711000	2.06976800
O	-2.11478000	-3.98721500	-0.21704400
C	-3.37105500	-4.03126600	-0.36054800
O	-4.06333900	-3.13860600	-0.93061100

C	-4.10887600	-5.23239900	0.22588200
H	-4.40293100	-4.98962700	1.25333000
H	-5.01711100	-5.45442100	-0.33868600
H	-3.46662600	-6.11294000	0.25805700
H	0.73072800	1.19948600	-2.04580800
H	-3.26126000	1.79816800	1.69471300
N	1.62739700	1.71617800	0.08776800
C	2.17215800	0.94668300	-0.81159900
H	2.17782900	1.84379300	0.92927200
C	3.47483100	0.29437500	-0.62630500
O	1.57382600	0.70223300	-1.95386100
C	4.01109300	-0.46107700	-1.67870600
C	4.17377500	0.38587300	0.58532200
C	5.22813900	-1.11135900	-1.52010300
H	3.47238800	-0.54194700	-2.61277400
C	5.39020800	-0.26642100	0.73686900
H	3.78472600	0.94711600	1.42597300
C	5.91902200	-1.01701100	-0.31272900
H	5.63488200	-1.69545600	-2.33697700
H	5.92088400	-0.19599800	1.67858500
H	6.86635400	-1.52892200	-0.18819000

IRC_TS1_point291

B	-2.69195700	3.97808700	0.34256800
B	-1.59537300	3.82993000	1.73714300
B	-0.71121200	2.29922800	1.58377300
B	-2.48417100	2.54251800	-0.68516800
B	-1.25595100	1.56521400	0.08685100
B	-1.15186600	4.87042900	0.36491300
B	-1.69636800	4.08220700	-1.13287500
H	-3.74150700	4.53197000	0.42273300
B	0.07334800	3.83240500	1.12350900
H	-1.86503400	4.27746600	2.80590800
B	0.28004000	2.41075000	0.09783700
H	-0.33776200	1.65665800	2.50645800
B	-0.80947800	2.56050500	-1.29913800
H	-3.36085800	2.05879500	-1.32341100
H	-1.11392200	6.05495600	0.46931700
B	0.01260800	3.99895800	-0.65290100
H	-2.04610400	4.69350800	-2.09063100
H	0.99476200	4.24994300	1.74919700
H	-0.56842500	2.08555300	-2.36632900
H	0.88666300	4.52918800	-1.25912400
B	-2.42434200	2.39414900	1.09906800

I	-1.45725200	-0.66123200	-0.19763600
C	0.37474600	-1.43354000	0.62231000
C	0.69918700	-1.15977200	1.94374400
C	1.15543600	-2.23887000	-0.19504500
C	1.87341600	-1.71018100	2.45697200
H	0.06478700	-0.53706200	2.55786800
C	2.31885300	-2.79088800	0.34325400
H	0.87582800	-2.43159200	-1.22184500
C	2.67891900	-2.52452400	1.66126500
H	2.15131100	-1.50028000	3.48346500
H	2.94590200	-3.41576200	-0.28131500
H	3.59051700	-2.94574300	2.06806200
O	-2.11368200	-3.99262900	-0.22238200
C	-3.37062100	-4.03523500	-0.36244900
O	-4.06328700	-3.14489000	-0.93548400
C	-4.10866500	-5.23125700	0.23249300
H	-4.40378200	-4.98060200	1.25793300
H	-5.01571400	-5.45602100	-0.33114100
H	-3.46735600	-6.11498100	0.27440700
H	0.73236200	1.20404000	-2.04602800
H	-3.26226200	1.79998100	1.69465900
N	1.62708100	1.71512800	0.08948000
C	2.17293100	0.94812700	-0.81117000
H	2.17615000	1.84177900	0.93034600
C	3.47516600	0.29499800	-0.62625200
O	1.57571000	0.70682100	-1.95446800
C	4.01063100	-0.46166800	-1.67819600
C	4.17439700	0.38648800	0.58527800
C	5.22701800	-1.11314300	-1.51928000
H	3.47176700	-0.54276500	-2.61214300
C	5.39019100	-0.26693700	0.73711000
H	3.78622100	0.94888700	1.42557400
C	5.91813400	-1.01876700	-0.31204800
H	5.63302500	-1.69826800	-2.33577400
H	5.92106100	-0.19638400	1.67873400
H	6.86496200	-1.53157100	-0.18725800
IRC_TS1_point292			
B	-2.69154600	3.97922900	0.34198200
B	-1.59539900	3.83101200	1.73690600
B	-0.71183900	2.29980300	1.58407300
B	-2.48403300	2.54325700	-0.68533800
B	-1.25615100	1.56584600	0.08701700
B	-1.15110400	4.87093200	0.36452600
B	-1.69546400	4.08255900	-1.13322600

H	-3.74087900	4.53356600	0.42167300
B	0.07351400	3.83257900	1.12369300
H	-1.86516500	4.27880400	2.80542500
B	0.27988500	2.41065600	0.09837300
H	-0.33885000	1.65731900	2.50700700
B	-0.80915300	2.56050800	-1.29872400
H	-3.36072900	2.05978600	-1.32376200
H	-1.11296000	6.05530400	0.46878300
B	0.01325800	3.99887600	-0.65269600
H	-2.04469700	4.69380100	-2.09119900
H	0.99487100	4.24997300	1.74950900
H	-0.56832800	2.08518000	-2.36583700
H	0.88701700	4.52935700	-1.25822200
B	-2.42477200	2.39533800	1.09894000
I	-1.45804500	-0.66086000	-0.19682200
C	0.37458000	-1.43294300	0.62220200
C	0.69999900	-1.15844900	1.94324700
C	1.15466700	-2.23855900	-0.19542100
C	1.87463800	-1.70855300	2.45582700
H	0.06608600	-0.53536600	2.55751300
C	2.31848800	-2.79031600	0.34229800
H	0.87432800	-2.43173200	-1.22193900
C	2.67952700	-2.52331300	1.65990200
H	2.15332900	-1.49809500	3.48199000
H	2.94508300	-3.41546400	-0.28244100
H	3.59143400	-2.94428200	2.06620900
O	-2.11326100	-3.99763100	-0.22711000
C	-3.37007300	-4.03945000	-0.36415600
O	-4.06247800	-3.15134800	-0.94122000
C	-4.10889000	-5.23110400	0.23984400
H	-4.39946500	-4.97568700	1.26449000
H	-5.01914200	-5.45767400	-0.31937600
H	-3.46886000	-6.11332400	0.28144100
H	0.73500200	1.20770300	-2.04715600
H	-3.26269300	1.80123600	1.69397800
N	1.62665600	1.71471500	0.09019600
C	2.17393000	0.94953000	-0.81097100
H	2.17410000	1.83788800	0.93389500
C	3.47564200	0.29563300	-0.62574800
O	1.57877900	0.71074800	-1.95615100
C	4.01010200	-0.46205600	-1.67748300
C	4.17515200	0.38709000	0.58553400
C	5.22577800	-1.11476900	-1.51844800
H	3.47091100	-0.54310200	-2.61123500

C	5.39028200	-0.26752400	0.73747400
H	3.78786100	0.95064400	1.42545500
C	5.91717600	-1.02051800	-0.31135400
H	5.63103600	-1.70075400	-2.33470000
H	5.92146400	-0.19693500	1.67890600
H	6.86347400	-1.53426700	-0.18644400
IRC_TS1_point293			
B	-2.69105200	3.98017300	0.34119400
B	-1.59537000	3.83178600	1.73646600
B	-0.71222100	2.30043400	1.58417800
B	-2.48380900	2.54407700	-0.68582500
B	-1.25678600	1.56625600	0.08727800
B	-1.15043500	4.87142400	0.36415800
B	-1.69457800	4.08301000	-1.13365300
H	-3.74026500	4.53458400	0.42062500
B	0.07366400	3.83288900	1.12385100
H	-1.86547500	4.27949400	2.80484000
B	0.27999400	2.41070400	0.09889500
H	-0.33977800	1.65793700	2.50734900
B	-0.80875000	2.56059900	-1.29875500
H	-3.36043700	2.06071700	-1.32440800
H	-1.11191700	6.05586500	0.46821300
B	0.01399400	3.99879000	-0.65261700
H	-2.04336000	4.69411800	-2.09187600
H	0.99496400	4.25001100	1.74993900
H	-0.56804800	2.08507400	-2.36574500
H	0.88893900	4.52798300	-1.25881800
B	-2.42497400	2.39631800	1.09842100
I	-1.45880100	-0.66056400	-0.19595200
C	0.37443800	-1.43227800	0.62205300
C	0.70077900	-1.15720500	1.94275700
C	1.15396900	-2.23830400	-0.19569500
C	1.87579800	-1.70700500	2.45477700
H	0.06725000	-0.53390000	2.55716600
C	2.31816000	-2.78982600	0.34150900
H	0.87291900	-2.43199300	-1.22192500
C	2.68013400	-2.52216500	1.65871400
H	2.15518000	-1.49607000	3.48064900
H	2.94429800	-3.41530300	-0.28336400
H	3.59231800	-2.94299100	2.06458500
O	-2.11168400	-4.00321100	-0.23245600
C	-3.36954600	-4.04334800	-0.36601600
O	-4.06207200	-3.15752100	-0.94626000
C	-4.10865700	-5.23001700	0.24638700

H	-4.39830800	-4.96572200	1.27030200
H	-5.01914100	-5.45871300	-0.31045500
H	-3.46983400	-6.11464500	0.29530200
H	0.73641800	1.21236500	-2.04773700
H	-3.26375000	1.80308300	1.69397500
N	1.62637500	1.71389500	0.09194800
C	2.17463400	0.95119600	-0.81116100
H	2.17242900	1.83543200	0.93594300
C	3.47589900	0.29604500	-0.62554800
O	1.58013200	0.71585300	-1.95705700
C	4.00962200	-0.46282900	-1.67681600
C	4.17578400	0.38762100	0.58558900
C	5.22466000	-1.11668300	-1.51750700
H	3.47025900	-0.54401500	-2.61047600
C	5.39033100	-0.26805700	0.73777100
H	3.78944500	0.95242900	1.42512300
C	5.91633800	-1.02233100	-0.31060300
H	5.62914600	-1.70360400	-2.33347200
H	5.92179800	-0.19719800	1.67902000
H	6.86218200	-1.53686000	-0.18554900
IRC_TS1_point294			
B	-2.69073200	3.98136300	0.34065800
B	-1.59549600	3.83290300	1.73628100
B	-0.71296000	2.30100500	1.58453000
B	-2.48375500	2.54479900	-0.68597100
B	-1.25705600	1.56681600	0.08747400
B	-1.14962300	4.87194100	0.36369900
B	-1.69368300	4.08335200	-1.13401600
H	-3.73972600	4.53661100	0.41947200
B	0.07378600	3.83305300	1.12399400
H	-1.86546900	4.28153700	2.80454200
B	0.27983700	2.41048800	0.09944200
H	-0.34091000	1.65859400	2.50787000
B	-0.80851400	2.56052400	-1.29840700
H	-3.36039700	2.06171900	-1.32474700
H	-1.11049200	6.05644300	0.46734000
B	0.01473200	3.99854600	-0.65255400
H	-2.04191700	4.69442700	-2.09244700
H	0.99508000	4.25002200	1.75018800
H	-0.56797800	2.08467300	-2.36530800
H	0.88911500	4.52816700	-1.25779200
B	-2.42560600	2.39756700	1.09845700
I	-1.45966700	-0.66014100	-0.19515400
C	0.37424000	-1.43166600	0.62191900

C	0.70156600	-1.15588800	1.94222300
C	1.15315900	-2.23793100	-0.19614100
C	1.87700300	-1.70541100	2.45357000
H	0.06855100	-0.53221700	2.55682000
C	2.31775600	-2.78921300	0.34045100
H	0.87136300	-2.43205700	-1.22207900
C	2.68071300	-2.52097000	1.65726100
H	2.15719900	-1.49394400	3.47911900
H	2.94342500	-3.41498600	-0.28458400
H	3.59319400	-2.94157500	2.06264800
O	-2.11115600	-4.00828600	-0.23697000
C	-3.36871600	-4.04756600	-0.36782300
O	-4.06100600	-3.16415500	-0.95221200
C	-4.10852700	-5.22946200	0.25359400
H	-4.39455200	-4.96088200	1.27612500
H	-5.02129800	-5.45987400	-0.29950500
H	-3.47100100	-6.11350800	0.30393600
H	0.73915700	1.21594900	-2.04852400
H	-3.26420100	1.80425900	1.69323900
N	1.62595300	1.71329600	0.09276400
C	2.17565600	0.95239700	-0.81043100
H	2.17049300	1.83204000	0.93863800
C	3.47640400	0.29681500	-0.62512300
O	1.58348600	0.71935100	-1.95838600
C	4.00907000	-0.46313900	-1.67615800
C	4.17654300	0.38830400	0.58579200
C	5.22339400	-1.11824700	-1.51670900
H	3.46935700	-0.54441400	-2.60957300
C	5.39040300	-0.26857700	0.73809500
H	3.79106600	0.95417700	1.42500400
C	5.91535800	-1.02401300	-0.30994100
H	5.62711100	-1.70616300	-2.33233300
H	5.92215000	-0.19774800	1.67919900
H	6.86063200	-1.53957500	-0.18468400

IRC_TS1_point295

B	-2.69022200	3.98232500	0.33983800
B	-1.59545700	3.83371700	1.73582300
B	-0.71335500	2.30163100	1.58461600
B	-2.48350500	2.54563600	-0.68645200
B	-1.25763400	1.56734300	0.08769800
B	-1.14900800	4.87245300	0.36337100
B	-1.69279500	4.08381400	-1.13445000
H	-3.73906600	4.53748400	0.41845400

B	0.07392800	3.83336400	1.12419100
H	-1.86590600	4.28187500	2.80382000
B	0.27987000	2.41061800	0.09995500
H	-0.34189600	1.65922400	2.50825500
B	-0.80803600	2.56067500	-1.29833200
H	-3.36007700	2.06267800	-1.32539900
H	-1.10988900	6.05678400	0.46706700
B	0.01537200	3.99861600	-0.65234400
H	-2.04058500	4.69475300	-2.09313300
H	0.99514100	4.25007200	1.75066100
H	-0.56758300	2.08443800	-2.36510100
H	0.89095500	4.52702900	-1.25824700
B	-2.42575200	2.39853900	1.09785400
I	-1.46047000	-0.65985300	-0.19427000
C	0.37403000	-1.43101300	0.62177500
C	0.70226900	-1.15469200	1.94175300
C	1.15239900	-2.23766900	-0.19642700
C	1.87808100	-1.70391900	2.45252400
H	0.06964900	-0.53078400	2.55648400
C	2.31736100	-2.78872800	0.33964300
H	0.86990600	-2.43225300	-1.22209500
C	2.68124300	-2.51985700	1.65605600
H	2.15898000	-1.49197500	3.47777100
H	2.94259000	-3.41476600	-0.28556800
H	3.59402400	-2.94027300	2.06097000
O	-2.10940200	-4.01390800	-0.24205700
C	-3.36789300	-4.05153300	-0.36967400
O	-4.06007300	-3.17043600	-0.95754600
C	-4.10822800	-5.22842200	0.26010000
H	-4.39163000	-4.95162800	1.28230200
H	-5.02256400	-5.46041300	-0.28940800
H	-3.47225500	-6.11432500	0.31537800
H	0.74059500	1.22044200	-2.04936700
H	-3.26527200	1.80613600	1.69320200
N	1.62561400	1.71266900	0.09429100
C	2.17632400	0.95414700	-0.81089100
H	2.16873000	1.82941300	0.94106900
C	3.47664000	0.29715400	-0.62479500
O	1.58474700	0.72448100	-1.95942500
C	4.00857300	-0.46394400	-1.67539100
C	4.17716500	0.38878500	0.58595400
C	5.22225500	-1.12018000	-1.51569400
H	3.46867100	-0.54527400	-2.60873000
C	5.39045800	-0.26914300	0.73847100

H	3.79262600	0.95592700	1.42475600
C	5.91451000	-1.02584700	-0.30912200
H	5.62519100	-1.70896100	-2.33108600
H	5.92250400	-0.19803300	1.67936900
H	6.85933700	-1.54215800	-0.18376900
IRC_TS1_point296			
B	-2.68995500	3.98346100	0.33929600
B	-1.59563600	3.83475100	1.73563100
B	-0.71407900	2.30221900	1.58494900
B	-2.48348200	2.54636300	-0.68667000
B	-1.25798300	1.56780700	0.08788600
B	-1.14825100	4.87295100	0.36292600
B	-1.69196300	4.08417900	-1.13479800
H	-3.73862200	4.53941100	0.41729600
B	0.07399800	3.83355800	1.12433200
H	-1.86593700	4.28393000	2.80359300
B	0.27977100	2.41040700	0.10050300
H	-0.34301500	1.65985800	2.50871500
B	-0.80789200	2.56059700	-1.29811100
H	-3.36005900	2.06364200	-1.32579100
H	-1.10822300	6.05755700	0.46601300
B	0.01611500	3.99829700	-0.65234800
H	-2.03920700	4.69509000	-2.09368300
H	0.99518200	4.25012400	1.75093600
H	-0.56758500	2.08436700	-2.36481900
H	0.89127700	4.52694100	-1.25744700
B	-2.42640900	2.39976700	1.09786600
I	-1.46141100	-0.65939500	-0.19344700
C	0.37377900	-1.43038700	0.62161600
C	0.70299100	-1.15341300	1.94120300
C	1.15154600	-2.23726700	-0.19690200
C	1.87921800	-1.70237700	2.45130400
H	0.07084600	-0.52921500	2.55615000
C	2.31690800	-2.78810200	0.33855300
H	0.86832200	-2.43227800	-1.22227800
C	2.68176300	-2.51868900	1.65458200
H	2.16088700	-1.48997600	3.47625600
H	2.94166400	-3.41445800	-0.28680800
H	3.59481400	-2.93896100	2.05903600
O	-2.10849700	-4.01916000	-0.24642600
C	-3.36681100	-4.05574400	-0.37153300
O	-4.05866200	-3.17710200	-0.96364100
C	-4.10786600	-5.22764700	0.26707000
H	-4.38889500	-4.94568500	1.28765400

H	-5.02337000	-5.46117500	-0.27969200
H	-3.47305500	-6.11340200	0.32555200
H	0.74325400	1.22400100	-2.04997200
H	-3.26573300	1.80728000	1.69245500
N	1.62523400	1.71201100	0.09522100
C	2.17734700	0.95528500	-0.81001300
H	2.16690300	1.82621500	0.94351900
C	3.47713200	0.29792300	-0.62436700
O	1.58808800	0.72794700	-1.96063400
C	4.00801000	-0.46427600	-1.67470900
C	4.17792200	0.38947700	0.58616200
C	5.22099200	-1.12174500	-1.51487300
H	3.46776200	-0.54575100	-2.60779000
C	5.39054300	-0.26962600	0.73879300
H	3.79425100	0.95762700	1.42468200
C	5.91355100	-1.02749300	-0.30845500
H	5.62316800	-1.71153300	-2.32991000
H	5.92288500	-0.19851900	1.67953800
H	6.85783500	-1.54479200	-0.18290100

IRC_TS1_point297

B	-2.68945000	3.98452600	0.33846300
B	-1.59562600	3.83567200	1.73516800
B	-0.71458400	2.30285100	1.58504200
B	-2.48325700	2.54724300	-0.68711300
B	-1.25857900	1.56847300	0.08811100
B	-1.14759100	4.87351300	0.36254900
B	-1.69102800	4.08465600	-1.13527000
H	-3.73792000	4.54060800	0.41620700
B	0.07413300	3.83385600	1.12451400
H	-1.86634700	4.28451800	2.80284100
B	0.27969400	2.41053300	0.10100800
H	-0.34408400	1.66051900	2.50911100
B	-0.80736300	2.56077400	-1.29795500
H	-3.35976500	2.06471400	-1.32645200
H	-1.10776200	6.05778800	0.46583400
B	0.01676000	3.99842700	-0.65212100
H	-2.03779900	4.69544500	-2.09440700
H	0.99527900	4.25012700	1.75137200
H	-0.56712300	2.08385500	-2.36451900
H	0.89293000	4.52608000	-1.25764900
B	-2.42664200	2.40080500	1.09728800
I	-1.46227400	-0.65910900	-0.19257700
C	0.37350900	-1.42973500	0.62146100

C	0.70364000	-1.15223800	1.94072200
C	1.15071700	-2.23697900	-0.19723500
C	1.88025000	-1.70091500	2.45021400
H	0.07192900	-0.52776100	2.55581900
C	2.31644900	-2.78760000	0.33766800
H	0.86678000	-2.43240900	-1.22234400
C	2.68224000	-2.51758500	1.65330100
H	2.16267200	-1.48799800	3.47484200
H	2.94076700	-3.41417700	-0.28790100
H	3.59562000	-2.93760300	2.05723800
O	-2.10658800	-4.02483500	-0.25117600
C	-3.36562100	-4.05978400	-0.37338800
O	-4.05723300	-3.18354400	-0.96916200
C	-4.10729300	-5.22648200	0.27336100
H	-4.38342200	-4.93792800	1.29384500
H	-5.02609000	-5.46128600	-0.26811600
H	-3.47462100	-6.11419600	0.33437400
H	0.74470300	1.22832700	-2.05088200
H	-3.26689700	1.80923700	1.69239500
N	1.62478300	1.71133100	0.09679100
C	2.17796200	0.95701200	-0.81042000
H	2.16505900	1.82374900	0.94578600
C	3.47735500	0.29829000	-0.62401200
O	1.58937900	0.73293100	-1.96160000
C	4.00751000	-0.46504100	-1.67391400
C	4.17850100	0.38993700	0.58637600
C	5.21983800	-1.12365400	-1.51380800
H	3.46707700	-0.54656600	-2.60692300
C	5.39054800	-0.27021700	0.73923400
H	3.79572600	0.95929000	1.42450800
C	5.91266800	-1.02932900	-0.30757000
H	5.62121800	-1.71433500	-2.32858800
H	5.92313700	-0.19889700	1.67981200
H	6.85646400	-1.54744300	-0.18187800
IRC_TS1_point298			
B	-2.68923200	3.98554800	0.33796000
B	-1.59583500	3.83656800	1.73501800
B	-0.71523600	2.30339000	1.58536000
B	-2.48323600	2.54793500	-0.68737100
B	-1.25889500	1.56881000	0.08824500
B	-1.14698000	4.87396700	0.36225200
B	-1.69030200	4.08504100	-1.13553100
H	-3.73757800	4.54206900	0.41517700
B	0.07415000	3.83404800	1.12474100

H	-1.86655800	4.28605200	2.80264400
B	0.27964100	2.41038400	0.10153700
H	-0.34521800	1.66107400	2.50959200
B	-0.80729400	2.56071800	-1.29775700
H	-3.35974700	2.06559200	-1.32686300
H	-1.10623400	6.05858700	0.46492900
B	0.01738600	3.99815000	-0.65202500
H	-2.03655000	4.69580600	-2.09486600
H	0.99518500	4.25022100	1.75178600
H	-0.56709900	2.08410900	-2.36426600
H	0.89329700	4.52590600	-1.25691900
B	-2.42723900	2.40193900	1.09724300
I	-1.46326500	-0.65864900	-0.19174400
C	0.37317900	-1.42915600	0.62128900
C	0.70424500	-1.15108200	1.94018800
C	1.14981600	-2.23658800	-0.19772100
C	1.88125000	-1.69951400	2.44902800
H	0.07295500	-0.52638600	2.55549600
C	2.31593300	-2.78700800	0.33658400
H	0.86518800	-2.43240700	-1.22255500
C	2.68265400	-2.51651800	1.65185500
H	2.16438200	-1.48623600	3.47339200
H	2.93978800	-3.41389300	-0.28914100
H	3.59627900	-2.93646600	2.05534900
O	-2.10532700	-4.03008300	-0.25529400
C	-3.36425700	-4.06391200	-0.37533700
O	-4.05531100	-3.19002400	-0.97546500
C	-4.10696500	-5.22564700	0.28028500
H	-4.38431300	-4.92939500	1.29854800
H	-5.02415000	-5.46183400	-0.26129500
H	-3.47469800	-6.11268600	0.34801800
H	0.74741500	1.23175400	-2.05156100
H	-3.26730400	1.81025200	1.69160500
N	1.62448900	1.71100400	0.09718200
C	2.17899300	0.95815200	-0.80966800
H	2.16328700	1.82027500	0.94853000
C	3.47781000	0.29898100	-0.62344800
O	1.59272700	0.73631400	-1.96287900
C	4.00691200	-0.46540700	-1.67313100
C	4.17924700	0.39061200	0.58668100
C	5.21856900	-1.12518100	-1.51294800
H	3.46609500	-0.54707700	-2.60586400
C	5.39066400	-0.27065600	0.73959700
H	3.79737600	0.96101900	1.42450700

C	5.91173700	-1.03090000	-0.30688500
H	5.61918400	-1.71682600	-2.32741400
H	5.92363200	-0.19924300	1.67995400
H	6.85504700	-1.54989800	-0.18107100

IRC_TS1_point299

B	-2.68881200	3.98669700	0.33714400
B	-1.59597900	3.83750600	1.73459800
B	-0.71599300	2.30398200	1.58550700
B	-2.48311500	2.54888300	-0.68783100
B	-1.25969900	1.56952300	0.08850400
B	-1.14624600	4.87451000	0.36183700
B	-1.68932900	4.08553300	-1.13599600
H	-3.73687500	4.54392300	0.41389300
B	0.07418000	3.83425000	1.12494300
H	-1.86689800	4.28733700	2.80199200
B	0.27942100	2.41033500	0.10215300
H	-0.34650700	1.66166800	2.50995800
B	-0.80680000	2.56088500	-1.29763800
H	-3.35956500	2.06690100	-1.32762500
H	-1.10520200	6.05894700	0.46445500
B	0.01811300	3.99812300	-0.65182500
H	-2.03490600	4.69628700	-2.09557900
H	0.99525100	4.25004900	1.75224300
H	-0.56670800	2.08361900	-2.36403000
H	0.89496900	4.52497700	-1.25691600
B	-2.42770800	2.40301000	1.09671200
I	-1.46410200	-0.65839100	-0.19110000
C	0.37285200	-1.42856400	0.62105100
C	0.70487100	-1.14996900	1.93960600
C	1.14889300	-2.23633500	-0.19819600
C	1.88229900	-1.69811000	2.44776000
H	0.07417800	-0.52480200	2.55507300
C	2.31540400	-2.78653300	0.33547600
H	0.86345000	-2.43252900	-1.22274600
C	2.68312000	-2.51544300	1.65033700
H	2.16643600	-1.48402500	3.47167100
H	2.93880600	-3.41354600	-0.29056000
H	3.59722800	-2.93490300	2.05314300
O	-2.10333900	-4.03540300	-0.25956300
C	-3.36289700	-4.06757400	-0.37682800
O	-4.05375600	-3.19626700	-0.98063700
C	-4.10575600	-5.22368200	0.28644800
H	-4.37439400	-4.92386400	1.30473800

H	-5.02940800	-5.46215500	-0.24646900
H	-3.47635800	-6.11312800	0.35388900
H	0.74885700	1.23607600	-2.05228400
H	-3.26867100	1.81218600	1.69137300
N	1.62376700	1.70955500	0.09990900
C	2.17955600	0.95966000	-0.80971000
H	2.16129800	1.81836400	0.95017200
C	3.47809100	0.29948200	-0.62319300
O	1.59404300	0.74105300	-1.96361200
C	4.00649400	-0.46602400	-1.67240300
C	4.17984100	0.39112400	0.58686400
C	5.21745200	-1.12703600	-1.51187400
H	3.46545800	-0.54785500	-2.60501100
C	5.39062900	-0.27126300	0.74006400
H	3.79887700	0.96259500	1.42441400
C	5.91081900	-1.03277400	-0.30594600
H	5.61712100	-1.71988100	-2.32590700
H	5.92369600	-0.19989800	1.68038900
H	6.85339200	-1.55301800	-0.17974700

IRC_TS1_point300

B	-2.68852700	3.98765800	0.33663400
B	-1.59620600	3.83820200	1.73449500
B	-0.71665700	2.30431100	1.58582800
B	-2.48302700	2.54959300	-0.68809500
B	-1.25999000	1.56985000	0.08861900
B	-1.14572500	4.87491900	0.36184500
B	-1.68851700	4.08598100	-1.13614800
H	-3.73644100	4.54494300	0.41297700
B	0.07418100	3.83431200	1.12544200
H	-1.86755200	4.28784100	2.80169100
B	0.27932600	2.41030900	0.10270300
H	-0.34790800	1.66198500	2.51058900
B	-0.80661000	2.56090200	-1.29721600
H	-3.35939000	2.06788900	-1.32824000
H	-1.10470200	6.05924800	0.46457400
B	0.01868600	3.99804700	-0.65136900
H	-2.03357000	4.69670000	-2.09594900
H	0.99504700	4.24989500	1.75309900
H	-0.56640900	2.08354700	-2.36350500
H	0.89565900	4.52469100	-1.25598000
B	-2.42829700	2.40399800	1.09652600
I	-1.46498100	-0.65808500	-0.19044100
C	0.37249400	-1.42817100	0.62081600

C	0.70537700	-1.14908200	1.93904500
C	1.14800800	-2.23612600	-0.19870200
C	1.88318000	-1.69697300	2.44658500
H	0.07504300	-0.52375900	2.55466600
C	2.31488300	-2.78612600	0.33440500
H	0.86192000	-2.43273300	-1.22298100
C	2.68347700	-2.51458400	1.64891400
H	2.16796900	-1.48259800	3.47025000
H	2.93784900	-3.41342800	-0.29178300
H	3.59786000	-2.93395300	2.05127200
O	-2.10172300	-4.04013100	-0.26351900
C	-3.36122200	-4.07124600	-0.37905100
O	-4.05147600	-3.20205800	-0.98679700
C	-4.10558300	-5.22247200	0.29388100
H	-4.37187300	-4.91248100	1.31186500
H	-5.02895100	-5.45952900	-0.23677700
H	-3.47771900	-6.11248600	0.36595400
H	0.75117000	1.23952400	-2.05306000
H	-3.26957400	1.81355100	1.69081200
N	1.62361800	1.71013500	0.09876800
C	2.18021600	0.96083000	-0.80906500
H	2.15942500	1.81423600	0.95361900
C	3.47825300	0.29989700	-0.62235100
O	1.59662800	0.74445000	-1.96455700
C	4.00575900	-0.46653300	-1.67141900
C	4.18041700	0.39168700	0.58733400
C	5.21613600	-1.12854700	-1.51086500
H	3.46436700	-0.54852400	-2.60380800
C	5.39066900	-0.27167700	0.74056100
H	3.80037700	0.96444900	1.42440300
C	5.90985200	-1.03430600	-0.30511900
H	5.61502100	-1.72230700	-2.32465100
H	5.92417400	-0.19999000	1.68057700
H	6.85199800	-1.55528700	-0.17890200

IRC_TS1_point301

B	-2.68834600	3.98860100	0.33597300
B	-1.59663700	3.83891000	1.73427600
B	-0.71763500	2.30477200	1.58609300
B	-2.48299100	2.55042300	-0.68861200
B	-1.26082100	1.57022900	0.08878600
B	-1.14516300	4.87527800	0.36161400
B	-1.68771800	4.08642100	-1.13642900
H	-3.73602400	4.54672400	0.41174200

B	0.07395800	3.83437900	1.12580600
H	-1.86799500	4.28929800	2.80141900
B	0.27903800	2.41004600	0.10352000
H	-0.34943900	1.66238500	2.51101400
B	-0.80630400	2.56106900	-1.29720600
H	-3.35939700	2.06906500	-1.32894700
H	-1.10281800	6.05997900	0.46370500
B	0.01929400	3.99781700	-0.65106200
H	-2.03196600	4.69727000	-2.09641900
H	0.99478000	4.24968000	1.75378600
H	-0.56615000	2.08390900	-2.36344400
H	0.89668600	4.52423200	-1.25528100
B	-2.42892900	2.40490100	1.09605900
I	-1.46574500	-0.65783900	-0.19009500
C	0.37219000	-1.42764000	0.62040500
C	0.70598600	-1.14808000	1.93831400
C	1.14711600	-2.23588000	-0.19939000
C	1.88417900	-1.69576500	2.44517300
H	0.07628200	-0.52226200	2.55414300
C	2.31434500	-2.78574100	0.33309400
H	0.86023300	-2.43270500	-1.22342700
C	2.68388500	-2.51370800	1.64723100
H	2.16995600	-1.48069700	3.46841600
H	2.93682100	-3.41318800	-0.29342800
H	3.59866400	-2.93276800	2.04893300
O	-2.10000500	-4.04447600	-0.26706700
C	-3.36002800	-4.07421500	-0.37964900
O	-4.04984300	-3.20784600	-0.99198700
C	-4.10412800	-5.21957900	0.30081500
H	-4.36935400	-4.90621800	1.31573600
H	-5.02902100	-5.45947000	-0.22697600
H	-3.47712500	-6.10968000	0.37861100
H	0.75331600	1.24368300	-2.05396100
H	-3.27049200	1.81463200	1.68991700
N	1.62254200	1.70760400	0.10340800
C	2.18116500	0.96222100	-0.80944600
H	2.15741100	1.81237300	0.95513900
C	3.47875800	0.30063100	-0.62229900
O	1.59873000	0.74857900	-1.96584500
C	4.00540700	-0.46700600	-1.67078300
C	4.18101600	0.39229900	0.58749600
C	5.21504600	-1.13026400	-1.50986900
H	3.46365000	-0.54918400	-2.60290900
C	5.39061300	-0.27219100	0.74100400

H	3.80186400	0.96585200	1.42447900
C	5.90894000	-1.03598800	-0.30425800
H	5.61304000	-1.72520000	-2.32318800
H	5.92422900	-0.20067800	1.68102100
H	6.85035600	-1.55822000	-0.17760000
IRC_TS1_point302			
B	-2.68809600	3.98956800	0.33549800
B	-1.59703100	3.83944000	1.73425600
B	-0.71856000	2.30476200	1.58644200
B	-2.48299200	2.55115800	-0.68887700
B	-1.26131200	1.57077600	0.08889200
B	-1.14454400	4.87561800	0.36179200
B	-1.68676900	4.08686700	-1.13646900
H	-3.73546900	4.54822000	0.41055000
B	0.07386800	3.83412000	1.12656600
H	-1.86892500	4.28984400	2.80104900
B	0.27883700	2.40983000	0.10411500
H	-0.35139600	1.66226200	2.51165400
B	-0.80599100	2.56107700	-1.29659400
H	-3.35915500	2.07045700	-1.32999100
H	-1.10221900	6.05985900	0.46419300
B	0.01993800	3.99767100	-0.65027800
H	-2.03015700	4.69786600	-2.09669900
H	0.99442800	4.24902600	1.75509900
H	-0.56576400	2.08360900	-2.36292900
H	0.89837500	4.52302800	-1.25446800
B	-2.42974100	2.40564400	1.09575100
I	-1.46640100	-0.65773400	-0.18977000
C	0.37182900	-1.42752100	0.62006900
C	0.70649700	-1.14748300	1.93763300
C	1.14621600	-2.23586300	-0.20006300
C	1.88509700	-1.69490900	2.44381100
H	0.07746600	-0.52100100	2.55342000
C	2.31380900	-2.78553200	0.33177800
H	0.85856900	-2.43301000	-1.22382400
C	2.68424900	-2.51309300	1.64556600
H	2.17206400	-1.47880700	3.46648100
H	2.93584400	-3.41299600	-0.29516000
H	3.59967200	-2.93150300	2.04640400
O	-2.09824800	-4.04858700	-0.27093600
C	-3.35821700	-4.07693200	-0.38199500
O	-4.04833900	-3.21282400	-0.99667600
C	-4.10323200	-5.21669200	0.30800900
H	-4.36205400	-4.89097600	1.32361000

H	-5.03225700	-5.45965800	-0.21213600
H	-3.47845800	-6.10838500	0.39125800
H	0.75525400	1.24772600	-2.05456000
H	-3.27244200	1.81631300	1.68946500
N	1.62263900	1.70885000	0.10021200
C	2.18111000	0.96290000	-0.80735400
H	2.15516400	1.80749100	0.95879200
C	3.47865900	0.30080700	-0.62114000
O	1.60036700	0.75198500	-1.96562200
C	4.00473800	-0.46739300	-1.66976900
C	4.18160000	0.39281300	0.58802200
C	5.21385400	-1.13163500	-1.50879700
H	3.46268600	-0.54995000	-2.60173000
C	5.39065500	-0.27263300	0.74160800
H	3.80345900	0.96797500	1.42432800
C	5.90798700	-1.03760400	-0.30326000
H	5.61066800	-1.72821900	-2.32152200
H	5.92442000	-0.20114400	1.68150500
H	6.84845000	-1.56144500	-0.17616300

IRC_TS1_point303

B	-2.68799200	3.99006500	0.33493500
B	-1.59750500	3.83955900	1.73413800
B	-0.71939200	2.30490100	1.58660600
B	-2.48286100	2.55175700	-0.68947800
B	-1.26186500	1.57062600	0.08886900
B	-1.14436900	4.87569000	0.36200500
B	-1.68615900	4.08729500	-1.13658100
H	-3.73531000	4.54858000	0.40996300
B	0.07354500	3.83403400	1.12710400
H	-1.86977100	4.28956000	2.80099100
B	0.27850500	2.40970800	0.10484600
H	-0.35264500	1.66209500	2.51182700
B	-0.80576700	2.56125500	-1.29663300
H	-3.35896400	2.07112900	-1.33074700
H	-1.10207700	6.06000500	0.46477200
B	0.02037200	3.99755400	-0.64986500
H	-2.02923200	4.69840800	-2.09677500
H	0.99402100	4.24855100	1.75610300
H	-0.56515000	2.08386100	-2.36267100
H	0.89859100	4.52326100	-1.25313000
B	-2.43033700	2.40620300	1.09526800
I	-1.46704600	-0.65756100	-0.18965400
C	0.37164800	-1.42715700	0.61952000

C	0.70695900	-1.14683800	1.93688100
C	1.14561600	-2.23579800	-0.20074600
C	1.88584900	-1.69405900	2.44258800
H	0.07797200	-0.52072400	2.55302000
C	2.31348300	-2.78531500	0.33068200
H	0.85756700	-2.43330300	-1.22431100
C	2.68462600	-2.51244200	1.64417000
H	2.17298600	-1.47831800	3.46528900
H	2.93521000	-3.41313300	-0.29621600
H	3.60004200	-2.93113200	2.04489300
O	-2.09663200	-4.05124300	-0.27423500
C	-3.35712900	-4.07894200	-0.38221700
O	-4.04620200	-3.21710100	-1.00207700
C	-4.10295100	-5.21379400	0.31642700
H	-4.35968300	-4.88445400	1.32914000
H	-5.03170800	-5.45646100	-0.20210100
H	-3.47919400	-6.10477400	0.40159800
H	0.75729900	1.25069600	-2.05536900
H	-3.27293700	1.81677500	1.68848300
N	1.62135900	1.70635500	0.10564400
C	2.18233700	0.96443200	-0.80910900
H	2.15353500	1.80648500	0.95978400
C	3.47915200	0.30147900	-0.62110700
O	1.60243700	0.75497100	-1.96720300
C	4.00436700	-0.46786200	-1.66905000
C	4.18200100	0.39336000	0.58831500
C	5.21289700	-1.13299400	-1.50786900
H	3.46205600	-0.55024400	-2.60084700
C	5.39058500	-0.27295100	0.74206500
H	3.80449700	0.96912000	1.42455400
C	5.90721900	-1.03882500	-0.30250900
H	5.60947600	-1.72956800	-2.32069800
H	5.92477700	-0.20107900	1.68170100
H	6.84761300	-1.56273400	-0.17553500
IRC_TS1_point304			
B	-2.68790200	3.99086300	0.33447900
B	-1.59814700	3.83995300	1.73417100
B	-0.72047900	2.30487500	1.58693400
B	-2.48284500	2.55245200	-0.68989500
B	-1.26251600	1.57129500	0.08888700
B	-1.14386300	4.87599700	0.36217500
B	-1.68525900	4.08769900	-1.13664500
H	-3.73511100	4.55011600	0.40877900
B	0.07328100	3.83375300	1.12786800

H	-1.87070700	4.29028500	2.80098700
B	0.27839200	2.40935700	0.10558000
H	-0.35451800	1.66195800	2.51232800
B	-0.80533100	2.56139900	-1.29622800
H	-3.35881300	2.07223700	-1.33167200
H	-1.10049800	6.06066000	0.46448200
B	0.02093900	3.99742400	-0.64899900
H	-2.02751100	4.69898600	-2.09713500
H	0.99354600	4.24798200	1.75728500
H	-0.56489000	2.08433400	-2.36257100
H	0.89996400	4.52269300	-1.25221900
B	-2.43107400	2.40674500	1.09473200
I	-1.46770700	-0.65750800	-0.18946800
C	0.37138700	-1.42686900	0.61889000
C	0.70744400	-1.14626800	1.93599500
C	1.14484000	-2.23564400	-0.20169700
C	1.88662300	-1.69342300	2.44110800
H	0.07885700	-0.51989300	2.55237400
C	2.31297100	-2.78516500	0.32919000
H	0.85608900	-2.43329000	-1.22507800
C	2.68489000	-2.51204000	1.64240200
H	2.17432300	-1.47751900	3.46360300
H	2.93413600	-3.41328000	-0.29799000
H	3.60045500	-2.93074100	2.04263100
O	-2.09494100	-4.05519100	-0.27766000
C	-3.35547400	-4.08130300	-0.38329700
O	-4.04508700	-3.22285900	-1.00667800
C	-4.10128000	-5.20934700	0.32359000
H	-4.35587000	-4.87117600	1.33483900
H	-5.03335100	-5.45348200	-0.18984600
H	-3.47943300	-6.10252500	0.41690100
H	0.75931100	1.25499700	-2.05654900
H	-3.27428600	1.81761900	1.68755600
N	1.62156900	1.70690100	0.10378000
C	2.18235800	0.96509200	-0.80650300
H	2.15134600	1.80228800	0.96345300
C	3.47912100	0.30163500	-0.62007000
O	1.60419500	0.75897600	-1.96742600
C	4.00379600	-0.46835400	-1.66805200
C	4.18251000	0.39368000	0.58888300
C	5.21187900	-1.13437000	-1.50676600
H	3.46136600	-0.55084800	-2.59976500
C	5.39060900	-0.27343300	0.74273500
H	3.80578800	0.97052800	1.42470900

C	5.90646900	-1.04022600	-0.30152900
H	5.60792100	-1.73168700	-2.31931400
H	5.92507700	-0.20134400	1.68220400
H	6.84663600	-1.56459100	-0.17449000

IRC_TS1_point305

B	-2.68774400	3.99158300	0.33386000
B	-1.59845700	3.84046000	1.73394800
B	-0.72119000	2.30514200	1.58707500
B	-2.48275400	2.55301200	-0.69035600
B	-1.26292900	1.57131700	0.08886800
B	-1.14349100	4.87628300	0.36207000
B	-1.68462600	4.08807200	-1.13686700
H	-3.73484100	4.55068900	0.40807300
B	0.07308800	3.83383500	1.12823800
H	-1.87119800	4.29070100	2.80065000
B	0.27808200	2.40935200	0.10612300
H	-0.35536900	1.66216600	2.51252000
B	-0.80512100	2.56143600	-1.29613800
H	-3.35859700	2.07277900	-1.33225700
H	-1.10068200	6.06043400	0.46480300
B	0.02144600	3.99733100	-0.64879100
H	-2.02668800	4.69925900	-2.09737000
H	0.99332400	4.24800600	1.75777200
H	-0.56463000	2.08420200	-2.36236500
H	0.90056000	4.52227300	-1.25190600
B	-2.43170500	2.40743200	1.09441500
I	-1.46863000	-0.65729700	-0.18902500
C	0.37118500	-1.42642500	0.61838200
C	0.70789400	-1.14549800	1.93525600
C	1.14424000	-2.23536400	-0.20241200
C	1.88729300	-1.69254300	2.43993200
H	0.07948900	-0.51913500	2.55180500
C	2.31257500	-2.78483800	0.32808800
H	0.85526800	-2.43308400	-1.22566400
C	2.68510200	-2.51145600	1.64106600
H	2.17526200	-1.47658000	3.46236500
H	2.93355300	-3.41305600	-0.29910300
H	3.60063900	-2.93032900	2.04121900
O	-2.09287100	-4.05906700	-0.28138000
C	-3.35370600	-4.08382600	-0.38453000
O	-4.04249600	-3.22797300	-1.01284100
C	-4.10096900	-5.20658000	0.33157400
H	-4.35306500	-4.86194700	1.34100200

H	-5.03234000	-5.45240800	-0.18099200
H	-3.48056300	-6.09885000	0.42606900
H	0.76110700	1.25775200	-2.05651000
H	-3.27508800	1.81841200	1.68718000
N	1.62054500	1.70542800	0.10715500
C	2.18346100	0.96666800	-0.80767500
H	2.14980100	1.80036900	0.96472400
C	3.47951800	0.30216100	-0.61964600
O	1.60638900	0.76208900	-1.96811500
C	4.00337600	-0.46881100	-1.66718500
C	4.18296600	0.39407700	0.58934700
C	5.21093400	-1.13565900	-1.50576300
H	3.46086000	-0.55121300	-2.59885900
C	5.39067000	-0.27379300	0.74327000
H	3.80669600	0.97136400	1.42507700
C	5.90584700	-1.04136800	-0.30074700
H	5.60660700	-1.73329300	-2.31825000
H	5.92536000	-0.20167600	1.68261400
H	6.84585900	-1.56603700	-0.17378000

IRC_TS1_point306

B	-2.68762800	3.99227400	0.33330500
B	-1.59884900	3.84101400	1.73376000
B	-0.72188900	2.30552100	1.58731200
B	-2.48270000	2.55362600	-0.69072500
B	-1.26345000	1.57181000	0.08900100
B	-1.14322100	4.87653900	0.36195400
B	-1.68396700	4.08836000	-1.13711900
H	-3.73468700	4.55163800	0.40712300
B	0.07293400	3.83394400	1.12856700
H	-1.87171500	4.29141300	2.80034800
B	0.27803600	2.40919100	0.10676800
H	-0.35641000	1.66258900	2.51292700
B	-0.80482300	2.56147200	-1.29594100
H	-3.35848700	2.07341700	-1.33275700
H	-1.09959500	6.06115500	0.46401800
B	0.02188500	3.99716800	-0.64843000
H	-2.02567900	4.69943600	-2.09789000
H	0.99309700	4.24802800	1.75824500
H	-0.56417500	2.08406200	-2.36204400
H	0.90107500	4.52199000	-1.25139100
B	-2.43216800	2.40818200	1.09402400
I	-1.46963100	-0.65711500	-0.18849000
C	0.37080200	-1.42593600	0.61778700

C	0.70824600	-1.14468900	1.93441400
C	1.14344500	-2.23501100	-0.20325700
C	1.88790500	-1.69159900	2.43858200
H	0.08012800	-0.51826400	2.55120300
C	2.31202500	-2.78444500	0.32680400
H	0.85397400	-2.43296900	-1.22633900
C	2.68522900	-2.51079500	1.63952700
H	2.17631700	-1.47548500	3.46086800
H	2.93267900	-3.41291400	-0.30049400
H	3.60084500	-2.92973400	2.03943100
O	-2.09053100	-4.06367000	-0.28484600
C	-3.35158500	-4.08663700	-0.38547300
O	-4.03986600	-3.23427700	-1.01903200
C	-4.09972100	-5.20271300	0.33828800
H	-4.35045600	-4.85345500	1.34554200
H	-5.03304400	-5.44974300	-0.17156100
H	-3.48126100	-6.09721500	0.43750100
H	0.76297100	1.26117600	-2.05736900
H	-3.27570800	1.81935700	1.68667200
N	1.62045400	1.70529100	0.10726800
C	2.18393900	0.96764000	-0.80606500
H	2.14789800	1.79747300	0.96754000
C	3.47964000	0.30238000	-0.61868300
O	1.60872300	0.76652100	-1.96914900
C	4.00273000	-0.46944200	-1.66606300
C	4.18350500	0.39435100	0.59000000
C	5.20979100	-1.13719800	-1.50461500
H	3.45994800	-0.55188800	-2.59755400
C	5.39074000	-0.27435500	0.74395100
H	3.80792400	0.97262300	1.42537600
C	5.90506600	-1.04286100	-0.29980100
H	5.60487300	-1.73539600	-2.31698600
H	5.92582200	-0.20197100	1.68302200
H	6.84486200	-1.56792300	-0.17294100

IRC_TS1_point307

B	-2.68745900	3.99321600	0.33264200
B	-1.59919600	3.84175300	1.73347200
B	-0.72270400	2.30586700	1.58746900
B	-2.48265600	2.55426100	-0.69109600
B	-1.26399300	1.57217100	0.08910600
B	-1.14268300	4.87701000	0.36163400
B	-1.68321200	4.08870700	-1.13745300
H	-3.73433600	4.55314300	0.40599900

B	0.07281100	3.83403300	1.12886100
H	-1.87224100	4.29257700	2.79990700
B	0.27771100	2.40917700	0.10727600
H	-0.35768700	1.66287800	2.51324100
B	-0.80449900	2.56147100	-1.29566800
H	-3.35834200	2.07438500	-1.33348100
H	-1.09919300	6.06122600	0.46397000
B	0.02243600	3.99716900	-0.64816200
H	-2.02430400	4.69980300	-2.09839100
H	0.99286800	4.24780700	1.75888500
H	-0.56399200	2.08400000	-2.36175800
H	0.90216100	4.52155800	-1.25093000
B	-2.43283200	2.40902900	1.09368300
I	-1.47067500	-0.65692600	-0.18783300
C	0.37038700	-1.42551000	0.61739600
C	0.70856600	-1.14392800	1.93376700
C	1.14255600	-2.23476200	-0.20391300
C	1.88855100	-1.69064400	2.43737100
H	0.08080100	-0.51732400	2.55075700
C	2.31145200	-2.78404200	0.32562800
H	0.85246700	-2.43300400	-1.22676500
C	2.68542200	-2.51003100	1.63805300
H	2.17760100	-1.47418100	3.45940800
H	2.93173800	-3.41263900	-0.30189800
H	3.60135100	-2.92871900	2.03745500
O	-2.08831700	-4.06851200	-0.28806800
C	-3.34935800	-4.08957400	-0.38733100
O	-4.03685400	-3.24027600	-1.02560200
C	-4.09879300	-5.19978100	0.34501500
H	-4.34830600	-4.84199400	1.35101500
H	-5.03173000	-5.44852700	-0.16375900
H	-3.48113800	-6.09336700	0.44883000
H	0.76486900	1.26436200	-2.05784500
H	-3.27676900	1.82042100	1.68600500
N	1.61961500	1.70426200	0.10930600
C	2.18486400	0.96923600	-0.80662600
H	2.14596200	1.79475500	0.96965500
C	3.48002500	0.30301400	-0.61828300
O	1.61121300	0.77033000	-1.96978900
C	4.00234100	-0.46991400	-1.66519600
C	4.18401800	0.39491600	0.59039300
C	5.20877200	-1.13871300	-1.50344500
H	3.45937400	-0.55253000	-2.59658500
C	5.39069200	-0.27478400	0.74460500

H	3.80921000	0.97411400	1.42547300
C	5.90425300	-1.04433100	-0.29875200
H	5.60314100	-1.73785000	-2.31546000
H	5.92590400	-0.20239000	1.68363200
H	6.84350300	-1.57034300	-0.17158300

IRC_TS1_point308

B	-2.68732900	3.99380500	0.33205700
B	-1.59955100	3.84218100	1.73329700
B	-0.72339500	2.30617800	1.58767300
B	-2.48266000	2.55482700	-0.69154800
B	-1.26461100	1.57238500	0.08915400
B	-1.14246700	4.87714000	0.36159400
B	-1.68266900	4.08898600	-1.13766500
H	-3.73413000	4.55348000	0.40519500
B	0.07260400	3.83405500	1.12920200
H	-1.87295200	4.29277100	2.79957400
B	0.27756900	2.40889100	0.10788100
H	-0.35883000	1.66307200	2.51351000
B	-0.80442400	2.56149100	-1.29564100
H	-3.35825600	2.07498800	-1.33410400
H	-1.09835800	6.06166100	0.46356800
B	0.02282600	3.99684200	-0.64789100
H	-2.02340600	4.70023500	-2.09858900
H	0.99259700	4.24771900	1.75938600
H	-0.56378200	2.08384600	-2.36159500
H	0.90275200	4.52100300	-1.25042700
B	-2.43335500	2.40972400	1.09329400
I	-1.47174100	-0.65674600	-0.18724300
C	0.37001600	-1.42508400	0.61686300
C	0.70877600	-1.14324200	1.93301600
C	1.14181800	-2.23446800	-0.20462900
C	1.88891700	-1.68989600	2.43628100
H	0.08111100	-0.51684400	2.55026000
C	2.31094800	-2.78364800	0.32454500
H	0.85135300	-2.43288800	-1.22731500
C	2.68545000	-2.50940500	1.63675800
H	2.17823600	-1.47352400	3.45824900
H	2.93097400	-3.41243800	-0.30301400
H	3.60148100	-2.92814900	2.03594700
O	-2.08550300	-4.07295900	-0.29136700
C	-3.34704900	-4.09205800	-0.38839500
O	-4.03309300	-3.24576400	-1.03254900
C	-4.09814800	-5.19570200	0.35201800

H	-4.34476200	-4.83457000	1.35577300
H	-5.03348400	-5.44579000	-0.15292800
H	-3.48266000	-6.09110000	0.45902000
H	0.76688800	1.26760300	-2.05869300
H	-3.27772000	1.82153300	1.68551200
N	1.61923600	1.70364700	0.10980400
C	2.18539100	0.97009600	-0.80549800
H	2.14416200	1.79198100	0.97160700
C	3.48021600	0.30333500	-0.61745000
O	1.61378400	0.77449700	-1.97111100
C	4.00181100	-0.47044600	-1.66415700
C	4.18454700	0.39544400	0.59091800
C	5.20774300	-1.14007600	-1.50229000
H	3.45869000	-0.55311100	-2.59544500
C	5.39067500	-0.27517200	0.74529300
H	3.81041600	0.97575900	1.42554000
C	5.90345700	-1.04567300	-0.29774000
H	5.60160400	-1.73979700	-2.31413900
H	5.92615900	-0.20252100	1.68411200
H	6.84241100	-1.57213800	-0.17055500

IRC_TS1_point309

B	-2.68711100	3.99491300	0.33139000
B	-1.59995000	3.84298300	1.73302900
B	-0.72443000	2.30647100	1.58789600
B	-2.48267400	2.55558200	-0.69188600
B	-1.26536400	1.57292600	0.08935800
B	-1.14175200	4.87757000	0.36125200
B	-1.68169800	4.08931900	-1.13804200
H	-3.73361900	4.55593800	0.40378800
B	0.07251600	3.83398400	1.12953300
H	-1.87340600	4.29435700	2.79920000
B	0.27715400	2.40872800	0.10847600
H	-0.36053800	1.66337900	2.51406400
B	-0.80398900	2.56138800	-1.29528300
H	-3.35824700	2.07620400	-1.33481100
H	-1.09732300	6.06190200	0.46317400
B	0.02349500	3.99672000	-0.64753500
H	-2.02162500	4.70051000	-2.09939400
H	0.99244400	4.24726400	1.76006100
H	-0.56341300	2.08342200	-2.36114100
H	0.90374100	4.52068100	-1.24964300
B	-2.43418000	2.41069800	1.09294100
I	-1.47269300	-0.65665500	-0.18667800

C	0.36957000	-1.42466000	0.61647400
C	0.70906100	-1.14253800	1.93239800
C	1.14092600	-2.23413000	-0.20535100
C	1.88952500	-1.68902700	2.43504800
H	0.08188200	-0.51572200	2.54980900
C	2.31035200	-2.78323700	0.32328500
H	0.84984400	-2.43266100	-1.22786600
C	2.68558900	-2.50875600	1.63523800
H	2.17960300	-1.47216600	3.45671000
H	2.92999600	-3.41208600	-0.30461600
H	3.60193500	-2.92726600	2.03387600
O	-2.08362100	-4.07769500	-0.29367500
C	-3.34469000	-4.09504700	-0.39048200
O	-4.03029000	-3.25197500	-1.03858000
C	-4.09661400	-5.19228700	0.35785800
H	-4.34154400	-4.82077200	1.36051400
H	-5.03233000	-5.44344900	-0.14460100
H	-3.48238400	-6.08745000	0.47142800
H	0.76900600	1.27172800	-2.05995000
H	-3.27881300	1.82272500	1.68468900
N	1.61826200	1.70228600	0.11188300
C	2.18616200	0.97173100	-0.80602100
H	2.14159400	1.78775500	0.97496600
C	3.48051800	0.30394200	-0.61714800
O	1.61622400	0.77918000	-1.97217500
C	4.00146000	-0.47095200	-1.66330600
C	4.18493900	0.39602800	0.59126900
C	5.20673700	-1.14167800	-1.50098600
H	3.45813600	-0.55386800	-2.59444100
C	5.39045900	-0.27562500	0.74606700
H	3.81159800	0.97744400	1.42549100
C	5.90252800	-1.04725300	-0.29648600
H	5.59984600	-1.74248200	-2.31237700
H	5.92599900	-0.20295700	1.68487800
H	6.84083500	-1.57481600	-0.16884400

IRC_TS1_point310

B	-2.68701000	3.99546900	0.33081200
B	-1.60032200	3.84327400	1.73286400
B	-0.72520500	2.30659400	1.58810400
B	-2.48275400	2.55613000	-0.69240300
B	-1.26597500	1.57294500	0.08936100
B	-1.14153100	4.87769200	0.36134900
B	-1.68122500	4.08963200	-1.13815100

H	-3.73338400	4.55588700	0.40311500
B	0.07225000	3.83384500	1.13002000
H	-1.87418200	4.29416100	2.79886100
B	0.27687300	2.40829300	0.10907000
H	-0.36175500	1.66334600	2.51426300
B	-0.80408900	2.56137000	-1.29515200
H	-3.35821200	2.07699800	-1.33563200
H	-1.09688900	6.06202300	0.46335100
B	0.02382500	3.99634400	-0.64712100
H	-2.02075200	4.70090600	-2.09947500
H	0.99200800	4.24692300	1.76089900
H	-0.56344500	2.08385100	-2.36105800
H	0.90485700	4.51942700	-1.24943000
B	-2.43475500	2.41127200	1.09250700
I	-1.47368200	-0.65654000	-0.18621200
C	0.36908100	-1.42447500	0.61615300
C	0.70914800	-1.14220500	1.93188400
C	1.14012600	-2.23388600	-0.20598000
C	1.88994900	-1.68845400	2.43399700
H	0.08212600	-0.51554300	2.54952200
C	2.30981300	-2.78288300	0.32219000
H	0.84864000	-2.43258400	-1.22832900
C	2.68566800	-2.50822900	1.63392200
H	2.18045300	-1.47151300	3.45551200
H	2.92922900	-3.41177900	-0.30586000
H	3.60218200	-2.92671300	2.03222900
O	-2.08043600	-4.08146400	-0.29715900
C	-3.34252000	-4.09704600	-0.39129600
O	-4.02623700	-3.25670100	-1.04579600
C	-4.09650700	-5.18788900	0.36561400
H	-4.33852500	-4.81307200	1.36534600
H	-5.03406100	-5.44009900	-0.13355000
H	-3.48446600	-6.08412300	0.48203500
H	0.77129400	1.27498200	-2.06060300
H	-3.28009600	1.82397400	1.68442100
N	1.61774600	1.70168900	0.11199100
C	2.18673400	0.97254900	-0.80495700
H	2.13972000	1.78539300	0.97584500
C	3.48073800	0.30436100	-0.61635800
O	1.61887600	0.78266100	-1.97309100
C	4.00100600	-0.47132200	-1.66235200
C	4.18542000	0.39666300	0.59176600
C	5.20573800	-1.14293900	-1.49984500
H	3.45756500	-0.55432300	-2.59343000

C	5.39042600	-0.27584100	0.74673600
H	3.81270600	0.97917900	1.42551800
C	5.90169100	-1.04849400	-0.29543600
H	5.59835000	-1.74444600	-2.31097900
H	5.92621700	-0.20292900	1.68536300
H	6.83962800	-1.57663900	-0.16765600

IRC_TS1_point311

B	-2.68685500	3.99633700	0.33023200
B	-1.60077700	3.84380600	1.73268200
B	-0.72626600	2.30673800	1.58828500
B	-2.48281700	2.55681400	-0.69277500
B	-1.26690000	1.57337600	0.08951700
B	-1.14090600	4.87784900	0.36111500
B	-1.68032500	4.08987100	-1.13846000
H	-3.73302900	4.55801400	0.40182000
B	0.07208900	3.83359300	1.13034100
H	-1.87469800	4.29536000	2.79864200
B	0.27651100	2.40799500	0.10964400
H	-0.36352800	1.66340200	2.51473100
B	-0.80373100	2.56127400	-1.29505300
H	-3.35830100	2.07805100	-1.33627600
H	-1.09528700	6.06239000	0.46265900
B	0.02447900	3.99598300	-0.64684400
H	-2.01918400	4.70120700	-2.10004100
H	0.99180600	4.24632300	1.76154900
H	-0.56321500	2.08304300	-2.36088600
H	0.90512600	4.51951700	-1.24808600
B	-2.43564300	2.41211200	1.09217600
I	-1.47450600	-0.65647600	-0.18582000
C	0.36867500	-1.42414000	0.61571700
C	0.70935400	-1.14174700	1.93127200
C	1.13935900	-2.23356300	-0.20674100
C	1.89044300	-1.68787200	2.43282800
H	0.08264600	-0.51499800	2.54917300
C	2.30931600	-2.78248900	0.32092700
H	0.84735900	-2.43223900	-1.22896100
C	2.68580100	-2.50770300	1.63243200
H	2.18151800	-1.47078700	3.45414600
H	2.92840700	-3.41139800	-0.30744400
H	3.60258500	-2.92606400	2.03023200
O	-2.07901200	-4.08566600	-0.29868100
C	-3.34000600	-4.09966200	-0.39355200
O	-4.02371100	-3.26262900	-1.05124300

C	-4.09489000	-5.18340300	0.37119800
H	-4.33266500	-4.79750700	1.37026000
H	-5.03517900	-5.43615600	-0.12275700
H	-3.48541700	-6.08096700	0.49405300
H	0.77364600	1.27984100	-2.06232300
H	-3.28098100	1.82485700	1.68335100
N	1.61672800	1.69986700	0.11466000
C	2.18746400	0.97404500	-0.80539400
H	2.13663700	1.77964400	0.98061000
C	3.48095900	0.30473700	-0.61593800
O	1.62126200	0.78795700	-1.97473000
C	4.00066900	-0.47190100	-1.66142000
C	4.18579500	0.39718100	0.59217700
C	5.20484800	-1.14441000	-1.49854000
H	3.45700800	-0.55512500	-2.59231400
C	5.39028900	-0.27617300	0.74752000
H	3.81383800	0.98080900	1.42550100
C	5.90090000	-1.04986700	-0.29421500
H	5.59679800	-1.74680700	-2.30930700
H	5.92624900	-0.20304100	1.68604900
H	6.83833800	-1.57881600	-0.16611100

IRC_TS1_point312

B	-2.68669200	3.99717400	0.32960100
B	-1.60121500	3.84428200	1.73250400
B	-0.72727800	2.30676900	1.58863500
B	-2.48292800	2.55735200	-0.69315800
B	-1.26745900	1.57344700	0.08960000
B	-1.14047800	4.87811300	0.36112100
B	-1.67963100	4.09013500	-1.13864500
H	-3.73257400	4.55900100	0.40087100
B	0.07185200	3.83335200	1.13094300
H	-1.87550300	4.29579500	2.79821100
B	0.27601900	2.40745400	0.11043000
H	-0.36515000	1.66337300	2.51526200
B	-0.80366200	2.56102600	-1.29451500
H	-3.35830400	2.07895400	-1.33702200
H	-1.09518700	6.06222700	0.46306700
B	0.02486300	3.99565700	-0.64619500
H	-2.01774000	4.70145500	-2.10052600
H	0.99148300	4.24574900	1.76245500
H	-0.56274000	2.08320000	-2.36019300
H	0.90706400	4.51760600	-1.24824300
B	-2.43636600	2.41272300	1.09174400

I	-1.47543700	-0.65649300	-0.18546900
C	0.36821900	-1.42398500	0.61537600
C	0.70948600	-1.14145900	1.93074400
C	1.13859200	-2.23329800	-0.20745600
C	1.89089200	-1.68741800	2.43174100
H	0.08308200	-0.51459600	2.54886200
C	2.30881100	-2.78216600	0.31970100
H	0.84619900	-2.43200000	-1.22955200
C	2.68589700	-2.50728900	1.63102100
H	2.18248900	-1.47011800	3.45287000
H	2.92767700	-3.41104600	-0.30891000
H	3.60290400	-2.92550700	2.02841800
O	-2.07577500	-4.08917400	-0.30222400
C	-3.33825700	-4.10141400	-0.39392000
O	-4.01986700	-3.26714000	-1.05841500
C	-4.09472900	-5.17892700	0.37913100
H	-4.33149800	-4.78917600	1.37451900
H	-5.03438400	-5.43216500	-0.11409700
H	-3.48661700	-6.07607800	0.50575900
H	0.77603600	1.28329500	-2.06309300
H	-3.28273000	1.82632100	1.68320900
N	1.61607400	1.69938000	0.11450900
C	2.18795800	0.97503500	-0.80439200
H	2.13440400	1.77717800	0.98116700
C	3.48118500	0.30535000	-0.61530400
O	1.62378500	0.79117800	-1.97513400
C	4.00023100	-0.47221400	-1.66052400
C	4.18623300	0.39790100	0.59260100
C	5.20386200	-1.14566100	-1.49734800
H	3.45647500	-0.55563700	-2.59137400
C	5.39017100	-0.27638500	0.74823100
H	3.81489300	0.98261000	1.42546200
C	5.90005600	-1.05108900	-0.29308800
H	5.59529000	-1.74890600	-2.30776100
H	5.92624600	-0.20316200	1.68668400
H	6.83705700	-1.58078300	-0.16472200

IRC_TS1_point313

B	-2.68664500	3.99759800	0.32906400
B	-1.60169600	3.84445700	1.73237100
B	-0.72819400	2.30683500	1.58875900
B	-2.48300000	2.55789200	-0.69369000
B	-1.26837000	1.57355900	0.08961600
B	-1.14015600	4.87796500	0.36111900

B	-1.67904100	4.09030300	-1.13877000
H	-3.73246700	4.55938900	0.39997700
B	0.07155900	3.83302900	1.13131600
H	-1.87620400	4.29599900	2.79803400
B	0.27580300	2.40705800	0.11089800
H	-0.36660400	1.66321300	2.51539600
B	-0.80362100	2.56108300	-1.29470700
H	-3.35831800	2.07969400	-1.33780700
H	-1.09361900	6.06260000	0.46248500
B	0.02540800	3.99505100	-0.64599900
H	-2.01677800	4.70179700	-2.10053600
H	0.99097800	4.24522500	1.76324200
H	-0.56335400	2.08315400	-2.36064200
H	0.90678700	4.51774000	-1.24664100
B	-2.43713600	2.41333200	1.09136700
I	-1.47627900	-0.65640700	-0.18510500
C	0.36782600	-1.42374200	0.61489400
C	0.70956000	-1.14121000	1.93014400
C	1.13792400	-2.23298100	-0.20823800
C	1.89121100	-1.68703300	2.43066200
H	0.08324100	-0.51459100	2.54852100
C	2.30836100	-2.78179200	0.31850600
H	0.84514800	-2.43166500	-1.23022800
C	2.68594200	-2.50687900	1.62965400
H	2.18314100	-1.46986000	3.45170900
H	2.92697200	-3.41069300	-0.31033200
H	3.60307500	-2.92519600	2.02671300
O	-2.07416200	-4.09307900	-0.30384500
C	-3.33537800	-4.10352900	-0.39627300
O	-4.01703700	-3.27254800	-1.06376800
C	-4.09371500	-5.17344200	0.38498300
H	-4.32641100	-4.77326400	1.37923700
H	-5.03750100	-5.42811200	-0.10223400
H	-3.48882700	-6.07297100	0.51821000
H	0.77861300	1.28783900	-2.06449700
H	-3.28337100	1.82688800	1.68208600
N	1.61523000	1.69761100	0.11703300
C	2.18888600	0.97634000	-0.80463000
H	2.13144800	1.77162400	0.98546300
C	3.48148300	0.30562600	-0.61464500
O	1.62652300	0.79623200	-1.97690800
C	3.99988400	-0.47274600	-1.65951600
C	4.18673100	0.39848800	0.59311400
C	5.20299400	-1.14698200	-1.49611300

H	3.45588500	-0.55622500	-2.59019200
C	5.39019300	-0.27656900	0.74897400
H	3.81610900	0.98438200	1.42547400
C	5.89933600	-1.05228600	-0.29196500
H	5.59386500	-1.75088500	-2.30628300
H	5.92658800	-0.20299900	1.68721100
H	6.83597400	-1.58252500	-0.16344100

IRC_TS1_point314

B	-2.68648300	3.99854000	0.32845800
B	-1.60217100	3.84500700	1.73217800
B	-0.72931800	2.30680200	1.58907000
B	-2.48312900	2.55840600	-0.69394900
B	-1.26902400	1.57384400	0.08979400
B	-1.13955300	4.87828300	0.36092500
B	-1.67817000	4.09048000	-1.13909700
H	-3.73201000	4.56164300	0.39873600
B	0.07136300	3.83273500	1.13181300
H	-1.87679000	4.29706600	2.79768700
B	0.27523400	2.40655400	0.11169800
H	-0.36832700	1.66319400	2.51603000
B	-0.80328700	2.56064700	-1.29412700
H	-3.35839900	2.08058100	-1.33839600
H	-1.09328100	6.06241200	0.46259600
B	0.02583700	3.99481300	-0.64538400
H	-2.01517700	4.70187300	-2.10134700
H	0.99086400	4.24453200	1.76393400
H	-0.56236600	2.08222200	-2.35965200
H	0.90866000	4.51618100	-1.24678100
B	-2.43798800	2.41394700	1.09099300
I	-1.47718900	-0.65648400	-0.18480400
C	0.36741000	-1.42350600	0.61445400
C	0.70967300	-1.14094300	1.92956200
C	1.13724500	-2.23261500	-0.20905200
C	1.89159800	-1.68666900	2.42956000
H	0.08365400	-0.51420300	2.54821000
C	2.30791400	-2.78141800	0.31721400
H	0.84411000	-2.43124400	-1.23095200
C	2.68602200	-2.50650800	1.62821700
H	2.18397500	-1.46937500	3.45046900
H	2.92631700	-3.41027700	-0.31186600
H	3.60334500	-2.92468700	2.02490500
O	-2.07141700	-4.09689000	-0.30677600
C	-3.33387900	-4.10529700	-0.39651500

O	-4.01324800	-3.27722400	-1.07104200
C	-4.09325100	-5.16883700	0.39240400
H	-4.32469100	-4.76411600	1.38336400
H	-5.03552400	-5.42380700	-0.09465000
H	-3.48932300	-6.06698200	0.52922100
H	0.78072600	1.29163400	-2.06554500
H	-3.28500700	1.82810400	1.68183000
N	1.61449000	1.69680200	0.11765700
C	2.18927400	0.97751000	-0.80370200
H	2.12866400	1.76758500	0.98777600
C	3.48166700	0.30621000	-0.61410400
O	1.62883000	0.80025300	-1.97741600
C	3.99950800	-0.47316600	-1.65856700
C	4.18717500	0.39916800	0.59351200
C	5.20213100	-1.14826600	-1.49481300
H	3.45542500	-0.55701000	-2.58916700
C	5.39014000	-0.27672200	0.74972100
H	3.81715400	0.98602700	1.42546700
C	5.89864700	-1.05343700	-0.29077500
H	5.59249100	-1.75300000	-2.30462700
H	5.92667100	-0.20294600	1.68786800
H	6.83492400	-1.58430900	-0.16202400

IRC_TS1_point315

B	-2.68643200	3.99899500	0.32784100
B	-1.60266200	3.84521800	1.73202300
B	-0.73023500	2.30686600	1.58931700
B	-2.48320000	2.55887500	-0.69451500
B	-1.26976500	1.57371200	0.08976500
B	-1.13934800	4.87817100	0.36101000
B	-1.67764900	4.09063300	-1.13918900
H	-3.73183700	4.56131600	0.39800000
B	0.07104200	3.83242700	1.13230100
H	-1.87772400	4.29693400	2.79736100
B	0.27492600	2.40597500	0.11229500
H	-0.36982000	1.66308700	2.51633500
B	-0.80338500	2.56059900	-1.29404900
H	-3.35839700	2.08126900	-1.33921300
H	-1.09229800	6.06262900	0.46236700
B	0.02631300	3.99414400	-0.64503200
H	-2.01409300	4.70218600	-2.10140200
H	0.99025600	4.24409200	1.76483200
H	-0.56279700	2.08278500	-2.35975600
H	0.90882800	4.51571900	-1.24552300

B	-2.43869100	2.41452600	1.09056800
I	-1.47819300	-0.65642900	-0.18436400
C	0.36690500	-1.42332500	0.61402400
C	0.70961600	-1.14076900	1.92902000
C	1.13650300	-2.23225400	-0.20984100
C	1.89180000	-1.68634400	2.42852500
H	0.08370800	-0.51421100	2.54791000
C	2.30739100	-2.78101000	0.31600300
H	0.84304300	-2.43080200	-1.23165900
C	2.68596200	-2.50613100	1.62686300
H	2.18453100	-1.46911000	3.44933900
H	2.92559400	-3.40980500	-0.31333400
H	3.60343100	-2.92436700	2.02320100
O	-2.06902200	-4.10100100	-0.30918500
C	-3.33084100	-4.10718200	-0.39879000
O	-4.00997700	-3.28242700	-1.07646100
C	-4.09265700	-5.16297000	0.39827900
H	-4.32244700	-4.74896700	1.38706300
H	-5.03789600	-5.41966500	-0.08459800
H	-3.49162600	-6.06364900	0.54265000
H	0.78371900	1.29551600	-2.06682900
H	-3.28603100	1.82900500	1.68104600
N	1.61361300	1.69542100	0.11912800
C	2.19041700	0.97886200	-0.80385900
H	2.12579100	1.76349700	0.98991300
C	3.48215400	0.30674300	-0.61333200
O	1.63226500	0.80468400	-1.97895100
C	3.99915700	-0.47359600	-1.65746600
C	4.18783700	0.40002400	0.59408700
C	5.20119300	-1.14958300	-1.49349600
H	3.45478700	-0.55746400	-2.58789600
C	5.39023000	-0.27682500	0.75053600
H	3.81857600	0.98830300	1.42541100
C	5.89789100	-1.05462400	-0.28956200
H	5.59098300	-1.75505100	-2.30302800
H	5.92707700	-0.20279100	1.68848400
H	6.83377400	-1.58612800	-0.16062000

IRC_TS1_point316

B	-2.68634700	3.99966400	0.32732800
B	-1.60313100	3.84555000	1.73185300
B	-0.73126500	2.30680700	1.58945400
B	-2.48337200	2.55936500	-0.69480000
B	-1.27069700	1.57410200	0.08999100

B	-1.13878600	4.87825500	0.36078700
B	-1.67688100	4.09072000	-1.13947900
H	-3.73156400	4.56349900	0.39678300
B	0.07082100	3.83206500	1.13265000
H	-1.87812900	4.29797200	2.79716200
B	0.27454800	2.40559400	0.11286200
H	-0.37127300	1.66290100	2.51654400
B	-0.80312100	2.56027400	-1.29390500
H	-3.35846500	2.08204100	-1.33983700
H	-1.09140500	6.06254500	0.46210300
B	0.02676900	3.99378600	-0.64468100
H	-2.01287400	4.70225300	-2.10191600
H	0.99008900	4.24334400	1.76542600
H	-0.56270500	2.08152600	-2.35952400
H	0.90999100	4.51480900	-1.24525100
B	-2.43957300	2.41506300	1.09024300
I	-1.47906300	-0.65646400	-0.18405300
C	0.36650200	-1.42310500	0.61354400
C	0.70963100	-1.14064200	1.92845500
C	1.13591800	-2.23188100	-0.21064500
C	1.89205500	-1.68610700	2.42750900
H	0.08385300	-0.51421900	2.54763600
C	2.30701700	-2.78060700	0.31478800
H	0.84215000	-2.43038400	-1.23238400
C	2.68601300	-2.50578200	1.62553500
H	2.18506800	-1.46894100	3.44826000
H	2.92505000	-3.40936600	-0.31474600
H	3.60362000	-2.92395700	2.02158100
O	-2.06692200	-4.10512200	-0.31111400
C	-3.32914400	-4.10893400	-0.39925500
O	-4.00574800	-3.28692100	-1.08402000
C	-4.09220400	-5.15819900	0.40503500
H	-4.31940600	-4.73940800	1.39123900
H	-5.03710500	-5.41522200	-0.07655400
H	-3.49238500	-6.05721400	0.55184000
H	0.78544200	1.29980400	-2.06783700
H	-3.28712100	1.82966700	1.68038100
N	1.61297500	1.69406000	0.12088100
C	2.19078900	0.98004500	-0.80301000
H	2.12277900	1.75737200	0.99460100
C	3.48227300	0.30709000	-0.61286000
O	1.63436900	0.80989100	-1.97991900
C	3.99885300	-0.47419400	-1.65651900
C	4.18827100	0.40066700	0.59439400

C	5.20047200	-1.15091100	-1.49213500
H	3.45443100	-0.55856600	-2.58686100
C	5.39025000	-0.27681200	0.75124400
H	3.81949600	0.98978900	1.42530700
C	5.89733500	-1.05567600	-0.28834200
H	5.58974000	-1.75723800	-2.30127900
H	5.92723500	-0.20237900	1.68907200
H	6.83287900	-1.58771500	-0.15915100

IRC_TS1_point317

B	-2.68623500	4.00033300	0.32667900
B	-1.60368100	3.84585400	1.73171900
B	-0.73236500	2.30671600	1.58986400
B	-2.48342900	2.55977900	-0.69527300
B	-1.27120100	1.57390300	0.08995500
B	-1.13849300	4.87830500	0.36091900
B	-1.67617200	4.09086700	-1.13961100
H	-3.73120200	4.56382800	0.39587500
B	0.07051400	3.83166800	1.13331000
H	-1.87924200	4.29788000	2.79677700
B	0.27389200	2.40475800	0.11371500
H	-0.37320500	1.66276400	2.51736400
B	-0.80304900	2.55992900	-1.29328100
H	-3.35854600	2.08288600	-1.34062800
H	-1.09097300	6.06251700	0.46235700
B	0.02719800	3.99321500	-0.64397600
H	-2.01130300	4.70250000	-2.10232600
H	0.98957800	4.24270000	1.76649600
H	-0.56170400	2.08180400	-2.35853300
H	0.91090500	4.51370500	-1.24427100
B	-2.44033700	2.41559800	1.08979800
I	-1.48009900	-0.65653700	-0.18367000
C	0.36589900	-1.42305000	0.61318400
C	0.70945400	-1.14062400	1.92799100
C	1.13512400	-2.23150700	-0.21145300
C	1.89218100	-1.68591400	2.42650600
H	0.08385400	-0.51427200	2.54744300
C	2.30646800	-2.78017200	0.31351000
H	0.84104500	-2.42980800	-1.23314400
C	2.68591600	-2.50545100	1.62414100
H	2.18565000	-1.46870900	3.44712000
H	2.92436000	-3.40869600	-0.31638900
H	3.60377500	-2.92351200	2.01971800
O	-2.06391700	-4.10935800	-0.31428700

C	-3.32641500	-4.11048900	-0.40128900
O	-4.00263200	-3.29171800	-1.08869900
C	-4.09176200	-5.15187200	0.41071700
H	-4.31878400	-4.72370800	1.39413800
H	-5.03803300	-5.41076100	-0.06815300
H	-3.49438700	-6.05335200	0.56694300
H	0.78901000	1.30347700	-2.06956800
H	-3.28879400	1.83097300	1.67994200
N	1.61174200	1.69279700	0.12142700
C	2.19193600	0.98149000	-0.80323900
H	2.11959200	1.75420900	0.99478800
C	3.48287300	0.30798200	-0.61214700
O	1.63839800	0.81383900	-1.98131000
C	3.99850200	-0.47448200	-1.65539100
C	4.18901900	0.40188900	0.59492600
C	5.19947100	-1.15218400	-1.49073200
H	3.45368600	-0.55901700	-2.58549400
C	5.39032900	-0.27674500	0.75211000
H	3.82119700	0.99285000	1.42503600
C	5.89650800	-1.05680100	-0.28701600
H	5.58807700	-1.75948900	-2.29946200
H	5.92763800	-0.20205400	1.68974500
H	6.83153800	-1.58968700	-0.15750600

IRC_TS1_point318

B	-2.68625400	4.00062800	0.32625100
B	-1.60416500	3.84584300	1.73162800
B	-0.73327300	2.30658000	1.58993100
B	-2.48363500	2.56021400	-0.69568000
B	-1.27238500	1.57409100	0.09016800
B	-1.13812500	4.87806100	0.36089000
B	-1.67564500	4.09089900	-1.13971100
H	-3.73114800	4.56465000	0.39503400
B	0.07020900	3.83116900	1.13368300
H	-1.87973500	4.29834500	2.79670500
B	0.27379200	2.40438700	0.11410300
H	-0.37440900	1.66232000	2.51715000
B	-0.80304700	2.55984300	-1.29355300
H	-3.35852800	2.08349900	-1.34139300
H	-1.08971300	6.06248400	0.46201100
B	0.02765500	3.99260900	-0.64374900
H	-2.01042900	4.70267100	-2.10235200
H	0.98913700	4.24193000	1.76722500
H	-0.56299400	2.08122800	-2.35930500

H	0.91139200	4.51321800	-1.24346000
B	-2.44118700	2.41597800	1.08947100
I	-1.48089000	-0.65653500	-0.18340100
C	0.36550300	-1.42294000	0.61272000
C	0.70937500	-1.14071400	1.92749300
C	1.13462800	-2.23118300	-0.21222200
C	1.89233100	-1.68585900	2.42559800
H	0.08377200	-0.51467700	2.54722800
C	2.30617300	-2.77979400	0.31237400
H	0.84031700	-2.42938700	-1.23386100
C	2.68595800	-2.50518200	1.62292200
H	2.18596300	-1.46883600	3.44619600
H	2.92395200	-3.40824100	-0.31771100
H	3.60393200	-2.92322600	2.01825700
O	-2.06242700	-4.11334600	-0.31546300
C	-3.32440900	-4.11207600	-0.40192600
O	-3.99815100	-3.29559300	-1.09609800
C	-4.09163700	-5.14694700	0.41722100
H	-4.31654100	-4.71383800	1.39778300
H	-5.03844400	-5.40618100	-0.05994100
H	-3.49581800	-6.04662500	0.57571700
H	0.79064200	1.30814500	-2.07054000
H	-3.28951500	1.83123700	1.67898100
N	1.61131300	1.69115000	0.12367600
C	2.19244900	0.98265800	-0.80259900
H	2.11662900	1.74686400	1.00079200
C	3.48301700	0.30816800	-0.61172500
O	1.64049600	0.81975900	-1.98270800
C	3.99826800	-0.47518800	-1.65448400
C	4.18951200	0.40264500	0.59511100
C	5.19884700	-1.15353700	-1.48936500
H	3.45342000	-0.56022000	-2.58451800
C	5.39042500	-0.27653700	0.75274600
H	3.82209600	0.99450100	1.42469900
C	5.89601200	-1.05778000	-0.28579000
H	5.58694600	-1.76170000	-2.29768800
H	5.92787600	-0.20134000	1.69024800
H	6.83069100	-1.59117200	-0.15597200

IRC_TS1_point319

B	-2.68611500	4.00141800	0.32568000
B	-1.60472300	3.84618900	1.73151500
B	-0.73452800	2.30634500	1.59030400
B	-2.48378300	2.56058600	-0.69599800

B	-1.27287100	1.57407300	0.09014800
B	-1.13761700	4.87816600	0.36090300
B	-1.67478000	4.09096900	-1.13992900
H	-3.73066900	4.56648800	0.39386000
B	0.06995100	3.83065800	1.13429400
H	-1.88058300	4.29870700	2.79640600
B	0.27292500	2.40341800	0.11501900
H	-0.37647400	1.66203400	2.51801000
B	-0.80286600	2.55920400	-1.29279000
H	-3.35877900	2.08436600	-1.34202400
H	-1.08928300	6.06226100	0.46229100
B	0.02808800	3.99206900	-0.64303500
H	-2.00880300	4.70277000	-2.10293000
H	0.98889700	4.24100500	1.76814900
H	-0.56158300	2.08052000	-2.35791400
H	0.91275800	4.51172100	-1.24294900
B	-2.44208700	2.41646100	1.08908800
I	-1.48188900	-0.65670800	-0.18311900
C	0.36493100	-1.42290400	0.61233800
C	0.70915100	-1.14080100	1.92703800
C	1.13393600	-2.23074200	-0.21307500
C	1.89240400	-1.68578100	2.42462900
H	0.08368000	-0.51490900	2.54708500
C	2.30571400	-2.77930000	0.31107000
H	0.83939200	-2.42869000	-1.23469900
C	2.68587900	-2.50487700	1.62154500
H	2.18640700	-1.46884400	3.44514300
H	2.92340300	-3.40747800	-0.31936900
H	3.60408000	-2.92282200	2.01644500
O	-2.05924300	-4.11781900	-0.31889900
C	-3.32218200	-4.11340200	-0.40354400
O	-3.99503800	-3.29985200	-1.10048000
C	-4.09120200	-5.14040100	0.42267800
H	-4.31486400	-4.69813100	1.40057200
H	-5.03895700	-5.40159400	-0.05178800
H	-3.49762900	-6.04191000	0.59013700
H	0.79410800	1.31223700	-2.07216900
H	-3.29125600	1.83236200	1.67857400
N	1.60986500	1.68949200	0.12452900
C	2.19339300	0.98410500	-0.80248900
H	2.11301200	1.74281300	1.00121400
C	3.48355200	0.30914000	-0.61114500
O	1.64447000	0.82410700	-1.98389700
C	3.99790000	-0.47553200	-1.65337500

C	4.19025400	0.40402100	0.59550100
C	5.19788100	-1.15480300	-1.48788500
H	3.45267000	-0.56103000	-2.58313700
C	5.39054300	-0.27620600	0.75355400
H	3.82375600	0.99768400	1.42427900
C	5.89526700	-1.05871300	-0.28443700
H	5.58534400	-1.76405900	-2.29569900
H	5.92834100	-0.20054300	1.69082600
H	6.82949900	-1.59283000	-0.15429800

IRC_TS1_point320

B	-2.68607800	4.00169300	0.32513500
B	-1.60521400	3.84615300	1.73141900
B	-0.73545000	2.30618000	1.59056700
B	-2.48389900	2.56096900	-0.69649100
B	-1.27399100	1.57389500	0.09037600
B	-1.13735500	4.87784500	0.36100900
B	-1.67424100	4.09095900	-1.13998000
H	-3.73054400	4.56604700	0.39321000
B	0.06961700	3.83009000	1.13483800
H	-1.88140800	4.29867200	2.79619400
B	0.27278300	2.40283800	0.11559600
H	-0.37787300	1.66168000	2.51819200
B	-0.80285600	2.55908800	-1.29284200
H	-3.35869500	2.08492700	-1.34282500
H	-1.08821300	6.06221400	0.46208600
B	0.02857000	3.99127200	-0.64260800
H	-2.00767900	4.70288900	-2.10303300
H	0.98827900	4.24029300	1.76907400
H	-0.56221400	2.08047700	-2.35825800
H	0.91308600	4.51112100	-1.24175700
B	-2.44287000	2.41684100	1.08871600
I	-1.48280000	-0.65674600	-0.18279800
C	0.36443400	-1.42285500	0.61192300
C	0.70892700	-1.14098600	1.92661700
C	1.13339400	-2.23037600	-0.21383600
C	1.89241000	-1.68581200	2.42379900
H	0.08346600	-0.51535500	2.54693300
C	2.30536700	-2.77889700	0.30995700
H	0.83866700	-2.42813500	-1.23544100
C	2.68581000	-2.50465600	1.62038100
H	2.18657400	-1.46902400	3.44429900
H	2.92298600	-3.40692500	-0.32069000
H	3.60411600	-2.92258100	2.01505600

O	-2.05769900	-4.12190300	-0.32011200
C	-3.31964800	-4.11505900	-0.40468400
O	-3.99046500	-3.30369600	-1.10738900
C	-4.09124700	-5.13534800	0.42863900
H	-4.31559700	-4.68746400	1.40269100
H	-5.03863800	-5.39706500	-0.04559800
H	-3.49931200	-6.03573100	0.60083000
H	0.79645500	1.31699400	-2.07360700
H	-3.29237400	1.83311500	1.67795200
N	1.60931700	1.68807000	0.12617100
C	2.19427900	0.98563600	-0.80240000
H	2.10978900	1.73593000	1.00638300
C	3.48390000	0.30957600	-0.61063100
O	1.64731200	0.83020200	-1.98569300
C	3.99762300	-0.47619500	-1.65232300
C	4.19092300	0.40513800	0.59574200
C	5.19712700	-1.15621400	-1.48639900
H	3.45223600	-0.56201800	-2.58197800
C	5.39071200	-0.27585700	0.75426500
H	3.82499000	1.00013300	1.42378900
C	5.89469400	-1.05968700	-0.28310700
H	5.58404800	-1.76630200	-2.29383600
H	5.92875400	-0.19968900	1.69134900
H	6.82858900	-1.59430800	-0.15269500

IRC_TS1_point321

B	-2.68601700	4.00229600	0.32468300
B	-1.60577600	3.84636700	1.73132400
B	-0.73668800	2.30591200	1.59077900
B	-2.48416800	2.56128500	-0.69674100
B	-1.27467700	1.57405900	0.09038900
B	-1.13676000	4.87779400	0.36091600
B	-1.67344800	4.09090600	-1.14017700
H	-3.73021100	4.56852600	0.39194500
B	0.06936300	3.82949200	1.13529900
H	-1.88194100	4.29941500	2.79605400
B	0.27207900	2.40195800	0.11626500
H	-0.37966300	1.66125100	2.51855900
B	-0.80283300	2.55844600	-1.29241300
H	-3.35897900	2.08565700	-1.34341400
H	-1.08731900	6.06197700	0.46205500
B	0.02901800	3.99063300	-0.64213400
H	-2.00635500	4.70289700	-2.10336900
H	0.98810600	4.23925800	1.76982900

H	-0.56229100	2.07944700	-2.35774400
H	0.91444900	4.50958800	-1.24146900
B	-2.44386400	2.41726400	1.08841700
I	-1.48382900	-0.65695200	-0.18253800
C	0.36383500	-1.42283800	0.61152600
C	0.70860500	-1.14113600	1.92617300
C	1.13276300	-2.22989600	-0.21468200
C	1.89237700	-1.68576200	2.42289200
H	0.08317000	-0.51580000	2.54680600
C	2.30496300	-2.77831800	0.30870100
H	0.83786200	-2.42741100	-1.23628300
C	2.68570300	-2.50430700	1.61908700
H	2.18678500	-1.46916100	3.44336100
H	2.92253800	-3.40608400	-0.32225200
H	3.60418800	-2.92218000	2.01340600
O	-2.05449100	-4.12683900	-0.32353900
C	-3.31766900	-4.11637500	-0.40595000
O	-3.98696100	-3.30747500	-1.11195400
C	-4.09105100	-5.12902700	0.43373000
H	-4.31244400	-4.67286200	1.40558000
H	-5.04036100	-5.39263300	-0.03705400
H	-3.50146000	-6.03010800	0.61199700
H	0.79955900	1.32145000	-2.07473400
H	-3.29345800	1.83351900	1.67703000
N	1.60811200	1.68601400	0.12782900
C	2.19525600	0.98709200	-0.80179700
H	2.10625200	1.73059900	1.00801900
C	3.48446600	0.31055100	-0.61013100
O	1.65125800	0.83543700	-1.98681300
C	3.99732300	-0.47658400	-1.65123000
C	4.19179600	0.40671300	0.59598600
C	5.19624900	-1.15750300	-1.48483600
H	3.45162200	-0.56304500	-2.58062200
C	5.39096400	-0.27524800	0.75500800
H	3.82666100	1.00337900	1.42320000
C	5.89405100	-1.06051400	-0.28170500
H	5.58252900	-1.76878100	-2.29169300
H	5.92933200	-0.19852800	1.69186700
H	6.82747900	-1.59588500	-0.15090700

IRC_TS1_point322

B	-2.68585300	4.00271200	0.32403200
B	-1.60623600	3.84637200	1.73120000
B	-0.73768800	2.30560400	1.59117500

B	-2.48420700	2.56162200	-0.69724200
B	-1.27570100	1.57367400	0.09064900
B	-1.13647100	4.87751900	0.36107400
B	-1.67274700	4.09086700	-1.14028300
H	-3.72986000	4.56786100	0.39127400
B	0.06905100	3.82885100	1.13598100
H	-1.88299600	4.29893600	2.79567000
B	0.27169700	2.40109700	0.11716200
H	-0.38141000	1.66083100	2.51920600
B	-0.80260500	2.55808200	-1.29212300
H	-3.35893200	2.08629100	-1.34421700
H	-1.08676700	6.06168400	0.46224500
B	0.02953200	3.98978900	-0.64147500
H	-2.00488600	4.70292600	-2.10375300
H	0.98752900	4.23837400	1.77092000
H	-0.56121000	2.07912600	-2.35705500
H	0.91493700	4.50876200	-1.24014800
B	-2.44460300	2.41759400	1.08796900
I	-1.48477400	-0.65707200	-0.18221100
C	0.36327600	-1.42287400	0.61115400
C	0.70826200	-1.14146000	1.92581900
C	1.13222100	-2.22950800	-0.21544300
C	1.89229000	-1.68588700	2.42212100
H	0.08279900	-0.51642600	2.54674000
C	2.30463200	-2.77786700	0.30758900
H	0.83718200	-2.42673900	-1.23706000
C	2.68560800	-2.50408500	1.61794500
H	2.18686200	-1.46944500	3.44257900
H	2.92220000	-3.40535100	-0.32363400
H	3.60426000	-2.92183500	2.01197900
O	-2.05306700	-4.13083500	-0.32453500
C	-3.31492700	-4.11787000	-0.40740400
O	-3.98249900	-3.31115000	-1.11826700
C	-4.09092700	-5.12365600	0.43897400
H	-4.31663100	-4.66104600	1.40581600
H	-5.03736300	-5.38890200	-0.03425500
H	-3.50225400	-6.02411600	0.62680200
H	0.80215400	1.32623700	-2.07636100
H	-3.29544200	1.83499200	1.67702900
N	1.60718700	1.68450500	0.12907300
C	2.19614500	0.98885500	-0.80217800
H	2.10237100	1.72320400	1.01288000
C	3.48490000	0.31122500	-0.60972600
O	1.65434000	0.84165400	-1.98868300

C	3.99701500	-0.47725000	-1.65016100
C	4.19261000	0.40819000	0.59608700
C	5.19541700	-1.15896800	-1.48329100
H	3.45100500	-0.56424100	-2.57933800
C	5.39121700	-0.27465500	0.75564600
H	3.82833600	1.00666000	1.42239400
C	5.89346200	-1.06141800	-0.28035500
H	5.58100200	-1.77135200	-2.28963000
H	5.92993100	-0.19720500	1.69223300
H	6.82648700	-1.59737200	-0.14922300

IRC_TS1_point323

B	-2.68593200	4.00303000	0.32365000
B	-1.60691400	3.84634300	1.73119400
B	-0.73893600	2.30527300	1.59139800
B	-2.48448300	2.56188200	-0.69754600
B	-1.27647200	1.57378000	0.09063900
B	-1.13598500	4.87724100	0.36109700
B	-1.67207300	4.09074200	-1.14034000
H	-3.72977500	4.56977300	0.39008100
B	0.06871600	3.82809300	1.13650200
H	-1.88359200	4.29976300	2.79571400
B	0.27113300	2.40018800	0.11771700
H	-0.38318000	1.66024400	2.51939300
B	-0.80272600	2.55763100	-1.29183800
H	-3.35908900	2.08697000	-1.34496800
H	-1.08518300	6.06164200	0.46188800
B	0.02997100	3.98899500	-0.64096400
H	-2.00358000	4.70297500	-2.10384800
H	0.98710100	4.23727800	1.77185300
H	-0.56246000	2.07853300	-2.35720100
H	0.91614400	4.50734300	-1.23950100
B	-2.44567900	2.41793000	1.08771900
I	-1.48571700	-0.65730600	-0.18203200
C	0.36267400	-1.42295600	0.61079500
C	0.70785800	-1.14177400	1.92545100
C	1.13166900	-2.22903200	-0.21625600
C	1.89219400	-1.68594800	2.42130200
H	0.08235600	-0.51710000	2.54669800
C	2.30431400	-2.77725900	0.30638000
H	0.83650600	-2.42595500	-1.23789800
C	2.68552200	-2.50375300	1.61672700
H	2.18695900	-1.46971800	3.44174600
H	2.92189700	-3.40440000	-0.32517400

H	3.60437500	-2.92140600	2.01040700
O	-2.04993100	-4.13565300	-0.32790800
C	-3.31318300	-4.11892600	-0.40823900
O	-3.97890500	-3.31424400	-1.12258900
C	-4.09136100	-5.11753500	0.44421500
H	-4.31399900	-4.64687300	1.40880800
H	-5.04080600	-5.38472400	-0.02496700
H	-3.50495100	-6.01686800	0.63525000
H	0.80506000	1.33051800	-2.07729200
H	-3.29596700	1.83478000	1.67549200
N	1.60605700	1.68221000	0.13087500
C	2.19719300	0.99015700	-0.80135800
H	2.09865800	1.71738900	1.01467700
C	3.48553600	0.31223200	-0.60926000
O	1.65840500	0.84708400	-1.98996100
C	3.99664600	-0.47772700	-1.64906800
C	4.19379200	0.41023100	0.59607300
C	5.19450400	-1.16029300	-1.48176700
H	3.45016700	-0.56551100	-2.57788300
C	5.39170200	-0.27368800	0.75617600
H	3.83063700	1.01093300	1.42125100
C	5.89285500	-1.06217200	-0.27904000
H	5.57933700	-1.77402600	-2.28745100
H	5.93085900	-0.19553400	1.69246700
H	6.82532800	-1.59902100	-0.14744300

IRC_TS1_point324

B	-2.68570700	4.00353000	0.32309100
B	-1.60733700	3.84630900	1.73109500
B	-0.74005900	2.30478200	1.59170400
B	-2.48466100	2.56214800	-0.69794200
B	-1.27755000	1.57339400	0.09085900
B	-1.13550300	4.87695700	0.36124700
B	-1.67127500	4.09064800	-1.14046200
H	-3.72917000	4.57043000	0.38925400
B	0.06845000	3.82731900	1.13716900
H	-1.88447100	4.29921000	2.79533600
B	0.27057000	2.39919300	0.11858700
H	-0.38497400	1.65954800	2.51985300
B	-0.80254800	2.55699600	-1.29154900
H	-3.35928800	2.08761300	-1.34565000
H	-1.08523400	6.06081100	0.46264600
B	0.03052200	3.98812100	-0.64036800
H	-2.00221900	4.70295700	-2.10413200

H	0.98680500	4.23604500	1.77286300
H	-0.56135500	2.07754300	-2.35636300
H	0.91701400	4.50607200	-1.23861200
B	-2.44648900	2.41810900	1.08725700
I	-1.48662400	-0.65756100	-0.18180000
C	0.36211700	-1.42311300	0.61044300
C	0.70745100	-1.14224000	1.92512900
C	1.13121700	-2.22865400	-0.21702200
C	1.89207600	-1.68614400	2.42057400
H	0.08183900	-0.51799400	2.54667800
C	2.30410200	-2.77673000	0.30526700
H	0.83599200	-2.42524300	-1.23870600
C	2.68548600	-2.50349300	1.61561000
H	2.18695400	-1.47014200	3.44103300
H	2.92176600	-3.40347800	-0.32657900
H	3.60453500	-2.92098500	2.00899800
O	-2.04864100	-4.13951100	-0.32891800
C	-3.31070400	-4.12000600	-0.40969800
O	-3.97496100	-3.31742700	-1.12801600
C	-4.09100100	-5.11139000	0.44883300
H	-4.31759500	-4.63386700	1.40829400
H	-5.03718500	-5.38173300	-0.02246000
H	-3.50531200	-6.01121100	0.65248900
H	0.80738500	1.33501800	-2.07830000
H	-3.29819300	1.83608800	1.67559100
N	1.60487000	1.68020300	0.13247500
C	2.19801900	0.99191400	-0.80166300
H	2.09401900	1.70848200	1.02007800
C	3.48605100	0.31307000	-0.60899300
O	1.66150000	0.85339400	-1.99144900
C	3.99624400	-0.47852000	-1.64798800
C	4.19496700	0.41225600	0.59587300
C	5.19361000	-1.16183200	-1.48020600
H	3.44925100	-0.56722800	-2.57642400
C	5.39225700	-0.27261700	0.75656600
H	3.83304900	1.01527900	1.41987400
C	5.89235000	-1.06292100	-0.27778400
H	5.57761500	-1.77689700	-2.28525700
H	5.93199100	-0.19335600	1.69241400
H	6.82439000	-1.60037300	-0.14585100

IRC_TS1_point325

B	-2.68571400	4.00384700	0.32258000
B	-1.60802000	3.84624400	1.73109200

B	-0.74132800	2.30440000	1.59212600
B	-2.48478100	2.56246300	-0.69835500
B	-1.27836200	1.57330400	0.09094400
B	-1.13509500	4.87659200	0.36138500
B	-1.67051500	4.09052200	-1.14050700
H	-3.72907900	4.57078100	0.38831200
B	0.06809800	3.82646100	1.13787200
H	-1.88534700	4.29966200	2.79532000
B	0.27001700	2.39806800	0.11946500
H	-0.38702100	1.65902800	2.52055000
B	-0.80245700	2.55660200	-1.29109000
H	-3.35930700	2.08834300	-1.34645900
H	-1.08304200	6.06115900	0.46192400
B	0.03103800	3.98713800	-0.63959400
H	-2.00051500	4.70299300	-2.10445800
H	0.98618700	4.23497300	1.77400900
H	-0.56139500	2.07719400	-2.35594900
H	0.91789800	4.50486100	-1.23732800
B	-2.44754700	2.41852400	1.08697900
I	-1.48758600	-0.65782400	-0.18165000
C	0.36149000	-1.42319600	0.61009900
C	0.70697600	-1.14261400	1.92481100
C	1.13069700	-2.22815100	-0.21780900
C	1.89191700	-1.68622900	2.41982000
H	0.08132300	-0.51868700	2.54667700
C	2.30381600	-2.77610400	0.30411400
H	0.83537300	-2.42443500	-1.23952900
C	2.68539700	-2.50313700	1.61445600
H	2.18695600	-1.47041100	3.44027300
H	2.92151300	-3.40253300	-0.32802800
H	3.60464000	-2.92048300	2.00753400
O	-2.04585200	-4.14396400	-0.33193900
C	-3.30882200	-4.12112400	-0.41045400
O	-3.97121000	-3.32036400	-1.13248700
C	-4.09161600	-5.10603500	0.45418700
H	-4.31978600	-4.62006700	1.40986600
H	-5.03818100	-5.37827900	-0.01651200
H	-3.50712300	-6.00262100	0.66188300
H	0.81011100	1.33903700	-2.07952600
H	-3.29927000	1.83666200	1.67456100
N	1.60365200	1.67791200	0.13405700
C	2.19904900	0.99328700	-0.80101300
H	2.08975200	1.70212800	1.02205800
C	3.48674300	0.31414900	-0.60853500

O	1.66546300	0.85912400	-1.99310300
C	3.99569200	-0.47928900	-1.64674800
C	4.19653000	0.41486500	0.59560400
C	5.19253200	-1.16342700	-1.47858700
H	3.44804200	-0.56898500	-2.57470300
C	5.39307100	-0.27120400	0.75685200
H	3.83609200	1.02069200	1.41820800
C	5.89180700	-1.06362700	-0.27653500
H	5.57564900	-1.77998500	-2.28293400
H	5.93345500	-0.19096800	1.69225700
H	6.82334700	-1.60190400	-0.14420700

IRC_TS1_point326

B	-2.68556900	4.00420100	0.32212700
B	-1.60853900	3.84610800	1.73105100
B	-0.74258400	2.30385000	1.59238400
B	-2.48509200	2.56264300	-0.69867800
B	-1.27953400	1.57296200	0.09113100
B	-1.13446400	4.87621300	0.36150100
B	-1.66969900	4.09033000	-1.14055300
H	-3.72856000	4.57273300	0.38715400
B	0.06780800	3.82555700	1.13854600
H	-1.88606500	4.29963100	2.79507800
B	0.26943800	2.39705600	0.12015200
H	-0.38874800	1.65818100	2.52063400
B	-0.80251100	2.55590900	-1.29086000
H	-3.35950300	2.08896300	-1.34724700
H	-1.08335600	6.05985200	0.46298900
B	0.03161900	3.98621000	-0.63905600
H	-1.99925900	4.70293300	-2.10444200
H	0.98585800	4.23358700	1.77511200
H	-0.56195400	2.07611900	-2.35578200
H	0.91925800	4.50314300	-1.23675600
B	-2.44853300	2.41863100	1.08659800
I	-1.48852600	-0.65817900	-0.18145300
C	0.36089500	-1.42343900	0.60978100
C	0.70650500	-1.14309900	1.92451200
C	1.13026200	-2.22778000	-0.21854300
C	1.89176900	-1.68636500	2.41912500
H	0.08071600	-0.51962700	2.54666300
C	2.30364600	-2.77549100	0.30304000
H	0.83490600	-2.42372800	-1.24031000
C	2.68537400	-2.50278900	1.61338900
H	2.18689600	-1.47077300	3.43960000

H	2.92145400	-3.40149900	-0.32938400
H	3.60481200	-2.91999100	2.00619300
O	-2.04429800	-4.14799500	-0.33337300
C	-3.30665000	-4.12186100	-0.41174800
O	-3.96764400	-3.32308800	-1.13716900
C	-4.09126900	-5.09932300	0.45814000
H	-4.32115400	-4.60724000	1.40909900
H	-5.03680400	-5.37683500	-0.01215300
H	-3.50768500	-5.99668300	0.67783900
H	0.81236400	1.34299600	-2.07986300
H	-3.30068800	1.83696000	1.67375000
N	1.60241100	1.67547300	0.13594000
C	2.20010700	0.99505800	-0.80118000
H	2.08458100	1.69179800	1.02773800
C	3.48747600	0.31526100	-0.60840000
O	1.66906000	0.86529200	-1.99425100
C	3.99514900	-0.48027800	-1.64559200
C	4.19819500	0.41765000	0.59506000
C	5.19148000	-1.16518200	-1.47692400
H	3.44671200	-0.57131400	-2.57295100
C	5.39400600	-0.26952300	0.75697500
H	3.83935900	1.02638800	1.41615200
C	5.89135500	-1.06424400	-0.27531900
H	5.57355500	-1.78346900	-2.28043100
H	5.93518500	-0.18787200	1.69179200
H	6.82238200	-1.60326900	-0.14255400

IRC_TS1_point327

B	-2.68541200	4.00467000	0.32162800
B	-1.60904400	3.84601200	1.73104900
B	-0.74376800	2.30334800	1.59277300
B	-2.48518100	2.56302500	-0.69908100
B	-1.28039000	1.57285600	0.09123700
B	-1.13401700	4.87580100	0.36176400
B	-1.66886500	4.09023600	-1.14058900
H	-3.72819600	4.57247300	0.38655500
B	0.06756500	3.82461500	1.13926700
H	-1.88688900	4.29940500	2.79500700
B	0.26885100	2.39575500	0.12114600
H	-0.39083600	1.65750100	2.52145000
B	-0.80229300	2.55544600	-1.29041700
H	-3.35969000	2.08977500	-1.34789100
H	-1.08080700	6.06043000	0.46223800
B	0.03221800	3.98511500	-0.63824400

H	-1.99749200	4.70300000	-2.10482800
H	0.98550800	4.23228800	1.77618900
H	-0.56084400	2.07547000	-2.35487400
H	0.91985800	4.50210700	-1.23522800
B	-2.44943600	2.41899000	1.08622600
I	-1.48943400	-0.65846100	-0.18134600
C	0.36027000	-1.42356800	0.60945900
C	0.70596700	-1.14354100	1.92424100
C	1.12981200	-2.22732900	-0.21925400
C	1.89156100	-1.68644000	2.41846500
H	0.08003100	-0.52050500	2.54669800
C	2.30344000	-2.77485900	0.30201700
H	0.83441300	-2.42300900	-1.24106700
C	2.68532200	-2.50236200	1.61236300
H	2.18676500	-1.47103900	3.43895600
H	2.92134900	-3.40049800	-0.33067600
H	3.60498400	-2.91929400	2.00488200
O	-2.04201500	-4.15186700	-0.33589000
C	-3.30476600	-4.12294000	-0.41256000
O	-3.96402800	-3.32583000	-1.14151300
C	-4.09188800	-5.09469200	0.46333700
H	-4.32812300	-4.59221500	1.40923300
H	-5.03398300	-5.37461200	-0.01038400
H	-3.50808500	-5.98722400	0.69024500
H	0.81458200	1.34684300	-2.08115300
H	-3.30275800	1.83849800	1.67367800
N	1.60105200	1.67285700	0.13753300
C	2.20082200	0.99622100	-0.80043400
H	2.07974300	1.68453200	1.02960900
C	3.48806900	0.31617400	-0.60791600
O	1.67242700	0.87138400	-1.99606100
C	3.99436600	-0.48144500	-1.64421700
C	4.20014300	0.42075800	0.59448900
C	5.19027900	-1.16699800	-1.47527800
H	3.44501800	-0.57387300	-2.57091700
C	5.39523900	-0.26755900	0.75689700
H	3.84333600	1.03304800	1.41385900
C	5.89095900	-1.06480400	-0.27424400
H	5.57126100	-1.78699200	-2.27799600
H	5.93742000	-0.18437700	1.69100200
H	6.82153300	-1.60453500	-0.14116400

IRC_TS1_point328

B	-2.68534800	4.00492300	0.32116400
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B	-1.60971100	3.84582100	1.73109200
B	-0.74519400	2.30272300	1.59323300
B	-2.48546700	2.56318700	-0.69943500
B	-1.28159300	1.57232900	0.09149200
B	-1.13332500	4.87539000	0.36187800
B	-1.66798800	4.08999700	-1.14059800
H	-3.72785100	4.57436800	0.38522600
B	0.06721000	3.82354200	1.14009900
H	-1.88776600	4.29981600	2.79488100
B	0.26815200	2.39456500	0.12196900
H	-0.39298800	1.65662400	2.52187900
B	-0.80233100	2.55470600	-1.28995200
H	-3.35975600	2.09055400	-1.34886700
H	-1.08067600	6.05907700	0.46312400
B	0.03279200	3.98406500	-0.63747700
H	-1.99575900	4.70296900	-2.10492700
H	0.98486800	4.23081000	1.77760600
H	-0.56130600	2.07461300	-2.35449000
H	0.92155400	4.50005300	-1.23442400
B	-2.45065400	2.41920400	1.08599900
I	-1.49030100	-0.65889500	-0.18123400
C	0.35967500	-1.42388800	0.60920300
C	0.70549100	-1.14405200	1.92399100
C	1.12937500	-2.22700000	-0.21994400
C	1.89146400	-1.68652400	2.41778500
H	0.07946600	-0.52137500	2.54672500
C	2.30330300	-2.77423200	0.30095900
H	0.83390500	-2.42231300	-1.24180500
C	2.68537000	-2.50194400	1.61129400
H	2.18686300	-1.47121000	3.43824200
H	2.92132300	-3.39939700	-0.33208100
H	3.60533000	-2.91860300	2.00344400
O	-2.04034400	-4.15558800	-0.33765600
C	-3.30293000	-4.12323300	-0.41334900
O	-3.96113800	-3.32805000	-1.14509300
C	-4.09172000	-5.08768100	0.46689400
H	-4.33018100	-4.58131900	1.40729100
H	-5.03393700	-5.37471000	-0.00556200
H	-3.50842400	-5.97998000	0.70495000
H	0.81703000	1.35020400	-2.08136400
H	-3.30356100	1.83824700	1.67206900
N	1.59956400	1.67033000	0.13913600
C	2.20208300	0.99801400	-0.80100600
H	2.07368500	1.67293900	1.03582400

C	3.48897100	0.31758300	-0.60798800
O	1.67651900	0.87685000	-1.99714500
C	3.99361200	-0.48272200	-1.64296400
C	4.20222100	0.42432900	0.59355400
C	5.18901000	-1.16906300	-1.47351500
H	3.44306700	-0.57699900	-2.56874800
C	5.39647900	-0.26531400	0.75671500
H	3.84769500	1.04049700	1.41096300
C	5.89050300	-1.06534900	-0.27308700
H	5.56863000	-1.79136100	-2.27509900
H	5.93974500	-0.18031900	1.69003900
H	6.82043900	-1.60607200	-0.13940700

IRC_TS1_point329

B	-2.68508800	4.00529300	0.32081600
B	-1.61004000	3.84556200	1.73109400
B	-0.74620200	2.30217700	1.59337600
B	-2.48564000	2.56351700	-0.69973200
B	-1.28247200	1.57241000	0.09149000
B	-1.13284900	4.87481800	0.36227200
B	-1.66720500	4.08988700	-1.14051700
H	-3.72721000	4.57496000	0.38467200
B	0.06707400	3.82259600	1.14072300
H	-1.88830300	4.29922800	2.79481200
B	0.26775300	2.39341200	0.12262900
H	-0.39451200	1.65568000	2.52195700
B	-0.80231500	2.55435600	-1.28982500
H	-3.35998600	2.09120500	-1.34943200
H	-1.07936600	6.05898700	0.46335800
B	0.03347100	3.98304300	-0.63690400
H	-1.99462100	4.70300700	-2.10480200
H	0.98479000	4.22935000	1.77860300
H	-0.56181400	2.07369000	-2.35445100
H	0.92217300	4.49899600	-1.23325900
B	-2.45130800	2.41925300	1.08550100
I	-1.49110000	-0.65915800	-0.18115300
C	0.35911200	-1.42407200	0.60893400
C	0.70496600	-1.14451500	1.92378200
C	1.12904800	-2.22663900	-0.22052300
C	1.89125900	-1.68657700	2.41726100
H	0.07865900	-0.52244200	2.54680100
C	2.30321800	-2.77362600	0.30013900
H	0.83364000	-2.42175000	-1.24243600
C	2.68537800	-2.50149500	1.61047400

H	2.18656200	-1.47160900	3.43780600
H	2.92141400	-3.39843900	-0.33306500
H	3.60548600	-2.91796900	2.00246800
O	-2.03894100	-4.15867700	-0.33928200
C	-3.30134300	-4.12411500	-0.41431200
O	-3.95784000	-3.33024500	-1.14953300
C	-4.09209700	-5.08375400	0.47163100
H	-4.33982100	-4.56375600	1.40640100
H	-5.02836900	-5.37591500	-0.00620600
H	-3.50734200	-5.97044500	0.72136300
H	0.81872300	1.35388100	-2.08238700
H	-3.30577200	1.83957000	1.67232000
N	1.59836100	1.66722400	0.14100800
C	2.20245600	0.99868900	-0.79975100
H	2.06883400	1.66506000	1.03694900
C	3.48943200	0.31814900	-0.60747500
O	1.67915500	0.88306500	-1.99879500
C	3.99258800	-0.48433800	-1.64155000
C	4.20455000	0.42779200	0.59264500
C	5.18771200	-1.17108400	-1.47194500
H	3.44091000	-0.58044400	-2.56652400
C	5.39816200	-0.26281800	0.75617300
H	3.85260100	1.04800300	1.40803700
C	5.89028700	-1.06573300	-0.27228500
H	5.56611200	-1.79520100	-2.27267500
H	5.94280800	-0.17567700	1.68848900
H	6.81989400	-1.60687900	-0.13841900

IRC_TS1_point330

B	-2.68502500	4.00573300	0.32037100
B	-1.61067800	3.84542300	1.73121800
B	-0.74764600	2.30144700	1.59395400
B	-2.48588300	2.56377400	-0.70012700
B	-1.28361300	1.57168300	0.09177200
B	-1.13213700	4.87450500	0.36243800
B	-1.66631600	4.08971200	-1.14055100
H	-3.72693000	4.57555900	0.38380500
B	0.06675300	3.82141100	1.14160900
H	-1.88921000	4.29932500	2.79480100
B	0.26685500	2.39198600	0.12370100
H	-0.39697700	1.65484400	2.52298600
B	-0.80219500	2.55345100	-1.28916500
H	-3.36029200	2.09218700	-1.35020600
H	-1.07716000	6.05879700	0.46299600

B	0.03396100	3.98183400	-0.63593900
H	-1.99244900	4.70314700	-2.10525100
H	0.98429200	4.22783200	1.77982900
H	-0.56009000	2.07311200	-2.35299600
H	0.92342800	4.49723100	-1.23199100
B	-2.45264500	2.41968900	1.08540700
I	-1.49190400	-0.65966100	-0.18115700
C	0.35854400	-1.42436600	0.60867700
C	0.70447700	-1.14500400	1.92353900
C	1.12861900	-2.22633700	-0.22117400
C	1.89115200	-1.68661300	2.41660400
H	0.07816000	-0.52312200	2.54679200
C	2.30307600	-2.77303300	0.29914200
H	0.83306300	-2.42114800	-1.24311700
C	2.68543800	-2.50102300	1.60944500
H	2.18675400	-1.47150700	3.43704700
H	2.92133600	-3.39741500	-0.33442400
H	3.60592100	-2.91703100	2.00101400
O	-2.03674200	-4.16194200	-0.34181600
C	-3.29962900	-4.12417100	-0.41461200
O	-3.95567500	-3.33234600	-1.15167300
C	-4.09237900	-5.07705400	0.47516300
H	-4.34598100	-4.55542600	1.40259600
H	-5.02705800	-5.37710400	-0.00358500
H	-3.50692900	-5.96073700	0.73493300
H	0.82128500	1.35703600	-2.08288000
H	-3.30703200	1.84016100	1.67118300
N	1.59668700	1.66514600	0.14213400
C	2.20379800	1.00063300	-0.80078800
H	2.06220500	1.65340000	1.04354800
C	3.49035100	0.31964900	-0.60752500
O	1.68332200	0.88799600	-1.99993300
C	3.99159900	-0.48594300	-1.64003400
C	4.20681800	0.43165500	0.59162800
C	5.18624600	-1.17344000	-1.47002500
H	3.43845900	-0.58410400	-2.56387600
C	5.39969100	-0.26023500	0.75580900
H	3.85729800	1.05585600	1.40502600
C	5.88993300	-1.06618400	-0.27120000
H	5.56308300	-1.80008300	-2.26954500
H	5.94565900	-0.17112600	1.68718300
H	6.81894800	-1.60833300	-0.13681500

IRC_TS1_point331

B	-2.68474700	4.00588400	0.32003000
B	-1.61103400	3.84513900	1.73119600
B	-0.74868500	2.30092900	1.59421100
B	-2.48605600	2.56400200	-0.70035800
B	-1.28451700	1.57173700	0.09185000
B	-1.13149300	4.87390000	0.36268100
B	-1.66548100	4.08950900	-1.14046700
H	-3.72636300	4.57726900	0.38282300
B	0.06661200	3.82045500	1.14226800
H	-1.88971300	4.29954600	2.79470800
B	0.26666900	2.39094300	0.12425900
H	-0.39859900	1.65395500	2.52306400
B	-0.80222300	2.55319000	-1.28898300
H	-3.36025000	2.09275900	-1.35093400
H	-1.07758000	6.05733800	0.46433400
B	0.03471300	3.98087100	-0.63539800
H	-1.99124500	4.70303100	-2.10504200
H	0.98389700	4.22642300	1.78112600
H	-0.56172300	2.07188600	-2.35348600
H	0.92485800	4.49546300	-1.23131500
B	-2.45327900	2.41964100	1.08495600
I	-1.49271600	-0.65996700	-0.18101600
C	0.35797800	-1.42459900	0.60846300
C	0.70402100	-1.14537300	1.92334700
C	1.12827400	-2.22603700	-0.22169700
C	1.89106100	-1.68650300	2.41606800
H	0.07745700	-0.52405000	2.54685700
C	2.30302300	-2.77240100	0.29834900
H	0.83277000	-2.42067700	-1.24367300
C	2.68553900	-2.50046200	1.60861900
H	2.18662200	-1.47168500	3.43657300
H	2.92144800	-3.39645200	-0.33536200
H	3.60619600	-2.91631300	2.00002000
O	-2.03621500	-4.16462300	-0.34230700
C	-3.29826000	-4.12488900	-0.41545300
O	-3.95252800	-3.33410300	-1.15641600
C	-4.09221500	-5.07335100	0.47866100
H	-4.35665500	-4.53746100	1.39983600
H	-5.02098000	-5.38240700	-0.00498200
H	-3.50470500	-5.95180100	0.75391400
H	0.82331100	1.36068000	-2.08377000
H	-3.30817500	1.84030600	1.67046700
N	1.59584200	1.66200600	0.14402300

C	2.20429400	1.00123200	-0.79949600
H	2.05818600	1.64594900	1.04361600
C	3.49087100	0.32026700	-0.60725800
O	1.68610500	0.89395900	-2.00148600
C	3.99042100	-0.48781400	-1.63869100
C	4.20910000	0.43529600	0.59049200
C	5.18474900	-1.17577000	-1.46839400
H	3.43597100	-0.58812900	-2.56156600
C	5.40149800	-0.25726000	0.75498600
H	3.86134900	1.06272000	1.40196800
C	5.88974800	-1.06632500	-0.27051500
H	5.56016100	-1.80475800	-2.26672700
H	5.94883900	-0.16592500	1.68534300
H	6.81845100	-1.60883400	-0.13581100

IRC_TS1_point332

B	-2.68456000	4.00642200	0.31966900
B	-1.61148700	3.84490800	1.73134800
B	-0.74986300	2.30016100	1.59457200
B	-2.48623700	2.56426400	-0.70068200
B	-1.28545400	1.57112800	0.09199900
B	-1.13093200	4.87342900	0.36312100
B	-1.66460300	4.08935300	-1.14036300
H	-3.72581600	4.57737200	0.38235100
B	0.06640000	3.81931700	1.14312100
H	-1.89039900	4.29873400	2.79468600
B	0.26596100	2.38962700	0.12522900
H	-0.40030400	1.65302600	2.52354400
B	-0.80220000	2.55228200	-1.28853900
H	-3.36057100	2.09348900	-1.35147500
H	-1.07495000	6.05786400	0.46368400
B	0.03527300	3.97962900	-0.63454700
H	-1.98967500	4.70313900	-2.10509300
H	0.98384800	4.22496900	1.78205800
H	-0.56096500	2.07159500	-2.35252800
H	0.92525600	4.49445600	-1.22980500
B	-2.45432000	2.41989700	1.08471300
I	-1.49364500	-0.66051300	-0.18103000
C	0.35735000	-1.42481900	0.60818700
C	0.70342600	-1.14578000	1.92309400
C	1.12782600	-2.22573200	-0.22227300
C	1.89082500	-1.68643800	2.41547600
H	0.07679100	-0.52471400	2.54682300
C	2.30284500	-2.77177800	0.29750300

H	0.83221300	-2.42025900	-1.24424600
C	2.68551600	-2.49989500	1.60773600
H	2.18653300	-1.47158800	3.43594000
H	2.92134100	-3.39555600	-0.33640200
H	3.60641300	-2.91539500	1.99889500
O	-2.03358500	-4.16774200	-0.34538500
C	-3.29641700	-4.12503600	-0.41608900
O	-3.95029600	-3.33632800	-1.15837600
C	-4.09302800	-5.06754000	0.48285500
H	-4.36390900	-4.52909200	1.39647800
H	-5.01796800	-5.38386900	-0.00331300
H	-3.50450500	-5.94098400	0.76589400
H	0.82584600	1.36428800	-2.08471100
H	-3.31030700	1.84170700	1.67052800
N	1.59465000	1.66048300	0.14477100
C	2.20564700	1.00327200	-0.80050200
H	2.05284200	1.63568400	1.04923700
C	3.49170400	0.32144300	-0.60710200
O	1.69004600	0.89940700	-2.00284600
C	3.98935700	-0.48978600	-1.63692400
C	4.21126500	0.43895400	0.58961900
C	5.18324800	-1.17836900	-1.46618300
H	3.43374600	-0.59185900	-2.55890900
C	5.40321200	-0.25437500	0.75465000
H	3.86508800	1.06940700	1.39950800
C	5.88958800	-1.06652700	-0.26933300
H	5.55734000	-1.80943900	-2.26348700
H	5.95178800	-0.16110300	1.68408100
H	6.81803200	-1.60944200	-0.13439700

IRC_TS1_point333

B	-2.68428600	4.00660800	0.31931100
B	-1.61182600	3.84471400	1.73137200
B	-0.75095600	2.29954200	1.59504200
B	-2.48636200	2.56446300	-0.70094500
B	-1.28645100	1.57080800	0.09225800
B	-1.13001000	4.87301600	0.36312400
B	-1.66370000	4.08908100	-1.14041900
H	-3.72538500	4.57863700	0.38147600
B	0.06632300	3.81822000	1.14375100
H	-1.89079100	4.29947600	2.79472700
B	0.26562600	2.38830200	0.12595500
H	-0.40236400	1.65226300	2.52441800
B	-0.80197900	2.55172800	-1.28811900

H	-3.36066900	2.09415300	-1.35206100
H	-1.07418600	6.05668400	0.46431600
B	0.03592800	3.97854200	-0.63386200
H	-1.98787500	4.70300900	-2.10541900
H	0.98347400	4.22352000	1.78318200
H	-0.56012300	2.07018900	-2.35183200
H	0.92715600	4.49215700	-1.22934900
B	-2.45521600	2.42015100	1.08458300
I	-1.49466600	-0.66097100	-0.18083600
C	0.35665300	-1.42505200	0.60792800
C	0.70291400	-1.14601700	1.92281000
C	1.12731900	-2.22544200	-0.22285400
C	1.89073300	-1.68610200	2.41480500
H	0.07613500	-0.52532800	2.54676000
C	2.30268600	-2.77106900	0.29660600
H	0.83161600	-2.41985900	-1.24482400
C	2.68559900	-2.49913000	1.60676200
H	2.18656700	-1.47125400	3.43523600
H	2.92126900	-3.39454700	-0.33750000
H	3.60677000	-2.91429800	1.99765300
O	-2.03292500	-4.17055800	-0.34543200
C	-3.29498200	-4.12569200	-0.41635500
O	-3.94707400	-3.33836700	-1.16310200
C	-4.09233400	-5.06314200	0.48504500
H	-4.37385300	-4.51422700	1.39172400
H	-5.01299800	-5.38837800	-0.00450300
H	-3.50206000	-5.93249100	0.78391000
H	0.82853700	1.36839900	-2.08566300
H	-3.31068600	1.84152200	1.66920700
N	1.59377600	1.65761900	0.14658700
C	2.20654900	1.00438000	-0.79988800
H	2.04950500	1.62940900	1.04933300
C	3.49239900	0.32245000	-0.60711700
O	1.69359400	0.90545000	-2.00455300
C	3.98822600	-0.49171100	-1.63548700
C	4.21336600	0.44273200	0.58845400
C	5.18169600	-1.18091000	-1.46421100
H	3.43131100	-0.59596500	-2.55642300
C	5.40494200	-0.25115400	0.75393500
H	3.86842600	1.07584000	1.39672700
C	5.88944000	-1.06649100	-0.26840900
H	5.55435200	-1.81466000	-2.26008600
H	5.95466600	-0.15587000	1.68250000
H	6.81753700	-1.60993200	-0.13290800

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B	-2.68393800	4.00684200	0.31899300
B	-1.61210800	3.84428600	1.73144500
B	-0.75184800	2.29879900	1.59527300
B	-2.48641100	2.56459900	-0.70119500
B	-1.28712500	1.57044600	0.09228400
B	-1.12952700	4.87231300	0.36365200
B	-1.66279600	4.08885400	-1.14021900
H	-3.72467200	4.57937400	0.38081000
B	0.06619100	3.81718000	1.14456500
H	-1.89133100	4.29854300	2.79458300
B	0.26527600	2.38730800	0.12669400
H	-0.40351700	1.65126800	2.52434000
B	-0.80197100	2.55110300	-1.28778000
H	-3.36057500	2.09466900	-1.35276800
H	-1.07354400	6.05611000	0.46493500
B	0.03664800	3.97748000	-0.63317200
H	-1.98669100	4.70294500	-2.10507500
H	0.98336400	4.22209600	1.78430400
H	-0.56127100	2.06967100	-2.35188000
H	0.92750800	4.49138800	-1.22788900
B	-2.45574500	2.41997700	1.08407300
I	-1.49580200	-0.66154700	-0.18072500
C	0.35587300	-1.42531000	0.60767600
C	0.70215800	-1.14635200	1.92256300
C	1.12677200	-2.22519000	-0.22334100
C	1.89036800	-1.68585000	2.41426700
H	0.07515900	-0.52610900	2.54672400
C	2.30244700	-2.77037200	0.29589700
H	0.83105100	-2.41960600	-1.24529600
C	2.68549700	-2.49837900	1.60599500
H	2.18622000	-1.47106100	3.43470400
H	2.92119900	-3.39355400	-0.33830800
H	3.60689500	-2.91321200	1.99671700
O	-2.03044700	-4.17378700	-0.34823300
C	-3.29283300	-4.12611800	-0.41793100
O	-3.94421900	-3.34073900	-1.16596700
C	-4.09344500	-5.05798300	0.48976200
H	-4.37926500	-4.50333700	1.39008200
H	-5.01030600	-5.38905200	-0.00165300
H	-3.50327700	-5.92239300	0.79440400
H	0.83123700	1.37251100	-2.08663500
H	-3.31272900	1.84256200	1.66939800

N	1.59310100	1.65633700	0.14683300
C	2.20784600	1.00633100	-0.80053700
H	2.04573600	1.62088600	1.05335400
C	3.49318400	0.32342900	-0.60685100
O	1.69751500	0.91155200	-2.00599100
C	3.98719000	-0.49376300	-1.63367100
C	4.21543100	0.44628000	0.58764200
C	5.18023100	-1.18353100	-1.46184100
H	3.42916300	-0.59986700	-2.55376800
C	5.40666500	-0.24807900	0.75364500
H	3.87179200	1.08210200	1.39436800
C	5.88934500	-1.06650700	-0.26710800
H	5.55156700	-1.81944500	-2.25658800
H	5.95761400	-0.15062100	1.68124100
H	6.81727200	-1.61008000	-0.13140400