Syntheses, photophysical, electroluminescence and computational studies of rhenium(I) diimine triarylamine-containing alkynyl complexes

Wai-Kin Chung,^a Keith Man-Chung Wong,^a Wai Han Lam,^a Xiuling Zhu,^b Nianyong Zhu,^a Hoi-Sing Kwok^b and Vivian Wing-Wah Yam^{*a}

^a Institute of Molecular Functional Materials (Areas of Excellence Scheme, University Grants Committee, Hong Kong) and Department of Chemistry, The University of Hong Kong, Pokfulam Road, Hong Kong.

Fax: +(852) 2857-1586; Tel: +(852) 2859-2153; E-mail: wwwam@hku.hk

^b Department of Electrical & Electronic Engineering, The Hong Kong University of Science and Technology, Clear Water Bay, Kowloon, Hong Kong.

Supplementary Information

	1	2	2 ^b	5	9	12
Re–C(1)	2.106	2.106	(2.182)	2.107	2.106	2.106
Re–N(1)	2.184	2.184	(2.177)	2.185	2.191	2.232
Re–N(2)	2.184	2.184	(2.178)	2.185	2.191	2.232
Re-CO _{trans to C(1)}	1.965	1.966	(1.991)	1.964	1.965	1.962
Re-CO _{trans to N(2)}	1.922	1.922	(1.900)	1.921	1.921	1.915
Re-CO _{trans to N(1)}	1.922	1.922	(1.938)	1.921	1.921	1.915
C(1)–C(2)	1.230	1.230	(1.108)	1.230	1.230	1.230
C(2)–C(3)	1.423	1.423	(1.469)	1.423	1.423	1.423
N–C ^c	1.412	1.411	(1.425)	1.412	1.412	1.412
ϕ_{NPh}^{d}	39.8	39.6	(43.4)	39.8	39.8	39.9

Table S1Selected structural parameters of the PBE0 optimized geometries for 1, 2, 5, 9 and 12^a

^{*a*}The atomic numbering is shown in Figure S1. Bond distances and angles are in Å and °, respectively

^bThe structural parameters in parentheses are from X-ray crystallographic data

^cAverage N–C distances of the triarylamine ligand

^{*d*}Average interplanar angles between the NC₃ plane of the triarylamine ligand and the phenyl rings.

Complex Sn (Coefficient) ^b wavelength (nm) J Character 1 S1 $H \rightarrow L(0.68)$ 572 0.001 LLCT S2 $H-2 \rightarrow L(0.66)$ 433 0.053 MLCT/LLCT S3 $H-1 \rightarrow L(0.63)$ 417 0.007 MLCT/LLCT S4 $H \rightarrow L+1(0.69)$ 389 0.002 LLCT S5 $H \rightarrow L+2(0.68)$ 374 0.096 LLCT S6 $H \rightarrow L-3(0.65)$ 363 0.704 IL/LCT S2 $H-2 \rightarrow L(0.68)$ 430 0.057 MLC7/LLCT S2 $H-2 \rightarrow L(0.68)$ 430 0.057 MLC7/LLCT S4 $H \rightarrow L(0.67)$ 543 0.001 LLCT S2 $H-2 \rightarrow L(0.68)$ 375 0.004 LLCT S4 $H \rightarrow L+3(0.66)$ 360 0.551 IL S5 $H \rightarrow L+2(0.43)$ 367 0.866 LLCT S6 $H \rightarrow L+2(0.65)$ 431 0.057 MLCT/LLCT S6		C	Excitation ^{<i>a</i>}	Vertical excitation	E	
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	Complex	Sn	(Coefficient) ^b	wavelength (nm)	ſ	Character [®]
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	1	S_1	$H \rightarrow L (0.68)$	572	0.001	LLCT
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$		S_2	$H-2 \rightarrow L(0.66)$	433	0.053	MLCT/LLCT
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$		S_3	$H-1 \rightarrow L(0.63)$	417	0.007	MLCT/LLCT
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$		S_4	$H \to L+1 \ (0.69)$	389	0.002	LLCT
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$		S_5	$H \rightarrow L+2 (0.68)$	374	0.096	LLCT
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$		S_6	$H \rightarrow L+3 (0.65)$	363	0.704	IL/LLCT
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$		S_7	$H-3 \rightarrow L(0.70)$	359	0.018	MLCT
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	2	S ₁	$H \rightarrow L(0.67)$	543	0.001	LLCT
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	-	\mathbf{S}_{1}	$H=2 \rightarrow L_{1}(0.68)$	430	0.057	MLCT/LLCT
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		S_2	$H_{-1} \rightarrow I_{-1} (0.64)$	414	0.005	MLCT/LLCT
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		S,	$H \rightarrow L+1 (0.68)$	375	0.005	LLCT
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$		S ₅	$H \rightarrow L + 2 (0.43)$	367	0.866	LLCT
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		D'J	$H \rightarrow L + 4 (0.50)$	201	0.000	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		Sc	$H \rightarrow L+3 (0.66)$	360	0 551	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		S_{7}	$H^{-3} \rightarrow L(0.62)$	359	0.088	MLCT
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$		27	II 5 E (0.02)		0.000	111201
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	5	S_1	$\mathrm{H} \rightarrow \mathrm{L} \left(0.68 \right)$	562	0.001	LLCT
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		S_2	$H-2 \rightarrow L(0.65)$	431	0.057	MLCT/LLCT
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		S_3	$H-1 \rightarrow L(0.62)$	413	0.010	MLCT/LLCT
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		S_4	$H \rightarrow L+1 \ (0.69)$	378	0.004	LLCT
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		S_5	$\mathrm{H} \rightarrow \mathrm{L+2}\;(0.52)$	366	0.583	LLCT
$\begin{array}{cccccccccccccccccccccccccccccccccccc$			$H \to L+3 (-0.41)$			IL/LLCT
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		S_6	$H \rightarrow L+2 (0.44)$	359	0.220	LLCT
$\begin{array}{cccccccccccccccccccccccccccccccccccc$			$H \rightarrow L+3 \ (0.51)$			IL/LLCT
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		S_7	$H-3 \rightarrow L (0.70)$	357	0.007	MLCT
	9	S_1	$H \rightarrow L (0.68)$	564	0.001	LLCT
S_3 $H-2 \rightarrow L (0.69)$ 4280.066MLCT/LLCT S_4 $H-1 \rightarrow L (0.66)$ 4130.002MLCT/LLCT S_5 $H-2 \rightarrow L+1 (0.70)$ 3980.016MLCT/LLCT S_6 $H-1 \rightarrow L+1 (0.68)$ 3850.011MLCT/LLCT S_7 $H \rightarrow L+2 (0.66)$ 3650.799IL/LLCT		\mathbf{S}_2	$H \rightarrow L+1 (0.69)$	515	0.001	LLCT
S_4 $H-1 \rightarrow L (0.66)$ 4130.002MLCT/LLCT S_5 $H-2 \rightarrow L+1 (0.70)$ 3980.016MLCT/LLCT S_6 $H-1 \rightarrow L+1 (0.68)$ 3850.011MLCT/LLCT S_7 $H \rightarrow L+2 (0.66)$ 3650.799IL/LLCT		$\bar{S_3}$	$H-2 \rightarrow L(0.69)$	428	0.066	MLCT/LLCT
S_5 $H-2 \rightarrow L+1 (0.70)$ 3980.016MLCT/LLCT S_6 $H-1 \rightarrow L+1 (0.68)$ 3850.011MLCT/LLCT S_7 $H \rightarrow L+2 (0.66)$ 3650.799IL/LLCT		S_4	$H-1 \rightarrow L(0.66)$	413	0.002	MLCT/LLCT
S_6 H-1 \rightarrow L+1 (0.68)3850.011MLCT/LLCT S_7 H \rightarrow L+2 (0.66)3650.799IL/LLCT		S_5	$H-2 \rightarrow L+1 (0.70)$	398	0.016	MLCT/LLCT
S_7 H \rightarrow L+2 (0.66) 365 0.799 IL/LLCT		S_6	$H-1 \rightarrow L+1 (0.68)$	385	0.011	MLCT/LLCT
		\mathbf{S}_7	$H \to L+2 (0.66)$	365	0.799	IL/LLCT
12 S_1 $H \rightarrow L(0.68)$ 544 0.001 LLCT	12	S_1	$H \rightarrow L (0.68)$	544	0.001	LLCT
$S_2 H \to L^+1 (0.69) 478 0.007 LLCT$		S ₂	$H \rightarrow L+1 (0.69)$	478	0.007	LLCT
$S_3 \qquad H-2 \rightarrow L(0.69) \qquad 411 \qquad 0.056 \qquad MLCT/LLCT$		S_2	$H-2 \rightarrow L(0.69)$	411	0.056	MLCT/LLCT
S_4 H-1 \rightarrow L (0.67) 402 0.001 MLCT/LLCT		S₄	$H-1 \rightarrow L(0.67)$	402	0.001	MLCT/LLCT
S ₅ $H-2 \rightarrow L+1$ (0.69) 369 0.022 MLCT/LLCT		S ₅	$H-2 \rightarrow L+1 (0.69)$	369	0.022	MLCT/LLCT
$S_6 = H^{-1} \rightarrow L^{+1} (0.64)$ 363 0.075 MLCT/LLCT		55 S6	$H-1 \rightarrow L+1 (0.64)$	363	0.075	MLCT/LLCT
$S_7 \qquad H \rightarrow L+2 (0.62) \qquad 360 \qquad 0.745 \qquad IL/LLCT$		S ₇	$H \rightarrow L+2 (0.62)$	360	0.745	IL/LLCT

Table S2	Selected singlet excited states (S _n) of the complexes computed by TDDFT/CPCM
	(CH_2Cl_2)

^{*a*}The orbitals involved in the excitations (H = HOMO and L = LUMO)

^bThe coefficients in the configuration interaction (CI) expansion that are less than absolute value of 0.3 are not listed ^cOscillator strengths

^dCharacter of the transition

MOs	0⁄0				%				
	1					2			
	Re	CO	N^N	C≡CR	_	Re	CO	N^N	C≡CR
L+4	13	48	2	37		11	19	11	58
L+3	18	34	6	42		0	0	0	100
L+2	3	3	93	1		3	5	86	5
L+1	1	2	97	0		1	2	97	0
L	2	3	94	1		2	3	94	1
Н	5	3	0	92		6	3	0	91
H–1	25	12	1	62		23	11	1	65
Н–2	37	17	4	42		38	17	4	41
Н–3	67	31	2	0		67	31	2	0
	5				_			9	
	Re	CO	N^N	C≡CR		Re	CO	N^N	C≡CR
L+4	12	46	2	40		1	3	0	96
L+3	16	31	12	41		1	2	96	0
L+2	4	5	87	4		19	35	3	42
L+1	2	2	96	0		1	1	99	0
L	2	3	95	1		2	3	94	1
Н	5	3	0	92		5	3	0	92
H-1	25	12	1	61		24	11	1	63
H–2	37	17	4	42		37	17	5	41
Н–3	67	31	2	0		68	31	2	0
		1	2						
	Re	CO	N^N	C≡CR					
L+4	0	0	0	99					
L+3	1	4	94	1					
L+2	16	29	6	49					
L+1	0	1	99	0					
L	2	3	95	1					
Н	5	3	0	92					
H–1	24	11	1	63					

Table S3Mulliken percentage compositions^a of selected molecular orbitals (H = HOMO and L= LUMO) in the complexes

^{*a*}The compositions were expressed in terms of contributions from the Re atom (Re), three carbonyl ligands (CO), diimine ligand (N^N), and triphenylamine alkynyl ligand (C=C-C₆H₄-R)

H-2

H-3

Electronic Supplementary Material (ESI) for New Journal of Chemistry This journal is © The Royal Society of Chemistry and The Centre National de la Recherche Scientifique 2013



Figure S1 Optimized geometry of 2.



Figure S2 Spatial plots (isovalue = 0.03 au) of selected frontier molecular orbitals of 1 obtained from PBE0/CPCM calculation.



Figure S3 Orbital energy diagram of the frontier molecular orbitals (H = HOMO and L = LUMO) in 1, 2, 5 and 9 and 12.



Figure S4 The change in bond distances (in Å) in triplet-excited state of **1** relative to the ground state. Only difference in bond distances larger than 0.013 Å were shown. The positive and negative values indicate bond elongation and contraction in the excited state, respectively. For clarity, all hydrogen atoms are omitted



Figure S5 A plot of $1/\Delta OD$ versus time monitored at 640 nm (\blacksquare) after laser flash of 11 and triphenylamine (2.01 × 10⁻² M) in degassed dichloromethane solution (0.1 M $^{n}Bu_{4}NPF_{6}$) and its theoretical fit (—).



Figure S6 Electroluminescence spectra of 3 at different DC voltages applied (from bottom to top: 8, 10, 12, 14 and 16 V). The device structure was ITO/MoO_x (2.5 nm)/MCP (8 wt% 3) (20 nm)/TPBi (50 nm)/LiF (1 nm)/Al (80 nm).



Figure S7 Electroluminescence spectra of **3** and the photoluminescence spectra of 50 nm thin-film MCP and 60 nm thin-film MCP with 8wt% **3** as dopant.



Figure S8 Electroluminescence spectra of 4 at different DC voltages applied (from bottom to top: 8, 10, 12, 14, 16 V). The device structure was ITO/MoO_x (2.5 nm)/NPB (50 nm)/MCP (8 wt% 4) (25 nm)/TPBi (50 nm)/LiF (1 nm)/Al (80 nm).



Figure S9 Current density-voltage curve for 3 and 4.



Figure S10 Luminance-voltage relationship curve for 3 and 4.



Figure S11 Current efficiency-current density relationship curve for 3 and 4.



Figure S12 Power efficiency versus luminance for 3 and 4.



Figure S13 Electroluminescence spectrum of complex 11 at bias voltage 10 V. The device structure was ITO/MoO_x (2.5 nm)/NPB (50 nm)/MCP (8 wt% 11) (20 nm)/TPBi (50 nm)/LiF (1 nm)/Al (80 nm).



Figure S14 Electroluminescence spectrum of 12 at bias voltage 10 V. The device structure was ITO/MoO_x (2.5 nm)/NPB (50 nm)/MCP (8wt% 12)/TPBi (50 nm)/LiF (1 nm)/Al (80 nm)



Figure S15 Current density-voltage relationship curve for 11 and 12.



Figure S16 Luminance-voltage relationship curve for 11 and 12.



Figure S17 Current efficiency versus current density for 11 and 12.

Cartesian coordinates for the optimized geometries

1 (S ₀)	2 (S ₀)				
1 C 7.496385 -1.375128 -0.525935	1 C 4.980292 2.255154 -0.900501				
2 C 6.271880 -1.204796 0.133986	2 C 5.533051 1.235885 -0.110533				
3 C 5.818668 -2.215963 0.991656	3 C 6.675155 1.522030 0.652992				
4 C 6.572044 -3.369343 1.176341	4 C 7.250077 2.781704 0.617346				
5 C 7.794183 -3.531463 0.527565	5 C 6.698484 3.805764 -0.169016				
6 C 8.250373 -2.524556 -0.320346	6 C 5.550407 3.517152 -0.923954				
7 N 5.503114 -0.038362 -0.065913	7 N 4.940374 -0.038792 -0.076470				
8 C 6.132165 1.218813 -0.183458	8 C 5.726015 -1.201793 0.023757				
9 C 7.236157 1.543449 0.616701	9 C 5.275218 -2.301662 0.768397				
10 C 7.853808 2.782343 0.491612	10 C 6.038717 -3.454012 0.856561				
11 C 7.376281 3.726248 -0.415049	11 C 7.284075 -3.546285 0.215065				
12 C 6.272765 3.409840 -1.204524	12 C 7.731749 -2.442078 -0.527538				
13 C 5.658334 2.167521 -1.099694	13 C 6.964526 -1.293314 -0.629097				
14 C 4.094094 -0.130053 -0.150588	14 C 8.0/1452 -4.7292/1 0.312559				
15 C 3.278001 0.805605 0.497415	15 C 8./40883 -5./34117 0.395/10				
16 C 1.897444 0.720015 0.405628	16 C 7.287030 5.102527 -0.198858				
17 C 1.273929 -0.311692 -0.319203	17 C 7.787012 6.204527 -0.223810				
18 C 2.105379 -1.250330 -0.957675					
19 C 3.486390 -1.157432 -0.883444					
20 C -0.143520 -0.406012 -0.406314	20 C 1.543852 -1.191182 -1.052944				
21 C -1.366653 -0.504051 -0.493178					
22 Re -3.468085 -0.613111 -0.586653	22 C 1.555950 0.550454 0.595958				
23 C -3.398077 -2.533606 -0.580792					
24 O -3.338923 -3.690300 -0.527319					
25 N -3.375979 1.550319 -0.302236	25 C -1.520445 -0.004050 -0.550810 $26 R_{0} -4.027171 -0.732636 -0.478559$				
26 C -3.384318 2.431420 -1.312236	20 (2 -4.027171 -0.732030 -0.478333				
27 C -3.253080 3.797497 -1.118009	$27 \ C \ -3.933240 \ -2.020419 \ -0.130834$				
28 C -3.102823 4.274897 0.179405	29 N -3 936867 -0 068963 1 600216				
29 C -3.089030 3.367071 1.227511	30 C -3 937770 -0 906506 2 646730				
30 C -3.224791 2.003955 0.962112	30 C -3.810793 -0.471577 -3.956663				
31 C -3.221122 0.970385 2.009491	32 C -3 673379 0 891316 4 196117				
32 N -3.367614 -0.300491 1.572984	33 C -3.667940 1.761738 3.116616				
33 C -3.368890 -1.298777 2.467303	34 C -3.798788 1.257362 1.822264				
34 C -3.234777 -1.085915 3.830324	35 C -3.804176 2.104978 0.619359				
35 C -3.089659 0.218387 4.290180	36 N -3.946014 1.448848 -0.553985				
36 C -3.083451 1.254474 3.368600	37 C -3.956034 2.152227 -1.694912				
37 H -2.995164 5.337626 0.373595	38 C -3.835018 3.532630 -1.726978				
38 H -2.980114 0.427101 5.349949	39 C -3.694135 4.217518 -0.525002				
39 C -5.433140 -0.633956 -0.594705	40 C -3.679254 3.494106 0.657975				
	41 C -5.992513 -0.761125 -0.491594				
41 C -3.411303 -0.031418 -2.307773	42 O -7.151859 -0.782777 -0.502765				
42 0 -3.301474 -0.392483 -3.003392 A2 H 1.276683 1.453311 0.012800	43 C -3.960902 -1.066519 -2.370285				
45 H 1.270005 1.455511 0.512805	44 O -3.904330 -1.218387 -3.518182				
45 H 4 108563 -1 885936 -1 305232	45 H -4.039732 -1.959206 2.409624				
46 H 1.647085 -2.051002 -1.530531	46 H -3.816691 -1.194466 4.765236				
47 H 4 871592 -2 090211 1 507617	47 H -3.569686 1.272125 5.207504				
48 H 6.203076 -4.142795 1.845037	48 H -3.558602 2.826996 3.282391				
49 H 8.382622 -4.431811 0.679159	49 H -3.566883 4.009294 1.604626				
50 H 9.197047 -2.638704 -0.842222	50 H -3.594775 5.298475 -0.507436				
51 H 7.850008 -0.600939 -1.200224	51 H -3.848002 4.050653 -2.679800				
52 H 7.604751 0.817041 1.334741	52 H -4.060310 1.574074 -2.605769				
53 H 8.708958 3.015043 1.121092	53 H 1.085138 -1.909882 -1.725242				
54 H 7.858172 4.695560 -0.505475	54 H 3.548624 -1.704049 -1.629423				
55 H 5.891690 4.131224 -1.922884	55 H 3.176257 1.369911 1.340113				
56 H 4.806460 1.921222 -1.726313	56 H 0./12071 1.182741 1.223116				
57 H -3.476611 -2.297606 2.060468	57 H 4.318648 -2.244080 1.278175				
58 H -3.240871 -1.931979 4.508953	58 H 5.678948 -4.296622 1.439200				
59 H -2.967603 2.277419 3.706792	59 H 8.686391 -2.500829 -1.041526				
60 H -2.968816 3.718942 2.245330	DU H /.319393 -U.456543 -1.222740				
61 H -3.265296 4.464857 -1.972929	61 H 9.329939 -6.620598 0.467741				
62 H -3.495357 2.011194 -2.305136					
	03 H 8.131255 2.989921 1.216696				
	04 П Э.11ЭЭЭЭ 4.294ЭЭХ -1.944/Х2 АС Н А.000078 Э.045946 1.409740				
	со п 4.055076 2.045840 -1.458/45 66 н 8.220061 7.177607 0.277260				
	00 N 0.223301 /.1/403/ -U.24/203				

5 (S ₀)					9 (S ₀)				
1	c	-3 035628	1 071/131	3 1/12/69	1	С	-3.062550	2.040944	2.670477
2	c	-3.140948	0.768532	1.785036	2	С	-3.175587	1.282096	1.487067
3	N	-3.253373	-0.507658	1.359600	3	Ν	-3.271559	-0.072134	1.486565
4	С	-3.252286	-1.488929	2.273421	4	С	-3.245536	-0.706397	2.653983
5	c	-3.148702	-1.251347	3.631797	5	С	-3.136069	-0.034284	3.877999
6	C	-3.035247	0.061129	4.098724	6	С	-3.045724	1.340987	3.891141
7	С	-3.144491	1.789745	0.724343	7	С	-3.190893	1.938329	0.217277
8	Ν	-3.261912	1.316118	-0.534346	8	Ν	-3.299942	1.153578	-0.885219
9	С	-3.267387	2.192266	-1.549483	9	С	-3.302823	1.739185	-2.078077
10	С	-3.166002	3.558874	-1.363929	10	C	-3.210679	3.127461	-2.239667
11	С	-3.047357	4.075330	-0.070578	11	C	-3.10/100	3.934622	-1.12/243
12	С	-3.040179	3.157922	0.975094	12	0	-3.093308	3.343/10	0.149817
13	Re	-3.303530	-0.852260	-0.797771	13	ке	-3.338294	-1.002498	-0.496360
14	С	-3.209337	-0.892244	-2.716433	14		-3.250374	1 006646	-2.320333
15	0	-3.138459	-0.865984	-3.873721	15	c	-3.191772	-1.000040	-3.443023
16	С	-1.206713	-0.695519	-0.662133	10	c	-0.022600	-0.813737	-0.424217
17	С	0.011691	-0.567405	-0.549910	18	c	1 3902/5	-0.0033333	-0.337031
18	С	1.423735	-0.436407	-0.431245	10	c	1.950245	0.500401	0.233948
19	С	2.004680	0.648667	0.250114	20	c	3 350431	0.806392	0 313222
20	С	3.380074	0.771550	0.372679	20	c	4 201288	-0 207366	-0 144435
21	C	4.233490	-0.179755	-0.199562	22	č	3.633260	-1.372524	-0.674926
22	C	3.669083	-1.260754	-0.888137	23	c	2.256601	-1.522321	-0.736019
23	С	2.292882	-1.389848	-0.993334	24	N	5.606235	-0.057845	-0.070315
24	N	5.638087	-0.049512	-0.083944	25	с	6.199816	1.172196	-0.422239
25	C	6.241352	1.210400	-0.278266	26	С	7.285184	1.677472	0.306689
26	C	7.318818	1.619281	0.519666	27	С	7.867788	2.888041	-0.049720
27	c	7.909818	2.801180	0.652424	28	С	7.372953	3.626525	-1.122456
28	c	7.431250	3.725714	-0.003434	29	С	6.287568	3.131601	-1.842290
29	c	0.333700 E 766202	3.320007	-1.431009	30	С	5.708367	1.913968	-1.505069
30	c	6 121258	-1 180504	0.2210/1	31	С	6.404144	-1.138740	0.361525
31	c	7 67513/	-1.160504	-0 383190	32	С	7.643653	-1.397026	-0.239248
32	c	8 444988	-2 481774	-0.074222	33	С	8.425648	-2.461008	0.194806
34	c	7,979945	-3.440050	0.823751	34	С	7.983571	-3.296991	1.217856
35	c	6.732023	-3.263171	1 417211	35	С	6.746826	-3.048899	1.809216
36	c	5.961815	-2.142682	1.128904	36	С	5.964981	-1.976983	1.394931
37	c	-3.195157	-2.769954	-0.765752	37	С	-3.227573	-2.829221	0.088188
38	0	-3.114162	-3.924883	-0.695844	38	0	-3.144649	-3.915480	0.484784
39	С	-5.266204	-0.912083	-0.842296	39	С	-5.301925	-1.071205	-0.508831
40	0	-6.425475	-0.951249	-0.872372	40	0	-6.461031	-1.115771	-0.518436
41	С	-2.926358	5.549767	0.171682	41	н	-3.032269	5.014456	-1.223318
42	С	-2.909962	0.359521	5.562446	42	н	-2.95/946	1.88/9/5	4.826002
43	н	1.353970	1.394554	0.697937	43	п	1.325///	1.454697	0.593457
44	н	3.807077	1.611753	0.912963	44	н	3.773737 A 282111	-2 163/83	-1 038206
45	н	4.321263	-2.002166	-1.340848	46	н	1 828967	-2 430587	-1 150086
46	н	1.867855	-2.231808	-1.531587	43	н	5.006363	-1.782199	1.866170
47	Н	4.994149	-2.005133	1.601800	48	н	6.388304	-3.688275	2.611819
48	н	6.355156	-3.998608	2.123376	49	н	8.594125	-4.132327	1.548471
49	н	8.581183	-4.314335	1.056141	50	н	9.383618	-2.645746	-0.284524
50	п	9.411892	-2.008554	-0.554469	51	н	7.986788	-0.758456	-1.047699
51		0.030000 7.697062	-0.051/35	-1.090190	52	н	7.667029	1.113334	1.152277
52	н	7.007903 8.744610	3 150582	0.947850	53	н	8.708910	3.262647	0.528098
50	н	7 892306	1 697800	-0.813273	54	н	7.827460	4.575000	-1.394090
55	н	5.972273	3,984349	-2.227431	55	Н	5.893344	3.690637	-2.687132
56	н	4.934962	1.767900	-1.895037	56	н	4.870712	1.526699	-2.077230
57	н	-3.333206	-2.497415	1.884202	57	н	-3.309443	-1.788201	2.612606
58	н	-3.152318	-2.091228	4.320100	58	н	-3.120155	-0.609915	4.797283
59	н	-2.947705	2.103475	3.463925	59	С	-2.966843	3.466385	2.574263
60	н	-2.947181	3.518246	1.993776	60	C	-2.981660	4.090723	1.366280
61	н	-3.175198	4.214870	-2.229245	61	H	-3.218464	3.544468	-3.241036
62	н	-3.351556	1.765082	-2.542203	62	H	-3.3/6661	1.0/9058	-2.935340
63	н	-2.885674	5.781752	1.239419	63	H U	-2.900234	5.1/2825 1 011751	1.303377
64	н	-2.017867	5.946020	-0.296499	64	н	-2.0/9340	4.041/51	3.471007
65	н	-3.775877	6.088651	-0.262740					
66	н	-2.897235	1.435639	5.755720					
67	H	-3.742102	-0.079031	6.124401					
68	Н	-1.984999	-0.068223	5.966465					

1 C -2.15743 1.43426 0.50999 2 C -5.3246 -0.47134 1.34426 0.50999 3 N -3.1784 -1.13487 0.20099 3 C 5.9183 -2.00211 1.17821 4 C 2.3486 0.48077 4 C 5.99183 -2.00211 1.17821 5 C 2.34887 0.48077 3.49273 0.60433 0.60433 6 C 2.34887 0.48077 N 5.00077 0.10035 0.00544 7 N 3.20275 0.60433 0.00199 0 C 2.34887 0.00199 0.01035 0.00199 1 C 7.3780 11 C 4.31044 0.00199 0.01037 2.27847 0.43893 0.00247 1 C 7.23154 0.03916 0.23239 0.110 7.714783 1.10374 0.44111 1.11398 1.11398 1.11398 1.11398 1.11398 1.1139	12 (S ₀)	1 (T ₁)					
2 C 2.61270 1.10404 1.57887 2 C 6.23285 -1.17946 1.20099 3 N 1.71244 0.20171 2.91273 3.00281 5 C 6.591093 -1.01505 0.01512 6 C 2.21397 0.81712 0.90281 0.91712 0.90281 0.91712 0.91733 0.9575 7 N 3.11534 4.01712 0.91733 0.91733 0.91735 0.01512 7 N 3.11534 4.01713 0.91733 0.01512 0.91735 <	1 C -2.154743 1.691097 2.892904	1 C 7.477361 -1.334826 -0.569590					
3 N -3.1248 0.24398 1.278888 3 C 5.01211 1.12521 4 C 2.333462 0.357112 3.90028 C 7.05734 3.32725 0.04363 6 C 2.310441 0.857112 3.90028 C 7.05734 3.32725 0.04363 7 N 5.00027 0.01555 0.00254 0.01555 0.00254 9 C 2.34554 0.008145 0.178700 D C 7.77728 2.32524 0.00817 11 C 2.34554 0.008146 0.178700 D C 7.77728 2.32524 0.00847 12 C 2.34554 0.00814 0.17870 D C 7.77728 2.32524 0.00477 13 Re 3.0028 0.0158 0.0158 0.01677 0.01677 0.01677 0.01687 0.04278 14 C 3.02028 0.01518 0.02078 0.01678 0.02078 0.01711 0.01874 0.02078 0.01875 0.01875 0.01876 0.01876	2 C -2.616270 1.143049 1.676837	2 C 6.323545 -1.157016 0.200099					
A C 3.348.0 0.349/99 1.349/97 4.2 C 7.50773 3.39755 S C 2.31830 0.35711 3.99756 5.5 C 7.50773 3.99756 C 2.31830 0.35794 0.049652 C 2.82682 2.44602 0.31735 D C 2.349962 2.06937 1.73730 B C 1.34781 1.03976 0.01735 D C 2.349962 2.06937 1.73706 D C 7.14784 1.03976 0.017351 D C 2.32687 1.237871 1.33002 D C 0.349877 1.37244 0.018271 D 0.32027 0.323801 1.32721 1.32724 0.30827 0.328302 D 0.32024 0.35024 1.32704 1.3222 0.35302 0.36220 0.35302 D 0.30896 0.42764 1.11806 2.31806 2.31806 3.37755 0.34849 0.353202 0.3622	3 N -3.117844 -0.120439 1.578888	3 C 5.991693 -2.100211 1.178521					
b c 2.810847 3.81142 3.91083 c c 2.810847 3.810184 1.421108 0.611233 7 c 2.810847 3.810184 1.421108 0.611233 9 C 2.810847 3.810184 1.421108 0.611233 9 C 2.810847 3.81014 3.91092 2.020244 10 C 2.80868 3.54612 1.77206 3.92744 0.008471 11 C -2.81554 0.008170 0.121254 0.708471 12 C -2.81584 0.00816 0.137870 11 C 7.93973 0.272444 0.308471 13 Re 3.20187 0.72812 3.32704 11 C 0.12268 0.12368 </td <td>4 C -3.253662 -0.847469 2.692787</td> <td>4 C 6.799544 -3.215465 1.369755</td>	4 C -3.253662 -0.847469 2.692787	4 C 6.799544 -3.215465 1.369755					
b c 2.85974 0.96652 C 8.80677 C 8.80776 C 8.80777 C 8.80778 C S.80778 C S.80778 C S.80778 <th< td=""><td>5 C -2.813073 -0.357712 3.940288</td><td>5 C 7.950173 -3.392735 0.604363</td></th<>	5 C -2.813073 -0.357712 3.940288	5 C 7.950173 -3.392735 0.604363					
8 N 3.11310 0.613203 A N 5.2007 4.00358 0.002149 9 C 2.349882 2.00514 0.107306 9 C 7.177282 3.2352 0.700711 11 C 2.249358 0.00614 0.378760 10 C 7.177282 3.23524 0.700711 12 C 2.249358 0.00616 0.578760 11 C 7.007732 3.23687 1.14885 13 C 3.20028 1.27214 3.10180 0.113980 1.13980 1.13980 1.13980 15 C 3.20028 1.27214 3.12701 0.48360 1.07331 0.48360 1.07331 0.48360 1.07331 0.48360 1.07331 0.48360 1.07331 0.48360 1.07331 0.48360 0.07331 0.21483 0.300512 0.30512 0.30512 0.30512 0.30512 0.30512 0.30512 0.47131 0.44474 0.47131 10 C 3.40600	7 C -2 615447 1 958794 0 496652	6 C 8.286238 -2.446062 -0.361122					
9 C 3.20637 1.72500 8 C 6.14313 1.24333 1.050376 0.12555 11 C 2.240886 3.28711 0.50192 11 C 7.47784 2.33545 0.070071 12 C 2.15256 3.28711 0.580192 11 C 7.40733 2.43526 0.14443 14 C 2.126106 0.17781 0.488406 16 5 0.93202 0.935809 15 C 0.30028 1.57781 0.488406 16 C 1.13026 0.439345 0.209318 16 C 1.245341 0.45059 0.67149 0.44716 19 0.2 0.439345 0.209313 0.2 C 1.33025 0.35944 0.55344 16 C 2.426507 0.457495 0.442165 0.20933 20 C 0.329169 0.55464 17 C 1.34560 0.57246 0.440276 0.33164 0.11786 0.324164	8 N -3.116334 1.421108 -0.651293	/ N 5.5090// -0.010535 0.002564					
10 C 2.48138 4.6412 1.707366 1 C 7.77878 2.83734 1.70434 1.80237 11 C 2.24313 4.06416 0.578700 11 C 7.78738 3.72744 <t< td=""><td>9 C -3.249926 2.206397 -1.725200</td><td>8 C 6.146513 1.254330 -0.098199</td></t<>	9 C -3.249926 2.206397 -1.725200	8 C 6.146513 1.254330 -0.098199					
11 C 2.21339 4.389/15 0.578760 1.0 0.27247 0.30987 12 C 2.15395 3.25811 0.58912 1.1 0.27247 0.30887 13 Re 3.26288 1.25848 2.40238 11 C 5.79838 0.213488 1.11988 15 C 3.26288 1.27161 0.42446 1.11988 0.23348 0.233591 0.233591 15 C 1.26106 0.17761 0.42446 15 C 3.28879 0.235507 0.268620 15 C 2.42510 0.26484 0.429067 16 C 1.31027 0.35507 0.268620 12 C 2.42660 0.57749 0.40276 18 C 1.31027 0.35140 0.41766 12 C 2.44604 0.434487 4.32130 0.21 0.432149 0.44424 13 C 2.34034 0.45749 0.44224 0.331814 0.44176 12 C 2.46080 0.357860 0.21785 0.324181 0.441766	10 C -2.808862 3.546122 -1.707306	9 C 7.147843 1.005970 0.812355 10 C 7.787285 2.825254 0.700471					
12 C 2.5390 3.38711 0.580192 12 C 6.41404 3.37627 1.114285 14 C 3.20017 0.717261 -4.21724 1.114285 1.11939 15 G 3.20012 0.717261 -4.21724 1.11935 0.066362 16 C 1.21064 0.717261 -4.21724 0.066362 0.066362 16 C 1.21062 0.832945 0.200537 0.066326 0.07572 0.066326 16 C 1.21062 0.832954 0.000563 0.07714 0.041706 17 C 0.340564 0.40476 19 C 1.312827 0.55994 12 C 0.440567 0.933302 21 C 1.312827 0.55994 12 C 0.56133 0.41706 1.12129 0.55910 0.41706 12 C 0.342584 0.232898 21 C 1.328247 0.44424 12 C 0.56138 0.327848 0.24979 26 C 3.328438 1.94567	11 C -2.243158 4.080416 -0.578760	10 C 7 430373 3 727444 -0 308427					
18 Re -3.20187 -0.799108 -0.33002 11 12 C 7.75587 2.149308 -1.119308 15 C 3.20287 1.27741 -3.42404 13 C 1.217318 -0.466225 16 C 1.20028 -0.20171 -0.44404 15 C 3.20277 0.949128 0.20652 16 C 1.00028 -0.20171 -0.44404 16 C 1.50027 -0.20202 0.266220 17 C 1.00086 -0.10293 0.30104 118 C 2.10027 -0.20202 0.266217 18 C 2.40027 -0.422020 0.42017 0.44014 0.47765 19 C 2.40329 -0.43330 -0.33301 22 C -0.32336 0.41766 12 C 2.40320 -0.42320 -0.44389 0.40775 0.44424 12 C 3.20241 -0.47389 2.2077 0.44424 0.40785 0.44424 12 C 3.20255 -1.45558 2.20 0.443939	12 C -2.152956 3.289711 0.580192	12 C 6.431494 3.376867 -1.214285					
11 C -3.20023 -2.00130 14 C 4.127064 0.123303 0.086826 15 C -1.20106 -0.71730 -0.435494 15 C 1.92777 0.943355 0.293589 16 C 1.00165 -0.17730 -0.435494 10 C 1.92052 0.82377 0.494355 0.293589 17 C 1.00165 -0.01739 0.17746 11 C 1.30077 0.424355 0.293599 18 C 2.10650 0.12786 0.11313 12 C 0.007349 0.17766 19 C 3.44060 0.127869 0.11313 12 C 0.127189 0.1147766 21 C 3.42057 0.44126 0 3.22389 1.014654 22 C 3.20186 1.201789 0.411276 2.222 0.53916 0.417266 23 C 3.20280 1.22587 0.43429 0.11786 0 3.22389 1.010564 24 C 3.2016 0.23530 0.44129 2.012	13 Re -3.320187 -0.799108 -0.538302	13 C 5.795887 2.143985 -1.119308					
16 C 1.11100 1.11100 1.11100 1.5 C 3.28773 0.48355 0.293589 17 C 0.00855 0.00095 0.100007 16 C 1.9020 0.20552 0.20753 0.20763 0.20763 0.20763 0.20763 0.20763 0.20763 0.20763 0.20764	14 C -3.202887 -1.234084 -2.402138 15 O -3.200428 -1.527812 -3.522704	14 C 4.127064 -0.123403 -0.086826					
17 C 0.02866 0.02007 16 C 1.92062 0.83270 0.266820 18 C 1.42510 0.50284 0.320424 18 C 1.90022 0.832702 0.266820 10 C 2.40265 0.65739 0.40276 19 C 2.10087 0.335122 0.266820 22 C 3.40369 0.28436 0.10393 20 C 0.007343 0.447766 23 C 2.64045 1.94087 0.933929 21 C 3.32308 4.50776 0.444424 26 C 3.26392 26 N 3.23280 3.25598 1.34642 0.44178 27 C 7.36940 1.46770 0.444399 25 C 3.1634 3.2660 1.10700 1.11651 28 C 7.31684 1.30204 1.32607 1.40180 1.30706 1.40180 29 C 5.36640 0.21183 3.4843 2.26812	16 C -1.216106 -0.717361 -0.483496	15 C 3.289737 0.948355 0.293589					
18 C 1.42510 0.206820 17 C 1.310259 0.266820 19 C 2.40569 0.66734 0.42476 18 C 1.42502 0.55944 21 C 3.43466 0.243468 0.203783 20 C 0.067743 0.467785 0.35106 22 C 3.64405 1.34960 0.83530 22 RC 3.323168 -1.32122 0.658275 24 N 5.65213 0.14106 23 C -3.233168 -3.48511 0.44158 25 C 7.36950 0.479789 26 N -3.323168 1.493135 0.461178 26 C 7.36950 0.479755 26 C -3.36401 0.41506 27 C 7.36960 3.2556 1.458968 27 C -3.36402 0.46178 28 C 7.46960 3.2976 0.44293 3.8164 0.41992 21 C 4.36960 1.42807 0.42985 2.3113 0.41795 216 6.36282	17 C 0.008566 -0.619995 -0.420407	16 C 1.920622 0.832943 0.206532					
19 C 2.402691 0.551060 0.227244 18 C 2.16027 -0.42700 -0.647191 20 C 3.42606 0.224436 0.210393 20 C -0.079143 -0.47785 -0.354166 21 C 3.64404 1.34867 0.893929 21 C -0.079143 -0.47785 -0.34186 24 N 5.65312 1.07660 0.41406 22 C -3.32916 1.49135 -0.461178 25 C 7.369540 2.20427 2.23807 -248807 2 C -3.16344 3.06067 -1.401902 26 C 7.669540 2.204975 2.22 C -3.46407 2.03808 -1.23808 -1.401902 27 C 7.66913 1.53338 0.54718 31 C -3.42423 1.527280 30 C 7.46913 1.5338 0.54718 31 C -3.62424 2.49854 31 C <td< td=""><td>18 C 1.425510 -0.508284 -0.349068</td><td>17 C 1.310259 -0.355072 -0.266820</td></td<>	18 C 1.425510 -0.508284 -0.349068	17 C 1.310259 -0.355072 -0.266820					
20 C 3.43069 0.66734 0.44276 19 C 3.50184 -1.31222 0.553494 21 C 3.44065 0.32365 0.235305 21 C -0.47745 0.44776 22 C 2.66327 1.46305 0.953300 22 Re -3.32192 0.564295 0.44424 25 C 6.263251 0.44785 0.432588 24 0 -3.328168 1.491135 -0.44424 26 C 7.369540 0.44789 25 N -3.328168 1.491135 -0.41756 27 C 7.46649 1.31644 0.10791 20 C -3.46400 -0.11684 30 C 5.66755 1.98038 -0.547618 31 C -3.46400 0.065018 31 C 6.46898 -1.31644 0.10791 30 C -3.46400 0.065018 32 C 7.460131 1.05333 0.547618 31 C	19 C 2.040591 0.561008 0.327424	18 C 2.160627 -1.422602 -0.647191					
21 C 4.28400 0.284300 0.284300 0.284300 0.234300 22 C 3.64404 1.48607 0.935330 22 Re -3.32129 -0.55160 -0.41706 23 C 2.53277 1.46300 0.935330 22 Re -3.32308 -2.59475 -0.44424 24 N 5.56213 0.107060 0.14206 23 C -3.23508 -3.44501 -0.346554 26 C 7.36940 2.704526 0.244290 26 C -3.38441 4.56400 -0.461178 27 C 7.66940 1.31644 0.10291 29 C -3.38443 4.65480 -0.461178 30 C 5.766755 27 C -3.16844 4.26480 -0.11884 31 C 6.46409 0.20201 0.30207 2 3.32443 4.26480 -0.11884 31 C 7.6039 3.40449 1.00291 30 C -3.42192 0.20281 0.30207 32 C 7.60393 3.404	20 C 3.420569 0.667349 0.404276	19 C 3.530184 -1.312822 -0.559494					
22 C 3.44403 1.43680 0.35350 22 12 C 1.42169 0.56275 24 N 5.652132 0.17090 0.141206 23 C 3.232105 0.6626927 25 C 6.263232 0.06550 0.32789 26 C 3.23508 3.74453 0.346554 26 C 7.30954 1.465702 0.44299 25 N 3.23508 3.066667 1.401090 27 C 6.30824 0.250975 27 C 3.168017 2.338443 4.263480 0.116854 30 C 5.466353 1.920194 1.25067 28 C 3.38443 4.263480 0.116854 31 C 6.30339 0.547618 30 C 3.460124 0.26921 0.808007 32 C 7.60133 1.50339 0.547618 30 C 3.46123 3.48442 0.26921 0.27228 1.527280 33 C 5.26013 1.25368 31 C 3.46123 3.48444 0.245345	21 C 4.243609 -0.284586 -0.210393	20 C -0.0/9143 -0.46/785 -0.354196					
24 N 565132 2.0000839 0.339113 24 N 565232 1.0000839 0.34243 25 C 6262952 1.0000839 0.34249 26 C 7.370494 1.465702 0.44424 27 C 7.99540 2.704926 0.244799 26 C 3.183841 0.66554 27 C 7.99540 2.704926 0.244799 26 C 3.163844 3.06667 1.401902 28 C 7.450840 0.10281 0.0576755 1.25087 1.097247 1.871445 30 C 7.660133 1.05339 0.567618 30 C 3.48440 0.008207 32 C 7.66133 0.506660 32 N 3.562843 0.066661 33 C 6.676349 3.424519 1.25869 33 C 3.368732 0.318744 36 C 6.793493 3.62643 0.666669 33 C 3.367853 0.37474 37 C 3.317838 0.484755	22 C 3.044045 -1.349807 -0.893929 23 C 2.263727 -1.463050 -0.953530	21 C -1.321929 -0.559160 -0.41/606					
15 C 6 5.22952 1.08550 0.327889 2.0 0.346554 16 C 7.37044 1.465702 0.44299 25 N 3.32818 1.493135 0.461178 17 C 7.36484 0.399354 0.029755 27 C 3.168017 2.338443 4.263400 0.116854 18 C 5.366057 1.982084 1.285087 29 C 3.464003 0.0116854 10 C 5.76755 1.982084 1.285087 29 C 3.464009 2.026207 0.605018 13 C 7.660193 1.50339 0.547618 30 C 3.46440 0.48544 0.48544 13 C 7.660193 1.253689 33 C 3.66655 1.17784 4.498544 14 C 7.322070 1.010319 34 C 3.87138 0.487755 4.40332 15 C 6.60075 2.20730 1.010319 34 C 3.87138 0.487755 4.404332 16 -	24 N 5.652132 -0.170960 -0.141206	22 RE -5.557115 -0.004899 -0.509275					
26 C 7.370494 1.465702 0.442989 25 N -3.328166 1.493135 0.461178 27 C 7.465960 3.595874 0.657955 27 C -3.163840 3.66667 1.4101902 28 C 7.465960 3.595874 0.657955 27 C -3.163840 3.66667 1.4101902 29 C 6.362462 3.22566 -1.435668 28 C -3.34844 0.66671 1.4101902 30 C 5.46679 1.313444 0.10291 30 C -3.44402 0.965018 31 C 6.46098 -1.31333 0.32454 0.384207 1.572720 32 C 7.90033 3.020243 0.060669 32 N -3.56600 -0.47935 1.537728 34 C 6.70073 3.486073 -0.61622 36 C -3.87938 0.47755 3.24074 0.42735 32.4374 35 C -3.22016 -0.74813 -0.51637 37 H -3.348807 5.44035 3.2	25 C 6.262952 1.086590 -0.327889	25 C -3.283508 -2.554775 -0.444424					
27 C 7.969540 2.7095540 2.523809 1.507066 28 C 7.46980 3.359874 0.6679755 27 C 3.16840 0.116554 30 C 5.643663 3.252565 1.455568 28 C -3.318443 0.965018 31 C 6.446998 -1.31644 0.110291 30 C -3.64800 2.02521 0.80307 32 C 7.600193 1.503339 0.547618 31 C -3.648055 -1.177844 2.489444 33 C 7.90033 3.602643 0.06669 32 N -3.66855 -1.177844 2.489444 36 C 6.00077 2.290730 1.18019 34 C -3.48875 3.81634 37 C 3.282067 0.748431 0.224538 0.3755 2.30744 38 O 3.19440 -3.48407 0.163622 36 C -3.77755 2.0737 37 H -3.39274 0.707883 5.24764 39 C -3.262067 <td< td=""><td>26 C 7.370494 1.465702 0.442989</td><td>25 N -3.328168 1.493135 -0.461178</td></td<>	26 C 7.370494 1.465702 0.442989	25 N -3.328168 1.493135 -0.461178					
28 C 7.469800 355874 -0.697555 27 C -3.138443 3.696667 -1.011002 29 C 6.32626 .128556 28 C -3.338443 4.263480 -0.116854 30 C 5.76755 1.982034 -1.285087 29 C -3.338443 4.263480 -0.116854 31 C 7.660133 -1.316340 0.0127247 1.871415 32 C 7.660133 -1.6026669 31 C -3.613373 1.092747 1.871484 34 C 7.99033 -6.02475 -2.290730 1.018019 34 C -3.81738 -0.87556 3.81634 35 C 6.00075 -2.290730 1.018019 34 C -3.81738 -0.87556 3.81634 36 C 5.32006 -0.74831 -0.52137 37 H -3.438497 5.420786 -0.42337 0.12755 38 0 -6.43335 1.72481 -0.52137 37 H -3.38773 0.41754 -0.81728 <t< td=""><td>27 C 7.969540 2.704926 0.249479</td><td>26 C -3.168017 2.323809 -1.507096</td></t<>	27 C 7.969540 2.704926 0.249479	26 C -3.168017 2.323809 -1.507096					
29 C 5.36286 3.22585 -1.438586 28 C C 3.3844.3 4.26340 0.016854 31 C 5.43699 -1.316444 0.110291 20 C -3.494123 3.438422 0.965018 32 C 7.60193 -1.60380 0.038207 1.871415 3.48402 0.965018 33 C 7.60193 -3.60264 0.60669 3.2 N -3.568205 0.247251 1.527280 34 C -3.60494 -3.424519 1.253689 34 C -3.66552 -1.17784 2.498544 35 C -5.32607 -0.74851 0.281237 37 7 H -3.48887 3.7474 36 C -5.32604 -0.521357 37 H -3.348837 0.17255 3.24743 3.424319 3.24743 41 H -1.880689 5.10699 -0.51322 39 C -5.356401 0.71231 3.4 42 H -1.41380 1.36774 0.80802 41 C -3.34775 <t< td=""><td>28 C 7.469860 3.595874 -0.697955</td><td>27 C -3.163844 3.696667 -1.401902</td></t<>	28 C 7.469860 3.595874 -0.697955	27 C -3.163844 3.696667 -1.401902					
30 C 5.76075 1.283004 1.283007 22 C 7.460193 1.50333 0.547618 30 C 3.483042 0.605018 31 C 7.80033 3.06243 0.60669 31 N 3.566052 1.247843 1.871415 32 C 7.90033 3.60243 0.60669 32 N 7.3568025 0.247924 1.871415 33 C 6.600775 2.290730 1.018019 34 C -3.871938 0.487755 4.249544 34 C 5.36205 0.747451 0.25137 37 H -3.48837 5.342078 0.012755 40 0 -6.43355 0.71832 0.51317 38 H -3.992744 0.616302 39 C -3.367932 1.45150 3.237474 41 H -1.88668 5.10693 -0.51302 39 C -5.356401 0.631037 0.711231 42 H -1.880685 5.10693 -0.51302 41 H 3.81634 -3.426205 -0.62657 -0.812728 <td>29 C 6.362862 3.225565 -1.458568</td> <td>28 C -3.338443 4.263480 -0.116854</td>	29 C 6.362862 3.225565 -1.458568	28 C -3.338443 4.263480 -0.116854					
33 C 7.601039 -1.50339 -0.547618 311 C -3.613373 1.09247 1.871415 33 C 7.422186 -0.291213 31 C -3.613373 1.09247 1.871415 34 C 7.90333 -3.602640 32 N -3.568205 -0.247925 1.527280 35 C 6.705499 -3.424519 1.253689 33 C -3.817938 0.878556 3.31634 36 C -3.262016 -0.696344 -0.26198 36 C -3.871938 0.87755 4.204332 37 C -3.262016 -0.771832 -0.513174 38 H -3.348837 5.342078 0.012755 38 O -5.3262067 -0.771832 -0.513127 37 H -3.348837 0.631037 -0.711231 41 H -1.880108 1.64979 420 C -3.03752 -0.650827 -0.61567 -0.510827 42 H -1.891058 1.46491 0.41979 42 C -3.03752 -0.650657 <td>30 C 5.766755 1.982034 -1.285087 31 C 6.436998 -1.316444 0.110291</td> <td>29 C -3.494123 3.438482 0.965018</td>	30 C 5.766755 1.982034 -1.285087 31 C 6.436998 -1.316444 0.110291	29 C -3.494123 3.438482 0.965018					
33 C 8.429557 -2.632186 -0.291213 33 C -3.643373 1.09247 1.871415 34 C 7.990333 -3.002643 0.606669 32 C -3.666552 -1.177884 2.498544 35 C -3.20730 1.018019 34 C -3.666552 -1.177884 2.498544 36 C -3.20730 1.018019 34 C -3.87033 0.48755 4.204332 37 C -3.22007 0.71481 0.51622 36 C -3.87133 0.48755 -3.20217 0.71481 0.52157 37 H -3.38837 0.301275 0.23275 0.21755 0.22757 0.25957 0.31278 41 H 1.886689 5.10693 0.551302 39 C -5.36401 0.631037 0.711231 42 H 1.89141 1.49891 0.941979 42 C -3.36372 0.65657 0.81238 43 H 1.811418 2.239191 1.487918 44 H 3.733227 1.654440	32 C 7.660193 -1.503339 -0.547618	30 C -3.484009 2.026921 0.808207					
34 C 790333 -3.626243 0.606669 32 N 35 C -3.79925 1.527280 35 C 6.769499 -3.424519 1.253689 33 C -3.66652 -1.177884 -2.498544 36 C 6.00775 -2.290730 0.108019 34 C -3.81733 0.487755 4.204332 37 C -3.262016 -0.696344 0.281387 37 T -3.348837 5.42078 0.012755 38 O -6.443355 0.771832 -0.51137 37 H -3.348837 5.42078 0.012755 41 H -1.88068 5.106930 0.661562 -0.711221 -0.631037 -0.711221 42 H -1.89108 1.449691 0.941979 42 C -3.087752 -0.65567 -5.05641 -0.817574 43 H 1.413810 1.397740 0.808902 41 K 1.823502 1.664941 0.510827 44 H 3.282075 -4.487355 0.780856 47 H <t< td=""><td>33 C 8.429557 -2.632186 -0.291213</td><td>31 C -3.613373 1.097247 1.871415</td></t<>	33 C 8.429557 -2.632186 -0.291213	31 C -3.613373 1.097247 1.871415					
35 C 6.76949 -3.242519 1.235869 -3.060532 -1.117/88 2.498544 36 C -3.060532 -1.117/88 0.8755 4.204332 37 C -3.262016 -2.696344 -0.286198 35 C -3.371938 0.487755 4.204332 38 O -5.326207 -0.77481 -0.511357 37 H -3.348847 5.342078 0.012755 40 O -6.44333 -0.771832 -0.511307 371 H -3.348873 5.342078 0.012755 41 H -1.886689 5.10699 -0.961522 40 O -6.500827 -0.626957 -0.817278 42 H 1.413810 1.306704 0.80902 41 C -3.37532 0.965596 -3.50461 44 H 3.84733 -1.487733 43 H 1.283502 1.654941 0.518023 45 H 4.272001 -2091814 -1.378753 43 H 1.283502 1.664941 1.810418 -2.92751 0.51867 -5.91865	34 C 7.990333 -3.602643 0.606669	32 N -3.568205 -0.247925 1.527280					
36 C 6.00077 5.290730 1.018019 34 C 3.01838 0.03833 3.1034 37 C 3.220073 0.163622 36 C -3.76252 1.451350 3.237474 38 O 5.28207 0.774851 0.521357 37 H -3.34837 5.342078 0.012755 40 O 6.44335 0.774851 0.51132 37 H -3.34837 5.342078 0.012755 41 H 1.891058 1.64979 4.996552 40 O 6.500827 -0.652082 -0.65508 -2.501865 43 H 1.418180 1.30704 0.80902 41 C -3.177503 -0.81557 -2.501865 44 H 3.874271 0.79683 5.24614 0.51023 -0.812728 45 H 1.811418 2.29191 -1.487918 44 H 3.733227 1.861893 0.675388 47 H 5.06473 0.727848 4487356 0.79083 -1.201814 1.785281 48 H <td>35 C 6.769499 -3.424519 1.253689</td> <td>33 C -3.000552 -1.17/884 2.498544 24 C 2.917929 0.979505 2.921524</td>	35 C 6.769499 -3.424519 1.253689	33 C -3.000552 -1.17/884 2.498544 24 C 2.917929 0.979505 2.921524					
37 C -3.76016 -2.99644 -0.286198 -3.76922 1.451350 3.237474 38 O -3.769252 1.451350 3.237474 39 C 5.282067 0.774851 0.521357 37 H -3.348837 5.342078 0.012755 40 O -6.443335 0.0771832 0.519174 38 H -3.92744 0.76883 5.246384 41 H 1.88669 5.106993 0.561302 39 C -5.356401 0.631037 0.711231 42 H 1.431450 1.04679 40 O -6.600827 -0.626557 -0.631032 0.71728 43 H 1.4378051 1.434661 0.941979 42 O -3.083752 -0.95559 -6.500421 44 H 3.874951 1.434661 0.941979 42 O -3.083752 -0.812727 0.81207 45 H 4.151064 -1.18141 1.232104 1.53274 45 H 1.16164 -2.13807 0.8727572 48 F	36 C 6.000775 -2.290730 1.018019	34 C -5.01/050 -0.070590 5.051054 35 C -3.871938 0.487755 4.204332					
38 0 5.153430 5.143430 1.013022 39 C 5.2607 .0774851 -0.51357 37 H -3.348837 5.342078 0.012755 40 0 -6.43335 .0771832 -0.519174 38 H -3.392744 0.631037 0.711231 41 H -1.881058 1.264979 4.996552 40 O -6.500827 -0.621957 0.811278 43 H 1.432101 1.306704 0.808902 41 C -3.177503 -0.861567 -5.50461 44 H 3.73745 1.4378753 43 H 1.23502 1.654941 0.510823 45 H 4.272001 -0.98056 44 H 3.73327 1.861893 0.673388 47 H 5.05476 0.78139 1.92688 -48736 -9.97272 46 H 1.711656 -3.314204 1.128281 50 H 9.379517 4.56527 0.842010 51 H 8.512037 -4.26108 0.760581 51 H	37 C -3.262016 -2.696344 -0.286198	36 C -3.769252 1.451350 3.237474					
40 0 -6.443335 -0.771822 -0.519174 38 H -3.992744 0.769883 5.246384 41 H -1.886689 5.106993 -0.561302 39 C -5.356401 -0.631037 -0.711231 42 H -1.891058 1.264974 0.808902 41 C -3.177503 -0.626957 0.861567 -2.501865 44 H 3.874951 1.494691 0.941979 42 O -3.083752 -0.65596 -3.650461 45 H 1.811418 -2.29114 -1.378753 43 H 1.283507 1.654941 0.57328 46 H 1.811418 -2.93114 1.378753 45 H 4.161064 -2.138076 0.872572 48 H 6.533674 3.94248 2.132290 1.171656 -2.34804 -1.027881 50 H 9.374930 -2.75683 0.78139 1.92268 50 H 7.93152 -0.557927 0.42248 2.132290 51 H 8.827793 2.980157 0.85720	39 C -5.282067 -0.774851 -0.521357	37 H -3.348837 5.342078 0.012755					
41 H -1.886689 5.106993 -0.561302 39 C -5.356401 -0.631037 -7.11231 42 H -1.891058 1.264979 -9.96552 40 0 -6.500827 -0.631037 -7.11231 43 H 1.31810 1.30704 0.80902 41 C -3.177503 -0.851567 -2.501865 44 H 3.874951 1.449191 0.941979 42 O -3.083752 -0.965996 -3.650401 0.57388 45 H 4.272001 -2.01814 -1.378753 43 H 1.233502 1.651403 0.675388 46 H 5.05473 -4.167104 1.532574 45 H 4.161064 -2.138076 0.872572 48 H 6.43505 -4.16910 1.960732 46 H 1.711256 -3.34204 1.027881 49 H 8.50773 0.75838 -0.260466 49 H 8.582773 -2.02108 .760851 51 H 7.937517 4.56567 0.842100 52	40 O -6.443335 -0.771832 -0.519174	38 H -3.992744 0.769883 5.246384					
42 H -1.891058 1.264979 4.996552 40 0 -6.50827 -0.626957 -0.817278 43 H 1.413810 1.306704 0.808902 41 C -3.108752 -0.965596 -3.50461 44 H 3.277503 -0.815147 -1.518023 -4.61914 -0.518023 45 H 4.272001 -2.091814 -1.378753 43 H 1.283502 1.654914 0.518023 46 H 1.811418 -2.291104 1.532574 45 H 4.61064 -2.138076 0.872572 478 H 6.613505 -4.69130 -7.9683 0.81258 46 H 1.711656 -2.334604 -1.027881 49 H 8.500758 -4.487366 0.798056 0.781258 -6.533674 -3.942248 2.132290 50 H 9.75578 0.78139 1.120268 50 H 9.17929 -2.577060 0.965843 51 H 7.937517 4.56172 0.84110 2.20819 51 H 7.3152 <td< td=""><td>41 H -1.886689 5.106993 -0.561302</td><td>39 C -5.356401 -0.631037 -0.711231</td></td<>	41 H -1.886689 5.106993 -0.561302	39 C -5.356401 -0.631037 -0.711231					
43 H 1.413810 1.036704 0.808902 41 C 3.177503 0.861567 2.501865 44 H 3.874951 1.49491 0.941979 42 O -0.801567 2.501865 45 H 2.72001 -2.091814 -1.378753 43 H 1.283502 1.654941 0.518023 46 H 1.811418 2.23191 -1.487918 44 H 3.73327 1.861893 0.675388 47 H 5.054736 -2.152104 1.532574 45 H 4.161064 -2.138076 0.872572 48 H 6.533674 -3.942248 2.132290 -1.951481 1.785281 50 H 9.374930 -2.75688 0.812358 48 H 6.533674 -3.942248 2.132290 51 H 8.807793 2.980157 0.857200 51 H 7.47145 0.91218 1.603082 54 H 7.937517 4.56672 0.84010 52 H 7.417415 0.91218 1.603082 5	42 H -1.891058 1.264979 4.996552	40 O -6.500827 -0.626957 -0.817278					
44 H 3.874951 1.494691 0.941979 42 O -3.083752 -0.965596 -3.650461 45 H 4.272001 -2.091814 -1.378753 43 H 1.283502 1.654941 0.518023 46 H 1.811418 -2.293191 -1.487918 44 H 3.733327 1.861893 0.675388 47 H 5.054736 -4.16704 1.960732 46 H 1.711656 -2.334804 -1.027881 49 H 8.500758 -4.487356 0.78056 47 H 5.103226 -1.951481 1.785281 50 H 9.374930 -2.756578 0.781139 1.192268 48 H 6.533674 -3.942248 2.132290 51 H 8.82773 2.980157 0.857200 51 H 7.731552 0.59927 -1.327593 54 H 7.937517 4.565672 0.842010 52 H 7.417415 0.91218 1.603082 55 H 5.964721 3.904248 2.132290 2.57766 <td>43 H 1.413810 1.306704 0.808902</td> <td>41 C -3.177503 -0.861567 -2.501865</td>	43 H 1.413810 1.306704 0.808902	41 C -3.177503 -0.861567 -2.501865					
43 H 1.28302 1.054941 0.518023 46 H 1.81148 -223191 1.487918 44 H 3.73327 1.861893 0.675388 47 H 5.054736 -2.152104 1.532574 45 H 4.161064 -2.138076 -0.872572 48 H 6.413505 -4.169410 1.960732 46 H 1.711656 -2.334804 -1.027881 49 H 8.590758 -4.87356 0.758389 -1.260466 47 H 5.103226 -1.951481 1.785281 50 H 9.373930 -758389 -1.260466 49 H 8.52073 -3.42248 2.132290 51 H 8.000753 -0.758389 -1.260466 49 H 8.52073 -2.62706 -0.66881 52 H 7.75578 0.87113 1.192268 50 H 9.17929 -2.57706 -0.965843 53 H 8.26073 -3.07143 2.08109 51 H 7.471415 0.91219 1.603082 55	44 H 3.874951 1.494691 0.941979	42 O -3.083752 -0.965596 -3.650461					
44 n 5.7532/ 1.60139 0.073386 44 n 5.7532/ 1.60139 0.073386 48 H 6.413505 -4.169410 1.960732 46 H 1.1711656 2.334804 -1.027881 49 H 8.590758 -4.487356 0.798056 47 H 5.103226 -1.951481 1.785281 50 H 9.374930 -2.75968 0.812358 48 H 6.533674 -3.942248 2.132290 51 H 8.000753 0.78139 1.192268 50 H 9.179292 -2.577060 0.965843 52 H 7.756578 0.781139 1.92268 50 H 9.179292 -2.577060 0.965843 53 H 8.827793 2.980157 0.857200 51 H 7.731552 0.59927 1.327593 54 H 9.937431 2.080199 52 H 7.471415 0.912198 1.603082 55 H 5.964721 3.904811 -2.08109 54 H 7.92073	46 H 1 811418 -2 293191 -1 487918	43 H 1.283502 1.654941 0.518023					
48 H 6.413505 4.169410 1.960732 46 H 1.711656 2.334804 -1.027881 49 H 8.590758 -4.487356 0.798056 47 H 5.103226 -1.951481 1.785281 50 H 9.374930 2.759638 -0.812358 48 H 6.533674 -3.942248 2.132290 51 H 8.00753 -0.758389 -1.260466 49 H 8.582073 -4.26108 0.760851 52 H 7.756578 0.781139 1.92268 50 H 9.179292 -2.577060 -0.965843 53 H 8.82773 2.980157 0.857200 51 H 7.731552 0.599927 -1.327593 54 H -9.32792 -0.90683 4.814105 54 H 7.929073 4.68842 -0.389787 55 H 5.94721 3.092011 2.929644 55 H 5.028771 1.86162 -1.834492 50 H -1.26208 3.05733 3.874271 59 H -3.6	47 H 5.054736 -2.152104 1.532574	44 F 5.755527 1.601695 0.075566 45 H 4.161064 -2.138076 -0.872572					
49H8.590758-4.4873560.7980561.78528150H9.374930-2.759683-0.81235848H5.103226-1.9514811.78528151H8.000753-0.758389-1.26046649H8.582073-4.2621080.76085152H7.7565780.7811391.19226850H9.179292-2.577060-0.96584353H8.827732.9801570.85720051H7.731552-0.599927-1.32759354H7.9375174.565672-0.84201052H7.4174150.9121981.60308255H5.9647213.904811-2.20810953H8.5623663.1005081.41412157H-2.927923-0.9906834.81410554H7.9290734.688842-0.38978756H4.9121661.693258-1.88948253H6.1526694.06039-2.01121359C-1.637463.0220112.92964455H6.1526694.06039-2.01121359C-1.6368813.793911.81283456H-3.021711.861682-1.83449260H-2.9215404.13993-2.60835057H-3.616521-2.2089962.16275361H-1.2622863.4057333.87427159H-3.8066152.4999153.51257262C-3.8743711.672244-2.972530	48 H 6.413505 -4.169410 1.960732	45 H 1 711656 -2 334804 -1 027881					
50 H 9.374930 -2.759683 -0.812358 48 H 6.533674 -3.942248 2.132290 51 H 8.000753 -0.758389 -1.260466 49 H 8.582073 -4.262108 0.760851 52 H 7.756578 0.781139 1.192268 50 H 9.179292 -2.577060 -0.965843 53 H 8.2827733 2.980157 0.857200 51 H 7.731552 -0.599927 -1.327593 54 H 7.937517 4.565672 -0.842010 52 H 7.417415 0.912198 1.603082 55 H 5.964721 3.904811 -2.08109 53 H 8.56266 3.100508 1.41421 56 H 4.912166 1.693258 -1.889482 55 H 6.152669 4.060639 -2.011213 57 H -2.327540 4.139939 -2.608350 57 H -3.616521 -2.20896 2.162753 50 H -1.260788 4.813031 1.838415 58 H	49 H 8.590758 -4.487356 0.798056	47 H 5.103226 -1.951481 1.785281					
51 H 8.000753 -0.758389 -1.260466 49 H 8.582073 -4.262108 0.760851 52 H 7.756578 0.781139 1.192268 50 H 9.179292 -2.577060 -0.965843 53 H 8.827793 2.980157 0.857200 51 H 7.731552 -0.599927 -1.327593 54 H 7.937517 4.565672 -0.842010 52 H 7.417415 0.912198 1.603082 55 H 5.964721 3.90481 -2.08109 53 H 8.562366 3.100508 1.414121 56 H 4.912166 1.693258 -1.889482 55 H 6.152669 4.060639 -2.011213 57 H -2.927923 0.990683 4.814105 55 H 6.152669 4.060639 -2.01213 58 C -1.63681 3.79391 1.812834 56 H -3.20171 1.861682 -1.834492 60 H -2.20289 4.139993 -2.608350 57 H <t< td=""><td>50 H 9.374930 -2.759683 -0.812358</td><td>48 H 6.533674 -3.942248 2.132290</td></t<>	50 H 9.374930 -2.759683 -0.812358	48 H 6.533674 -3.942248 2.132290					
52 H 7.756578 0.781139 1.192288 50 H 9.179292 -2.577060 -0.965843 53 H 8.827793 2.980157 0.857200 51 H 7.731552 -0.599927 -1.327593 54 H 7.937517 4.565672 -0.842010 52 H 7.417415 0.912198 1.603082 55 H 5.964721 3.904811 -2.208109 52 H 7.417415 0.912198 1.603082 56 H 4.912166 1.693258 -1.889482 53 H 8.562366 3.100508 1.414121 57 H -2.927923 -0.990683 4.814105 54 H 7.929073 4.688842 -0.389787 58 C -1.637746 3.02011 2.929644 55 H 6.152669 4.060639 -2.011213 59 K -2.921540 4.139993 -2.608550 57 H -3.616521 -2.20896 2.162753 61 H -1.262286 3.405733 3.874271 59 H	51 H 8.000753 -0.758389 -1.260466	49 H 8.582073 -4.262108 0.760851					
54 H 7.937517 4.565672 -0.842010 51 H 7.731552 -0.599927 -1.327593 55 H 5.964721 3.904811 -2.208109 52 H 7.417415 0.912198 1.603082 56 H 4.912166 1.693258 -1.889482 53 H 8.562366 3.100508 1.414121 57 H -2.927923 -0.990683 4.814105 54 H 7.929073 4.688842 -0.389787 58 C -1.637746 3.022011 2.929644 55 H 6.152669 4.060639 -2.011213 59 C -1.636881 3.793991 1.812834 56 H 5.028771 1.861682 -1.834492 60 H -2.921540 4.139993 -2.608350 57 H -3.616521 -2.208996 2.162753 61 H -1.262286 3.405733 3.874271 59 H -3.80615 2.499915 3.512572 63 C -3.874371 1.67224 2.972530 60 H	52 H 8 827793 2 980157 0 857200	50 H 9.179292 -2.577060 -0.965843					
55H5.9647213.904811-2.20810952H7.4174150.9121981.60308256H4.9121661.693258-1.88948253H8.5623663.1005081.41412157H-2.927923-0.9906834.81410554H7.9290734.688842-0.38978758C-1.6377463.0220112.92964455H6.1526694.060639-2.01121359C-1.6368813.7939911.81283456H5.0287711.861682-1.83449260H-2.9215404.139993-2.60835057H-3.616521-2.2089962.16275361H-1.2627683.4057333.87427158H-3.8066152.4999153.51257263C-3.8743711.672244-2.9725060H-3.6263763.8624901.95459364H-3.1540351.083321-3.5018461H-3.0334324.309513-2.28649165H-4.7239671.024787-2.74145962H-3.0390731.840364-2.47077566H-4.7239672.204772.63294867C-3.879403-2.021772.63294868H-4.727715-2.214431.943965	54 H 7.937517 4.565672 -0.842010	51 H 7.731552 -0.599927 -1.327593					
56 H 4.912166 1.693258 -1.889482 53 H 8.562366 3.100508 1.414121 57 H -2.927923 -0.90683 4.814105 54 H 7.929073 4.688842 -0.389787 58 C -1.637746 3.022011 2.929644 55 H 6.152669 4.060639 -2.011213 59 C -1.636881 3.793991 1.812834 56 H 5.028771 1.861682 -1.834492 60 H -2.921540 4.13993 -2.608350 57 H -3.616521 -2.20896 2.162753 61 H -1.262786 3.405733 3.874271 59 H -3.806615 2.499915 3.512572 63 C -3.874371 1.672244 -2.972530 60 H -3.033432 4.30951 -2.286491 64 H -3.154035 1.08321 -3.50184 61 H -3.039073 1.840364 -2.470775 66 H -4.216576 2.496506 -3.604528 -2.470775 -	55 H 5.964721 3.904811 -2.208109	52 H 7.417415 0.912198 1.603082					
57 H -2.927923 -0.990683 4.814105 54 H 7.929073 4.888842 -0.389787 58 C -1.637746 3.022011 2.929644 55 H 6.152669 4.060639 -2.011213 59 C -1.636881 3.793991 1.812834 56 H 5.028771 1.861682 -1.834492 60 H -2.921540 4.139993 -2.608350 57 H -3.616521 -2.20896 2.162753 61 H -1.260789 4.813031 1.838415 58 H -3.891733 -1.675523 4.562648 62 H -1.262286 3.405733 3.874271 59 H -3.806155 2.499915 3.512572 63 C -3.874371 1.672244 -2.972530 60 H -3.033432 4.309513 -2.286491 64 H -3.154035 1.08321 -3.50184 61 H -3.039073 1.840364 -2.470775 66 H -4.216576 2.496506 -3.604528 -2.470775	56 H 4.912166 1.693258 -1.889482	53 H 8.562366 3.100508 1.414121					
58 C -1.637746 3.022011 2.929644 53 H 0.152009 4.00039 -2.011213 59 C -1.636881 3.793991 1.812834 56 H 5.028771 1.861682 -1.834492 60 H -2.921540 4.139993 -2.608350 57 H -3.616521 -2.208996 2.162753 61 H -1.262286 3.405733 3.874271 59 H -3.806155 2.499915 3.512572 63 C -3.874371 1.672244 -2.972530 60 H -3.626376 3.862490 1.954593 64 H -3.154035 1.024787 -2.741459 62 H -3.033432 4.309513 -2.286491 65 H -4.216576 2.496506 -3.604528 62 H -3.039073 1.840364 -2.470775 66 H -4.223775 -2.21434 1.943965 -2.470775 -2.470775 -2.470775 67 C -3.874903 -2.202477 2.632948 -4.727715 -2.21434 1.94	57 H -2.927923 -0.990683 4.814105	54 H 7.929073 4.688842 -0.389787					
59 C -1.030881 3.793991 1.812834 50 H -3.031071 1.601071 <td< td=""><td>58 C -1.637746 3.022011 2.929644</td><td>56 H 5 028771 1 861682 -1 834492</td></td<>	58 C -1.637746 3.022011 2.929644	56 H 5 028771 1 861682 -1 834492					
61 H -1.260789 4.813031 1.838415 58 H -3.891733 -1.675523 4.562648 62 H -1.262286 3.405733 3.874271 59 H -3.806615 2.499915 3.512572 63 C -3.874371 1.672244 -2.972530 60 H -3.626376 3.862490 1.954593 64 H -3.154035 1.083321 -3.550184 61 H -3.033432 4.309513 -2.286491 65 H -4.216576 2.496506 -3.604528 62 H -3.039073 1.840364 -2.470775 66 H -4.227715 -2.214434 1.943965 62 H -3.039073 1.840364 -2.470775 68 H -4.727715 -2.214434 1.943965 -	54 C -1.030881 3.793991 1.812834 60 H -2 921540 4.139993 -2 608350	57 H -3.616521 -2.208996 2.162753					
62 H -1.262286 3.405733 3.874271 59 H -3.806615 2.499915 3.512572 63 C -3.874371 1.672244 -2.972530 60 H -3.626376 3.862490 1.954593 64 H -3.154035 1.083321 -3.550184 61 H -3.033432 4.309513 -2.286491 65 H -4.723967 1.024787 -2.741459 62 H -3.039073 1.840364 -2.470775 66 H -4.216576 2.496506 -3.604528 62 H -3.039073 1.840364 -2.470775 66 H -4.727715 -2.214434 1.943965 62 H -3.039073 1.840364 -2.470775 67 C -3.879403 -2.202477 2.632948 64 H -4.727715 -2.214434 1.943965 69 H -3.159207 -2.951779 2.287588 H H H H H H H H H H H H H H H	61 H -1.260789 4.813031 1.838415	58 H -3.891733 -1.675523 4.562648					
63 C -3.874371 1.672244 -2.972530 60 H -3.626376 3.862490 1.954593 64 H -3.154035 1.083321 -3.550184 61 H -3.033432 4.309513 -2.286491 65 H -4.723967 1.024787 -2.741459 62 H -3.039073 1.840364 -2.470775 66 H -4.216576 2.496506 -3.604528 62 H -3.039073 1.840364 -2.470775 67 C -3.879403 -2.202477 2.632948 1.943965 5 5 5 5 5.214434 1.943965 68 H -4.727715 -2.214434 1.943965 5	62 H -1.262286 3.405733 3.874271	59 H -3.806615 2.499915 3.512572					
64 H -3.154035 1.083321 -3.550184 61 H -3.033432 4.309513 -2.286491 65 H -4.723967 1.024787 -2.741459 62 H -3.039073 1.840364 -2.470775 66 H -4.216576 2.496506 -3.604528 62 H -3.039073 1.840364 -2.470775 67 C -3.879403 -2.202477 2.632948 64 H -4.727715 -2.214434 1.943965 68 H -4.727715 -2.214434 1.943965 64 H -3.159207 -2.951779 2.287588 70 H -4.223725 -2.501842 3.626809 H	63 C -3.874371 1.672244 -2.972530	60 H -3.626376 3.862490 1.954593					
65 H -4.723967 1.024787 -2.741459 62 H -3.039073 1.840364 -2.470775 66 H -4.216576 2.496506 -3.604528 62 H -3.039073 1.840364 -2.470775 67 C -3.879403 -2.202477 2.632948 68 H -4.727715 -2.214434 1.943965 68 H -4.727715 -2.951779 2.287588 - <td>64 H -3.154035 1.083321 -3.550184</td> <td>61 H -3.033432 4.309513 -2.286491</td>	64 H -3.154035 1.083321 -3.550184	61 H -3.033432 4.309513 -2.286491					
bb H -4.216576 2.496506 -3.604528 67 C -3.879403 -2.202477 2.632948 68 H -4.727715 -2.214434 1.943965 69 H -3.159207 -2.951779 2.287588 70 H -4.223725 -2.501842 3.626809	65 H -4.723967 1.024787 -2.741459	62 H -3.039073 1.840364 -2.470775					
67 C -3.073403 -2.202477 2.032346 68 H -4.727715 -2.214434 1.943965 69 H -3.159207 -2.951779 2.287588 70 H -4.223725 -2.501842 3.626809	66 H -4.216576 2.496506 -3.604528						
69 H -3.159207 -2.951779 2.287588 70 H -4.223725 -2.501842 3.626809	07 C -3.079403 -2.202477 2.032948 68 H -4 727715 -2 214434 1 943965						
70 H -4.223725 -2.501842 3.626809	69 H -3.159207 -2.951779 2.287588						
	70 H -4.223725 -2.501842 3.626809						