

*Supporting Information for*

**Insights to Lewis Bases-Catalyzed Chemoselective [3+2] and [3+4]  
Annulation Reactions of MBH Carbonates**

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**Table of Contents**

1.	Test results of computational methods .....	1
2.	The local activity indexes for predicting chemoselectivity .....	1
3.	Distances of C $\alpha$ –O <sub>3</sub> , and single-point energies of IRC in TS5 .....	2
4.	Distances of C1 <sup>b</sup> –C2 <sup>b</sup> , and single-point energies of IRC in TSb <sub>[3+2]</sub> .....	2
5.	Distances of C1 <sup>c</sup> –C2 <sup>c</sup> , and single-point energies of IRC in TSc <sub>[3+4]</sub> .....	3
6.	The orbital changes along several representative IRC points of TS5 .....	4
7.	The orbital changes along several representative IRC points of TSb <sub>[3+2]</sub> .....	5
8.	The orbital changes along several representative IRC points of TSc <sub>[3+4]</sub> .....	6
9.	Absolute single-point energies and Gibbs free energy (GFE) of the optimized structures by the B3LYP .....	6
10.	Coordinates of stationary points of DABCO catalyzed cyclization and IRC points in TS5 (IRC-1 is transition state) in acetonitrile solvent .....	7
11.	Coordinates of M2b, TSb <sub>[3+2]</sub> , TSb <sub>[3+4]</sub> and IRC points in TSb <sub>[3+2]</sub> (IRC-1 is transition state) .....	62
12.	Coordinates of M2c, TSc <sub>[3+4]</sub> , TSc <sub>[3+2]</sub> and IRC points in TSc <sub>[3+4]</sub> (IRC-1 is transition state) .....	100

## 1. Test results of computational methods

B3LYP method was employed for optimization and the frequency calculation of all intermediates, and transition states. In order to test the reliability of the selected method, different computational levels including B3LYP/6-31G(d) (L1), M06-2X/6-31G(d) (L2), and  $\omega$ B97X-D/6-31G(d) (L3) were used for additionally computing the key step, and the calculated results had been shown in **Table S1**. There are small differences between the calculated results obtained by L1-3, but the trend and conclusions should be the same, indicating the computational method is reliable.

**Table S1.** Comparison of relative Gibbs free energies ( $\Delta\Delta G^\ddagger$ ) of the key step calculated by using different levels including B3LYP/6-31G(d) (L1), M06-2X/6-31G(d) (L2) and  $\omega$ B97X-D/6-31G(d) (L3) (Unit: kcal/mol).

	L1	L2	L3
<b>M2a</b>	0.0	0.0	0.0
<b>TSa<sub>[3+4]</sub></b>	10.7	8.3	9.8

## 2. The local activity indexes for predicting chemoselectivity

Generally, the electrophilic and nucleophilic Parr function ( $P_k^+$  and  $P_k^-$ ) can be used to predict the electrophilicity and nucleophilicity of the reaction sites, respectively. The bigger nucleophilic Parr function values are corresponding to the stronger nucleophilicity of the reaction sites. In order to explore the general principle for predicting chemoselectivity, the nucleophilic Parr function  $P_k^-$  analysis were performed for the selected three reactions. For the first reaction (Scheme S1a), the data summarized in Table S2a shows  $P_k^-(O3)$  (0.324) <  $P_k^-(C2)$  (0.357), which is not agreement with the computed energy barriers and experimental results. For the second reaction (Scheme S1b), the data summarized in Table S2b shows  $P_k^-(C2)^b$  (0.711) >  $P_k^-(O1)^b$  (0.404), which is consistent with the computed energy barriers and experimental results. For the third reaction (Scheme S1c), the data summarized in Table S2c shows  $P_k^-(C2)^c$  (0.077) <  $P_k^-(N1)^c$  (0.269), which is not agreement with the computed energy barriers and experimental results. In summary, the Parr function analysis is not suitable to predict the origin of chemoselectivity for these kinds of reactions.

**Table S2a.** The nucleophilic Parr functions ( $P_k^-$ ) of the ring-closure sites and the energy barrier ( $\Delta\Delta G^\ddagger$ ) of the ring-closure step in the first reaction model.

	O3	C2
$P_k^-$	0.324	0.357
$\Delta\Delta G^\ddagger$ (kcal/mol)	10.7	19.2

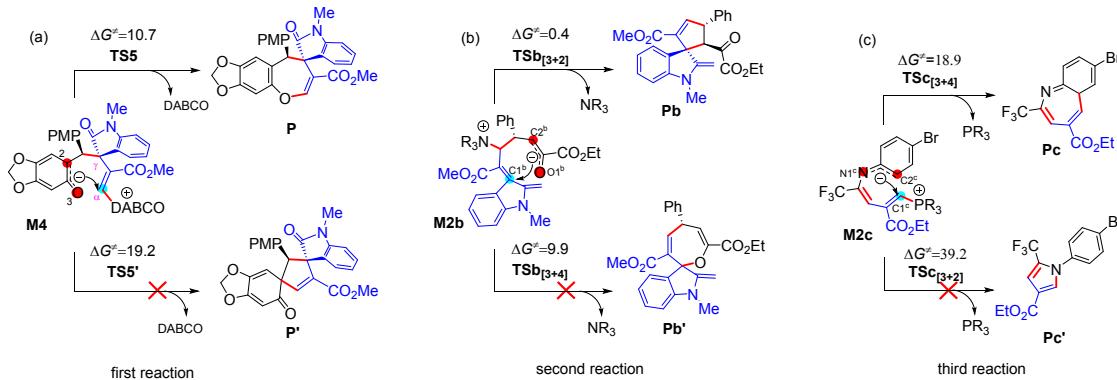
**Table S2b.** The nucleophilic Parr functions ( $P_k^-$ ) of the ring-closure sites and the energy

barrier ( $\Delta\Delta G^\ddagger$ ) of the ring-closure step in the second reaction model.

	C2 <sup>b</sup>	O1 <sup>b</sup>
$P_k^-$	0.711	0.404
$\Delta\Delta G^\ddagger$ (kcal/mol)	0.4	9.9

**Table S2c.** The nucleophilic Parr functions ( $P_k^-$ ) of the ring-closure sites and the energy barrier ( $\Delta\Delta G^\ddagger$ ) of the ring-closure step in the third reaction model.

	C2 <sup>c</sup>	N1 <sup>c</sup>
$P_k^-$	0.077	0.269
$\Delta\Delta G^\ddagger$ (kcal/mol)	18.9	39.2



**Scheme S1.** The chemoselective step of the selected three reaction models.

### 3. Distances of C $\alpha$ –O3, and single-point energies of IRC in TS5

**Table S3.** The distances of C $\alpha$ –O3 (unit: Å) and single-point energies E (unit: a.u.) of several IRC points in TS5 at B3LYP/6-311+G(d, p) level in acetonitrile using IEF-PCM model.

	C $\alpha$ –O3	E	C $\alpha$ –O3	E
IRC-F-61	2.69	-2007.954593	IRC-F-16	2.40
IRC-F-52	2.67	-2007.953837	IRC-F-11	2.31
IRC-F-46	2.65	-2007.953766	IRC-F-7	2.19
IRC-F-41	2.63	-2007.953363	IRC-1	1.95
IRC-F-36	2.61	-2007.952721	IRC-R-8	1.62
IRC-F-31	2.57	-2007.951857	IRC-R-23	1.46
IRC-F-26	2.54	-2007.951179	IRC-R-38	1.46
IRC-F-21	2.48	-2007.949949	IRC-R-53	1.46

### 4. Distances of C1<sup>b</sup>–C2<sup>b</sup>, and single-point energies of IRC in TSb<sub>[3+2]</sub>

**Table S4.** The distances of C1<sup>b</sup>–C2<sup>b</sup> (unit: Å) and single-point energies E (unit: a.u.) of several IRC points in TSb<sub>[3+2]</sub> at B3LYP/6-311+G(d, p) level in dichloromethane using IEF-PCM model.

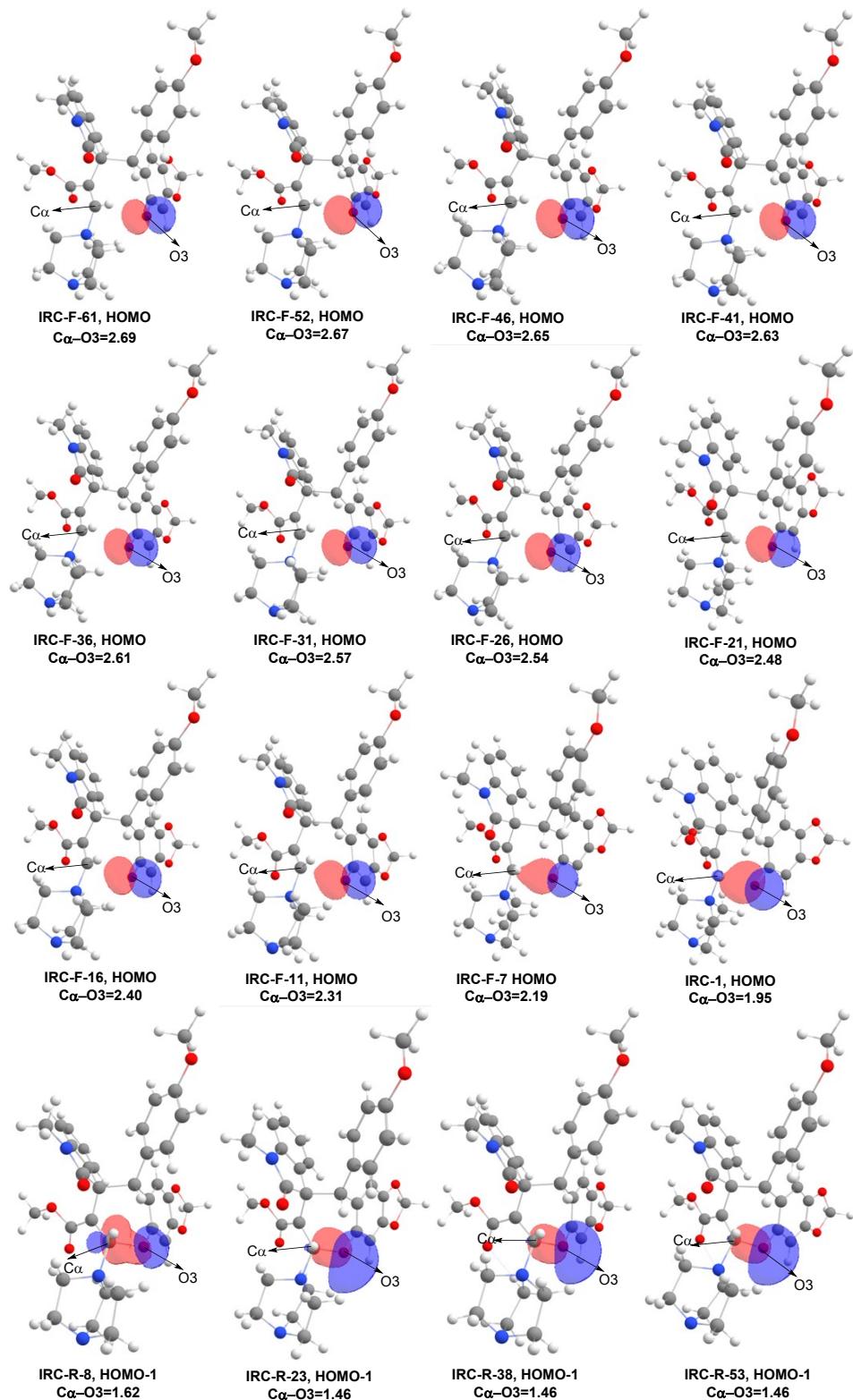
	C1 <sup>b</sup> –C2 <sup>b</sup>	E		C1 <sup>b</sup> –C2 <sup>b</sup>	E
IRC-F-61	2.79	-2069.572408	IRC-F-16	2.58	-2069.568448
IRC-F-51	2.78	-2069.572268	IRC-F-10	2.51	-2069.567242
IRC-F-46	2.77	-2069.572103	IRC-F-4	2.35	-2069.565501
IRC-F-40	2.75	-2069.571857	IRC-1	2.20	-2069.564583
IRC-F-36	2.73	-2069.571485	IRC-R-16	1.69	-2069.572422
IRC-F-30	2.69	-2069.570601	IRC-R-31	1.66	-2069.577244
IRC-F-28	2.66	-2069.570056	IRC-F-45	1.64	-2069.580735
IRC-F-20	2.62	-2069.569200	IRC-R-61	1.61	-2069.583791

## 5. Distances of C1<sup>c</sup>–C2<sup>c</sup>, and single-point energies of IRC in TSc<sub>[3+4]</sub>

**Table S5.** The distances of C1<sup>c</sup>–C2<sup>c</sup> (unit: Å) and single-point energies E (unit: a.u.) of several IRC points in TSc<sub>[3+4]</sub> at B3LYP/6-311+G(d, p) level in chloroform using IEF-PCM model.

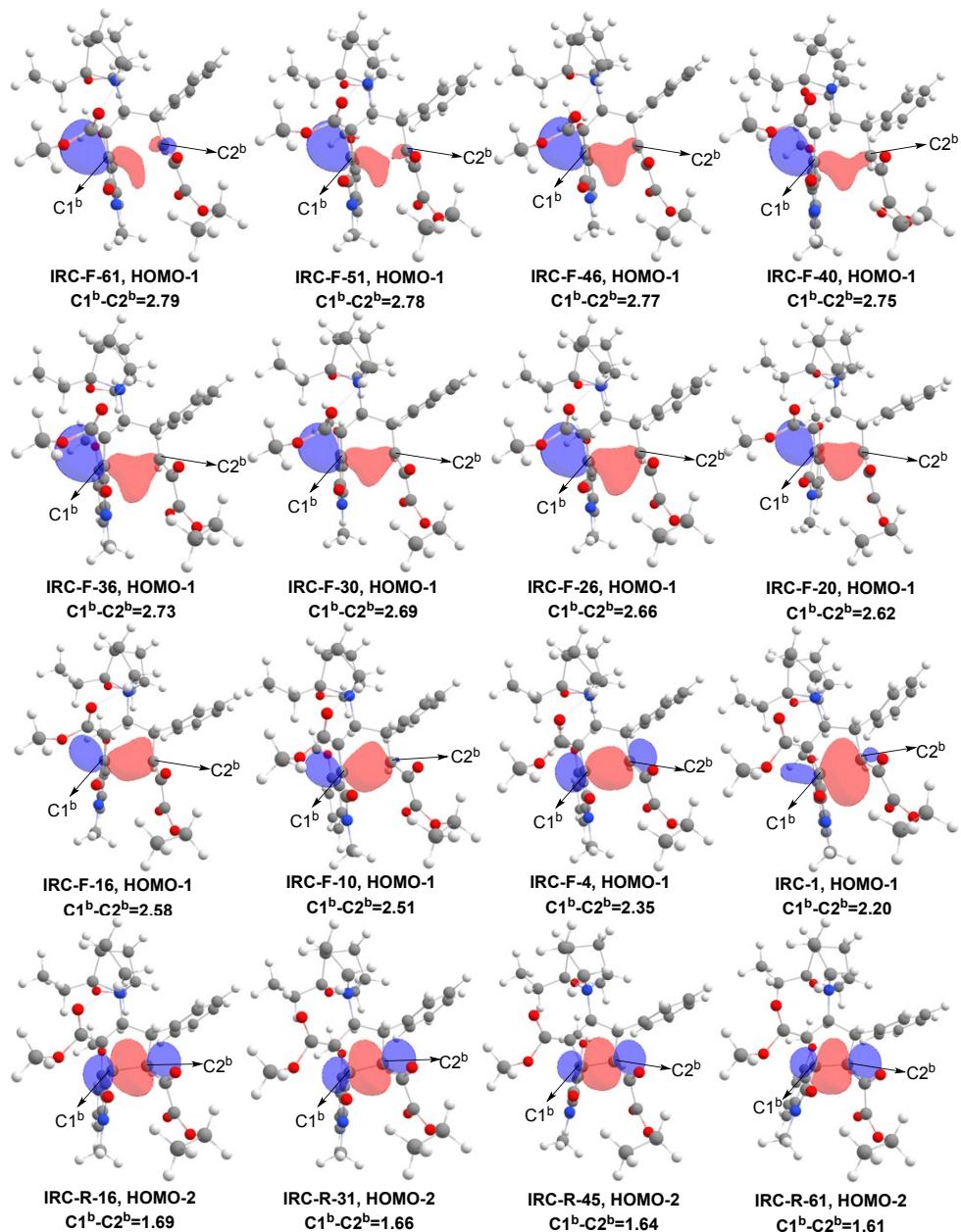
	C1 <sup>c</sup> –C2 <sup>c</sup>	E		C1 <sup>c</sup> –C2 <sup>c</sup>	E
IRC-F-61	2.99	-4655.749474	IRC-F-17	2.64	-4655.740316
IRC-F-52	2.98	-4655.748755	IRC-F-11	2.45	-4655.73445
IRC-F-47	2.97	-4655.748379	IRC-F-5	2.12	-4655.724053
IRC-F-42	2.96	-4655.747858	IRC-1	1.88	-4655.720977
IRC-F-37	2.93	-4655.747206	IRC-R-5	1.72	-4655.721701
IRC-F-32	2.89	-4655.746461	IRC-R-9	1.71	-4655.721934
IRC-F-27	2.83	-4655.745184	IRC-R-12	1.70	-4655.722063
IRC-F-22	2.74	-4655.743224	IRC-R-15	1.69	-4655.722173

## 6. The orbital changes along several representative IRC points of TS5



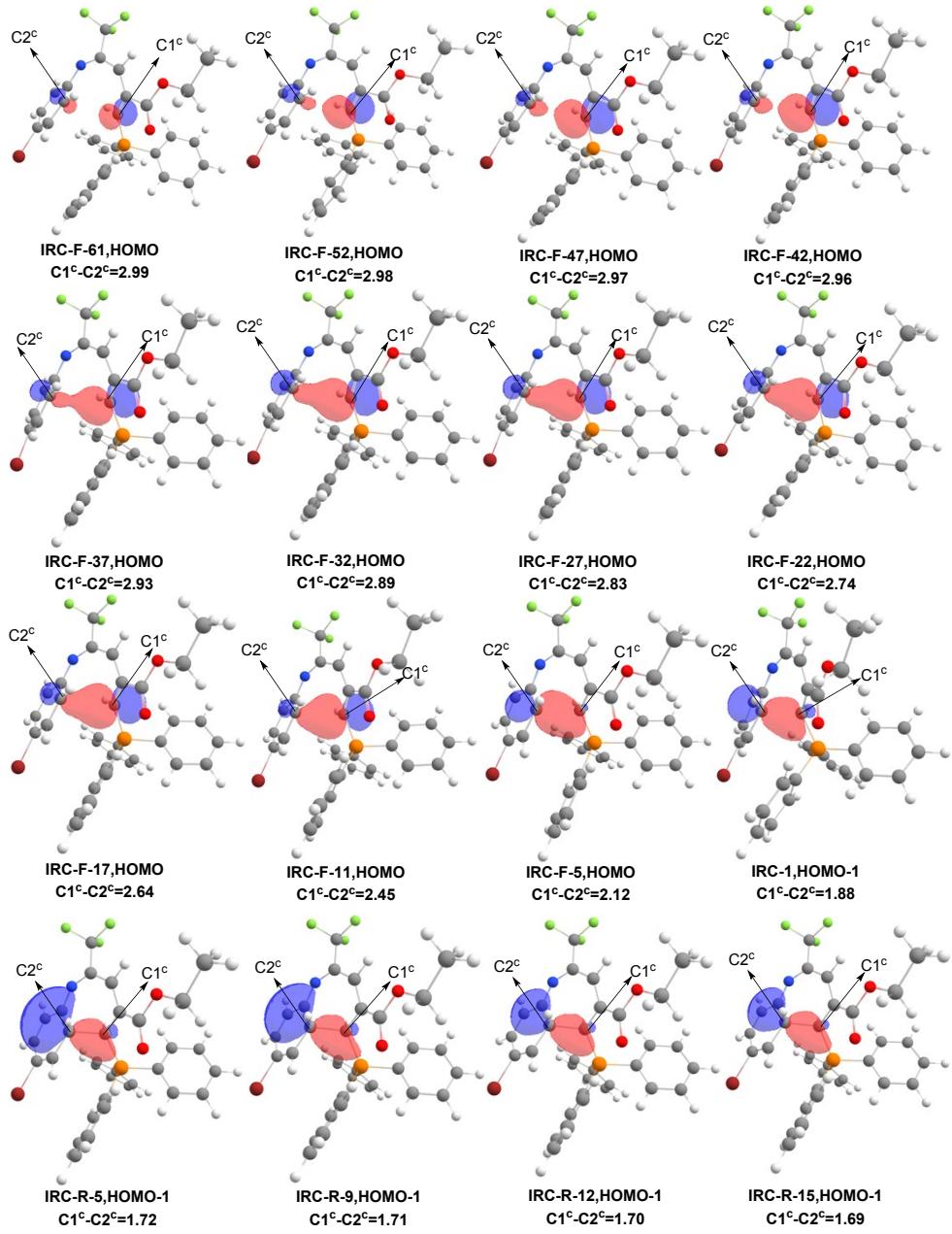
**Figure S1.** The orbital structures of several representative IRC points of TS5 calculated at the B3LYP/6-311G+(d, p) level in acetonitrile solvent, (F represents forward, R represents reverse, IRC-1 is the structure of TS5, and only the orbital pictures of the C $\alpha$  and O $3$  atoms are shown, length unit is in Å) (The basis set has little effect on the orbital structures).

## 7. The orbital changes along several representative IRC points of $\text{TSb}_{[3+2]}$



**Figure S2.** The orbital structures of several representative IRC points of  $\text{TSb}_{[3+2]}$  calculated at the B3LYP/6-311G+(d, p) level in dichloromethane solvent, (F represents forward, R represents reverse, IRC-1 is the structure of  $\text{TSb}_{[3+2]}$ , and only the orbital pictures of the  $C1^b$  and  $C2^b$  atoms are shown, length is in Å) (The basis set has little effect on the orbital structures).

## 8. The orbital changes along several representative IRC points of $\text{TSc}_{[3+4]}$



**Figure S3.** The orbital structures of several representative IRC points of  $\text{TSc}_{[3+4]}$  calculated at the B3LYP/6-311G+(d, p) level in chloroform solvent, (F represents forward, R represents reverse, IRC-1 is the structure of  $\text{TSc}_{[3+4]}$ , and only the orbital pictures of the C1<sup>c</sup> and C2<sup>c</sup> atoms are shown, length is in Å) (The basis set has little effect on the orbital structures).

## 9. Absolute single-point energies and Gibbs free energy (GFE) of the optimized structures by the B3LYP

**Table S6.** The single-point, Gibbs free energy corrections (GFEC) and GFE (=E+GFEC) energies

of the stationary points involved in DABCO catalyzed cyclization (first representative example).

(unit: a.u.)

	GFEC (B3LYP/6-31G(d) /IEF-PCM <sub>acetonitrile</sub> )	E (B3LYP-D3/6-311+G(d, p)/IEF-PCM <sub>acetonitrile</sub> )	GFE
DABCO	0.154749	-345.4433091	-345.2885601
R1	0.313590	-1205.083621	-1204.770031
TS1	0.494464	-1550.536178	-1550.041714
TS1'	0.489232	-1550.511056	-1550.021824
M1	0.493567	-1550.537141	-1550.043574
TS2	0.493163	-1550.526268	-1550.033105
M2	0.491393	-1550.556940	-1550.065547
TS3	0.483022	-1550.524128	-1550.041106
M3	0.353884	-1128.114870	-1127.760986
<i>t</i> -BuOH+CO <sub>2</sub>	0.110313	-422.4221274	-422.3118144
R2	0.194986	-879.9372029	-879.7422169
TS4	0.571303	-2008.051740	-2007.480437
TS4'	0.574619	-2008.046574	-2007.471955
M4	0.575726	-2008.069169	-2007.493443
TS5	0.580343	-2008.056784	-2007.476441
TS5'	0.578221	-2008.041065	-2007.462844
P	0.398486	-1662.645748	-1662.247262

**Table S7** The single-point, Gibbs free energy corrections (GFEC) and GFE (=E+GFEC) energies of the stationary points involved in ring-closure step

	GFEC B3LYP/6-31G(d)	E B3LYP-D3/6-311+ G(d, p)	GFE
<b>M2b</b>	0.428331	-4655.8417046	-4655.413374
<b>TSb<sub>[3+2]</sub></b>	0.433282	-4655.8165027	-4655.383221
<b>TSb<sub>[3+4]</sub></b>	0.431122	-4655.7820035	-4655.350882
<b>M2c</b>	0.632144	-2069.6996144	-2069.067470
<b>TSc<sub>[3+4]</sub></b>	0.633333	-2069.7002027	-2069.066870
<b>TSc<sub>[3+2]</sub></b>	0.634909	-2069.6866587	-2069.051750

## 10. Coordinates of stationary points of DABCO catalyzed cyclization and IRC points in TS5 (IRC-1 is transition state) in acetonitrile solvent

### DABCO

O 1  
C 1. 19958900 0. 78180100 -0. 69278200

C	1.19946400	-0.78193500	-0.69289100
C	0.00004700	-0.78141600	1.38544900
C	-0.00004700	0.78141600	1.38544900
H	1.19728400	-1.18073100	-1.71410600
H	2.08364000	-1.18158600	-0.18253000
H	2.08372500	1.18124200	-0.18219300
H	1.19765400	1.18073300	-1.71394600
H	-0.88432900	-1.18103500	1.89560000
H	0.88457800	-1.18091600	1.89542200
H	-0.88457800	1.18091600	1.89542200
H	0.88432900	1.18103500	1.89560000
N	0.00004700	1.29213000	0.00044300
N	-0.00004700	-1.29213000	0.00044300
C	-1.19946400	0.78193500	-0.69289100
C	-1.19958900	-0.78180100	-0.69278200
H	-1.19728400	1.18073100	-1.71410600
H	-2.08364000	1.18158600	-0.18253000
H	-1.19765400	-1.18073300	-1.71394600
H	-2.08372500	-1.18124200	-0.18219300

### R1

0 1			
C	-2.01532700	-1.58059400	0.36691100
C	-1.40898900	-0.95413100	-0.72899400
C	-1.69339000	-1.35951800	-2.02192300
C	-2.59891500	-2.41474700	-2.21244600
C	-3.19739900	-3.03408400	-1.11308900
C	-2.91661200	-2.62565700	0.19928800
C	-0.73942900	0.07509700	1.32950300
C	-0.45030500	0.10768000	-0.22100500
H	-1.22823700	-0.86706300	-2.87120000
H	-2.83619000	-2.74747200	-3.21821500
H	-3.89909100	-3.84812100	-1.27151500
H	-3.39006300	-3.11020100	1.04675700
N	-1.58127200	-0.98807200	1.56286900
C	-2.04350600	-1.36182800	2.88735800
H	-3.12580700	-1.21720000	2.97544100
H	-1.80431500	-2.40988300	3.09399300
H	-1.53280200	-0.72312800	3.60831600
O	-0.27418500	0.81134100	2.18016900
C	-0.62966600	1.45314800	-0.90616500
C	-1.79004000	2.32480600	-0.53480600
C	0.14293900	1.86327800	-1.91761800
O	-1.95519300	3.46302800	-0.93175300

O	-2.65115800	1.69231700	0.28184700
C	-3.80534200	2.44790500	0.70313100
H	-4.40384000	2.73581400	-0.16394500
H	-4.36758000	1.77914600	1.35329700
H	-3.49285800	3.34206200	1.24689600
H	-0.06824400	2.80735800	-2.40793100
H	0.98503900	1.28508000	-2.27936200
C	4.41022200	-0.33718700	0.01831200
C	5.15719200	-1.58404100	-0.45766100
H	4.98856700	-1.75322300	-1.52597800
H	6.23161200	-1.45700700	-0.29224600
H	4.82385100	-2.46945600	0.09298500
C	4.81986200	0.89102400	-0.79734100
H	4.62754900	0.72358700	-1.86254900
H	4.28101600	1.78343400	-0.47420700
H	5.89305000	1.06725700	-0.66910500
C	4.58652100	-0.13453100	1.52479800
H	4.04158200	0.74326000	1.87641200
H	4.23498700	-1.01556800	2.07227600
H	5.64980800	0.00299000	1.74799600
O	2.99603800	-0.68773700	-0.27805300
C	2.00433500	0.16208600	-0.01158500
O	2.07176700	1.26048600	0.48901900
O	0.87122800	-0.46036100	-0.44850500

### TS1

O 1			
C	-2.90276600	-1.23771400	-0.48196400
C	-2.15254400	-0.88096200	0.64714100
C	-2.72707200	-0.90125700	1.90551800
C	-4.07496500	-1.27727300	2.03048100
C	-4.81169600	-1.63303400	0.89930100
C	-4.23453500	-1.62144700	-0.38058900
C	-0.85531300	-0.68181500	-1.34747900
C	-0.74169800	-0.52534000	0.21228400
H	-2.14083200	-0.63464600	2.78114100
H	-4.54320100	-1.29536700	3.01032800
H	-5.85225500	-1.92761700	1.00533900
H	-4.81482100	-1.90120400	-1.25414000
N	-2.11212800	-1.14286000	-1.63981600
C	-2.57843900	-1.41454800	-2.98492500
H	-1.74000600	-1.25699000	-3.66430600
H	-2.92767600	-2.44899600	-3.07163700
H	-3.39694100	-0.73839400	-3.25677500

O	0.03522100	-0.45966200	-2.15894200
C	0.38685100	-1.34682300	0.82431900
C	0.41383700	-2.77138400	0.71838800
C	1.47412400	-0.74462400	1.52268700
O	1.26380300	-3.53850700	1.19629400
O	-0.64409300	-3.28414000	-0.00448700
C	-0.68838700	-4.70678100	-0.12273500
H	-0.76588300	-5.18508800	0.85858400
H	-1.57881700	-4.92689900	-0.71470900
H	0.20210300	-5.09108300	-0.62986400
H	1.31101100	0.23479000	1.96361100
C	-1.12805000	4.32992800	0.17169000
C	-0.28935500	5.26348100	1.04598500
H	0.77682800	5.14398700	0.82825400
H	-0.56821000	6.30372900	0.85112200
H	-0.45478600	5.05328900	2.10748200
C	-0.85228500	4.57549100	-1.31346000
H	0.21274200	4.44191800	-1.53141200
H	-1.43104700	3.89751500	-1.94305900
H	-1.12474300	5.60538500	-1.56737400
C	-2.61328200	4.43704300	0.52463500
H	-3.21790600	3.76263500	-0.08409700
H	-2.77239900	4.20183600	1.58240900
H	-2.95220200	5.46347800	0.34927200
O	-0.61425400	2.99109200	0.56038000
C	-1.09976600	1.87647600	0.01063200
O	-1.97769900	1.77610200	-0.82252400
O	-0.41239200	0.85434000	0.55577800
C	3.95489300	1.25056100	-1.06749300
C	2.65597300	0.89638700	-0.28103600
C	3.29528300	-1.44796400	-0.32978100
C	4.58066500	-1.05651100	-1.11983700
H	2.34303400	1.70297600	0.38609800
H	1.82364100	0.64699500	-0.94144300
H	3.76771100	1.22682700	-2.14557500
H	4.29846600	2.25715300	-0.80961600
H	3.43481700	-2.32644500	0.30218000
H	2.43749000	-1.62954900	-0.98035700
H	5.39047200	-1.76020700	-0.90371300
H	4.39374300	-1.08272700	-2.19783000
N	5.03425300	0.29814400	-0.76253700
N	2.91592500	-0.31139000	0.56298700
C	5.31037800	0.34384300	0.68142000
C	4.03765800	-0.02442600	1.50509700

H	5.65492600	1.35048600	0.93670500
H	6.12296500	-0.35489900	0.90212200
H	3.71566400	0.79028900	2.15968200
H	4.18944500	-0.91713800	2.11739300
H	1.97857900	-1.43494200	2.19608300

### TS1'

0 1

C	0.38932000	-1.67389700	0.60273300
C	-0.04118600	-1.09031500	-0.61904300
C	0.10813200	-1.81356400	-1.81283600
C	0.72014700	-3.06519500	-1.78098800
C	1.16831800	-3.60393300	-0.56637200
C	1.00524200	-2.91986200	0.64118500
C	-0.42152300	0.35290100	1.21754900
C	-0.63747800	0.18934100	-0.28925800
H	-0.26148600	-1.43046700	-2.75673200
H	0.84371500	-3.62720800	-2.70078000
H	1.64641700	-4.57911300	-0.55900600
H	1.35058500	-3.34815000	1.57523300
N	0.08712300	-0.84076500	1.67720600
C	0.58196100	-1.02216000	3.03367500
H	0.27125100	-1.99649200	3.42072100
H	1.67211600	-0.93438700	3.02244500
H	0.14670200	-0.23582200	3.65140100
O	-0.72385200	1.32285800	1.89385200
C	-0.66927200	1.39614400	-1.11822100
C	-0.99391300	2.75396500	-0.52203900
C	-0.29784000	1.41999200	-2.41223100
O	-0.20870600	3.67741100	-0.50995000
O	-2.27349800	2.85954600	-0.12868800
C	-2.65411400	4.13532400	0.43376800
H	-2.49848400	4.93125200	-0.29702200
H	-3.71067100	4.03902100	0.67960800
H	-2.06546700	4.33537000	1.33144100
H	-0.27654000	2.35706100	-2.95921100
H	0.02544000	0.54072700	-2.95222600
C	5.40548400	0.28110300	-0.33021700
C	6.13732200	0.97621200	-1.48695600
H	6.16097300	2.06060900	-1.33130400
H	7.16936700	0.61585500	-1.56422400
H	5.63043000	0.77819600	-2.43804400
C	6.10505000	0.60709900	0.99773100
H	6.12186500	1.69198600	1.15771600

H	5. 57948000	0. 13820800	1. 83061900
H	7. 14221100	0. 25100100	0. 97977000
C	5. 34695600	-1. 23233100	-0. 58426900
H	4. 79516700	-1. 72921100	0. 21474400
H	4. 84417700	-1. 43493900	-1. 53769400
H	6. 35921000	-1. 65099800	-0. 63888900
O	4. 07872000	0. 86574300	-0. 37912400
C	3. 05847700	0. 51435000	0. 53487100
O	3. 29485100	-0. 34247500	1. 41521100
O	2. 00453300	1. 15687600	0. 30897400
C	-3. 42070200	0. 04419400	-1. 35682200
C	-4. 89552700	-0. 50584100	-1. 36777000
C	-4. 34355600	-2. 30715200	0. 08491100
C	-2. 82791100	-1. 88738200	-0. 03429200
H	-5. 59374300	0. 31781000	-1. 54209200
H	-5. 02377700	-1. 23737900	-2. 17051300
H	-2. 85401200	-0. 32901800	-2. 21320800
H	-3. 40098100	1. 13319600	-1. 37121400
H	-4. 53664500	-2. 74751100	1. 06712200
H	-4. 57819300	-3. 05528000	-0. 67742400
H	-2. 25775400	-2. 21966300	0. 83500700
H	-2. 37502200	-2. 30834000	-0. 93239600
N	-2. 75177100	-0. 41056500	-0. 11515800
N	-5. 21709500	-1. 14696200	-0. 09167000
C	-3. 43364900	0. 16310200	1. 07363900
C	-4. 96356300	-0. 19481700	0. 99161200
H	-3. 26581100	1. 23693300	1. 08695200
H	-2. 97590800	-0. 27342700	1. 96264100
H	-5. 55576500	0. 70649700	0. 80965100
H	-5. 29006500	-0. 63162100	1. 93990400

### M1

0 1			
C	2. 88411800	-1. 27133100	0. 46706500
C	2. 11863700	-0. 90843500	-0. 64961800
C	2. 67086500	-0. 94126000	-1. 91758300
C	4. 01101600	-1. 33663500	-2. 06508600
C	4. 76273700	-1. 69884100	-0. 94593600
C	4. 20830400	-1. 67448200	0. 34386300
C	0. 86240700	-0. 67778600	1. 36719600
C	0. 71987000	-0. 53106800	-0. 19145800
H	2. 07279900	-0. 67036800	-2. 78392400
H	4. 46150500	-1. 36465100	-3. 05305200
H	5. 79700100	-2. 00857000	-1. 06925900

H	4.79991900	-1.95912600	1.20823200
N	2.11596400	-1.16008000	1.63876200
C	2.60194800	-1.43605200	2.97586600
H	1.77811500	-1.26467900	3.66962400
H	2.93722300	-2.47547500	3.05872600
H	3.43527400	-0.77190600	3.23213500
O	-0.00838700	-0.43654600	2.19510400
C	-0.43387600	-1.33690000	-0.77313900
C	-0.46863100	-2.75330100	-0.69064300
C	-1.53830200	-0.71197200	-1.46973200
O	-1.33236500	-3.51365800	-1.16556900
O	0.59865000	-3.28948900	0.01220900
C	0.63313300	-4.71258400	0.10267900
H	0.69660400	-5.17579900	-0.88731100
H	1.52853100	-4.95161500	0.68041500
H	-0.25364900	-5.10246700	0.61277800
H	-1.32805500	0.24645500	-1.94107200
C	1.17609800	4.32036800	-0.17742100
C	0.33659100	5.26244200	-1.04180500
H	-0.72755400	5.15899200	-0.80654200
H	0.63328700	6.29936400	-0.855578100
H	0.48182300	5.04584500	-2.10498300
C	0.92750500	4.57489600	1.31104500
H	-0.13570700	4.45752400	1.54658400
H	1.50639900	3.89064000	1.93369800
H	1.21900300	5.60150900	1.55683800
C	2.65699300	4.40658100	-0.55394600
H	3.26227500	3.72731800	0.04868200
H	2.79666900	4.16425700	-1.61287700
H	3.01178600	5.42936600	-0.38902200
O	0.63803900	2.98765000	-0.55300400
C	1.11784000	1.86777800	-0.00780000
O	2.00825700	1.75906600	0.81103400
O	0.40827300	0.85368500	-0.53814400
C	-3.89559900	1.23598000	1.12258500
C	-2.60670100	0.88993600	0.31953500
C	-3.31905700	-1.44218300	0.30077800
C	-4.62098600	-1.04081600	1.05393200
H	-2.28592000	1.70910900	-0.32718900
H	-1.77470500	0.60646300	0.96599300
H	-3.71429600	1.13400600	2.19681500
H	-4.19792900	2.26996500	0.93125700
H	-3.44597600	-2.30737800	-0.35061600
H	-2.48340800	-1.64308600	0.97266500

H	-5.44643200	-1.69818200	0.76474700
H	-4.48088600	-1.13613100	2.13494000
N	-5.00789000	0.34712400	0.75489800
N	-2.88825600	-0.29251800	-0.56528600
C	-5.25642800	0.47217600	-0.68833600
C	-4.00083900	0.05458100	-1.51074200
H	-5.52793900	1.50960200	-0.90447400
H	-6.10906500	-0.16016400	-0.95263000
H	-3.63855800	0.85792400	-2.15729800
H	-4.18623500	-0.82769300	-2.12803700
H	-2.00621900	-1.40493300	-2.16951200

## TS2

0 1

C	1.19032200	-2.92902300	0.82004700
C	1.34343300	-1.91053500	-0.13654700
C	2.31735900	-2.05843500	-1.11965200
C	3.07192100	-3.23782300	-1.17034800
C	2.86435700	-4.25899100	-0.24000100
C	1.91793100	-4.11379000	0.78128200
C	-0.19135800	-1.26713600	1.57434000
C	0.43410000	-0.76906400	0.23859100
H	2.48945500	-1.26084500	-1.82714100
H	3.82712200	-3.35592100	-1.94228700
H	3.45045400	-5.17225500	-0.29599000
H	1.77148200	-4.89198500	1.52325500
N	0.25145700	-2.54572400	1.79110200
C	-0.14011700	-3.35237000	2.93198300
H	-0.59337100	-4.29230900	2.60029800
H	0.72674000	-3.57791900	3.56273700
H	-0.86787300	-2.78014700	3.50753300
O	-0.97882700	-0.67596200	2.30889800
C	-0.48953400	-0.09062400	-0.64169200
C	-0.52799000	-0.13830400	-2.07823300
C	-1.26902500	1.03757200	-0.05137100
O	-1.23347200	0.60738100	-2.77774400
O	0.20640000	-1.11911700	-2.67818100
C	0.11339900	-1.18552100	-4.10380200
H	0.43951300	-0.25055700	-4.56851200
H	0.77467900	-2.00159600	-4.40055200
H	-0.91130100	-1.39856200	-4.42333400
C	3.73263200	3.08443200	0.53448500
C	4.13926700	3.85873700	1.79205400
H	4.64012300	3.19848500	2.50781000

H	4. 82652000	4. 66974800	1. 52967000
H	3. 26024200	4. 29396200	2. 27906200
C	4. 95826300	2. 43052100	-0. 11244600
H	5. 45096100	1. 75890800	0. 59950800
H	4. 67800700	1. 86051600	-0. 99942200
H	5. 67754500	3. 20432000	-0. 40315200
C	2. 97832200	3. 99815700	-0. 43725400
H	2. 67077800	3. 45251300	-1. 33054900
H	2. 08831900	4. 41516400	0. 04732900
H	3. 62363000	4. 83144900	-0. 73702800
O	2. 82730400	2. 05628600	1. 07284100
C	2. 23607800	1. 13242100	0. 26632100
O	2. 37970300	1. 07540700	-0. 94826500
O	1. 50490600	0. 34645100	1. 02451700
H	-0. 94502400	1. 23559300	0. 96521500
H	-1. 16901500	1. 94465200	-0. 65062000
C	-3. 28966300	1. 48473700	1. 40666200
C	-4. 84394000	1. 50521800	1. 46979900
H	-2. 83646400	0. 86067400	2. 17693000
H	-2. 85909300	2. 48669700	1. 46784000
H	-5. 18394100	1. 03882100	2. 39898100
H	-5. 21698300	2. 53327300	1. 45477200
C	-3. 32800800	-0. 53355400	0. 00977300
H	-3. 07128700	-0. 89788400	-0. 98432000
H	-2. 76008400	-1. 09221500	0. 75025500
C	-4. 85919200	-0. 56977600	0. 28644400
H	-5. 36524700	-1. 14135000	-0. 49703200
H	-5. 06215400	-1. 06144200	1. 24237800
C	-5. 07658900	1. 48263800	-0. 91036000
H	-5. 45017500	0. 89386000	-1. 75334800
H	-5. 58365300	2. 45196200	-0. 92915400
C	-3. 54077600	1. 68465500	-1. 02230100
H	-3. 11129400	1. 33475400	-1. 96002500
H	-3. 25353500	2. 72842600	-0. 87573700
N	-2. 85583500	0. 89901000	0. 07949100
N	-5. 43138500	0. 78282800	0. 33247300

## M2

0 1

C	1. 55439600	2. 88363700	-0. 40234300
C	1. 17600100	1. 95545400	0. 59610200
C	1. 88402500	1. 94697800	1. 80099400
C	2. 91662200	2. 86821300	2. 00299400
C	3. 25129400	3. 79206100	1. 00938100

C	2. 57402500	3. 80812600	-0. 21573300
C	-0. 08659800	1. 64916900	-1. 39507200
C	0. 10687500	1. 12220900	0. 02735900
H	1. 64764000	1. 23783900	2. 58231800
H	3. 46159000	2. 86121200	2. 94188700
H	4. 05359600	4. 50390300	1. 18131300
H	2. 84660800	4. 51258700	-0. 99435300
N	0. 77454100	2. 70640700	-1. 54673800
C	0. 90984300	3. 46296400	-2. 77635000
H	0. 75799300	4. 53074900	-2. 58911900
H	1. 90204000	3. 31261600	-3. 21552300
H	0. 14888200	3. 10504700	-3. 46993600
O	-0. 91824200	1. 30712600	-2. 23394000
C	-0. 61260700	0. 08268200	0. 52874800
C	-0. 52779700	-0. 39020500	1. 94853300
C	-1. 42181500	-0. 82884500	-0. 36277900
O	-0. 49378900	-1. 56704800	2. 26424200
O	-0. 59376600	0. 61307400	2. 83758600
C	-0. 56387000	0. 22900000	4. 23147800
H	0. 36951500	-0. 28846500	4. 46367400
H	-0. 63479200	1. 16276300	4. 78715100
H	-1. 41018800	-0. 42227700	4. 45950600
C	3. 79326200	-2. 84199800	-0. 32680900
C	5. 32161500	-2. 77283600	-0. 19762500
H	5. 62046900	-1. 88184600	0. 36593100
H	5. 70683100	-3. 65664500	0. 32368000
H	5. 79096900	-2. 72445900	-1. 18682700
C	3. 15393000	-2. 88191800	1. 06944800
H	3. 47267600	-2. 01027900	1. 65409600
H	2. 06597200	-2. 86999700	0. 99033300
H	3. 46632000	-3. 78406800	1. 60949400
C	3. 39920200	-4. 06725900	-1. 16536800
H	2. 31561400	-4. 11776300	-1. 27566100
H	3. 85227000	-4. 00248200	-2. 16215800
H	3. 75842800	-4. 98784200	-0. 68929600
O	3. 46045600	-1. 60728100	-1. 00896800
C	2. 12706000	-1. 25053700	-1. 33441600
O	1. 20196200	-2. 05385900	-1. 07684500
O	2. 07154800	-0. 11817600	-1. 86497800
H	-1. 14829100	-0. 67730600	-1. 39889900
H	-1. 22078500	-1. 86211400	-0. 08387100
C	-3. 52319200	-1. 28525400	-1. 56316500
C	-5. 07454500	-1. 25976400	-1. 48803400
H	-3. 13104700	-0. 69099500	-2. 38995100

H	-3.11690500	-2.29590100	-1.63308200
H	-5.48115600	-0.80006200	-2.39272300
H	-5.47120600	-2.27600100	-1.41856600
C	-3.39124100	0.78852800	-0.23961500
H	-3.03172200	1.18672200	0.71016100
H	-2.87923400	1.29788000	-1.05519300
C	-4.94212200	0.84433100	-0.35546000
H	-5.35405600	1.43443800	0.46748600
H	-5.23513100	1.32409900	-1.29310500
C	-5.08786800	-1.18534100	0.90040500
H	-5.39103700	-0.58829400	1.76452800
H	-5.59034700	-2.15396600	0.96725500
C	-3.54506900	-1.39123200	0.90089300
H	-3.07722700	-0.98550500	1.79667500
H	-3.25860200	-2.43980900	0.80417700
N	-2.95402500	-0.66561600	-0.29510000
N	-5.53188900	-0.49985700	-0.31810000

### TS3

0 1

H	-0.93743100	0.61465500	0.38918100
C	3.89395500	0.43801900	-0.76311300
C	2.48543100	0.60833000	-0.79085800
C	1.97064100	1.80893100	-1.28928100
C	2.84653900	2.78090900	-1.79193600
C	4.22701300	2.57267500	-1.78393700
C	4.77213600	1.39391000	-1.25608900
C	3.05965100	-1.44618800	0.23259100
C	1.90369000	-0.59594400	-0.19045600
H	0.91010200	2.02620200	-1.26282500
H	2.44116700	3.71069100	-2.17994800
H	4.89257000	3.33669400	-2.17565700
H	5.84610600	1.23992800	-1.22794700
N	4.20896400	-0.78482200	-0.16277200
C	5.54833600	-1.29670700	0.04921400
H	6.07006400	-1.42837500	-0.90490500
H	6.12994100	-0.61670000	0.68129800
H	5.45626000	-2.26269700	0.54689400
O	3.03929800	-2.54484800	0.79069900
C	0.61066900	-1.02710200	-0.05833200
C	0.40449700	-2.33576900	0.67946900
C	-0.52945200	-0.20048200	-0.49031100
O	0.18087900	-3.40397600	0.13961700
O	0.41575800	-2.15037300	2.00383500

C	0. 31943100	-3. 34518400	2. 81085600
H	1. 18622900	-3. 98077900	2. 61881300
H	0. 31622300	-2. 99623600	3. 84239100
H	-0. 59989100	-3. 88994200	2. 58535300
H	-0. 22517900	0. 42187000	-1. 33124800
C	-2. 59635000	-1. 49007000	0. 18131000
C	-3. 92884900	-2. 07383400	-0. 36879400
C	-4. 03190400	-0. 36952000	-2. 03575600
C	-2. 69193700	0. 24064900	-1. 54096800
H	-3. 96432700	-3. 15402800	-0. 20244500
H	-4. 77851800	-1. 62560400	0. 15401000
H	-2. 73150700	-0. 67815100	0. 89696700
H	-1. 97877800	-2. 26816800	0. 62065200
H	-4. 16325000	-0. 18048400	-3. 10491400
H	-4. 87185700	0. 09141000	-1. 50828300
H	-2. 12130900	0. 69292400	-2. 35441900
H	-2. 81255200	0. 96604400	-0. 73577600
N	-1. 81535500	-0. 87168300	-0. 96671000
N	-4. 07539800	-1. 81870800	-1. 80657300
C	-1. 58638900	-1. 89944600	-2. 06189900
C	-2. 96471100	-2. 45413400	-2. 52764900
H	-0. 94040100	-2. 67108000	-1. 64537900
H	-1. 05241400	-1. 37938400	-2. 85989100
H	-3. 01258200	-3. 53302700	-2. 35553900
H	-3. 09957400	-2. 27865900	-3. 59864600
C	-1. 87926900	3. 78437700	-0. 55021500
O	-0. 73890000	4. 04651300	-0. 50841200
O	-1. 68574000	1. 58026600	1. 07874400
C	-1. 33658200	1. 85086000	2. 41112700
C	0. 17747000	2. 13893300	2. 54016600
H	0. 76226300	1. 25773200	2. 24887600
H	0. 45802100	2. 96504800	1. 87701000
H	0. 46263600	2. 40761200	3. 56633000
C	-2. 12436500	3. 09510700	2. 88093900
H	-3. 20013100	2. 93067100	2. 74534100
H	-1. 94205900	3. 32275600	3. 93977400
H	-1. 83857300	3. 97563200	2. 29302400
C	-1. 70402900	0. 66170200	3. 33061400
H	-1. 45989800	0. 85989500	4. 38328000
H	-2. 77987200	0. 45473800	3. 26592600
H	-1. 16346400	-0. 24035000	3. 02251000
O	-3. 03119800	3. 62185900	-0. 67668200

### M3

0	1		
C	-3.64073300	-0.62237100	-0.07831100
C	-2.27703300	-1.02213700	0.08174200
C	-2.02531100	-2.36482500	0.40249400
C	-3.09208900	-3.26509600	0.53550500
C	-4.41472400	-2.85009600	0.35357700
C	-4.70219600	-1.51099900	0.04733300
C	-2.36831500	1.26408000	-0.37340600
C	-1.46946100	0.16569400	-0.09344100
H	-1.01420900	-2.71924400	0.57486700
H	-2.88197400	-4.30275800	0.78344400
H	-5.22859600	-3.56352900	0.45310000
H	-5.72834700	-1.17785300	-0.08232300
N	-3.67441100	0.73780100	-0.34948100
C	-4.86040500	1.52509000	-0.59617400
H	-5.41242400	1.15340900	-1.46840100
H	-5.53376400	1.51700400	0.27004600
H	-4.53528300	2.54929500	-0.78778000
O	-2.12686500	2.46502600	-0.61797200
C	-0.05165400	0.33501400	-0.09102300
C	0.82765700	-0.71038700	-0.16350600
C	0.41985200	1.77438600	-0.02398100
O	1.03081500	2.34977800	-0.90829500
O	0.15547500	2.31547100	1.17297700
C	0.43778600	3.72274200	1.30081700
H	1.49142500	3.92872000	1.09814700
H	-0.19123400	4.28198300	0.60472000
H	0.19036700	3.97649500	2.33118800
C	4.45383800	-0.16434000	-1.33598100
C	2.90384400	-0.19934800	-1.45403800
C	2.80625300	-2.09084100	0.12533300
C	4.35597000	-2.12207200	0.03782600
H	2.46103700	0.77414600	-1.65826700
H	2.55041900	-0.91392200	-2.19943900
H	4.90384700	-0.70831900	-2.17118600
H	2.42457200	-2.37918400	1.10625800
H	2.33686400	-2.71996700	-0.63211200
H	4.76805600	-2.60060000	0.93048700
H	4.67669400	-2.70135200	-0.83231500
N	4.90786300	-0.76742800	-0.07499300
N	2.31207800	-0.66798900	-0.12120900
C	4.41863100	0.03695600	1.04968800
C	2.87182700	0.20078000	1.00037700
H	4.89468200	1.02084400	1.01553800

H	4.71995800	-0.45017600	1.98106200
H	2.59142200	1.22678900	0.77941100
H	2.37231800	-0.11876800	1.91550500
H	4.81543900	0.86696100	-1.37232300
H	0.47219100	-1.71225600	-0.34252600

### *t*-BuOH + CO<sub>2</sub>

0 1

H	0.11325900	-1.57301000	-0.00078800
C	-2.51227300	0.02088900	0.01895200
O	-2.30175600	1.16881400	-0.05578300
O	0.16885900	-0.74095700	0.49774000
C	1.31579700	-0.01244200	-0.00061500
C	1.11806000	0.29700700	-1.49122500
H	1.04285600	-0.63000800	-2.07372300
H	0.19945100	0.87359300	-1.64168800
H	1.95949100	0.87478600	-1.89031200
C	1.35428300	1.27424300	0.82652600
H	1.47468900	1.04156700	1.89028200
H	2.18942600	1.91000900	0.51485700
H	0.42219700	1.83415800	0.69884000
C	2.58209300	-0.85050000	0.22376000
H	3.47734100	-0.30912800	-0.10251800
H	2.69385800	-1.09671200	1.28522500
H	2.53375600	-1.78884100	-0.34336600
O	-2.77386400	-1.11680600	0.08289400

### R2

0 1

C	-2.63263100	-0.98366000	-0.13851200
C	-3.74043900	-0.08422700	0.05230300
C	-3.59608700	1.25373500	0.20219400
C	-2.24842700	1.81236600	0.17892000
C	-1.08672800	0.84983900	0.02228200
C	-1.34996500	-0.56700700	-0.16248200
C	-4.54136600	-2.17955900	-0.16845400
H	-4.43812500	1.92485500	0.32373700
H	-0.54642500	-1.26289800	-0.36442100
H	-4.84877300	-2.74726800	0.71443100
O	-4.89065000	-0.79697700	0.01712400
O	-3.12260500	-2.24741200	-0.31954500
H	-5.02651000	-2.55192300	-1.07382000
O	-2.06790100	3.03463400	0.30073900
C	0.15813800	1.42280800	0.03378600

C	2. 55297700	1. 64532900	-0. 46854200
C	1. 48850900	0. 84174400	0. 00968900
C	1. 81796900	-0. 44756700	0. 47697800
C	3. 12258000	-0. 93158800	0. 43480100
C	4. 14943300	-0. 12862500	-0. 08571800
C	3. 85105500	1. 17161200	-0. 53208900
H	2. 33890800	2. 65486500	-0. 80945500
H	1. 05657200	-1. 07199300	0. 93002600
H	3. 33138700	-1. 92245400	0. 82033100
H	4. 65712200	1. 78996800	-0. 91452300
O	5. 44940200	-0. 50264900	-0. 18114300
C	5. 81994000	-1. 81033900	0. 25960800
H	5. 29228000	-2. 58459100	-0. 30876700
H	6. 89197200	-1. 89057600	0. 07695700
H	5. 62024600	-1. 93942600	1. 32942600
H	0. 13563500	2. 51150000	0. 05008000

#### TS4

0 1

C	0. 37829800	3. 84118000	0. 05890700
C	-0. 80731500	4. 15671000	-0. 62698200
C	-1. 45149600	3. 26195000	-1. 43509500
C	-0. 91112100	1. 92359000	-1. 58588000
C	0. 32941400	1. 60884200	-0. 84840900
C	0. 95732600	2. 60846700	-0. 04236300
C	-0. 26390900	5. 88567700	0. 68744700
H	-2. 35990000	3. 51876400	-1. 97016800
H	1. 87631100	2. 40522700	0. 48982200
H	0. 10713600	6. 88902800	0. 46891500
O	-1. 14234300	5. 46497600	-0. 37133900
O	0. 82741900	4. 97074000	0. 73652800
H	-0. 81718300	5. 86603200	1. 63706400
O	-1. 49869500	1. 09097200	-2. 34826400
C	0. 87227700	0. 28991600	-1. 05636700
C	2. 65877000	-0. 79329100	-2. 37308600
C	2. 31163900	-0. 01478700	-1. 24513300
C	3. 36999100	0. 41890800	-0. 42838500
C	4. 70258700	0. 12496200	-0. 72679600
C	5. 01681900	-0. 62386800	-1. 86747200
C	3. 97699100	-1. 08699400	-2. 68892600
H	1. 86903600	-1. 16344900	-3. 02076100
H	3. 17204400	0. 96870900	0. 48258900
H	5. 48066200	0. 48162100	-0. 06183500
H	4. 22476600	-1. 67384200	-3. 56844600

O	6.28016700	-0.95586400	-2.25785600
C	7.37296800	-0.51603900	-1.45462100
H	7.31710200	-0.93226200	-0.44155200
H	8.27312100	-0.88442000	-1.94874200
H	7.41122900	0.57831500	-1.39601600
C	2.10957800	-1.65282700	1.77525100
C	1.06787700	-0.69691700	1.69658900
C	1.05243000	0.35455900	2.61666000
C	2.04922600	0.42490000	3.60070400
C	3.06241200	-0.53614600	3.66308500
C	3.10657300	-1.59244400	2.74263000
C	0.81157000	-2.31018300	0.00506200
C	0.23936700	-1.03377500	0.52714000
H	0.28539100	1.11997800	2.57224300
H	2.03336500	1.24025500	4.31868700
H	3.82853400	-0.46678100	4.43051300
H	3.89549600	-2.33708600	2.78541200
N	1.93938000	-2.59711800	0.76279400
C	2.83333700	-3.70316400	0.48767500
H	2.41690800	-4.26032300	-0.35239300
H	3.83359300	-3.34139600	0.22352800
H	2.91356800	-4.36508000	1.35713000
O	0.41952400	-3.00249400	-0.94102400
C	-1.23895600	-0.90484200	0.53139400
C	-1.95069400	-1.32605400	-0.52642400
C	-1.84387000	-0.30905400	1.78155100
O	-2.19625000	0.84800100	1.90882500
O	-1.91239200	-1.22442200	2.75787100
C	-2.38391700	-0.75336300	4.04344600
H	-1.69237900	-0.00735700	4.44040300
H	-3.38152200	-0.32080400	3.94656800
H	-2.40515500	-1.63592000	4.68068300
C	-5.22763000	-1.93324400	-2.34349700
C	-3.69383800	-1.86637400	-2.11501100
C	-3.98540100	0.12339500	-0.69377700
C	-5.49517400	0.06300800	-1.05642700
H	-3.22025000	-2.84873900	-2.15305100
H	-3.18133100	-1.19508700	-2.80546100
H	-5.48933300	-1.40913700	-3.26660700
H	-3.81045700	0.50922800	0.30773600
H	-3.37236400	0.68506400	-1.40382300
H	-6.08735800	0.53478900	-0.26726300
H	-5.68355600	0.60466400	-1.98770600
N	-5.95682300	-1.32139100	-1.22652300

N	-3.42020000	-1.30232400	-0.72136000
C	-5.68565100	-2.07826400	0.00077600
C	-4.15872500	-2.17395400	0.28672900
H	-6.10518000	-3.08285000	-0.10121200
H	-6.19498900	-1.58281000	0.83153700
H	-3.76342500	-3.18349400	0.16165700
H	-3.89485600	-1.82320800	1.28286900
H	-5.55142900	-2.97281900	-2.44291300
H	-1.43417400	-1.74270800	-1.37543000
H	0.26010800	-0.24442800	-1.77868700

#### TS4'

O 1

C	-3.91505600	-1.94029800	-1.41908700
C	-4.95833800	-0.99571200	-1.34754100
C	-4.73747800	0.31630600	-1.04273100
C	-3.38436900	0.76484500	-0.76447400
C	-2.29802500	-0.20065900	-0.96052000
C	-2.61603600	-1.57769900	-1.22274400
C	-5.81945900	-2.95760700	-2.00831000
H	-5.54499500	1.03383400	-0.94533600
H	-1.81886900	-2.31358700	-1.27217000
H	-6.45344200	-3.67352200	-1.48112600
O	-6.15352800	-1.62509000	-1.58025400
O	-4.45177700	-3.19251800	-1.67551100
H	-5.96024700	-3.02858600	-3.09504100
O	-3.20731600	1.94687300	-0.32688900
C	-0.87585600	0.09255800	-0.89664400
C	1.05000600	0.98424400	-2.15533200
C	-0.17454700	1.25720700	-1.50084400
C	-0.63604800	2.58387100	-1.55233500
C	0.07890200	3.58590500	-2.21003300
C	1.29382100	3.28848800	-2.84053800
C	1.77207000	1.96969700	-2.81115400
H	1.43619800	-0.03080900	-2.16231200
H	-1.58138000	2.82070700	-1.07999500
H	-0.32110900	4.59370500	-2.22255300
H	2.70584500	1.73731400	-3.31463000
O	2.07078300	4.19215600	-3.50254000
C	1.62390800	5.54450200	-3.57120500
H	1.53445000	5.98680900	-2.57177500
H	2.38522900	6.08157000	-4.13880100
H	0.66062100	5.62118800	-4.08944100
C	3.48238400	-2.94543600	-0.47909500

C	3. 31435100	-1. 59201800	-0. 09189600
C	4. 38650300	-0. 71182500	-0. 27449100
C	5. 59930500	-1. 19306200	-0. 78000600
C	5. 74933300	-2. 54159600	-1. 11902500
C	4. 68140100	-3. 43756100	-0. 98108600
C	1. 28744600	-2. 76804500	0. 15101400
C	1. 93389400	-1. 44256000	0. 36922900
H	4. 28770300	0. 34614800	-0. 05778000
H	6. 42937300	-0. 50598900	-0. 91655500
H	6. 69826900	-2. 90000700	-1. 50785300
H	4. 78681100	-4. 47958600	-1. 26612700
N	2. 27823300	-3. 62777600	-0. 30116000
C	2. 04700600	-5. 02130700	-0. 62522300
H	1. 00186700	-5. 24139900	-0. 40530200
H	2. 24296700	-5. 21353400	-1. 68619500
H	2. 68975000	-5. 67221900	-0. 02271800
O	0. 11446200	-3. 11910800	0. 34228600
C	1. 30398000	-0. 35427400	0. 96300700
C	-0. 13367900	-0. 29524100	1. 06907300
C	2. 17180800	0. 81352800	1. 36132800
O	2. 07273600	1. 95144300	0. 94285400
O	3. 07643400	0. 44270100	2. 28512200
C	3. 98533000	1. 47138100	2. 73689700
H	4. 62121300	1. 80262400	1. 91241800
H	3. 43029000	2. 32333000	3. 13515700
H	4. 58443000	1. 00189000	3. 51561600
C	-2. 95438400	0. 77715200	3. 42221000
C	-2. 17840700	-0. 12116400	2. 42773400
C	-0. 96701800	1. 95990300	1. 92133000
C	-1. 48909600	2. 64969100	3. 20753500
H	-2. 01805600	-1. 12995100	2. 81360300
H	-2. 66045000	-0. 18752000	1. 45672700
H	-3. 68167200	1. 39554300	2. 88895000
H	-0. 00778800	2. 34902700	1. 58797800
H	-1. 68873800	2. 01731600	1. 10246900
H	-0. 69141000	3. 20065400	3. 71489700
H	-2. 27123400	3. 36649500	2. 93933900
N	-2. 03882000	1. 66521700	4. 15339900
N	-0. 78857200	0. 47112200	2. 20611500
C	-0. 93124700	0. 85830800	4. 68183700
C	-0. 04753700	0. 29818700	3. 53127300
H	-1. 34974500	0. 04314000	5. 27858700
H	-0. 31732200	1. 47673800	5. 34273600
H	0. 16637700	-0. 76610100	3. 63991300

H	0. 89413200	0. 83604800	3. 45113400
H	-3. 49965300	0. 14956400	4. 13329200
H	-0. 57176200	-1. 28594600	1. 05420300
H	-0. 31708900	-0. 80473100	-1. 14922500

#### M4

0 1

C	0. 62193600	3. 69892100	0. 44000600
C	-0. 49636600	4. 14976800	-0. 25238400
C	-1. 20237000	3. 34338200	-1. 11455800
C	-0. 77967900	1. 97715400	-1. 31567800
C	0. 37443700	1. 52217800	-0. 55591200
C	1. 07892500	2. 40627000	0. 28811900
C	0. 15270900	5. 74658200	1. 16053100
H	-2. 06189300	3. 70991700	-1. 66797500
H	1. 98109500	2. 09036000	0. 80010300
H	0. 59475700	6. 73985900	1. 06056600
O	-0. 70213100	5. 49066000	0. 03514300
O	1. 18182200	4. 76157100	1. 16001400
H	-0. 44146300	5. 66886900	2. 08493500
O	-1. 42423600	1. 21947600	-2. 13884100
C	0. 84546000	0. 09178900	-0. 80540100
C	2. 66366800	-0. 29910200	-2. 50335700
C	2. 32679600	-0. 05047800	-1. 15893400
C	3. 39175200	0. 07780400	-0. 25621700
C	4. 72690200	-0. 03095800	-0. 66208000
C	5. 03044600	-0. 27205100	-2. 00602900
C	3. 98231900	-0. 40519800	-2. 92817700
H	1. 86872300	-0. 41031600	-3. 23679700
H	3. 20030600	0. 25856100	0. 79502200
H	5. 51201300	0. 07427600	0. 07804300
H	4. 22120200	-0. 59673600	-3. 97028900
O	6. 29373200	-0. 39544800	-2. 51227400
C	7. 39225700	-0. 27279000	-1. 61363500
H	7. 36184100	-1. 04543000	-0. 83561600
H	8. 29025400	-0. 40446500	-2. 21930500
H	7. 41476600	0. 71641000	-1. 14018900
C	1. 72061500	-2. 18206600	1. 79213100
C	1. 03790300	-0. 96521700	1. 62107700
C	1. 09569400	-0. 00880600	2. 62947700
C	1. 84237700	-0. 27447700	3. 78835100
C	2. 51866200	-1. 48683300	3. 93310700
C	2. 46596100	-2. 46483200	2. 93124700
C	0. 73668500	-2. 39164900	-0. 26652400

C	0. 34123100	-0. 97928000	0. 26924400
H	0. 57787200	0. 93676300	2. 52105200
H	1. 89337100	0. 47233000	4. 57508900
H	3. 09403100	-1. 68138100	4. 83379700
H	2. 98996700	-3. 40819400	3. 04498800
N	1. 52959200	-3. 00426700	0. 67154900
C	2. 11606000	-4. 32088000	0. 49631400
H	1. 78531100	-4. 70411500	-0. 46926500
H	3. 20940700	-4. 25989900	0. 50984900
H	1. 78541200	-4. 99810700	1. 29061400
O	0. 41485300	-2. 87127300	-1. 34596100
C	-1. 20497100	-0. 91585400	0. 38114900
C	-1. 91058700	-1. 06317000	-0. 74211200
C	-1. 78198100	-0. 82584600	1. 76949000
O	-2. 01396800	-1. 80599200	2. 45090700
O	-1. 98553900	0. 43447000	2. 17582700
C	-2. 47088600	0. 59198400	3. 53263900
H	-3. 43037700	0. 08494800	3. 65077500
H	-1. 74359700	0. 18047100	4. 23517700
H	-2. 58028400	1. 66593700	3. 67304200
C	-5. 18616600	-1. 04765000	-2. 66511000
C	-3. 65371600	-1. 10926300	-2. 42736600
C	-3. 96598900	0. 32519000	-0. 45651200
C	-5. 49730800	0. 31085200	-0. 72163300
H	-3. 21681900	-2. 05398600	-2. 75573000
H	-3. 10287200	-0. 27851800	-2. 86953600
H	-5. 43448700	-0. 19044800	-3. 29678200
H	-3. 72685600	0. 43221400	0. 59899200
H	-3. 41397000	1. 07422300	-1. 02706700
H	-6. 04538500	0. 39223100	0. 22093300
H	-5. 77451000	1. 16404200	-1. 34692500
N	-5. 91752100	-0. 92267200	-1. 39831000
N	-3. 38076500	-1. 00824400	-0. 92469600
C	-5. 60988000	-2. 07513700	-0. 54415000
C	-4. 08718800	-2. 16788900	-0. 23167200
H	-5. 94299900	-2. 98514000	-1. 05026400
H	-6. 17525900	-1. 98034100	0. 38667800
H	-3. 62743900	-3. 07993400	-0. 61625300
H	-3. 86737800	-2. 09230300	0. 83189500
H	-5. 52456200	-1. 95244500	-3. 17718600
H	-1. 40756500	-1. 25768100	-1. 67247800
H	0. 30775600	-0. 19810700	-1. 71085000

**TS5**

0	1		
C	0.91528800	3.74277100	0.65427400
C	-0.34129300	4.21597700	0.29847600
C	-1.25384800	3.42607800	-0.36590700
C	-0.87150800	2.09771000	-0.71432500
C	0.41397400	1.60804600	-0.32653200
C	1.31337600	2.45704800	0.35352000
C	0.82743200	5.91491600	1.15468900
H	-2.23247300	3.79473700	-0.65424200
H	2.30610500	2.11963000	0.62349300
H	1.28085600	6.53265100	0.36589700
O	-0.48944000	5.51525000	0.74189700
O	1.60479600	4.72998300	1.34698100
H	0.76011200	6.46500700	2.09540000
O	-1.72260300	1.36950700	-1.42590100
C	0.78931000	0.18686500	-0.75634400
C	2.47426700	-0.22900600	-2.57533500
C	2.23872500	-0.01557900	-1.20318300
C	3.36626800	0.00928700	-0.36927700
C	4.66249800	-0.16328000	-0.86741800
C	4.86420900	-0.36946700	-2.23610200
C	3.75302800	-0.40147100	-3.09054300
H	1.62998100	-0.26052500	-3.25992400
H	3.25590800	0.15644100	0.69828800
H	5.49811800	-0.13484700	-0.17758000
H	3.91139500	-0.56446800	-4.15258100
O	6.08173200	-0.54861000	-2.82815100
C	7.24199300	-0.52343700	-2.00129800
H	7.21588300	-1.32175900	-1.24960600
H	8.08896000	-0.68384200	-2.67015700
H	7.35428500	0.44446400	-1.49776800
C	1.74527300	-2.19020700	1.58331100
C	1.06312200	-0.96373800	1.53955500
C	1.24952100	-0.04633500	2.56447100
C	2.13095400	-0.35508500	3.61264400
C	2.80940300	-1.57548800	3.63182900
C	2.62160100	-2.51867000	2.61190100
C	0.51381700	-2.30761300	-0.34585500
C	0.23321100	-0.91029800	0.26871100
H	0.71520400	0.89754600	2.56186700
H	2.28122100	0.36030400	4.41625100
H	3.48934400	-1.80444900	4.44785400
H	3.14366000	-3.47015000	2.62967700
N	1.39838700	-2.97287600	0.46912700

C	1. 91117800	-4. 30155800	0. 19407100
H	2. 99975700	-4. 27880000	0. 07379200
H	1. 65753100	-4. 99111800	1. 00650700
H	1. 45142800	-4. 64711400	-0. 73251200
O	0. 04352200	-2. 75245700	-1. 38970900
C	-1. 29655400	-0. 69824600	0. 45802000
C	-1. 96664100	-0. 44182900	-0. 73235500
C	-1. 94722200	-0. 83573900	1. 75001300
O	-3. 00809500	-0. 31439100	2. 11105800
O	-1. 30891600	-1. 71004000	2. 57170400
C	-1. 86278300	-1. 86137100	3. 88644700
H	-1. 89653700	-0. 90170300	4. 40904400
H	-2. 87260800	-2. 27776600	3. 83793900
H	-1. 19503600	-2. 55035700	4. 40464600
H	-1. 48019500	-0. 81975700	-1. 61755300
C	-5. 45954500	-2. 00681200	-1. 01117000
C	-4. 01240500	-1. 83942400	-0. 46983500
C	-3. 66315400	-0. 48822700	-2. 49651900
C	-5. 18521500	-0. 43707700	-2. 78697200
H	-3. 98408800	-1. 78440000	0. 61532700
H	-3. 33694900	-2. 62426100	-0. 81293400
H	-5. 49649800	-2. 77777700	-1. 78592100
H	-6. 11689000	-2. 31986800	-0. 19486900
H	-3. 11983500	0. 37982300	-2. 86406500
H	-3. 19955300	-1. 39707200	-2. 88544200
H	-5. 47877500	0. 55615200	-3. 13810700
H	-5. 43186700	-1. 15607500	-3. 57357600
N	-5. 96453500	-0. 75087600	-1. 58184500
N	-3. 44952100	-0. 51466500	-0. 98170600
C	-5. 76540300	0. 32690800	-0. 59988400
C	-4. 26188600	0. 64467300	-0. 39845800
H	-6. 22822000	0. 01787100	0. 34219400
H	-6. 28327600	1. 22674600	-0. 94566800
H	-3. 97638700	0. 72759000	0. 64638500
H	-3. 92750900	1. 52252600	-0. 94466000
H	0. 21271700	0. 01768100	-1. 66720200

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C	-1. 48847600	3. 30873800	-0. 42153200
C	-1. 70664600	3. 39330900	0. 98501200
C	-1. 35567900	2. 39731900	1. 84190700
C	-0. 64525600	1. 24121000	1. 31059400
C	-0. 53632700	1. 07497400	-0. 17304100

C	-0.92477000	2.22426100	-1.00061700
C	-2.33627400	5.33796100	0.04767100
H	-1.48637300	2.47550500	2.91563200
H	-0.75750100	2.19241000	-2.07368300
H	-3.35125300	5.70542000	-0.11817300
O	-2.30310700	4.58330200	1.27211700
O	-1.96419900	4.45765900	-1.01393100
H	-1.61943300	6.16384000	0.11726900
O	-0.16545900	0.38419300	2.08427900
C	0.70673000	0.35637000	-0.75552900
C	2.88962400	1.17490800	-1.69671300
C	2.04520600	1.06031500	-0.57784400
C	2.49924700	1.61919800	0.62363100
C	3.73480900	2.26587900	0.71515900
C	4.56077500	2.35977700	-0.41174000
C	4.12720800	1.80565800	-1.62364400
H	2.56841900	0.76552900	-2.65208000
H	1.88762100	1.54892300	1.51440700
H	4.04008000	2.68597200	1.66682300
H	4.76649300	1.88783800	-2.49780900
O	5.78513300	2.96677500	-0.43319800
C	6.26689000	3.55084600	0.77352000
H	6.37759700	2.80089000	1.56630300
H	7.24528300	3.96981100	0.53302900
H	5.60461900	4.35212900	1.12372000
C	2.62558900	-2.60403300	-0.39834900
C	1.85569100	-1.74214800	0.39847100
C	2.25578700	-1.50057900	1.70581200
C	3.41675100	-2.11738500	2.19705700
C	4.16961600	-2.96918800	1.38653700
C	3.77930300	-3.22716500	0.06573300
C	0.92580900	-1.94786900	-1.78503800
C	0.68355300	-1.22758200	-0.42335100
H	1.66043600	-0.84764600	2.33121300
H	3.73072400	-1.92978600	3.22053100
H	5.06717200	-3.44081600	1.77791900
H	4.35721300	-3.89273800	-0.56793900
N	2.04849700	-2.72776800	-1.67450500
C	2.57296000	-3.54859800	-2.74913500
H	3.59345000	-3.24363400	-3.00562200
H	2.58111000	-4.60616000	-2.46285900
H	1.92530500	-3.41185500	-3.61575200
O	0.24381600	-1.83837700	-2.80255800
C	-0.73878200	-1.52516400	0.06063500

C	-1.58890400	-0.53930400	-0.54556600
C	-1.07549200	-2.54614800	0.99375600
O	-2.14736700	-2.69868200	1.61507900
O	-0.09321300	-3.49635400	1.12799300
C	-0.34436800	-4.52135200	2.09125900
H	-0.47474900	-4.10269400	3.09412000
H	-1.23674000	-5.09944000	1.83333400
H	0.53702700	-5.16485400	2.06853900
H	-1.42702000	-0.44218500	-1.61815100
C	-5.20545800	-1.79057100	-0.92375600
C	-3.65793100	-1.88864100	-0.83739600
C	-3.69636900	0.50289500	-1.34683700
C	-5.22690800	0.58420600	-1.10214600
H	-3.32980100	-2.60214300	-0.08648800
H	-3.19250900	-2.11420600	-1.79819900
H	-5.54158200	-1.80860800	-1.96441500
H	-5.65198500	-2.64833300	-0.41224400
H	-3.19240800	1.44851500	-1.16444200
H	-3.45479000	0.16595700	-2.35688000
H	-5.48363100	1.50747000	-0.57531100
H	-5.75015800	0.59018100	-2.06275700
N	-5.69543200	-0.55304700	-0.30135400
N	-3.09871700	-0.52915000	-0.39696200
C	-5.12547500	-0.44571300	1.05065800
C	-3.59510600	-0.20003700	1.00521600
H	-5.35051100	-1.37114200	1.58893700
H	-5.61208000	0.37791700	1.58172400
H	-3.04561000	-0.84105800	1.68962100
H	-3.33838700	0.84527100	1.17386600
H	0.52472600	0.38726800	-1.83503700

## P

0 1			
C	0.96778500	3.63954800	0.35054500
C	-0.10272200	4.38831100	-0.13145300
C	-1.11298600	3.80250400	-0.86275400
C	-0.99594800	2.41947900	-1.09036600
C	0.07064200	1.64270700	-0.63426300
C	1.08188600	2.28632800	0.11702200
C	1.31966700	5.78932000	0.88238300
H	-1.96009300	4.35593500	-1.24966900
H	1.94000700	1.73832000	0.48217600
H	1.99992200	6.34977200	0.23029800
O	0.02786700	5.69554800	0.25356300

O	1.81616600	4.45398800	1.06173200
H	1.21333900	6.27275300	1.85592700
O	-2.01854300	1.89278300	-1.87920400
C	0.12024100	0.16476100	-1.01052500
C	2.16883600	-0.76187000	-2.14772200
C	1.51764900	-0.44593100	-0.94249700
C	2.21141300	-0.70502700	0.24705400
C	3.49614300	-1.25717800	0.24699300
C	4.12345600	-1.56065600	-0.96693600
C	3.44631900	-1.30727900	-2.16899400
H	1.66214000	-0.57849800	-3.09191100
H	1.75398500	-0.48263100	1.20490100
H	3.99042700	-1.44093800	1.19377900
H	3.93649400	-1.54707100	-3.10777500
O	5.37180000	-2.09701100	-1.08551400
C	6.10256400	-2.37478100	0.10676600
H	5.58114600	-3.10814800	0.73363200
H	7.05723500	-2.79030700	-0.21891700
H	6.28158900	-1.46212200	0.68780400
C	-0.52957800	-1.96002900	1.67018000
C	-0.92209700	-0.67877400	1.24472600
C	-1.16614900	0.31393400	2.18258000
C	-0.99122100	0.02486400	3.54592700
C	-0.58510000	-1.24783900	3.95059500
C	-0.35075400	-2.26605300	3.01477300
C	-0.72740600	-2.17224900	-0.60251100
C	-1.01456800	-0.67389200	-0.27162600
H	-1.49344700	1.30087100	1.87011300
H	-1.17690100	0.79626900	4.28747900
H	-0.45368900	-1.46145000	5.00778100
H	-0.04602900	-3.25726500	3.33499800
N	-0.37058700	-2.80589400	0.56458900
C	-0.01504300	-4.20937300	0.63737300
H	0.97231700	-4.33328300	1.09439700
H	-0.75348700	-4.76768200	1.22374300
H	0.00593100	-4.59759900	-0.38149400
O	-0.74763000	-2.67635500	-1.71599800
C	-2.39150400	-0.29390700	-0.81181600
C	-2.72835400	0.79477300	-1.53821700
C	-3.48271700	-1.26774200	-0.54047900
O	-3.32999500	-2.28788400	0.11327600
O	-4.67712600	-0.92385600	-1.06942400
C	-5.75642600	-1.84684100	-0.83489900
H	-5.52654800	-2.82371700	-1.26711700

H	-5.93887500	-1.95756900	0.23661400
H	-6.62388900	-1.40706800	-1.32627400
H	-3.72129800	0.86210900	-1.96638300
H	-0.17066800	0.10022300	-2.06483700

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C	-0.68515900	0.00003400	0.00000100
C	0.68515900	-0.00003400	0.00000000
C	-1.43244100	1.21956100	0.00000100
C	1.43256200	1.21941700	-0.00000100
C	-1.43256200	-1.21941700	-0.00000100
C	1.43244100	-1.21956000	0.00000100
N	-2.05419100	2.20126200	0.00000100
N	2.05441900	2.20105200	-0.00000200
N	-2.05441900	-2.20105200	-0.00000200
N	2.05419100	-2.20126200	0.00000100

### IRC-R-53

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C	1.00245100	3.82857700	0.38598600
C	-0.31731900	4.23083300	0.22627400
C	-1.28604800	3.36001400	-0.22911500
C	-0.87433700	2.04949700	-0.53652300
C	0.45884600	1.62008600	-0.38200700
C	1.41336100	2.54396400	0.09435300
C	0.88447700	6.02023700	0.81665000
H	-2.32037800	3.65622700	-0.36113900
H	2.45165200	2.26220400	0.20902500
H	1.17654300	6.65725200	-0.02883100
O	-0.45676400	5.54318500	0.60949500
O	1.74976400	4.87861900	0.88122000
H	0.93136400	6.56785400	1.76007700
O	-1.84683100	1.25877600	-1.11645200
C	0.80739400	0.18138600	-0.76495200
C	2.47770200	-0.41040200	-2.54757800
C	2.25042800	-0.07658800	-1.19836600
C	3.37945100	-0.00461000	-0.36882000
C	4.67048900	-0.24447800	-0.85148200
C	4.86486900	-0.57064300	-2.19794000
C	3.75143800	-0.65330600	-3.04622700
H	1.63170200	-0.48296000	-3.22695800
H	3.27224000	0.23433600	0.68228900
H	5.50812200	-0.17423300	-0.16708800

H	3.90415800	-0.90936800	-4.09053100
O	6.07680300	-0.82275600	-2.77292900
C	7.23937400	-0.75255400	-1.95132300
H	7.19817800	-1.48483000	-1.13596200
H	8.08119200	-0.98552300	-2.60494300
H	7.37235600	0.25142300	-1.53043300
C	1.69014000	-2.16002100	1.63130700
C	1.08100500	-0.89828400	1.55664200
C	1.36725500	0.05364000	2.52458500
C	2.26850300	-0.26070200	3.55363900
C	2.86846800	-1.52123900	3.60927800
C	2.58322900	-2.49645600	2.64347700
C	0.40198600	-2.27100000	-0.26096200
C	0.20809100	-0.84595900	0.31590400
H	0.88937300	1.02726300	2.49382200
H	2.49563700	0.48044400	4.31500500
H	3.56384600	-1.75527700	4.41086100
H	3.04698900	-3.47706000	2.68799800
N	1.25750800	-2.96529600	0.56305100
C	1.66111500	-4.34029000	0.34083500
H	2.74474500	-4.40891700	0.19584400
H	1.37666600	-4.97102300	1.18990800
H	1.15312200	-4.69102200	-0.55792000
O	-0.11629200	-2.72605900	-1.28067200
C	-1.29158300	-0.54568200	0.54394800
C	-1.95257900	-0.14610100	-0.72264900
C	-1.96356000	-0.69584600	1.76943200
O	-3.12723200	-0.32398300	2.06302900
O	-1.26121800	-1.41025000	2.72849600
C	-1.85464300	-1.45900200	4.02331900
H	-2.01225400	-0.45676800	4.43550400
H	-2.81631700	-1.98129000	4.00765900
H	-1.14757500	-2.00698400	4.65008700
H	-1.50169300	-0.72616800	-1.52887100
C	-5.22151600	-2.18851500	-1.08432000
C	-3.82427100	-1.82540300	-0.51085800
C	-3.67263200	-0.39340500	-2.49896200
C	-5.19154900	-0.52213300	-2.78871000
H	-3.82547600	-1.77526900	0.57518800
H	-3.03363300	-2.49744400	-0.84898200
H	-5.13676900	-2.91432600	-1.89844700
H	-5.82902400	-2.64200400	-0.29552700
H	-3.24623000	0.54119900	-2.86090500
H	-3.10321700	-1.22798600	-2.91296600

H	-5.61313400	0.44170800	-3.08748800
H	-5.34755700	-1.22527500	-3.61194300
N	-5.91207800	-0.99602000	-1.59951100
N	-3.45725900	-0.43060300	-0.98832200
C	-5.85703700	0.05755400	-0.57171900
C	-4.41308100	0.59043400	-0.38233000
H	-6.24111900	-0.36041000	0.36363000
H	-6.51500800	0.88166800	-0.86436400
H	-4.12622700	0.69500700	0.66175000
H	-4.24117700	1.52050800	-0.92077200
H	0.23636700	-0.02139300	-1.67330300

### IRC-R-38

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C	0.98482100	3.80213900	0.44388200
C	-0.33298000	4.20233000	0.27129500
C	-1.29093000	3.33655500	-0.21414200
C	-0.86855000	2.03363200	-0.53675400
C	0.46281100	1.60717500	-0.37225600
C	1.40662200	2.52535700	0.13350300
C	0.85256500	5.98494400	0.91269600
H	-2.32236000	3.63217800	-0.35703000
H	2.44411500	2.24627700	0.25771600
H	1.15616000	6.63723100	0.08434000
O	-0.48293300	5.50713300	0.67548000
O	1.71971400	4.84574500	0.97010700
H	0.88321200	6.51603600	1.86569800
O	-1.82380300	1.24255900	-1.14362300
C	0.81474000	0.17408400	-0.77079200
C	2.49591900	-0.37616100	-2.55663800
C	2.26052400	-0.07095700	-1.20212700
C	3.38589700	-0.00280300	-0.36733900
C	4.68142900	-0.21600600	-0.85060000
C	4.88427300	-0.51005600	-2.20318400
C	3.77428200	-0.59214700	-3.05599600
H	1.65292200	-0.44558200	-3.24006900
H	3.27226300	0.21430800	0.68782400
H	5.51597900	-0.14878300	-0.16217400
H	3.93332700	-0.82546500	-4.10463400
O	6.10152800	-0.73008400	-2.78026300
C	7.26117600	-0.65507300	-1.95506000
H	7.23234500	-1.40483500	-1.15506700
H	8.10835300	-0.85883500	-2.61168100
H	7.37443300	0.34229100	-1.51317300

C	1. 69800300	-2. 17247300	1. 61501400
C	1. 07764500	-0. 91587500	1. 54540800
C	1. 34689400	0. 03068000	2. 52331900
C	2. 24371900	-0. 28307700	3. 55660300
C	2. 85604200	-1. 53774300	3. 60635200
C	2. 58713100	-2. 50806300	2. 63082900
C	0. 41864800	-2. 28335700	-0. 28370300
C	0. 21232500	-0. 86267900	0. 29885300
H	0. 85915000	0. 99940500	2. 49736200
H	2. 45840700	0. 45416900	4. 32534600
H	3. 54834600	-1. 77140900	4. 41072000
H	3. 05955000	-3. 48470500	2. 67106500
N	1. 27826800	-2. 97442400	0. 53925100
C	1. 69128700	-4. 34575700	0. 31276000
H	2. 77591200	-4. 40732300	0. 17052500
H	1. 40784700	-4. 98186900	1. 15864000
H	1. 18748800	-4. 69564600	-0. 58908700
O	-0. 09289400	-2. 73782900	-1. 30687400
C	-1. 28947500	-0. 56664300	0. 52120900
C	-1. 95039400	-0. 15893600	-0. 74440900
C	-1. 96275100	-0. 74502800	1. 74259900
O	-3. 12669200	-0. 37765800	2. 04913400
O	-1. 26079400	-1. 48848600	2. 68055000
C	-1. 84580100	-1. 56156000	3. 97799600
H	-2. 02784300	-0. 56751000	4. 39720600
H	-2. 79302300	-2. 10910600	3. 96467100
H	-1. 12206100	-2. 09491500	4. 59713900
H	-1. 51123400	-0. 74533500	-1. 55356000
C	-5. 25762900	-2. 14224500	-1. 10285200
C	-3. 84796700	-1. 81290000	-0. 53913700
C	-3. 69199100	-0. 35335900	-2. 50720200
C	-5. 21698100	-0. 45053200	-2. 78066800
H	-3. 83801300	-1. 78112600	0. 54762500
H	-3. 07276300	-2. 49333900	-0. 89709400
H	-5. 19384800	-2. 85556600	-1. 92988400
H	-5. 86374300	-2. 59943100	-0. 31500800
H	-3. 25329400	0. 57951900	-2. 85996100
H	-3. 14160800	-1. 19167000	-2. 94046400
H	-5. 62429600	0. 52517700	-3. 06039400
H	-5. 39501100	-1. 13858800	-3. 61201600
N	-5. 93265100	-0. 92942100	-1. 59056700
N	-3. 46129400	-0. 41700100	-0. 99928900
C	-5. 84714600	0. 10649700	-0. 54666300
C	-4. 39277200	0. 61353100	-0. 36937100

H	-6.22385800	-0.32348200	0.38740900
H	-6.49831100	0.94532000	-0.81509300
H	-4.09384600	0.70041400	0.67293400
H	-4.21183100	1.54655300	-0.89987100
H	0.24555500	-0.02044400	-1.68236300

### IRC-R-23

0 1

C	0.89472500	3.75907700	0.56444800
C	-0.41073300	4.15611100	0.30227500
C	-1.33027800	3.29235700	-0.25750800
C	-0.87679600	1.99636200	-0.56383100
C	0.44822600	1.58342300	-0.33467100
C	1.35025500	2.49380400	0.25377400
C	0.71281600	5.93086900	1.06817100
H	-2.35612600	3.58270900	-0.45694100
H	2.38070900	2.21892500	0.43995600
H	1.07745000	6.60453700	0.28149100
O	-0.59714900	5.45402800	0.71298600
O	1.57958100	4.79366100	1.16964300
H	0.66349800	6.43910100	2.03326700
O	-1.78053500	1.18153100	-1.21628500
C	0.82843200	0.16689500	-0.75662400
C	2.51804000	-0.25796300	-2.56222500
C	2.27859900	-0.03232600	-1.19273500
C	3.40241000	0.01602700	-0.35529600
C	4.70150500	-0.14493600	-0.85041800
C	4.90800900	-0.36157400	-2.21714300
C	3.79919400	-0.41892300	-3.07334800
H	1.67554600	-0.30662700	-3.24800300
H	3.28508700	0.17613000	0.70997000
H	5.53596700	-0.09782900	-0.16021900
H	3.96204900	-0.59079400	-4.13321400
O	6.12773300	-0.52696800	-2.80710800
C	7.28766800	-0.48166100	-1.98043800
H	7.27178400	-1.27590300	-1.22420700
H	8.13662500	-0.63474700	-2.64845200
H	7.38711000	0.49060700	-1.48271500
C	1.74886900	-2.17233300	1.60108300
C	1.07137200	-0.94435300	1.55040000
C	1.27291400	-0.01462800	2.56041800
C	2.16044800	-0.31484000	3.60586000
C	2.83229100	-1.53910000	3.63485700
C	2.63184500	-2.49312900	2.62708300

C	0.49629800	-2.30016400	-0.31514500
C	0.23036000	-0.89795700	0.28633000
H	0.73778100	0.92896800	2.55106900
H	2.32092100	0.40915700	4.39999400
H	3.51708200	-1.76231200	4.44856800
H	3.14893500	-3.44735400	2.65256100
N	1.38563800	-2.96528000	0.49868900
C	1.88974500	-4.29861900	0.23316900
H	2.97837100	-4.28352100	0.11008500
H	1.63480900	-4.98217900	1.05063200
H	1.42565700	-4.64841900	-0.68988800
O	0.01387100	-2.75663100	-1.35089200
C	-1.27762900	-0.61717900	0.48174900
C	-1.93308100	-0.21038800	-0.78798200
C	-1.95618900	-0.81454500	1.69760500
O	-3.09328600	-0.39966200	2.03305500
O	-1.28891700	-1.64473700	2.58751400
C	-1.84687200	-1.73315200	3.89594700
H	-1.86972000	-0.75749500	4.39463100
H	-2.86441600	-2.13502900	3.87287800
H	-1.19283100	-2.41095500	4.44979000
H	-1.50773900	-0.81350000	-1.59262500
C	-5.31686700	-2.09735800	-1.05986400
C	-3.88339800	-1.81119100	-0.53105100
C	-3.69690600	-0.40079300	-2.52887500
C	-5.22574800	-0.46149100	-2.79031600
H	-3.85335500	-1.76328700	0.55392700
H	-3.14279800	-2.52664800	-0.89286700
H	-5.29928800	-2.84293700	-1.86036200
H	-5.92861200	-2.49679000	-0.24543900
H	-3.23650800	0.51183000	-2.90418100
H	-3.17308200	-1.26193700	-2.94855100
H	-5.60428900	0.51619600	-3.10217600
H	-5.43059000	-1.17239800	-3.59612800
N	-5.94834300	-0.87578000	-1.58037800
N	-3.45422600	-0.43940900	-1.02243400
C	-5.81826400	0.18795800	-0.57088100
C	-4.34278000	0.63274600	-0.40062700
H	-6.21965300	-0.19063400	0.37411100
H	-6.42669900	1.04613600	-0.87248700
H	-4.03679400	0.71568800	0.64026800
H	-4.12461300	1.55258100	-0.93910700
H	0.26501000	-0.01991700	-1.67323100

**IRC-R-8**

0 1

C	0.89308400	3.73986700	0.64015800
C	-0.37104200	4.19494600	0.28453300
C	-1.28289700	3.37531600	-0.35906700
C	-0.87663600	2.04959200	-0.65399600
C	0.41865500	1.59496300	-0.32499500
C	1.31248900	2.46141300	0.33934800
C	0.78169700	5.91145200	1.14077400
H	-2.27609700	3.71962100	-0.62553900
H	2.31388900	2.14114200	0.59534600
H	1.23039700	6.54269000	0.36146200
O	-0.52904700	5.49543500	0.71733400
O	1.57410100	4.73250300	1.32173100
H	0.70198900	6.44772800	2.08806800
O	-1.75977400	1.23533300	-1.31701400
C	0.80102200	0.17893100	-0.75449900
C	2.48201100	-0.22176700	-2.57372200
C	2.24812700	-0.00972000	-1.20143200
C	3.37346100	0.02269100	-0.36637600
C	4.66977200	-0.14284500	-0.86515600
C	4.87128900	-0.34945300	-2.23384400
C	3.76086000	-0.38803600	-3.08897100
H	1.63717500	-0.25781500	-3.25737400
H	3.26051800	0.16876000	0.70113400
H	5.50577000	-0.10947400	-0.17613800
H	3.92051700	-0.55093400	-4.15076400
O	6.08916500	-0.52300900	-2.82552100
C	7.24885500	-0.49171200	-1.99809800
H	7.22586300	-1.28942400	-1.24571100
H	8.09686400	-0.64887900	-2.66634900
H	7.35631700	0.47721800	-1.49553800
C	1.75560800	-2.18161100	1.58566100
C	1.06759600	-0.95897100	1.54121100
C	1.25010800	-0.03951100	2.56451000
C	2.13308400	-0.34194200	3.61313300
C	2.81692700	-1.55944100	3.63413200
C	2.63310100	-2.50486900	2.61526000
C	0.52071400	-2.30317900	-0.34173200
C	0.23288500	-0.91020300	0.27338800
H	0.70571600	0.89868600	2.56303600
H	2.27952000	0.37488000	4.41635900
H	3.49761800	-1.78450900	4.45073000
H	3.15891600	-3.45437600	2.63501500

N	1. 40945000	-2. 96715100	0. 47297500
C	1. 92775800	-4. 29354100	0. 19965700
H	3. 01654400	-4. 26678000	0. 08024700
H	1. 67698900	-4. 98488000	1. 01173800
H	1. 47037400	-4. 64146800	-0. 72735800
O	0. 05277600	-2. 75302900	-1. 38634800
C	-1. 28379800	-0. 66182000	0. 46916300
C	-1. 93664700	-0. 28454200	-0. 77238300
C	-1. 94006500	-0. 82826400	1. 72033900
O	-3. 02881100	-0. 34235900	2. 09293100
O	-1. 29615600	-1. 70744400	2. 56739400
C	-1. 85468700	-1. 84984000	3. 87451000
H	-1. 89787600	-0. 89098900	4. 40080200
H	-2. 86364400	-2. 27198900	3. 83246400
H	-1. 18836900	-2. 53368300	4. 40433200
H	-1. 49042600	-0. 82642600	-1. 60289400
C	-5. 41138300	-2. 03068900	-1. 00862400
C	-3. 96066200	-1. 82077600	-0. 47454300
C	-3. 67105100	-0. 48351000	-2. 50923700
C	-5. 19415400	-0. 46228600	-2. 79078900
H	-3. 93015100	-1. 75411600	0. 60971400
H	-3. 26568600	-2. 58863100	-0. 81707000
H	-5. 43363100	-2. 80587200	-1. 77985500
H	-6. 05318800	-2. 35827600	-0. 18560200
H	-3. 15120000	0. 38570800	-2. 90735200
H	-3. 19302900	-1. 38966700	-2. 88704500
H	-5. 50920300	0. 52524900	-3. 13958700
H	-5. 43130500	-1. 18569600	-3. 57638500
N	-5. 95768000	-0. 79219900	-1. 57999900
N	-3. 44584200	-0. 48058600	-0. 99924800
C	-5. 78192300	0. 29195300	-0. 60083700
C	-4. 28689500	0. 64380900	-0. 40374000
H	-6. 23462000	-0. 02659200	0. 34294400
H	-6. 32225600	1. 17826200	-0. 94695200
H	-3. 99335800	0. 71806000	0. 64150100
H	-3. 99691900	1. 54267500	-0. 94104700
H	0. 23286400	0. 00148900	-1. 66889300

### IRC-1

0 1			
C	0. 91528800	3. 74277100	0. 65427400
C	-0. 34129300	4. 21597700	0. 29847600
C	-1. 25384800	3. 42607800	-0. 36590700
C	-0. 87150800	2. 09771000	-0. 71432500

C	0. 41397400	1. 60804600	-0. 32653200
C	1. 31337600	2. 45704800	0. 35352000
C	0. 82743200	5. 91491600	1. 15468900
H	-2. 23247300	3. 79473700	-0. 65424200
H	2. 30610500	2. 11963000	0. 62349300
H	1. 28085600	6. 53265100	0. 36589700
O	-0. 48944000	5. 51525000	0. 74189700
O	1. 60479600	4. 72998300	1. 34698100
H	0. 76011200	6. 46500700	2. 09540000
O	-1. 72260300	1. 36950700	-1. 42590100
C	0. 78931000	0. 18686500	-0. 75634400
C	2. 47426700	-0. 22900600	-2. 57533500
C	2. 23872500	-0. 01557900	-1. 20318300
C	3. 36626800	0. 00928700	-0. 36927700
C	4. 66249800	-0. 16328000	-0. 86741800
C	4. 86420900	-0. 36946700	-2. 23610200
C	3. 75302800	-0. 40147100	-3. 09054300
H	1. 62998100	-0. 26052500	-3. 25992400
H	3. 25590800	0. 15644100	0. 69828800
H	5. 49811800	-0. 13484700	-0. 17758000
H	3. 91139500	-0. 56446800	-4. 15258100
O	6. 08173200	-0. 54861000	-2. 82815100
C	7. 24199300	-0. 52343700	-2. 00129800
H	7. 21588300	-1. 32175900	-1. 24960600
H	8. 08896000	-0. 68384200	-2. 67015700
H	7. 35428500	0. 44446400	-1. 49776800
C	1. 74527300	-2. 19020700	1. 58331100
C	1. 06312200	-0. 96373800	1. 53955500
C	1. 24952100	-0. 04633500	2. 56447100
C	2. 13095400	-0. 35508500	3. 61264400
C	2. 80940300	-1. 57548800	3. 63182900
C	2. 62160100	-2. 51867000	2. 61190100
C	0. 51381700	-2. 30761300	-0. 34585500
C	0. 23321100	-0. 91029800	0. 26871100
H	0. 71520400	0. 89754600	2. 56186700
H	2. 28122100	0. 36030400	4. 41625100
H	3. 48934400	-1. 80444900	4. 44785400
H	3. 14366000	-3. 47015000	2. 62967700
N	1. 39838700	-2. 97287600	0. 46912700
C	1. 91117800	-4. 30155800	0. 19407100
H	2. 99975700	-4. 27880000	0. 07379200
H	1. 65753100	-4. 99111800	1. 00650700
H	1. 45142800	-4. 64711400	-0. 73251200
O	0. 04352200	-2. 75245700	-1. 38970900

C	-1.29655400	-0.69824600	0.45802000
C	-1.96664100	-0.44182900	-0.73235500
C	-1.94722200	-0.83573900	1.75001300
O	-3.00809500	-0.31439100	2.11105800
O	-1.30891600	-1.71004000	2.57170400
C	-1.86278300	-1.86137100	3.88644700
H	-1.89653700	-0.90170300	4.40904400
H	-2.87260800	-2.27776600	3.83793900
H	-1.19503600	-2.55035700	4.40464600
H	-1.48019500	-0.81975700	-1.61755300
C	-5.45954500	-2.00681200	-1.01117000
C	-4.01240500	-1.83942400	-0.46983500
C	-3.66315400	-0.48822700	-2.49651900
C	-5.18521500	-0.43707700	-2.78697200
H	-3.98408800	-1.78440000	0.61532700
H	-3.33694900	-2.62426100	-0.81293400
H	-5.49649800	-2.77777700	-1.78592100
H	-6.11689000	-2.31986800	-0.19486900
H	-3.11983500	0.37982300	-2.86406500
H	-3.19955300	-1.39707200	-2.88544200
H	-5.47877500	0.55615200	-3.13810700
H	-5.43186700	-1.15607500	-3.57357600
N	-5.96453500	-0.75087600	-1.58184500
N	-3.44952100	-0.51466500	-0.98170600
C	-5.76540300	0.32690800	-0.59988400
C	-4.26188600	0.64467300	-0.39845800
H	-6.22822000	0.01787100	0.34219400
H	-6.28327600	1.22674600	-0.94566800
H	-3.97638700	0.72759000	0.64638500
H	-3.92750900	1.52252600	-0.94466000
H	0.21271700	0.01768100	-1.66720200

### IRC-F-7

0 1			
C	0.93930400	3.74434800	0.67048700
C	-0.30682200	4.23826000	0.30610700
C	-1.21844100	3.47684600	-0.38706800
C	-0.85607000	2.14466300	-0.76983800
C	0.41455700	1.62247900	-0.33344300
C	1.31618200	2.45241000	0.36738500
C	0.88147500	5.91555900	1.16994300
H	-2.18113300	3.87114000	-0.69590400
H	2.29797100	2.09556900	0.65367000
H	1.34488100	6.51320000	0.37042800

O	-0.44256500	5.53569500	0.76465600
O	1.63599300	4.72076500	1.38004200
H	0.82595900	6.48230000	2.10156700
O	-1.68238800	1.46392200	-1.51974200
C	0.77858000	0.19584400	-0.75931400
C	2.46322400	-0.23694800	-2.57915500
C	2.22766100	-0.02086400	-1.20730000
C	3.35648000	-0.00469500	-0.37401700
C	4.65196600	-0.18643800	-0.87154800
C	4.85317600	-0.39325200	-2.24016000
C	3.74137400	-0.41785600	-3.09410600
H	1.61921500	-0.26315000	-3.26432800
H	3.24832600	0.14347900	0.69354200
H	5.48732400	-0.16389800	-0.18108700
H	3.89836600	-0.58196100	-4.15621700
O	6.06992800	-0.57975100	-2.83237200
C	7.23073000	-0.56095200	-2.00605400
H	7.20080900	-1.35923500	-1.25443000
H	8.07652900	-0.72578600	-2.67534700
H	7.34852200	0.40622200	-1.50234400
C	1.73424500	-2.19787300	1.58081200
C	1.05786200	-0.96783200	1.53856400
C	1.24795700	-0.05298300	2.56527800
C	2.12796000	-0.36807200	3.61281500
C	2.80076100	-1.59154700	3.62993800
C	2.60890500	-2.53218600	2.60862200
C	0.50662100	-2.30893000	-0.35080500
C	0.23059400	-0.90792900	0.26644800
H	0.72136300	0.89519900	2.56247800
H	2.28203500	0.34552600	4.41717100
H	3.47973400	-1.82474400	4.44549100
H	3.12687600	-3.48583500	2.62448800
N	1.38632200	-2.97707700	0.46487000
C	1.89295200	-4.30842700	0.18891400
H	2.98138300	-4.29033700	0.06765500
H	1.63646500	-4.99579600	1.00214100
H	1.43065400	-4.65204300	-0.73699800
O	0.03460400	-2.74920400	-1.39441000
C	-1.30417300	-0.72220000	0.45516900
C	-1.98961700	-0.54368400	-0.71087600
C	-1.94996000	-0.83974400	1.77370000
O	-2.98331800	-0.28026800	2.13473900
O	-1.32341200	-1.72332600	2.57617400
C	-1.86951100	-1.87502700	3.89850400

H	-1.88338600	-0.91559600	4.42098100
H	-2.88505700	-2.27590500	3.85092400
H	-1.20660800	-2.57600000	4.40511700
H	-1.48176700	-0.80425200	-1.62154800
C	-5.51621700	-1.97344400	-1.00786600
C	-4.06942100	-1.85384800	-0.45778300
C	-3.66057600	-0.50801500	-2.48414700
C	-5.17871100	-0.41315900	-2.78351900
H	-4.04347000	-1.80163100	0.62828600
H	-3.41795000	-2.66031500	-0.79753500
H	-5.57191900	-2.74277600	-1.78305500
H	-6.18967500	-2.26490900	-0.19679000
H	-3.08808300	0.34845800	-2.83476800
H	-3.21940500	-1.42725400	-2.87481800
H	-5.44142700	0.58741400	-3.13812200
H	-5.44210400	-1.12631900	-3.56990400
N	-5.97414000	-0.70138400	-1.58226900
N	-3.45894900	-0.54948700	-0.96665900
C	-5.74632600	0.37133900	-0.60077100
C	-4.23425400	0.64374400	-0.39394900
H	-6.22200600	0.07796100	0.33994400
H	-6.23507000	1.28617000	-0.94973900
H	-3.95334300	0.72757100	0.65134600
H	-3.85698300	1.50167600	-0.94582200
H	0.19480200	0.03128900	-1.66656600

### IRC-F-11

0	1		
C	0.95456200	3.74282100	0.68588400
C	-0.28038500	4.25385400	0.30675500
C	-1.18858100	3.51159200	-0.41065400
C	-0.83985100	2.17513300	-0.80439500
C	0.41707900	1.63216600	-0.33855600
C	1.31760700	2.44728800	0.38103900
C	0.91931700	5.91182300	1.18832300
H	-2.13921400	3.92296600	-0.73478100
H	2.28963500	2.07587800	0.68227900
H	1.39743300	6.49539500	0.38657300
O	-0.40744300	5.54957300	0.77653100
O	1.65256700	4.70765700	1.41386600
H	0.86607700	6.48756800	2.11445800
O	-1.65429700	1.51528200	-1.57474000
C	0.77137200	0.20217200	-0.76126000
C	2.45371100	-0.23957000	-2.58297700

C	2. 21911000	-0. 02284200	-1. 21106700
C	3. 34832000	-0. 01303200	-0. 37808000
C	4. 64292600	-0. 20107400	-0. 87550000
C	4. 84320900	-0. 40790500	-2. 24417200
C	3. 73114000	-0. 42643300	-3. 09797600
H	1. 60959800	-0. 26138600	-3. 26816800
H	3. 24148200	0. 13479500	0. 68959300
H	5. 47826800	-0. 18329500	-0. 18486400
H	3. 88723800	-0. 59074800	-4. 16020100
O	6. 05923700	-0. 60005700	-2. 83637600
C	7. 22009200	-0. 58612400	-2. 01003800
H	7. 18707700	-1. 38452000	-1. 25864800
H	8. 06525600	-0. 75408800	-2. 67937000
H	7. 34173300	0. 38040500	-1. 50599000
C	1. 72679600	-2. 20230000	1. 57804600
C	1. 05279700	-0. 97063400	1. 53789600
C	1. 24357600	-0. 05874900	2. 56722700
C	2. 12255600	-0. 37817200	3. 61442400
C	2. 79301200	-1. 60289300	3. 62903400
C	2. 59996600	-2. 54083100	2. 60553700
C	0. 50341400	-2. 30738300	-0. 35638300
C	0. 22741400	-0. 90596700	0. 26479500
H	0. 72022200	0. 89123000	2. 56576100
H	2. 27781800	0. 33338700	4. 42029700
H	3. 47118500	-1. 83917000	4. 44433200
H	3. 11618500	-3. 49541900	2. 61931700
N	1. 37960400	-2. 97817600	0. 45983000
C	1. 88298200	-4. 31067300	0. 18238900
H	2. 97135300	-4. 29512800	0. 06073800
H	1. 62482900	-4. 99755100	0. 99541800
H	1. 41944400	-4. 65247700	-0. 74352000
O	0. 03230600	-2. 74379600	-1. 40131600
C	-1. 30933700	-0. 73659300	0. 45432800
C	-2. 00219300	-0. 59119500	-0. 70204500
C	-1. 94953800	-0. 84483000	1. 78608600
O	-2. 96009000	-0. 25544400	2. 15536300
O	-1. 33627400	-1. 74503500	2. 57356500
C	-1. 87194400	-1. 89306000	3. 90267100
H	-1. 86172700	-0. 93509700	4. 42740300
H	-2. 89507400	-2. 27441600	3. 86165500
H	-1. 21675900	-2. 60859500	4. 39823500
H	-1. 48606000	-0. 79141500	-1. 62218500
C	-5. 55748400	-1. 94380800	-0. 99928500
C	-4. 10913700	-1. 85882100	-0. 44555100

C	-3. 66158200	-0. 52740900	-2. 47668500
C	-5. 17581900	-0. 40038700	-2. 78188900
H	-4. 08337100	-1. 80435800	0. 64086000
H	-3. 47672800	-2. 68190100	-0. 78160100
H	-5. 62966700	-2. 71530000	-1. 77092400
H	-6. 24056800	-2. 21429700	-0. 18906600
H	-3. 06985100	0. 31830400	-2. 82258700
H	-3. 23723400	-1. 45574500	-2. 86436800
H	-5. 41462900	0. 60388700	-3. 14275200
H	-5. 45308900	-1. 11183200	-3. 56497000
N	-5. 98114900	-0. 66352300	-1. 58140400
N	-3. 46680200	-0. 57157500	-0. 95786400
C	-5. 73114500	0. 40882300	-0. 60490900
C	-4. 21363300	0. 64362000	-0. 39147600
H	-6. 21865500	0. 13299700	0. 33505400
H	-6. 19485700	1. 33358800	-0. 96164200
H	-3. 93613900	0. 72312200	0. 65503800
H	-3. 80614000	1. 48858300	-0. 94343400
H	0. 18332800	0. 04045800	-1. 66622900

### IRC-F-16

0 1

C	0. 96678700	3. 73789200	0. 70907600
C	-0. 25119300	4. 26972000	0. 30424400
C	-1. 15281700	3. 54740200	-0. 44204000
C	-0. 81959500	2. 20411900	-0. 83415300
C	0. 41962200	1. 64057200	-0. 33986300
C	1. 31563200	2. 43854800	0. 40438900
C	0. 95520100	5. 90382500	1. 22006100
H	-2. 08438700	3. 98156700	-0. 79218300
H	2. 27284600	2. 04925800	0. 72979400
H	1. 46089500	6. 47739300	0. 42790800
O	-0. 36942600	5. 56427700	0. 78233800
O	1. 66169000	4. 68754700	1. 46150600
H	0. 89331800	6. 48184400	2. 14433200
O	-1. 62531200	1. 55632700	-1. 62378100
C	0. 76380500	0. 20861700	-0. 76164800
C	2. 44221100	-0. 23725900	-2. 58740400
C	2. 20947000	-0. 02240600	-1. 21497300
C	3. 33906600	-0. 01938600	-0. 38261400
C	4. 63248100	-0. 21251800	-0. 88077300
C	4. 83120100	-0. 41784700	-2. 24985300
C	3. 71867500	-0. 42898800	-3. 10328300
H	1. 59742800	-0. 25329900	-3. 27201600

H	3.23349000	0.12672600	0.68537200
H	5.46799800	-0.19967600	-0.19037900
H	3.87318200	-0.59131900	-4.16605400
O	6.04633800	-0.61531400	-2.84230100
C	7.20674900	-0.60746000	-2.01535900
H	7.16896600	-1.40581300	-1.26414000
H	8.05130600	-0.77960000	-2.68428200
H	7.33261600	0.35836800	-1.51102400
C	1.72057300	-2.20593800	1.57385900
C	1.04538500	-0.97461800	1.53735700
C	1.23177100	-0.06753200	2.57182300
C	2.10927800	-0.39044300	3.61928900
C	2.78194700	-1.61389700	3.62936100
C	2.59219200	-2.54770700	2.60146200
C	0.50344900	-2.30432600	-0.36480300
C	0.22318800	-0.90517300	0.26261000
H	0.70617000	0.88130900	2.57448200
H	2.25973100	0.31707300	4.42967600
H	3.45847300	-1.85240100	4.44532900
H	3.11040900	-3.50114400	2.61203700
N	1.37683900	-2.97752300	0.45181000
C	1.88310900	-4.30812700	0.17016300
H	2.97176500	-4.28902500	0.05007500
H	1.62597200	-4.99807700	0.98069100
H	1.42230200	-4.64746800	-0.75787800
O	0.03586100	-2.73589300	-1.41288100
C	-1.31380000	-0.75011500	0.45269400
C	-2.01120200	-0.62247000	-0.70121800
C	-1.94713500	-0.85401600	1.79315100
O	-2.92906200	-0.23042100	2.17890800
O	-1.35362700	-1.78289600	2.56032800
C	-1.87218500	-1.92989100	3.89731300
H	-1.78442800	-0.98745500	4.44538000
H	-2.92045600	-2.24112600	3.86804200
H	-1.25545500	-2.70245100	4.35895600
H	-1.49515500	-0.78510300	-1.61994200
C	-5.60277700	-1.90418000	-0.97552200
C	-4.14860500	-1.85727300	-0.42802800
C	-3.66551500	-0.55427900	-2.47080500
C	-5.17521600	-0.39790300	-2.78154100
H	-4.11803200	-1.79780200	0.65849400
H	-3.54238300	-2.70120200	-0.76091600
H	-5.70628900	-2.68820100	-1.73064000
H	-6.29128900	-2.13365600	-0.15649600

H	-3. 05519400	0. 27661200	-2. 82053700
H	-3. 25865800	-1. 49444900	-2. 84905700
H	-5. 38943000	0. 60458600	-3. 16161200
H	-5. 46783200	-1. 11799100	-3. 55116000
N	-5. 98797100	-0. 62163900	-1. 57811900
N	-3. 47494300	-0. 59097600	-0. 95126500
C	-5. 71191300	0. 45894500	-0. 61808600
C	-4. 18929600	0. 64672300	-0. 39237100
H	-6. 21837200	0. 21997900	0. 32172000
H	-6. 13844800	1. 39210100	-0. 99956300
H	-3. 91713600	0. 71834900	0. 65645600
H	-3. 74670400	1. 47669000	-0. 94200200
H	0. 17037200	0. 05169500	-1. 66385100

### IRC-F-21

0 1

C	0. 97076900	3. 73000400	0. 73879900
C	-0. 22790700	4. 28170900	0. 30335900
C	-1. 11980700	3. 57682000	-0. 47061000
C	-0. 80019600	2. 22744400	-0. 86086300
C	0. 42161300	1. 64631000	-0. 33628200
C	1. 30933100	2. 42805700	0. 43440300
C	0. 97822500	5. 89223300	1. 26055400
H	-2. 03834000	4. 02357500	-0. 83788400
H	2. 25415000	2. 02540000	0. 77881000
H	1. 51312700	6. 45785400	0. 48153400
O	-0. 33969200	5. 57574000	0. 78645100
O	1. 65679700	4. 66453600	1. 52021600
H	0. 90128000	6. 47134900	2. 18297300
O	-1. 59441300	1. 59449000	-1. 66576300
C	0. 75891100	0. 21433000	-0. 76009800
C	2. 43402300	-0. 22799700	-2. 58947900
C	2. 20284900	-0. 01863100	-1. 21600900
C	3. 33228100	-0. 02209200	-0. 38384000
C	4. 62485000	-0. 21709300	-0. 88303900
C	4. 82223200	-0. 41742800	-2. 25298700
C	3. 70973600	-0. 42121900	-3. 10646300
H	1. 58890300	-0. 23911600	-3. 27362400
H	3. 22746300	0. 11919900	0. 68490100
H	5. 46073100	-0. 21037100	-0. 19292000
H	3. 86407800	-0. 58006400	-4. 16979400
O	6. 03665700	-0. 61709000	-2. 84623900
C	7. 19687800	-0. 61717800	-2. 01905400
H	7. 15662700	-1. 41913200	-1. 27178400

H	8.04116600	-0.78877300	-2.68857700
H	7.32623900	0.34566900	-1.50987800
C	1.71682400	-2.20870100	1.56928600
C	1.03532800	-0.98048800	1.53790100
C	1.21052500	-0.08033500	2.58050000
C	2.08522600	-0.40579900	3.62969900
C	2.76545100	-1.62498700	3.63357800
C	2.58559500	-2.55270100	2.59836600
C	0.50959400	-2.30093600	-0.37583700
C	0.22064100	-0.90615700	0.25873400
H	0.68132500	0.86640200	2.58678500
H	2.22952400	0.29723400	4.44494300
H	3.44055000	-1.86547000	4.45014100
H	3.10874900	-3.50352400	2.60460400
N	1.38276400	-2.97431900	0.44042800
C	1.89615100	-4.30097100	0.15244500
H	2.98474400	-4.27685600	0.03443200
H	1.63983900	-4.99622100	0.95876600
H	1.43800100	-4.63769600	-0.77792800
O	0.04888500	-2.72695400	-1.42865000
C	-1.31773400	-0.76527900	0.44386700
C	-2.01842500	-0.65016200	-0.70149400
C	-1.94478800	-0.86944800	1.79332300
O	-2.89112800	-0.20819500	2.19922700
O	-1.38039400	-1.83620000	2.53105900
C	-1.87951500	-1.98220800	3.87711800
H	-1.75233400	-1.04833200	4.43104200
H	-2.93681600	-2.25958100	3.86347100
H	-1.27890800	-2.77671000	4.31964600
H	-1.49665200	-0.76730000	-1.63083000
C	-5.63625000	-1.86651700	-0.94808900
C	-4.17690500	-1.84813700	-0.41128900
C	-3.67101300	-0.57483600	-2.46961500
C	-5.17910000	-0.40373600	-2.78194500
H	-4.13626600	-1.78167600	0.67450700
H	-3.59030000	-2.70618900	-0.74272200
H	-5.76145600	-2.66029300	-1.68928400
H	-6.32454100	-2.06603600	-0.12215100
H	-3.05372300	0.24942800	-2.82430800
H	-3.27158600	-1.52036000	-2.84191900
H	-5.37837200	0.59368500	-3.18317900
H	-5.48482700	-1.13534300	-3.53522000
N	-5.99294600	-0.58688000	-1.57273300
N	-3.47998200	-0.60178300	-0.94958000

C	-5.69334400	0.50502500	-0.63300200
C	-4.16736700	0.65526400	-0.39868200
H	-6.21090800	0.29610700	0.30778900
H	-6.09438300	1.44044500	-1.03415300
H	-3.89985900	0.72140400	0.65211600
H	-3.70082000	1.47418300	-0.94580700
H	0.16297000	0.06238700	-1.66123700

### IRC-F-26

0 1

C	0.96682900	3.71958100	0.77611500
C	-0.21057100	4.28961800	0.30813600
C	-1.08895600	3.60149000	-0.49594900
C	-0.78024300	2.24707900	-0.88219500
C	0.42291100	1.65052300	-0.32936100
C	1.29797100	2.41607400	0.47105700
C	0.98837900	5.87770700	1.31132000
H	-1.98905700	4.06524600	-0.89068300
H	2.22729400	1.99900800	0.84001500
H	1.55558700	6.43825300	0.55204600
O	-0.31872100	5.58295700	0.79512100
O	1.63974900	4.63963900	1.58613400
H	0.89139000	6.45436200	2.23330100
O	-1.56268700	1.62508400	-1.70408200
C	0.75750800	0.22036400	-0.75777000
C	2.43208100	-0.21160300	-2.58922300
C	2.20086700	-0.01113800	-1.21452300
C	3.32928300	-0.02139700	-0.38145300
C	4.62176900	-0.21556100	-0.88107300
C	4.81938700	-0.40763700	-2.25219400
C	3.70768300	-0.40343100	-3.10666000
H	1.58711500	-0.21665400	-3.27359300
H	3.22368000	0.11329000	0.68815000
H	5.45734600	-0.21475400	-0.19058500
H	3.86256500	-0.55534000	-4.17093000
O	6.03372500	-0.60651200	-2.84591700
C	7.19300000	-0.61598900	-2.01764600
H	7.14918900	-1.42272000	-1.27573900
H	8.03737000	-0.78604900	-2.68745700
H	7.32511200	0.34303900	-1.50200800
C	1.71370500	-2.21206200	1.56393800
C	1.02360500	-0.98845500	1.53790200
C	1.18045700	-0.09809700	2.59185600
C	2.04820300	-0.42690500	3.64581900

C	2.73964300	-1.63964900	3.64281100
C	2.57664900	-2.55865600	2.59702500
C	0.52040400	-2.29688400	-0.39027900
C	0.21969800	-0.90803400	0.25255400
H	0.64223700	0.84355700	2.60366800
H	2.17729300	0.26831300	4.47033100
H	3.40919800	-1.88251000	4.46321100
H	3.10771600	-3.50505000	2.59899000
N	1.39355800	-2.97011800	0.42612800
C	1.92117000	-4.28940400	0.12959800
H	3.01030000	-4.25339600	0.01873900
H	1.66685200	-4.99410600	0.92823200
H	1.47247700	-4.62228800	-0.80671900
O	0.06914600	-2.71674900	-1.44921200
C	-1.31898300	-0.77800300	0.43011000
C	-2.02059200	-0.66546700	-0.71134900
C	-1.94177500	-0.88671100	1.78452100
O	-2.85095600	-0.19589800	2.21157900
O	-1.41226000	-1.89224300	2.49052600
C	-1.90040500	-2.05440300	3.83913200
H	-1.73980100	-1.13815000	4.41104300
H	-2.96426400	-2.30037500	3.82916200
H	-1.32034900	-2.87728600	4.25699800
H	-1.49865800	-0.75143300	-1.64426600
C	-5.66089300	-1.83118000	-0.92284500
C	-4.19540800	-1.83704500	-0.40087600
C	-3.67807800	-0.58878100	-2.47290600
C	-5.18555800	-0.40621600	-2.78214900
H	-4.14418400	-1.76473500	0.68423400
H	-3.62804400	-2.70820800	-0.73154200
H	-5.81220900	-2.63596900	-1.64806800
H	-6.34568700	-1.99872400	-0.08572100
H	-3.05520600	0.22829000	-2.83510000
H	-3.28742500	-1.54010600	-2.84026100
H	-5.37450700	0.58475900	-3.20373600
H	-5.50422100	-1.15010400	-3.51793600
N	-5.99557600	-0.55496600	-1.56604000
N	-3.48183800	-0.60727900	-0.95340300
C	-5.67362900	0.54713100	-0.64602000
C	-4.14466100	0.66435400	-0.40654700
H	-6.20115600	0.37130800	0.29698500
H	-6.04859800	1.48468000	-1.06962900
H	-3.87848600	0.72526300	0.64532000
H	-3.65764700	1.47322400	-0.95225700

H	0.16108300	0.07439400	-1.65942800
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### IRC-F-31

0 1

C	0.95995900	3.71184800	0.80381700
C	-0.20318200	4.29294000	0.31408500
C	-1.07089500	3.61519900	-0.51061500
C	-0.76716300	2.25840000	-0.89405400
C	0.42355800	1.65269500	-0.32351600
C	1.28828500	2.40793600	0.49780100
C	0.98617100	5.86693900	1.35146400
H	-1.95907300	4.08865500	-0.92195200
H	2.20750400	1.98277200	0.88203300
H	1.57441900	6.42788500	0.60856900
O	-0.31112000	5.58527500	0.80398700
O	1.62201200	4.62244600	1.63365000
H	0.87231400	6.43904300	2.27443200
O	-1.54118500	1.64224700	-1.72818400
C	0.75832000	0.22452100	-0.75604600
C	2.43508300	-0.19650800	-2.58740500
C	2.20227900	-0.00394600	-1.21186100
C	3.32932500	-0.01853400	-0.37723300
C	4.62245600	-0.21028400	-0.87625800
C	4.82168400	-0.39501300	-2.24819900
C	3.71125300	-0.38547800	-3.10423600
H	1.59092100	-0.19767100	-3.27273300
H	3.22211700	0.11031500	0.69302000
H	5.45725300	-0.21355500	-0.18481900
H	3.86766500	-0.53142500	-4.16912100
O	6.03656900	-0.59152700	-2.84160600
C	7.19476000	-0.60771000	-2.01200400
H	7.14894700	-1.41894800	-1.27512500
H	8.03974500	-0.77481600	-2.68179700
H	7.32761000	0.34792800	-1.49030800
C	1.71241300	-2.21395000	1.56019300
C	1.01404800	-0.99481300	1.53789500
C	1.15435400	-0.11240600	2.60097800
C	2.01497400	-0.44386500	3.66014500
C	2.71591000	-1.65102800	3.65265400
C	2.56905100	-2.56248600	2.59781100
C	0.53150400	-2.29403200	-0.40188500
C	0.21987900	-0.91067500	0.24670000
H	0.60958600	0.82545700	2.61580900
H	2.13118600	0.24516000	4.49170500

H	3.37990100	-1.89588400	4.47696600
H	3.10677700	-3.50512500	2.59703300
N	1.40608400	-2.96560500	0.41445400
C	1.95027900	-4.27607200	0.10911200
H	3.04065200	-4.22802200	0.01752700
H	1.68930400	-4.99458700	0.89318500
H	1.52089900	-4.59984700	-0.83937400
O	0.08756800	-2.71003600	-1.46514300
C	-1.31931000	-0.78903800	0.41660200
C	-2.02021100	-0.67407400	-0.72285300
C	-1.94098100	-0.90616400	1.77200400
O	-2.81966300	-0.18009600	2.22309400
O	-1.44055300	-1.94265900	2.45161100
C	-1.92297800	-2.11832400	3.80137400
H	-1.64326200	-1.25763600	4.41517400
H	-3.00849800	-2.23826100	3.80382800
H	-1.43462300	-3.02389800	4.16331700
H	-1.49901600	-0.74043300	-1.65787700
C	-5.67943100	-1.79910800	-0.89223400
C	-4.20521400	-1.82829600	-0.39493600
C	-3.68290200	-0.59932500	-2.47777100
C	-5.19201700	-0.42232000	-2.78449600
H	-4.13659300	-1.75811900	0.68932100
H	-3.65680100	-2.70782400	-0.73484100
H	-5.86272900	-2.61796300	-1.59298700
H	-6.35261100	-1.92816600	-0.03995000
H	-3.06308400	0.21823200	-2.84496400
H	-3.29001300	-1.55085100	-2.84240900
H	-5.38009500	0.55549000	-3.23607800
H	-5.51723900	-1.18810000	-3.49446200
N	-5.99640900	-0.53253800	-1.56099100
N	-3.48192500	-0.61025800	-0.95900300
C	-5.65557900	0.58418700	-0.66656000
C	-4.12628100	0.67196200	-0.41501800
H	-6.19428600	0.44614100	0.27584300
H	-6.00504000	1.51792700	-1.11827300
H	-3.86704000	0.72492000	0.63930900
H	-3.61967400	1.47319600	-0.95408600
H	0.16321400	0.08254100	-1.65911200

### IRC-F-36

0 1

C	0.95032900	3.70282800	0.83467900
C	-0.19891800	4.29467200	0.32467300

C	-1.05471100	3.62738400	-0.52006300
C	-0.75383500	2.27006200	-0.90604900
C	0.42414400	1.65496500	-0.31754300
C	1.27714500	2.39926400	0.52570500
C	0.98020000	5.85357900	1.39608600
H	-1.93359400	4.10720700	-0.94078300
H	2.18641000	1.96520700	0.92579000
H	1.58814600	6.41192700	0.66659800
O	-0.30821400	5.58463600	0.82121500
O	1.59956900	4.60292900	1.68701400
H	0.85245500	6.42373300	2.31853200
O	-1.51730500	1.66227100	-1.75466600
C	0.76023300	0.22939100	-0.75521100
C	2.44077300	-0.17708500	-2.58554300
C	2.20512000	0.00515300	-1.20912000
C	3.32999300	-0.01470800	-0.37193300
C	4.62432400	-0.20247100	-0.86952900
C	4.82645600	-0.37723800	-2.24240100
C	3.71804800	-0.36160000	-3.10091900
H	1.59799300	-0.17363700	-3.27252100
H	3.22007200	0.10655200	0.69904300
H	5.45768100	-0.21055400	-0.17639300
H	3.87706500	-0.49976200	-4.16645200
O	6.04252500	-0.56951700	-2.83484400
C	7.19888000	-0.59314600	-2.00295700
H	7.15047900	-1.40957300	-1.27199200
H	8.04516900	-0.75646700	-2.67204100
H	7.33185200	0.35852400	-1.47403700
C	1.71073800	-2.21720700	1.55445300
C	1.00309800	-1.00320500	1.53640800
C	1.12373900	-0.13070000	2.61024100
C	1.97507900	-0.46615200	3.67582000
C	2.68691600	-1.66681600	3.66318500
C	2.55965800	-2.56850900	2.59740700
C	0.54534700	-2.29064700	-0.41727300
C	0.22091800	-0.91348200	0.23833400
H	0.57206900	0.80310800	2.62804900
H	2.07681200	0.21544600	4.51536100
H	3.34477000	-1.91424200	4.49164200
H	3.10614900	-3.50605900	2.59248500
N	1.42010700	-2.96125900	0.39980600
C	1.97857600	-4.26380200	0.08623400
H	3.06367400	-4.19777200	-0.04828500
H	1.76069900	-4.97683400	0.88768600

H	1. 51886000	-4. 60668000	-0. 84127900
O	0. 11110000	-2. 70175700	-1. 48611900
C	-1. 31843000	-0. 80108800	0. 39939900
C	-2. 01972700	-0. 68341900	-0. 73774500
C	-1. 93768500	-0. 92481300	1. 75739600
O	-2. 78045400	-0. 17605900	2. 23008100
O	-1. 47395200	-1. 99870900	2. 40437200
C	-1. 93978900	-2. 18576100	3. 75859800
H	-1. 60537700	-1. 35763800	4. 38450100
H	-3. 02606100	-2. 25215100	3. 77935900
H	-1. 49264000	-3. 12375200	4. 08929600
H	-1. 49995100	-0. 72509600	-1. 67520000
C	-5. 69743600	-1. 76569700	-0. 86414500
C	-4. 21708700	-1. 81505600	-0. 38469800
C	-3. 69039800	-0. 61292800	-2. 48344300
C	-5. 20016500	-0. 43226800	-2. 78522000
H	-4. 13546000	-1. 73892900	0. 69829700
H	-3. 68662600	-2. 70573000	-0. 72478300
H	-5. 90413100	-2. 59506200	-1. 54687600
H	-6. 36370900	-1. 86462200	-0. 00145000
H	-3. 07026100	0. 20063500	-2. 85909500
H	-3. 30103700	-1. 56751200	-2. 84344400
H	-5. 38219800	0. 53666800	-3. 25853600
H	-5. 53689800	-1. 21209300	-3. 47455900
N	-5. 99757600	-0. 50630200	-1. 55458800
N	-3. 48203800	-0. 61264600	-0. 96578000
C	-5. 63538700	0. 62075600	-0. 68252900
C	-4. 10537900	0. 68291800	-0. 42773500
H	-6. 17492700	0. 50843300	0. 26000600
H	-5. 96924200	1. 54947700	-1. 14929400
H	-3. 84770800	0. 73326500	0. 62753300
H	-3. 58193400	1. 47407000	-0. 96675700
H	0. 16717700	0. 09199200	-1. 66028000

### IRC-F-41

0 1			
C	0. 93876300	3. 69303800	0. 86641800
C	-0. 19758900	4. 29429500	0. 33884300
C	-1. 04103300	3. 63756900	-0. 52649400
C	-0. 74182900	2. 28011000	-0. 91480700
C	0. 42439900	1. 65672300	-0. 31110500
C	1. 26548000	2. 39068400	0. 55265900
C	0. 96887600	5. 83943700	1. 44402600
H	-1. 90832300	4. 12711900	-0. 96389700

H	2.16527000	1.94901700	0.96575400
H	1.59390500	6.40005500	0.73111600
O	-0.30942400	5.58166200	0.84180500
O	1.57582100	4.58367300	1.73779900
H	0.82583300	6.40328200	2.36806800
O	-1.49525800	1.67994000	-1.77723200
C	0.76345500	0.23448400	-0.75546800
C	2.44991900	-0.15556000	-2.58344700
C	2.20993000	0.01576500	-1.20639500
C	3.33189400	-0.00909800	-0.36565700
C	4.62796800	-0.19229800	-0.86053800
C	4.83445300	-0.35664600	-2.23409300
C	3.72891000	-0.33497400	-3.09612500
H	1.60929000	-0.14723300	-3.27298300
H	3.21818400	0.10429100	0.70588400
H	5.45926700	-0.20486200	-0.16498900
H	3.89166400	-0.46434200	-4.16220600
O	6.05238700	-0.54382600	-2.82438200
C	7.20622500	-0.57404400	-1.98931200
H	7.15621700	-1.39692600	-1.26574100
H	8.05466800	-0.73075700	-2.65726100
H	7.33704200	0.37299100	-1.45156900
C	1.70689200	-2.22293100	1.54842100
C	0.99294000	-1.01253900	1.53285400
C	1.09467500	-0.14954600	2.61637700
C	1.93485400	-0.49002400	3.68931500
C	2.65388800	-1.68627400	3.67406800
C	2.54458200	-2.57911200	2.59873500
C	0.56000800	-2.28753100	-0.43459100
C	0.22348500	-0.91651200	0.22777700
H	0.53661900	0.78040700	2.63623700
H	2.02066400	0.18351300	4.53710100
H	3.30116500	-1.93857000	4.50934500
H	3.09386600	-3.51502400	2.59364200
N	1.43457000	-2.95753300	0.38350000
C	2.00573400	-4.25371100	0.06525400
H	3.09799100	-4.19437200	0.03992700
H	1.70707100	-5.00205200	0.80563200
H	1.63606800	-4.54689300	-0.91635200
O	0.13569300	-2.69315700	-1.50919400
C	-1.31613500	-0.81284800	0.38053400
C	-2.01778400	-0.69030800	-0.75444200
C	-1.93307500	-0.94438100	1.74010900
O	-2.73874800	-0.17308200	2.23572400

O	-1.50773300	-2.05586300	2.35416200
C	-1.96356300	-2.25478400	3.71055000
H	-1.57277800	-1.46005400	4.35291300
H	-3.05806700	-2.25783200	3.75004700
H	-1.55869400	-3.21609500	4.01062400
H	-1.49989600	-0.70916600	-1.69383300
C	-5.71110500	-1.73446200	-0.84133700
C	-4.22528400	-1.80261300	-0.37939400
C	-3.69820900	-0.62109900	-2.49053600
C	-5.20896000	-0.43590900	-2.78534700
H	-4.13034900	-1.72373800	0.70228600
H	-3.71164700	-2.70245200	-0.72185900
H	-5.93768900	-2.56919100	-1.50938100
H	-6.36778000	-1.81168600	0.02896800
H	-3.07747300	0.18822400	-2.87473000
H	-3.31407900	-1.57874400	-2.84781200
H	-5.38749800	0.52538300	-3.27670000
H	-5.55620200	-1.22728400	-3.45667300
N	-5.99819500	-0.48064900	-1.54744700
N	-3.48086300	-0.61329000	-0.97421800
C	-5.61552200	0.65394600	-0.69423700
C	-4.08460600	0.69253800	-0.43858000
H	-6.15534300	0.56493600	0.24903700
H	-5.93450700	1.57948000	-1.17470300
H	-3.82697700	0.73857200	0.61733100
H	-3.54705900	1.47538400	-0.97663200
H	0.17326400	0.10182200	-1.66309000

#### IRC-F-46

O 1			
C	0.92979800	3.68508000	0.89032600
C	-0.19742300	4.29282700	0.35119300
C	-1.03146800	3.64412700	-0.52998800
C	-0.73266400	2.28701100	-0.92047200
C	0.42543100	1.65780000	-0.30670100
C	1.25704500	2.38409700	0.57205200
C	0.95938100	5.82800000	1.47931200
H	-1.89113700	4.13898100	-0.97606000
H	2.15023800	1.93900800	0.99064800
H	1.59505000	6.38856100	0.77632800
O	-0.31170800	5.57779700	0.85984300
O	1.55721100	4.56861900	1.77577100
H	0.80684900	6.38938300	2.40316400
O	-1.47855300	1.69236300	-1.79323200

C	0.76690600	0.23824800	-0.75633700
C	2.45873700	-0.13875100	-2.58191900
C	2.21468500	0.02364800	-1.20451400
C	3.33395400	-0.00548200	-0.36047500
C	4.63164600	-0.18481200	-0.85261600
C	4.84225300	-0.34036300	-2.22658600
C	3.73935700	-0.31388000	-3.09186000
H	1.62015700	-0.12651700	-3.27387000
H	3.21677600	0.10168900	0.71137300
H	5.46092800	-0.20134800	-0.15473700
H	3.90560800	-0.43617200	-4.15824300
O	6.06203500	-0.52300000	-2.81450100
C	7.21325200	-0.55909500	-1.97606800
H	7.16229100	-1.38897200	-1.26051200
H	8.06415300	-0.70798600	-2.64268000
H	7.34080800	0.38292700	-1.42880900
C	1.70632200	-2.22686000	1.54200700
C	0.98673600	-1.01959800	1.52904800
C	1.07223100	-0.16495300	2.62070700
C	1.90287300	-0.50973700	3.69962600
C	2.63043500	-1.70082100	3.68062600
C	2.53807300	-2.58502500	2.59644900
C	0.57090700	-2.28492000	-0.44809000
C	0.22622900	-0.91857300	0.21920900
H	0.50775500	0.76118200	2.64271000
H	1.97401400	0.15629700	4.55475900
H	3.27164400	-1.95555000	4.51979000
H	3.09637300	-3.51557100	2.58792800
N	1.44212200	-2.95681500	0.37207500
C	2.01373300	-4.25161400	0.05057900
H	3.09677000	-4.17484500	-0.08319800
H	1.80352700	-4.97108500	0.84731500
H	1.55765800	-4.59406100	-0.87718800
O	0.15440300	-2.68626100	-1.52721200
C	-1.31331500	-0.82079500	0.36601400
C	-2.01524200	-0.69408200	-0.76760100
C	-1.92923000	-0.95961200	1.72603300
O	-2.71224400	-0.17678700	2.23745800
O	-1.52823300	-2.09319100	2.31782400
C	-1.98363400	-2.30186000	3.67349100
H	-1.60107200	-1.51419200	4.32084600
H	-3.07361600	-2.31489000	3.71007900
H	-1.57873300	-3.27548900	3.96117500
H	-1.49889300	-0.69753200	-1.70856600

C	-5.71931700	-1.71364400	-0.82872000
C	-4.22957500	-1.79397200	-0.37837300
C	-3.70327100	-0.62177400	-2.49592500
C	-5.21462800	-0.43035100	-2.78397100
H	-4.12769200	-1.71243000	0.70272300
H	-3.72580700	-2.69961900	-0.72134600
H	-5.96047800	-2.55097600	-1.48675500
H	-6.36796700	-1.77653000	0.04655300
H	-3.08183900	0.18530400	-2.88360200
H	-3.32395600	-1.58067800	-2.85421900
H	-5.38962900	0.52905400	-3.27924800
H	-5.57144700	-1.22257500	-3.44794700
N	-5.99798300	-0.46183500	-1.54217600
N	-3.47901300	-0.61268000	-0.98089500
C	-5.60221100	0.67590200	-0.69863600
C	-4.06965700	0.69918000	-0.44527400
H	-6.14401700	0.60261700	0.24679800
H	-5.90927400	1.60242900	-1.18919000
H	-3.80854200	0.74504800	0.60996600
H	-3.52479000	1.47640800	-0.98594800
H	0.17903100	0.10906500	-1.66595200

### IRC-F-52

0 1

C	0.92007900	3.67913100	0.90933500
C	-0.19986200	4.29234600	0.36010400
C	-1.02504800	3.65012400	-0.53402200
C	-0.72612500	2.29296100	-0.92551300
C	0.42509200	1.65915700	-0.30371700
C	1.24923400	2.38001100	0.58592600
C	0.94606100	5.81787800	1.51469600
H	-1.87995700	4.14346300	-0.97884500
H	2.13853700	1.92940100	1.01233800
H	1.59148900	6.38427700	0.82530000
O	-0.31714500	5.57393400	0.87665600
O	1.53879700	4.55562500	1.80896900
H	0.78170400	6.37128100	2.44139600
O	-1.46609700	1.70250900	-1.80470900
C	0.76937000	0.24161400	-0.75702500
C	2.46623600	-0.12361700	-2.58019700
C	2.21858100	0.03191100	-1.20268200
C	3.33583500	0.00270400	-0.35611800
C	4.63520400	-0.17052700	-0.84601600
C	4.84917800	-0.32268100	-2.21988000

C	3. 74836700	-0. 29444200	-3. 08775000
H	1. 62916000	-0. 11068400	-3. 27394000
H	3. 21571600	0. 10652000	0. 71583100
H	5. 46345600	-0. 18241700	-0. 14684800
H	3. 91711800	-0. 41401900	-4. 15404600
O	6. 07002300	-0. 50652600	-2. 80527100
C	7. 22009400	-0. 54238600	-1. 96527500
H	7. 14266500	-1. 33488900	-1. 21056100
H	8. 06482600	-0. 75272300	-2. 62396400
H	7. 37924700	0. 42090600	-1. 46394900
C	1. 70033900	-2. 23360400	1. 53945200
C	0. 98013600	-1. 02673200	1. 52616700
C	1. 05711800	-0. 17673600	2. 62206600
C	1. 88024200	-0. 52559800	3. 70550900
C	2. 60594700	-1. 71762400	3. 68833200
C	2. 51979800	-2. 59829500	2. 60116600
C	0. 58200900	-2. 28288300	-0. 46053500
C	0. 22873400	-0. 92088500	0. 21119900
H	0. 49451000	0. 75034300	2. 64261100
H	1. 94833200	0. 13869600	4. 56187800
H	3. 24006000	-1. 97672700	4. 53155800
H	3. 07078600	-3. 53309800	2. 59733600
N	1. 45504800	-2. 95332200	0. 35908600
C	2. 03347600	-4. 24447500	0. 03319300
H	3. 11513400	-4. 22349400	0. 19063900
H	1. 59746000	-5. 03825000	0. 64974200
H	1. 82345300	-4. 44760500	-1. 01657800
O	0. 17223400	-2. 68097300	-1. 54327800
C	-1. 31165300	-0. 83020100	0. 35263100
C	-2. 01358700	-0. 69760800	-0. 77900300
C	-1. 92565400	-0. 97788700	1. 71334200
O	-2. 68242600	-0. 17887400	2. 24341600
O	-1. 54825100	-2. 12554400	2. 28440000
C	-1. 99569500	-2. 35098300	3. 63982600
H	-1. 54697600	-1. 61561100	4. 30365700
H	-3. 09026500	-2. 27499600	3. 69633200
H	-1. 66155500	-3. 35735200	3. 89081500
H	-1. 49939900	-0. 68561400	-1. 72037600
C	-5. 72721800	-1. 69080100	-0. 80936500
C	-4. 23205300	-1. 78983500	-0. 38147400
C	-3. 70827000	-0. 61799100	-2. 50051600
C	-5. 22252300	-0. 43997500	-2. 78344700
H	-4. 11293600	-1. 71901500	0. 69862100
H	-3. 74424700	-2. 69856100	-0. 73989400

H	-5. 99042200	-2. 53337500	-1. 45285300
H	-6. 36545600	-1. 73122500	0. 07655800
H	-3. 09670900	0. 19750600	-2. 88552700
H	-3. 31919800	-1. 57013400	-2. 86501300
H	-5. 40346800	0. 50624700	-3. 30355800
H	-5. 58144700	-1. 25217900	-3. 42385100
N	-5. 99806100	-0. 44537000	-1. 53615400
N	-3. 47816200	-0. 61259200	-0. 98650600
C	-5. 58852600	0. 70105700	-0. 71204400
C	-4. 05751300	0. 70195000	-0. 44564700
H	-6. 14121400	0. 66072900	0. 23156300
H	-5. 87341800	1. 62320800	-1. 22836200
H	-3. 80630900	0. 73473000	0. 61264900
H	-3. 49778500	1. 47680900	-0. 97492500
H	0. 18383900	0. 11518100	-1. 66850800

### IRC-F-61

O 1

C	0. 90223500	3. 66822500	0. 94329800
C	-0. 20743000	4. 28814300	0. 38123500
C	-1. 02006500	3. 65402700	-0. 52891400
C	-0. 71668000	2. 30069400	-0. 93026400
C	0. 42511300	1. 66061900	-0. 29641300
C	1. 23485500	2. 37154700	0. 61367500
C	0. 92141400	5. 80087700	1. 56817400
H	-1. 87057500	4. 15348500	-0. 98009300
H	2. 11475500	1. 91601000	1. 05226900
H	1. 58019800	6. 36989300	0. 89332200
O	-0. 33175100	5. 56560100	0. 90659600
O	1. 50510200	4. 53455300	1. 86354500
H	0. 74314800	6. 34836900	2. 49592400
O	-1. 44409500	1. 71859300	-1. 82631400
C	0. 77523200	0. 24796700	-0. 75890000
C	2. 48176600	-0. 09580500	-2. 57705900
C	2. 22697800	0. 04663300	-1. 19945000
C	3. 33955100	0. 01000400	-0. 34715700
C	4. 64156000	-0. 15899100	-0. 83174800
C	4. 86315400	-0. 29359100	-2. 20630900
C	3. 76681200	-0. 25882400	-3. 07960200
H	1. 64803200	-0. 07803700	-3. 27468700
H	3. 21320000	0. 10012000	0. 72541100
H	5. 46511500	-0. 18772300	-0. 12744400
H	3. 94150500	-0. 36612500	-4. 14624200
O	6. 08804200	-0. 46182600	-2. 78799300

C	7.23306300	-0.50896100	-1.94166100
H	7.19834200	-1.37611300	-1.26975800
H	8.09349900	-0.59968300	-2.60723300
H	7.33035200	0.40700800	-1.34565700
C	1.69780900	-2.24139300	1.52911000
C	0.97157600	-1.03814600	1.51919200
C	1.02644900	-0.20105900	2.62662700
C	1.83462500	-0.55885900	3.71849400
C	2.56948100	-1.74523500	3.69665000
C	2.50675100	-2.61238400	2.59668800
C	0.59942200	-2.27910100	-0.48243600
C	0.23412800	-0.92398700	0.19712700
H	0.45812500	0.72243000	2.65014900
H	1.88611800	0.09507300	4.58426200
H	3.19465700	-2.00976900	4.54494800
H	3.06807000	-3.54107800	2.58664300
N	1.46469400	-2.95380600	0.34223600
C	2.06412600	-4.23323000	0.00817000
H	3.15350300	-4.14983200	-0.02034700
H	1.78457100	-4.99426100	0.74040500
H	1.69858600	-4.52499400	-0.97401300
O	0.20340600	-2.66829900	-1.57329800
C	-1.30565000	-0.84177900	0.33068700
C	-2.00938900	-0.70304100	-0.79851800
C	-1.91653800	-0.99770000	1.69307700
O	-2.64329100	-0.19460100	2.24175400
O	-1.57894800	-2.18264900	2.22890500
C	-2.02898000	-2.42277000	3.58141300
H	-1.60350900	-1.67401400	4.25339800
H	-3.11763400	-2.38984700	3.62928500
H	-1.66089000	-3.41520300	3.83274500
H	-1.49841100	-0.67153800	-1.74091000
C	-5.73280300	-1.66419000	-0.79903500
C	-4.23678500	-1.77897900	-0.38268600
C	-3.71500100	-0.61984200	-2.50869200
C	-5.22976000	-0.42770000	-2.78089000
H	-4.11199000	-1.70916700	0.69605400
H	-3.76098000	-2.69334900	-0.74244700
H	-6.01148400	-2.50623600	-1.43592200
H	-6.36351000	-1.69200500	0.09151800
H	-3.09804700	0.18904300	-2.90225400
H	-3.33691800	-1.57753600	-2.87332400
H	-5.40524200	0.51821200	-3.29495700
H	-5.59908000	-1.23087900	-3.42020300

N	-5. 99601100	-0. 42076400	-1. 53018200
N	-3. 47490600	-0. 61091800	-0. 99644100
C	-5. 56906100	0. 72582800	-0. 71403400
C	-4. 03710900	0. 71165500	-0. 45558100
H	-6. 11490700	0. 69329300	0. 23157800
H	-5. 84834500	1. 64691900	-1. 23139600
H	-3. 78005300	0. 74472100	0. 60137800
H	-3. 47305000	1. 47983200	-0. 98929300
H	0. 19357300	0. 12649600	-1. 67358900

## 11. Coordinates of M2b, TSb<sub>[3+2]</sub>, TSb<sub>[3+4]</sub> and IRC points in TSb<sub>[3+2]</sub> (IRC-1 is transition state)

### M2b

0 1			
C	-2. 38822100	1. 54934400	-0. 45983500
C	0. 09272200	1. 54303200	-0. 09745500
C	-1. 30284300	1. 34288700	0. 39271700
H	-1. 48118500	1. 23116300	1. 45362800
C	0. 70974500	2. 67510100	0. 71828100
C	1. 07638500	3. 87640700	0. 09284500
C	0. 87609500	2. 57721400	2. 11174300
C	1. 61190100	4. 93832900	0. 82786900
H	0. 93218700	3. 98584700	-0. 97947500
C	1. 41547000	3. 63280000	2. 84588900
H	0. 57859200	1. 66815700	2. 62918300
C	1. 79066000	4. 81922600	2. 20666500
H	1. 88757300	5. 85827400	0. 31891900
H	1. 53795600	3. 53179400	3. 92114000
H	2. 20961100	5. 64171100	2. 77955400
O	-2. 33561800	1. 76692600	-1. 70573700
H	0. 02073500	1. 85250500	-1. 14372000
C	-3. 75309300	1. 49152600	0. 25510300
O	-3. 90198300	0. 97461500	1. 35281200
O	-4. 86424500	1. 99655800	-0. 32685400
C	-4. 91211000	2. 78129100	-1. 54677500
H	-5. 68871100	3. 52769400	-1. 34694900
H	-3. 95829300	3. 27670000	-1. 71090900
C	-5. 29015000	1. 90637800	-2. 72949800
H	-6. 23639500	1. 38552200	-2. 54540800
H	-5. 40890100	2. 52529700	-3. 62708100
H	-4. 49903500	1. 17482000	-2. 90930500
C	-2. 46990400	-2. 05217800	1. 57178400

C	-1.09791800	-1.73658900	1.40049000
C	-0.23601100	-1.98079000	2.48578900
C	-0.77000900	-2.36545300	3.72662100
C	-2.14327100	-2.56943300	3.87103400
C	-3.01702200	-2.44104200	2.78840500
C	-2.24135500	-1.66806200	-0.67174100
C	-0.88777800	-1.43185500	-0.01411800
H	-0.11706700	-2.51375700	4.57777100
H	-2.53341900	-2.86133500	4.84192300
H	-4.07498200	-2.65480200	2.89080300
N	-3.12197600	-1.98525000	0.34608300
O	-2.56245800	-1.53367600	-1.84715600
O	1.10570200	-1.85581300	2.26592400
C	1.99749500	-2.47849900	3.19757500
H	1.68690800	-3.50894100	3.39839500
H	2.97297800	-2.47648400	2.71258000
H	2.04798400	-1.92030200	4.13927300
C	0.17073500	-0.92427800	-0.74547100
C	-4.54798300	-2.15641800	0.15079800
H	-5.09804000	-1.40116200	0.72044600
H	-4.75074300	-2.02784100	-0.91297000
H	-4.86783700	-3.15702000	0.46231300
C	0.12164500	-1.16045800	-2.21469300
O	0.29454400	-0.34756400	-3.11255800
C	0.97922600	0.17055400	-0.08369000
H	1.10208100	-0.11116500	0.95788600
O	-0.04642000	-2.47785600	-2.46795900
C	-0.29610100	-2.81911100	-3.84077500
H	0.52538200	-2.48642600	-4.48018100
H	-0.37904500	-3.90600500	-3.86045100
H	-1.23004200	-2.35805200	-4.17120900
C	3.38934600	1.11967200	0.41875400
C	4.55517100	0.01708900	-1.35809000
C	4.72010000	1.18962300	-0.36222300
H	4.86277100	2.14192900	-0.87862500
H	5.55803800	1.05680700	0.32489800
C	2.53329800	1.13546700	-1.93320100
H	1.64304800	0.91920200	-2.51284400
H	2.57486100	2.20234400	-1.71411500
C	3.83139600	0.60065700	-2.57415700
H	3.61516900	-0.14920700	-3.33944300
H	4.40682500	1.40295100	-3.04294700
H	5.46892800	-0.53565700	-1.57549000
C	3.45322000	-0.83865700	-0.67726200

N	2.43107200	0.40413700	-0.59277000
O	3.70483000	-1.14710600	0.67039700
C	3.00688200	-2.10720800	-1.38090400
H	2.16069600	-2.52057800	-0.82893000
H	2.66291300	-1.87777900	-2.39117100
C	4.13533300	-3.14990700	-1.44807900
H	4.97479700	-2.80696500	-2.06146400
H	4.51254100	-3.38913200	-0.44990100
H	3.74986400	-4.07045400	-1.89674500
H	2.97814300	2.06160500	0.75852300
C	3.57372500	0.04796100	1.47229300
H	4.48367200	0.21197700	2.05456100
H	2.73027200	-0.07182700	2.15327000

### TSb<sub>[3+2]</sub>

0 1

C	-2.27168700	1.58269700	-0.55299700
C	0.21179700	1.43569100	-0.26693300
C	-1.17043300	1.10563700	0.23841400
H	-1.32715500	1.12294500	1.30887000
C	0.69547000	2.70152900	0.43025200
C	0.98083800	3.85081100	-0.32190400
C	0.83595300	2.77131100	1.82786900
C	1.41243100	5.02779000	0.29658600
H	0.85591900	3.82575100	-1.40172100
C	1.27252200	3.94236700	2.44628600
H	0.60064800	1.90398400	2.43995700
C	1.56540300	5.07699400	1.68265700
H	1.62575200	5.90533100	-0.30799500
H	1.37739900	3.97178000	3.52757700
H	1.90151400	5.99014800	2.16576200
O	-2.18498200	1.91387200	-1.74810900
H	0.12009600	1.64097900	-1.33739700
C	-3.61962900	1.64119300	0.20390900
O	-3.69270300	1.32312000	1.37976700
O	-4.74694900	2.06738000	-0.39089400
C	-4.90886100	2.50151600	-1.77207900
H	-5.78715300	3.15183500	-1.72250500
H	-4.04220500	3.08012900	-2.08079000
C	-5.15824800	1.32143600	-2.69499300
H	-6.03789700	0.75397300	-2.37132700
H	-5.34388100	1.68737000	-3.71187300
H	-4.28988900	0.65843500	-2.71441500
C	-2.66477100	-1.84219900	1.45105200

C	-1.29351500	-1.50238000	1.39856500
C	-0.51564900	-1.75170300	2.54176300
C	-1.13196400	-2.22442100	3.71323900
C	-2.50289700	-2.48648200	3.73543300
C	-3.29401500	-2.31660600	2.59781700
C	-2.28886800	-1.31115100	-0.74748500
C	-0.98559700	-1.07414800	0.01419600
H	-0.54526500	-2.39252200	4.60797000
H	-2.95568500	-2.84823200	4.65433600
H	-4.35112900	-2.55821700	2.60583700
N	-3.23432700	-1.69656700	0.18787500
O	-2.52744700	-1.12453800	-1.93460400
O	0.83145900	-1.53495800	2.45335800
C	1.67400300	-2.08832600	3.46667100
H	1.44118000	-3.14575000	3.63186300
H	2.68977500	-1.99541700	3.08318000
H	1.57962100	-1.54091200	4.41166800
C	0.26397800	-1.00418500	-0.68118100
C	-4.62640100	-1.94455800	-0.12763100
H	-5.27528000	-1.25023400	0.41703400
H	-4.75139800	-1.79327100	-1.20017600
H	-4.90612800	-2.97259700	0.12868100
C	0.35357400	-1.62289100	-1.97555100
O	1.01013400	-1.28799400	-2.97226300
C	1.10533000	0.12546000	-0.11224500
H	1.20737500	-0.06361900	0.95479300
O	-0.32444000	-2.82103000	-1.98658300
C	-0.56529900	-3.38307600	-3.27846800
H	0.37003000	-3.54864300	-3.81973300
H	-1.06783100	-4.33520900	-3.09732000
H	-1.21395100	-2.72617100	-3.86639100
C	3.44679300	1.20217200	0.32702200
C	4.71083200	-0.13856600	-1.20003300
C	4.81554000	1.17563600	-0.39113000
H	4.97412000	2.03991100	-1.04064200
H	5.61989500	1.16457300	0.34723800
C	2.69200000	0.82898600	-2.02743000
H	1.84572000	0.46296500	-2.59935500
H	2.69117300	1.91881400	-1.98081200
C	4.02872600	0.23603100	-2.51987900
H	3.85185500	-0.62856300	-3.16422200
H	4.61316700	0.96799300	-3.08352000
H	5.64178000	-0.69695700	-1.29613400
C	3.59587700	-0.90489500	-0.43784100

N	2. 55320500	0. 31197800	-0. 59759800
O	3. 78589800	-0. 98325500	0. 95677100
C	3. 21807400	-2. 28818700	-0. 93579900
H	2. 33306600	-2. 61165800	-0. 38298400
H	2. 94314600	-2. 24428900	-1. 98957200
C	4. 36033700	-3. 29634400	-0. 72742000
H	5. 24908300	-3. 03798100	-1. 31329800
H	4. 65021100	-3. 36074600	0. 32522100
H	4. 02894400	-4. 28828800	-1. 05026300
H	3. 00353600	2. 17737900	0. 48744100
C	3. 59769300	0. 31922500	1. 54905500
H	4. 47647900	0. 59653700	2. 13677700
H	2. 72743300	0. 29163800	2. 20804800

### TSb<sub>[3+4]</sub>

0 1

C	-1. 04983500	2. 43238300	-0. 43461600
C	1. 37586000	1. 44540800	-0. 94290100
C	0. 20577400	2. 41429500	-0. 96230300
H	0. 48230400	3. 34697400	-1. 44369600
C	2. 55925400	2. 17782800	-0. 30326800
C	3. 72138800	2. 44572400	-1. 03899200
C	2. 48285600	2. 65003000	1. 01700500
C	4. 79304900	3. 13732600	-0. 46544800
H	3. 78699900	2. 12030500	-2. 07500500
C	3. 55169000	3. 33377300	1. 59581700
H	1. 57130500	2. 48741000	1. 58618800
C	4. 71418000	3. 57682700	0. 85650100
H	5. 68409700	3. 33617700	-1. 05503900
H	3. 47485700	3. 68775800	2. 62053400
H	5. 54492000	4. 11447600	1. 30518900
O	-1. 72602300	1. 52126900	0. 25176000
H	1. 63027400	1. 25480900	-1. 98985700
C	-1. 73614200	3. 79407000	-0. 56411200
O	-1. 09760700	4. 83440000	-0. 60070000
O	-3. 08067100	3. 90908000	-0. 52655900
C	-4. 00658400	2. 86168300	-0. 90709100
H	-4. 65902800	3. 33096400	-1. 65250900
H	-3. 47868200	2. 03578100	-1. 37673000
C	-4. 81204000	2. 40818100	0. 29773200
H	-5. 32963500	3. 25392300	0. 76406100
H	-5. 56657400	1. 67697300	-0. 01566400
H	-4. 15328500	1. 94169700	1. 03406000
C	-2. 94915700	-1. 55928300	1. 15346600

C	-1.77107800	-0.78706100	1.23138800
C	-1.20925200	-0.59359300	2.49999500
C	-1.73308100	-1.28950300	3.60622500
C	-2.84074300	-2.12227100	3.46072700
C	-3.48659400	-2.25755000	2.22983800
C	-2.81126100	-0.54471200	-0.89193800
C	-1.49529600	-0.25300000	-0.15072000
H	-1.28598400	-1.16969200	4.58520900
H	-3.22252700	-2.65175200	4.32904300
H	-4.38473000	-2.85643300	2.12703000
N	-3.52457400	-1.43563900	-0.12052100
O	-3.20144900	-0.05926100	-1.94489500
O	-0.18554300	0.30614400	2.62841000
C	0.11279400	0.80599100	3.93468700
H	0.58086100	0.04106800	4.56490300
H	0.81561500	1.62658000	3.78425000
H	-0.79235900	1.18165200	4.42292900
C	-0.30744800	-0.43225600	-0.91638700
C	-4.84545900	-1.91768900	-0.47463700
H	-5.60461300	-1.52082000	0.20977000
H	-5.05909400	-1.57515400	-1.48750900
H	-4.87714000	-3.01167500	-0.44544800
C	-0.36915200	-0.75553100	-2.33474900
O	0.33371400	-0.29964500	-3.24340400
C	0.98399100	0.06608500	-0.31967000
H	0.82258900	0.20366600	0.74492400
O	-1.23275500	-1.78512700	-2.59835100
C	-1.57071900	-1.98892800	-3.97526100
H	-0.67403400	-2.14206200	-4.58014700
H	-2.19967000	-2.88035700	-3.99611200
H	-2.12853900	-1.12952700	-4.35920900
C	3.29052300	-0.75335000	0.70576100
C	3.41492100	-2.89870100	-0.33510300
C	4.31368600	-1.86165900	0.38235400
H	5.12854000	-1.51906400	-0.26060900
H	4.75895600	-2.23866000	1.30544100
C	2.85813700	-1.07601000	-1.75478400
H	2.11455200	-0.87063400	-2.51782900
H	3.63461200	-0.31256500	-1.80375000
C	3.42826600	-2.51054400	-1.81368100
H	2.80334200	-3.16420900	-2.42766700
H	4.43843300	-2.52362300	-2.23118500
H	3.65108300	-3.94024600	-0.11961200
C	1.98352600	-2.47638400	0.10724900

N	2.19334200	-0.96178400	-0.38266200
O	1.81400300	-2.35101500	1.49390900
C	0.82255500	-3.28857400	-0.44711800
H	-0.10135600	-2.85426300	-0.06612200
H	0.77971000	-3.21054600	-1.53498000
C	0.91414900	-4.76617700	-0.03034000
H	1.77240800	-5.27345000	-0.48337800
H	0.99070200	-4.86602800	1.05666800
H	0.01032300	-5.29071300	-0.35572500
H	3.65983800	0.26599600	0.71021500
C	2.56357200	-1.20659500	1.96089300
H	3.26954300	-1.50924600	2.73876500
H	1.86269900	-0.48168700	2.37039300

### IRC-R-61

0 1

C	-2.12449400	1.71881300	-0.50279400
C	0.36057500	1.39078300	-0.29337400
C	-1.02729000	0.93351700	0.21402000
H	-1.14439700	1.15141900	1.27653200
C	0.79533100	2.67206800	0.39995200
C	1.01887600	3.83187200	-0.35793200
C	0.95142200	2.74978300	1.79420400
C	1.41359700	5.02579400	0.25027100
H	0.87572700	3.79762300	-1.43505100
C	1.34833200	3.94042100	2.40440100
H	0.76088900	1.87338700	2.40928400
C	1.58507300	5.08269700	1.63443700
H	1.58098800	5.91078000	-0.35774400
H	1.46750400	3.97725500	3.48398100
H	1.89177600	6.00944100	2.11133000
O	-1.92529900	2.39350800	-1.49492600
H	0.26618900	1.59861000	-1.36298900
C	-3.50322900	1.72425900	0.21593500
O	-3.55878600	1.34588400	1.37192500
O	-4.61084500	2.18835300	-0.36511600
C	-4.77497900	2.64124800	-1.74739300
H	-5.59798700	3.35585300	-1.67047100
H	-3.87590400	3.15666400	-2.07212200
C	-5.13841500	1.48192500	-2.65831500
H	-6.04873500	0.98413500	-2.30717400
H	-5.32610800	1.86551100	-3.66794900
H	-4.32866300	0.74918300	-2.70389600
C	-2.70740500	-1.91115800	1.29516900

C	-1.41392500	-1.37373300	1.36988100
C	-0.68685900	-1.58353400	2.54665100
C	-1.28727000	-2.25612500	3.62795700
C	-2.59162800	-2.73847800	3.52207300
C	-3.32639100	-2.58634800	2.34451000
C	-2.35782300	-1.01253100	-0.78835100
C	-1.08777200	-0.67223000	0.04286300
H	-0.74054300	-2.39798000	4.55244500
H	-3.03606700	-3.24970200	4.36950100
H	-4.33194900	-2.97725000	2.25453100
N	-3.24663100	-1.67538400	0.02237300
O	-2.59991700	-0.64043700	-1.93159300
O	0.60085100	-1.11208500	2.60086400
C	1.46657900	-1.62307800	3.61549500
H	1.40951500	-2.71495000	3.66657200
H	2.47267200	-1.32844500	3.32028000
H	1.23023000	-1.19915000	4.59816500
C	0.226666000	-0.98248600	-0.65536800
C	-4.56985700	-2.09013500	-0.39827300
H	-5.33987100	-1.59491100	0.20315500
H	-4.68731000	-1.80480900	-1.44500200
H	-4.68474900	-3.17544500	-0.30108000
C	0.29778600	-1.90186100	-1.69706700
O	1.13936200	-2.03569800	-2.62389600
C	1.20403700	0.07991600	-0.15849000
H	1.38980900	-0.10005100	0.90094100
O	-0.75882900	-2.83007500	-1.64298900
C	-1.09509900	-3.43909500	-2.88625800
H	-0.22612400	-3.92407300	-3.33985200
H	-1.86280000	-4.18502100	-2.65925900
H	-1.50333300	-2.70315400	-3.58887900
C	3.53037700	1.23126800	-0.05688200
C	4.74104600	-0.39683300	-1.32131400
C	4.86984600	1.05720200	-0.80701700
H	4.99304100	1.76511900	-1.63077100
H	5.70432800	1.20201500	-0.11759500
C	2.67615300	0.36963300	-2.25444200
H	1.82117800	-0.14096900	-2.68997700
H	2.64728800	1.44229900	-2.45366200
C	4.00672400	-0.30069400	-2.66304700
H	3.81234100	-1.28057900	-3.10522500
H	4.56281600	0.30162200	-3.38607200
H	5.67111200	-0.96479500	-1.33742400
C	3.65714200	-0.98845000	-0.37961800

N	2. 60967500	0. 17575900	-0. 74540300
O	3. 89662900	-0. 78327600	0. 99641200
C	3. 24917400	-2. 43598700	-0. 56831900
H	2. 42519600	-2. 63370900	0. 12391300
H	2. 85140400	-2. 58457700	-1. 57185700
C	4. 41313500	-3. 39962200	-0. 28877600
H	5. 22523200	-3. 28509000	-1. 01574700
H	4. 82869300	-3. 25499700	0. 71347100
H	4. 05312200	-4. 43089000	-0. 35967400
H	3. 08668100	2. 22050400	-0. 08216800
C	3. 73915300	0. 61481600	1. 31496600
H	4. 64587900	0. 99921800	1. 78912500
H	2. 90280800	0. 73606300	2. 00563900

### IRC-R-45

0 1			
C	-2. 15803200	1. 66187400	-0. 52270200
C	0. 32778800	1. 38744300	-0. 28525900
C	-1. 05478500	0. 90839200	0. 21205400
H	-1. 18822800	1. 11883200	1. 27334600
C	0. 75049500	2. 66872800	0. 41390000
C	0. 99836200	3. 82453100	-0. 34227000
C	0. 89050300	2. 74590400	1. 81001100
C	1. 40117500	5. 01399800	0. 26963100
H	0. 87084400	3. 79073500	-1. 42147300
C	1. 29448300	3. 93198800	2. 42399900
H	0. 68743200	1. 87103500	2. 42322700
C	1. 55607300	5. 07019000	1. 65570000
H	1. 58867200	5. 89565800	-0. 33732900
H	1. 40145600	3. 96845500	3. 50483200
H	1. 86965100	5. 99320700	2. 13526900
O	-1. 97498100	2. 27977700	-1. 55447700
H	0. 23470500	1. 59739200	-1. 35438600
C	-3. 52815100	1. 70024600	0. 21081700
O	-3. 57928200	1. 35216400	1. 37662300
O	-4. 63740300	2. 15827000	-0. 37342400
C	-4. 80638800	2. 59463500	-1. 76007600
H	-5. 64697800	3. 28936900	-1. 69160300
H	-3. 91881200	3. 12946400	-2. 08547700
C	-5. 13866800	1. 42209500	-2. 66596400
H	-6. 03972600	0. 90649300	-2. 31658200
H	-5. 32983800	1. 79563100	-3. 67869400
H	-4. 31382500	0. 70615200	-2. 70446600
C	-2. 70135500	-1. 89134000	1. 33993600

C	-1.38762800	-1.40063600	1.37817000
C	-0.64282500	-1.62870800	2.54153800
C	-1.24920200	-2.25278800	3.64805100
C	-2.57632500	-2.67566100	3.58175400
C	-3.32709200	-2.51691900	2.41530000
C	-2.35681400	-1.06450700	-0.77535000
C	-1.07596100	-0.71979200	0.03801900
H	-0.68744300	-2.40614600	4.56156000
H	-3.02528900	-3.15287600	4.44908000
H	-4.34991100	-2.87322900	2.35041400
N	-3.25164600	-1.67614600	0.06855600
O	-2.60637600	-0.73124300	-1.92838000
O	0.66834500	-1.23004500	2.56067300
C	1.53544300	-1.80249200	3.54184900
H	1.40567000	-2.88858200	3.59217800
H	2.54801200	-1.57439100	3.20886400
H	1.36390600	-1.36798600	4.53367600
C	0.23776300	-0.98748600	-0.66843200
C	-4.59672700	-2.05565700	-0.31671800
H	-5.33827600	-1.50294700	0.27091600
H	-4.71880400	-1.81565300	-1.37247900
H	-4.75256600	-3.12972700	-0.16782400
C	0.31835400	-1.83064800	-1.77357900
O	1.14975400	-1.86488000	-2.72048900
C	1.18866800	0.08837300	-0.15053900
H	1.35175800	-0.10089400	0.91009100
O	-0.68238000	-2.81575500	-1.75418900
C	-0.99931400	-3.38252400	-3.02239600
H	-0.10927700	-3.79435100	-3.50843200
H	-1.72014500	-4.18277900	-2.82414900
H	-1.45892100	-2.63647500	-3.68327400
C	3.50671000	1.22927900	0.07655000
C	4.75394300	-0.30248000	-1.26833800
C	4.86283700	1.11280000	-0.65341800
H	5.00101900	1.87685700	-1.42242700
H	5.68080700	1.21240600	0.06313200
C	2.70169800	0.50829700	-2.19293400
H	1.86197300	0.01423200	-2.67517300
H	2.66056300	1.59083700	-2.32353200
C	4.04918700	-0.11756100	-2.61665200
H	3.87878700	-1.06477900	-3.13350900
H	4.61496200	0.54089500	-3.28087100
H	5.68743200	-0.86385000	-1.30241000
C	3.65321100	-0.96264200	-0.39320900

N	2. 60673400	0. 21692000	-0. 70129100
O	3. 86238100	-0. 85056900	0. 99861700
C	3. 26234600	-2. 39629400	-0. 69232900
H	2. 42661800	-2. 64879500	-0. 03341100
H	2. 88593400	-2. 47491600	-1. 71151900
C	4. 42990500	-3. 36790100	-0. 45975900
H	5. 25133300	-3. 19955400	-1. 16556100
H	4. 83031300	-3. 28547900	0. 55598300
H	4. 07997300	-4. 39562700	-0. 60247100
H	3. 05771500	2. 21565600	0. 10803700
C	3. 68898700	0. 52216900	1. 40785600
H	4. 58292100	0. 87788100	1. 92682000
H	2. 83751300	0. 59123600	2. 08787900

### IRC-R-31

0 1

C	-2. 19530500	1. 60707100	-0. 54336700
C	0. 29048300	1. 38892700	-0. 27632100
C	-1. 08628900	0. 88836900	0. 21043600
H	-1. 23642000	1. 08872900	1. 27021500
C	0. 70440700	2. 67002600	0. 42677300
C	0. 98413400	3. 81818500	-0. 32981500
C	0. 82880600	2. 74907800	1. 82442000
C	1. 40287400	5. 00172100	0. 28303600
H	0. 87182600	3. 78274300	-1. 41076200
C	1. 24894700	3. 92895100	2. 43930100
H	0. 60476500	1. 87993400	2. 43843400
C	1. 54297100	5. 05917200	1. 67058600
H	1. 61454100	5. 87775900	-0. 32420000
H	1. 34396200	3. 96678400	3. 52124000
H	1. 86851900	5. 97746100	2. 15137500
O	-2. 03275600	2. 14719100	-1. 61514000
H	0. 19929200	1. 60011200	-1. 34524800
C	-3. 55840600	1. 67520500	0. 20151600
O	-3. 60912300	1. 35048600	1. 37425600
O	-4. 66787300	2. 12827200	-0. 38752600
C	-4. 83601300	2. 55251600	-1. 77726900
H	-5. 69256900	3. 22846300	-1. 71797000
H	-3. 95850100	3. 10640000	-2. 09901200
C	-5. 13531400	1. 37006500	-2. 68177700
H	-6. 02998600	0. 83864200	-2. 33964000
H	-5. 32300900	1. 73556100	-3. 69807300
H	-4. 29671200	0. 66978200	-2. 70917700
C	-2. 69525900	-1. 86971000	1. 38044700

C	-1.36480300	-1.42259700	1.38491800
C	-0.60485800	-1.66517500	2.53615500
C	-1.21516600	-2.24001600	3.66733400
C	-2.55988400	-2.60590400	3.63744700
C	-3.32496400	-2.44539700	2.48066900
C	-2.35378600	-1.11810400	-0.76538900
C	-1.06592600	-0.76221100	0.03222600
H	-0.64055800	-2.40059700	4.57150300
H	-3.01083200	-3.04499900	4.52355700
H	-4.36082000	-2.76611300	2.44007100
N	-3.25554200	-1.67760100	0.11048600
O	-2.60709500	-0.83425100	-1.93006400
O	0.72498400	-1.33507600	2.52106800
C	1.58438600	-1.95420100	3.48076200
H	1.38499600	-3.02931700	3.54674500
H	2.59814800	-1.79500700	3.11226800
H	1.47360600	-1.50068700	4.47318000
C	0.24932400	-0.98922200	-0.67629800
C	-4.61495300	-2.03293400	-0.24744700
H	-5.33426400	-1.44874000	0.33870100
H	-4.74413200	-1.81196700	-1.30767100
H	-4.79532100	-3.10074200	-0.07397600
C	0.34690500	-1.75790900	-1.83762600
O	1.15395100	-1.67715500	-2.79567800
C	1.17000700	0.10175000	-0.13916900
H	1.31213400	-0.09346600	0.92296700
O	-0.58363100	-2.80328000	-1.85587400
C	-0.85307900	-3.35744000	-3.14049500
H	0.06061300	-3.71618500	-3.62011100
H	-1.53642700	-4.19326200	-2.96897700
H	-1.33695700	-2.62374700	-3.79466900
C	3.48425200	1.21889500	0.19909200
C	4.75628400	-0.22013100	-1.22241000
C	4.85224500	1.15173800	-0.51459400
H	5.00220700	1.96488300	-1.22971600
H	5.65835300	1.20467700	0.22021900
C	2.71651100	0.64515300	-2.12430200
H	1.88573600	0.17924700	-2.64877400
H	2.67225900	1.73387300	-2.18491200
C	4.07231800	0.05210400	-2.56697200
H	3.91452000	-0.85959300	-3.14865200
H	4.64654100	0.75401300	-3.17750500
H	5.69149400	-0.77684000	-1.27891900
C	3.64429400	-0.93843700	-0.40898300

N	2. 59862400	0. 25749100	-0. 65668900
O	3. 83147600	-0. 91546000	0. 98993600
C	3. 26878200	-2. 35276500	-0. 80648200
H	2. 41176500	-2. 64623700	-0. 19398000
H	2. 93119100	-2. 37179700	-1. 84178800
C	4. 43011600	-3. 33552000	-0. 59063900
H	5. 28410000	-3. 11374100	-1. 24054100
H	4. 78044000	-3. 32736600	0. 44668300
H	4. 09328100	-4. 35058900	-0. 82530000
H	3. 03261100	2. 20065900	0. 28567500
C	3. 64659300	0. 42755200	1. 48427800
H	4. 53116900	0. 75119200	2. 03940500
H	2. 78360800	0. 45219200	2. 15267500

### IRC-R-16

0 1			
C	-2. 24341000	1. 52903600	-0. 55752900
C	0. 24442000	1. 40016500	-0. 26669600
C	-1. 12240800	0. 87198600	0. 21585900
H	-1. 28570100	1. 05612000	1. 27489300
C	0. 65850400	2. 67836300	0. 44077100
C	0. 95868100	3. 82377200	-0. 31247500
C	0. 79155400	2. 75013400	1. 83817600
C	1. 40754600	4. 99524700	0. 30256900
H	0. 84187000	3. 79512800	-1. 39324500
C	1. 24295900	3. 91738300	2. 45520100
H	0. 55262000	1. 88379400	2. 45055000
C	1. 55927000	5. 04359200	1. 68925700
H	1. 63709800	5. 86781700	-0. 30315600
H	1. 34626800	3. 94817000	3. 53657300
H	1. 91216300	5. 95111100	2. 17109800
O	-2. 10392500	1. 98466000	-1. 68152300
H	0. 14750600	1. 61340100	-1. 33466200
C	-3. 59578800	1. 63978200	0. 19748300
O	-3. 65130600	1. 33871000	1. 37653400
O	-4. 70254200	2. 09622400	-0. 39803800
C	-4. 86333500	2. 52494600	-1. 78637000
H	-5. 72858200	3. 19032300	-1. 73136200
H	-3. 99007300	3. 09166300	-2. 09821500
C	-5. 14120600	1. 34684700	-2. 70329600
H	-6. 03358800	0. 80322800	-2. 37482100
H	-5. 32232800	1. 71803200	-3. 71874100
H	-4. 29478300	0. 65607900	-2. 72952300
C	-2. 68327900	-1. 84122100	1. 42009400

C	-1.33540700	-1.44687600	1.39091100
C	-0.56037600	-1.70942100	2.52865100
C	-1.17310900	-2.23611300	3.68237000
C	-2.53443700	-2.53539100	3.68885500
C	-3.31579700	-2.36375100	2.54473700
C	-2.33923100	-1.18621400	-0.75815800
C	-1.04882200	-0.81068600	0.02613000
H	-0.58697600	-2.41143200	4.57621200
H	-2.98582500	-2.93123400	4.59426300
H	-4.36561700	-2.63520300	2.53260700
N	-3.25383100	-1.66986600	0.15253800
O	-2.58693100	-0.98146300	-1.93911000
O	0.78424300	-1.45307800	2.47565100
C	1.62658400	-2.06818100	3.45259900
H	1.39525500	-3.13421700	3.55123700
H	2.64280700	-1.95128000	3.07679200
H	1.53297700	-1.58248600	4.43100800
C	0.26292900	-0.98042700	-0.68580900
C	-4.62604100	-1.99830800	-0.17897700
H	-5.31962800	-1.36260500	0.38211000
H	-4.75791600	-1.82733100	-1.24763800
H	-4.83949000	-3.04817200	0.04976300
C	0.37045000	-1.66302900	-1.90694000
O	1.12556300	-1.44531500	-2.88551700
C	1.14701400	0.12759800	-0.13068300
H	1.27036900	-0.07121400	0.93334400
O	-0.44114400	-2.79696800	-1.94728500
C	-0.65891600	-3.34518000	-3.24467200
H	0.28484500	-3.59179600	-3.73820100
H	-1.24708500	-4.25331100	-3.09093900
H	-1.22118500	-2.65058300	-3.87906000
C	3.46611900	1.20537300	0.30398400
C	4.74363300	-0.15925500	-1.18753900
C	4.84214300	1.16795400	-0.39832400
H	5.00762000	2.02123500	-1.06088200
H	5.63968200	1.16879500	0.34761200
C	2.72606900	0.78307300	-2.05602600
H	1.89226500	0.37073300	-2.61792300
H	2.70321000	1.87386900	-2.04341400
C	4.07648800	0.19667400	-2.52085400
H	3.91273000	-0.67782700	-3.15513700
H	4.66527600	0.92501000	-3.08490200
H	5.67514900	-0.71967300	-1.26576100
C	3.61825400	-0.91427100	-0.42825900

N	2. 58389200	0. 30394900	-0. 61738300
O	3. 79182000	-0. 97315400	0. 97073600
C	3. 23883000	-2. 30215800	-0. 90936700
H	2. 35557800	-2. 61320600	-0. 34666100
H	2. 94584100	-2. 26599500	-1. 95785300
C	4. 37747700	-3. 31219000	-0. 69942200
H	5. 26198500	-3. 06831500	-1. 29860300
H	4. 68088700	-3. 36676700	0. 35052100
H	4. 03737700	-4. 30676000	-1. 00551000
H	3. 01978700	2. 18293700	0. 44705400
C	3. 60849300	0. 33874000	1. 54156100
H	4. 48800400	0. 62199200	2. 12593100
H	2. 73783500	0. 32649400	2. 20012000

### IRC-1

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C	-2. 27168700	1. 58269700	-0. 55299700
C	0. 21179700	1. 43569100	-0. 26693300
C	-1. 17043300	1. 10563700	0. 23841400
H	-1. 32715500	1. 12294500	1. 30887000
C	0. 69547000	2. 70152900	0. 43025200
C	0. 98083800	3. 85081100	-0. 32190400
C	0. 83595300	2. 77131100	1. 82786900
C	1. 41243100	5. 02779000	0. 29658600
H	0. 85591900	3. 82575100	-1. 40172100
C	1. 27252200	3. 94236700	2. 44628600
H	0. 60064800	1. 90398400	2. 43995700
C	1. 56540300	5. 07699400	1. 68265700
H	1. 62575200	5. 90533100	-0. 30799500
H	1. 37739900	3. 97178000	3. 52757700
H	1. 90151400	5. 99014800	2. 16576200
O	-2. 18498200	1. 91387200	-1. 74810900
H	0. 12009600	1. 64097900	-1. 33739700
C	-3. 61962900	1. 64119300	0. 20390900
O	-3. 69270300	1. 32312000	1. 37976700
O	-4. 74694900	2. 06738000	-0. 39089400
C	-4. 90886100	2. 50151600	-1. 77207900
H	-5. 78715300	3. 15183500	-1. 72250500
H	-4. 04220500	3. 08012900	-2. 08079000
C	-5. 15824800	1. 32143600	-2. 69499300
H	-6. 03789700	0. 75397300	-2. 37132700
H	-5. 34388100	1. 68737000	-3. 71187300
H	-4. 28988900	0. 65843500	-2. 71441500
C	-2. 66477100	-1. 84219900	1. 45105200

C	-1.29351500	-1.50238000	1.39856500
C	-0.51564900	-1.75170300	2.54176300
C	-1.13196400	-2.22442100	3.71323900
C	-2.50289700	-2.48648200	3.73543300
C	-3.29401500	-2.31660600	2.59781700
C	-2.28886800	-1.31115100	-0.74748500
C	-0.98559700	-1.07414800	0.01419600
H	-0.54526500	-2.39252200	4.60797000
H	-2.95568500	-2.84823200	4.65433600
H	-4.35112900	-2.55821700	2.60583700
N	-3.23432700	-1.69656700	0.18787500
O	-2.52744700	-1.12453800	-1.93460400
O	0.83145900	-1.53495800	2.45335800
C	1.67400300	-2.08832600	3.46667100
H	1.44118000	-3.14575000	3.63186300
H	2.68977500	-1.99541700	3.08318000
H	1.57962100	-1.54091200	4.41166800
C	0.26397800	-1.00418500	-0.68118100
C	-4.62640100	-1.94455800	-0.12763100
H	-5.27528000	-1.25023400	0.41703400
H	-4.75139800	-1.79327100	-1.20017600
H	-4.90612800	-2.97259700	0.12868100
C	0.35357400	-1.62289100	-1.97555100
O	1.01013400	-1.28799400	-2.97226300
C	1.10533000	0.12546000	-0.11224500
H	1.20737500	-0.06361900	0.95479300
O	-0.32444000	-2.82103000	-1.98658300
C	-0.56529900	-3.38307600	-3.27846800
H	0.37003000	-3.54864300	-3.81973300
H	-1.06783100	-4.33520900	-3.09732000
H	-1.21395100	-2.72617100	-3.86639100
C	3.44679300	1.20217200	0.32702200
C	4.71083200	-0.13856600	-1.20003300
C	4.81554000	1.17563600	-0.39113000
H	4.97412000	2.03991100	-1.04064200
H	5.61989500	1.16457300	0.34723800
C	2.69200000	0.82898600	-2.02743000
H	1.84572000	0.46296500	-2.59935500
H	2.69117300	1.91881400	-1.98081200
C	4.02872600	0.23603100	-2.51987900
H	3.85185500	-0.62856300	-3.16422200
H	4.61316700	0.96799300	-3.08352000
H	5.64178000	-0.69695700	-1.29613400
C	3.59587700	-0.90489500	-0.43784100

N	2. 55320500	0. 31197800	-0. 59759800
O	3. 78589800	-0. 98325500	0. 95677100
C	3. 21807400	-2. 28818700	-0. 93579900
H	2. 33306600	-2. 61165800	-0. 38298400
H	2. 94314600	-2. 24428900	-1. 98957200
C	4. 36033700	-3. 29634400	-0. 72742000
H	5. 24908300	-3. 03798100	-1. 31329800
H	4. 65021100	-3. 36074600	0. 32522100
H	4. 02894400	-4. 28828800	-1. 05026300
H	3. 00353600	2. 17737900	0. 48744100
C	3. 59769300	0. 31922500	1. 54905500
H	4. 47647900	0. 59653700	2. 13677700
H	2. 72743300	0. 29163800	2. 20804800

#### IRC-F-4

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C	-2. 27582800	1. 60341500	-0. 55324000
C	0. 20645300	1. 44605000	-0. 26736300
C	-1. 17885800	1. 18082400	0. 24567200
H	-1. 33407600	1. 15453400	1. 31517100
C	0. 71010500	2. 70660100	0. 42720000
C	0. 99014300	3. 85665100	-0. 32512200
C	0. 84995400	2. 77633000	1. 82510200
C	1. 41560800	5. 03548000	0. 29411000
H	0. 86385600	3. 83156300	-1. 40474600
C	1. 28081000	3. 94892100	2. 44360700
H	0. 61531200	1. 90883200	2. 43709500
C	1. 56791500	5. 08532000	1. 68008400
H	1. 62477400	5. 91422200	-0. 31023400
H	1. 38497500	3. 97884000	3. 52497300
H	1. 89908400	6. 00018400	2. 16336400
O	-2. 19944700	1. 91115600	-1. 76220100
H	0. 11703100	1. 64845600	-1. 33863000
C	-3. 62219400	1. 64462100	0. 20473500
O	-3. 69925600	1. 32110000	1. 37954800
O	-4. 75552300	2. 06141900	-0. 38975700
C	-4. 91633600	2. 49823900	-1. 76893300
H	-5. 79592400	3. 14748200	-1. 72082600
H	-4. 04916400	3. 07655100	-2. 07650100
C	-5. 16184400	1. 31841600	-2. 69341700
H	-6. 03972700	0. 74734300	-2. 37091400
H	-5. 34774700	1. 68360200	-3. 71064700
H	-4. 28958500	0. 66041400	-2. 71109800
C	-2. 66263100	-1. 84469500	1. 45703500

C	-1.28584400	-1.51742100	1.40016900
C	-0.50822500	-1.75928200	2.54654400
C	-1.12529500	-2.21949900	3.72138700
C	-2.49790400	-2.47604800	3.74518800
C	-3.29081300	-2.30810300	2.60839400
C	-2.27862200	-1.34284200	-0.74444000
C	-0.96960900	-1.15119600	0.01267300
H	-0.53945300	-2.38322400	4.61745500
H	-2.95125300	-2.83034800	4.66670100
H	-4.34911400	-2.54421800	2.62050100
N	-3.23106100	-1.70538500	0.19495300
O	-2.51578600	-1.15064500	-1.93147700
O	0.83831900	-1.54770000	2.45082200
C	1.68258500	-2.08922900	3.46957000
H	1.44989300	-3.14468700	3.64665400
H	2.69777600	-2.00007200	3.08384400
H	1.58835300	-1.53082000	4.40800700
C	0.25977300	-1.00947300	-0.67930900
C	-4.62667900	-1.93531400	-0.11864500
H	-5.26572800	-1.23271200	0.42681600
H	-4.75091400	-1.78122300	-1.19088200
H	-4.91933300	-2.96002000	0.13707700
C	0.34799500	-1.61974200	-1.98896100
O	0.98493800	-1.26371700	-2.98655700
C	1.09445800	0.12380300	-0.10745800
H	1.19386000	-0.06419800	0.95965900
O	-0.30455000	-2.82654200	-1.99303300
C	-0.55341800	-3.39162200	-3.28333300
H	0.37855400	-3.55060200	-3.83213500
H	-1.04778600	-4.34643900	-3.09604900
H	-1.21153800	-2.73702300	-3.86249000
C	3.44352500	1.20106300	0.32804800
C	4.70413200	-0.13800800	-1.20369100
C	4.81057000	1.17500800	-0.39357200
H	4.96793600	2.04009400	-1.04220600
H	5.61637400	1.16279300	0.34316300
C	2.68481400	0.83303600	-2.02450500
H	1.83605200	0.47632000	-2.59784000
H	2.68857100	1.92255400	-1.97334400
C	4.01897600	0.23790100	-2.52137300
H	3.83989900	-0.62590800	-3.16623100
H	4.60241500	0.96965800	-3.08622500
H	5.63471300	-0.69652600	-1.30249200
C	3.59136500	-0.90502300	-0.43928900

N	2. 54619500	0. 31124800	-0. 59525900
O	3. 78462100	-0. 98469800	0. 95435100
C	3. 21346600	-2. 28811300	-0. 93797700
H	2. 32950900	-2. 61402300	-0. 38460200
H	2. 94013400	-2. 24459100	-1. 99231600
C	4. 35658900	-3. 29586400	-0. 73036700
H	5. 24460300	-3. 03632600	-1. 31660200
H	4. 64649400	-3. 35986700	0. 32218200
H	4. 02562500	-4. 28786600	-1. 05328600
H	3. 00150600	2. 17625600	0. 49010800
C	3. 59642800	0. 31723100	1. 54848800
H	4. 47553400	0. 59399200	2. 13583400
H	2. 72666300	0. 28837600	2. 20816300

### IRC-F-10

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C	-2. 28937100	1. 62498600	-0. 55431700
C	0. 19461000	1. 46668500	-0. 26520400
C	-1. 19338100	1. 25553700	0. 25247900
H	-1. 34854800	1. 19855600	1. 32044700
C	0. 72715400	2. 71861800	0. 42720700
C	1. 00804700	3. 86924100	-0. 32422100
C	0. 87350000	2. 78648100	1. 82489100
C	1. 43452400	5. 04753700	0. 29580500
H	0. 87772900	3. 84665800	-1. 40343700
C	1. 30685300	3. 95785500	2. 44368700
H	0. 63785600	1. 91925400	2. 43693300
C	1. 59000800	5. 09623500	1. 68136300
H	1. 64158100	5. 92706800	-0. 30817600
H	1. 41443700	3. 98587200	3. 52480200
H	1. 92103700	6. 01089200	2. 16511200
O	-2. 22567300	1. 91144300	-1. 77529900
H	0. 10856000	1. 66759900	-1. 33708000
C	-3. 63418900	1. 64651800	0. 20636600
O	-3. 71353500	1. 31532700	1. 37953700
O	-4. 77563800	2. 04992900	-0. 38655100
C	-4. 93785300	2. 49228000	-1. 76237600
H	-5. 82275000	3. 13480300	-1. 71425400
H	-4. 07377200	3. 07675900	-2. 06692500
C	-5. 17185100	1. 31374200	-2. 69163700
H	-6. 04567300	0. 73389000	-2. 37348200
H	-5. 35738800	1. 67926100	-3. 70890000
H	-4. 29258900	0. 66493000	-2. 70721900
C	-2. 65005400	-1. 85210000	1. 47376300

C	-1.26761500	-1.54367500	1.40614000
C	-0.48688000	-1.77798600	2.55310100
C	-1.10435400	-2.20925300	3.73811500
C	-2.48080900	-2.44570100	3.77156500
C	-3.27777600	-2.28619200	2.63601400
C	-2.26282100	-1.40559700	-0.73665000
C	-0.94895500	-1.23309600	0.01388000
H	-0.51729100	-2.36670900	4.63445300
H	-2.93457100	-2.77811900	4.70097800
H	-4.33886000	-2.50861200	2.65760100
N	-3.21982700	-1.73073600	0.21154600
O	-2.49848200	-1.22766300	-1.92664000
O	0.86073700	-1.58815400	2.44171900
C	1.70496400	-2.10610400	3.47316900
H	1.46658400	-3.15477400	3.68004000
H	2.71938900	-2.03299500	3.08225300
H	1.61575100	-1.52077800	4.39545500
C	0.25271800	-1.00988500	-0.68119600
C	-4.62388900	-1.91997100	-0.09239500
H	-5.23638900	-1.19584800	0.45496400
H	-4.74985000	-1.76445300	-1.16416500
H	-4.94640500	-2.93459300	0.16759400
C	0.33216300	-1.59038800	-2.01823900
O	0.90490000	-1.17270000	-3.02618400
C	1.07507000	0.12897300	-0.10309500
H	1.16899700	-0.06128200	0.96392100
O	-0.24204400	-2.83097900	-2.01783300
C	-0.49723100	-3.39839100	-3.30748500
H	0.42818500	-3.51185200	-3.87831200
H	-0.94419400	-4.37498500	-3.11470000
H	-1.19681800	-2.76738200	-3.86328000
C	3.43688500	1.19329200	0.33850000
C	4.68556000	-0.13832900	-1.21039800
C	4.80079900	1.16690200	-0.38919400
H	4.95929400	2.03705500	-1.03068600
H	5.60942700	1.14456400	0.34417900
C	2.67017700	0.85250600	-2.01380400
H	1.81486000	0.51651200	-2.58953500
H	2.68600400	1.94107100	-1.94922700
C	3.99687100	0.25122100	-2.52203800
H	3.80993300	-0.60651300	-3.17295100
H	4.58204800	0.98326000	-3.08465700
H	5.61321000	-0.70016900	-1.31735600
C	3.57294000	-0.90637700	-0.44744400

N	2. 53100400	0. 31562900	-0. 58925300
O	3. 77182300	-0. 99865200	0. 94411300
C	3. 18824600	-2. 28418000	-0. 95590700
H	2. 30496900	-2. 61309800	-0. 40346000
H	2. 91613400	-2. 23297900	-2. 01074100
C	4. 32923800	-3. 29673500	-0. 75681100
H	5. 21707400	-3. 03508200	-1. 34213900
H	4. 61936600	-3. 36756100	0. 29510700
H	3. 99540200	-4. 28570600	-1. 08573500
H	3. 00141200	2. 16944000	0. 51009000
C	3. 58873500	0. 29865900	1. 55036000
H	4. 46942000	0. 56697000	2. 13914400
H	2. 71929400	0. 26656800	2. 21041400

### IRC-F-16

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C	-2. 30274800	1. 62564400	-0. 55382300
C	0. 18196200	1. 48007900	-0. 25918000
C	-1. 20623800	1. 28241600	0. 25977600
H	-1. 36325600	1. 22166500	1. 32652000
C	0. 73073500	2. 72578100	0. 43232100
C	1. 02116400	3. 87424200	-0. 31912700
C	0. 88148400	2. 79210100	1. 82970800
C	1. 45980800	5. 04847300	0. 30029300
H	0. 88865400	3. 85356100	-1. 39814800
C	1. 32756200	3. 95910900	2. 44786700
H	0. 63915600	1. 92697500	2. 44213400
C	1. 61936500	5. 09530900	1. 68543700
H	1. 67447800	5. 92594000	-0. 30411400
H	1. 43868600	3. 98556100	3. 52868200
H	1. 96135700	6. 00630700	2. 16853500
O	-2. 24237800	1. 90023000	-1. 77964100
H	0. 09595700	1. 68161200	-1. 33093800
C	-3. 64874500	1. 63710300	0. 20513100
O	-3. 73182200	1. 29751600	1. 37590700
O	-4. 79228800	2. 03655700	-0. 38830100
C	-4. 95318300	2. 48702400	-1. 76106800
H	-5. 83697100	3. 13110000	-1. 71074700
H	-4. 08739900	3. 07050600	-2. 06282900
C	-5. 18866900	1. 31361700	-2. 69646900
H	-6. 05929700	0. 72902700	-2. 37826200
H	-5. 37942000	1. 68429900	-3. 71096700
H	-4. 30697600	0. 66877600	-2. 71960500
C	-2. 63464000	-1. 85560300	1. 49278700

C	-1.25059000	-1.55748600	1.41351200
C	-0.46446300	-1.78636200	2.55794100
C	-1.07891700	-2.19343100	3.75318700
C	-2.45770200	-2.41323700	3.79884400
C	-3.25987900	-2.26390600	2.66538500
C	-2.25481100	-1.45020400	-0.72623800
C	-0.93820600	-1.26738600	0.01696600
H	-0.48791600	-2.34306900	4.64834800
H	-2.90944900	-2.72391300	4.73683000
H	-4.32316100	-2.47427800	2.69735600
N	-3.20905400	-1.75311800	0.23078800
O	-2.49324100	-1.29229800	-1.91859900
O	0.88443500	-1.61610300	2.43378400
C	1.72912000	-2.13074400	3.46692700
H	1.47480600	-3.17132500	3.69398100
H	2.74111300	-2.08160900	3.06628500
H	1.65784300	-1.52819000	4.37949300
C	0.24551000	-1.00419100	-0.68367400
C	-4.61871300	-1.92047800	-0.06074700
H	-5.21108200	-1.16584200	0.46772900
H	-4.74705600	-1.79487100	-1.13615400
H	-4.96192500	-2.91942700	0.23184500
C	0.31477100	-1.54981600	-2.04268300
O	0.82512600	-1.07253300	-3.05581600
C	1.06056400	0.13611900	-0.09964000
H	1.15124700	-0.05835300	0.96679900
O	-0.18385300	-2.82014500	-2.05178100
C	-0.42142000	-3.38533300	-3.34659700
H	0.50193500	-3.43384300	-3.92948200
H	-0.80447300	-4.38967800	-3.16220300
H	-1.16344500	-2.78986100	-3.88484300
C	3.43147200	1.18186000	0.35609400
C	4.66981700	-0.13784800	-1.21220900
C	4.79433600	1.15578500	-0.37385000
H	4.95776500	2.03339000	-1.00375600
H	5.60354100	1.11804400	0.35827500
C	2.66153700	0.87771000	-1.99983900
H	1.80111700	0.56138500	-2.57915000
H	2.68797600	1.96495100	-1.91920200
C	3.98252800	0.27271100	-2.51796500
H	3.78915900	-0.57523700	-3.17985600
H	4.57197300	1.00766900	-3.07218400
H	5.59342800	-0.70480500	-1.32672600
C	3.55299800	-0.90773600	-0.45784900

N	2. 51887200	0. 32256400	-0. 58226700
O	3. 75392000	-1. 01992900	0. 93158400
C	3. 15635400	-2. 27516000	-0. 98480100
H	2. 27169400	-2. 60579700	-0. 43606400
H	2. 88391000	-2. 20672100	-2. 03905000
C	4. 28881500	-3. 30043700	-0. 80289100
H	5. 17767800	-3. 03855700	-1. 38636900
H	4. 57936600	-3. 38892300	0. 24745800
H	3. 94474600	-4. 28129000	-1. 14547400
H	3. 00297700	2. 15854200	0. 54145300
C	3. 57816200	0. 27017600	1. 55560400
H	4. 46032100	0. 52476500	2. 14817000
H	2. 70817000	0. 23363000	2. 21469900

### IRC-F-20

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C	-2. 31039900	1. 62177200	-0. 55088700
C	0. 17361400	1. 48769600	-0. 25303300
C	-1. 21495300	1. 30216500	0. 26700400
H	-1. 37183700	1. 23245300	1. 33411500
C	0. 73270200	2. 72859800	0. 43907900
C	1. 03061100	3. 87571700	-0. 31147500
C	0. 88466600	2. 79271900	1. 83642400
C	1. 47783900	5. 04633500	0. 30868200
H	0. 89670100	3. 85711200	-1. 39037300
C	1. 33937800	3. 95600100	2. 45530600
H	0. 63690700	1. 92853400	2. 44808800
C	1. 63875100	5. 09085200	1. 69372900
H	1. 69718500	5. 92306200	-0. 29506600
H	1. 45099100	3. 98063100	3. 53612300
H	1. 98636400	5. 99925200	2. 17762300
O	-2. 25275900	1. 88416700	-1. 78173900
H	0. 08768000	1. 69048100	-1. 32454000
C	-3. 65771600	1. 62532200	0. 20494900
O	-3. 74577900	1. 27628000	1. 37283000
O	-4. 80144300	2. 02595100	-0. 38895400
C	-4. 95955100	2. 49001800	-1. 75697100
H	-5. 83993000	3. 13849100	-1. 70129800
H	-4. 09032000	3. 07101600	-2. 05385100
C	-5. 20142800	1. 32602400	-2. 70251600
H	-6. 07060800	0. 73890500	-2. 38496200
H	-5. 39703300	1. 70607800	-3. 71256800
H	-4. 31969500	0. 68193500	-2. 73584600
C	-2. 62471700	-1. 85702900	1. 50531500

C	-1.23969600	-1.56396600	1.41826800
C	-0.44956800	-1.78986200	2.56070500
C	-1.06096900	-2.18373900	3.76175300
C	-2.44076500	-2.39503600	3.81529600
C	-3.24688800	-2.25151300	2.68389200
C	-2.25071000	-1.47589400	-0.71861100
C	-0.93115900	-1.29245700	0.01780100
H	-0.46659300	-2.33155100	4.65485400
H	-2.89003800	-2.69699000	4.75708700
H	-4.31054900	-2.45853500	2.72098100
N	-3.20269100	-1.76678400	0.24430400
O	-2.49276200	-1.32890300	-1.91176100
O	0.89990300	-1.63126600	2.42827800
C	1.74524600	-2.15101000	3.45858300
H	1.48146600	-3.18834500	3.69011900
H	2.75547000	-2.11271000	3.05224200
H	1.68455600	-1.54474700	4.36965000
C	0.24026900	-0.99931700	-0.68517500
C	-4.61462400	-1.92550400	-0.04055600
H	-5.19771600	-1.15922600	0.48026400
H	-4.74585500	-1.81227000	-1.11687100
H	-4.96535000	-2.91745600	0.26498400
C	0.30199200	-1.52076700	-2.05892600
O	0.77271500	-1.00448000	-3.07220500
C	1.05219300	0.13998300	-0.09655800
H	1.14228800	-0.05776000	0.96902100
O	-0.14983000	-2.80635000	-2.07764500
C	-0.38088300	-3.36503600	-3.37712000
H	0.53494200	-3.36257700	-3.97391700
H	-0.71575700	-4.38752500	-3.19959000
H	-1.15834400	-2.79589500	-3.89468100
C	3.42852500	1.17272700	0.36838300
C	4.66098200	-0.13633600	-1.21366000
C	4.79054800	1.14890800	-0.36309900
H	4.95586500	2.03170200	-0.98531900
H	5.60060100	1.10231000	0.36747300
C	2.65685800	0.89467400	-1.99060900
H	1.79405800	0.58977000	-2.57243300
H	2.68827300	1.98079600	-1.89984300
C	3.97507600	0.28912700	-2.51521600
H	3.77874500	-0.55192000	-3.18512700
H	4.56701800	1.02671000	-3.06322700
H	5.58246300	-0.70565600	-1.33355200
C	3.54105400	-0.90890900	-0.46677000

N	2. 51187700	0. 32672500	-0. 57809400
O	3. 74194300	-1. 03661800	0. 92099000
C	3. 13707400	-2. 26857300	-1. 00827700
H	2. 25315000	-2. 60234300	-0. 46066200
H	2. 86303200	-2. 18753000	-2. 06136100
C	4. 26558600	-3. 30072500	-0. 84121800
H	5. 15310900	-3. 03755500	-1. 42622800
H	4. 56072200	-3. 39909000	0. 20701700
H	3. 91595700	-4. 27716600	-1. 19021700
H	3. 00401000	2. 14921500	0. 56385300
C	3. 57248100	0. 24811200	1. 55826700
H	4. 45642800	0. 49332800	2. 15206600
H	2. 70294700	0. 20878900	2. 21759800

### IRC-F-26

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C	-2. 32054700	1. 61096800	-0. 54595900
C	0. 16326300	1. 49722800	-0. 24187300
C	-1. 22540700	1. 31916000	0. 27868300
H	-1. 38373800	1. 25120400	1. 34585300
C	0. 73434000	2. 73124600	0. 45256600
C	1. 04531800	3. 87650200	-0. 29567400
C	0. 88606300	2. 79159200	1. 85011300
C	1. 50501700	5. 04112400	0. 32668300
H	0. 91290700	3. 86126600	-1. 37483800
C	1. 35294100	3. 94886900	2. 47130400
H	0. 62918000	1. 92890900	2. 46010800
C	1. 66551500	5. 08162400	1. 71188900
H	1. 73575400	5. 91598200	-0. 27563300
H	1. 46454500	3. 97044500	3. 55219500
H	2. 02398600	5. 98502300	2. 19735600
O	-2. 26504600	1. 85467000	-1. 78231200
H	0. 07705400	1. 70284700	-1. 31270400
C	-3. 66983400	1. 60779000	0. 20602300
O	-3. 76349400	1. 24747800	1. 37020300
O	-4. 81295000	2. 00957900	-0. 38975900
C	-4. 96084200	2. 50247700	-1. 74843600
H	-5. 83235500	3. 16228800	-1. 68416100
H	-4. 08245200	3. 07661400	-2. 03185600
C	-5. 21484900	1. 36012000	-2. 71715300
H	-6. 09954900	0. 78450900	-2. 42164100
H	-5. 38930600	1. 76192400	-3. 72290000
H	-4. 34452400	0. 70067500	-2. 75106500
C	-2. 61162600	-1. 86487600	1. 52000900

C	-1.22651800	-1.57509100	1.42339300
C	-0.43092700	-1.79632700	2.56286100
C	-1.03770100	-2.17246800	3.77188800
C	-2.41820600	-2.37551200	3.83561300
C	-3.22926200	-2.24366200	2.70611600
C	-2.24784900	-1.50509800	-0.70913900
C	-0.92534900	-1.31471100	0.01916600
H	-0.43877000	-2.31100100	4.66357000
H	-2.86415400	-2.66092900	4.78435500
H	-4.29364300	-2.44561300	2.75159800
N	-3.19501300	-1.78687400	0.26056600
O	-2.49531500	-1.36780800	-1.90244200
O	0.91914700	-1.65135100	2.42095900
C	1.76580300	-2.18724500	3.44240500
H	1.48192200	-3.21738300	3.67958200
H	2.77132200	-2.17228000	3.02419200
H	1.72997600	-1.57830000	4.35239100
C	0.23176600	-0.99135100	-0.68776400
C	-4.60936500	-1.94076200	-0.01535700
H	-5.18591200	-1.17966100	0.52083100
H	-4.74855100	-1.81282200	-1.08929800
H	-4.95996400	-2.93660100	0.27967300
C	0.28327700	-1.47976500	-2.07796300
O	0.70580800	-0.91341200	-3.08604800
C	1.04134900	0.14459900	-0.09172700
H	1.13031100	-0.05854300	0.97261600
O	-0.11454800	-2.77696700	-2.11946000
C	-0.32460600	-3.32647000	-3.42717100
H	0.56178900	-3.19989000	-4.05139700
H	-0.53062600	-4.38586500	-3.27098800
H	-1.18130000	-2.83798200	-3.89967200
C	3.42417800	1.15754300	0.38858700
C	4.64954900	-0.13202300	-1.21519900
C	4.78532500	1.13925700	-0.34447200
H	4.95389300	2.03113900	-0.95273100
H	5.59570300	1.07744900	0.38465200
C	2.65056700	0.91978600	-1.97521000
H	1.78476700	0.63064700	-2.56058000
H	2.68751800	2.00411300	-1.86759300
C	3.96598100	0.31686300	-2.50987700
H	3.76692400	-0.51221500	-3.19380700
H	4.56085100	1.06105300	-3.04564700
H	5.56813500	-0.70416500	-1.34348600
C	3.52578900	-0.91067300	-0.48060600

N	2. 50279500	0. 33177200	-0. 57106200
O	3. 72728600	-1. 06285100	0. 90404000
C	3. 11212800	-2. 25710400	-1. 04696700
H	2. 22697800	-2. 59656000	-0. 50526800
H	2. 83718600	-2. 15337500	-2. 09805600
C	4. 23296100	-3. 30083300	-0. 90422700
H	5. 12486700	-3. 02762700	-1. 47765900
H	4. 52202300	-3. 43097800	0. 14199100
H	3. 87786800	-4. 26409500	-1. 28273000
H	3. 00434400	2. 13247100	0. 60171100
C	3. 56468900	0. 21225900	1. 56274200
H	4. 45044100	0. 44258300	2. 15972400
H	2. 69543400	0. 16554000	2. 22174600

### IRC-F-30

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C	-2. 32355500	1. 60386100	-0. 53976100
C	0. 16065700	1. 50405300	-0. 23092200
C	-1. 22806900	1. 33037500	0. 28993500
H	-1. 38721000	1. 26726400	1. 35727700
C	0. 74147600	2. 73109100	0. 46741600
C	1. 06140200	3. 87665600	-0. 27660900
C	0. 89471700	2. 78499900	1. 86503600
C	1. 53113400	5. 03508000	0. 34979600
H	0. 92744200	3. 86684800	-1. 35566300
C	1. 37142800	3. 93605100	2. 49035700
H	0. 63161400	1. 92191500	2. 47181800
C	1. 69298700	5. 06901100	1. 73504100
H	1. 76767200	5. 91052000	-0. 24927300
H	1. 48362200	3. 95254300	3. 57128800
H	2. 05863200	5. 96766200	2. 22378300
O	-2. 26944900	1. 83244300	-1. 77956900
H	0. 07550200	1. 71247500	-1. 30129200
C	-3. 67330300	1. 60121700	0. 21058600
O	-3. 77138000	1. 23305700	1. 37195500
O	-4. 81417100	2. 00955700	-0. 38519700
C	-4. 95768200	2. 52158700	-1. 73684000
H	-5. 82442500	3. 18663400	-1. 66353300
H	-4. 07529200	3. 09322800	-2. 01353200
C	-5. 22066600	1. 39325100	-2. 71921300
H	-6. 08811100	0. 79967500	-2. 40855500
H	-5. 42930600	1. 80838000	-3. 71275500
H	-4. 34194300	0. 74786200	-2. 78545700
C	-2. 60462600	-1. 87060300	1. 52806300

C	-1.21948100	-1.58372900	1.42564200
C	-0.41998000	-1.80655900	2.56195300
C	-1.02337300	-2.17661200	3.77458300
C	-2.40438300	-2.37340000	3.84456100
C	-3.21924300	-2.24275600	2.71769400
C	-2.24843000	-1.51938800	-0.70354200
C	-0.92391100	-1.32457200	0.02016300
H	-0.42118700	-2.31705500	4.66363700
H	-2.84764900	-2.65550300	4.79512400
H	-4.28396000	-2.44105000	2.76732300
N	-3.19191500	-1.79829800	0.26987800
O	-2.49968000	-1.38553900	-1.89643900
O	0.93047600	-1.67017500	2.41401700
C	1.77729000	-2.21906000	3.42854800
H	1.48858000	-3.25050900	3.65700300
H	2.78222200	-2.20476700	3.00761400
H	1.74654100	-1.61784200	4.34451000
C	0.22362900	-0.98394000	-0.68985900
C	-4.60793800	-1.94904100	-0.00027100
H	-5.17731400	-1.15737000	0.49730300
H	-4.74576800	-1.87249600	-1.07885900
H	-4.96786100	-2.92516600	0.34279500
C	0.26076400	-1.44009200	-2.09456200
O	0.64649500	-0.84022400	-3.09363000
C	1.03536500	0.14662600	-0.08812000
H	1.12499100	-0.06275600	0.97480000
O	-0.09637600	-2.75108900	-2.15429000
C	-0.31291600	-3.27955200	-3.46980200
H	0.56718600	-3.12993100	-4.10189200
H	-0.50554000	-4.34458700	-3.33003700
H	-1.17894500	-2.79204700	-3.92579100
C	3.42444100	1.14200200	0.39989800
C	4.64153200	-0.13518300	-1.22016000
C	4.78430100	1.12572400	-0.33545000
H	4.95577200	2.02324000	-0.93439000
H	5.59571200	1.05257900	0.39133500
C	2.64683300	0.93392100	-1.96613600
H	1.77826200	0.65643900	-2.55313100
H	2.68894200	2.01678700	-1.84739700
C	3.95896300	0.33099700	-2.50895300
H	3.75605200	-0.49009500	-3.20140100
H	4.55639900	1.07801300	-3.03771500
H	5.55695200	-0.71081500	-1.35552200
C	3.51433200	-0.91611700	-0.49362800

N	2.49767600	0.33200600	-0.56788100
O	3.71730300	-1.08582700	0.88865000
C	3.09121200	-2.25417600	-1.07288100
H	2.21482600	-2.59889700	-0.52053500
H	2.80029800	-2.13841600	-2.11855000
C	4.21408000	-3.29995500	-0.95999600
H	5.07782200	-3.04277300	-1.58238600
H	4.55353700	-3.40738600	0.07433000
H	3.83859200	-4.27073600	-1.29808900
H	3.00964200	2.11644900	0.62490500
C	3.56225600	0.18222800	1.56250800
H	4.45022100	0.40173900	2.16017200
H	2.69395000	0.13237200	2.22231900

### IRC-F-36

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C	-2.32442000	1.59718600	-0.52317000
C	0.15823800	1.51695600	-0.20747500
C	-1.23072200	1.35254300	0.31347200
H	-1.39095800	1.29060600	1.38084500
C	0.75626900	2.72837100	0.50282100
C	1.09089800	3.87711100	-0.22977700
C	0.91222800	2.76583300	1.90058700
C	1.57758600	5.02240700	0.40760600
H	0.95497600	3.88048200	-1.30865500
C	1.40550600	3.90381200	2.53698800
H	0.63865200	1.89996300	2.49872700
C	1.74191600	5.03984100	1.79287900
H	1.82555400	5.90056200	-0.18288700
H	1.51957900	3.90763200	3.61784300
H	2.12098900	5.92818100	2.29023200
O	-2.27067700	1.80180700	-1.76882900
H	0.07303500	1.73832900	-1.27527200
C	-3.67607900	1.59426300	0.22325100
O	-3.78218300	1.21155900	1.37941900
O	-4.81301000	2.01448900	-0.37327000
C	-4.93881100	2.56158900	-1.71252400
H	-5.78542900	3.25104000	-1.62759500
H	-4.03858900	3.11154400	-1.97569700
C	-5.23147000	1.46248300	-2.71944900
H	-6.12793800	0.89965400	-2.43527100
H	-5.40400500	1.90309300	-3.70897300
H	-4.37788000	0.78363100	-2.78212100
C	-2.59451700	-1.88855300	1.53666700

C	-1.20946600	-1.60432200	1.42589100
C	-0.40345300	-1.83381600	2.55605100
C	-1.00050700	-2.20029300	3.77283300
C	-2.38177900	-2.39099500	3.85210600
C	-3.20299100	-2.25894200	2.72992600
C	-2.25179800	-1.53774300	-0.69660400
C	-0.92283700	-1.34383400	0.01838800
H	-0.39264800	-2.34275400	4.65777800
H	-2.82018800	-2.67053500	4.80580000
H	-4.26776500	-2.45532300	2.78556400
N	-3.18902200	-1.81577100	0.28172800
O	-2.51031500	-1.40287500	-1.88763000
O	0.94695900	-1.70851500	2.39877800
C	1.79561700	-2.28162200	3.39868800
H	1.48822300	-3.30818500	3.62425300
H	2.79522100	-2.28528500	2.96481700
H	1.78931000	-1.68599300	4.31882900
C	0.20841100	-0.96965700	-0.69555100
C	-4.60821000	-1.95557300	0.02111800
H	-5.16914800	-1.18252900	0.55614900
H	-4.75738700	-1.83514100	-1.05170300
H	-4.96718700	-2.94425000	0.32782200
C	0.22156900	-1.37305400	-2.12105200
O	0.54267400	-0.71235500	-3.10329600
C	1.02600900	0.14912900	-0.08240700
H	1.11743400	-0.07236100	0.97757000
O	-0.07771800	-2.69412200	-2.22153100
C	-0.30175700	-3.17990500	-3.55307400
H	0.57703700	-3.01088400	-4.18416000
H	-0.49537200	-4.24795100	-3.44575300
H	-1.16584600	-2.67465400	-3.98900000
C	3.42550800	1.11278200	0.41803200
C	4.62874100	-0.13800400	-1.23205300
C	4.78235700	1.10362000	-0.32210700
H	4.95708200	2.01220800	-0.90331500
H	5.59593900	1.01093300	0.40006500
C	2.63957100	0.95793000	-1.95174500
H	1.76623800	0.70057400	-2.54109700
H	2.68827600	2.03801800	-1.81269300
C	3.94760600	0.35945100	-2.50970900
H	3.74102200	-0.44495400	-3.22050800
H	4.54818900	1.11507700	-3.02246100
H	5.53984100	-0.71709400	-1.38077100
C	3.49666700	-0.92588400	-0.52030300

N	2.48955700	0.33117100	-0.56427400
O	3.70136700	-1.12911600	0.85635700
C	3.05995000	-2.24398600	-1.13370900
H	2.18070500	-2.59678600	-0.59140600
H	2.76928000	-2.09608100	-2.17561700
C	4.17227200	-3.30345000	-1.05299800
H	5.05096100	-3.02332100	-1.64353500
H	4.48916300	-3.46594500	-0.01900500
H	3.79564700	-4.25227700	-1.44745100
H	3.01819400	2.08462600	0.66707900
C	3.56046400	0.12575700	1.55844700
H	4.45310300	0.32453100	2.15635400
H	2.69479800	0.06826300	2.22078700

### IRC-F-40

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C	-2.32428200	1.59390400	-0.51161600
C	0.15779300	1.52561100	-0.19132100
C	-1.23150500	1.36519300	0.32886900
H	-1.39320300	1.30843100	1.39650200
C	0.76761300	2.72667500	0.52616600
C	1.11372900	3.87643100	-0.19972100
C	0.92557800	2.75418100	1.92389300
C	1.61361700	5.01255700	0.44379100
H	0.97712400	3.88785400	-1.27846600
C	1.43154300	3.88316700	2.56658600
H	0.64376700	1.88761900	2.51718500
C	1.77964600	5.01987900	1.82897600
H	1.87173700	5.89109800	-0.14188700
H	1.54709300	3.87935000	3.64729100
H	2.17009000	5.90067400	2.33104000
O	-2.27046500	1.78484900	-1.75948900
H	0.07270600	1.75520800	-1.25730500
C	-3.67732500	1.59304600	0.23188300
O	-3.78895800	1.20301900	1.38508000
O	-4.81070200	2.02113100	-0.36655500
C	-4.92286600	2.59142100	-1.69731500
H	-5.75309200	3.29946600	-1.60421200
H	-4.00963900	3.12334300	-1.95211100
C	-5.23832000	1.51368200	-2.72036300
H	-6.15428500	0.97440000	-2.45313800
H	-5.38643900	1.97120300	-3.70627200
H	-4.40422900	0.81099500	-2.78273800
C	-2.58828000	-1.89742600	1.54335400

C	-1.20321600	-1.61599800	1.42562000
C	-0.39248300	-1.85007200	2.55143500
C	-0.98484800	-2.21364600	3.77151100
C	-2.36624700	-2.39915700	3.85795900
C	-3.19217200	-2.26596800	2.73928600
C	-2.25582100	-1.54952000	-0.69220700
C	-0.92345800	-1.35237500	0.01692200
H	-0.37283600	-2.35688900	4.65361900
H	-2.80125500	-2.67350400	4.81544800
H	-4.25771800	-2.45728100	2.80119700
N	-3.18917500	-1.82314000	0.29216100
O	-2.52007700	-1.41922200	-1.88276500
O	0.95782100	-1.73196500	2.38825000
C	1.80737000	-2.32000500	3.37894100
H	1.49627200	-3.34587700	3.59446500
H	2.80426700	-2.32441500	2.94285600
H	1.80834500	-1.73604200	4.30461700
C	0.19875400	-0.96026100	-0.69885400
C	-4.60833700	-1.96818200	0.03773100
H	-5.16867600	-1.18211000	0.55329600
H	-4.75941900	-1.87827800	-1.03868800
H	-4.96510500	-2.94862900	0.37265800
C	0.19976400	-1.33242300	-2.13476800
O	0.48252300	-0.63529100	-3.10588800
C	1.02035600	0.15092400	-0.07842300
H	1.11331400	-0.07806300	0.97969600
O	-0.07136000	-2.65607300	-2.26282700
C	-0.30789200	-3.11349600	-3.60244000
H	0.57478800	-2.95280300	-4.22969500
H	-0.52372400	-4.17850600	-3.51236000
H	-1.16219600	-2.58447300	-4.03061200
C	3.42780300	1.09211700	0.42670800
C	4.61851500	-0.14402400	-1.24338000
C	4.78204100	1.08497300	-0.31796400
H	4.95999200	1.99994100	-0.88800100
H	5.59738500	0.97821800	0.40027300
C	2.63380800	0.97202100	-1.94335500
H	1.75632300	0.72894200	-2.53283300
H	2.68917600	2.05004300	-1.79107300
C	3.93707400	0.37375000	-2.51269700
H	3.72479300	-0.41994800	-3.23380400
H	4.54024500	1.13313900	-3.01673300
H	5.52561100	-0.72676800	-1.40187100
C	3.48364200	-0.93435500	-0.53891100

N	2. 48405300	0. 32953600	-0. 56290500
O	3. 69139600	-1. 15779400	0. 83374000
C	3. 03514600	-2. 23975200	-1. 17062900
H	2. 15684000	-2. 59601200	-0. 62927200
H	2. 73881200	-2. 07252500	-2. 20816200
C	4. 13999200	-3. 30846300	-1. 11575400
H	5. 01959800	-3. 02146200	-1. 70127200
H	4. 45672200	-3. 49726100	-0. 08635800
H	3. 75549600	-4. 24488800	-1. 53153800
H	3. 02689000	2. 06271600	0. 69106600
C	3. 56077000	0. 08864800	1. 55310800
H	4. 45681200	0. 27347500	2. 15045200
H	2. 69704100	0. 02729900	2. 21744100

### IRC-F-46

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C	-2. 32867500	1. 59488200	-0. 50043400
C	0. 15400900	1. 53325500	-0. 17784800
C	-1. 23553100	1. 37637300	0. 34259900
H	-1. 39774300	1. 31392300	1. 40975700
C	0. 77325600	2. 72490000	0. 54720700
C	1. 12814500	3. 87660400	-0. 17136500
C	0. 93290700	2. 74194600	1. 94487300
C	1. 63878300	5. 00411700	0. 47883100
H	0. 98937600	3. 89671900	-1. 24969700
C	1. 44927600	3. 86241400	2. 59434800
H	0. 64497500	1. 87351900	2. 53261200
C	1. 80670600	5. 00085200	1. 86380600
H	1. 90274300	5. 88462200	-0. 10126700
H	1. 56578300	3. 85039500	3. 67490100
H	2. 20465600	5. 87510300	2. 37139600
O	-2. 27746700	1. 78129500	-1. 75053200
H	0. 06903200	1. 77049300	-1. 24213800
C	-3. 68241700	1. 58896600	0. 24007300
O	-3. 79927800	1. 18914700	1. 38947100
O	-4. 81363100	2. 02183400	-0. 35925900
C	-4. 92439800	2. 61214200	-1. 68093800
H	-5. 75657000	3. 31637900	-1. 57678200
H	-4. 01266200	3. 15082900	-1. 92715500
C	-5. 23872000	1. 55028600	-2. 72078800
H	-6. 12941500	0. 97819400	-2. 43768700
H	-5. 43156000	2. 02499400	-3. 69060000
H	-4. 38724900	0. 87418200	-2. 82275900
C	-2. 57907700	-1. 91210600	1. 54750400

C	-1.19491900	-1.62871600	1.42369200
C	-0.37973100	-1.86397800	2.54615700
C	-0.96748300	-2.22391600	3.76981700
C	-2.34850100	-2.40899900	3.86261400
C	-3.17830300	-2.27997100	2.74615100
C	-2.25730100	-1.56466600	-0.68955500
C	-0.92244600	-1.36324300	0.01316700
H	-0.35138500	-2.36717500	4.64878600
H	-2.77946000	-2.68428500	4.82082600
H	-4.24236700	-2.47799600	2.80983900
N	-3.18501900	-1.83902600	0.29817800
O	-2.52847700	-1.43560300	-1.87853200
O	0.97053400	-1.75206700	2.37663300
C	1.82124000	-2.35187200	3.35940800
H	1.50427200	-3.37491000	3.57091100
H	2.81456500	-2.36161300	2.91947900
H	1.83196700	-1.77488200	4.28727000
C	0.18932000	-0.95072400	-0.70503600
C	-4.60670500	-1.97483800	0.05010700
H	-5.16373100	-1.27531700	0.68244600
H	-4.78005800	-1.73241100	-0.99995300
H	-4.94753200	-2.99904200	0.24644000
C	0.18361300	-1.29987800	-2.14758500
O	0.44131400	-0.57588700	-3.10614700
C	1.01385800	0.15331100	-0.07740900
H	1.10888100	-0.08389500	0.97845100
O	-0.06254700	-2.62254600	-2.29926500
C	-0.29900200	-3.06318600	-3.64528300
H	0.53171200	-2.80213500	-4.29715000
H	-0.40628600	-4.14407600	-3.58252300
H	-1.23268100	-2.61327800	-4.01567700
C	3.42608500	1.07729900	0.43453300
C	4.61060800	-0.13844500	-1.25413500
C	4.77860000	1.07778900	-0.31265000
H	4.95706000	2.00009000	-0.87087500
H	5.59528700	0.96048900	0.40247100
C	2.62699700	0.99066700	-1.93659500
H	1.74812600	0.75704800	-2.52781800
H	2.68384100	2.06670900	-1.77140500
C	3.92919000	0.39883200	-2.51537800
H	3.71602100	-0.38360800	-3.24837900
H	4.53327600	1.16487800	-3.00827700
H	5.51602900	-0.72130900	-1.42188700
C	3.47447100	-0.93588500	-0.55942600

N	2.47784700	0.33163200	-0.56395100
O	3.68221100	-1.17979200	0.80928100
C	3.02195900	-2.23032400	-1.20963100
H	2.13507300	-2.58476700	-0.68186500
H	2.73890100	-2.05069000	-2.24845700
C	4.11565600	-3.31012400	-1.15196200
H	5.00687900	-3.02752300	-1.71884000
H	4.41404300	-3.51410600	-0.12262100
H	3.72897400	-4.23604200	-1.58384500
H	3.02824300	2.04492500	0.71426300
C	3.55900200	0.05720100	1.54614300
H	4.45781100	0.23057800	2.14276700
H	2.69728000	-0.01007700	2.21217100

### IRC-F-51

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C	-2.33002100	1.59842500	-0.49697400
C	0.15246500	1.53624700	-0.17438400
C	-1.23750100	1.38076800	0.34579600
H	-1.39967000	1.31636300	1.41285700
C	0.77599300	2.72447900	0.55228600
C	1.13542400	3.87605300	-0.16429000
C	0.93710600	2.73790900	1.94975700
C	1.65190700	4.99984700	0.48774400
H	0.99562200	3.89892200	-1.24244300
C	1.45927100	3.85463000	2.60107700
H	0.64576300	1.86953000	2.53585200
C	1.82132200	4.99286700	1.87254100
H	1.91894400	5.88034700	-0.09072500
H	1.57674300	3.83979900	3.68148200
H	2.22378700	5.86415900	2.38151500
O	-2.27962300	1.78447400	-1.74759900
H	0.06777400	1.77504500	-1.23836900
C	-3.68469400	1.59034100	0.24179900
O	-3.80332900	1.18633200	1.38963000
O	-4.81556300	2.02345800	-0.35855800
C	-4.92156100	2.61835600	-1.67859500
H	-5.74907400	3.32765300	-1.57405800
H	-4.00618300	3.15101500	-1.92258900
C	-5.24062500	1.56050000	-2.72086000
H	-6.14592700	1.00674600	-2.45130900
H	-5.40853900	2.03623900	-3.69404500
H	-4.40159500	0.86797600	-2.80908200
C	-2.57605200	-1.91262700	1.55178500

C	-1.19169900	-1.63134300	1.42465400
C	-0.37463600	-1.86722100	2.54583800
C	-0.96026400	-2.22720300	3.77055900
C	-2.34119700	-2.41026600	3.86616100
C	-3.17342400	-2.27787500	2.75206500
C	-2.25887500	-1.56924100	-0.68650100
C	-0.92254300	-1.36659300	0.01355100
H	-0.34264900	-2.37023700	4.64886300
H	-2.77097900	-2.68347100	4.82645000
H	-4.23867400	-2.46866700	2.81972000
N	-3.18452500	-1.84307000	0.30384500
O	-2.53187200	-1.44288800	-1.87549600
O	0.97524600	-1.75660700	2.37456000
C	1.82681000	-2.35943400	3.35511100
H	1.49005700	-3.37668900	3.58629500
H	2.81700500	-2.39453700	2.89867500
H	1.85989700	-1.76457100	4.27679000
C	0.18604600	-0.94623000	-0.70753500
C	-4.60663000	-1.98015900	0.05901000
H	-5.15738100	-1.17855900	0.55888800
H	-4.76086600	-1.91092500	-1.01668500
H	-4.97071300	-2.94879600	0.41529900
C	0.17646600	-1.28690900	-2.15276300
O	0.43141800	-0.56202600	-3.10444800
C	1.01126600	0.15501300	-0.07666600
H	1.10653900	-0.08429600	0.97876400
O	-0.06208800	-2.61209700	-2.31034700
C	-0.30923900	-3.04361300	-3.65750000
H	0.52790100	-2.77996300	-4.31588100
H	-0.43424600	-4.11890100	-3.59729900
H	-1.23132900	-2.57689300	-4.02588300
C	3.42687500	1.07402500	0.43340100
C	4.60558700	-0.14405700	-1.25782700
C	4.77808100	1.07124200	-0.31642500
H	4.95790300	1.99291400	-0.87492000
H	5.59581400	0.95156500	0.39690500
C	2.62460800	0.99120700	-1.93606200
H	1.74366100	0.76233200	-2.52573800
H	2.68668400	2.06667100	-1.77003000
C	3.92291200	0.39413200	-2.51776400
H	3.70479300	-0.38871200	-3.24872800
H	4.52833000	1.15700000	-3.01360900
H	5.50972900	-0.72825600	-1.42709300
C	3.46915300	-0.93907800	-0.56101400

N	2. 47527000	0. 33143400	-0. 56377200
O	3. 67934200	-1. 18368700	0. 80686300
C	3. 01276800	-2. 23188700	-1. 21212900
H	2. 13428800	-2. 59361400	-0. 67519300
H	2. 71552300	-2. 04616200	-2. 24603900
C	4. 11156400	-3. 30781400	-1. 17914700
H	5. 00620000	-3. 00103100	-1. 73134300
H	4. 40411100	-3. 54351100	-0. 15204900
H	3. 73236000	-4. 22304400	-1. 64460100
H	3. 03208600	2. 04263300	0. 71381600
C	3. 55925800	0. 05336300	1. 54443900
H	4. 45909500	0. 22517100	2. 13984300
H	2. 69823600	-0. 01259400	2. 21150700

### IRC-F-61

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C	-2. 33376800	1. 60489400	-0. 48908400
C	0. 14967600	1. 53856100	-0. 16764100
C	-1. 24100100	1. 38075800	0. 35019300
H	-1. 40342100	1. 30973800	1. 41728700
C	0. 77894700	2. 72003900	0. 56588500
C	1. 14742300	3. 87273900	-0. 14447300
C	0. 94049800	2. 72527900	1. 96346400
C	1. 67460900	4. 98848300	0. 51298500
H	1. 00753600	3. 90260100	-1. 22244500
C	1. 47297200	3. 83400300	2. 62032300
H	0. 64222500	1. 85644100	2. 54542100
C	1. 84535600	4. 97261400	1. 89755800
H	1. 95020200	5. 86928000	-0. 06133100
H	1. 59106600	3. 81239000	3. 70056000
H	2. 25737100	5. 83708800	2. 41068700
O	-2. 28376500	1. 80749400	-1. 73421500
H	0. 06566000	1. 78392700	-1. 23010500
C	-3. 68939300	1. 58937100	0. 24847500
O	-3. 80803300	1. 17878300	1. 39370700
O	-4. 82066400	2. 02350800	-0. 35083000
C	-4. 92490800	2. 63073200	-1. 66571300
H	-5. 75092700	3. 34183500	-1. 55660800
H	-4. 00713100	3. 16262300	-1. 90400900
C	-5. 24516600	1. 58289600	-2. 71799400
H	-6. 17403800	1. 05087700	-2. 47593200
H	-5. 37210200	2. 06655200	-3. 69555500
H	-4. 42059500	0. 86849300	-2. 78484000
C	-2. 56907200	-1. 92014000	1. 55457600

C	-1.18564400	-1.63841200	1.42267400
C	-0.36483500	-1.87679200	2.54050900
C	-0.94664700	-2.23536600	3.76751900
C	-2.32775000	-2.41378500	3.86929700
C	-3.16332300	-2.28188200	2.75755100
C	-2.26062700	-1.57644700	-0.68548800
C	-0.92160800	-1.36929500	0.01020800
H	-0.32604300	-2.38068400	4.64332200
H	-2.75479500	-2.68315200	4.83172500
H	-4.22892200	-2.46859900	2.82992500
N	-3.18142000	-1.85393900	0.30789500
O	-2.53898600	-1.44861000	-1.87308000
O	0.98491000	-1.76933100	2.36542300
C	1.83698700	-2.37625700	3.34287900
H	1.51475200	-3.40174800	3.55183000
H	2.83071200	-2.38773000	2.89610900
H	1.85318700	-1.79929200	4.27476600
C	0.18189900	-0.94772000	-0.70815700
C	-4.60472700	-1.99384300	0.07137900
H	-5.15061600	-1.17429700	0.54962200
H	-4.76434600	-1.95832400	-1.00633100
H	-4.96935400	-2.95016600	0.46099500
C	0.16347500	-1.26422600	-2.16254200
O	0.40880800	-0.52648400	-3.10437500
C	1.00726600	0.15477600	-0.07737700
H	1.10416600	-0.08792500	0.97699900
O	-0.06540000	-2.59170300	-2.33638800
C	-0.31634500	-3.00413000	-3.68856300
H	0.49745700	-2.69650200	-4.35087900
H	-0.38953000	-4.09144500	-3.65104200
H	-1.26075500	-2.56811500	-4.03209700
C	3.42574500	1.06450200	0.43657500
C	4.60074500	-0.14102800	-1.26550500
C	4.77574300	1.06667400	-0.31481700
H	4.95531000	1.99280300	-0.86618600
H	5.59434300	0.94111700	0.39663900
C	2.62054200	1.00161400	-1.93334000
H	1.73908800	0.77763800	-2.52392700
H	2.68264800	2.07570300	-1.75960700
C	3.91858000	0.40922800	-2.52059300
H	3.70116400	-0.36577700	-3.26016800
H	4.52462500	1.17716500	-3.00812800
H	5.50402100	-0.72507900	-1.44014000
C	3.46296200	-0.94015600	-0.57509900

N	2. 47146300	0. 33197200	-0. 56580000
O	3. 67243600	-1. 19775400	0. 79026600
C	3. 00555700	-2. 22426000	-1. 24213700
H	2. 11546100	-2. 58469100	-0. 72392800
H	2. 72672100	-2. 02647400	-2. 27904000
C	4. 09594300	-3. 30839600	-1. 20099800
H	5. 00885000	-3. 00013300	-1. 71601200
H	4. 35435100	-3. 56702900	-0. 17322700
H	3. 72610700	-4. 20856500	-1. 69518700
H	3. 03270000	2. 03093400	0. 72680300
C	3. 55811000	0. 03379500	1. 53838900
H	4. 46014000	0. 19747400	2. 13284900
H	2. 69864600	-0. 03534800	2. 20694900

**12. Coordinates of M2c, TSc<sub>|3+4|</sub>, TSc<sub>|3+2|</sub> and IRC points in TSc<sub>|3+4|</sub> (IRC-1 is transition state)**

**M2c**

0 1			
C	1. 08023000	2. 90828200	0. 31720200
C	1. 25089300	2. 29814600	-0. 94612900
C	2. 47827600	1. 74921500	-1. 31831200
C	3. 53992600	1. 77437600	-0. 41794800
C	3. 41243700	2. 38096900	0. 83312700
C	2. 19814500	2. 95723900	1. 18185300
H	0. 42183100	2. 28148700	-1. 64517900
H	2. 59591600	1. 28332500	-2. 29130600
H	4. 25147300	2. 40426500	1. 52028700
H	2. 08334700	3. 45262000	2. 14113000
Br	5. 18825600	0. 90175000	-0. 87156100
N	-0. 06025000	3. 57199700	0. 73085900
C	-1. 28893900	3. 33527700	0. 36115000
C	-2. 23496300	4. 48859700	0. 74127400
F	-1. 59555800	5. 61204200	1. 09992100
F	-3. 06009100	4. 81890200	-0. 28814200
F	-3. 03963400	4. 14064700	1. 77880200
C	-2. 74438800	0. 04367700	-1. 04356900
C	-1. 73619000	0. 87861400	-0. 30162800
C	-0. 66539400	0. 17763500	0. 27116100
H	0. 05258900	0. 72464200	0. 86523200
O	-2. 54508000	-1. 13017800	-1. 32858700
O	-3. 87650800	0. 67796400	-1. 36957500
C	-4. 86845000	-0. 09406900	-2. 09593600

H	-4.41841500	-0.44498800	-3.02942600
H	-5.13141700	-0.97049800	-1.49660000
C	-6.05880300	0.81234000	-2.33928800
H	-5.77225700	1.68642400	-2.93250100
H	-6.83061200	0.26166300	-2.88732600
H	-6.48804100	1.15822200	-1.39372900
C	-1.99906900	2.25446200	-0.24579400
H	-2.97483400	2.53583400	-0.61780100
P	-0.34716300	-1.54804900	0.30478600
C	0.29223200	-2.30147900	-1.24275500
C	0.94089200	-3.54641800	-1.19354800
C	0.21853200	-1.61109600	-2.45892900
C	1.47801700	-4.10420400	-2.35420700
C	0.76527900	-2.16835100	-3.61517000
H	-0.26236300	-0.64111900	-2.49965200
C	1.38923200	-3.41663100	-3.56644900
H	1.97398000	-5.06936600	-2.30710700
H	0.70375500	-1.62535200	-4.55394500
H	1.81370800	-3.84838400	-4.46843600
C	1.06482900	-1.73046400	1.46355500
C	0.93367700	-2.32706600	2.72529900
C	2.31870500	-1.24178800	1.06120500
C	2.04111700	-2.42632500	3.57109200
H	-0.02454100	-2.71583700	3.05256100
C	3.41981700	-1.33878700	1.90991900
H	2.44390900	-0.78353700	0.08571200
C	3.28271600	-1.93344700	3.16666600
H	1.92961900	-2.89149000	4.54640800
H	4.37763900	-0.94859500	1.57807500
H	4.14127300	-2.01379600	3.82761200
C	-1.70614000	-2.57357000	0.98537700
C	-2.45442800	-2.04544300	2.04911100
C	-2.00717800	-3.85174300	0.49720200
C	-3.47960800	-2.79555200	2.62608900
H	-2.24356100	-1.04603700	2.41894500
C	-3.03554100	-4.59648900	1.07661100
H	-1.45633900	-4.26331800	-0.34131300
C	-3.77058300	-4.07280200	2.14184900
H	-4.05278300	-2.37823900	3.44898500
H	-3.26519600	-5.58474800	0.68848100
H	-4.57141300	-4.65497000	2.58894300
H	1.04155000	-4.07793200	-0.25164000

**TSc<sub>[3+4]</sub>**

0	1		
C	0.02895400	2.86788000	0.07809800
C	0.23913000	1.69880400	-0.81543900
C	1.62463500	1.46859600	-1.24730700
C	2.65250700	2.16359700	-0.69616600
C	2.45864900	3.22377600	0.24319800
C	1.17591100	3.56225900	0.58499600
H	-0.45843300	1.67784800	-1.65118800
H	1.81077900	0.73453600	-2.02138100
H	3.31293600	3.75538800	0.64613700
H	0.98398000	4.38837100	1.26380100
Br	4.46022000	1.76658200	-1.22934900
N	-1.15853200	3.30403000	0.49060100
C	-2.36024900	2.75861400	0.22403300
C	-3.46198500	3.73814000	0.57933300
F	-3.28737600	4.94973900	-0.00493200
F	-4.69939100	3.31533700	0.21313900
F	-3.52011700	3.97587400	1.91744400
C	-2.51380800	-0.75860700	-1.20184400
C	-2.01051600	0.32045300	-0.36682000
C	-0.63034100	0.31391800	0.11460300
H	-0.59034200	0.77268800	1.10096700
O	-1.81458800	-1.67744200	-1.63858400
O	-3.83813600	-0.69487300	-1.46861200
C	-4.38011400	-1.74600700	-2.29911400
H	-3.86934700	-1.73267400	-3.26747200
H	-4.17620600	-2.71204900	-1.82672200
C	-5.86821500	-1.48851900	-2.44281000
H	-6.05458100	-0.51728600	-2.91229100
H	-6.31804000	-2.26628100	-3.06922800
H	-6.36396600	-1.50259100	-1.46679800
C	-2.76432900	1.49423600	-0.24267000
H	-3.80800000	1.41127100	-0.51927600
P	0.26712800	-1.27836900	0.37610900
C	1.47585300	-1.75927600	-0.91538900
C	2.83594800	-1.84396300	-0.57137900
C	1.08159000	-2.02979500	-2.23889000
C	3.78453800	-2.19008200	-1.53394100
C	2.03885600	-2.37803700	-3.19115300
H	0.03678900	-1.96485500	-2.51158300
C	3.38959700	-2.45810500	-2.84428200
H	4.83230500	-2.24398200	-1.25436600
H	1.72423900	-2.58441500	-4.21012400
H	4.12990200	-2.72521300	-3.59301300

C	1.23676800	-1.02589000	1.91366900
C	1.50973600	-2.12650000	2.74513800
C	1.74365200	0.23568400	2.26117800
C	2.27020600	-1.96272500	3.90222300
H	1.12668800	-3.11037700	2.49654900
C	2.50008700	0.39337700	3.42315300
H	1.56331800	1.10285500	1.63899100
C	2.76458300	-0.70249600	4.24523000
H	2.46997900	-2.82063800	4.53745400
H	2.88029700	1.37745900	3.68032600
H	3.35217800	-0.57586500	5.14995700
C	-0.81690200	-2.69074700	0.78757400
C	-1.84360100	-2.50218700	1.72570800
C	-0.59440900	-3.96077400	0.24149200
C	-2.64641500	-3.57805600	2.10204000
H	-2.02602900	-1.52188900	2.15524000
C	-1.39840400	-5.03421900	0.62865200
H	0.19350700	-4.11341100	-0.48815600
C	-2.42511900	-4.84465600	1.55488800
H	-3.44406000	-3.42539900	2.82307400
H	-1.22304500	-6.01649500	0.19968400
H	-3.05156400	-5.68117100	1.85112400
H	3.16479200	-1.63103800	0.43838000

### TSc<sub>[3+2]</sub>

0 1

C	-1.69080500	0.83292300	-0.86211600
C	-2.38566700	-0.21390800	-1.49517400
C	-3.51318900	-0.78677000	-0.90934900
C	-3.95274300	-0.30617300	0.32485600
C	-3.30705200	0.75200400	0.96262100
C	-2.18008600	1.31388400	0.36809700
H	-2.01903200	-0.58158700	-2.44797800
H	-4.03701400	-1.60073900	-1.39907600
H	-3.66449000	1.11439300	1.92065400
H	-1.65673700	2.12370000	0.86667500
Br	-5.44055900	-1.15186900	1.19098600
N	-0.48539000	1.29772400	-1.45088200
C	-0.21917700	2.67551100	-1.28309200
C	-1.15563400	3.66523100	-1.90666100
F	-1.31745000	3.44214600	-3.23825300
F	-2.40754700	3.65013700	-1.37892400
F	-0.69956400	4.93531000	-1.78073200
C	2.20511700	1.82320100	1.29005800

C	1. 62149000	1. 96511900	-0. 00943800
C	1. 27658700	0. 78993900	-0. 75427000
H	1. 58387800	0. 78985600	-1. 79819800
O	2. 53077800	0. 70544100	1. 73190000
O	2. 49059900	2. 86358700	2. 12421000
C	2. 35262000	4. 24437700	1. 75665200
H	2. 88073200	4. 43009900	0. 81413100
H	1. 29409500	4. 49051700	1. 61894400
C	2. 95496300	5. 06864200	2. 88191500
H	4. 01422900	4. 82705200	3. 01569600
H	2. 86767300	6. 13572800	2. 65057200
H	2. 43366100	4. 87486600	3. 82482600
C	0. 90654100	3. 07091500	-0. 62565000
H	1. 17937500	4. 11375900	-0. 56624800
P	1. 52620500	-0. 92462600	-0. 15179400
C	0. 72941800	-1. 48523900	1. 39192800
C	-0. 66480000	-1. 63268500	1. 42904300
C	1. 49242200	-1. 81229000	2. 52356100
C	-1. 29292400	-2. 08558100	2. 59025400
H	-1. 26498600	-1. 40765300	0. 55694800
C	0. 86042000	-2. 28483800	3. 67219100
H	2. 56702500	-1. 68201600	2. 51067100
C	-0. 53091700	-2. 41565000	3. 71114400
H	-2. 37553800	-2. 17500500	2. 60485100
H	1. 45708900	-2. 54058000	4. 54293400
H	-1. 01756800	-2. 77502700	4. 61357100
C	0. 78992400	-1. 99184800	-1. 46733700
C	0. 34963600	-3. 28950000	-1. 15458100
C	0. 76199500	-1. 57654200	-2. 80966600
C	-0. 11457700	-4. 14401100	-2. 15525300
H	0. 35446900	-3. 63792600	-0. 12769100
C	0. 29397300	-2. 43313800	-3. 80654600
H	1. 08600200	-0. 58297200	-3. 09352700
C	-0. 14558100	-3. 71794000	-3. 48338500
H	-0. 45475800	-5. 14124200	-1. 89158900
H	0. 27276700	-2. 09062800	-4. 83698800
H	-0. 50953700	-4. 38219200	-4. 26200200
C	3. 30143500	-1. 37185700	-0. 20437300
C	4. 28003500	-0. 40185000	-0. 45716100
C	3. 67453800	-2. 71627500	-0. 05768200
C	5. 61917700	-0. 77679700	-0. 56321400
H	3. 99624400	0. 63947500	-0. 56488300
C	5. 01763100	-3. 08156600	-0. 14782400
H	2. 92641500	-3. 48149700	0. 12471800

C	5. 99061400	-2. 11334000	-0. 40419300
H	6. 37257300	-0. 02030200	-0. 76248600
H	5. 29994500	-4. 12302200	-0. 02444400
H	7. 03542200	-2. 40056200	-0. 48134000

### IRC-F-61

0 1

C	0. 72826700	2. 92199600	0. 23477100
C	0. 86048000	2. 21111800	-0. 98196100
C	2. 09760300	1. 72550200	-1. 40346000
C	3. 22025500	1. 92044200	-0. 60680800
C	3. 13825900	2. 64445000	0. 58814600
C	1. 90684400	3. 14958200	0. 98837200
H	-0. 00859700	2. 06536600	-1. 61232200
H	2. 17695200	1. 17015000	-2. 33105200
H	4. 02454800	2. 81133500	1. 19098000
H	1. 82421800	3. 72681800	1. 90429600
Br	4. 89261500	1. 13958600	-1. 13068200
N	-0. 43466800	3. 49270000	0. 71172100
C	-1. 66663900	3. 16226600	0. 40413200
C	-2. 62205800	4. 27863800	0. 86129000
F	-2. 22070200	5. 49852400	0. 44332700
F	-3. 89512000	4. 12377700	0. 42138700
F	-2. 68601400	4. 33065400	2. 21425400
C	-2. 73514500	-0. 18998200	-1. 15799200
C	-1. 89977200	0. 69450100	-0. 27983600
C	-0. 80628700	0. 12698800	0. 36984500
H	-0. 27537300	0. 75460600	1. 07173000
O	-2. 32943500	-1. 24749700	-1. 61887100
O	-3. 96683900	0. 27310500	-1. 40511200
C	-4. 79659600	-0. 52658600	-2. 28844200
H	-4. 28294200	-0. 62607800	-3. 24906800
H	-4. 90180100	-1. 52504800	-1. 85552900
C	-6. 13015000	0. 18190800	-2. 42426200
H	-6. 00477800	1. 17619900	-2. 86487600
H	-6. 78926400	-0. 40282600	-3. 07410500
H	-6. 61739600	0. 29231100	-1. 45006300
C	-2. 30957700	2. 03876100	-0. 18725400
H	-3. 31416900	2. 23060300	-0. 53601000
P	-0. 14702000	-1. 50536900	0. 37855900
C	0. 98127700	-1. 94997800	-1. 01032300
C	2. 29168600	-2. 37339600	-0. 73097500
C	0. 57447000	-1. 82348900	-2. 35067300
C	3. 17847100	-2. 65894400	-1. 77067200

C	1. 46432700	-2. 11833500	-3. 38264600
H	-0. 43327000	-1. 49939000	-2. 57695500
C	2. 76806600	-2. 53291100	-3. 09739500
H	4. 18875200	-2. 98240600	-1. 53708600
H	1. 13732800	-2. 01569800	-4. 41412100
H	3. 45907200	-2. 75317300	-3. 90598800
C	0. 89872500	-1. 55476900	1. 88314600
C	0. 81967900	-2. 62802100	2. 78395700
C	1. 81629200	-0. 51800300	2. 12748400
C	1. 63618900	-2. 65628800	3. 91639900
H	0. 12134900	-3. 43960400	2. 61083500
C	2. 62478500	-0. 54995600	3. 26265700
H	1. 91216000	0. 31158600	1. 43536200
C	2. 53720400	-1. 61792400	4. 15923900
H	1. 56143200	-3. 48991000	4. 61084600
H	3. 32934100	0. 26076000	3. 43900600
H	3. 16821300	-1. 64012100	5. 04327800
C	-1. 38046400	-2. 83643600	0. 58802400
C	-2. 47295300	-2. 60821300	1. 43861500
C	-1. 23063300	-4. 08180100	-0. 03388400
C	-3. 40653400	-3. 61905100	1. 66107100
H	-2. 59698200	-1. 64136000	1. 91726200
C	-2. 16941000	-5. 09027200	0. 19280800
H	-0. 39100000	-4. 26595100	-0. 69630600
C	-3. 25637400	-4. 86065900	1. 03763400
H	-4. 25193600	-3. 43700800	2. 31797900
H	-2. 04936200	-6. 05424000	-0. 29358100
H	-3. 98463100	-5. 64814000	1. 21063200
H	2. 62957300	-2. 48092300	0. 29338900

### IRC-F-52

0 1

C	0. 60452000	2. 97311600	0. 19168300
C	0. 75953300	2. 26111100	-1. 01984600
C	2. 00941500	1. 80380500	-1. 43528300
C	3. 12328100	2. 02610900	-0. 63249800
C	3. 02046100	2. 76000800	0. 55570100
C	1. 77599600	3. 23852700	0. 94821100
H	-0. 10285900	2. 08869700	-1. 65155700
H	2. 10526600	1. 24502000	-2. 36004700
H	3. 90030300	2. 95361400	1. 15773500
H	1. 67607500	3. 82156000	1. 85640900
Br	4. 80997800	1. 26371500	-1. 13508800
N	-0. 57715700	3. 50148200	0. 67148500

C	-1.79562100	3.11058300	0.37759400
C	-2.80015100	4.17846600	0.84233800
F	-2.47297000	5.41439800	0.40668300
F	-4.07115700	3.95112300	0.42881500
F	-2.84128300	4.23985800	2.19592100
C	-2.70238300	-0.29592500	-1.16757500
C	-1.91130000	0.63430800	-0.29730300
C	-0.78888300	0.11837700	0.35816400
H	-0.28919300	0.77753900	1.05356500
O	-2.24659500	-1.33849500	-1.61970600
O	-3.95518200	0.10479100	-1.41988600
C	-4.74551600	-0.75096800	-2.28675600
H	-4.22837000	-0.84541500	-3.24674400
H	-4.80226900	-1.74505600	-1.83326100
C	-6.11129800	-0.10966500	-2.43379700
H	-6.03229000	0.88272700	-2.88927500
H	-6.74182800	-0.73427300	-3.07517400
H	-6.60354400	-0.00819400	-1.46141200
C	-2.38645100	1.95541300	-0.20618000
H	-3.40067800	2.09622600	-0.55117900
P	-0.07050000	-1.48706400	0.38466400
C	1.07531200	-1.91979000	-0.99555300
C	2.41386800	-2.23696000	-0.70786000
C	0.65310100	-1.89509000	-2.33721600
C	3.31129000	-2.51965700	-1.73911200
C	1.55453900	-2.18691400	-3.36026500
H	-0.37500300	-1.65180000	-2.57135900
C	2.88484600	-2.49720000	-3.06651800
H	4.34333800	-2.75699200	-1.49837600
H	1.21437300	-2.16557800	-4.39198200
H	3.58389300	-2.71597800	-3.86881300
C	0.97549200	-1.48762200	1.89027100
C	0.97678000	-2.58783300	2.76102600
C	1.81879600	-0.39698800	2.16154300
C	1.79903700	-2.59071700	3.88934900
H	0.33562900	-3.44039600	2.56773900
C	2.63300800	-0.40351400	3.29316100
H	1.85629300	0.45430800	1.49161400
C	2.62525800	-1.49934200	4.15941600
H	1.78586000	-3.44567400	4.55911100
H	3.27743800	0.44754600	3.49163200
H	3.26138800	-1.50217100	5.03992400
C	-1.26768000	-2.84649500	0.61768000
C	-2.34723600	-2.63408300	1.48907800

C	-1.11063100	-4.08946700	-0.00719700
C	-3.26192100	-3.65800600	1.72864900
H	-2.47763600	-1.66824400	1.96861300
C	-2.03168900	-5.11069600	0.23554700
H	-0.28129200	-4.26073800	-0.68586400
C	-3.10607000	-4.89686900	1.10067600
H	-4.09792800	-3.48752300	2.40078100
H	-1.90783900	-6.07227100	-0.25449700
H	-3.82096100	-5.69384900	1.28526900
H	2.76686300	-2.26244700	0.31609900

### IRC-F-47

0 1

C	0.54280700	2.99386900	0.16960700
C	0.70892800	2.28287200	-1.04467900
C	1.96538700	1.83634000	-1.45303600
C	3.07365300	2.07361300	-0.64763100
C	2.95984800	2.81568900	0.53014400
C	1.70937900	3.28129800	0.91998500
H	-0.15140400	2.09775900	-1.67615400
H	2.06882800	1.27885600	-2.38021000
H	3.83621900	3.01878200	1.13769200
H	1.60044500	3.86524500	1.82820700
Br	4.76714600	1.31862100	-1.13953700
N	-0.64849300	3.50222100	0.64760100
C	-1.85835000	3.08286100	0.35909700
C	-2.88495700	4.12854700	0.82611800
F	-2.59248800	5.36921300	0.37930700
F	-4.15358900	3.86680700	0.42619500
F	-2.91477900	4.19803300	2.17949800
C	-2.68333100	-0.35080800	-1.17351200
C	-1.91648300	0.60249300	-0.30670000
C	-0.78159700	0.11775400	0.34776200
H	-0.29927200	0.79130200	1.04139300
O	-2.19955500	-1.38216800	-1.62131900
O	-3.94669800	0.01373400	-1.42640500
C	-4.71563300	-0.87452100	-2.27977700
H	-4.19267500	-0.97714200	-3.23513700
H	-4.75293700	-1.86014000	-1.80665600
C	-6.09362000	-0.26549500	-2.44499700
H	-6.03139000	0.72382700	-2.90909700
H	-6.70323100	-0.90945000	-3.08756100
H	-6.59810300	-0.16548500	-1.47888400
C	-2.42426000	1.91206100	-0.21923400

H	-3.44279500	2.02718100	-0.56152300
P	-0.03262500	-1.47325100	0.38811300
C	1.12172200	-1.90631600	-0.98551300
C	2.46880400	-2.17916500	-0.69176500
C	0.69837400	-1.92906700	-2.32696400
C	3.37242300	-2.46744300	-1.71595700
C	1.60644400	-2.22597800	-3.34278100
H	-0.33553200	-1.71884100	-2.56679600
C	2.94438400	-2.49423000	-3.04266100
H	4.41072000	-2.66975400	-1.47016800
H	1.26479700	-2.24332300	-4.37402700
H	3.64799100	-2.71868700	-3.83943400
C	1.01250500	-1.44584700	1.89454700
C	1.06592300	-2.56109000	2.74476400
C	1.80661600	-0.32378500	2.18471000
C	1.89007300	-2.54775300	3.87146800
H	0.46458100	-3.43880400	2.53531600
C	2.62158400	-0.31361600	3.31588400
H	1.80621100	0.54001400	1.52991700
C	2.66563700	-1.42448100	4.16147300
H	1.91910000	-3.41572600	4.52375700
H	3.22664800	0.56254500	3.52964900
H	3.30315900	-1.41482400	5.04095200
C	-1.21272000	-2.84482800	0.63897800
C	-2.27968200	-2.63757200	1.52717000
C	-1.06174800	-4.08546600	0.00855000
C	-3.18828400	-3.66416900	1.77747700
H	-2.40544000	-1.67329900	2.01110100
C	-1.97730500	-5.10931100	0.26146500
H	-0.24278000	-4.25219300	-0.68375400
C	-3.03934000	-4.90051700	1.14289700
H	-4.01400900	-3.49758300	2.46313000
H	-1.85935300	-6.06883900	-0.23404500
H	-3.75017300	-5.69930200	1.33514600
H	2.82374600	-2.16528200	0.33154300

### IRC-F-42

0 1

C	0.48731000	3.00934000	0.13839200
C	0.66151800	2.29116700	-1.06485000
C	1.92257500	1.85606200	-1.47123800
C	3.02834500	2.10901800	-0.66499700
C	2.90683000	2.86109400	0.50627900
C	1.65034500	3.31875800	0.88655300

H	-0.19543900	2.09110400	-1.69630300
H	2.03253600	1.29040500	-2.39144300
H	3.77944200	3.08219600	1.10763100
H	1.53385400	3.90570600	1.79648200
Br	4.72749100	1.36070700	-1.14635100
N	-0.71085200	3.50004700	0.61863600
C	-1.91447900	3.05634200	0.33898400
C	-2.95742000	4.08662700	0.80388400
F	-2.69145400	5.32806600	0.34281500
F	-4.22376900	3.79710200	0.41613500
F	-2.97869400	4.16922500	2.15667600
C	-2.66413700	-0.40094200	-1.17990500
C	-1.92252600	0.57392400	-0.31562500
C	-0.77573800	0.11966200	0.33904100
H	-0.31053500	0.80739700	1.03122500
O	-2.15204000	-1.41990700	-1.62404900
O	-3.93667600	-0.07229700	-1.43524800
C	-4.67904500	-0.98853300	-2.28305300
H	-4.15523100	-1.07895800	-3.23854500
H	-4.68376400	-1.97186000	-1.80508200
C	-6.07644200	-0.42697300	-2.44829700
H	-6.04919900	0.56092900	-2.91861100
H	-6.66472800	-1.09585700	-3.08568400
H	-6.58188900	-0.33843500	-1.48134000
C	-2.46004600	1.87200400	-0.23156500
H	-3.48216200	1.96382800	-0.57079100
P	0.00172700	-1.45794500	0.39286900
C	1.16337500	-1.89577500	-0.97403600
C	2.51593500	-2.13270800	-0.67367000
C	0.74152100	-1.96293400	-2.31463600
C	3.42555800	-2.43088900	-1.68962600
C	1.65596400	-2.26933100	-3.32201200
H	-0.29583500	-1.77945000	-2.56061200
C	2.99868500	-2.50317500	-3.01499100
H	4.46756200	-2.60505400	-1.43821900
H	1.31498600	-2.32152200	-4.35230400
H	3.70680600	-2.73585400	-3.80535800
C	1.04541700	-1.40025800	1.89968200
C	1.14915400	-2.52519100	2.73264000
C	1.78939300	-0.24909700	2.20707500
C	1.97201000	-2.49249300	3.85968300
H	0.58716500	-3.42575100	2.50920300
C	2.60302200	-0.21973300	3.33899000
H	1.75172800	0.62392200	1.56594200

C	2. 69644600	-1. 34002700	4. 16764000
H	2. 03990600	-3. 36841700	4. 49853500
H	3. 16863200	0. 67927000	3. 56616800
H	3. 33270600	-1. 31543600	5. 04774700
C	-1. 16447200	-2. 83789100	0. 66400500
C	-2. 21803700	-2. 63135300	1. 56846300
C	-1. 02338600	-4. 07756400	0. 02993000
C	-3. 12321400	-3. 65774100	1. 83108100
H	-2. 33684500	-1. 66749400	2. 05490100
C	-1. 93575000	-5. 10122100	0. 29493100
H	-0. 21520400	-4. 24335500	-0. 67521100
C	-2. 98453300	-4. 89311200	1. 19224100
H	-3. 93847800	-3. 49183800	2. 52939900
H	-1. 82571400	-6. 06009900	-0. 20367200
H	-3. 69281400	-5. 69188200	1. 39382800
H	2. 87028400	-2. 08363300	0. 34869800

### IRC-F-37

0 1

C	0. 43320200	3. 01518500	0. 11610500
C	0. 61549000	2. 28079200	-1. 08151500
C	1. 88205100	1. 85477300	-1. 48258100
C	2. 98444100	2. 13871300	-0. 68853300
C	2. 85567200	2. 90761500	0. 47596100
C	1. 59406400	3. 35581700	0. 84960100
H	-0. 24051400	2. 06331000	-1. 70888200
H	1. 99721000	1. 27513300	-2. 39167600
H	3. 72688900	3. 14929800	1. 07154600
H	1. 47246800	3. 95826800	1. 74702100
Br	4. 69101400	1. 39717300	-1. 15442200
N	-0. 77088600	3. 49190000	0. 59179900
C	-1. 96961100	3. 02762800	0. 31952700
C	-3. 02414700	4. 04896500	0. 77606700
F	-2. 77620200	5. 28765500	0. 29708300
F	-4. 28822200	3. 73776500	0. 39772600
F	-3. 04120500	4. 15029100	2. 12781300
C	-2. 64604400	-0. 44905300	-1. 18689500
C	-1. 93297000	0. 54421500	-0. 32123700
C	-0. 77190800	0. 12158400	0. 33228100
H	-0. 32546600	0. 82251100	1. 02181400
O	-2. 10377600	-1. 45277400	-1. 63124400
O	-3. 92631800	-0. 15610900	-1. 44805800
C	-4. 63366200	-1. 09077800	-2. 30672200
H	-4. 11966000	-1. 13299000	-3. 27187200

H	-4.58089600	-2.08409400	-1.85120300
C	-6.06096700	-0.59862800	-2.43845200
H	-6.09489500	0.39204200	-2.90418400
H	-6.63037900	-1.29377900	-3.06465100
H	-6.54727900	-0.53938500	-1.45901100
C	-2.49831300	1.83040300	-0.23882300
H	-3.52323600	1.90105400	-0.57546700
P	0.03477500	-1.44158700	0.39820900
C	1.20344000	-1.88479200	-0.96213600
C	2.55947100	-2.09304400	-0.65530500
C	0.78481000	-1.99177200	-2.30133700
C	3.47464800	-2.40410300	-1.66240100
C	1.70517100	-2.31025600	-3.29970600
H	-0.25442900	-1.82984600	-2.55353400
C	3.05059900	-2.51729600	-2.98576500
H	4.51884100	-2.55554800	-1.40546300
H	1.36615900	-2.39301900	-4.32860000
H	3.76300400	-2.75973900	-3.76921900
C	1.07613000	-1.35188000	1.90546000
C	1.22149200	-2.47881500	2.72964900
C	1.77501900	-0.17591900	2.22397200
C	2.04003600	-2.42395200	3.85884600
H	0.69406300	-3.39808900	2.49821400
C	2.58411300	-0.12444500	3.35852900
H	1.70613200	0.70044700	1.59042200
C	2.71852900	-1.24680100	4.17843800
H	2.13979900	-3.30157900	4.49101900
H	3.11458600	0.79355300	3.59392600
H	3.35112800	-1.20491400	5.06056700
C	-1.11796700	-2.82849900	0.69060500
C	-2.16033300	-2.61836300	1.60733800
C	-0.98487600	-4.07012000	0.05906300
C	-3.06311600	-3.64287100	1.88418400
H	-2.27289200	-1.65295500	2.09176700
C	-1.89530700	-5.09182500	0.33803500
H	-0.18526900	-4.23875900	-0.65505300
C	-2.93335400	-4.87992300	1.24688800
H	-3.86983000	-3.47463400	2.59175400
H	-1.79213100	-6.05247100	-0.15858400
H	-3.63983700	-5.67768700	1.45882100
H	2.91213300	-2.01234800	0.36555100

IRC-F-32

0 1

C	0. 37303200	3. 01336700	0. 08741600
C	0. 56232500	2. 25289400	-1. 08815400
C	1. 83498500	1. 83831300	-1. 48579000
C	2. 93661200	2. 16042700	-0. 70271900
C	2. 79989700	2. 96083900	0. 43517100
C	1. 53260600	3. 39255300	0. 80936100
H	-0. 28968100	2. 00841800	-1. 71010300
H	1. 95546700	1. 23685600	-2. 38087800
H	3. 67063800	3. 23293200	1. 02272600
H	1. 40489500	4. 01785300	1. 68657700
Br	4. 65319400	1. 44053200	-1. 16579500
N	-0. 83617900	3. 47478600	0. 56423800
C	-2. 03040100	2. 99058400	0. 30198200
C	-3. 09564300	4. 00719900	0. 74413100
F	-2. 86074700	5. 23975200	0. 24309200
F	-4. 35680500	3. 67649500	0. 37247800
F	-3. 11298200	4. 13256000	2. 09381400
C	-2. 63082100	-0. 50541400	-1. 18775300
C	-1. 94854200	0. 50594300	-0. 31922900
C	-0. 77405700	0. 12110400	0. 32866000
H	-0. 34858200	0. 83427700	1. 01829200
O	-2. 05437600	-1. 48679600	-1. 63860400
O	-3. 92029600	-0. 25526600	-1. 44774100
C	-4. 58637000	-1. 20196700	-2. 32688600
H	-4. 07318400	-1. 19422500	-3. 29327500
H	-4. 48406800	-2. 20261900	-1. 89778600
C	-6. 03553000	-0. 77647500	-2. 44728900
H	-6. 11708800	0. 23056000	-2. 86847700
H	-6. 56448000	-1. 47055400	-3. 10896800
H	-6. 53035600	-0. 78692500	-1. 47095000
C	-2. 54400200	1. 77963300	-0. 23927100
H	-3. 57296700	1. 82681800	-0. 56805000
P	0. 07210800	-1. 42177700	0. 40248400
C	1. 24771200	-1. 86680900	-0. 95208400
C	2. 60598000	-2. 05043800	-0. 63862900
C	0. 83333900	-2. 01149900	-2. 28923100
C	3. 52621600	-2. 37868700	-1. 63561100
C	1. 75925400	-2. 34565000	-3. 27751900
H	-0. 20687700	-1. 86846400	-2. 54785800
C	3. 10589200	-2. 53197800	-2. 95608500
H	4. 57141800	-2. 51230300	-1. 37283900
H	1. 42299200	-2. 45922600	-4. 30437300
H	3. 82198700	-2. 78972300	-3. 73137400
C	1. 11028200	-1. 29749700	1. 90960500

C	1. 29287900	-2. 42201900	2. 72982200
C	1. 76422700	-0. 09845200	2. 23636100
C	2. 10302300	-2. 34233000	3. 86334900
H	0. 80101600	-3. 35928300	2. 49149100
C	2. 56455900	-0. 02225400	3. 37586600
H	1. 66537300	0. 77854600	1. 60787900
C	2. 73542200	-1. 14215900	4. 19202900
H	2. 23294800	-3. 21892400	4. 49146900
H	3. 05804300	0. 91425900	3. 61899600
H	3. 36059100	-1. 08056600	5. 07829400
C	-1. 06396900	-2. 81653300	0. 71780600
C	-2. 09718400	-2. 59904200	1. 64332900
C	-0. 93528900	-4. 06305900	0. 09590800
C	-2. 99640500	-3. 62109900	1. 93827800
H	-2. 20511600	-1. 62953800	2. 12048500
C	-1. 84246000	-5. 08267200	0. 39316900
H	-0. 14355900	-4. 23639400	-0. 62588800
C	-2. 87194400	-4. 86327300	1. 31004900
H	-3. 79583800	-3. 44682300	2. 65266700
H	-1. 74502000	-6. 04714900	-0. 09704800
H	-3. 57673700	-5. 65893800	1. 53491600
H	2. 95646100	-1. 93842700	0. 37999400

### IRC-F-27

0 1

C	0. 30369500	2. 99783100	0. 06952200
C	0. 50682400	2. 19976000	-1. 08266000
C	1. 78289300	1. 80100200	-1. 47389200
C	2. 88253800	2. 18057200	-0. 71491600
C	2. 73478600	3. 02002600	0. 39486300
C	1. 46017000	3. 43264400	0. 76485300
H	-0. 34248300	1. 92084400	-1. 69136600
H	1. 91111100	1. 16999500	-2. 34712200
H	3. 60259400	3. 34064100	0. 95778800
H	1. 32404800	4. 08803000	1. 61785300
Br	4. 61346300	1. 49734500	-1. 17923100
N	-0. 91184600	3. 44513400	0. 54070700
C	-2. 10105600	2. 94238000	0. 28625300
C	-3. 17725300	3. 95621200	0. 70750200
F	-2. 95191600	5. 18016300	0. 18136100
F	-4. 43445700	3. 60663600	0. 33902000
F	-3. 20052700	4. 10994500	2. 05413300
C	-2. 61430900	-0. 56878000	-1. 19141200
C	-1. 96934000	0. 46066200	-0. 31740700

C	-0.78198800	0.11469800	0.32914500
H	-0.38952400	0.83935100	1.02607200
O	-2.00056000	-1.52362700	-1.64980600
O	-3.91173900	-0.36474600	-1.45016600
C	-4.54090100	-1.32959100	-2.33706500
H	-4.02641200	-1.29638600	-3.30217600
H	-4.40236800	-2.32854300	-1.91428400
C	-6.00452000	-0.95747700	-2.45796000
H	-6.12267800	0.04830800	-2.87327000
H	-6.50582300	-1.66669400	-3.12506800
H	-6.50056500	-0.99243400	-1.48286800
C	-2.59895600	1.71814800	-0.23629300
H	-3.63124200	1.74005500	-0.55715500
P	0.11375200	-1.39607400	0.40462500
C	1.29804400	-1.83773200	-0.94476600
C	2.65751400	-1.99927200	-0.62324700
C	0.89022100	-2.01923100	-2.27961500
C	3.58376200	-2.34726200	-1.60798700
C	1.82272600	-2.37083800	-3.25587100
H	-0.15014000	-1.89347200	-2.54574400
C	3.16934800	-2.53988300	-2.92511900
H	4.62903100	-2.46518300	-1.33804100
H	1.49091000	-2.51331200	-4.28054300
H	3.88986000	-2.81394400	-3.69063800
C	1.14733000	-1.23628200	1.91147800
C	1.35941500	-2.35538900	2.73215000
C	1.75973700	-0.01727400	2.24393100
C	2.15619200	-2.25108800	3.87275500
H	0.89941700	-3.30757100	2.48942100
C	2.54682400	0.08322100	3.39103100
H	1.63690200	0.85687500	1.61584000
C	2.74569600	-1.03111300	4.20834500
H	2.30872400	-3.12365200	4.50134400
H	3.00716000	1.03497900	3.63968700
H	3.35949900	-0.94985800	5.10092700
C	-1.00007300	-2.80112600	0.74224900
C	-2.02850900	-2.57560600	1.67133400
C	-0.86682800	-4.05478400	0.13751100
C	-2.91957900	-3.59765500	1.98731100
H	-2.13879600	-1.59989200	2.13470300
C	-1.76611100	-5.07491700	0.45615300
H	-0.07891200	-4.23324300	-0.58726100
C	-2.79108000	-4.84787800	1.37623300
H	-3.71544100	-3.41762700	2.70421500

H	-1. 66675900	-6. 04596700	-0. 02040700
H	-3. 48971200	-5. 64432100	1. 61681200
H	3. 00426300	-1. 85644300	0. 39273800

### IRC-F-22

0 1

C	0. 23384300	2. 97412900	0. 05510600
C	0. 45069500	2. 12597600	-1. 05899300
C	1. 73530600	1. 74177200	-1. 44100500
C	2. 82855300	2. 19001500	-0. 71493900
C	2. 66739900	3. 07845300	0. 35499300
C	1. 38546300	3. 46983300	0. 71985600
H	-0. 39076900	1. 81859400	-1. 66567500
H	1. 87493300	1. 08023800	-2. 28899000
H	3. 53272900	3. 44724500	0. 89989300
H	1. 23791000	4. 15676100	1. 55000500
Br	4. 57524400	1. 56197700	-1. 19314900
N	-0. 98590200	3. 41060400	0. 51949200
C	-2. 17171200	2. 89053100	0. 27196600
C	-3. 25798100	3. 90100100	0. 67106400
F	-3. 04043400	5. 11652700	0. 12211900
F	-4. 51051000	3. 53360900	0. 30315100
F	-3. 29025300	4. 08137000	2. 01435000
C	-2. 59485800	-0. 62961700	-1. 19671000
C	-1. 99105400	0. 41406600	-0. 31413800
C	-0. 79249500	0. 11306400	0. 33278100
H	-0. 43679200	0. 84225900	1. 04619800
O	-1. 94741100	-1. 56054300	-1. 65884100
O	-3. 89749000	-0. 46656000	-1. 45822900
C	-4. 49914600	-1. 45313500	-2. 33927400
H	-3. 98563900	-1. 41265800	-3. 30458500
H	-4. 33484600	-2. 44548500	-1. 91000900
C	-5. 97183600	-1. 11889400	-2. 46183900
H	-6. 11467600	-0. 11786100	-2. 88051100
H	-6. 45550100	-1. 84240300	-3. 12639800
H	-6. 46677200	-1. 16253700	-1. 48668500
C	-2. 65338500	1. 65488900	-0. 23379100
H	-3. 68749300	1. 65325300	-0. 54973100
P	0. 15440800	-1. 36690400	0. 40412700
C	1. 34715800	-1. 80619800	-0. 94008000
C	2. 70696200	-1. 94898900	-0. 61006200
C	0. 94691800	-2. 02017300	-2. 27259100
C	3. 64004400	-2. 31228700	-1. 58282400
C	1. 88688900	-2. 38469600	-3. 23718200

H	-0.09324800	-1.91041100	-2.54602700
C	3.23318600	-2.53684500	-2.89722000
H	4.68484500	-2.41629400	-1.30556800
H	1.56049300	-2.55170900	-4.25985900
H	3.95897600	-2.82262000	-3.65334200
C	1.18048400	-1.17576800	1.91151500
C	1.41251400	-2.28944200	2.73406100
C	1.75835500	0.05834700	2.24907100
C	2.19476100	-2.16592400	3.88222800
H	0.97811400	-3.25247700	2.48744300
C	2.53177300	0.17765000	3.40391800
H	1.61749800	0.92928700	1.62045300
C	2.75006700	-0.93150700	4.22328900
H	2.36249900	-3.03440800	4.51255600
H	2.96541400	1.14051100	3.65757900
H	3.35231000	-0.83478800	5.12217000
C	-0.93724800	-2.78150500	0.76029800
C	-1.96461400	-2.55137500	1.68951800
C	-0.79148500	-4.04164000	0.17436600
C	-2.84257500	-3.57732500	2.02589700
H	-2.08353100	-1.56966000	2.13706700
C	-1.67784200	-5.06618000	0.51370300
H	-0.00451800	-4.22213500	-0.55091500
C	-2.70117700	-4.83565100	1.43470800
H	-3.63760400	-3.39494600	2.74312500
H	-1.57010900	-6.04386300	0.05269000
H	-3.38914800	-5.63636300	1.69136000
H	3.04876900	-1.77957100	0.40347600

### IRC-F-17

0 1

C	0.17655100	2.94795300	0.04825100
C	0.40798200	2.04356900	-1.02067600
C	1.69890400	1.66759300	-1.39238800
C	2.78391100	2.18482500	-0.70279600
C	2.60972000	3.12865900	0.31904600
C	1.32245300	3.50496200	0.67554800
H	-0.42876300	1.71525900	-1.62952600
H	1.85054900	0.98449700	-2.22036300
H	3.46974000	3.55104500	0.82819200
H	1.16361100	4.23157800	1.46693600
Br	4.54182200	1.62062500	-1.20446900
N	-1.04538700	3.37809300	0.50401400
C	-2.22877300	2.84628800	0.25829000

C	-3.32364600	3.85268600	0.63938900
F	-3.11344800	5.06197300	0.07346900
F	-4.57158500	3.46982900	0.27067200
F	-3.36480200	4.05378000	1.97966900
C	-2.57439100	-0.67799900	-1.20250400
C	-2.00539100	0.37712300	-0.31637900
C	-0.79406000	0.11973600	0.32668700
H	-0.47605500	0.83982100	1.05448100
O	-1.90331400	-1.59436300	-1.66094400
O	-3.87903900	-0.54373700	-1.46916500
C	-4.46393300	-1.55442100	-2.33179200
H	-3.95113900	-1.52532300	-3.29795700
H	-4.28695200	-2.53652900	-1.88397100
C	-5.94063700	-1.24078500	-2.46023700
H	-6.09569600	-0.25241500	-2.90431000
H	-6.41793300	-1.98655700	-3.10476100
H	-6.43327000	-1.26458900	-1.48302300
C	-2.69527400	1.60268800	-0.23676700
H	-3.72943500	1.58215500	-0.55216400
P	0.18684800	-1.33997800	0.40123200
C	1.38756200	-1.78584800	-0.93453100
C	2.74734900	-1.91398800	-0.59791400
C	0.99329600	-2.02345800	-2.26482500
C	3.68665100	-2.28212000	-1.56301100
C	1.93976200	-2.39122200	-3.22188600
H	-0.04695800	-1.92732800	-2.54285200
C	3.28649500	-2.52542800	-2.87620900
H	4.73141000	-2.37234900	-1.28085400
H	1.61785300	-2.57404900	-4.24324600
H	4.01762900	-2.81253300	-3.62660900
C	1.20235700	-1.12378000	1.91109100
C	1.44617600	-2.23395200	2.73495200
C	1.75523200	0.12014900	2.25383400
C	2.21746200	-2.09872700	3.88861500
H	1.02941400	-3.20397500	2.48568700
C	2.51897800	0.25068600	3.41408700
H	1.60247200	0.98908300	1.62561700
C	2.75037800	-0.85560000	4.23366400
H	2.39490300	-2.96422100	4.52038700
H	2.93486900	1.22041000	3.67136600
H	3.34510300	-0.74911600	5.13646000
C	-0.89099400	-2.75750500	0.77127100
C	-1.91935400	-2.52772800	1.69962600
C	-0.72846700	-4.02127400	0.20018600

C	-2.77992100	-3.56199700	2.05331700
H	-2.04928700	-1.54274600	2.13612000
C	-1.59734800	-5.05402700	0.55715200
H	0.06016800	-4.20077600	-0.52343100
C	-2.61929700	-4.82634400	1.48009100
H	-3.57551600	-3.38323100	2.77081800
H	-1.47739500	-6.03663600	0.10987100
H	-3.29353400	-5.63426300	1.75047500
H	3.08439000	-1.72580500	0.41397100

### IRC-F-11

0 1

C	0.11305900	2.90970600	0.05172500
C	0.35604500	1.93530200	-0.96125700
C	1.66105600	1.57418400	-1.32333600
C	2.73059000	2.17215200	-0.68782000
C	2.54166700	3.17576200	0.27717600
C	1.25218600	3.53234800	0.63085600
H	-0.45592300	1.62424800	-1.59764700
H	1.82349400	0.84593800	-2.10912300
H	3.39696000	3.66624900	0.72961200
H	1.07929800	4.31139700	1.36760400
Br	4.50277000	1.68916800	-1.21541200
N	-1.10547700	3.34000100	0.49526500
C	-2.28888700	2.80031900	0.24395300
C	-3.39212400	3.79959200	0.60797600
F	-3.19475000	5.00591200	0.02907500
F	-4.63416100	3.39799900	0.23819800
F	-3.44152300	4.01889000	1.94549400
C	-2.54694700	-0.72307200	-1.20846800
C	-2.00758900	0.34538400	-0.33321700
C	-0.76502000	0.14714500	0.27564600
H	-0.51134200	0.83539000	1.06688400
O	-1.85881600	-1.63416800	-1.65516600
O	-3.85537600	-0.61766900	-1.47411500
C	-4.42247100	-1.65127600	-2.31798400
H	-3.90876100	-1.63374400	-3.28399800
H	-4.23236200	-2.62260300	-1.85194600
C	-5.90337300	-1.36159700	-2.45374200
H	-6.07129800	-0.38319300	-2.91482200
H	-6.36928900	-2.12509500	-3.08561200
H	-6.39632900	-1.37519300	-1.47651800
C	-2.73288800	1.54915800	-0.24071800
H	-3.77064700	1.49980800	-0.54099300

P	0.22154500	-1.31056200	0.39356600
C	1.43006700	-1.77073100	-0.92550100
C	2.79020500	-1.88059400	-0.58396800
C	1.03903300	-2.02789500	-2.25288800
C	3.73524600	-2.24228000	-1.54585400
C	1.99135900	-2.38953300	-3.20597300
H	-0.00223300	-1.94774800	-2.53219600
C	3.33970600	-2.49858900	-2.85809000
H	4.78094200	-2.31735500	-1.26284100
H	1.67364100	-2.58587100	-4.22609900
H	4.07602500	-2.77857300	-3.60613400
C	1.21913100	-1.07102300	1.91144900
C	1.47477800	-2.17744000	2.73758400
C	1.74940800	0.18142300	2.25810600
C	2.23891500	-2.03100600	3.89428900
H	1.07394600	-3.15337400	2.48564200
C	2.50760200	0.32254300	3.42110000
H	1.58360800	1.04971800	1.63249400
C	2.75359000	-0.78039200	4.24060900
H	2.42541700	-2.89435700	4.52630400
H	2.90641300	1.29856000	3.68143800
H	3.34388700	-0.66605000	5.14529300
C	-0.85077400	-2.72562700	0.78066900
C	-1.88171300	-2.50729700	1.70895500
C	-0.66323800	-3.99027000	0.22119200
C	-2.71516500	-3.55919900	2.07734400
H	-2.03470200	-1.52062500	2.13454700
C	-1.50305700	-5.04030500	0.59398100
H	0.12505500	-4.15648400	-0.50567700
C	-2.52469800	-4.82706200	1.52041800
H	-3.51217100	-3.39061000	2.79572800
H	-1.35980100	-6.02419200	0.15673700
H	-3.17538400	-5.64824400	1.80746400
H	3.12300800	-1.67991800	0.42699800

### IRC-F-5

0 1

C	0.06182200	2.88014400	0.06703800
C	0.29199600	1.79618500	-0.87348000
C	1.63585200	1.50773500	-1.27588800
C	2.68252000	2.16530000	-0.69057600
C	2.48960200	3.20531700	0.25412100
C	1.20397200	3.55064600	0.60138700
H	-0.46862500	1.64601400	-1.63074600

H	1.81134300	0.77731700	-2.05629100
H	3.34396100	3.72541800	0.67272900
H	1.01952100	4.36295700	1.29849000
Br	4.47599500	1.73744500	-1.22391100
N	-1.13922700	3.31561900	0.49295200
C	-2.33178000	2.77336900	0.23157700
C	-3.43575100	3.76184100	0.58972700
F	-3.25209300	4.97070500	0.00693100
F	-4.67463100	3.34677900	0.22169800
F	-3.49035900	3.99236500	1.92707600
C	-2.52627400	-0.74617600	-1.20564300
C	-2.00702200	0.32906000	-0.35287500
C	-0.68522900	0.23960700	0.17646200
H	-0.56633900	0.79770300	1.09907000
O	-1.83106700	-1.66109100	-1.64463500
O	-3.84338100	-0.66551500	-1.47093900
C	-4.39579300	-1.71068800	-2.30614200
H	-3.88344100	-1.69588500	-3.27326600
H	-4.19681100	-2.67815700	-1.83521300
C	-5.88104600	-1.44083400	-2.44705400
H	-6.06037900	-0.46706800	-2.91382200
H	-6.33663000	-2.21352000	-3.07543100
H	-6.37600800	-1.45454100	-1.47074300
C	-2.75289600	1.51418700	-0.24130600
H	-3.79476100	1.44332800	-0.52518000
P	0.24896100	-1.28915300	0.38277800
C	1.45836200	-1.76230400	-0.91909400
C	2.81854400	-1.85763900	-0.57574000
C	1.06578000	-2.02908000	-2.24389700
C	3.76600100	-2.21041500	-1.53782000
C	2.02113200	-2.38311100	-3.19625200
H	0.02257900	-1.95868000	-2.51975300
C	3.37099700	-2.47406500	-2.84889200
H	4.81295900	-2.27248900	-1.25670400
H	1.70530700	-2.58615300	-4.21556700
H	4.10986300	-2.74630700	-3.59723000
C	1.22974800	-1.04205000	1.91266800
C	1.49607100	-2.14508100	2.74209100
C	1.74556600	0.21602100	2.26001500
C	2.25789200	-1.98805600	3.89914300
H	1.10626800	-3.12596500	2.49212900
C	2.50274700	0.36712400	3.42251100
H	1.57038400	1.08334100	1.63618800
C	2.76017900	-0.73150600	4.24354100

H	2. 45250500	-2. 84813300	4. 53311900
H	2. 89017800	1. 34812600	3. 68096100
H	3. 34892300	-0. 60968200	5. 14822500
C	-0. 82931800	-2. 70274200	0. 78544600
C	-1. 85839000	-2. 50242600	1. 71933200
C	-0. 62063100	-3. 97037800	0. 23420800
C	-2. 67243900	-3. 56959400	2. 09297900
H	-2. 02996200	-1. 51934100	2. 14711700
C	-1. 43764300	-5. 03539200	0. 61601400
H	0. 16774800	-4. 12789400	-0. 49417800
C	-2. 46226100	-4. 83699900	1. 54249500
H	-3. 46996900	-3. 41129200	2. 81303300
H	-1. 27415200	-6. 01848400	0. 18415500
H	-3. 09753600	-5. 66795700	1. 83569500
H	3. 14890100	-1. 64907200	0. 43443600

### IRC-1

0 1

C	0. 02895500	2. 86788000	0. 07809800
C	0. 23913000	1. 69880400	-0. 81543900
C	1. 62463500	1. 46859600	-1. 24730700
C	2. 65250800	2. 16359600	-0. 69616600
C	2. 45865000	3. 22377500	0. 24319800
C	1. 17591200	3. 56225900	0. 58499600
H	-0. 45843300	1. 67784800	-1. 65118800
H	1. 81077900	0. 73453600	-2. 02138100
H	3. 31293700	3. 75538700	0. 64613700
H	0. 98398100	4. 38837100	1. 26380100
Br	4. 46022000	1. 76658100	-1. 22934900
N	-1. 15853100	3. 30403000	0. 49060100
C	-2. 36024800	2. 75861400	0. 22403300
C	-3. 46198400	3. 73814100	0. 57933300
F	-3. 28737500	4. 94974000	-0. 00493200
F	-4. 69939000	3. 31533800	0. 21313900
F	-3. 52011600	3. 97587500	1. 91744400
C	-2. 51380800	-0. 75860700	-1. 20184400
C	-2. 01051600	0. 32045300	-0. 36682000
C	-0. 63034100	0. 31391800	0. 11460300
H	-0. 59034200	0. 77268800	1. 10096700
O	-1. 81458800	-1. 67744200	-1. 63858400
O	-3. 83813600	-0. 69487200	-1. 46861200
C	-4. 38011400	-1. 74600600	-2. 29911400
H	-3. 86934700	-1. 73267300	-3. 26747200
H	-4. 17620700	-2. 71204800	-1. 82672200

C	-5.86821500	-1.48851800	-2.44281000
H	-6.05458100	-0.51728500	-2.91229100
H	-6.31804000	-2.26628000	-3.06922800
H	-6.36396600	-1.50259000	-1.46679800
C	-2.76432900	1.49423700	-0.24267000
H	-3.80800000	1.41127200	-0.51927600
P	0.26712800	-1.27836900	0.37610900
C	1.47585300	-1.75927600	-0.91538900
C	2.83594800	-1.84396400	-0.57137900
C	1.08159000	-2.02979500	-2.23889000
C	3.78453800	-2.19008300	-1.53394100
C	2.03885600	-2.37803700	-3.19115300
H	0.03678900	-1.96485500	-2.51158300
C	3.38959700	-2.45810600	-2.84428200
H	4.83230500	-2.24398300	-1.25436600
H	1.72423900	-2.58441500	-4.21012400
H	4.12990100	-2.72521400	-3.59301300
C	1.23676800	-1.02589000	1.91366900
C	1.50973600	-2.12650000	2.74513800
C	1.74365200	0.23568400	2.26117800
C	2.27020600	-1.96272600	3.90222300
H	1.12668700	-3.11037700	2.49654900
C	2.50008700	0.39337600	3.42315300
H	1.56331800	1.10285500	1.63899100
C	2.76458300	-0.70249700	4.24523000
H	2.46997800	-2.82063900	4.53745400
H	2.88029700	1.37745800	3.68032600
H	3.35217800	-0.57586600	5.14995700
C	-0.81690300	-2.69074700	0.78757400
C	-1.84360100	-2.50218700	1.72570800
C	-0.59441000	-3.96077400	0.24149200
C	-2.64641600	-3.57805600	2.10204000
H	-2.02602900	-1.52188900	2.15524000
C	-1.39840500	-5.03421900	0.62865200
H	0.19350600	-4.11341100	-0.48815600
C	-2.42512000	-4.84465600	1.55488800
H	-3.44406100	-3.42539800	2.82307400
H	-1.22304600	-6.01649500	0.19968400
H	-3.05156500	-5.68117000	1.85112400
H	3.16479200	-1.63103900	0.43838000

### IRC-R-5

0 1

C	-0.01945600	2.84944300	0.08666400
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C	0.19139900	1.62082900	-0.76873200
C	1.60759500	1.41787000	-1.19875600
C	2.61292400	2.16549700	-0.69207600
C	2.40632700	3.25576500	0.21994500
C	1.12295800	3.57995000	0.55868200
H	-0.44715600	1.67091500	-1.65562300
H	1.80860200	0.67282800	-1.95729000
H	3.25477600	3.81425500	0.59733300
H	0.91893700	4.42360400	1.21197200
Br	4.42993300	1.81727300	-1.23754100
N	-1.20221300	3.28300100	0.48380000
C	-2.40694400	2.72849100	0.21507600
C	-3.51323800	3.69720600	0.56184600
F	-3.35111900	4.90934000	-0.02826000
F	-4.74602100	3.25953200	0.19645900
F	-3.57780800	3.94621900	1.89922400
C	-2.49532700	-0.78730100	-1.20229200
C	-2.01533100	0.30070400	-0.38173800
C	-0.60282500	0.35504900	0.07892100
H	-0.61207700	0.74971600	1.09746100
O	-1.78290100	-1.70209300	-1.63480900
O	-3.82503200	-0.74935500	-1.46891900
C	-4.35006400	-1.81270900	-2.29105300
H	-3.83972000	-1.80141700	-3.25993300
H	-4.13559900	-2.77368700	-1.81249200
C	-5.84174900	-1.57596200	-2.43890900
H	-6.03980600	-0.61024700	-2.91510100
H	-6.28141600	-2.36349700	-3.06041100
H	-6.33858000	-1.58912500	-1.46335900
C	-2.78795100	1.45794300	-0.24803700
H	-3.83098800	1.35614700	-0.52225400
P	0.29543600	-1.26132100	0.36907000
C	1.50804400	-1.75415500	-0.91006600
C	2.86821900	-1.82290800	-0.56390800
C	1.11509100	-2.03319600	-2.23203900
C	3.82044100	-2.15849000	-1.52607500
C	2.07654000	-2.37154400	-3.18334000
H	0.06901000	-1.97876600	-2.50336800
C	3.42824300	-2.43255300	-2.83622300
H	4.86891000	-2.19910500	-1.24702500
H	1.76482900	-2.58386400	-4.20194400
H	4.17197900	-2.69009700	-3.58485300
C	1.25253900	-0.99458000	1.91353100
C	1.53549000	-2.09163000	2.74702600

C	1. 74054700	0. 27329500	2. 26494600
C	2. 28959200	-1. 91815900	3. 90687400
H	1. 16569700	-3. 08035600	2. 49763100
C	2. 49157000	0. 44050800	3. 42900500
H	1. 55064000	1. 13983200	1. 64519200
C	2. 76787500	-0. 65204200	4. 25129000
H	2. 49724400	-2. 77340000	4. 54315400
H	2. 85753600	1. 42957600	3. 68759200
H	3. 35116300	-0. 51823500	5. 15775100
C	-0. 78809600	-2. 67279800	0. 79131500
C	-1. 81398400	-2. 49639300	1. 73246100
C	-0. 54647300	-3. 94379700	0. 25336300
C	-2. 59849300	-3. 58391000	2. 11624400
H	-2. 01120900	-1. 51806900	2. 15953600
C	-1. 33040200	-5. 02841900	0. 64988600
H	0. 24170000	-4. 08936200	-0. 47713500
C	-2. 35819600	-4. 85034100	1. 57714500
H	-3. 39661800	-3. 43962900	2. 83843900
H	-1. 13854600	-6. 01021500	0. 22694300
H	-2. 96984400	-5. 69510600	1. 88079700
H	3. 19362800	-1. 60265700	0. 44543800

### IRC-R-9

0 1

C	-0. 05988300	2. 84942600	0. 07947200
C	0. 16676900	1. 61758600	-0. 76855000
C	1. 58658000	1. 42352700	-1. 19114200
C	2. 58129600	2. 19094900	-0. 69555900
C	2. 36047800	3. 29052300	0. 20180900
C	1. 07346100	3. 60068300	0. 53985000
H	-0. 46620900	1. 65906000	-1. 65906800
H	1. 79691500	0. 67062200	-1. 93974700
H	3. 20168200	3. 86590600	0. 56956700
H	0. 85917000	4. 44903400	1. 18343300
Br	4. 39961500	1. 85917700	-1. 24378300
N	-1. 24774000	3. 26849500	0. 47516300
C	-2. 44587600	2. 69662400	0. 20957500
C	-3. 56380900	3. 65581800	0. 54517900
F	-3. 41237200	4. 86432500	-0. 05561400
F	-4. 79064100	3. 20193300	0. 17953700
F	-3. 63617700	3. 91722300	1. 87984400
C	-2. 47798100	-0. 82035100	-1. 20587700
C	-2. 01881300	0. 27363300	-0. 38270000
C	-0. 60586100	0. 35116000	0. 07703200

H	-0.62231300	0.74293700	1.09658600
O	-1.74766700	-1.72078000	-1.63944800
O	-3.80794000	-0.80705300	-1.47436400
C	-4.31251900	-1.88604000	-2.28878500
H	-3.79860300	-1.87590000	-3.25569300
H	-4.08435800	-2.83887700	-1.80026500
C	-5.80727200	-1.67531200	-2.44435100
H	-6.01920500	-0.71965700	-2.93380200
H	-6.23199300	-2.47778000	-3.05653800
H	-6.30703500	-1.68369000	-1.47056400
C	-2.80882700	1.41937900	-0.24947700
H	-3.85027200	1.30170800	-0.52387700
P	0.32188800	-1.24829200	0.36718700
C	1.53933100	-1.74419900	-0.90782700
C	2.89854300	-1.81129600	-0.55637000
C	1.15182800	-2.03236000	-2.22958300
C	3.85424800	-2.15487400	-1.51243400
C	2.11697700	-2.37731200	-3.17493700
H	0.10689400	-1.97998900	-2.50553300
C	3.46728900	-2.43730600	-2.82233200
H	4.90148600	-2.19549700	-1.22865800
H	1.80898200	-2.59622600	-4.19326900
H	4.21371300	-2.70107200	-3.56614200
C	1.27528100	-0.96512600	1.91171400
C	1.57815700	-2.06141400	2.73937400
C	1.73130800	0.31110500	2.27550700
C	2.31956400	-1.87952400	3.90585300
H	1.23269500	-3.05650500	2.48036200
C	2.46925400	0.48683300	3.44691300
H	1.52495400	1.17801600	1.66135700
C	2.76472700	-0.60495700	4.26348500
H	2.54264800	-2.73463300	4.53706300
H	2.80935600	1.48226200	3.71622100
H	3.33709600	-0.46414000	5.17580300
C	-0.75284500	-2.66018000	0.80179600
C	-1.77612000	-2.47800000	1.74460800
C	-0.50941800	-3.93398400	0.27248600
C	-2.55691400	-3.56400600	2.13919100
H	-1.97355800	-1.49685300	2.16500400
C	-1.28925000	-5.01723300	0.68027700
H	0.27643500	-4.08235200	-0.45999000
C	-2.31458300	-4.83398300	1.60935200
H	-3.35321800	-3.41587000	2.86263500
H	-1.09660900	-6.00195300	0.26461200

H	-2.92322500	-5.67773500	1.92169700
H	3.22074700	-1.58447700	0.45255500

### IRC-R-12

0 1

C	-0.08764200	2.85212800	0.06847600
C	0.14967700	1.62003800	-0.77647300
C	1.57030800	1.43330600	-1.19700600
C	2.55899700	2.21014300	-0.70449100
C	2.32927100	3.31344200	0.18669200
C	1.03992000	3.61522600	0.52421800
H	-0.48333700	1.65465800	-1.66754200
H	1.78652300	0.67695800	-1.93998900
H	3.16591900	3.89819700	0.55051100
H	0.81969700	4.46550800	1.16357900
Br	4.37854000	1.88485500	-1.25032300
N	-1.27942700	3.26008900	0.46409800
C	-2.47190200	2.67463100	0.20046300
C	-3.60000500	3.62354100	0.53152000
F	-3.46273500	4.82970700	-0.07753400
F	-4.82220100	3.15371900	0.17036800
F	-3.67392500	3.89312500	1.86440700
C	-2.46327200	-0.84507000	-1.20910600
C	-2.01931400	0.25499100	-0.38637300
C	-0.60753000	0.34966600	0.07232900
H	-0.62747600	0.74346500	1.09046500
O	-1.71953600	-1.73507300	-1.64154800
O	-3.79280700	-0.85087600	-1.47871500
C	-4.27998500	-1.93496400	-2.29710100
H	-3.76989600	-1.90972400	-3.26587400
H	-4.03223200	-2.88598400	-1.81470200
C	-5.77890000	-1.75138700	-2.44622200
H	-6.01052300	-0.79500000	-2.92617300
H	-6.19028300	-2.55631400	-3.06485400
H	-6.27539000	-1.77818900	-1.47066300
C	-2.82160300	1.39245300	-0.25546300
H	-3.86166900	1.26315000	-0.52999800
P	0.33920500	-1.23710700	0.36666200
C	1.55962700	-1.74122700	-0.90343900
C	2.91801900	-1.80559600	-0.54753500
C	1.17626800	-2.04492800	-2.22302000
C	3.87591800	-2.16409600	-1.49591400
C	2.14372100	-2.40411900	-3.16074400
H	0.13248000	-1.99457900	-2.50323000

C	3.49265300	-2.46329200	-2.80314000
H	4.92213900	-2.20280700	-1.20809200
H	1.83825000	-2.63525000	-4.17714200
H	4.24078700	-2.73862300	-3.54100700
C	1.29228500	-0.93885900	1.90894400
C	1.61527200	-2.03292600	2.73211100
C	1.72461000	0.34383300	2.27808800
C	2.35323100	-1.84273800	3.89926200
H	1.28724500	-3.03298700	2.46920000
C	2.45875000	0.52798700	3.45076900
H	1.50231100	1.20955600	1.66775600
C	2.77434600	-0.56159100	4.26263700
H	2.59179400	-2.69630100	4.52692400
H	2.78044400	1.52833500	3.72446300
H	3.34370900	-0.41408500	5.17577300
C	-0.73193700	-2.64584900	0.81706900
C	-1.74784500	-2.45349200	1.76589400
C	-0.49718800	-3.92339500	0.29355500
C	-2.53015000	-3.53369300	2.17284700
H	-1.93816600	-1.46898300	2.18172100
C	-1.27851400	-5.00085000	0.71365200
H	0.28247700	-4.07906400	-0.44405600
C	-2.29640500	-4.80774100	1.64896500
H	-3.32071300	-3.37811500	2.90100800
H	-1.09288300	-5.98894500	0.30276100
H	-2.90581100	-5.64734600	1.97086400
H	3.23802800	-1.56625400	0.45913000

### IRC-R-15

O 1			
C	-0.10049800	2.85396700	0.05222700
C	0.14261400	1.61690600	-0.78608600
C	1.56585000	1.43263500	-1.20232100
C	2.55003700	2.21750000	-0.71444500
C	2.31441200	3.32727000	0.16756700
C	1.02362400	3.62584800	0.50189000
H	-0.48668700	1.64757300	-1.67984800
H	1.78655100	0.67068800	-1.93845000
H	3.14822700	3.91826200	0.52766900
H	0.79921100	4.47959400	1.13515600
Br	4.37208000	1.89441400	-1.25307800
N	-1.29348700	3.25680500	0.44824000
C	-2.48403700	2.66413300	0.19026200
C	-3.61620600	3.60669600	0.52435700

F	-3.49118100	4.81147700	-0.09027200
F	-4.83742800	3.12701300	0.17290400
F	-3.68364500	3.88123200	1.85665700
C	-2.45453000	-0.85773300	-1.21300800
C	-2.01828400	0.24704000	-0.39365200
C	-0.60564200	0.35263000	0.06364600
H	-0.62978500	0.74702300	1.08199900
O	-1.70486800	-1.74640100	-1.63850100
O	-3.78288300	-0.87104700	-1.48846400
C	-4.26094300	-1.96247600	-2.30248300
H	-3.74927600	-1.93820700	-3.27044900
H	-4.00736300	-2.90939900	-1.81516800
C	-5.76085700	-1.79065300	-2.45541900
H	-5.99877000	-0.83888800	-2.94138800
H	-6.16521300	-2.60217400	-3.07003400
H	-6.25883600	-1.81546000	-1.48067100
C	-2.82744200	1.37939900	-0.26306100
H	-3.86729800	1.24331700	-0.53533700
P	0.34632300	-1.23013800	0.36670400
C	1.56595100	-1.74882600	-0.89907500
C	2.92371300	-1.81610800	-0.54050100
C	1.18386800	-2.06402300	-2.21637000
C	3.88125000	-2.19085100	-1.48289400
C	2.15104800	-2.43909500	-3.14817400
H	0.14108400	-2.01102700	-2.49948300
C	3.49883400	-2.50284800	-2.78734200
H	4.92667400	-2.23219000	-1.19246400
H	1.84597900	-2.67926900	-4.16259100
H	4.24667600	-2.79123400	-3.52048400
C	1.30286200	-0.92008900	1.90470100
C	1.64407000	-2.01208100	2.72339500
C	1.71994500	0.36698200	2.27531400
C	2.38570900	-1.81566700	3.88704800
H	1.32752800	-3.01562500	2.45929600
C	2.45732700	0.55752800	3.44508300
H	1.48322500	1.23147900	1.66872500
C	2.79171300	-0.52999900	4.25196200
H	2.63884700	-2.66772700	4.51100600
H	2.76699700	1.56126500	3.72017300
H	3.36381800	-0.37752700	5.16257800
C	-0.72792900	-2.63054200	0.83525300
C	-1.73324400	-2.42452900	1.79250000
C	-0.50948700	-3.91243700	0.31569900
C	-2.52149300	-3.49552800	2.21201400

H	-1. 91074300	-1. 43659600	2. 20581800
C	-1. 29663200	-4. 98069900	0. 74830800
H	0. 26143300	-4. 07845800	-0. 42883800
C	-2. 30414900	-4. 77398700	1. 69196100
H	-3. 30376300	-3. 32928800	2. 94673400
H	-1. 12381600	-5. 97239700	0. 34052200
H	-2. 91818700	-5. 60653400	2. 02325900
H	3. 24382600	-1. 56734500	0. 46374900