SUPPLEMENTARY INFORMATION

for

Fluorine interaction controlled AIEE phenomenon in an expanded calixbenzophyrin and its vapoluminescent response: Turn on emission with volatile ketones and esters

P. S. Salini, M. G. Derry Holaday, M. L. P. Reddy, C. H. Suresh* and A. Srinivasan*

Table of Contents:

1. **General Information : 2**
2. **ChemDraw structure of M-I and M-III : 3**
3. **Aggregation Properties (Figures S1–S12) : 3-10**
4. **Disaggregation Studies (Figures S13–S20) : 11-15**
5. **Spectral analyses of Calix[2]-*m*-benzo[4]phyrin : 16**
6. **Optimized geometries and energies : 17-65**

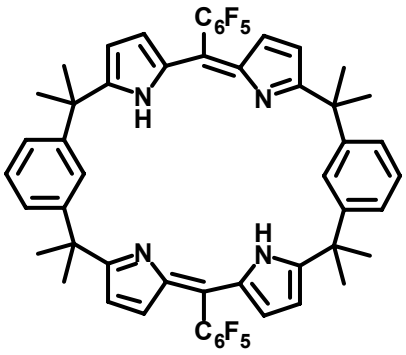
P. S. Salini, M. G. Derry Holaday
Photosciences and Photonics Section,
Dr. M. L. P. Reddy, Dr. C. H. Suresh
Inorganic Chemistry Section,
Chemical Sciences and Technology Division,
National Institute for Interdisciplinary Science and Technology (CSIR–NIIST),
Thiruvananthapuram – 695 019, Kerala, India.

Dr. A. Srinivasan
School of Chemical Sciences,
National Institute of Science Education and Research,
IOP Campus, Sainik School – P. O.,
Bhubaneswar – 751 005, Odisha, India.
Fax: (+91)674-2302436
E-mail: srini@niser.ac.in

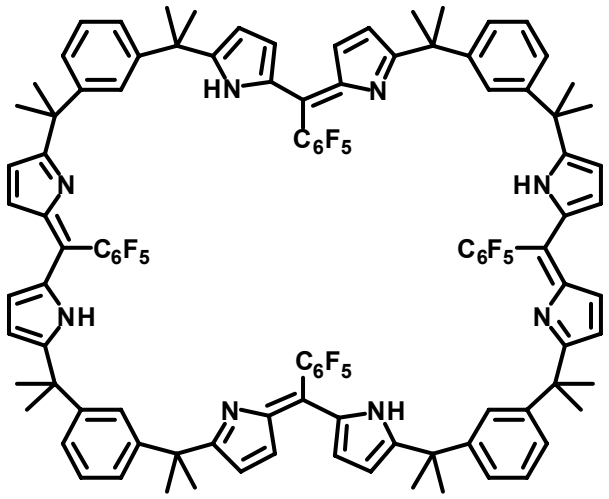
1. General Information:

The fluorescence spectra were recorded on a SPEX-Fluorolog F112X spectrofluorimeter. Electronic absorption spectra were recorded with Shimadzu 3101PC UV-Vis-NIR Scanning spectrophotometer. The single crystal X-ray diffraction data of **M-II** was collected on a Bruker AXS Kappa Apex 2 CCD diffractometer at 273(2) K. Good quality single crystal was grown by slow evaporation of *n*-hexane into chloroform solutions of **M-II**. All the solvents used were purified and distilled before use and doubly distilled water was used for all the experiments. Fluorescence quantum yields in solution state were determined using fluorescein in 0.1M NaOH (Φ_f = 0.95) as a reference. Fluorescence lifetimes were measured using IBH (FluoroCube) time-correlated picosecond single photon counting (TCSPC) system. Samples were excited with a pulsed diode laser (<100 ps pulse duration) at a wavelength of 440 nm (NanoLED-10) with a repetition rate of 1 MHz. The detection system consists of a microchannel plate photomultiplier (5000U-09B, Hamamatsu) with a 38.6 ps response time coupled to a monochromator (5000M) and TCSPC electronics (DataStation Hub including Hub-NL, NanoLED controller and preinstalled Fluorescence Measurement and Analysis Studio (FMAS) software). The fluorescence lifetime values were obtained using DAS6 decay analysis software. SEM analysis was carried out using scanning electron microscope JEOL JSM 5600LV. HR-TEM measurements were carried out using JEOL JEM1011 with an accelerating voltage of 100 kV. Samples were prepared by drop casting of 40:60 acetonitrile / water solutions of **M-II** on to carbon coated copper grids at the required concentrations at ambient conditions. The solvent was removed under vacuum. DLS analyses were carried out with a Zetasizer Nano S from Malvern Instruments at 25°C. The average hydrodynamic radii were calculated from Stork-Einstein equation ($R_h = kBT/(6\pi\eta D)$). The fluorescence measurement of **M-II** films with various VOCs was carried out by exposing organic vapors for 5 min in the closed environment and immediately measured the emission spectrum. All experiments were carried out at room temperature (25 ±1°C), unless otherwise mentioned.

2. ChemDraw structure of M-I and M-III:



M-I



M-III

3. Aggregation Properties:

(A) (B)

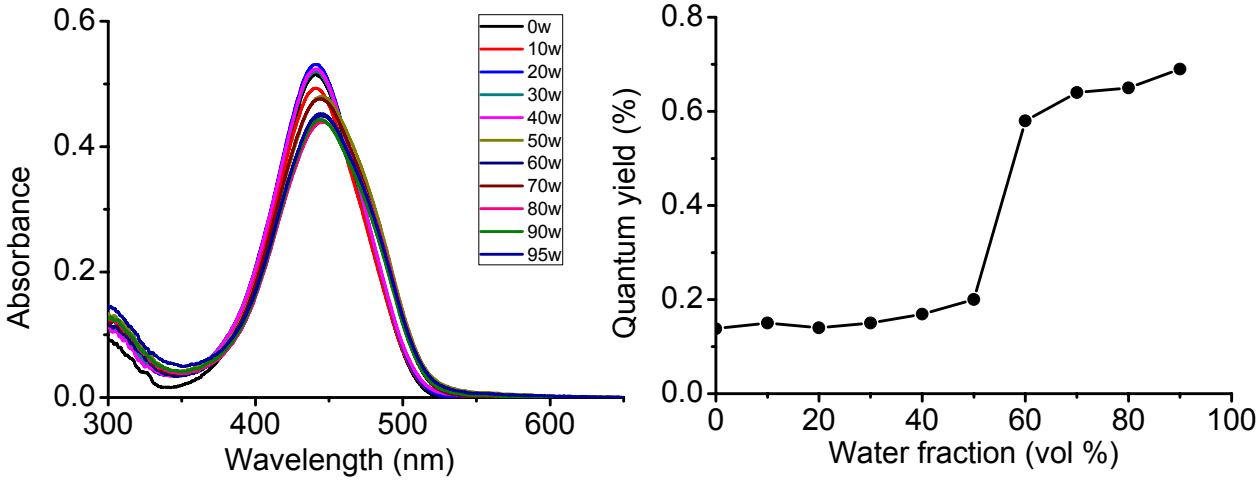


Figure S1. (A) Absorption spectra of **M-II** (8.2 μM) in acetonitrile and acetonitrile/water mixture. (B) Variation in quantum yield with increase in water contents in the acetonitrile/water mixtures (f_w = 0-90 vol %).

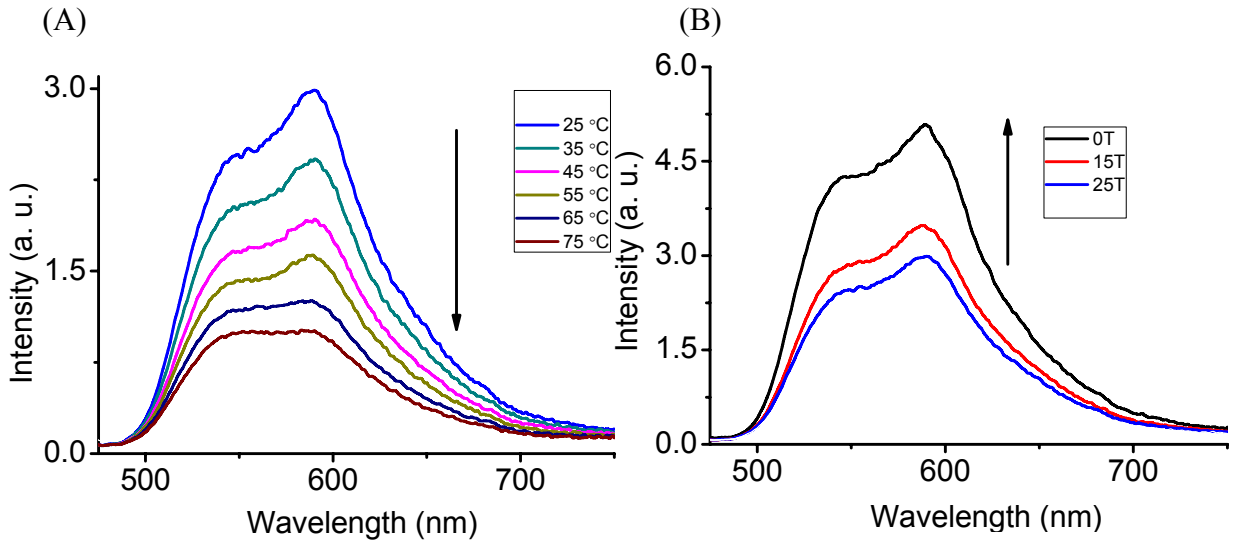


Figure S2. Temperature effect on the emission intensity of **M-II** in acetonitrile/water (1:9 v/v), (λ_{ex} = 440 nm). (A) Temperature increases from 25 °C-75 °C. (B) Temperature decreases from 25 °C-0 °C.

3.1. Single Crystal Analyses of M-II:

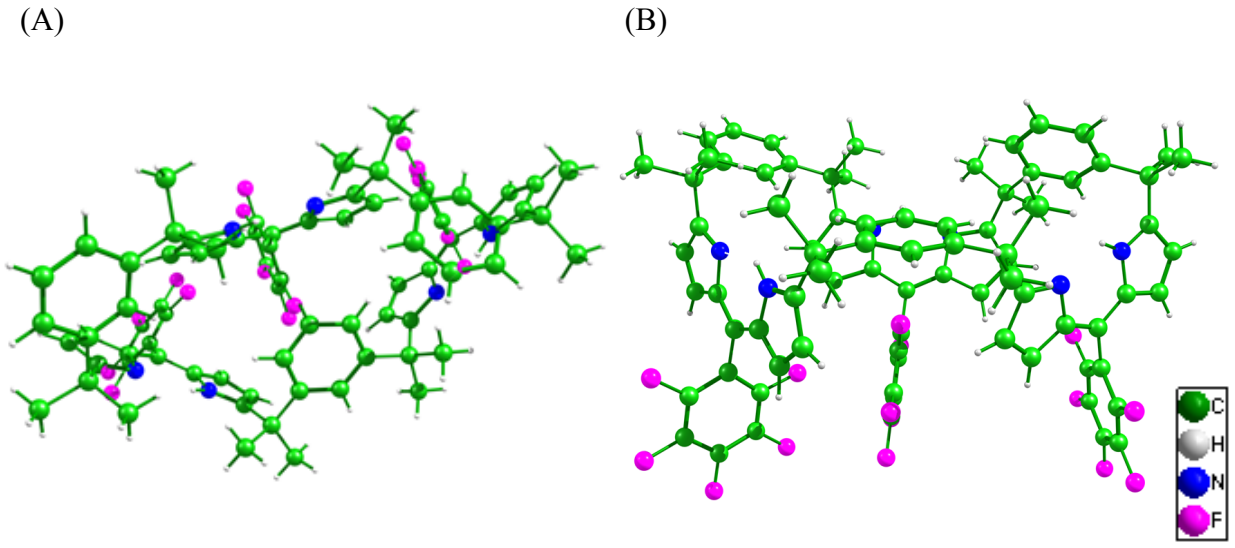


Figure S3. Single crystal X-ray structure of **M-II**: (A) Top view and (B) Side view

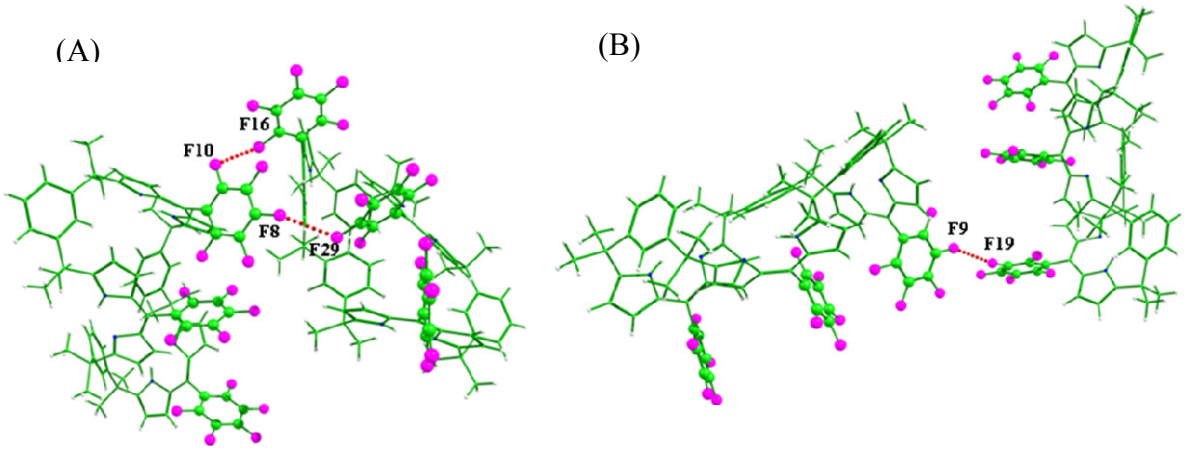


Figure S4. Single crystal X-ray analysis of **M-II:** Self-assembled dimer (A) and (B) formed by F…F interactions with the distances of F10…F16: 2.892 Å, F8…F29: 2.876 Å, and F9…F19: 2.785 Å, respectively.

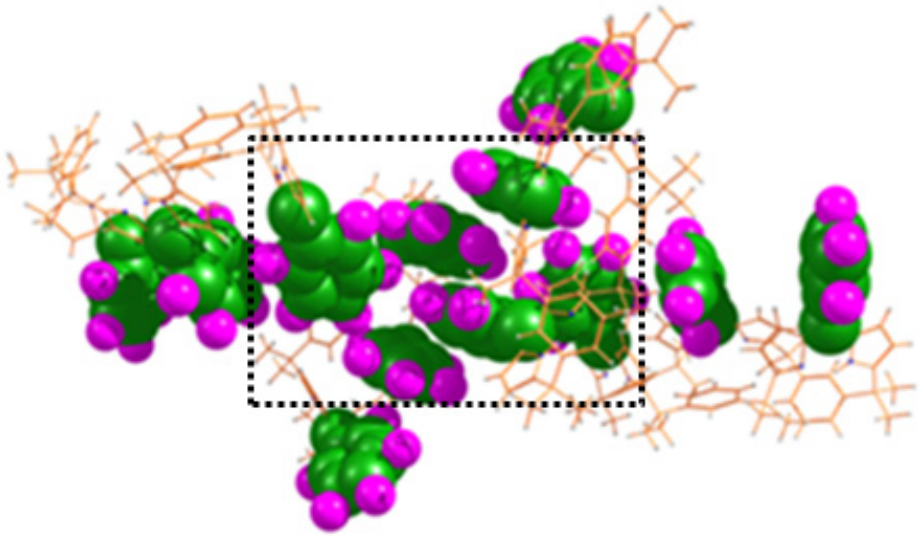


Figure S5. Single crystal X-ray analysis of tetramer cluster of **M-II** showing six-pack pattern.

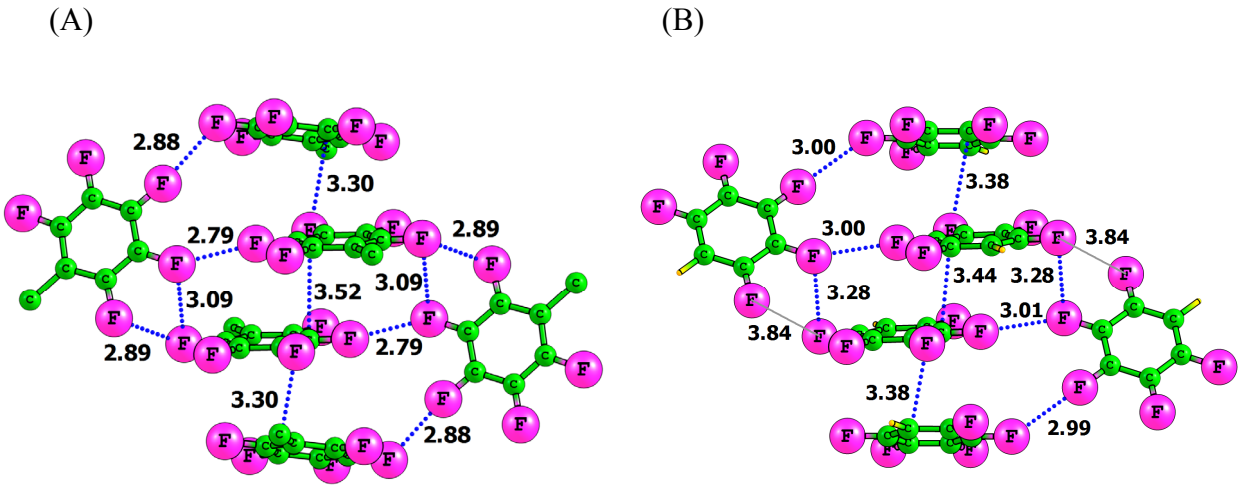


Figure S6. F...F, C-F...π_F and π_F...π_F stacking interactions in the 'six-pack' fluorophore cluster. (A) X-ray structure **M-II** and (B) optimized geometry of $(C_6F_5H)_6$ cluster using DFT (Distances in Å).

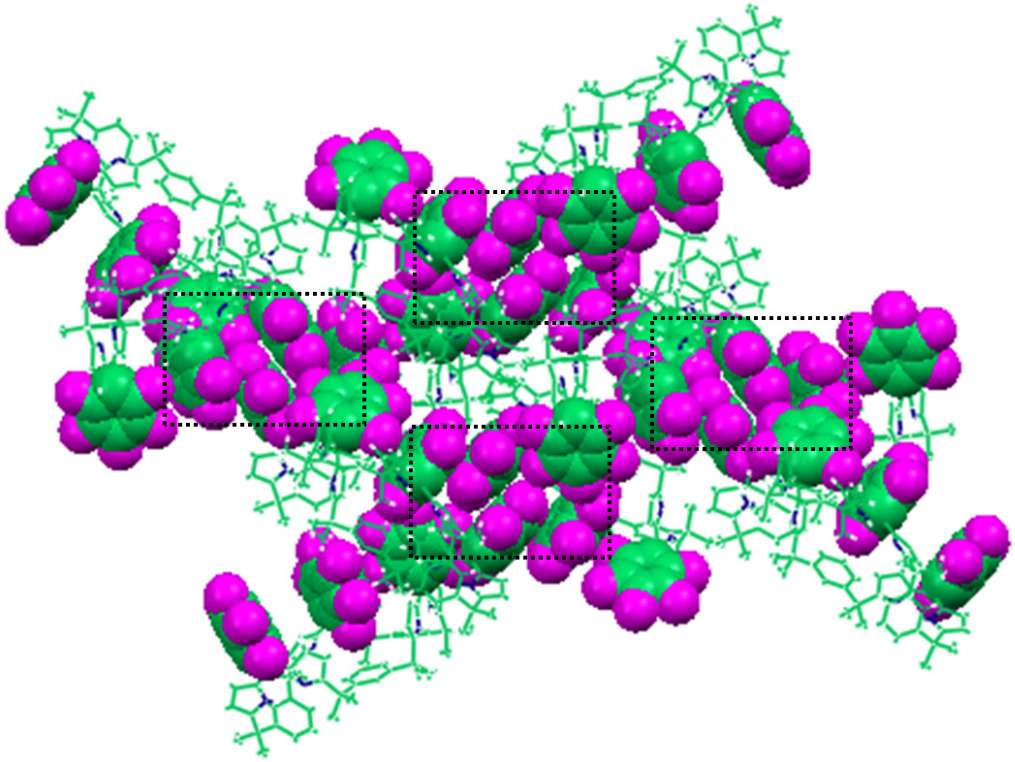


Figure S7. Single crystal X-ray analysis of dodecamer cluster of **M-II** showing repeated six-pack pattern.

(A)

(B)

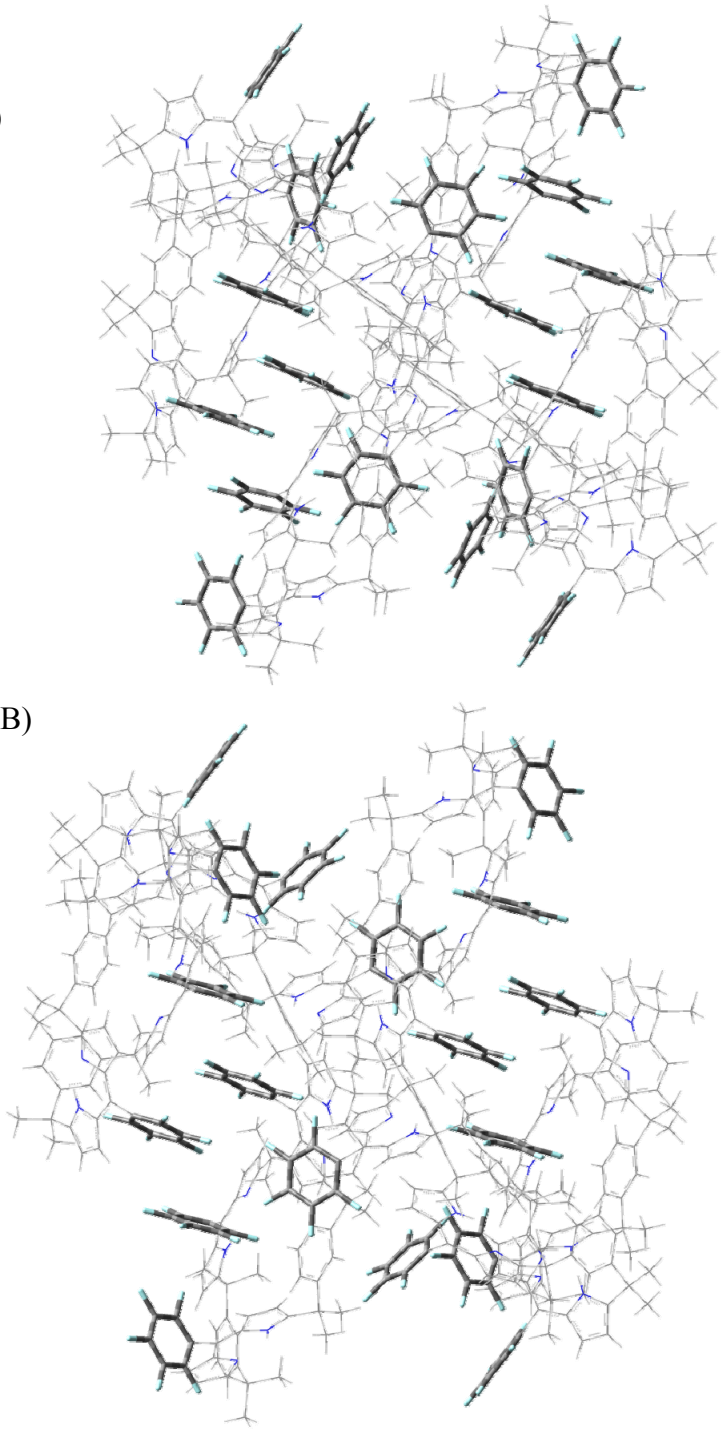


Figure S8. (A) X-ray geometry of a cluster composed of six molecules of M-II. (B) Optimized geometry of the same cluster using a two layer QM/MM ONIOM method. For the inner QM layer PM6 method (for all fluorinated aromatics) and outer MM layer universal force field (UFF) is used.

Crystallographic Data of M-II:

Crystallographic data of **M-II** in $CHCl_3$/n-hexane : $C_{81}H_{63}F_{15}N_6$, Mw = 1405.37, monoclinic, space group P21/n, a = 17.4183(12) Å, b = 14.7839(11) Å, c = 29.239(2) Å, α = 90.00º, β= 107.106(3)º, γ = 90.00º, V = 7196.2(9) $Å^3$, Z = 4, Dcalc = 1.297 mg/m^3, T = 273(2) K, R1 = 0.0432 {I > 2σ (I)}, R2w = 0.1240, GOF = 1.089.

CCDC- 882799 contains the supplementary crystallographic data for **M-II**. These data can be obtained free of charge from the Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

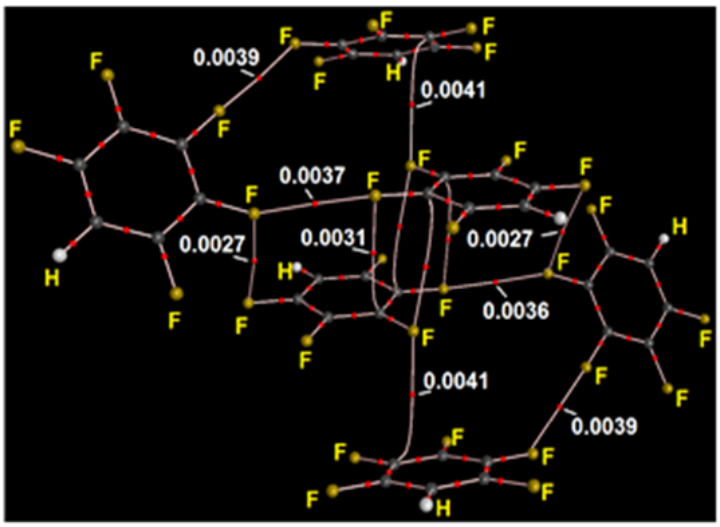


Figure S9. Electron density bond critical points for F...F, C-F...π_F and stacking π_F…π_F interactions (distances in Å and density in a.u.).

(A) (B)

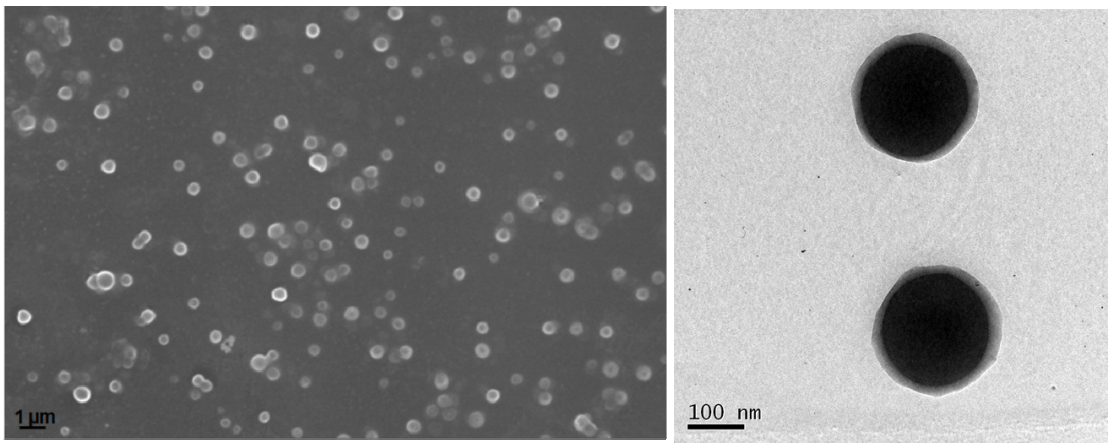


Figure S10. (A) SEM (scale bar=1μm) and (B) TEM (scale bar=100 nm) images of **M-II** aggregates

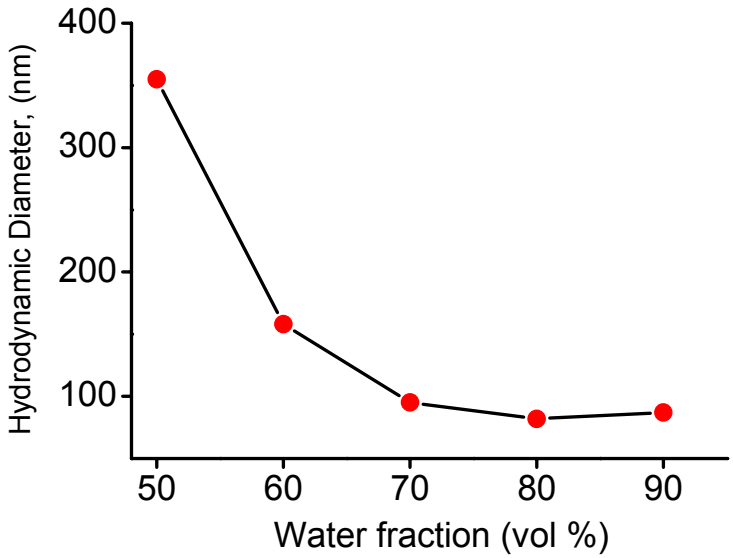


Figure S11. Hydrodynamic diameter of **M-II** (8.2 μM) in different acetonitrile/water mixture.

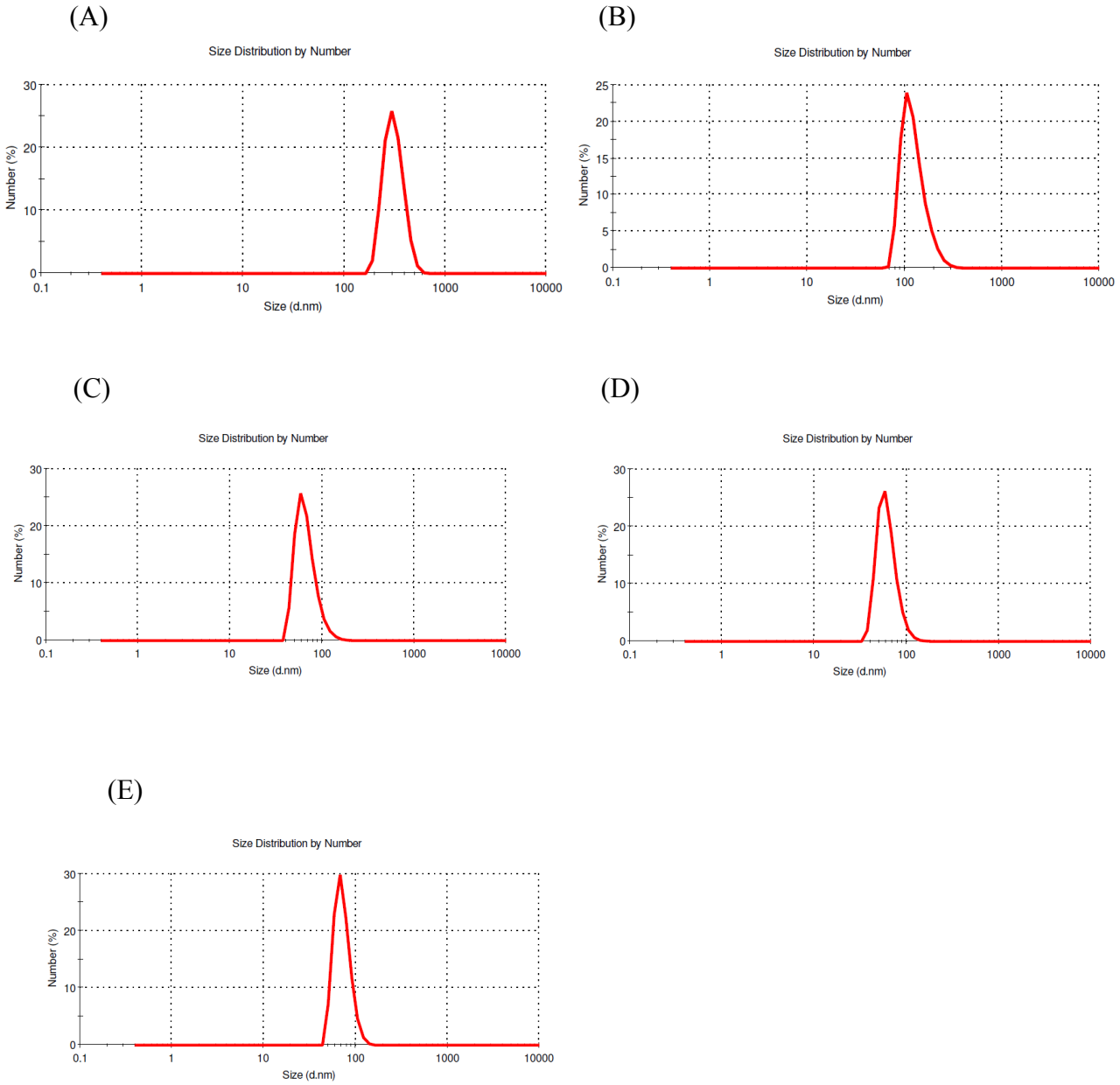


Figure S12. DLS measurements of **M-II** nanoparticle (8.2 μM) hydrodynamic size at room temperature in different acetonitrile/water mixture [(A) 50:50 (B) 40:60 (C) 30:70 (D) 20:80 (E) 10:90].

.

4. Disaggregation Studies:

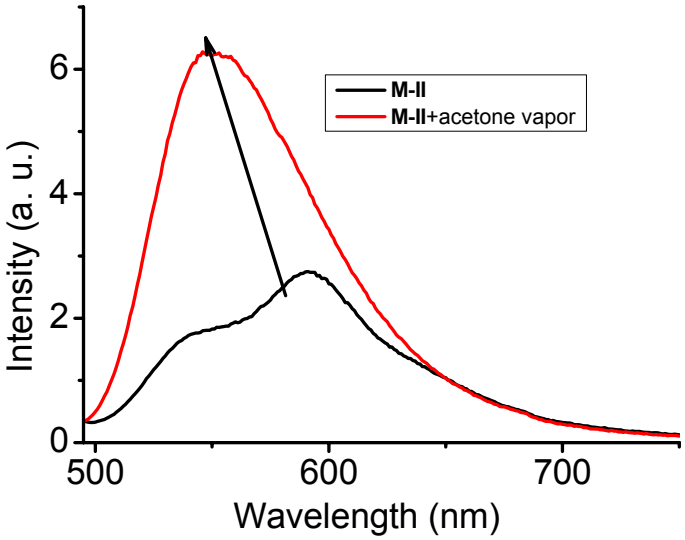


Figure S13. Changes in the emission spectrum of **M-II** film after exposure to acetone.

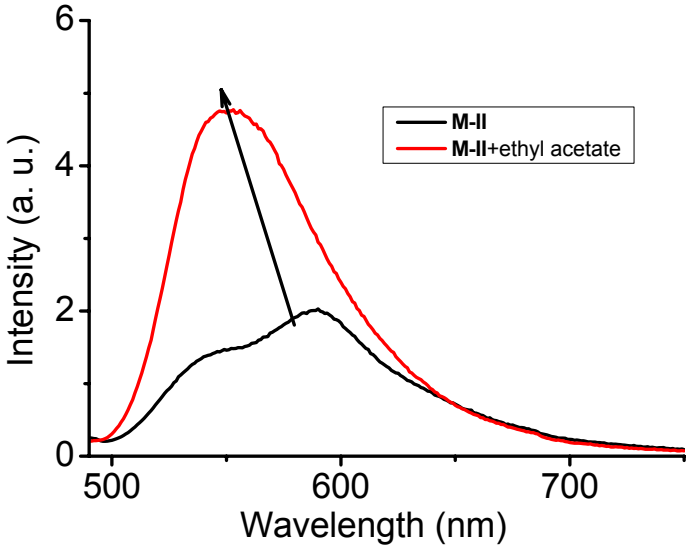


Figure S14. Emission Spectral changes of **M-II** film before and after exposure to ethyl acetate vapor.

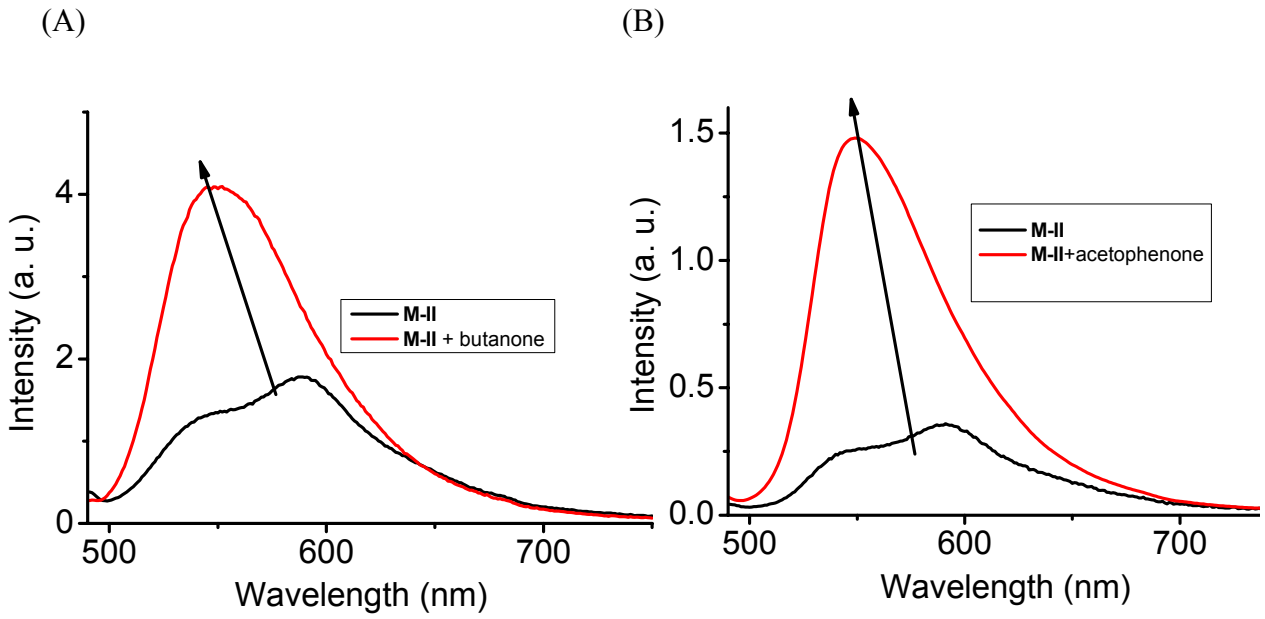


Figure S15. Emission Spectral changes of **M-II** film before and after exposure to (A) butanone and (B) acetophenone vapor

.

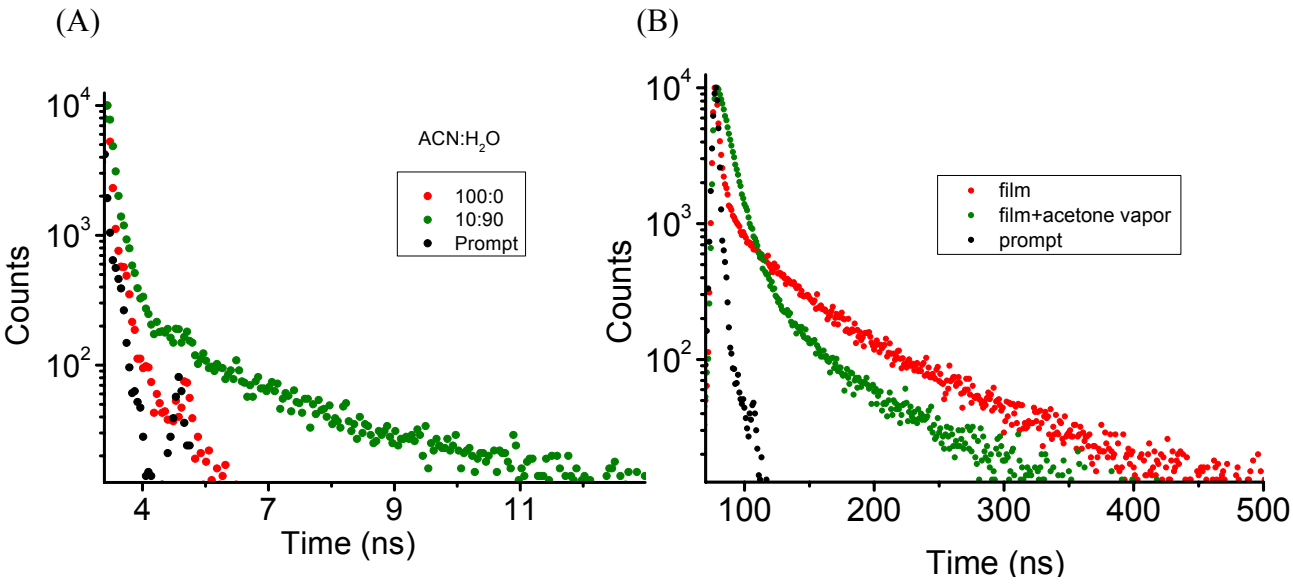


Figure S16. Lifetime decay profiles (λ_{ex}= 440 nm, monitored at 590 nm) of **M-II** in (A) solution and (B) film state.

Table S1. Fluorescence decay parameters of **M-II** in solution and film state.

M-II	τ_1 (ns)/A_1 [a]	τ_2 (ns)/A_2	τ_3 (ns)/A_3
ACN: H_2O (100:0) [b]	0.011/100	-	-
ACN: H_2O (10:90)	0.06/66.78	1.28/10.32	5.34/22.9
Film	0.16/46.34	1.72/27.86	6.26/25.81
Film with vapor	0.55/85.67	-	4.25/14.33

[a] where A and τ represents the percentage fractional amount and fluorescence lifetime of the shorter (1)- and longer (2 and 3)- lived species, respectively. [b] Volume ratios given in parentheses for solvent mixtures.

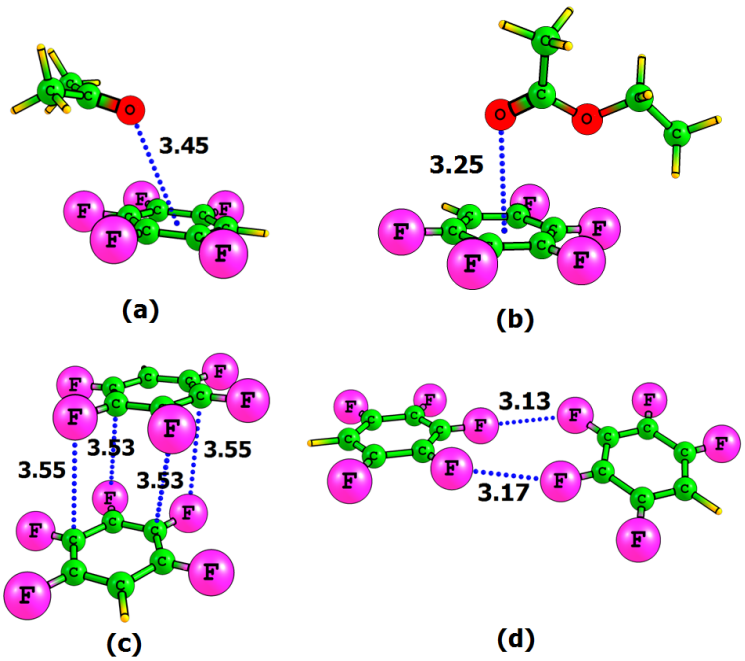


Figure S17. PW91PW91/6-311++G(d,p) optimized geometry of a) $(CH_3)_2CO...C_6F_5H$. b) $CH_3CH_2COCH_3...C_6F_5H$. (c) Stacked $(C_6F_5H)_2$. d) $(C_6F_5H)_2$ showing F...F interactions. All distances in Å. Interaction energy is computed using B97D/6-311++G(d,p) method.

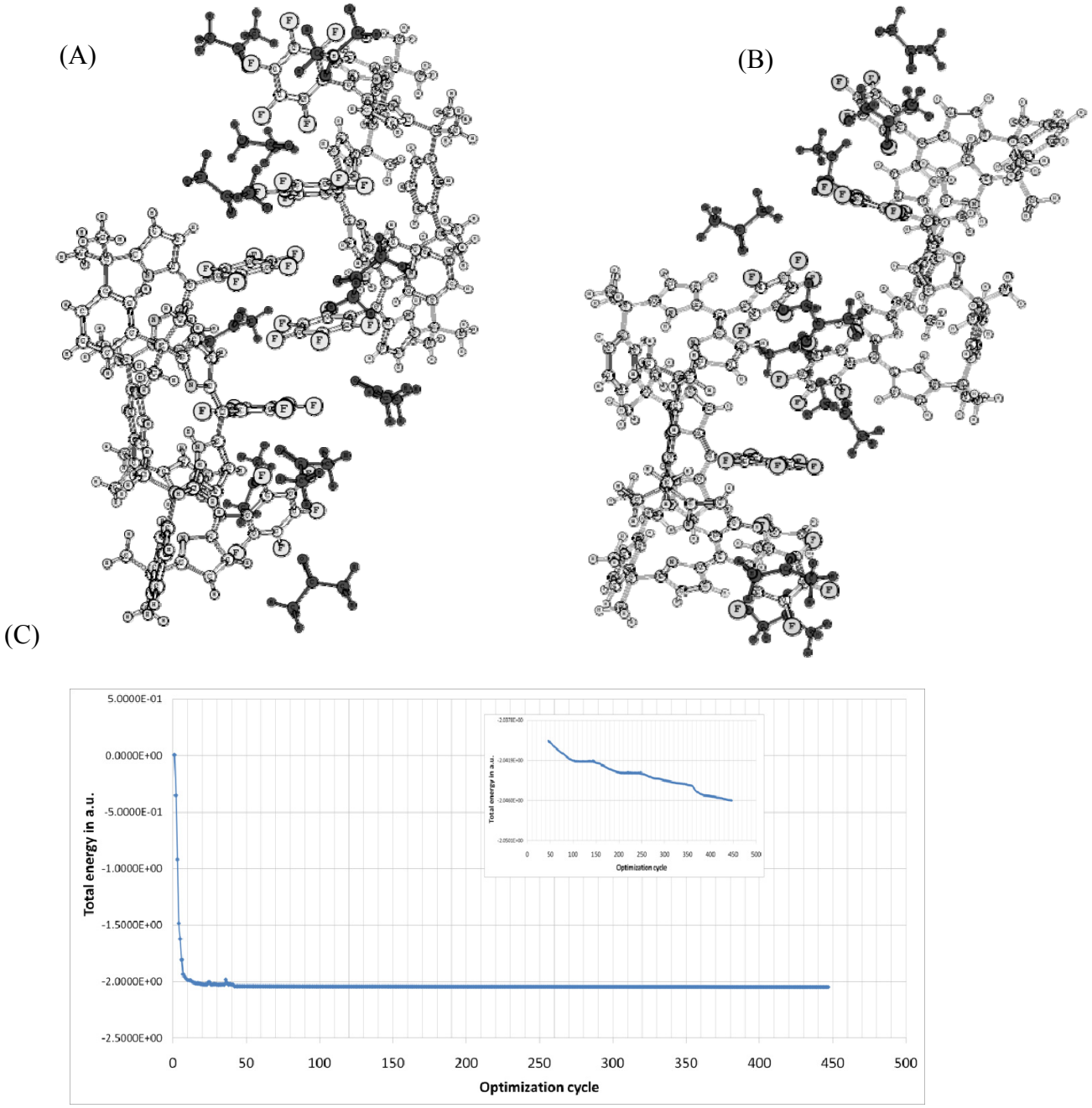


Figure S18. (A) X-ray geometry of a M-II dimer (grey shade) with ten acetone molecules (black shade) randomly oriented around pentalfluorophenylmoieties. Initial distance of carbonyl oxygen to the centre of the phenyl ring is selected to be 3.00 Å. (B) PM6 level optimized geometry of the same dimer with acetone (no geometry constraints are applied). (C) Energy convergence plot for 447 optimization cycles. In the inset, the same plot is shown, but without first 50 optimization cycles to indicate the slow convergence of the system.

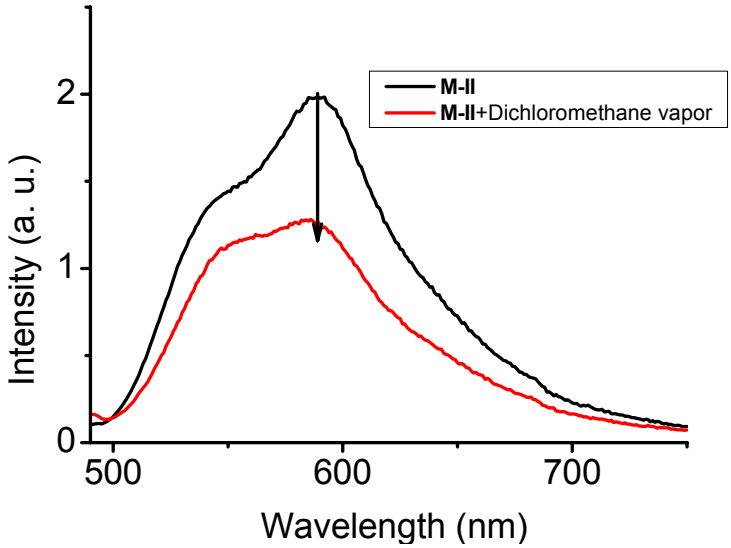


Figure S19. Changes in the emission spectrum of **M-II** film after exposure to dichloromethane vapor.

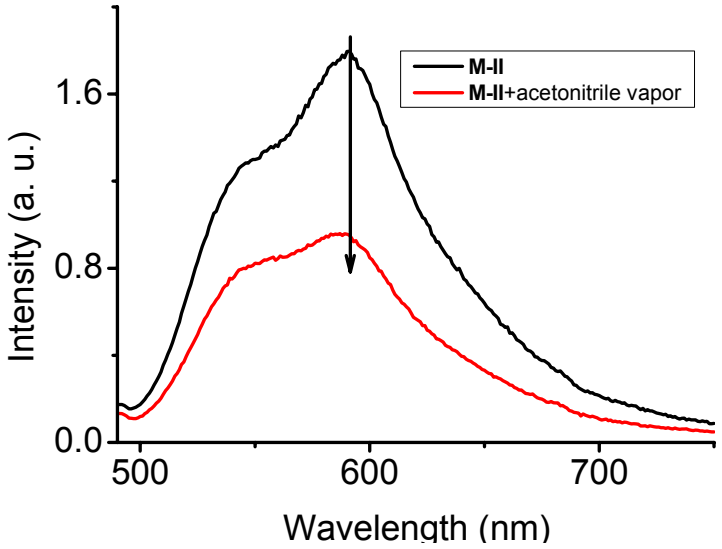


Figure S20. Changes in the emission spectrum of **M-II** film after exposure to acetonitrile vapor.

5. Spectral analyses of Calix[2]-*m*-benzo[4]phyrin containing C_6H_5 groups at *meso* position:

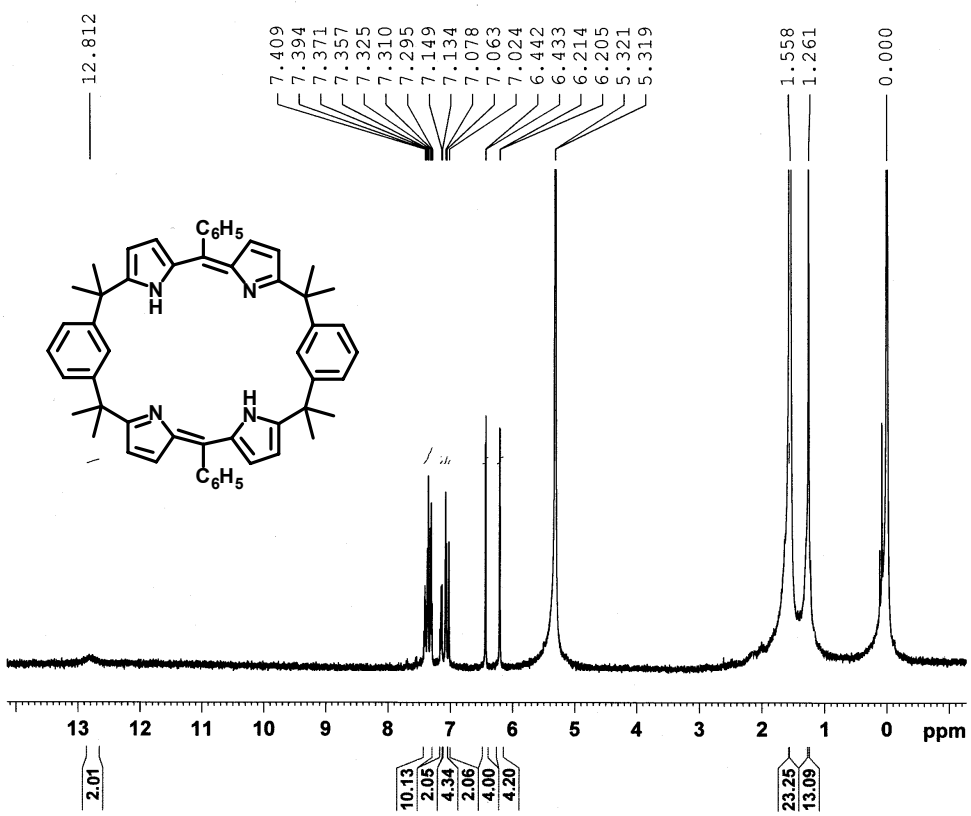


Figure S21. ^{1}H-NMR Spectrum in $CDCl_3$

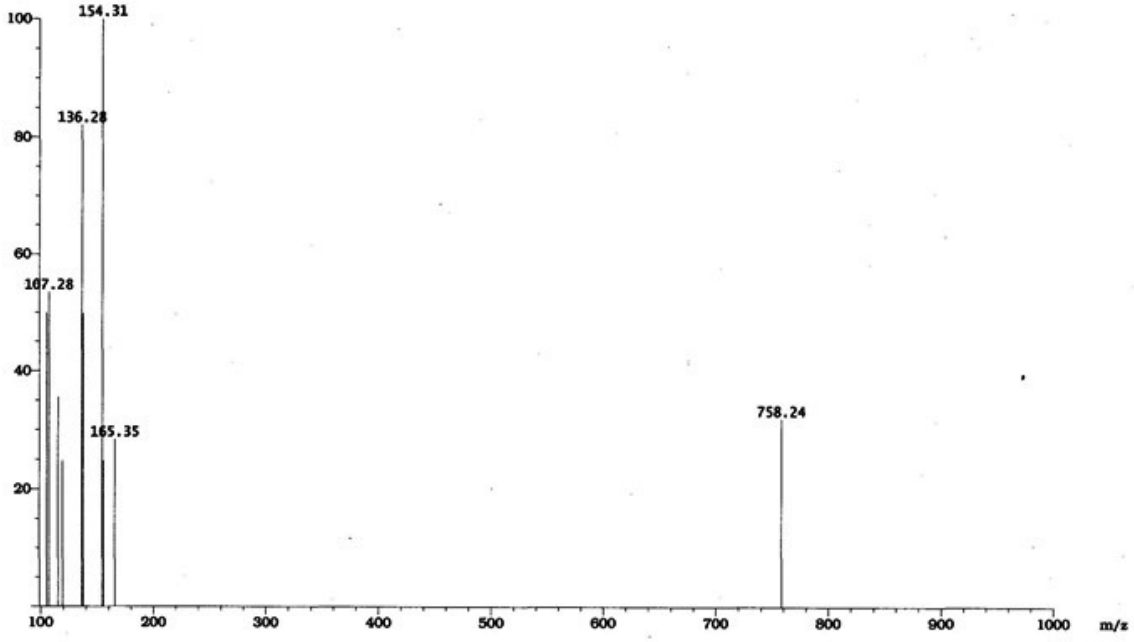


Figure S22. FAB MS Spectrum

6. Optimized geometries and energies:

Optimized Geometry of $(C_6F_5H)_6$ cluster at

PW91PW91/6-311++G(d,p). Coordinates in Angstrom unit

Atom	X	Y	Z
C	-7.263230	3.059728	0.538188
C	-8.161102	2.009878	0.373191
C	-7.720047	0.695076	0.202979
C	-6.346541	0.433723	0.196818
C	-5.428890	1.476179	0.360010
C	-5.899994	2.780662	0.529291
F	-9.487558	2.250035	0.376444
F	-8.594154	-0.311476	0.046359
F	-5.904670	-0.821380	0.038624
F	-4.112627	1.213362	0.352505
F	-5.007208	3.776454	0.689387
C	1.474767	-1.036896	3.089828
C	1.931698	-2.013781	2.211119
C	1.192613	-2.380597	1.084350
C	-0.029814	-1.747248	0.842079
C	-0.511248	-0.770544	1.717364
C	0.253399	-0.423094	2.833003
C	2.052061	5.553197	1.551862
C	1.317899	5.676109	0.376803
C	1.767702	5.115311	-0.820409
C	2.978768	4.417273	-0.836214
C	3.733091	4.286308	0.333059
C	3.255156	4.855855	1.516081
F	3.109492	-2.6274150	2.442051
F	1.633553	-3.3248030	0.240994
F	-0.749264	-2.078487	-0.244983
F	-1.689841	-0.175590	1.471888
F	-0.213828	0.527042	3.666374
F	0.146902	6.3413710	0.378029
F	1.043538	5.2244930	-1.947876
F	3.414326	3.8646910	-1.978137
F	4.898078	3.6220170	0.310643
F	3.988137	4.7189550	2.639307
C	-1.468348	1.034048	-3.080866
C	-1.927727	2.010763	-2.203273
C	-1.191033	2.378736	-1.075334
C	0.031520	1.746681	-0.830698
C	0.515480	0.770153	-1.704728
C	-0.246805	0.421576	-2.821689
C	-2.051880	-5.547651	-1.548573
C	-1.322041	-5.673924	-0.371152
C	-1.775660	-5.115576	0.825757
C	-2.986436	-4.416975	0.838977
C	-3.736716	-4.283180	-0.332634
C	-3.254798	-4.849893	-1.515385
F	-3.105847	2.622905	-2.436311
F	-1.634343	3.322868	-0.233215
F	0.748691	2.0789740	0.257530
F	1.694421	0.1767230	-1.456918
F	0.222911	-0.5283140	-3.653934
F	-0.151652	-6.340249	-0.369730
F	-1.055369	-5.227845	1.955379
F	-3.425962	-3.867061	1.980661
F	-4.901820	-3.619065	-0.312341
F	-3.983978	-4.710335	-2.640779
C	7.264667	-3.059749	-0.555388
C	8.162381	-2.008998	-0.395781
C	7.720940	-0.694754	-0.222582
C	6.347212	-0.434686	-0.207962
C	5.429656	-1.478117	-0.365468
C	5.901282	-2.782062	-0.537890
F	9.489035	-2.2477200	-0.407381
F	8.594935	0.3126790	-0.071219
F	5.905681	0.8202280	-0.046929
F	4.113068	-1.2171050	-0.349633
F	5.008587	-3.7787730	-0.692398
H	7.621240	-4.079352	-0.689571
H	1.689962	5.989708	2.480738
H	-2.053592	0.755047	-3.955012
H	-7.619638	4.079701	0.670018
H	-1.686706	-5.982171	-2.477176
H	2.061765	-0.758738	3.963070

Total Energy at PW91PW91/6-311++G(d,p) level = -4370.55499370 A.U.
Total Energy at B97D/6-311++G(d,p) level = -4369.25986210 A.U.
BSSE correction at B97D/6-311++G(d,p) level = 7.9 kcal/mol

Optimized Geometry of C6F5H at
PW91PW91/6-311++G(d,p). Coordinates in Angstrom unit

Atom	X	Y	Z
H	-0.000038	-2.768786	-0.000893
C	-0.000121	-1.680631	0.000203
C	-1.196499	-0.970765	0.000138
C	-1.212804	0.426159	0.000182
C	0.000016	1.121534	0.000023
C	1.212981	0.425983	0.000120
C	1.196399	-0.970726	0.000166
F	-2.371977	-1.629385	-0.000132
F	-2.371857	1.102223	-0.000054
F	0.000291	2.461486	-0.000095
F	2.371857	1.102179	-0.000059
F	2.371709	-1.629896	-0.000116

Total Energy = -728.422175365 A.U.

Optimized Geometry of (CH3)2CO...C6F5H complex at
PW91PW91/6-311++G(d,p). Coordinates in Angstrom unit

H	-3.299462	0.428786	1.466111
C	-2.468239	0.278340	0.780219
C	-1.756097	1.363205	0.279934
C	-0.685899	1.185282	-0.597870
C	-0.325996	-0.109339	-0.976170
C	-1.026011	-1.212343	-0.483979
C	-2.092455	-1.003250	0.391951
F	-2.093017	2.617373	0.643430
F	0.007558	2.2362620	-1.066413
F	0.713544	-0.296217	-1.807076
F	-0.658952	-2.453260	-0.844728
F	-2.761571	-2.074971	0.863994
C	2.856633	-0.102875	0.772309
O	1.757883	-0.018360	1.303214
C	3.489145	-1.445070	0.461810
H	4.547121	-1.468520	0.761740
H	2.934486	-2.249975	0.956046
H	3.463041	-1.609267	-0.627562
C	3.648574	1.128612	0.380143
H	4.016294	1.046517	-0.653507
H	3.032984	2.027646	0.491658
H	4.536486	1.213645	1.026860

Total Energy PW91PW91/6-311++G(d,p) level = -921.562195091 a.u.
Total Energy at B97D/6-311++G(d,p) level = -921.299052269 A.U.
BSSE correction at B97D/6-311++G(d,p) level = 0.9 kcal/mol

Optimized Geometry of (CH3)2CO at
PW91PW91/6-311++G(d,p). Coordinates in Angstrom unit

C	-0.000003	0.184125	0.000002
O	0.000003	1.404835	0.000000
C	-1.290374	-0.615442	-0.002853
H	-2.147198	0.051468	-0.145953
H	-1.274975	-1.386920	-0.787286
H	-1.398107	-1.143599	0.957898
C	1.290373	-0.615447	0.002854
H	1.274951	-1.386982	0.787228
H	1.398146	-1.143521	-0.957938
H	2.147183	0.051464	0.146034

Total Energy = -193.134721662 A.U.

Optimized Geometry of (C6F5H)2 showing F...F interactions.
PW91PW91/6-311++G(d,p). Coordinates in Angstrom unit

H	6.216062000	1.040856000	0.158456000
C	5.212096000	0.625253000	0.099870000
C	5.017987000	-0.733055000	-0.129414000
C	3.735349000	-1.280525000	-0.207148000
C	2.625891000	-0.443742000	-0.050741000
C	2.800301000	0.924473000	0.179807000
C	4.096088000	1.441626000	0.252497000
F	6.079130000	-1.549993000	-0.281702000
F	3.557429000	-2.592076000	-0.428229000
F	1.390824000	-0.956578000	-0.120823000
F	1.731319000	1.720603000	0.328307000
F	4.252358000	2.761490000	0.475975000
H	-5.891507000	1.612395000	-0.387336000
C	-5.015083000	0.984766000	-0.238902000

C	-5.151194000	-0.376441000	0.013632000
C	-4.035578000	-1.194533000	0.205909000
C	-2.757487000	-0.630780000	0.142732000
C	-2.599699000	0.735678000	-0.109262000
C	-3.735405000	1.527313000	-0.297648000
F	-6.377704000	-0.931668000	0.076474000
F	-4.176130000	-2.506778000	0.449142000
F	-1.679668000	-1.404723000	0.324890000
F	-1.370548000	1.268659000	-0.166012000
F	-3.571916000	2.842905000	-0.540147000

Total Energy PW91PW91/6-311++G(d,p) level = -1456.84602589 a.u.
Total Energy at B97D/6-311++G(d,p) level = -1456.40901115 A.U.
BSSE correction at B97D/6-311++G(d,p) level = 0.5 kcal/mol

Optimized Geometry of (C6F5H)2 showing stacking interactions.
PW91PW91/6-311++G(d,p). Coordinates in Angstrom unit

H	-3.767340000	1.824065000	-1.113419000
C	-3.129459000	1.215075000	-0.475825000
C	-3.360067000	-0.150078000	-0.338946000
C	-2.548451000	-0.947315000	0.471743000
C	-1.482786000	-0.355465000	1.155839000
C	-1.235506000	1.014848000	1.031843000
C	-2.064416000	1.785640000	0.213475000
F	-4.382158000	-0.730009000	-0.996863000
F	-2.774691000	-2.263194000	0.595580000
F	-0.686995000	-1.108027000	1.931308000
F	-0.203205000	1.569591000	1.689550000
F	-1.812894000	3.103443000	0.097971000
H	3.766518000	-1.823443000	1.114719000
C	3.128838000	-1.214670000	0.476717000
C	3.359513000	0.150428000	0.339556000
C	2.548352000	0.947428000	-0.471843000
C	1.483322000	0.355176000	-1.156522000
C	1.235866000	-1.015073000	-1.032113000
C	2.064420000	-1.785674000	-0.213230000
F	4.381061000	0.730590000	0.998115000
F	2.774459000	2.263313000	-0.595767000
F	0.687489000	1.107379000	-1.932318000
F	0.203736000	-1.569774000	-1.690161000
F	1.813539000	-3.103595000	-0.098023000

Total Energy PW91PW91/6-311++G(d,p) level = -1456.84866622 A.U.
Total Energy at B97D/6-311++G(d,p) level = -1456.41626243 A.U.
BSSE correction at B97D/6-311++G(d,p) level = 1.7 kcal/mol

Aniline

C	-0.221699000	-1.210826000	-0.003693000
C	1.173766000	-1.204998000	0.003014000
C	-0.941718000	-0.000034000	-0.005992000
H	1.709924000	-2.155499000	0.006695000
C	1.885417000	0.000039000	0.006560000
C	-0.221762000	1.210774000	-0.003628000
H	2.975279000	0.000013000	0.012846000
H	-0.764616000	2.158834000	-0.011520000
C	1.173743000	1.205022000	0.003008000
H	1.709766000	2.155597000	0.006894000
H	-0.764612000	-2.158851000	-0.011476000
N	-2.337599000	-0.000054000	-0.073966000
H	-2.794422000	0.843598000	0.258821000
H	-2.794610000	-0.843180000	0.259894000

Total energy = = -287.567187604 A.U.

CF_3COOH

H	-2.495215000	-0.915053000	0.000612000
O	-1.526856000	-1.054435000	-0.000189000
O	-1.509592000	1.226000000	-0.000003000
C	-0.948293000	0.160388000	-0.000230000
C	0.599827000	0.000561000	-0.000014000
F	1.008024000	-0.681970000	1.097166000
F	1.008685000	-0.679924000	-1.098142000
F	1.191914000	1.203764000	0.001242000

E = = -526.831487803 A.U.

CH_3OH

C	0.668301000	-0.020194000	0.000012000
H	1.037835000	-0.540542000	0.900964000
H	1.084082000	0.994558000	-0.005913000
O	-0.753072000	0.122654000	0.000014000
H	-1.144420000	-0.763532000	-0.000001000
H	1.037275000	-0.550555000	-0.895237000

Total Energy = -115.714808559 A.U.

Propanal

O	1.826134000	-0.036660000	-0.292177000
C	0.781873000	-0.236016000	0.295093000
C	-0.473383000	0.589613000	0.151221000

H	-0.635899000	1.090905000	1.122967000
H	-0.301843000	1.368183000	-0.604623000
H	0.691296000	-1.097085000	1.011243000
C	-1.696288000	-0.280555000	-0.179613000
H	-2.612018000	0.324735000	-0.191030000
H	-1.590371000	-0.752792000	-1.166084000
H	-1.833445000	-1.078920000	0.564738000

Total energy = -193.122251124 A.U.

CH_3CN

C	0.276461000	0.000003000	-0.000051000
N	1.440140000	0.000001000	0.000024000
C	-1.177296000	0.000000000	0.000007000
H	-1.558649000	-0.768822000	-0.685274000
H	-1.558626000	-0.209106000	1.008484000
H	-1.558698000	0.977905000	-0.323113000

Total energy PW91PW91/6-311++G(d,p) level = -132.736765392 A.U.
Total Energy at B97D/6-311++G(d,p) level = -132.700060665 A.U.

Ethylacetate

C	1.112785000	-0.234830000	-0.000029000
O	1.918660000	-1.138884000	0.000097000
C	1.490452000	1.231686000	-0.000186000
H	1.092257000	1.747266000	0.885614000
H	2.581556000	1.305075000	-0.000357000
H	1.091944000	1.747230000	-0.885855000
O	-0.220905000	-0.550013000	-0.000094000
C	-1.237001000	0.483343000	0.000450000
H	-1.122651000	1.116827000	0.894901000
H	-1.122436000	1.118118000	-0.893054000
C	-2.585511000	-0.209879000	-0.000239000
H	-2.698313000	-0.842511000	0.889794000
H	-2.698030000	-0.841250000	-0.891205000
H	-3.390704000	0.538498000	0.000160000

Total energy PW91PW91/6-311++G(d,p) level = -307.672466041 A.U.
Total Energy at B97D/6-311++G(d,p) level = -307.591731035 A.U.

Methanol-C_6F_5H complex

H	-2.696066000	1.055612000	-1.294598000
C	-1.878061000	0.700341000	-0.671248000
C	-0.905669000	1.579110000	-0.206069000
C	0.147117000	1.137293000	0.596489000
C	0.226521000	-0.215076000	0.934319000
C	-0.739804000	-1.113368000	0.477417000
C	-1.780905000	-0.643131000	-0.324119000
F	-0.967541000	2.887130000	-0.530085000
F	1.092357000	1.990575000	1.027734000
F	1.239971000	-0.653463000	1.693876000
F	-0.646572000	-2.415576000	0.795014000
F	-2.704878000	-1.522368000	-0.765405000
C	3.394721000	-0.476719000	-1.114172000
H	3.847417000	-1.210450000	-0.426042000
H	3.328284000	0.486663000	-0.594239000
O	2.058954000	-0.835628000	-1.485379000
H	2.094831000	-1.682405000	-1.955485000
H	4.050343000	-0.351780000	-1.992510000

Total energy = -844.141673957 A.U.

$CF_3COOH...C_6F_5H$ complex

H	-3.197665000	0.341587000	-2.162806000
C	-2.667044000	0.173755000	-1.227743000
C	-2.367053000	1.235358000	-0.381446000
C	-1.683681000	1.035778000	0.818803000
C	-1.291604000	-0.257376000	1.172821000
C	-1.581890000	-1.337767000	0.335788000
C	-2.267064000	-1.106240000	-0.858588000
F	-2.730887000	2.490205000	-0.717305000
F	-1.383891000	2.069726000	1.622976000
F	-0.619989000	-0.459763000	2.316051000
F	-1.194105000	-2.575507000	0.680702000
F	-2.538947000	-2.155286000	-1.661212000
H	2.784004000	2.602281000	-1.261069000
O	3.210944000	1.809623000	-0.877623000
O	1.079090000	1.006015000	-0.944259000
C	2.251760000	0.888656000	-0.687789000
C	2.872576000	-0.397163000	-0.068347000
F	3.814574000	-0.914502000	-0.892283000
F	3.454216000	-0.117972000	1.121444000
F	1.920961000	-1.323455000	0.127176000

Total energy PW91PW91/6-311++G(d,p) level = -1255.25787912 A.U.
Total Energy at B97D/6-311++G(d,p) level = -1254.89039815 A.U.
BSSE correction at B97D/6-311++G(d,p) level = 1.1 kcal/mol

$CH_3CN...C_6F_5H$ complex

H	2.322540000	0.350265000	-2.130212000
C	1.774427000	0.238271000	-1.197005000
C	1.250113000	1.348168000	-0.544391000
C	0.535862000	1.218830000	0.647213000
C	0.342441000	-0.053051000	1.189659000
C	0.859930000	-1.180573000	0.549184000
C	1.570210000	-1.019497000	-0.641030000
F	1.423784000	2.581467000	-1.063626000
F	0.019663000	2.295436000	1.264930000
F	-0.361619000	-0.194294000	2.324426000
F	0.654931000	-2.400968000	1.072818000
F	2.059494000	-2.116467000	-1.255383000
C	-3.115937000	-0.231410000	-0.920816000
N	-1.977503000	-0.221329000	-1.161831000
C	-4.536958000	-0.244599000	-0.617914000
H	-5.074756000	0.443779000	-1.283438000
H	-4.945372000	-1.255055000	-0.752877000
H	-4.706696000	0.066903000	0.421459000

Total energy PW91PW91/6-311++G(d,p) level = -132.736765392 a.u.
Total Energy at B97D/6-311++G(d,p) level = -860.909440011 A.U.

Propanal...C_6F_5H complex

H	-3.271854000	1.193251000	-1.194379000
C	-2.465191000	0.764896000	-0.602922000
C	-1.467739000	1.575050000	-0.070645000
C	-0.427133000	1.038749000	0.687950000
C	-0.386994000	-0.338627000	0.911274000
C	-1.377347000	-1.170330000	0.384962000
C	-2.407385000	-0.604887000	-0.369204000
F	-1.491332000	2.906137000	-0.287625000
F	0.543883000	1.824889000	1.184803000
F	0.620604000	-0.868702000	1.623791000
F	-1.323537000	-2.494909000	0.599216000
F	-3.359124000	-1.416021000	-0.874128000
O	1.483931000	-0.326157000	-1.632704000
C	2.676927000	-0.512064000	-1.481772000
C	3.590985000	0.334428000	-0.633874000
H	4.328893000	0.790536000	-1.318876000
H	3.007486000	1.143668000	-0.174156000
H	3.178301000	-1.378893000	-1.988921000
C	4.331293000	-0.509646000	0.417620000
H	5.057592000	0.106381000	0.963439000
H	3.628033000	-0.932844000	1.147859000
H	4.881168000	-1.340816000	-0.048183000

Total energy PW91PW91/6-311++G(d,p) level = -921.549600924 A.U.
Total Energy at B97D/6-311++G(d,p) level = -921.286751852 A.U.
BSSE correction at B97D/6-311++G(d,p) level = 0.7 kcal/mol

Initial structure used for PM6 level optimization dimer M-II with ten acetone molecule.

C	-1.669907000	-7.683617000	-0.551465000
C	-0.351661000	-7.436643000	-0.225429000
H	0.239920000	-8.053911000	0.143193000
C	-0.054714000	-6.125968000	-0.534767000
H	0.767762000	-5.709075000	-0.404587000
C	-1.187956000	-5.533908000	-1.075914000
C	-1.485607000	-4.204479000	-1.473141000
C	-0.460386000	-3.162188000	-1.166233000
C	0.266539000	-2.536336000	-2.141556000
C	1.156539000	-1.543033000	-1.896521000
C	1.369068000	-1.160732000	-0.591696000
C	0.676981000	-1.749150000	0.415392000
C	-0.204512000	-2.742534000	0.124985000
C	-2.652028000	-3.812997000	-2.076170000
C	-3.099258000	-2.497653000	-2.446318000
H	-2.642409000	-1.697335000	-2.312473000
C	-4.294010000	-2.646418000	-3.018860000
H	-4.834423000	-1.968744000	-3.359396000
C	-4.590156000	-4.056168000	-3.014160000
C	-5.801419000	-4.712514000	-3.625931000
C	-5.770309000	-4.411329000	-5.129499000
H	-6.550696000	-4.780482000	-5.548269000
H	-4.983913000	-4.799255000	-5.519043000
H	-5.756045000	-3.460374000	-5.265014000
C	-5.765897000	-6.230937000	-3.431039000
H	-5.770752000	-6.431988000	-2.491317000
H	-4.969514000	-6.586629000	-3.829921000
H	-6.535484000	-6.624676000	-3.846658000
C	-7.035809000	-4.134879000	-2.939610000
C	-8.015310000	-3.436419000	-3.620685000
H	-7.919851000	-3.321248000	-4.538481000
C	-9.131159000	-2.896655000	-3.001794000
C	-9.258814000	-3.097109000	-1.642952000
H	-9.997374000	-2.752334000	-1.194198000
C	-8.315900000	-3.796021000	-0.942818000
H	-8.427551000	-3.929733000	-0.027846000

C	-7.200672000	-4.307515000	-1.577656000
H	-6.557558000	-4.766689000	-1.085800000
C	-10.156320000	-2.055927000	-3.775637000
C	-9.914881000	-2.069135000	-5.278587000
H	-10.599978000	-1.559039000	-5.716034000
H	-9.935625000	-2.974350000	-5.596653000
H	-9.058458000	-1.682187000	-5.468422000
C	-11.591569000	-2.569540000	-3.507155000
H	-11.766235000	-2.553398000	-2.562415000
H	-11.676327000	-3.469441000	-3.831545000
H	-12.223676000	-2.004880000	-3.960112000
C	-10.013331000	-0.639470000	-3.265933000
C	-9.132422000	0.362673000	-3.667510000
H	-8.519542000	0.301559000	-4.363517000
C	-9.327723000	1.451906000	-2.861566000
H	-8.872246000	2.261327000	-2.916130000
C	-10.328420000	1.133113000	-1.950052000
C	-10.920758000	1.878849000	-0.915056000
C	-10.404524000	3.260118000	-0.777938000
C	-9.176815000	3.551612000	-0.248558000
C	-8.627617000	4.796259000	-0.247941000
C	-9.310201000	5.817643000	-0.796546000
C	-10.530413000	5.595928000	-1.329872000
C	-11.059449000	4.339606000	-1.298674000
C	-11.942012000	1.432782000	-0.104518000
C	-12.623268000	2.100255000	0.946765000
H	-12.442840000	2.954926000	1.266629000
C	-13.575031000	1.266898000	1.390844000
H	-14.173139000	1.432412000	2.084055000
C	-13.502631000	0.069625000	0.603091000
C	-14.378563000	-1.154952000	0.726734000
C	-14.141358000	-2.117760000	-0.440993000
H	-14.308530000	-1.662504000	-1.269683000
H	-14.734904000	-2.867960000	-0.360959000
H	-13.231432000	-2.425923000	-0.421335000
C	-15.857045000	-0.696427000	0.687880000
H	-16.026446000	-0.097507000	1.418525000
H	-16.431630000	-1.463453000	0.763300000
H	-16.030789000	-0.245395000	-0.139831000
C	-14.006911000	-1.845674000	2.036973000
C	-14.911751000	-2.033489000	3.045875000
H	-15.801309000	-1.778236000	2.933574000
C	-14.494329000	-2.603277000	4.220136000
H	-15.116769000	-2.758560000	4.892393000
C	-13.172902000	-2.953940000	4.434320000
H	-12.914545000	-3.310325000	5.252820000
C	-12.225251000	-2.772320000	3.424552000
C	-12.700956000	-2.242385000	2.240669000
H	-12.102215000	-2.144521000	1.537404000
C	-10.769244000	-3.175044000	3.578878000
C	-10.329006000	-3.263232000	5.054374000
H	-9.382652000	-3.416281000	5.095326000
H	-10.790521000	-3.987867000	5.483190000
H	-10.539446000	-2.441371000	5.500627000
C	-10.597208000	-4.553784000	2.922714000
H	-10.757465000	-4.480661000	1.978295000
H	-11.223273000	-5.171566000	3.306844000
H	-9.702170000	-4.869406000	3.072694000
C	-9.860277000	-2.166363000	2.924132000
C	-10.035636000	-0.822046000	2.581566000
H	-10.809288000	-0.322604000	2.710758000
C	-8.865129000	-0.365393000	2.020669000
H	-8.710098000	0.492611000	1.698588000
C	-7.955103000	-1.419337000	2.023135000
C	-6.641001000	-1.502758000	1.519804000
C	-6.111256000	-0.275212000	0.875132000
C	-5.544052000	0.740256000	1.590217000
C	-5.051574000	1.866857000	1.003251000
C	-5.113397000	2.002668000	-0.354876000
C	-5.669273000	1.023689000	-1.089745000
C	-6.153772000	-0.076256000	-0.479226000
C	-5.851859000	-2.628844000	1.549589000
C	-4.557428000	-2.853194000	0.994402000
H	-4.043509000	-2.239867000	0.520665000
C	-4.222179000	-4.121962000	1.282816000
H	-3.440075000	-4.559208000	1.038637000
C	-5.304838000	-4.671971000	2.041542000
C	-5.352352000	-6.062802000	2.659605000
C	-6.640021000	-6.226565000	3.471390000
H	-6.650888000	-5.583462000	4.185195000
H	-6.675951000	-7.113334000	3.836461000
H	-7.398471000	-6.082579000	2.900095000
C	-4.145992000	-6.204868000	3.605078000
H	-3.341044000	-5.969524000	3.137659000
H	-4.083493000	-7.113389000	3.910818000
H	-4.258789000	-5.621187000	4.360797000
C	-5.269354000	-7.079129000	1.507671000

C	-6.403817000	-7.455898000	0.784740000
H	-7.238075000	-7.124595000	1.028500000
C	-6.301462000	-8.298533000	-0.264897000
H	-7.072615000	-8.558686000	-0.716029000
C	-5.084687000	-8.786073000	-0.683790000
H	-5.038848000	-9.350134000	-1.421244000
C	-3.939954000	-8.437720000	-0.016582000
C	-4.067231000	-7.591625000	1.078847000
H	-3.298422000	-7.360363000	1.546827000
C	-2.543127000	-8.891872000	-0.419873000
C	-2.546297000	-9.648144000	-1.766075000
H	-2.823810000	-9.052049000	-2.466079000
H	-3.154295000	-10.388497000	-1.718060000
H	-1.663240000	-9.972085000	-1.954921000
C	-1.996274000	-9.833716000	0.674065000
H	-1.140532000	-10.174401000	0.400232000
H	-2.606038000	-10.564201000	0.799774000
H	-1.898622000	-9.349327000	1.495496000
N	-2.133096000	-6.530483000	-1.090405000
N	-3.636228000	-4.742987000	-2.447265000
N	-10.720152000	-0.163839000	-2.239836000
N	-12.513968000	0.164874000	-0.278537000
N	-8.602680000	-2.499179000	2.594139000
N	-6.268893000	-3.802009000	2.185564000
F	0.080793000	-2.905723000	-3.420269000
F	1.831342000	-0.956876000	-2.896598000
F	2.231444000	-0.167331000	-0.336567000
F	0.884045000	-1.360241000	1.684490000
F	-0.891556000	-3.281178000	1.140732000
F	-8.430305000	2.550075000	0.274486000
F	-7.403135000	5.019174000	0.256935000
F	-8.808508000	7.054569000	-0.821243000
F	-11.214573000	6.609220000	-1.889250000
F	-12.275417000	4.156160000	-1.840573000
F	-5.443566000	0.635341000	2.920405000
F	-4.497133000	2.843366000	1.749470000
F	-4.630071000	3.106880000	-0.938538000
F	-5.741743000	1.157200000	-2.431219000
F	-6.714709000	-1.016619000	-1.250906000
H	-11.351773000	-0.485231000	-1.756716000
H	-2.922672000	-6.399748000	-1.424390000
H	-8.179629000	-3.251290000	2.630670000
C	1.647097000	7.722635000	0.639679000
C	0.328853000	7.475662000	0.313642000
H	-0.262728000	8.092929000	-0.054979000
C	0.031904000	6.164987000	0.622981000
H	-0.790571000	5.748092000	0.492801000
C	1.165147000	5.572926000	1.164127000
C	1.462799000	4.243497000	1.561354000
C	0.437576000	3.201207000	1.254447000
C	-0.289348000	2.575354000	2.229770000
C	-1.179300000	1.581161000	1.984283000
C	-1.391877000	1.199749000	0.679910000
C	-0.699790000	1.788168000	-0.327179000
C	0.181703000	2.781553000	-0.036772000
C	2.629218000	3.852015000	2.164384000
C	3.076450000	2.536671000	2.534532000
H	2.619601000	1.736353000	2.400687000
C	4.271201000	2.685436000	3.107074000
H	4.811614000	2.007762000	3.447609000
C	4.567397000	4.094295000	3.101921000
C	5.778610000	4.751530000	3.714144000
C	5.747499000	4.450346000	5.217713000
H	6.527888000	4.819500000	5.636483000
H	4.961105000	4.838274000	5.607256000
H	5.733236000	3.499392000	5.353227000
C	5.743089000	6.269955000	3.519253000
H	5.747942000	6.471006000	2.579530000
H	4.946705000	6.625647000	3.918134000
H	6.512676000	6.663694000	3.934872000
C	7.013001000	4.173897000	3.027823000
C	7.992549000	3.474546000	3.708445000
H	7.897043000	3.360267000	4.626695000
C	9.108350000	2.935673000	3.090007000
C	9.236006000	3.136128000	1.731166000
H	9.974564000	2.791353000	1.282412000
C	8.293092000	3.835040000	1.031032000
H	8.404743000	3.968751000	0.116060000
C	7.177863000	4.346533000	1.665870000
H	6.534750000	4.805707000	1.174013000
C	10.133560000	2.094054000	3.863398000
C	9.892073000	2.108152000	5.366801000
H	10.577170000	1.598057000	5.804248000
H	9.912816000	3.013368000	5.684867000
H	9.035650000	1.721205000	5.556636000
C	11.568761000	2.608558000	3.595369000
H	11.743427000	2.592416000	2.650629000

H	11.653519000	3.508458000	3.919758000
H	12.200867000	2.043897000	4.048323000
C	9.990522000	0.678489000	3.354147000
C	9.109613000	-0.323654000	3.755723000
H	8.496734000	-0.262542000	4.451730000
C	9.304914000	-1.412888000	2.949779000
H	8.849438000	-2.222308000	3.004342000
C	10.305612000	-1.094096000	2.038266000
C	10.897949000	-1.839831000	1.003270000
C	10.381715000	-3.221099000	0.866151000
C	9.154007000	-3.512594000	0.336771000
C	8.604808000	-4.757240000	0.336154000
C	9.287393000	-5.778624000	0.884760000
C	10.507654000	-5.557801000	1.417633000
C	11.036641000	-4.300588000	1.386887000
C	11.919203000	-1.393765000	0.192730000
C	12.600460000	-2.061237000	-0.858553000
H	12.420030000	-2.915909000	-1.178415000
C	13.552223000	-1.227879000	-1.302631000
H	14.150379000	-1.394285000	-1.996293000
C	13.479872000	-0.031498000	-0.515331000
C	14.355803000	1.193080000	-0.638973000
C	14.118548000	2.156779000	0.529207000
H	14.285721000	1.701522000	1.357897000
H	14.712096000	2.906979000	0.449173000
H	13.208624000	2.464941000	0.509548000
C	15.834237000	0.735443000	-0.599667000
H	16.003685000	0.135633000	-1.330763000
H	16.408822000	1.502472000	-0.675086000
H	16.007980000	0.284413000	0.228045000
C	13.984103000	1.884690000	-1.948759000
C	14.888941000	2.072508000	-2.957661000
H	15.778501000	1.817254000	-2.845360000
C	14.471520000	2.642296000	-4.131923000
H	15.093961000	2.797578000	-4.804179000
C	13.150093000	2.992957000	-4.346107000
H	12.891737000	3.349343000	-5.164607000
C	12.202441000	2.811336000	-3.336338000
C	12.678148000	2.281403000	-2.152456000
H	12.079406000	2.183540000	-1.449191000
C	10.746484000	3.213170000	-3.491117000
C	10.306197000	3.302251000	-4.966160000
H	9.359843000	3.455298000	-5.007112000
H	10.767712000	4.026886000	-5.394976000
H	10.516685000	2.479497000	-5.412865000
C	10.574449000	4.591913000	-2.834954000
H	10.734656000	4.519680000	-1.890081000
H	11.200514000	5.209693000	-3.219082000
H	9.679361000	4.908423000	-2.984480000
C	9.837468000	2.205381000	-2.835919000
C	10.012826000	0.861064000	-2.493353000
H	10.786480000	0.361621000	-2.622544000
C	8.842320000	0.404411000	-1.932455000
H	8.687290000	-0.453593000	-1.610374000
C	7.932342000	1.457464000	-1.935373000
C	6.618192000	1.541776000	-1.431590000
C	6.088446000	0.314229000	-0.786918000
C	5.521243000	-0.701238000	-1.502003000
C	5.028814000	-1.828730000	-0.915489000
C	5.090587000	-1.963651000	0.443090000
C	5.646463000	-0.984670000	1.177959000
C	6.130964000	0.115274000	0.567440000
C	5.829050000	2.667861000	-1.461376000
C	4.534619000	2.892213000	-0.906188000
H	4.020700000	2.278885000	-0.432452000
C	4.199370000	4.160981000	-1.194602000
H	3.417266000	4.598227000	-0.950424000
C	5.282030000	4.710988000	-1.953329000
C	5.329543000	6.101819000	-2.571391000
C	6.617212000	6.265583000	-3.383176000
H	6.628079000	5.622480000	-4.096981000
H	6.653190000	7.151463000	-3.748700000
H	7.375661000	6.121595000	-2.811881000
C	4.123231000	6.242995000	-3.517316000
H	3.318236000	6.008541000	-3.049447000
H	4.060684000	7.152407000	-3.822605000
H	4.235979000	5.660206000	-4.272584000
C	5.246595000	7.117258000	-1.419910000
C	6.381008000	7.494916000	-0.696527000
H	7.215266000	7.163613000	-0.940287000
C	6.278653000	8.337552000	0.353110000
H	7.049806000	8.597703000	0.804242000
C	5.061879000	8.825092000	0.772003000
H	5.016040000	9.389153000	1.509458000
C	3.917145000	8.476738000	0.104796000
C	4.044421000	7.630643000	-0.990633000
H	3.275614000	7.399381000	-1.458613000

C	2.520318000	8.930889000	0.508086000
C	2.523487000	9.687162000	1.854288000
H	2.801001000	9.091067000	2.554292000
H	3.131486000	10.427516000	1.806273000
H	1.640431000	10.011101000	2.043134000
C	1.973465000	9.872734000	-0.585852000
H	1.117722000	10.213419000	-0.312019000
H	2.583228000	10.603218000	-0.711560000
H	1.875814000	9.388344000	-1.407282000
N	2.110287000	6.569502000	1.178619000
N	3.613419000	4.782004000	2.535477000
N	10.697342000	0.202857000	2.328050000
N	12.491159000	-0.125855000	0.366751000
N	8.579872000	2.538198000	-2.505925000
N	6.246085000	3.841026000	-2.097350000
F	-0.103601000	2.944742000	3.508483000
F	-1.854103000	0.995003000	2.984360000
F	-2.254254000	0.206348000	0.424781000
F	-0.906853000	1.399258000	-1.596276000
F	0.868748000	3.320195000	-1.052519000
F	8.407496000	-2.511057000	-0.186273000
F	7.380327000	-4.980156000	-0.168722000
F	8.785698000	-7.015551000	0.909457000
F	11.191765000	-6.570202000	1.977463000
F	12.252608000	-4.117142000	1.928787000
F	5.420758000	-0.596323000	-2.832192000
F	4.474325000	-2.804348000	-1.661256000
F	4.607262000	-3.067861000	1.026751000
F	5.718983000	-1.119072000	2.518980000
F	6.691899000	1.055637000	1.339120000
H	11.328963000	0.524248000	1.844929000
H	2.899862000	6.438767000	1.512602000
H	8.156821000	3.290308000	-2.542457000
C	-2.624194000	5.322405000	-0.629350000
O	-2.293625000	4.437920000	0.136543000
C	-2.792148000	5.068779000	-2.118268000
C	-2.890779000	6.738696000	-0.147211000
H	-2.575048000	4.023586000	-2.341641000
H	-2.738821000	6.796426000	0.931228000
H	-2.121424000	5.716023000	-2.695280000
H	-3.813793000	5.308875000	-2.435022000
H	-3.916043000	7.040077000	-0.391632000
H	-2.223675000	7.447224000	-0.651890000
C	7.265250000	-2.986397000	-2.171764000
O	7.032979000	-2.216650000	-1.259777000
C	6.751722000	-4.416634000	-2.160690000
C	8.084102000	-2.568005000	-3.381656000
H	6.182071000	-4.597426000	-1.248405000
H	8.394438000	-1.527843000	-3.275774000
H	7.586980000	-5.124140000	-2.219989000
H	6.116682000	-4.602536000	-3.034707000
H	7.497957000	-2.686066000	-4.300479000
H	8.968255000	-3.207671000	-3.485762000
C	12.102964000	-6.385500000	-1.718048000
O	11.277780000	-5.506020000	-1.563879000
C	11.745718000	-7.711177000	-2.369483000
C	13.544924000	-6.215912000	-1.269273000
H	10.690934000	-7.714022000	-2.646747000
H	13.678451000	-5.231189000	-0.819889000
H	11.948850000	-8.542085000	-1.683867000
H	12.361584000	-7.878400000	-3.260822000
H	14.226816000	-6.328262000	-2.120237000
H	13.814082000	-6.991948000	-0.543282000
C	-10.660933000	6.790271000	2.317059000
O	-9.794771000	6.136914000	1.768360000
C	-10.432277000	8.235381000	2.727892000
C	-12.028169000	6.204008000	2.627498000
H	-9.421759000	8.541492000	2.454754000
H	-12.071678000	5.168470000	2.288053000
H	-10.573781000	8.353512000	3.808522000
H	-11.161181000	8.892533000	2.239436000
H	-12.815637000	6.786613000	2.135358000
H	-12.228238000	6.247592000	3.704444000
C	8.637635000	-5.191803000	4.679634000
O	8.542955000	-4.689043000	3.576707000
C	9.984597000	-5.572723000	5.271245000
C	7.415130000	-5.471768000	5.537837000
H	10.780265000	-5.325414000	4.567537000
H	6.513758000	-5.157781000	5.010204000
H	10.013816000	-6.644685000	5.498804000
H	10.151216000	-5.043685000	6.216812000
H	7.487456000	-4.939025000	6.493187000
H	7.350055000	-6.540025000	5.775180000
C	-9.510409000	5.163036000	-4.681878000
O	-9.078387000	4.624320000	-3.681216000
C	-8.736150000	6.257136000	-5.398036000
C	-10.852564000	4.777087000	-5.281104000

H	-7.796083000	6.445176000	-4.878066000
H	-11.310311000	3.987608000	-4.683905000
H	-9.326007000	7.180264000	-5.438562000
H	-8.531976000	5.966104000	-6.435028000
H	-10.726057000	4.431740000	-6.313805000
H	-11.520088000	5.645901000	-5.317340000
C	-7.624339000	2.620759000	3.145877000
O	-7.659591000	2.192277000	2.008624000
C	-7.057971000	3.994346000	3.465086000
C	-8.144368000	1.810416000	4.321600000
H	-6.718886000	4.476364000	2.547408000
H	-8.522810000	0.850028000	3.969617000
H	-6.221012000	3.909830000	4.168006000
H	-7.817253000	4.618561000	3.950457000
H	-8.943519000	2.354487000	4.838403000
H	-7.347278000	1.645755000	5.055952000
C	2.523097000	-5.483496000	-2.335983000
O	2.370498000	-4.663749000	-1.451160000
C	2.322846000	-6.969934000	-2.091415000
C	2.923941000	-5.074626000	-3.743662000
H	2.039162000	-7.138230000	-1.051869000
H	3.037259000	-3.991141000	-3.795365000
H	3.242376000	-7.522625000	-2.316660000
H	1.544921000	-7.365988000	-2.754523000
H	2.168075000	-5.401128000	-4.467404000
H	3.865531000	-5.557764000	-4.029540000
C	1.746333000	0.133299000	3.677876000
O	1.474747000	0.612110000	2.593826000
C	0.947856000	-1.018509000	4.265397000
C	2.901814000	0.655705000	4.515352000
H	0.150993000	-1.304109000	3.577722000
H	3.395470000	1.475863000	3.992763000
H	0.515999000	-0.731961000	5.231383000
H	1.599288000	-1.880030000	4.452900000
H	3.624951000	-0.144376000	4.712029000
H	2.541663000	1.003694000	5.490511000
C	-1.329403000	-0.707974000	-4.171823000
O	-1.123008000	-0.593630000	-2.979134000
C	-0.175113000	-0.338912000	-5.088786000
C	-2.672196000	-1.214534000	-4.671536000
H	0.601855000	0.170609000	-4.517681000
H	-3.246466000	-1.621817000	-3.838596000
H	-0.522872000	0.311488000	-5.899824000
H	0.242291000	-1.236558000	-5.559685000
H	-2.529867000	-1.988668000	-5.434555000
H	-3.235748000	-0.402517000	-5.145643000

Final structure obtained from PM6 level optimization of dimer M-II with ten acetone molecule.

C	3.086499000	7.979282000	-0.028657000
C	1.826006000	7.919594000	0.595710000
H	1.401138000	8.665351000	1.233937000
C	1.226765000	6.690497000	0.241253000
H	0.259964000	6.334872000	0.565798000
C	2.118404000	5.998311000	-0.606572000
C	2.002652000	4.680267000	-1.196331000
C	0.787414000	3.923375000	-0.803791000
C	-0.289238000	3.765181000	-1.692394000
C	-1.453886000	3.073658000	-1.328455000
C	-1.567446000	2.528206000	-0.040937000
C	-0.508555000	2.669706000	0.867625000
C	0.650136000	3.362597000	0.478066000
C	2.904827000	4.111797000	-2.037687000
C	2.928068000	2.737965000	-2.605624000
H	2.170556000	1.990758000	-2.407906000
C	4.049517000	2.630098000	-3.358929000
H	4.421764000	1.783368000	-3.900081000
C	4.743872000	3.948367000	-3.298794000
C	6.029583000	4.279287000	-4.039196000
C	5.878467000	3.745362000	-5.476085000
H	6.704031000	4.076757000	-6.115063000
H	4.949781000	4.108173000	-5.932910000
H	5.853074000	2.650049000	-5.502147000
C	6.254993000	5.803943000	-4.090102000
H	6.327977000	6.227924000	-3.078783000
H	5.423380000	6.311847000	-4.590500000
H	7.179435000	6.048957000	-4.621091000
C	7.214095000	3.665357000	-3.289484000
C	8.274105000	3.051337000	-3.973234000
H	8.238477000	2.979600000	-5.058105000
C	9.373611000	2.532203000	-3.277863000
C	9.407297000	2.636029000	-1.877500000
H	10.239209000	2.218219000	-1.312749000
C	8.363526000	3.260343000	-1.193743000
H	8.397018000	3.339029000	-0.105548000
C	7.269980000	3.775972000	-1.892277000
H	6.464237000	4.262642000	-1.339559000
C	10.548145000	1.852892000	-3.991160000

C	10.397982000	1.828143000	-5.524599000
H	11.228501000	1.283101000	-5.988185000
H	10.392233000	2.840347000	-5.942392000
H	9.472568000	1.329039000	-5.834630000
C	11.843388000	2.622648000	-3.656638000
H	12.019342000	2.703845000	-2.578517000
H	11.789517000	3.648856000	-4.040404000
H	12.720641000	2.147600000	-4.108202000
C	10.605235000	0.419505000	-3.506526000
C	9.805675000	-0.671438000	-3.913938000
H	9.022722000	-0.636387000	-4.642982000
C	10.197419000	-1.799326000	-3.167778000
H	9.780205000	-2.791662000	-3.241529000
C	11.240062000	-1.404579000	-2.297719000
C	11.945328000	-2.187878000	-1.312153000
C	11.534635000	-3.615960000	-1.247913000
C	10.322277000	-4.015137000	-0.657733000
C	9.904045000	-5.358669000	-0.678263000
C	10.713388000	-6.333053000	-1.277203000
C	11.939985000	-5.961306000	-1.847880000
C	12.329587000	-4.614579000	-1.836648000
C	12.928769000	-1.742277000	-0.485171000
C	13.619832000	-2.480454000	0.600995000
H	13.383977000	-3.499009000	0.869024000
C	14.526111000	-1.637608000	1.153887000
H	15.198001000	-1.793862000	1.973864000
C	14.425408000	-0.351801000	0.406469000
C	15.329708000	0.837460000	0.678494000
C	14.915013000	2.064393000	-0.154563000
H	14.994997000	1.859329000	-1.228498000
H	15.544514000	2.929441000	0.077124000
H	13.872773000	2.347042000	0.038799000
C	16.749859000	0.406525000	0.264621000
H	17.112215000	-0.437350000	0.861969000
H	17.463955000	1.230354000	0.371061000
H	16.770848000	0.093692000	-0.787054000
C	15.214196000	1.203039000	2.159427000
C	16.333071000	1.321926000	2.991353000
H	17.336191000	1.144489000	2.611178000
C	16.168974000	1.680332000	4.333559000
H	17.042899000	1.773355000	4.976240000
C	14.897624000	1.921830000	4.854305000
H	14.791051000	2.204911000	5.899940000
C	13.764966000	1.802294000	4.032629000
C	13.936379000	1.451821000	2.688034000
H	13.063135000	1.359685000	2.035301000
C	12.371608000	2.116899000	4.586173000
C	12.247938000	1.717276000	6.070675000
H	11.220791000	1.851587000	6.430310000
H	12.902137000	2.314931000	6.712671000
H	12.503972000	0.660514000	6.215580000
C	12.164924000	3.637648000	4.436268000
H	12.152112000	3.938422000	3.381955000
H	12.980502000	4.191765000	4.916787000
H	11.232694000	3.973771000	4.901527000
C	11.311673000	1.333826000	3.844907000
C	11.320999000	-0.037663000	3.508649000
H	12.126749000	-0.717651000	3.696235000
C	10.102723000	-0.334697000	2.867459000
H	9.800266000	-1.295287000	2.472596000
C	9.338812000	0.852686000	2.815889000
C	8.022058000	1.057137000	2.258347000
C	7.346835000	-0.186243000	1.800482000
C	6.739839000	-1.053392000	2.726296000
C	6.127306000	-2.251938000	2.328514000
C	6.110969000	-2.605239000	0.971005000
C	6.700901000	-1.752962000	0.026611000
C	7.319010000	-0.564087000	0.447915000
C	7.376840000	2.247551000	2.142211000
C	6.045593000	2.520788000	1.542103000
H	5.430941000	1.761178000	1.094412000
C	5.808013000	3.849468000	1.666447000
H	4.962144000	4.424992000	1.340214000
C	6.987479000	4.432195000	2.364504000
C	7.078263000	5.893383000	2.766241000
C	8.458230000	6.232029000	3.361609000
H	8.631517000	5.679871000	4.292763000
H	8.541355000	7.301868000	3.577792000
H	9.272184000	5.960626000	2.678821000
C	6.010266000	6.118512000	3.854174000
H	5.000282000	5.884783000	3.495206000
H	6.013807000	7.155788000	4.205613000
H	6.196996000	5.475996000	4.723607000
C	6.850812000	6.742806000	1.513880000
C	7.830460000	6.742518000	0.503267000
H	8.720007000	6.121330000	0.607107000
C	7.661320000	7.526404000	-0.635569000

H	8.426956000	7.527602000	-1.410544000
C	6.508335000	8.305225000	-0.800222000
H	6.404867000	8.908941000	-1.699019000
C	5.510070000	8.288281000	0.177331000
C	5.696404000	7.508200000	1.334619000
H	4.904540000	7.495791000	2.085625000
C	4.176240000	9.029605000	0.015027000
C	4.097105000	9.851402000	-1.284876000
H	4.233617000	9.226289000	-2.174473000
H	4.850844000	10.645258000	-1.304867000
H	3.113613000	10.328110000	-1.381470000
C	3.972987000	9.975144000	1.212570000
H	3.065999000	10.578456000	1.095865000
H	4.820505000	10.661809000	1.316285000
H	3.877051000	9.422996000	2.154771000
N	3.250689000	6.817796000	-0.769108000
N	4.085997000	4.799443000	-2.529148000
N	11.473798000	-0.033016000	-2.528688000
N	13.493852000	-0.407842000	-0.530975000
N	10.106201000	1.867948000	3.423130000
N	7.902339000	3.511869000	2.625391000
F	-0.210146000	4.291285000	-2.910415000
F	-2.451659000	2.940854000	-2.199053000
F	-2.669346000	1.878487000	0.308692000
F	-0.598917000	2.144159000	2.083246000
F	1.647158000	3.484634000	1.345738000
F	9.563292000	-3.113274000	-0.057112000
F	8.740189000	-5.707744000	-0.142999000
F	10.328596000	-7.602933000	-1.300644000
F	12.720393000	-6.880600000	-2.410823000
F	13.486240000	-4.279128000	-2.398868000
F	6.740668000	-0.729472000	4.013971000
F	5.575300000	-3.053741000	3.233104000
F	5.537898000	-3.736528000	0.582593000
F	6.682062000	-2.075700000	-1.262856000
F	7.886046000	0.221069000	-0.457433000
H	12.172465000	0.512284000	-2.033724000
H	4.063397000	6.574292000	-1.332290000
H	9.798657000	2.830156000	3.517439000
C	-1.829676000	-6.734787000	1.274066000
C	-0.569118000	-6.462282000	0.706822000
H	0.027592000	-7.143905000	0.138823000
C	-0.230968000	-5.128963000	1.025368000
H	0.668457000	-4.607901000	0.731849000
C	-1.284355000	-4.583813000	1.792339000
C	-1.446578000	-3.248896000	2.322928000
C	-0.359238000	-2.297903000	1.977452000
C	0.792687000	-2.187866000	2.773928000
C	1.831149000	-1.300454000	2.452473000
C	1.736642000	-0.506750000	1.299872000
C	0.597423000	-0.596764000	0.487063000
C	-0.432209000	-1.486679000	0.832904000
C	-2.494486000	-2.811682000	3.069296000
C	-2.774560000	-1.439985000	3.565126000
H	-2.113738000	-0.598713000	3.393744000
C	-3.962163000	-1.480455000	4.217912000
H	-4.504168000	-0.683699000	4.685425000
C	-4.440072000	-2.890682000	4.163530000
C	-5.730518000	-3.389110000	4.793486000
C	-5.849800000	-2.735102000	6.182919000
H	-6.675380000	-3.166415000	6.759199000
H	-4.933834000	-2.886554000	6.766526000
H	-6.020747000	-1.655167000	6.110037000
C	-5.698718000	-4.921901000	4.960413000
H	-5.575174000	-5.422542000	3.989888000
H	-4.859485000	-5.234962000	5.590900000
H	-6.625185000	-5.289983000	5.410456000
C	-6.903877000	-3.052558000	3.869465000
C	-8.134288000	-2.614749000	4.382326000
H	-8.247757000	-2.482885000	5.456170000
C	-9.215697000	-2.352310000	3.531824000
C	-9.059475000	-2.542160000	2.148840000
H	-9.882293000	-2.333129000	1.466921000
C	-7.842337000	-2.989663000	1.634259000
H	-7.727021000	-3.136045000	0.558813000
C	-6.767336000	-3.248078000	2.487248000
H	-5.825920000	-3.605469000	2.066370000
C	-10.577264000	-1.886250000	4.059337000
C	-10.576866000	-1.594076000	5.572316000
H	-11.543873000	-1.184078000	5.888531000
H	-10.395660000	-2.500960000	6.158004000
H	-9.811938000	-0.857023000	5.842367000
C	-11.606926000	-3.003319000	3.787279000
H	-11.647433000	-3.287448000	2.730162000
H	-11.344747000	-3.911359000	4.343721000
H	-12.613656000	-2.705586000	4.099252000
C	-10.941056000	-0.601176000	3.345900000

C	-10.465029000	0.703317000	3.603019000
H	-9.760829000	0.971309000	4.362127000
C	-11.069076000	1.575781000	2.676460000
H	-10.925437000	2.640838000	2.602101000
C	-11.912596000	0.807595000	1.843108000
C	-12.711898000	1.241939000	0.722755000
C	-12.682621000	2.708474000	0.474930000
C	-11.690728000	3.311357000	-0.316376000
C	-11.655509000	4.703096000	-0.515440000
C	-12.626334000	5.518824000	0.080862000
C	-13.632388000	4.937774000	0.866779000
C	-13.644190000	3.548887000	1.062482000
C	-13.470239000	0.451755000	-0.081559000
C	-14.236918000	0.842676000	-1.291881000
H	-14.243390000	1.847515000	-1.690381000
C	-14.851873000	-0.271362000	-1.758173000
H	-15.474207000	-0.400106000	-2.620597000
C	-14.485173000	-1.382730000	-0.835248000
C	-15.041288000	-2.789311000	-0.967153000
C	-14.337389000	-3.766642000	-0.007428000
H	-14.489587000	-3.472765000	1.037877000
H	-14.714002000	-4.786279000	-0.135097000
H	-13.253772000	-3.784598000	-0.177377000
C	-16.532208000	-2.696630000	-0.587852000
H	-17.087012000	-2.044441000	-1.271252000
H	-17.008527000	-3.682802000	-0.593910000
H	-16.651077000	-2.285879000	0.422986000
C	-14.810756000	-3.280474000	-2.397321000
C	-15.845141000	-3.798109000	-3.185153000
H	-16.864244000	-3.848906000	-2.809283000
C	-15.573362000	-4.265994000	-4.475080000
H	-16.382139000	-4.667628000	-5.083234000
C	-14.276080000	-4.226820000	-4.985869000
H	-14.082254000	-4.603868000	-5.988201000
C	-13.228391000	-3.706594000	-4.208552000
C	-13.506189000	-3.239952000	-2.918231000
H	-12.700506000	-2.828822000	-2.303006000
C	-11.793370000	-3.718262000	-4.744677000
C	-11.755052000	-3.467361000	-6.265967000
H	-10.722755000	-3.369584000	-6.622389000
H	-12.221735000	-4.282276000	-6.827681000
H	-12.275700000	-2.537339000	-6.524775000
C	-11.210736000	-5.111579000	-4.433718000
H	-11.165180000	-5.297259000	-3.354105000
H	-11.838195000	-5.901407000	-4.864725000
H	-10.206055000	-5.238201000	-4.849723000
C	-10.979187000	-2.614688000	-4.108221000
C	-11.293480000	-1.238829000	-4.042500000
H	-12.192074000	-0.788749000	-4.411775000
C	-10.230841000	-0.583374000	-3.392457000
H	-10.163101000	0.470974000	-3.169193000
C	-9.258196000	-1.554344000	-3.062442000
C	-7.995660000	-1.373184000	-2.387317000
C	-7.650969000	0.043117000	-2.090438000
C	-7.039085000	0.851262000	-3.064627000
C	-6.726910000	2.197037000	-2.819679000
C	-7.034690000	2.765324000	-1.574533000
C	-7.636682000	1.978445000	-0.582890000
C	-7.948405000	0.634797000	-0.851795000
C	-7.125237000	-2.353972000	-2.030765000
C	-5.836330000	-2.222334000	-1.303663000
H	-5.454531000	-1.286326000	-0.939873000
C	-5.301665000	-3.463117000	-1.196749000
H	-4.390008000	-3.776653000	-0.723222000
C	-6.248051000	-4.397120000	-1.869398000
C	-5.972831000	-5.880776000	-2.035058000
C	-7.192437000	-6.622034000	-2.614513000
H	-7.427596000	-6.266179000	-3.624362000
H	-7.009361000	-7.700149000	-2.665301000
H	-8.090496000	-6.461447000	-2.006108000
C	-4.805999000	-5.998082000	-3.034992000
H	-3.903528000	-5.489785000	-2.674384000
H	-4.551902000	-7.045956000	-3.227534000
H	-5.069741000	-5.542622000	-3.997577000
C	-5.650479000	-6.461156000	-0.656689000
C	-6.656373000	-6.466150000	0.327482000
H	-7.633154000	-6.033858000	0.111164000
C	-6.402377000	-7.011772000	1.583759000
H	-7.186271000	-7.016297000	2.340432000
C	-5.142446000	-7.542897000	1.888025000
H	-4.972357000	-7.961919000	2.877646000
C	-4.123653000	-7.517697000	0.931148000
C	-4.391977000	-6.978065000	-0.340919000
H	-3.585127000	-6.953237000	-1.074606000
C	-2.692455000	-7.978364000	1.239064000
C	-2.570158000	-8.687667000	2.600623000
H	-2.876973000	-8.042280000	3.431290000

H	-3.175447000	-9.599215000	2.633716000
H	-1.528503000	-8.973833000	2.794771000
C	-2.211361000	-8.943409000	0.140129000
H	-1.220115000	-9.348689000	0.372988000
H	-2.901046000	-9.787778000	0.032767000
H	-2.137954000	-8.446924000	-0.834343000
N	-2.252164000	-5.595703000	1.941794000
N	-3.591612000	-3.658392000	3.498225000
N	-11.820036000	-0.529901000	2.278050000
N	-13.674370000	-0.969724000	0.124883000
N	-9.743585000	-2.799190000	-3.513005000
N	-7.309994000	-3.760534000	-2.336416000
F	0.899114000	-2.934818000	3.867317000
F	2.902116000	-1.212174000	3.236356000
F	2.719342000	0.326705000	0.983715000
F	0.503079000	0.142945000	-0.612521000
F	-1.507524000	-1.561290000	0.056289000
F	-10.774791000	2.554344000	-0.901876000
F	-10.702536000	5.250659000	-1.262973000
F	-12.603874000	6.832802000	-0.105902000
F	-14.563972000	5.702757000	1.430205000
F	-14.601066000	3.015621000	1.813631000
F	-6.737671000	0.326439000	-4.246540000
F	-6.146833000	2.933005000	-3.762917000
F	-6.749793000	4.039094000	-1.335448000
F	-7.912893000	2.504201000	0.605466000
F	-8.529497000	-0.092266000	0.091621000
H	-12.327732000	-1.298758000	1.852838000
H	-3.127848000	-5.484161000	2.448086000
H	-9.243329000	-3.674952000	-3.401411000
C	2.586436000	-3.385086000	-1.349062000
O	1.978623000	-3.207026000	-0.312883000
C	2.866391000	-2.275117000	-2.311073000
C	3.102153000	-4.745051000	-1.728699000
H	2.111926000	-1.465639000	-2.238734000
H	3.034204000	-5.445590000	-0.883096000
H	2.906183000	-2.598790000	-3.354729000
H	3.828894000	-1.792796000	-2.082807000
H	4.152684000	-4.713858000	-2.045827000
H	2.522357000	-5.176486000	-2.553488000
C	-10.725165000	3.139679000	-3.825751000
O	-9.948620000	2.599678000	-3.063291000
C	-10.323336000	4.341245000	-4.634277000
C	-12.127768000	2.654027000	-4.009673000
H	-9.351173000	4.735489000	-4.302791000
H	-12.262018000	1.637569000	-3.605717000
H	-11.055618000	5.153831000	-4.555648000
H	-10.224566000	4.089296000	-5.697803000
H	-12.447891000	2.645607000	-5.055946000
H	-12.846548000	3.293532000	-3.460708000
C	-15.567196000	4.461475000	-1.944313000
O	-14.560337000	3.891350000	-2.315357000
C	-15.803097000	5.913106000	-2.235636000
C	-16.633646000	3.754578000	-1.164811000
H	-15.036160000	6.318460000	-2.912914000
H	-16.347303000	2.715144000	-0.933286000
H	-15.765730000	6.516859000	-1.316514000
H	-16.781963000	6.094099000	-2.696281000
H	-17.582582000	3.711768000	-1.714970000
H	-16.841630000	4.250282000	-0.206016000
C	12.591009000	-6.912100000	1.853160000
O	11.690085000	-6.400076000	2.484085000
C	12.639788000	-8.387763000	1.592935000
C	13.724956000	-6.101866000	1.296896000
H	11.832772000	-8.916101000	2.123678000
H	13.456544000	-5.030489000	1.211414000
H	13.591385000	-8.833743000	1.908470000
H	12.518686000	-8.614264000	0.523727000
H	14.050186000	-6.441694000	0.305676000
H	14.603276000	-6.151675000	1.956212000
C	-10.137275000	5.153388000	3.527002000
O	-10.986706000	4.861728000	2.709910000
C	-10.401456000	6.154966000	4.614952000
C	-8.775009000	4.528153000	3.504688000
H	-11.424665000	6.555732000	4.547649000
H	-8.251876000	4.770082000	2.565428000
H	-9.711233000	7.006243000	4.560670000
H	-10.291837000	5.706588000	5.611007000
H	-8.848558000	3.426484000	3.519802000
H	-8.126001000	4.829242000	4.332891000
C	10.633848000	-4.851953000	-5.247668000
O	10.103513000	-4.847047000	-4.156750000
C	10.328810000	-5.912348000	-6.267517000
C	11.634386000	-3.811804000	-5.652553000
H	9.733009000	-6.726726000	-5.827884000
H	11.491353000	-2.876208000	-5.081016000
H	11.238190000	-6.356117000	-6.690080000

H	9.745463000	-5.503629000	-7.103359000
H	11.591155000	-3.558052000	-6.716644000
H	12.658487000	-4.147268000	-5.434498000
C	9.425074000	-4.089098000	3.034353000
O	9.089532000	-3.293333000	2.178252000
C	8.695857000	-5.379813000	3.252489000
C	10.611094000	-3.848992000	3.918856000
H	7.829634000	-5.477604000	2.583243000
H	11.023574000	-2.838986000	3.783991000
H	8.330894000	-5.480831000	4.279994000
H	9.366227000	-6.235117000	3.058558000
H	11.410839000	-4.573678000	3.675958000
H	10.376847000	-3.975911000	4.981609000
C	-2.514400000	6.487714000	-0.389455000
O	-1.840625000	5.826921000	0.373173000
C	-2.008093000	7.766141000	-0.990796000
C	-3.899841000	6.068804000	-0.784693000
H	-0.912491000	7.852313000	-0.881781000
H	-4.261925000	5.240706000	-0.154786000
H	-2.444702000	8.640040000	-0.489976000
H	-2.238153000	7.850830000	-2.059205000
H	-3.926379000	5.707062000	-1.823302000
H	-4.626797000	6.885592000	-0.709457000
C	0.148273000	0.715157000	4.851355000
O	-0.463931000	0.706198000	3.803236000
C	1.272410000	1.673180000	5.108428000
C	-0.172910000	-0.244962000	5.959898000
H	1.305169000	2.467544000	4.345484000
H	-0.959969000	-0.956163000	5.660601000
H	2.245712000	1.161377000	5.067498000
H	1.201760000	2.156796000	6.088998000
H	-0.528721000	0.273865000	6.858148000
H	0.703421000	-0.838788000	6.252900000
C	-0.023250000	0.233155000	-3.609934000
O	0.924158000	0.270903000	-2.850406000
C	-1.094551000	-0.806883000	-3.487743000
C	-0.183788000	1.232212000	-4.717925000
H	-0.747787000	-1.676072000	-2.906475000
H	0.599592000	2.005156000	-4.679413000
H	-1.461787000	-1.169034000	-4.453705000
H	-1.964399000	-0.406552000	-2.942274000
H	-1.153161000	1.747234000	-4.669198000
H	-0.122520000	0.757191000	-5.705165000

Input used for optimization of M-II cluster containing six molecules.
#T opt oniom(pm6:uff)=embed geom=connectivity test

test

0 1 0 1 0 1

C-C_R	0	-3.40800000	0.34300000	1.06800000	L
C-C_R	0	-2.47400000	0.64600000	2.03800000	L
H-H_	0	-2.40400000	0.23400000	2.87000000	L
C-C_R	0	-1.66200000	1.65900000	1.57300000	L
H-H_	0	-0.95700000	2.04900000	2.04000000	L
C-C_R	0	-2.07100000	1.99700000	0.29000000	L
C-C_R	0	-1.67100000	3.01600000	-0.61300000	L H-H_ 8
C-C_R	0	-0.70500000	4.03300000	-0.09900000	H
C-C_R	0	0.58500000	4.11400000	-0.54700000	H
C-C_R	0	1.46300000	5.06600000	-0.14500000	H
C-C_R	0	1.04900000	5.98600000	0.79100000	H
C-C_R	0	-0.21900000	5.95100000	1.27100000	H
C-C_R	0	-1.06600000	4.97800000	0.84200000	H
C-C_R	0	-2.13600000	3.14900000	-1.89500000	L
C-C_R	0	-1.87200000	4.17500000	-2.86700000	L
H-H_	0	-1.33400000	4.92600000	-2.75000000	L
C-C_R	0	-2.54600000	3.84200000	-3.96800000	L
H-H_	0	-2.57200000	4.31800000	-4.76800000	L
C-C_R	0	-3.22500000	2.60300000	-3.68700000	L
C-C_3	0	-4.05100000	1.80100000	-4.66000000	L
C-C_3	0	-3.12400000	1.38800000	-5.81000000	L
H-H_	0	-3.62600000	0.90800000	-6.47200000	L
H-H_	0	-2.42200000	0.82800000	-5.47200000	L
H-H_	0	-2.74000000	2.17300000	-6.20900000	L
C-C_3	0	-4.60700000	0.53500000	-4.00200000	L
H-H_	0	-5.17900000	0.78100000	-3.27000000	L
H-H_	0	-3.88200000	-0.00100000	-3.67500000	L
H-H_	0	-5.11000000	0.03400000	-4.64700000	L
C-C_R	0	-5.20300000	2.68600000	-5.12700000	L
C-C_R	0	-5.38300000	3.04800000	-6.44900000	L
H-H_	0	-4.77900000	2.73100000	-7.08100000	L
C-C_R	0	-6.41800000	3.86300000	-6.87800000	L
C-C_R	0	-7.31100000	4.30500000	-5.92400000	L
H-H_	0	-8.02100000	4.85100000	-6.17600000	L
C-C_R	0	-7.17000000	3.95300000	-4.61100000	L
H-H_	0	-7.79100000	4.25300000	-3.98500000	L
C-C_R	0	-6.11800000	3.15600000	-4.20300000	L

H-H_	0	-6.02400000	2.93800000	-3.30300000	L
C-C_3	0	-6.53900000	4.31200000	-8.34100000	L
C-C_3	0	-5.54700000	3.60900000	-9.25700000	L
H-H_	0	-5.68700000	3.89900000	-10.16100000	L
H-H_	0	-5.67800000	2.66000000	-9.20000000	L
H-H_	0	-4.65300000	3.82600000	-8.98700000	L
C-C_3	0	-7.96800000	4.04600000	-8.87300000	L
H-H_	0	-8.60700000	4.49600000	-8.31400000	L
H-H_	0	-8.14400000	3.10200000	-8.86200000	L
H-H_	0	-8.04100000	4.37500000	-9.77300000	L
C-C_R	0	-6.25400000	5.79700000	-8.35300000	L
C-C_R	0	-5.03300000	6.46500000	-8.42000000	L
H-H_	0	-4.19900000	6.06600000	-8.51500000	L
C-C_R	0	-5.27500000	7.80900000	-8.32400000	L
H-H_	0	-4.63400000	8.48300000	-8.34500000	L
C-C_R	0	-6.64800000	7.98600000	-8.19200000	L
C-C_R	0	-7.43200000	9.14700000	-8.06700000	L H-H_ 55
C-C_R	0	-6.66600000	10.41400000	-8.10100000	H
C-C_R	0	-5.89800000	10.85300000	-7.05700000	H
C-C_R	0	-5.07600000	11.93500000	-7.12300000	H
C-C_R	0	-4.99300000	12.63000000	-8.27200000	H
C-C_R	0	-5.73100000	12.25100000	-9.33700000	H
C-C_R	0	-6.55800000	11.17200000	-9.23200000	H
C-C_R	0	-8.80700000	9.16600000	-7.97800000	L
C-C_R	0	-9.69400000	10.26900000	-7.87100000	L
H-H_	0	-9.45500000	11.16600000	-7.81100000	L
C-C_R	0	-10.94000000	9.77400000	-7.87300000	L
H-H_	0	-11.72800000	10.26400000	-7.80500000	L
C-C_R	0	-10.83800000	8.34800000	-7.99700000	L
C-C_3	0	-11.97600000	7.35600000	-8.05200000	L
C-C_3	0	-11.46700000	5.95900000	-8.42100000	L
H-H_	0	-11.00900000	5.99800000	-9.26400000	L
H-H_	0	-12.21100000	5.35600000	-8.48700000	L
H-H_	0	-10.86300000	5.64900000	-7.74100000	L
C-C_3	0	-12.96700000	7.81900000	-9.14800000	L
H-H_	0	-13.30300000	8.69100000	-8.92900000	L
H-H_	0	-13.69900000	7.19800000	-9.20000000	L
H-H_	0	-12.51600000	7.85500000	-9.99300000	L
C-C_R	0	-12.60700000	7.31500000	-6.66200000	L
C-C_R	0	-13.91600000	7.64800000	-6.44400000	L
H-H_	0	-14.47100000	7.86800000	-7.16000000	L
C-C_R	0	-14.40000000	7.65100000	-5.16200000	L
H-H_	0	-15.29700000	7.84700000	-5.01900000	L
C-C_R	0	-13.59200000	7.37100000	-4.07400000	L
H-H_	0	-13.94200000	7.41100000	-3.21400000	L
C-C_R	0	-12.25100000	7.03000000	-4.26400000	L
C-C_R	0	-11.82000000	6.99000000	-5.57600000	L
H-H_	0	-10.94300000	6.73000000	-5.73700000	L
C-C_3	0	-11.32200000	6.67000000	-3.11800000	L
C-C_3	0	-11.79800000	7.23700000	-1.76500000	L
H-H_	0	-11.12800000	7.07300000	-1.09800000	L
H-H_	0	-12.61800000	6.80800000	-1.50900000	L
H-H_	0	-11.94300000	8.18100000	-1.84700000	L
C-C_3	0	-11.27000000	5.13700000	-3.02700000	L
H-H_	0	-10.86500000	4.78300000	-3.82300000	L
H-H_	0	-12.16100000	4.79100000	-2.94000000	L
H-H_	0	-10.75000000	4.88000000	-2.26100000	L
C-C_R	0	-9.94100000	7.22800000	-3.35000000	L
C-C_R	0	-9.47000000	8.27900000	-4.14300000	L
H-H_	0	-9.98700000	8.82000000	-4.69500000	L
C-C_R	0	-8.10900000	8.37500000	-3.96500000	L
H-H_	0	-7.54400000	8.98600000	-4.37900000	L
C-C_R	0	-7.73100000	7.39300000	-3.05300000	L
C-C_R	0	-6.45900000	7.02700000	-2.56800000	L H-H_ 102
C-C_R	0	-5.31100000	7.80300000	-3.10000000	H
C-C_R	0	-4.93100000	9.00300000	-2.57100000	H
C-C_R	0	-3.87500000	9.71700000	-3.05200000	H
C-C_R	0	-3.15100000	9.22700000	-4.10200000	H
C-C_R	0	-3.50000000	8.05000000	-4.65000000	H
C-C_R	0	-4.55400000	7.37000000	-4.15600000	H
C-C_R	0	-6.21300000	5.99900000	-1.68800000	L
C-C_R	0	-4.97300000	5.48500000	-1.20600000	L
H-H_	0	-4.12300000	5.79200000	-1.42500000	L
C-C_R	0	-5.26600000	4.46900000	-0.37700000	L
H-H_	0	-4.66100000	3.93100000	0.07800000	L
C-C_R	0	-6.69400000	4.37500000	-0.32900000	L
C-C_3	0	-7.50200000	3.41800000	0.53700000	L
C-C_3	0	-8.99700000	3.70200000	0.36900000	L
H-H_	0	-9.18600000	4.59800000	0.66000000	L
H-H_	0	-9.50100000	3.07900000	0.89700000	L
H-H_	0	-9.23800000	3.60900000	-0.55600000	L
C-C_3	0	-7.11100000	3.66000000	2.00600000	L
H-H_	0	-6.15600000	3.61900000	2.09600000	L
H-H_	0	-7.51300000	2.98600000	2.56000000	L
H-H_	0	-7.42100000	4.52700000	2.28300000	L
C-C_R	0	-7.13900000	1.98800000	0.10100000	L
C-C_R	0	-7.75700000	1.38100000	-0.99500000	L

H-H_ 0 -8.43600000 1.82700000 -1.44800000 L
C-C_R 0 -7.37900000 0.15100000 -1.40300000 L
H-H_ 0 -7.82200000 -0.24700000 -2.11800000 L
C-C_R 0 -6.35600000 -0.53200000 -0.78600000 L
H-H_ 0 -6.10200000 -1.37000000 -1.09800000 L
C-C_R 0 -5.70900000 0.02400000 0.28600000 L
C-C_R 0 -6.13000000 1.27900000 0.71000000 L
H-H_ 0 -5.70700000 1.65900000 1.44500000 L
C-C_3 0 -4.54300000 -0.63100000 1.01500000 L
C-C_3 0 -4.06100000 -1.91300000 0.30200000 L
H-H_ 0 -3.71400000 -1.68500000 -0.56400000 L
H-H_ 0 -4.79600000 -2.52100000 0.20100000 L
H-H_ 0 -3.37100000 -2.33000000 0.82200000 L
C-C_3 0 -5.00000000 -1.00200000 2.44200000 L
H-H_ 0 -4.29100000 -1.47100000 2.89000000 L
H-H_ 0 -5.77500000 -1.56600000 2.39200000 L
H-H_ 0 -5.21200000 -0.20400000 2.92900000 L
N-N_R 0 -3.11700000 1.14900000 0.01900000 L
N-N_R 0 -3.00000000 2.20100000 -2.46600000 L
N-N_R 0 -7.20800000 6.71900000 -8.21700000 L
N-N_R 0 -9.56100000 7.98600000 -8.04200000 L
N-N_R 0 -8.88500000 6.72100000 -2.69500000 L
N-N_R 0 -7.25100000 5.26200000 -1.11000000 L
F-F_ 0 1.01000000 3.21600000 -1.45200000 H
F-F_ 0 2.71300000 5.10300000 -0.63000000 H
F-F_ 0 1.90000000 6.94400000 1.18300000 H
F-F_ 0 -0.61600000 6.86100000 2.17600000 H
F-F_ 0 -2.31900000 4.99100000 1.31500000 H
F-F_ 0 -5.91100000 10.16100000 -5.89300000 H
F-F_ 0 -4.31900000 12.30200000 -6.07600000 H
F-F_ 0 -4.19700000 13.69600000 -8.38300000 H
F-F_ 0 -5.64600000 12.93400000 -10.49200000 H
F-F_ 0 -7.27600000 10.82300000 -10.31300000 H
F-F_ 0 -5.60000000 9.50600000 -1.52700000 H
F-F_ 0 -3.53400000 10.89700000 -2.49600000 H
F-F_ 0 -2.11100000 9.92300000 -4.57900000 H
F-F_ 0 -2.79400000 7.56600000 -5.69400000 H
F-F_ 0 -4.87500000 6.21100000 -4.74600000 H
H-H_ 0 -8.06300000 6.68200000 -8.16000000 L
H-H_ 0 -3.51400000 1.15300000 -0.75200000 L
H-H_ 0 -8.81100000 6.04700000 -2.16000000 L
C-C_R 0 -1.00100000 7.73500000 -15.04000000 L
C-C_R 0 -1.93500000 8.03800000 -16.01100000 L
H-H_ 0 -2.00500000 7.62600000 -16.84300000 L
C-C_R 0 -2.74700000 9.05100000 -15.54600000 L
H-H_ 0 -3.45200000 9.44100000 -16.01300000 L
C-C_R 0 -2.33800000 9.38900000 -14.26300000 L
C-C_R 0 -2.73700000 10.40800000 -13.35900000 L H-H_ 173
C-C_R 0 -3.70400000 11.42500000 -13.87400000 H
C-C_R 0 -4.99400000 11.50600000 -13.42500000 H
C-C_R 0 -5.87200000 12.45800000 -13.82700000 H
C-C_R 0 -5.45800000 13.37800000 -14.76400000 H
C-C_R 0 -4.19000000 13.34200000 -15.24400000 H
C-C_R 0 -3.34300000 12.37000000 -14.81500000 H
C-C_R 0 -2.27300000 10.54100000 -12.07700000 L
C-C_R 0 -2.53700000 11.56700000 -11.10600000 L
H-H_ 0 -3.07400000 12.31800000 -11.22300000 L
C-C_R 0 -1.86300000 11.23400000 -10.00500000 L
H-H_ 0 -1.83700000 11.71000000 -9.20500000 L
C-C_R 0 -1.18400000 9.99500000 -10.28600000 L
C-C_3 0 -0.35800000 9.19300000 -9.31200000 L
C-C_3 0 -1.28500000 8.78000000 -8.16200000 L
H-H_ 0 -0.78300000 8.30000000 -7.50100000 L
H-H_ 0 -1.98700000 8.22000000 -8.50100000 L
H-H_ 0 -1.66900000 9.56500000 -7.76300000 L
C-C_3 0 0.19800000 7.92700000 -9.97100000 L
H-H_ 0 0.77000000 8.17300000 -10.70300000 L
H-H_ 0 -0.52700000 7.39000000 -10.29800000 L
H-H_ 0 0.70100000 7.42600000 -9.32500000 L
C-C_R 0 0.79400000 10.07800000 -8.84600000 L
C-C_R 0 0.97400000 10.44000000 -7.52400000 L
H-H_ 0 0.37000000 10.12300000 -6.89100000 L
C-C_R 0 2.00900000 11.25500000 -7.09500000 L
C-C_R 0 2.90200000 11.69700000 -8.04800000 L
H-H_ 0 3.61200000 12.24300000 -7.79700000 L
C-C_R 0 2.76100000 11.34500000 -9.36200000 L
H-H_ 0 3.38200000 11.64500000 -9.98800000 L
C-C_R 0 1.70900000 10.54800000 -9.77000000 L
H-H_ 0 1.61500000 10.33000000 -10.67000000 L
C-C_3 0 2.13000000 11.70400000 -5.63200000 L
C-C_3 0 1.13800000 11.00100000 -4.71600000 L
H-H_ 0 1.27800000 11.29000000 -3.81200000 L
H-H_ 0 1.26900000 10.05200000 -4.77300000 L
H-H_ 0 0.24400000 11.21800000 -4.98500000 L
C-C_3 0 3.55900000 11.43800000 -5.10000000 L
H-H_ 0 4.19800000 11.88800000 -5.65900000 L
H-H_ 0 3.73500000 10.49400000 -5.11100000 L

H-H_ 0 3.63200000 11.76700000 -4.20000000 L
C-C_R 0 1.84500000 13.18900000 -5.62000000 L
C-C_R 0 0.62400000 13.85700000 -5.55300000 L
H-H_ 0 -0.21000000 13.45800000 -5.45800000 L
C-C_R 0 0.86600000 15.20100000 -5.64800000 L
H-H_ 0 0.22500000 15.87500000 -5.62800000 L
C-C_R 0 2.23900000 15.37800000 -5.78100000 L
C-C_R 0 3.02300000 16.53900000 -5.90600000 L H-H_ 220
C-C_R 0 2.25700000 17.80600000 -5.87200000 H
C-C_R 0 1.48900000 18.24500000 -6.91600000 H
C-C_R 0 0.66700000 19.32700000 -6.84900000 H
C-C_R 0 0.58400000 20.02200000 -5.70100000 H
C-C_R 0 1.32200000 19.64300000 -4.63600000 H
C-C_R 0 2.14900000 18.56400000 -4.74100000 H
C-C_R 0 4.39800000 16.55800000 -5.99500000 L
C-C_R 0 5.28500000 17.66100000 -6.10200000 L
H-H_ 0 5.04600000 18.55800000 -6.16200000 L
C-C_R 0 6.53100000 17.16600000 -6.10000000 L
H-H_ 0 7.31900000 17.65600000 -6.16800000 L
C-C_R 0 6.42900000 15.74000000 -5.97600000 L
C-C_3 0 7.56700000 14.74800000 -5.92100000 L
C-C_3 0 7.05800000 13.35100000 -5.55200000 L
H-H_ 0 6.60000000 13.39000000 -4.70900000 L
H-H_ 0 7.80200000 12.74800000 -5.48600000 L
H-H_ 0 6.45400000 13.04100000 -6.23200000 L
C-C_3 0 8.55900000 15.21100000 -4.82500000 L
H-H_ 0 8.89400000 16.08300000 -5.04400000 L
H-H_ 0 9.29000000 14.59000000 -4.77300000 L
H-H_ 0 8.10700000 15.24700000 -3.97900000 L
C-C_R 0 8.19800000 14.70700000 -7.31100000 L
C-C_R 0 9.50700000 15.04000000 -7.52900000 L
H-H_ 0 10.06200000 15.26000000 -6.81300000 L
C-C_R 0 9.99100000 15.04300000 -8.81100000 L
H-H_ 0 10.88800000 15.23900000 -8.95400000 L
C-C_R 0 9.18300000 14.76300000 -9.89800000 L
H-H_ 0 9.53300000 14.80300000 -10.75900000 L
C-C_R 0 7.84300000 14.42200000 -9.70900000 L
C-C_R 0 7.41100000 14.38200000 -8.39700000 L
H-H_ 0 6.53400000 14.12200000 -8.23600000 L
C-C_3 0 6.91300000 14.06200000 -10.85400000 L
C-C_3 0 7.38900000 14.62900000 -12.20800000 L
H-H_ 0 6.72000000 14.46500000 -12.87500000 L
H-H_ 0 8.21000000 14.20000000 -12.46400000 L
H-H_ 0 7.53400000 15.57300000 -12.12600000 L
C-C_3 0 6.86100000 12.52900000 -10.94600000 L
H-H_ 0 6.45600000 12.17500000 -10.15000000 L
H-H_ 0 7.75200000 12.18300000 -11.03300000 L
H-H_ 0 6.34100000 12.27200000 -11.71200000 L
C-C_R 0 5.53200000 14.62000000 -10.62300000 L
C-C_R 0 5.06100000 15.67100000 -9.82900000 L
H-H_ 0 5.57800000 16.21200000 -9.27800000 L
C-C_R 0 3.70000000 15.76700000 -10.00800000 L
H-H_ 0 3.13500000 16.37800000 -9.59400000 L
C-C_R 0 3.32200000 14.78500000 -10.91900000 L
C-C_R 0 2.05000000 14.41900000 -11.40500000 L H-H_ 267
C-C_R 0 0.90200000 15.19500000 -10.87200000 H
C-C_R 0 0.52200000 16.39500000 -11.40100000 H
C-C_R 0 -0.53400000 17.10900000 -10.92100000 H
C-C_R 0 -1.25800000 16.61900000 -9.87000000 H
C-C_R 0 -0.90900000 15.44200000 -9.32300000 H
C-C_R 0 0.14500000 14.76200000 -9.81600000 H
C-C_R 0 1.80400000 13.39100000 -12.28500000 L
C-C_R 0 0.56400000 12.87700000 -12.76700000 L
H-H_ 0 -0.28600000 13.18400000 -12.54800000 L
C-C_R 0 0.85700000 11.86100000 -13.59600000 L
H-H_ 0 0.25200000 11.32300000 -14.05100000 L
C-C_R 0 2.28500000 11.76700000 -13.64400000 L
C-C_3 0 3.09300000 10.81000000 -14.50900000 L
C-C_3 0 4.58800000 11.09400000 -14.34200000 L
H-H_ 0 4.77700000 11.99000000 -14.63200000 L
H-H_ 0 5.09200000 10.47100000 -14.87000000 L
H-H_ 0 4.82900000 11.00100000 -13.41700000 L
C-C_3 0 2.70200000 11.05200000 -15.97900000 L
H-H_ 0 1.74700000 11.01100000 -16.06900000 L
H-H_ 0 3.10400000 10.37800000 -16.53300000 L
H-H_ 0 3.01200000 11.91900000 -16.25600000 L
C-C_R 0 2.73000000 9.38000000 -14.07300000 L
C-C_R 0 3.34800000 8.77300000 -12.97800000 L
H-H_ 0 4.02700000 9.21900000 -12.52500000 L
C-C_R 0 2.97000000 7.54300000 -12.57000000 L
H-H_ 0 3.41300000 7.14500000 -11.85400000 L
C-C_R 0 1.94700000 6.86000000 -13.18600000 L
H-H_ 0 1.69300000 6.02100000 -12.87500000 L
C-C_R 0 1.30000000 7.41600000 -14.25800000 L
C-C_R 0 1.72100000 8.67100000 -14.68200000 L
H-H_ 0 1.29800000 9.05100000 -15.41800000 L
C-C_3 0 0.13400000 6.76100000 -14.98800000 L

C-C_3	0	-0.34800000	5.47900000	-14.27500000	L
H-H_	0	-0.69500000	5.70700000	-13.40800000	L
H-H_	0	0.38700000	4.87100000	-14.17400000	L
H-H_	0	-1.03800000	5.06200000	-14.79400000	L
C-C_3	0	0.59100000	6.39000000	-16.41400000	L
H-H_	0	-0.11800000	5.92100000	-16.86200000	L
H-H_	0	1.36600000	5.82600000	-16.36500000	L
H-H_	0	0.80300000	7.18800000	-16.90100000	L
N-N_R	0	-1.29200000	8.54100000	-13.99100000	L
N-N_R	0	-1.40900000	9.59300000	-11.50700000	L
N-N_R	0	2.79900000	14.11100000	-5.75600000	L
N-N_R	0	5.15200000	15.37800000	-5.93100000	L
N-N_R	0	4.47600000	14.11300000	-11.27800000	L
N-N_R	0	2.84200000	12.65400000	-12.86300000	L
F-F_	0	-5.41900000	10.60800000	-12.52000000	H
F-F_	0	-7.12200000	12.49500000	-13.34300000	H
F-F_	0	-6.30900000	14.33600000	-15.15500000	H
F-F_	0	-3.79300000	14.25300000	-16.14900000	H
F-F_	0	-2.09000000	12.38300000	-15.28700000	H
F-F_	0	1.50200000	17.55300000	-8.08000000	H
F-F_	0	-0.09000000	19.69400000	-7.89700000	H
F-F_	0	-0.21200000	21.08800000	-5.58900000	H
F-F_	0	1.23700000	20.32600000	-3.48100000	H
F-F_	0	2.86700000	18.21500000	-3.66000000	H
F-F_	0	1.19100000	16.89800000	-12.44600000	H
F-F_	0	-0.87500000	18.28900000	-11.47700000	H
F-F_	0	-2.29800000	17.31500000	-9.39400000	H
F-F_	0	-1.61500000	14.95800000	-8.27900000	H
F-F_	0	0.46600000	13.60300000	-9.22700000	H
H-H_	0	3.65400000	14.07400000	-5.81300000	L
H-H_	0	-0.89500000	8.54500000	-13.22100000	L
H-H_	0	4.40200000	13.43900000	-11.81300000	L
C-C_R	0	-3.40800000	15.12700000	1.06800000	L
C-C_R	0	-2.47400000	15.43000000	2.03800000	L
H-H_	0	-2.40400000	15.01700000	2.87000000	L
C-C_R	0	-1.66200000	16.44300000	1.57300000	L
H-H_	0	-0.95700000	16.83300000	2.04000000	L
C-C_R	0	-2.07100000	16.78100000	0.29000000	L
C-C_R	0	-1.67100000	17.80000000	-0.61300000	L H-H_ 338
C-C_R	0	-0.70500000	18.81700000	-0.09900000	H
C-C_R	0	0.58500000	18.89800000	-0.54700000	H
C-C_R	0	1.46300000	19.85000000	-0.14500000	H
C-C_R	0	1.04900000	20.77000000	0.79100000	H
C-C_R	0	-0.21900000	20.73400000	1.27100000	H
C-C_R	0	-1.06600000	19.76200000	0.84200000	H
C-C_R	0	-2.13600000	17.93300000	-1.89500000	L
C-C_R	0	-1.87200000	18.95900000	-2.86700000	L
H-H_	0	-1.33400000	19.71000000	-2.75000000	L
C-C_R	0	-2.54600000	18.62600000	-3.96800000	L
H-H_	0	-2.57200000	19.10200000	-4.76800000	L
C-C_R	0	-3.22500000	17.38700000	-3.68700000	L
C-C_3	0	-4.05100000	16.58500000	-4.66000000	L
C-C_3	0	-3.12400000	16.17200000	-5.81000000	L
H-H_	0	-3.62600000	15.69200000	-6.47200000	L
H-H_	0	-2.42200000	15.61200000	-5.47200000	L
H-H_	0	-2.74000000	16.95700000	-6.20900000	L
C-C_3	0	-4.60700000	15.31900000	-4.00200000	L
H-H_	0	-5.17900000	15.56400000	-3.27000000	L
H-H_	0	-3.88200000	14.78200000	-3.67500000	L
H-H_	0	-5.11000000	14.81800000	-4.64700000	L
C-C_R	0	-5.20300000	17.47000000	-5.12700000	L
C-C_R	0	-5.38300000	17.83200000	-6.44900000	L
H-H_	0	-4.77900000	17.51400000	-7.08100000	L
C-C_R	0	-6.41800000	18.64700000	-6.87800000	L
C-C_R	0	-7.31100000	19.08900000	-5.92400000	L
H-H_	0	-8.02100000	19.63400000	-6.17600000	L
C-C_R	0	-7.17000000	18.73700000	-4.61100000	L
H-H_	0	-7.79100000	19.03700000	-3.98500000	L
C-C_R	0	-6.11800000	17.94000000	-4.20300000	L
H-H_	0	-6.02400000	17.72100000	-3.30300000	L
C-C_3	0	-6.53900000	19.09600000	-8.34100000	L
C-C_3	0	-5.54700000	18.39300000	-9.25700000	L
H-H_	0	-5.68700000	18.68200000	-10.16100000	L
H-H_	0	-5.67800000	17.44400000	-9.20000000	L
H-H_	0	-4.65300000	18.61000000	-8.98700000	L
C-C_3	0	-7.96800000	18.83000000	-8.87300000	L
H-H_	0	-8.60700000	19.28000000	-8.31400000	L
H-H_	0	-8.14400000	17.88600000	-8.86200000	L
H-H_	0	-8.04100000	19.15800000	-9.77300000	L
C-C_R	0	-6.25400000	20.58100000	-8.35300000	L
C-C_R	0	-5.03300000	21.24900000	-8.42000000	L
H-H_	0	-4.19900000	20.85000000	-8.51500000	L
C-C_R	0	-5.27500000	22.59300000	-8.32400000	L
H-H_	0	-4.63400000	23.26700000	-8.34500000	L
C-C_R	0	-6.64800000	22.77000000	-8.19200000	L
C-C_R	0	-7.43200000	23.93100000	-8.06700000	L H-H_ 385
C-C_R	0	-6.66600000	25.19800000	-8.10100000	H

C-C_R	0	-5.89800000	25.63700000	-7.05700000 H
C-C_R	0	-5.07600000	26.71900000	-7.12300000 H
C-C_R	0	-4.99300000	27.41400000	-8.27200000 H
C-C_R	0	-5.73100000	27.03500000	-9.33700000 H
C-C_R	0	-6.55800000	25.95600000	-9.23200000 H
C-C_R	0	-8.80700000	23.95000000	-7.97800000 L
C-C_R	0	-9.69400000	25.05300000	-7.87100000 L
H-H_	0	-9.45500000	25.95000000	-7.81100000 L
C-C_R	0	-10.94000000	24.55800000	-7.87300000 L
H-H_	0	-11.72800000	25.04800000	-7.80500000 L
C-C_R	0	-10.83800000	23.13200000	-7.99700000 L
C-C_3	0	-11.97600000	22.14000000	-8.05200000 L
C-C_3	0	-11.46700000	20.74300000	-8.42100000 L
H-H_	0	-11.00900000	20.78200000	-9.26400000 L
H-H_	0	-12.21100000	20.14000000	-8.48700000 L
H-H_	0	-10.86300000	20.43300000	-7.74100000 L
C-C_3	0	-12.96700000	22.60300000	-9.14800000 L
H-H_	0	-13.30300000	23.47500000	-8.92900000 L
H-H_	0	-13.69900000	21.98200000	-9.20000000 L
H-H_	0	-12.51600000	22.63900000	-9.99300000 L
C-C_R	0	-12.60700000	22.09900000	-6.66200000 L
C-C_R	0	-13.91600000	22.43200000	-6.44400000 L
H-H_	0	-14.47100000	22.65200000	-7.16000000 L
C-C_R	0	-14.40000000	22.43500000	-5.16200000 L
H-H_	0	-15.29700000	22.63100000	-5.01900000 L
C-C_R	0	-13.59200000	22.15500000	-4.07400000 L
H-H_	0	-13.94200000	22.19500000	-3.21400000 L
C-C_R	0	-12.25100000	21.81400000	-4.26400000 L
C-C_R	0	-11.82000000	21.77400000	-5.57600000 L
H-H_	0	-10.94300000	21.51400000	-5.73700000 L
C-C_3	0	-11.32200000	21.45400000	-3.11800000 L
C-C_3	0	-11.79800000	22.02100000	-1.76500000 L
H-H_	0	-11.12800000	21.85700000	-1.09800000 L
H-H_	0	-12.61800000	21.59200000	-1.50900000 L
H-H_	0	-11.94300000	22.96500000	-1.84700000 L
C-C_3	0	-11.27000000	19.92100000	-3.02700000 L
H-H_	0	-10.86500000	19.56600000	-3.82300000 L
H-H_	0	-12.16100000	19.57500000	-2.94000000 L
H-H_	0	-10.75000000	19.66400000	-2.26100000 L
C-C_R	0	-9.94100000	22.01200000	-3.35000000 L
C-C_R	0	-9.47000000	23.06300000	-4.14300000 L
H-H_	0	-9.98700000	23.60400000	-4.69500000 L
C-C_R	0	-8.10900000	23.15900000	-3.96500000 L
H-H_	0	-7.54400000	23.77000000	-4.37900000 L
C-C_R	0	-7.73100000	22.17700000	-3.05300000 L
C-C_R	0	-6.45900000	21.81100000	-2.56800000 L H-H_ 432
C-C_R	0	-5.31100000	22.58700000	-3.10000000 H
C-C_R	0	-4.93100000	23.78700000	-2.57100000 H
C-C_R	0	-3.87500000	24.50100000	-3.05200000 H
C-C_R	0	-3.15100000	24.01100000	-4.10200000 H
C-C_R	0	-3.50000000	22.83400000	-4.65000000 H
C-C_R	0	-4.55400000	22.15400000	-4.15600000 H
C-C_R	0	-6.21300000	20.78300000	-1.68800000 L
C-C_R	0	-4.97300000	20.26900000	-1.20600000 L
H-H_	0	-4.12300000	20.57600000	-1.42500000 L
C-C_R	0	-5.26600000	19.25300000	-0.37700000 L
H-H_	0	-4.66100000	18.71500000	0.07800000 L
C-C_R	0	-6.69400000	19.15800000	-0.32900000 L
C-C_3	0	-7.50200000	18.20200000	0.53700000 L
C-C_3	0	-8.99700000	18.48600000	0.36900000 L
H-H_	0	-9.18600000	19.38200000	0.66000000 L
H-H_	0	-9.50100000	17.86300000	0.89700000 L
H-H_	0	-9.23800000	18.39300000	-0.55600000 L
C-C_3	0	-7.11100000	18.44400000	2.00600000 L
H-H_	0	-6.15600000	18.40300000	2.09600000 L
H-H_	0	-7.51300000	17.77000000	2.56000000 L
H-H_	0	-7.42100000	19.31100000	2.28300000 L
C-C_R	0	-7.13900000	16.77200000	0.10100000 L
C-C_R	0	-7.75700000	16.16500000	-0.99500000 L
H-H_	0	-8.43600000	16.61100000	-1.44800000 L
C-C_R	0	-7.37900000	14.93500000	-1.40300000 L
H-H_	0	-7.82200000	14.53700000	-2.11800000 L
C-C_R	0	-6.35600000	14.25200000	-0.78600000 L
H-H_	0	-6.10200000	13.41300000	-1.09800000 L
C-C_R	0	-5.70900000	14.80800000	0.28600000 L
C-C_R	0	-6.13000000	16.06300000	0.71000000 L
H-H_	0	-5.70700000	16.44300000	1.44500000 L
C-C_3	0	-4.54300000	14.15300000	1.01500000 L
C-C_3	0	-4.06100000	12.87100000	0.30200000 L
H-H_	0	-3.71400000	13.09900000	-0.56400000 L
H-H_	0	-4.79600000	12.26300000	0.20100000 L
H-H_	0	-3.37100000	12.45400000	0.82200000 L
C-C_3	0	-5.00000000	13.78200000	2.44200000 L
H-H_	0	-4.29100000	13.31300000	2.89000000 L
H-H_	0	-5.77500000	13.21800000	2.39200000 L
H-H_	0	-5.21200000	14.58000000	2.92900000 L
N-N_R	0	-3.11700000	15.93300000	0.01900000 L

N-N_R 0 -3.00000000 16.98500000 -2.46600000 L
N-N_R 0 -7.20800000 21.50300000 -8.21700000 L
N-N_R 0 -9.56100000 22.77000000 -8.04200000 L
N-N_R 0 -8.88500000 21.50500000 -2.69500000 L
N-N_R 0 -7.25100000 20.04500000 -1.11000000 L
F-F_ 0 1.01000000 18.00000000 -1.45200000 H
F-F_ 0 2.71300000 19.88700000 -0.63000000 H
F-F_ 0 1.90000000 21.72800000 1.18300000 H
F-F_ 0 -0.61600000 21.64500000 2.17600000 H
F-F_ 0 -2.31900000 19.77500000 1.31500000 H
F-F_ 0 -5.91100000 24.94500000 -5.89300000 H
F-F_ 0 -4.31900000 27.08600000 -6.07600000 H
F-F_ 0 -4.19700000 28.48000000 -8.38300000 H
F-F_ 0 -5.64600000 27.71800000 -10.49200000 H
F-F_ 0 -7.27600000 25.60700000 -10.31300000 H
F-F_ 0 -5.60000000 24.29000000 -1.52700000 H
F-F_ 0 -3.53400000 25.68100000 -2.49600000 H
F-F_ 0 -2.11100000 24.70700000 -4.57900000 H
F-F_ 0 -2.79400000 22.35000000 -5.69400000 H
F-F_ 0 -4.87500000 20.99500000 -4.74600000 H
H-H_ 0 -8.06300000 21.46600000 -8.16000000 L
H-H_ 0 -3.51400000 15.93700000 -0.75200000 L
H-H_ 0 -8.81100000 20.83100000 -2.16000000 L
C-C_R 0 3.40800000 29.22500000 -1.06800000 L
C-C_R 0 2.47400000 28.92200000 -2.03800000 L
H-H_ 0 2.40400000 29.33400000 -2.87000000 L
C-C_R 0 1.66200000 27.90900000 -1.57300000 L
H-H_ 0 0.95700000 27.51900000 -2.04000000 L
C-C_R 0 2.07100000 27.57000000 -0.29000000 L
C-C_R 0 1.67100000 26.55200000 0.61300000 L H-H_ 503
C-C_R 0 0.70500000 25.53500000 0.09900000 H
C-C_R 0 -0.58500000 25.45300000 0.54700000 H
C-C_R 0 -1.46300000 24.50100000 0.14500000 H
C-C_R 0 -1.04900000 23.58200000 -0.79100000 H
C-C_R 0 0.21900000 23.61700000 -1.27100000 H
C-C_R 0 1.06600000 24.59000000 -0.84200000 H
C-C_R 0 2.13600000 26.41900000 1.89500000 L
C-C_R 0 1.87200000 25.39300000 2.86700000 L
H-H_ 0 1.33400000 24.64200000 2.75000000 L
C-C_R 0 2.54600000 25.72500000 3.96800000 L
H-H_ 0 2.57200000 25.24900000 4.76800000 L
C-C_R 0 3.22500000 26.96400000 3.68700000 L
C-C_3 0 4.05100000 27.76700000 4.66000000 L
C-C_3 0 3.12400000 28.18000000 5.81000000 L
H-H_ 0 3.62600000 28.66000000 6.47200000 L
H-H_ 0 2.42200000 28.74000000 5.47200000 L
H-H_ 0 2.74000000 27.39500000 6.20900000 L
C-C_3 0 4.60700000 29.03300000 4.00200000 L
H-H_ 0 5.17900000 28.78700000 3.27000000 L
H-H_ 0 3.88200000 29.56900000 3.67500000 L
H-H_ 0 5.11000000 29.53400000 4.64700000 L
C-C_R 0 5.20300000 26.88200000 5.12700000 L
C-C_R 0 5.38300000 26.51900000 6.44900000 L
H-H_ 0 4.77900000 26.83700000 7.08100000 L
C-C_R 0 6.41800000 25.70500000 6.87800000 L
C-C_R 0 7.31100000 25.26300000 5.92400000 L
H-H_ 0 8.02100000 24.71700000 6.17600000 L
C-C_R 0 7.17000000 25.61500000 4.61100000 L
H-H_ 0 7.79100000 25.31400000 3.98500000 L
C-C_R 0 6.11800000 26.41100000 4.20300000 L
H-H_ 0 6.02400000 26.63000000 3.30300000 L
C-C_3 0 6.53900000 25.25500000 8.34100000 L
C-C_3 0 5.54700000 25.95900000 9.25700000 L
H-H_ 0 5.68700000 25.66900000 10.16100000 L
H-H_ 0 5.67800000 26.90800000 9.20000000 L
H-H_ 0 4.65300000 25.74200000 8.98700000 L
C-C_3 0 7.96800000 25.52100000 8.87300000 L
H-H_ 0 8.60700000 25.07200000 8.31400000 L
H-H_ 0 8.14400000 26.46600000 8.86200000 L
H-H_ 0 8.04100000 25.19300000 9.77300000 L
C-C_R 0 6.25400000 23.77100000 8.35300000 L
C-C_R 0 5.03300000 23.10300000 8.42000000 L
H-H_ 0 4.19900000 23.50200000 8.51500000 L
C-C_R 0 5.27500000 21.75900000 8.32400000 L
H-H_ 0 4.63400000 21.08500000 8.34500000 L
C-C_R 0 6.64800000 21.58200000 8.19200000 L
C-C_R 0 7.43200000 20.42100000 8.06700000 L H-H_ 550
C-C_R 0 6.66600000 19.15400000 8.10100000 H
C-C_R 0 5.89800000 18.71500000 7.05700000 H
C-C_R 0 5.07600000 17.63300000 7.12300000 H
C-C_R 0 4.99300000 16.93800000 8.27200000 H
C-C_R 0 5.73100000 17.31600000 9.33700000 H
C-C_R 0 6.55800000 18.39600000 9.23200000 H
C-C_R 0 8.80700000 20.40200000 7.97800000 L
C-C_R 0 9.69400000 19.29900000 7.87100000 L
H-H_ 0 9.45500000 18.40200000 7.81100000 L
C-C_R 0 10.94000000 19.79400000 7.87300000 L

H-H_ 0 11.72800000 19.30300000 7.80500000 L
C-C_R 0 10.83800000 21.21900000 7.99700000 L
C-C_3 0 11.97600000 22.21100000 8.05200000 L
C-C_3 0 11.46700000 23.60800000 8.42100000 L
H-H_ 0 11.00900000 23.57000000 9.26400000 L
H-H_ 0 12.21100000 24.21200000 8.48700000 L
H-H_ 0 10.86300000 23.91900000 7.74100000 L
C-C_3 0 12.96700000 21.74900000 9.14800000 L
H-H_ 0 13.30300000 20.87600000 8.92900000 L
H-H_ 0 13.69900000 22.37000000 9.20000000 L
H-H_ 0 12.51600000 21.71300000 9.99300000 L
C-C_R 0 12.60700000 22.25300000 6.66200000 L
C-C_R 0 13.91600000 21.92000000 6.44400000 L
H-H_ 0 14.47100000 21.70000000 7.16000000 L
C-C_R 0 14.40000000 21.91700000 5.16200000 L
H-H_ 0 15.29700000 21.72100000 5.01900000 L
C-C_R 0 13.59200000 22.19700000 4.07400000 L
H-H_ 0 13.94200000 22.15700000 3.21400000 L
C-C_R 0 12.25100000 22.53800000 4.26400000 L
C-C_R 0 11.82000000 22.57800000 5.57600000 L
H-H_ 0 10.94300000 22.83800000 5.73700000 L
C-C_3 0 11.32200000 22.89700000 3.11800000 L
C-C_3 0 11.79800000 22.33100000 1.76500000 L
H-H_ 0 11.12800000 22.49500000 1.09800000 L
H-H_ 0 12.61800000 22.76000000 1.50900000 L
H-H_ 0 11.94300000 21.38600000 1.84700000 L
C-C_3 0 11.27000000 24.43000000 3.02700000 L
H-H_ 0 10.86500000 24.78500000 3.82300000 L
H-H_ 0 12.16100000 24.77600000 2.94000000 L
H-H_ 0 10.75000000 24.68800000 2.26100000 L
C-C_R 0 9.94100000 22.34000000 3.35000000 L
C-C_R 0 9.47000000 21.28900000 4.14300000 L
H-H_ 0 9.98700000 20.74800000 4.69500000 L
C-C_R 0 8.10900000 21.19300000 3.96500000 L
H-H_ 0 7.54400000 20.58200000 4.37900000 L
C-C_R 0 7.73100000 22.17400000 3.05300000 L
C-C_R 0 6.45900000 22.54100000 2.56800000 L H-H_ 597
C-C_R 0 5.31100000 21.76500000 3.10000000 H
C-C_R 0 4.93100000 20.56400000 2.57100000 H
C-C_R 0 3.87500000 19.85000000 3.05200000 H
C-C_R 0 3.15100000 20.34100000 4.10200000 H
C-C_R 0 3.50000000 21.51800000 4.65000000 H
C-C_R 0 4.55400000 22.19800000 4.15600000 H
C-C_R 0 6.21300000 23.56800000 1.68800000 L
C-C_R 0 4.97300000 24.08300000 1.20600000 L
H-H_ 0 4.12300000 23.77500000 1.42500000 L
C-C_R 0 5.26600000 25.09900000 0.37700000 L
H-H_ 0 4.66100000 25.63700000 -0.07800000 L
C-C_R 0 6.69400000 25.19300000 0.32900000 L
C-C_3 0 7.50200000 26.15000000 -0.53700000 L
C-C_3 0 8.99700000 25.86600000 -0.36900000 L
H-H_ 0 9.18600000 24.97000000 -0.66000000 L
H-H_ 0 9.50100000 26.48800000 -0.89700000 L
H-H_ 0 9.23800000 25.95900000 0.55600000 L
C-C_3 0 7.11100000 25.90700000 -2.00600000 L
H-H_ 0 6.15600000 25.94900000 -2.09600000 L
H-H_ 0 7.51300000 26.58100000 -2.56000000 L
H-H_ 0 7.42100000 25.04100000 -2.28300000 L
C-C_R 0 7.13900000 27.57900000 -0.10100000 L
C-C_R 0 7.75700000 28.18700000 0.99500000 L
H-H_ 0 8.43600000 27.74100000 1.44800000 L
C-C_R 0 7.37900000 29.41700000 1.40300000 L
H-H_ 0 7.82200000 29.81500000 2.11800000 L
C-C_R 0 6.35600000 30.10000000 0.78600000 L
H-H_ 0 6.10200000 30.93800000 1.09800000 L
C-C_R 0 5.70900000 29.54400000 -0.28600000 L
C-C_R 0 6.13000000 28.28900000 -0.71000000 L
H-H_ 0 5.70700000 27.90900000 -1.44500000 L
C-C_3 0 4.54300000 30.19900000 -1.01500000 L
C-C_3 0 4.06100000 31.48100000 -0.30200000 L
H-H_ 0 3.71400000 31.25300000 0.56400000 L
H-H_ 0 4.79600000 32.08800000 -0.20100000 L
H-H_ 0 3.37100000 31.89800000 -0.82200000 L
C-C_3 0 5.00000000 30.57000000 -2.44200000 L
H-H_ 0 4.29100000 31.03900000 -2.89000000 L
H-H_ 0 5.77500000 31.13300000 -2.39200000 L
H-H_ 0 5.21200000 29.77200000 -2.92900000 L
N-N_R 0 3.11700000 28.41900000 -0.01900000 L
N-N_R 0 3.00000000 27.36600000 2.46600000 L
N-N_R 0 7.20800000 22.84900000 8.21700000 L
N-N_R 0 9.56100000 21.58200000 8.04200000 L
N-N_R 0 8.88500000 22.84700000 2.69500000 L
N-N_R 0 7.25100000 24.30600000 1.11000000 L
F-F_ 0 -1.01000000 26.35200000 1.45200000 H
F-F_ 0 -2.71300000 24.46400000 0.63000000 H
F-F_ 0 -1.90000000 22.62400000 -1.18300000 H
F-F_ 0 0.61600000 22.70700000 -2.17600000 H

F-F_ 0 2.31900000 24.57700000 -1.31500000 H
F-F_ 0 5.91100000 19.40700000 5.89300000 H
F-F_ 0 4.31900000 17.26600000 6.07600000 H
F-F_ 0 4.19700000 15.87200000 8.38300000 H
F-F_ 0 5.64600000 16.63400000 10.49200000 H
F-F_ 0 7.27600000 18.74500000 10.31300000 H
F-F_ 0 5.60000000 20.06200000 1.52700000 H
F-F_ 0 3.53400000 18.67100000 2.49600000 H
F-F_ 0 2.11100000 19.64500000 4.57900000 H
F-F_ 0 2.79400000 22.00100000 5.69400000 H
F-F_ 0 4.87500000 23.35700000 4.74600000 H
H-H_ 0 8.06300000 22.88500000 8.16000000 L
H-H_ 0 3.51400000 28.41500000 0.75200000 L
H-H_ 0 8.81100000 23.52100000 2.16000000 L
C-C_R 0 1.00100000 21.83300000 15.04000000 L
C-C_R 0 1.93500000 21.53000000 16.01100000 L
H-H_ 0 2.00500000 21.94200000 16.84300000 L
C-C_R 0 2.74700000 20.51700000 15.54600000 L
H-H_ 0 3.45200000 20.12700000 16.01300000 L
C-C_R 0 2.33800000 20.17900000 14.26300000 L
C-C_R 0 2.73700000 19.16000000 13.35900000 L H-H_ 668
C-C_R 0 3.70400000 18.14300000 13.87400000 H
C-C_R 0 4.99400000 18.06100000 13.42500000 H
C-C_R 0 5.87200000 17.10900000 13.82700000 H
C-C_R 0 5.45800000 16.19000000 14.76400000 H
C-C_R 0 4.19000000 16.22500000 15.24400000 H
C-C_R 0 3.34300000 17.19800000 14.81500000 H
C-C_R 0 2.27300000 19.02700000 12.07700000 L
C-C_R 0 2.53700000 18.00100000 11.10600000 L
H-H_ 0 3.07400000 17.25000000 11.22300000 L
C-C_R 0 1.86300000 18.33400000 10.00500000 L
H-H_ 0 1.83700000 17.85700000 9.20500000 L
C-C_R 0 1.18400000 19.57200000 10.28600000 L
C-C_3 0 0.35800000 20.37500000 9.31200000 L
C-C_3 0 1.28500000 20.78800000 8.16200000 L
H-H_ 0 0.78300000 21.26800000 7.50100000 L
H-H_ 0 1.98700000 21.34800000 8.50100000 L
H-H_ 0 1.66900000 20.00300000 7.76300000 L
C-C_3 0 -0.19800000 21.64100000 9.97100000 L
H-H_ 0 -0.77000000 21.39500000 10.70300000 L
H-H_ 0 0.52700000 22.17700000 10.29800000 L
H-H_ 0 -0.70100000 22.14200000 9.32500000 L
C-C_R 0 -0.79400000 19.49000000 8.84600000 L
C-C_R 0 -0.97400000 19.12700000 7.52400000 L
H-H_ 0 -0.37000000 19.44500000 6.89100000 L
C-C_R 0 -2.00900000 18.31300000 7.09500000 L
C-C_R 0 -2.90200000 17.87100000 8.04800000 L
H-H_ 0 -3.61200000 17.32500000 7.79700000 L
C-C_R 0 -2.76100000 18.22300000 9.36200000 L
H-H_ 0 -3.38200000 17.92300000 9.98800000 L
C-C_R 0 -1.70900000 19.01900000 9.77000000 L
H-H_ 0 -1.61500000 19.23800000 10.67000000 L
C-C_3 0 -2.13000000 17.86300000 5.63200000 L
C-C_3 0 -1.13800000 18.56700000 4.71600000 L
H-H_ 0 -1.27800000 18.27700000 3.81200000 L
H-H_ 0 -1.26900000 19.51600000 4.77300000 L
H-H_ 0 -0.24400000 18.35000000 4.98500000 L
C-C_3 0 -3.55900000 18.12900000 5.10000000 L
H-H_ 0 -4.19800000 17.68000000 5.65900000 L
H-H_ 0 -3.73500000 19.07400000 5.11100000 L
H-H_ 0 -3.63200000 17.80100000 4.20000000 L
C-C_R 0 -1.84500000 16.37900000 5.62000000 L
C-C_R 0 -0.62400000 15.71100000 5.55300000 L
H-H_ 0 0.21000000 16.11000000 5.45800000 L
C-C_R 0 -0.86600000 14.36700000 5.64800000 L
H-H_ 0 -0.22500000 13.69300000 5.62800000 L
C-C_R 0 -2.23900000 14.19000000 5.78100000 L
C-C_R 0 -3.02300000 13.02900000 5.90600000 L H-H_ 715
C-C_R 0 -2.25700000 11.76200000 5.87200000 H
C-C_R 0 -1.48900000 11.32300000 6.91600000 H
C-C_R 0 -0.66700000 10.24100000 6.84900000 H
C-C_R 0 -0.58400000 9.54600000 5.70100000 H
C-C_R 0 -1.32200000 9.92400000 4.63600000 H
C-C_R 0 -2.14900000 11.00400000 4.74100000 H
C-C_R 0 -4.39800000 13.01000000 5.99500000 L
C-C_R 0 -5.28500000 11.90700000 6.10200000 L
H-H_ 0 -5.04600000 11.01000000 6.16200000 L
C-C_R 0 -6.53100000 12.40200000 6.10000000 L
H-H_ 0 -7.31900000 11.91100000 6.16800000 L
C-C_R 0 -6.42900000 13.82700000 5.97600000 L
C-C_3 0 -7.56700000 14.81900000 5.92100000 L
C-C_3 0 -7.05800000 16.21600000 5.55200000 L
H-H_ 0 -6.60000000 16.17800000 4.70900000 L
H-H_ 0 -7.80200000 16.82000000 5.48600000 L
H-H_ 0 -6.45400000 16.52700000 6.23200000 L
C-C_3 0 -8.55900000 14.35700000 4.82500000 L
H-H_ 0 -8.89400000 13.48400000 5.04400000 L

H-H_	0	-9.29000000	14.97800000	4.77300000 L
H-H_	0	-8.10700000	14.32100000	3.97900000 L
C-C_R	0	-8.19800000	14.86100000	7.31100000 L
C-C_R	0	-9.50700000	14.52800000	7.52900000 L
H-H_	0	-10.06200000	14.30800000	6.81300000 L
C-C_R	0	-9.99100000	14.52500000	8.81100000 L
H-H_	0	-10.88800000	14.32900000	8.95400000 L
C-C_R	0	-9.18300000	14.80500000	9.89800000 L
H-H_	0	-9.53300000	14.76500000	10.75900000 L
C-C_R	0	-7.84300000	15.14600000	9.70900000 L
C-C_R	0	-7.41100000	15.18600000	8.39700000 L
H-H_	0	-6.53400000	15.44600000	8.23600000 L
C-C_3	0	-6.91300000	15.50500000	10.85400000 L
C-C_3	0	-7.38900000	14.93900000	12.20800000 L
H-H_	0	-6.72000000	15.10300000	12.87500000 L
H-H_	0	-8.21000000	15.36800000	12.46400000 L
H-H_	0	-7.53400000	13.99400000	12.12600000 L
C-C_3	0	-6.86100000	17.03800000	10.94600000 L
H-H_	0	-6.45600000	17.39300000	10.15000000 L
H-H_	0	-7.75200000	17.38400000	11.03300000 L
H-H_	0	-6.34100000	17.29600000	11.71200000 L
C-C_R	0	-5.53200000	14.94800000	10.62300000 L
C-C_R	0	-5.06100000	13.89700000	9.82900000 L
H-H_	0	-5.57800000	13.35600000	9.27800000 L
C-C_R	0	-3.70000000	13.80100000	10.00800000 L
H-H_	0	-3.13500000	13.19000000	9.59400000 L
C-C_R	0	-3.32200000	14.78200000	10.91900000 L
C-C_R	0	-2.05000000	15.14900000	11.40500000 L H-H_ 762
C-C_R	0	-0.90200000	14.37300000	10.87200000 H
C-C_R	0	-0.52200000	13.17200000	11.40100000 H
C-C_R	0	0.53400000	12.45800000	10.92100000 H
C-C_R	0	1.25800000	12.94900000	9.87000000 H
C-C_R	0	0.90900000	14.12600000	9.32300000 H
C-C_R	0	-0.14500000	14.80600000	9.81600000 H
C-C_R	0	-1.80400000	16.17700000	12.28500000 L
C-C_R	0	-0.56400000	16.69100000	12.76700000 L
H-H_	0	0.28600000	16.38400000	12.54800000 L
C-C_R	0	-0.85700000	17.70700000	13.59600000 L
H-H_	0	-0.25200000	18.24500000	14.05100000 L
C-C_R	0	-2.28500000	17.80100000	13.64400000 L
C-C_3	0	-3.09300000	18.75800000	14.50900000 L
C-C_3	0	-4.58800000	18.47400000	14.34200000 L
H-H_	0	-4.77700000	17.57800000	14.63200000 L
H-H_	0	-5.09200000	19.09600000	14.87000000 L
H-H_	0	-4.82900000	18.56700000	13.41700000 L
C-C_3	0	-2.70200000	18.51500000	15.97900000 L
H-H_	0	-1.74700000	18.55700000	16.06900000 L
H-H_	0	-3.10400000	19.19000000	16.53300000 L
H-H_	0	-3.01200000	17.64900000	16.25600000 L
C-C_R	0	-2.73000000	20.18700000	14.07300000 L
C-C_R	0	-3.34800000	20.79500000	12.97800000 L
H-H_	0	-4.02700000	20.34900000	12.52500000 L
C-C_R	0	-2.97000000	22.02500000	12.57000000 L
H-H_	0	-3.41300000	22.42300000	11.85400000 L
C-C_R	0	-1.94700000	22.70800000	13.18600000 L
H-H_	0	-1.69300000	23.54600000	12.87500000 L
C-C_R	0	-1.30000000	22.15200000	14.25800000 L
C-C_R	0	-1.72100000	20.89700000	14.68200000 L
H-H_	0	-1.29800000	20.51700000	15.41800000 L
C-C_3	0	-0.13400000	22.80700000	14.98800000 L
C-C_3	0	0.34800000	24.08900000	14.27500000 L
H-H_	0	0.69500000	23.86100000	13.40800000 L
H-H_	0	-0.38700000	24.69700000	14.17400000 L
H-H_	0	1.03800000	24.50600000	14.79400000 L
C-C_3	0	-0.59100000	23.17800000	16.41400000 L
H-H_	0	0.11800000	23.64700000	16.86200000 L
H-H_	0	-1.36600000	23.74100000	16.36500000 L
H-H_	0	-0.80300000	22.38000000	16.90100000 L
N-N_R	0	1.29200000	21.02700000	13.99100000 L
N-N_R	0	1.40900000	19.97500000	11.50700000 L
N-N_R	0	-2.79900000	15.45700000	5.75600000 L
N-N_R	0	-5.15200000	14.19000000	5.93100000 L
N-N_R	0	-4.47600000	15.45500000	11.27800000 L
N-N_R	0	-2.84200000	16.91400000	12.86300000 L
F-F_	0	5.41900000	18.96000000	12.52000000 H
F-F_	0	7.12200000	17.07200000	13.34300000 H
F-F_	0	6.30900000	15.23200000	15.15500000 H
F-F_	0	3.79300000	15.31500000	16.14900000 H
F-F_	0	2.09000000	17.18500000	15.28700000 H
F-F_	0	-1.50200000	12.01500000	8.08000000 H
F-F_	0	0.09000000	9.87400000	7.89700000 H
F-F_	0	0.21200000	8.48000000	5.58900000 H
F-F_	0	-1.23700000	9.24200000	3.48100000 H
F-F_	0	-2.86700000	11.35300000	3.66000000 H
F-F_	0	-1.19100000	12.67000000	12.44600000 H
F-F_	0	0.87500000	11.27900000	11.47700000 H
F-F_	0	2.29800000	12.25300000	9.39400000 H

F-F_ 0 1.61500000 14.60900000 8.27900000 H
F-F_ 0 -0.46600000 15.96500000 9.22700000 H
H-H_ 0 -3.65400000 15.49400000 5.81300000 L
H-H_ 0 0.89500000 21.02300000 13.22100000 L
H-H_ 0 -4.40200000 16.12900000 11.81300000 L
C-C_R 0 3.40800000 14.44100000 -1.06800000 L
C-C_R 0 2.47400000 14.13800000 -2.03800000 L
H-H_ 0 2.40400000 14.55000000 -2.87000000 L
C-C_R 0 1.66200000 13.12500000 -1.57300000 L
H-H_ 0 0.95700000 12.73500000 -2.04000000 L
C-C_R 0 2.07100000 12.78700000 -0.29000000 L
C-C_R 0 1.67100000 11.76800000 0.61300000 L H-H_ 833
C-C_R 0 0.70500000 10.75100000 0.09900000 H
C-C_R 0 -0.58500000 10.67000000 0.54700000 H
C-C_R 0 -1.46300000 9.71700000 0.14500000 H
C-C_R 0 -1.04900000 8.79800000 -0.79100000 H
C-C_R 0 0.21900000 8.83300000 -1.27100000 H
C-C_R 0 1.06600000 9.80600000 -0.84200000 H
C-C_R 0 2.13600000 11.63500000 1.89500000 L
C-C_R 0 1.87200000 10.60900000 2.86700000 L
H-H_ 0 1.33400000 9.85800000 2.75000000 L
C-C_R 0 2.54600000 10.94200000 3.96800000 L
H-H_ 0 2.57200000 10.46600000 4.76800000 L
C-C_R 0 3.22500000 12.18000000 3.68700000 L
C-C_3 0 4.05100000 12.98300000 4.66000000 L
C-C_3 0 3.12400000 13.39600000 5.81000000 L
H-H_ 0 3.62600000 13.87600000 6.47200000 L
H-H_ 0 2.42200000 13.95600000 5.47200000 L
H-H_ 0 2.74000000 12.61100000 6.20900000 L
C-C_3 0 4.60700000 14.24900000 4.00200000 L
H-H_ 0 5.17900000 14.00300000 3.27000000 L
H-H_ 0 3.88200000 14.78500000 3.67500000 L
H-H_ 0 5.11000000 14.75000000 4.64700000 L
C-C_R 0 5.20300000 12.09800000 5.12700000 L
C-C_R 0 5.38300000 11.73500000 6.44900000 L
H-H_ 0 4.77900000 12.05300000 7.08100000 L
C-C_R 0 6.41800000 10.92100000 6.87800000 L
C-C_R 0 7.31100000 10.47900000 5.92400000 L
H-H_ 0 8.02100000 9.93300000 6.17600000 L
C-C_R 0 7.17000000 10.83100000 4.61100000 L
H-H_ 0 7.79100000 10.53100000 3.98500000 L
C-C_R 0 6.11800000 11.62800000 4.20300000 L
H-H_ 0 6.02400000 11.84600000 3.30300000 L
C-C_3 0 6.53900000 10.47100000 8.34100000 L
C-C_3 0 5.54700000 11.17500000 9.25700000 L
H-H_ 0 5.68700000 10.88500000 10.16100000 L
H-H_ 0 5.67800000 12.12400000 9.20000000 L
H-H_ 0 4.65300000 10.95800000 8.98700000 L
C-C_3 0 7.96800000 10.73800000 8.87300000 L
H-H_ 0 8.60700000 10.28800000 8.31400000 L
H-H_ 0 8.14400000 11.68200000 8.86200000 L
H-H_ 0 8.04100000 10.40900000 9.77300000 L
C-C_R 0 6.25400000 8.98700000 8.35300000 L
C-C_R 0 5.03300000 8.31900000 8.42000000 L
H-H_ 0 4.19900000 8.71800000 8.51500000 L
C-C_R 0 5.27500000 6.97500000 8.32400000 L
H-H_ 0 4.63400000 6.30100000 8.34500000 L
C-C_R 0 6.64800000 6.79800000 8.19200000 L
C-C_R 0 7.43200000 5.63700000 8.06700000 L H-H_ 880
C-C_R 0 6.66600000 4.37000000 8.10100000 H
C-C_R 0 5.89800000 3.93100000 7.05700000 H
C-C_R 0 5.07600000 2.84900000 7.12300000 H
C-C_R 0 4.99300000 2.15400000 8.27200000 H
C-C_R 0 5.73100000 2.53200000 9.33700000 H
C-C_R 0 6.55800000 3.61200000 9.23200000 H
C-C_R 0 8.80700000 5.61800000 7.97800000 L
C-C_R 0 9.69400000 4.51500000 7.87100000 L
H-H_ 0 9.45500000 3.61800000 7.81100000 L
C-C_R 0 10.94000000 5.01000000 7.87300000 L
H-H_ 0 11.72800000 4.51900000 7.80500000 L
C-C_R 0 10.83800000 6.43500000 7.99700000 L
C-C_3 0 11.97600000 7.42700000 8.05200000 L
C-C_3 0 11.46700000 8.82500000 8.42100000 L
H-H_ 0 11.00900000 8.78600000 9.26400000 L
H-H_ 0 12.21100000 9.42800000 8.48700000 L
H-H_ 0 10.86300000 9.13500000 7.74100000 L
C-C_3 0 12.96700000 6.96500000 9.14800000 L
H-H_ 0 13.30300000 6.09200000 8.92900000 L
H-H_ 0 13.69900000 7.58600000 9.20000000 L
H-H_ 0 12.51600000 6.92900000 9.99300000 L
C-C_R 0 12.60700000 7.46900000 6.66200000 L
C-C_R 0 13.91600000 7.13600000 6.44400000 L
H-H_ 0 14.47100000 6.91600000 7.16000000 L
C-C_R 0 14.40000000 7.13300000 5.16200000 L
H-H_ 0 15.29700000 6.93700000 5.01900000 L
C-C_R 0 13.59200000 7.41300000 4.07400000 L
H-H_ 0 13.94200000 7.37300000 3.21400000 L

C-C_R 0 12.25100000 7.75400000 4.26400000 L
C-C_R 0 11.82000000 7.79400000 5.57600000 L
H-H_ 0 10.94300000 8.05400000 5.73700000 L
C-C_3 0 11.32200000 8.11300000 3.11800000 L
C-C_3 0 11.79800000 7.54700000 1.76500000 L
H-H_ 0 11.12800000 7.71100000 1.09800000 L
H-H_ 0 12.61800000 7.97600000 1.50900000 L
H-H_ 0 11.94300000 6.60200000 1.84700000 L
C-C_3 0 11.27000000 9.64600000 3.02700000 L
H-H_ 0 10.86500000 10.00100000 3.82300000 L
H-H_ 0 12.16100000 9.99200000 2.94000000 L
H-H_ 0 10.75000000 9.90400000 2.26100000 L
C-C_R 0 9.94100000 7.55600000 3.35000000 L
C-C_R 0 9.47000000 6.50500000 4.14300000 L
H-H_ 0 9.98700000 5.96400000 4.69500000 L
C-C_R 0 8.10900000 6.40900000 3.96500000 L
H-H_ 0 7.54400000 5.79800000 4.37900000 L
C-C_R 0 7.73100000 7.39000000 3.05300000 L
C-C_R 0 6.45900000 7.75700000 2.56800000 L H-H_ 927
C-C_R 0 5.31100000 6.98100000 3.10000000 H
C-C_R 0 4.93100000 5.78100000 2.57100000 H
C-C_R 0 3.87500000 5.06600000 3.05200000 H
C-C_R 0 3.15100000 5.55700000 4.10200000 H
C-C_R 0 3.50000000 6.73400000 4.65000000 H
C-C_R 0 4.55400000 7.41400000 4.15600000 H
C-C_R 0 6.21300000 8.78500000 1.68800000 L
C-C_R 0 4.97300000 9.29900000 1.20600000 L
H-H_ 0 4.12300000 8.99200000 1.42500000 L
C-C_R 0 5.26600000 10.31500000 0.37700000 L
H-H_ 0 4.66100000 10.85300000 -0.07800000 L
C-C_R 0 6.69400000 10.40900000 0.32900000 L
C-C_3 0 7.50200000 11.36600000 -0.53700000 L
C-C_3 0 8.99700000 11.08200000 -0.36900000 L
H-H_ 0 9.18600000 10.18600000 -0.66000000 L
H-H_ 0 9.50100000 11.70400000 -0.89700000 L
H-H_ 0 9.23800000 11.17500000 0.55600000 L
C-C_3 0 7.11100000 11.12300000 -2.00600000 L
H-H_ 0 6.15600000 11.16500000 -2.09600000 L
H-H_ 0 7.51300000 11.79800000 -2.56000000 L
H-H_ 0 7.42100000 10.25700000 -2.28300000 L
C-C_R 0 7.13900000 12.79500000 -0.10100000 L
C-C_R 0 7.75700000 13.40300000 0.99500000 L
H-H_ 0 8.43600000 12.95700000 1.44800000 L
C-C_R 0 7.37900000 14.63300000 1.40300000 L
H-H_ 0 7.82200000 15.03100000 2.11800000 L
C-C_R 0 6.35600000 15.31600000 0.78600000 L
H-H_ 0 6.10200000 16.15400000 1.09800000 L
C-C_R 0 5.70900000 14.76000000 -0.28600000 L
C-C_R 0 6.13000000 13.50500000 -0.71000000 L
H-H_ 0 5.70700000 13.12500000 -1.44500000 L
C-C_3 0 4.54300000 15.41500000 -1.01500000 L
C-C_3 0 4.06100000 16.69700000 -0.30200000 L
H-H_ 0 3.71400000 16.46900000 0.56400000 L
H-H_ 0 4.79600000 17.30500000 -0.20100000 L
H-H_ 0 3.37100000 17.11400000 -0.82200000 L
C-C_3 0 5.00000000 15.78600000 -2.44200000 L
H-H_ 0 4.29100000 16.25500000 -2.89000000 L
H-H_ 0 5.77500000 16.35000000 -2.39200000 L
H-H_ 0 5.21200000 14.98800000 -2.92900000 L
N-N_R 0 3.11700000 13.63500000 -0.01900000 L
N-N_R 0 3.00000000 12.58300000 2.46600000 L
N-N_R 0 7.20800000 8.06500000 8.21700000 L
N-N_R 0 9.56100000 6.79800000 8.04200000 L
N-N_R 0 8.88500000 8.06300000 2.69500000 L
N-N_R 0 7.25100000 9.52200000 1.11000000 L
F-F_ 0 -1.01000000 11.56800000 1.45200000 H
F-F_ 0 -2.71300000 9.68000000 0.63000000 H
F-F_ 0 -1.90000000 7.84000000 -1.18300000 H
F-F_ 0 0.61600000 7.92300000 -2.17600000 H
F-F_ 0 2.31900000 9.79300000 -1.31500000 H
F-F_ 0 5.91100000 4.62300000 5.89300000 H
F-F_ 0 4.31900000 2.48200000 6.07600000 H
F-F_ 0 4.19700000 1.08800000 8.38300000 H
F-F_ 0 5.64600000 1.85000000 10.49200000 H
F-F_ 0 7.27600000 3.96100000 10.31300000 H
F-F_ 0 5.60000000 5.27800000 1.52700000 H
F-F_ 0 3.53400000 3.88700000 2.49600000 H
F-F_ 0 2.11100000 4.86100000 4.57900000 H
F-F_ 0 2.79400000 7.21700000 5.69400000 H
F-F_ 0 4.87500000 8.57300000 4.74600000 H
H-H_ 0 8.06300000 8.10200000 8.16000000 L
H-H_ 0 3.51400000 13.63100000 0.75200000 L
H-H_ 0 8.81100000 8.73700000 2.16000000 L

1 2 2.0 133 1.0 142 1.5
2 3 1.0 4 2.0
3

4 5 1.0 6 1.5
5
6 7 1.5 142 1.5
7 8 1.0 14 2.0
8 9 2.0 13 2.0
9 10 2.0 148 1.0
10 11 2.0 149 1.0
11 12 2.0 150 1.0
12 13 2.0 151 1.0
13 152 1.0
14 15 1.5 143 1.0
15 16 1.0 17 2.0
16
17 18 1.0 19 1.5
18
19 20 1.0 143 2.0
20 21 1.0 25 1.0 29 1.0
21 22 1.0 23 1.0 24 1.0
22
23
24
25 26 1.0 27 1.0 28 1.0
26
27
28
29 30 2.0 37 2.0
30 31 1.0 32 2.0
31
32 33 2.0 39 1.0
33 34 1.0 35 2.0
34
35 36 1.0 37 2.0
36
37 38 1.0
38
39 40 1.0 44 1.0 48 1.0
40 41 1.0 42 1.0 43 1.0
41
42
43
44 45 1.0 46 1.0 47 1.0
45
46
47
48 49 1.5 144 1.5
49 50 1.0 51 2.0
50
51 52 1.0 53 1.5
52
53 54 1.5 144 1.0
54 55 1.0 61 2.0
55 56 2.0 60 2.0
56 57 2.0 153 1.0
57 58 2.0 154 1.0
58 59 2.0 155 1.0
59 60 2.0 156 1.0
60 157 1.0
61 62 1.5 145 1.0
62 63 1.0 64 2.0
63
64 65 1.0 66 1.5
65
66 67 1.0 145 1.5
67 68 1.0 72 1.0 76 1.0
68 69 1.0 70 1.0 71 1.0
69
70
71
72 73 1.0 74 1.0 75 1.0
73
74
75
76 77 2.0 84 2.0
77 78 1.0 79 2.0
78
79 80 1.0 81 2.0
80
81 82 1.0 83 1.5
82
83 84 2.0 86 1.0
84 85 1.0
85
86 87 1.0 91 1.0 95 1.0
87 88 1.0 89 1.0 90 1.0
88
89
90

91 92 1.0 93 1.0 94 1.0
92
93
94
95 96 1.5 146 1.5
96 97 1.0 98 2.0
97
98 99 1.0 100 1.5
99
100 101 1.5 146 1.0
101 102 1.0 108 2.0
102 103 2.0 107 2.0
103 104 2.0 158 1.0
104 105 2.0 159 1.0
105 106 2.0 160 1.0
106 107 2.0 161 1.0
107 162 1.0
108 109 1.5 147 1.0
109 110 1.0 111 2.0
110
111 112 1.0 113 1.5
112
113 114 1.0 147 2.0
114 115 1.0 119 1.0 123 1.0
115 116 1.0 117 1.0 118 1.0
116
117
118
119 120 1.0 121 1.0 122 1.0
120
121
122
123 124 1.5 131 2.0
124 125 1.0 126 2.0
125
126 127 1.0 128 2.0
127
128 129 1.0 130 2.0
129
130 131 1.5 133 1.0
131 132 1.0
132
133 134 1.0 138 1.0
134 135 1.0 136 1.0 137 1.0
135
136
137
138 139 1.0 140 1.0 141 1.0
139
140
141
142 164 1.0
143
144 163 1.0
145
146 165 1.0
147
148
149
150
151
152
153
154
155
156
157
158
159
160
161
162
163
164
165
166 167 2.0 298 1.0 307 1.5
167 168 1.0 169 2.0
168
169 170 1.0 171 1.5
170
171 172 1.5 307 1.5
172 173 1.0 179 2.0
173 174 2.0 178 2.0
174 175 2.0 313 1.0
175 176 2.0 314 1.0
176 177 2.0 315 1.0
177 178 2.0 316 1.0

178 317 1.0
179 180 1.5 308 1.0
180 181 1.0 182 2.0
181
182 183 1.0 184 1.5
183
184 185 1.0 308 2.0
185 186 1.0 190 1.0 194 1.0
186 187 1.0 188 1.0 189 1.0
187
188
189
190 191 1.0 192 1.0 193 1.0
191
192
193
194 195 2.0 202 2.0
195 196 1.0 197 2.0
196
197 198 2.0 204 1.0
198 199 1.0 200 2.0
199
200 201 1.0 202 2.0
201
202 203 1.0
203
204 205 1.0 209 1.0 213 1.0
205 206 1.0 207 1.0 208 1.0
206
207
208
209 210 1.0 211 1.0 212 1.0
210
211
212
213 214 1.5 309 1.5
214 215 1.0 216 2.0
215
216 217 1.0 218 1.5
217
218 219 1.5 309 1.0
219 220 1.0 226 2.0
220 221 2.0 225 2.0
221 222 2.0 318 1.0
222 223 2.0 319 1.0
223 224 2.0 320 1.0
224 225 2.0 321 1.0
225 322 1.0
226 227 1.5 310 1.0
227 228 1.0 229 2.0
228
229 230 1.0 231 1.5
230
231 232 1.0 310 1.5
232 233 1.0 237 1.0 241 1.0
233 234 1.0 235 1.0 236 1.0
234
235
236
237 238 1.0 239 1.0 240 1.0
238
239
240
241 242 2.0 249 2.0
242 243 1.0 244 2.0
243
244 245 1.0 246 2.0
245
246 247 1.0 248 1.5
247
248 249 2.0 251 1.0
249 250 1.0
250
251 252 1.0 256 1.0 260 1.0
252 253 1.0 254 1.0 255 1.0
253
254
255
256 257 1.0 258 1.0 259 1.0
257
258
259
260 261 1.5 311 1.5
261 262 1.0 263 2.0
262
263 264 1.0 265 1.5
264

265 266 1.5 311 1.0
266 267 1.0 273 2.0
267 268 2.0 272 2.0
268 269 2.0 323 1.0
269 270 2.0 324 1.0
270 271 2.0 325 1.0
271 272 2.0 326 1.0
272 327 1.0
273 274 1.5 312 1.0
274 275 1.0 276 2.0
275
276 277 1.0 278 1.5
277
278 279 1.0 312 2.0
279 280 1.0 284 1.0 288 1.0
280 281 1.0 282 1.0 283 1.0
281
282
283
284 285 1.0 286 1.0 287 1.0
285
286
287
288 289 1.5 296 2.0
289 290 1.0 291 2.0
290
291 292 1.0 293 2.0
292
293 294 1.0 295 2.0
294
295 296 1.5 298 1.0
296 297 1.0
297
298 299 1.0 303 1.0
299 300 1.0 301 1.0 302 1.0
300
301
302
303 304 1.0 305 1.0 306 1.0
304
305
306
307 329 1.0
308
309 328 1.0
310
311 330 1.0
312
313
314
315
316
317
318
319
320
321
322
323
324
325
326
327
328
329
330
331 332 2.0 463 1.0 472 1.5
332 333 1.0 334 2.0
333
334 335 1.0 336 1.5
335
336 337 1.5 472 1.5
337 338 1.0 344 2.0
338 339 2.0 343 2.0
339 340 2.0 478 1.0
340 341 2.0 479 1.0
341 342 2.0 480 1.0
342 343 2.0 481 1.0
343 482 1.0
344 345 1.5 473 1.0
345 346 1.0 347 2.0
346
347 348 1.0 349 1.5
348
349 350 1.0 473 2.0
350 351 1.0 355 1.0 359 1.0
351 352 1.0 353 1.0 354 1.0

352
353
354
355 356 1.0 357 1.0 358 1.0
356
357
358
359 360 2.0 367 2.0
360 361 1.0 362 2.0
361
362 363 2.0 369 1.0
363 364 1.0 365 2.0
364
365 366 1.0 367 2.0
366
367 368 1.0
368
369 370 1.0 374 1.0 378 1.0
370 371 1.0 372 1.0 373 1.0
371
372
373
374 375 1.0 376 1.0 377 1.0
375
376
377
378 379 1.5 474 1.5
379 380 1.0 381 2.0
380
381 382 1.0 383 1.5
382
383 384 1.5 474 1.0
384 385 1.0 391 2.0
385 386 2.0 390 2.0
386 387 2.0 483 1.0
387 388 2.0 484 1.0
388 389 2.0 485 1.0
389 390 2.0 486 1.0
390 487 1.0
391 392 1.5 475 1.0
392 393 1.0 394 2.0
393
394 395 1.0 396 1.5
395
396 397 1.0 475 1.5
397 398 1.0 402 1.0 406 1.0
398 399 1.0 400 1.0 401 1.0
399
400
401
402 403 1.0 404 1.0 405 1.0
403
404
405
406 407 2.0 414 2.0
407 408 1.0 409 2.0
408
409 410 1.0 411 2.0
410
411 412 1.0 413 1.5
412
413 414 2.0 416 1.0
414 415 1.0
415
416 417 1.0 421 1.0 425 1.0
417 418 1.0 419 1.0 420 1.0
418
419
420
421 422 1.0 423 1.0 424 1.0
422
423
424
425 426 1.5 476 1.5
426 427 1.0 428 2.0
427
428 429 1.0 430 1.5
429
430 431 1.5 476 1.0
431 432 1.0 438 2.0
432 433 2.0 437 2.0
433 434 2.0 488 1.0
434 435 2.0 489 1.0
435 436 2.0 490 1.0
436 437 2.0 491 1.0
437 492 1.0
438 439 1.5 477 1.0

439 440 1.0 441 2.0
440
441 442 1.0 443 1.5
442
443 444 1.0 477 2.0
444 445 1.0 449 1.0 453 1.0
445 446 1.0 447 1.0 448 1.0
446
447
448
449 450 1.0 451 1.0 452 1.0
450
451
452
453 454 1.5 461 2.0
454 455 1.0 456 2.0
455
456 457 1.0 458 2.0
457
458 459 1.0 460 2.0
459
460 461 1.5 463 1.0
461 462 1.0
462
463 464 1.0 468 1.0
464 465 1.0 466 1.0 467 1.0
465
466
467
468 469 1.0 470 1.0 471 1.0
469
470
471
472 494 1.0
473
474 493 1.0
475
476 495 1.0
477
478
479
480
481
482
483
484
485
486
487
488
489
490
491
492
493
494
495
496 497 2.0 628 1.0 637 1.5
497 498 1.0 499 2.0
498
499 500 1.0 501 1.5
500
501 502 1.5 637 1.5
502 503 1.0 509 2.0
503 504 2.0 508 2.0
504 505 2.0 643 1.0
505 506 2.0 644 1.0
506 507 2.0 645 1.0
507 508 2.0 646 1.0
508 647 1.0
509 510 1.5 638 1.0
510 511 1.0 512 2.0
511
512 513 1.0 514 1.5
513
514 515 1.0 638 2.0
515 516 1.0 520 1.0 524 1.0
516 517 1.0 518 1.0 519 1.0
517
518
519
520 521 1.0 522 1.0 523 1.0
521
522
523
524 525 2.0 532 2.0
525 526 1.0 527 2.0

526
527 528 2.0 534 1.0
528 529 1.0 530 2.0
529
530 531 1.0 532 2.0
531
532 533 1.0
533
534 535 1.0 539 1.0 543 1.0
535 536 1.0 537 1.0 538 1.0
536
537
538
539 540 1.0 541 1.0 542 1.0
540
541
542
543 544 1.5 639 1.5
544 545 1.0 546 2.0
545
546 547 1.0 548 1.5
547
548 549 1.5 639 1.0
549 550 1.0 556 2.0
550 551 2.0 555 2.0
551 552 2.0 648 1.0
552 553 2.0 649 1.0
553 554 2.0 650 1.0
554 555 2.0 651 1.0
555 652 1.0
556 557 1.5 640 1.0
557 558 1.0 559 2.0
558
559 560 1.0 561 1.5
560
561 562 1.0 640 1.5
562 563 1.0 567 1.0 571 1.0
563 564 1.0 565 1.0 566 1.0
564
565
566
567 568 1.0 569 1.0 570 1.0
568
569
570
571 572 2.0 579 2.0
572 573 1.0 574 2.0
573
574 575 1.0 576 2.0
575
576 577 1.0 578 1.5
577
578 579 2.0 581 1.0
579 580 1.0
580
581 582 1.0 586 1.0 590 1.0
582 583 1.0 584 1.0 585 1.0
583
584
585
586 587 1.0 588 1.0 589 1.0
587
588
589
590 591 1.5 641 1.5
591 592 1.0 593 2.0
592
593 594 1.0 595 1.5
594
595 596 1.5 641 1.0
596 597 1.0 603 2.0
597 598 2.0 602 2.0
598 599 2.0 653 1.0
599 600 2.0 654 1.0
600 601 2.0 655 1.0
601 602 2.0 656 1.0
602 657 1.0
603 604 1.5 642 1.0
604 605 1.0 606 2.0
605
606 607 1.0 608 1.5
607
608 609 1.0 642 2.0
609 610 1.0 614 1.0 618 1.0
610 611 1.0 612 1.0 613 1.0
611
612

613
614 615 1.0 616 1.0 617 1.0
615
616
617
618 619 1.5 626 2.0
619 620 1.0 621 2.0
620
621 622 1.0 623 2.0
622
623 624 1.0 625 2.0
624
625 626 1.5 628 1.0
626 627 1.0
627
628 629 1.0 633 1.0
629 630 1.0 631 1.0 632 1.0
630
631
632
633 634 1.0 635 1.0 636 1.0
634
635
636
637 659 1.0
638
639 658 1.0
640
641 660 1.0
642
643
644
645
646
647
648
649
650
651
652
653
654
655
656
657
658
659
660
661 662 2.0 793 1.0 802 1.5
662 663 1.0 664 2.0
663
664 665 1.0 666 1.5
665
666 667 1.5 802 1.5
667 668 1.0 674 2.0
668 669 2.0 673 2.0
669 670 2.0 808 1.0
670 671 2.0 809 1.0
671 672 2.0 810 1.0
672 673 2.0 811 1.0
673 812 1.0
674 675 1.5 803 1.0
675 676 1.0 677 2.0
676
677 678 1.0 679 1.5
678
679 680 1.0 803 2.0
680 681 1.0 685 1.0 689 1.0
681 682 1.0 683 1.0 684 1.0
682
683
684
685 686 1.0 687 1.0 688 1.0
686
687
688
689 690 2.0 697 2.0
690 691 1.0 692 2.0
691
692 693 2.0 699 1.0
693 694 1.0 695 2.0
694
695 696 1.0 697 2.0
696
697 698 1.0
698
699 700 1.0 704 1.0 708 1.0

700 701 1.0 702 1.0 703 1.0
701
702
703
704 705 1.0 706 1.0 707 1.0
705
706
707
708 709 1.5 804 1.5
709 710 1.0 711 2.0
710
711 712 1.0 713 1.5
712
713 714 1.5 804 1.0
714 715 1.0 721 2.0
715 716 2.0 720 2.0
716 717 2.0 813 1.0
717 718 2.0 814 1.0
718 719 2.0 815 1.0
719 720 2.0 816 1.0
720 817 1.0
721 722 1.5 805 1.0
722 723 1.0 724 2.0
723
724 725 1.0 726 1.5
725
726 727 1.0 805 1.5
727 728 1.0 732 1.0 736 1.0
728 729 1.0 730 1.0 731 1.0
729
730
731
732 733 1.0 734 1.0 735 1.0
733
734
735
736 737 2.0 744 2.0
737 738 1.0 739 2.0
738
739 740 1.0 741 2.0
740
741 742 1.0 743 1.5
742
743 744 2.0 746 1.0
744 745 1.0
745
746 747 1.0 751 1.0 755 1.0
747 748 1.0 749 1.0 750 1.0
748
749
750
751 752 1.0 753 1.0 754 1.0
752
753
754
755 756 1.5 806 1.5
756 757 1.0 758 2.0
757
758 759 1.0 760 1.5
759
760 761 1.5 806 1.0
761 762 1.0 768 2.0
762 763 2.0 767 2.0
763 764 2.0 818 1.0
764 765 2.0 819 1.0
765 766 2.0 820 1.0
766 767 2.0 821 1.0
767 822 1.0
768 769 1.5 807 1.0
769 770 1.0 771 2.0
770
771 772 1.0 773 1.5
772
773 774 1.0 807 2.0
774 775 1.0 779 1.0 783 1.0
775 776 1.0 777 1.0 778 1.0
776
777
778
779 780 1.0 781 1.0 782 1.0
780
781
782
783 784 1.5 791 2.0
784 785 1.0 786 2.0
785
786 787 1.0 788 2.0

787
788 789 1.0 790 2.0
789
790 791 1.5 793 1.0
791 792 1.0
792
793 794 1.0 798 1.0
794 795 1.0 796 1.0 797 1.0
795
796
797
798 799 1.0 800 1.0 801 1.0
799
800
801
802 824 1.0
803
804 823 1.0
805
806 825 1.0
807
808
809
810
811
812
813
814
815
816
817
818
819
820
821
822
823
824
825
826 827 2.0 958 1.0 967 1.5
827 828 1.0 829 2.0
828
829 830 1.0 831 1.5
830
831 832 1.5 967 1.5
832 833 1.0 839 2.0
833 834 2.0 838 2.0
834 835 2.0 973 1.0
835 836 2.0 974 1.0
836 837 2.0 975 1.0
837 838 2.0 976 1.0
838 977 1.0
839 840 1.5 968 1.0
840 841 1.0 842 2.0
841
842 843 1.0 844 1.5
843
844 845 1.0 968 2.0
845 846 1.0 850 1.0 854 1.0
846 847 1.0 848 1.0 849 1.0
847
848
849
850 851 1.0 852 1.0 853 1.0
851
852
853
854 855 2.0 862 2.0
855 856 1.0 857 2.0
856
857 858 2.0 864 1.0
858 859 1.0 860 2.0
859
860 861 1.0 862 2.0
861
862 863 1.0
863
864 865 1.0 869 1.0 873 1.0
865 866 1.0 867 1.0 868 1.0
866
867
868
869 870 1.0 871 1.0 872 1.0
870
871
872
873 874 1.5 969 1.5

874 875 1.0 876 2.0
875
876 877 1.0 878 1.5
877
878 879 1.5 969 1.0
879 880 1.0 886 2.0
880 881 2.0 885 2.0
881 882 2.0 978 1.0
882 883 2.0 979 1.0
883 884 2.0 980 1.0
884 885 2.0 981 1.0
885 982 1.0
886 887 1.5 970 1.0
887 888 1.0 889 2.0
888
889 890 1.0 891 1.5
890
891 892 1.0 970 1.5
892 893 1.0 897 1.0 901 1.0
893 894 1.0 895 1.0 896 1.0
894
895
896
897 898 1.0 899 1.0 900 1.0
898
899
900
901 902 2.0 909 2.0
902 903 1.0 904 2.0
903
904 905 1.0 906 2.0
905
906 907 1.0 908 1.5
907
908 909 2.0 911 1.0
909 910 1.0
910
911 912 1.0 916 1.0 920 1.0
912 913 1.0 914 1.0 915 1.0
913
914
915
916 917 1.0 918 1.0 919 1.0
917
918
919
920 921 1.5 971 1.5
921 922 1.0 923 2.0
922
923 924 1.0 925 1.5
924
925 926 1.5 971 1.0
926 927 1.0 933 2.0
927 928 2.0 932 2.0
928 929 2.0 983 1.0
929 930 2.0 984 1.0
930 931 2.0 985 1.0
931 932 2.0 986 1.0
932 987 1.0
933 934 1.5 972 1.0
934 935 1.0 936 2.0
935
936 937 1.0 938 1.5
937
938 939 1.0 972 2.0
939 940 1.0 944 1.0 948 1.0
940 941 1.0 942 1.0 943 1.0
941
942
943
944 945 1.0 946 1.0 947 1.0
945
946
947
948 949 1.5 956 2.0
949 950 1.0 951 2.0
950
951 952 1.0 953 2.0
952
953 954 1.0 955 2.0
954
955 956 1.5 958 1.0
956 957 1.0
957
958 959 1.0 963 1.0
959 960 1.0 961 1.0 962 1.0
960

961
962
963 964 1.0 965 1.0 966 1.0
964
965
966
967 989 1.0
968
969 988 1.0
970
971 990 1.0
972
973
974
975
976
977
978
979
980
981
982
983
984
985
986
987
988
989
990

QM/MM ONIOM optimized geometry (PM6/UFF level) of M-II cluster containing six molecules (total 990 atoms).

C	-2.487017000	-13.234303000	4.898542000
C	-1.314083000	-13.216515000	4.265811000
H	-0.397648000	-13.691153000	4.589135000
C	-1.441700000	-12.474753000	3.172091000
H	-0.648461000	-12.253842000	2.469552000
C	-2.750958000	-12.015522000	3.134507000
C	-3.275245000	-11.078937000	2.204560000
C	-2.323787000	-10.390716000	1.282675000
C	-2.393766000	-10.560177000	-0.109044000
C	-1.538361000	-9.877148000	-0.991579000
C	-0.564139000	-9.011057000	-0.478219000
C	-0.447789000	-8.847967000	0.909100000
C	-1.328507000	-9.526576000	1.767639000
C	-4.591769000	-10.752956000	2.145516000
C	-5.167834000	-9.732285000	1.401888000
H	-4.667966000	-9.031077000	0.746244000
C	-6.466970000	-9.730338000	1.677717000
H	-7.191916000	-9.035799000	1.275702000
C	-6.724180000	-10.758012000	2.576725000
C	-8.080727000	-11.082348000	3.189091000
C	-9.047333000	-11.423073000	2.027952000
H	-10.045222000	-11.721037000	2.416680000
H	-8.651322000	-12.272620000	1.429596000
H	-9.171386000	-10.561026000	1.337895000
C	-7.992822000	-12.340583000	4.089811000
H	-7.242499000	-12.219407000	4.899540000
H	-7.698291000	-13.232005000	3.494183000
H	-8.977784000	-12.546725000	4.561834000
C	-8.527212000	-9.880224000	4.052039000
C	-9.679126000	-9.182037000	3.817056000
H	-10.322074000	-9.489567000	3.015379000
C	-10.011622000	-8.080578000	4.558076000
C	-9.155686000	-7.693737000	5.546115000
H	-9.332344000	-6.800866000	6.128529000
C	-8.046769000	-8.402396000	5.817524000
H	-7.393846000	-8.094089000	6.621904000
C	-7.727512000	-9.474765000	5.075781000
H	-6.802853000	-9.993274000	5.298083000
C	-11.269501000	-7.227643000	4.258658000
C	-12.296659000	-7.940765000	3.336367000
H	-13.209049000	-7.317523000	3.211374000
H	-12.603343000	-8.916014000	3.773133000
H	-11.899905000	-8.120427000	2.316042000
C	-12.039155000	-6.928464000	5.575280000
H	-11.444441000	-6.356767000	6.313611000
H	-12.349160000	-7.878684000	6.061727000
H	-12.953424000	-6.330321000	5.368873000
C	-10.816053000	-5.947172000	3.560357000
C	-10.291725000	-5.893645000	2.276008000
H	-10.135942000	-6.733064000	1.611461000
C	-9.986344000	-4.637609000	1.990296000
H	-9.551414000	-4.307488000	1.056717000
C	-10.292354000	-3.852883000	3.092066000
C	-10.048252000	-2.458882000	3.191134000
C	-9.397510000	-1.768356000	2.037983000

C	-8.048464000	-1.974156000	1.720181000
C	-7.415036000	-1.306444000	0.660695000
C	-8.148876000	-0.416093000	-0.134626000
C	-9.501946000	-0.190285000	0.154353000
C	-10.105929000	-0.864962000	1.229495000
C	-10.367140000	-1.724257000	4.282992000
C	-9.983099000	-0.412955000	4.535114000
H	-9.378746000	0.222977000	3.900610000
C	-10.433044000	-0.076272000	5.738452000
H	-10.247618000	0.871248000	6.225979000
C	-11.144897000	-1.148373000	6.261452000
C	-11.740667000	-1.231193000	7.659054000
C	-12.723051000	-2.425794000	7.758243000
H	-13.573877000	-2.293100000	7.054914000
H	-13.131118000	-2.504730000	8.789156000
H	-12.238371000	-3.392687000	7.509246000
C	-12.574472000	0.050751000	7.912948000
H	-11.945209000	0.964525000	7.873539000
H	-13.072894000	0.006952000	8.905637000
H	-13.366145000	0.159090000	7.139642000
C	-10.582373000	-1.438673000	8.659436000
C	-10.304215000	-0.552460000	9.657318000
H	-10.901549000	0.332763000	9.815763000
C	-9.261852000	-0.741150000	10.487767000
H	-9.061276000	-0.018751000	11.269706000
C	-8.465988000	-1.814473000	10.355282000
H	-7.642559000	-1.918351000	11.046184000
C	-8.723313000	-2.766956000	9.339178000
C	-9.787819000	-2.539378000	8.525073000
H	-9.990651000	-3.244395000	7.729624000
C	-7.874089000	-4.046522000	9.148686000
C	-6.694137000	-4.133164000	10.144545000
H	-6.105939000	-5.063377000	9.987128000
H	-7.060292000	-4.151327000	11.193759000
H	-6.003051000	-3.273122000	10.008637000
C	-8.789509000	-5.270677000	9.391222000
H	-9.549487000	-5.372180000	8.587236000
H	-9.319110000	-5.170903000	10.363557000
H	-8.207699000	-6.216413000	9.422365000
C	-7.282228000	-4.130903000	7.741187000
C	-7.294655000	-3.141642000	6.762568000
H	-7.700293000	-2.142977000	6.851933000
C	-6.723147000	-3.620475000	5.666892000
H	-6.594670000	-3.067722000	4.749672000
C	-6.298539000	-4.912654000	5.927388000
C	-5.690998000	-5.787570000	5.000283000
C	-5.730835000	-5.440726000	3.553539000
C	-4.811535000	-4.539769000	2.998244000
C	-4.764667000	-4.276218000	1.619186000
C	-5.667511000	-4.921696000	0.761979000
C	-6.609290000	-5.814055000	1.290617000
C	-6.625276000	-6.063745000	2.672277000
C	-5.036890000	-6.908583000	5.378616000
C	-4.461945000	-7.851906000	4.542575000
H	-4.491607000	-7.878591000	3.463737000
C	-3.852011000	-8.738964000	5.313712000
H	-3.305258000	-9.602907000	4.961198000
C	-4.028298000	-8.359533000	6.639187000
C	-3.455070000	-9.095741000	7.837081000
C	-3.916543000	-8.441174000	9.166669000
H	-3.477406000	-7.426644000	9.285112000
H	-3.598324000	-9.060420000	10.033008000
H	-5.016999000	-8.309051000	9.209166000
C	-1.911154000	-8.954415000	7.787914000
H	-1.497352000	-9.243973000	6.798620000
H	-1.437303000	-9.577902000	8.576698000
H	-1.606378000	-7.897839000	7.952139000
C	-3.932502000	-10.563445000	7.765662000
C	-5.263951000	-10.898648000	8.108612000
H	-5.954949000	-10.150645000	8.468733000
C	-5.714405000	-12.157001000	7.972215000
H	-6.735372000	-12.389235000	8.250013000
C	-4.933807000	-13.122633000	7.454809000
H	-5.376603000	-14.100239000	7.335307000
C	-3.662335000	-12.859424000	7.051206000
C	-3.155705000	-11.550639000	7.250175000
H	-2.156379000	-11.342031000	6.903926000
C	-2.804948000	-13.867096000	6.253135000
C	-3.524824000	-15.204354000	5.966081000
H	-4.459732000	-15.036894000	5.387947000
H	-3.768361000	-15.735174000	6.911722000
H	-2.874222000	-15.873422000	5.361438000
C	-1.525729000	-14.181714000	7.063525000
H	-0.921512000	-14.970868000	6.566185000
H	-1.794370000	-14.546944000	8.078382000
H	-0.885386000	-13.281734000	7.176911000
N	-3.396898000	-12.521378000	4.205345000

N	-5.635702000	-11.386606000	2.867068000
N	-10.826065000	-4.711803000	4.103971000
N	-11.116437000	-2.177439000	5.397404000
N	-6.652098000	-5.227141000	7.271318000
N	-4.724870000	-7.274050000	6.714871000
F	-3.292229000	-11.388604000	-0.630400000
F	-1.653157000	-10.049091000	-2.303429000
F	0.237235000	-8.339905000	-1.295350000
F	0.491899000	-8.049611000	1.405072000
F	-1.208480000	-9.315497000	3.073793000
F	-7.326907000	-2.828919000	2.434491000
F	-6.127441000	-1.513402000	0.413004000
F	-7.558704000	0.199990000	-1.147774000
F	-10.209356000	0.658653000	-0.582461000
F	-11.391563000	-0.631922000	1.470071000
F	-3.947963000	-3.926637000	3.797296000
F	-3.865197000	-3.433489000	1.123124000
F	-5.629136000	-4.703938000	-0.542564000
F	-7.471503000	-6.425123000	0.485632000
F	-7.512432000	-6.932671000	3.135057000
H	-11.083861000	-4.489611000	5.085424000
H	-4.358789000	-12.321615000	4.546241000
H	-6.567831000	-6.136756000	7.771296000
C	-14.401397000	-4.671910000	-6.327733000
C	-15.445191000	-3.866277000	-6.518945000
H	-16.324742000	-4.075664000	-7.112453000
C	-15.211254000	-2.724844000	-5.884076000
H	-15.870477000	-1.866692000	-5.882599000
C	-13.959538000	-2.828536000	-5.291843000
C	-13.272068000	-1.775931000	-4.628097000
C	-13.963728000	-0.462994000	-4.493583000
C	-14.455581000	-0.022644000	-3.255420000
C	-15.092980000	1.220400000	-3.105792000
C	-15.251431000	2.057423000	-4.219633000
C	-14.773023000	1.640432000	-5.470020000
C	-14.139051000	0.392577000	-5.591566000
C	-12.006293000	-1.886472000	-4.150338000
C	-11.234062000	-0.876896000	-3.591414000
H	-11.513972000	0.156764000	-3.433596000
C	-10.049206000	-1.402513000	-3.302552000
H	-9.216091000	-0.870463000	-2.867945000
C	-10.065377000	-2.741328000	-3.667425000
C	-8.917503000	-3.724234000	-3.491251000
C	-8.689472000	-3.891394000	-1.970073000
H	-7.908367000	-4.654094000	-1.768852000
H	-9.624140000	-4.229768000	-1.471998000
H	-8.393407000	-2.931572000	-1.500316000
C	-9.298845000	-5.120746000	-4.046444000
H	-9.595777000	-5.072151000	-5.115314000
H	-10.155633000	-5.551046000	-3.483275000
H	-8.438981000	-5.819584000	-3.958062000
C	-7.685240000	-3.201212000	-4.264784000
C	-6.486713000	-2.933314000	-3.664146000
H	-6.393092000	-3.087429000	-2.608153000
C	-5.414170000	-2.464789000	-4.376814000
C	-5.582581000	-2.257759000	-5.713245000
H	-4.788547000	-1.867340000	-6.330673000
C	-6.750052000	-2.537876000	-6.316227000
H	-6.853193000	-2.390896000	-7.380998000
C	-7.791787000	-2.995186000	-5.604141000
H	-8.722724000	-3.188410000	-6.122460000
C	-4.053696000	-2.132817000	-3.707659000
C	-3.910195000	-2.756058000	-2.292838000
H	-2.908074000	-2.544958000	-1.875698000
H	-4.025000000	-3.859966000	-2.344076000
H	-4.644877000	-2.357492000	-1.568049000
C	-2.875772000	-2.733419000	-4.521929000
H	-2.797004000	-2.336724000	-5.551801000
H	-2.979783000	-3.837654000	-4.596603000
H	-1.908561000	-2.505921000	-4.023182000
C	-3.902883000	-0.612998000	-3.629214000
C	-4.224299000	0.194800000	-2.540080000
H	-4.574987000	-0.125614000	-1.570108000
C	-4.057892000	1.463596000	-2.885019000
H	-4.228846000	2.313662000	-2.241580000
C	-3.624974000	1.500483000	-4.196653000
C	-3.402846000	2.667709000	-4.957890000
C	-3.993139000	3.952009000	-4.479980000
C	-5.382753000	4.112168000	-4.367250000
C	-5.968658000	5.301500000	-3.906617000
C	-5.150677000	6.383054000	-3.551133000
C	-3.758984000	6.257212000	-3.659799000
C	-3.200323000	5.051027000	-4.116919000
C	-2.679443000	2.646405000	-6.099038000
C	-2.501413000	3.692869000	-6.993114000
H	-2.952495000	4.675561000	-6.946284000
C	-1.684890000	3.274890000	-7.953553000

H	-1.378987000	3.861435000	-8.809696000
C	-1.310816000	1.965440000	-7.679675000
C	-0.445311000	1.087151000	-8.567722000
C	-0.137243000	-0.266620000	-7.878787000
H	0.478265000	-0.111844000	-6.968487000
H	0.428989000	-0.930648000	-8.567138000
H	-1.059496000	-0.799820000	-7.567293000
C	0.911735000	1.805371000	-8.773989000
H	0.780558000	2.792816000	-9.265294000
H	1.596200000	1.185105000	-9.392349000
H	1.408225000	1.986115000	-7.795172000
C	-1.230054000	0.830173000	-9.870103000
C	-0.781213000	1.234511000	-11.091681000
H	0.174279000	1.722156000	-11.214366000
C	-1.521680000	1.053749000	-12.200564000
H	-1.144058000	1.389880000	-13.158658000
C	-2.727006000	0.466255000	-12.130468000
H	-3.281445000	0.348320000	-13.049499000
C	-3.227125000	0.018127000	-10.882542000
C	-2.444417000	0.214945000	-9.790155000
H	-2.814267000	-0.101415000	-8.823275000
C	-4.580528000	-0.715325000	-10.731661000
C	-5.343416000	-0.830594000	-12.072965000
H	-6.306871000	-1.369121000	-11.943742000
H	-4.751368000	-1.403210000	-12.819150000
H	-5.575106000	0.177988000	-12.478862000
C	-4.293335000	-2.149775000	-10.226610000
H	-3.909883000	-2.140814000	-9.183863000
H	-3.536602000	-2.643967000	-10.873939000
H	-5.208815000	-2.778831000	-10.240304000
C	-5.512235000	-0.014585000	-9.739135000
C	-5.324699000	1.217451000	-9.119136000
H	-4.488706000	1.890750000	-9.250869000
C	-6.357561000	1.453949000	-8.318958000
H	-6.475189000	2.338295000	-7.705690000
C	-7.245082000	0.393082000	-8.426563000
C	-8.477069000	0.278103000	-7.736163000
C	-8.840125000	1.338467000	-6.758485000
C	-9.592136000	2.455861000	-7.150530000
C	-10.049840000	3.406755000	-6.223678000
C	-9.756198000	3.243023000	-4.862377000
C	-8.987282000	2.146315000	-4.447689000
C	-8.528593000	1.217040000	-5.396994000
C	-9.363064000	-0.726387000	-7.942393000
C	-10.586444000	-0.891248000	-7.311732000
H	-11.016591000	-0.265748000	-6.540819000
C	-11.164130000	-1.960055000	-7.844251000
H	-12.140415000	-2.334293000	-7.573558000
C	-10.309349000	-2.485515000	-8.807254000
C	-10.595122000	-3.689146000	-9.696712000
C	-9.334663000	-4.041226000	-10.535371000
H	-9.108225000	-3.242424000	-11.275032000
H	-9.488647000	-4.991306000	-11.091333000
H	-8.430196000	-4.135173000	-9.897896000
C	-11.698725000	-3.295286000	-10.712378000
H	-12.572633000	-2.820623000	-10.219944000
H	-12.043431000	-4.188203000	-11.277381000
H	-11.319177000	-2.547063000	-11.441789000
C	-11.033032000	-4.885003000	-8.814351000
C	-10.102016000	-5.843019000	-8.342071000
H	-9.056002000	-5.794765000	-8.602859000
C	-10.493370000	-6.845225000	-7.536336000
H	-9.762613000	-7.567797000	-7.193587000
C	-11.769772000	-6.951045000	-7.125231000
H	-12.005966000	-7.766920000	-6.458368000
C	-12.710069000	-6.048701000	-7.510048000
C	-12.317284000	-5.010818000	-8.391429000
H	-13.061372000	-4.284793000	-8.678695000
C	-14.152546000	-6.041300000	-6.956330000
C	-14.399746000	-7.095307000	-5.853142000
H	-13.697594000	-6.953143000	-5.002913000
H	-14.284820000	-8.125704000	-6.253525000
H	-15.433711000	-7.003663000	-5.454343000
C	-15.126685000	-6.333089000	-8.120764000
H	-16.174141000	-6.404238000	-7.755980000
H	-14.867256000	-7.299038000	-8.605742000
H	-15.082635000	-5.536067000	-8.893096000
N	-13.486946000	-4.067402000	-5.545746000
N	-11.208423000	-3.057041000	-4.172585000
N	-3.530210000	0.160901000	-4.670714000
N	-1.914445000	1.543101000	-6.557088000
N	-6.689425000	-0.542339000	-9.348852000
N	-9.235578000	-1.771794000	-8.891260000
F	-14.326295000	-0.794486000	-2.181462000
F	-15.543757000	1.602551000	-1.916063000
F	-15.850095000	3.233109000	-4.091857000
F	-14.918700000	2.422634000	-6.533837000

F	-13.702036000	0.029808000	-6.792774000
F	-6.188234000	3.118612000	-4.727594000
F	-7.289480000	5.405672000	-3.811807000
F	-5.691911000	7.513935000	-3.122631000
F	-2.972025000	7.275406000	-3.330645000
F	-1.877265000	4.971968000	-4.200437000
F	-9.898536000	2.626863000	-8.432125000
F	-10.765862000	4.449003000	-6.630613000
F	-10.207491000	4.115808000	-3.972522000
F	-8.700075000	1.992002000	-3.160801000
F	-7.786102000	0.199355000	-4.976616000
H	-3.386373000	-0.156385000	-5.651897000
H	-12.585206000	-4.507493000	-5.276946000
H	-7.049904000	-1.468976000	-9.652663000
C	-0.694783000	0.562059000	2.213010000
C	0.525039000	0.619453000	1.680514000
H	1.371423000	-0.003369000	1.932574000
C	0.549482000	1.617543000	0.808010000
H	1.415176000	1.933555000	0.245165000
C	-0.710497000	2.194211000	0.803284000
C	-1.068725000	3.399535000	0.149002000
C	0.025498000	4.287111000	-0.340272000
C	0.173807000	4.604518000	-1.698321000
C	1.181570000	5.468989000	-2.161201000
C	2.068089000	6.045776000	-1.242713000
C	1.953564000	5.740671000	0.120326000
C	0.943965000	4.866423000	0.551684000
C	-2.355508000	3.810664000	0.029784000
C	-2.806074000	5.044597000	-0.416783000
H	-2.209260000	5.878267000	-0.762545000
C	-4.128643000	5.049936000	-0.286452000
H	-4.777990000	5.884787000	-0.514504000
C	-4.520990000	3.818651000	0.224633000
C	-5.939831000	3.427277000	0.613431000
C	-6.805804000	3.454435000	-0.670247000
H	-7.844257000	3.120332000	-0.456597000
H	-6.393150000	2.768016000	-1.438483000
H	-6.835231000	4.473094000	-1.112473000
C	-5.975839000	1.980522000	1.163877000
H	-5.311203000	1.855822000	2.044840000
H	-5.636952000	1.259361000	0.389914000
H	-7.008243000	1.711960000	1.475023000
C	-6.424999000	4.387205000	1.722090000
C	-7.549610000	5.153513000	1.600138000
H	-8.141103000	5.076707000	0.708440000
C	-7.922768000	6.033188000	2.577954000
C	-7.136812000	6.129638000	3.686965000
H	-7.355723000	6.842823000	4.470055000
C	-6.055036000	5.347378000	3.837388000
H	-5.460500000	5.418310000	4.737090000
C	-5.695250000	4.492807000	2.866426000
H	-4.796601000	3.904765000	3.008803000
C	-9.156960000	6.955584000	2.441229000
C	-10.074918000	6.600758000	1.240365000
H	-10.965455000	7.266363000	1.220400000
H	-10.433549000	5.551158000	1.316678000
H	-9.560152000	6.730333000	0.265391000
C	-10.048919000	6.826046000	3.705537000
H	-9.527357000	7.125191000	4.636334000
H	-10.382613000	5.773304000	3.832489000
H	-10.953037000	7.467175000	3.617614000
C	-8.654067000	8.381456000	2.237872000
C	-7.957832000	8.815551000	1.119068000
H	-7.678879000	8.212627000	0.264804000
C	-7.677412000	10.101023000	1.263351000
H	-7.138597000	10.696307000	0.538155000
C	-8.168431000	10.519951000	2.492102000
C	-8.016103000	11.825189000	3.027250000
C	-7.338845000	12.858677000	2.189614000
C	-5.959053000	12.832913000	1.944959000
C	-5.316252000	13.813761000	1.170570000
C	-6.066148000	14.858341000	0.612569000
C	-7.449931000	14.907961000	0.835118000
C	-8.064956000	13.914450000	1.614593000
C	-8.456031000	12.184606000	4.257189000
C	-8.192667000	13.383422000	4.908468000
H	-7.606503000	14.213262000	4.534723000
C	-8.739147000	13.325382000	6.117398000
H	-8.660614000	14.099139000	6.868890000
C	-9.393003000	12.107117000	6.249920000
C	-10.072660000	11.583891000	7.506797000
C	-11.010399000	10.399799000	7.158299000
H	-11.819284000	10.729666000	6.470490000
H	-11.479808000	9.995289000	8.081112000
H	-10.473328000	9.567719000	6.657509000
C	-10.975346000	12.704981000	8.083844000
H	-10.385938000	13.598601000	8.377278000

H	-11.533013000	12.342569000	8.974607000
H	-11.720364000	13.032967000	7.326311000
C	-8.974001000	11.097420000	8.477130000
C	-8.793164000	11.640132000	9.714682000
H	-9.427680000	12.429075000	10.089301000
C	-7.805321000	11.217017000	10.524863000
H	-7.681721000	11.669082000	11.501548000
C	-6.971043000	10.240065000	10.135023000
H	-6.196053000	9.936891000	10.823209000
C	-7.128342000	9.638839000	8.862209000
C	-8.136084000	10.098801000	8.074655000
H	-8.259795000	9.668293000	7.089867000
C	-6.238729000	8.474509000	8.364938000
C	-5.145815000	8.082172000	9.386806000
H	-4.529463000	7.237441000	9.009301000
H	-5.599305000	7.752345000	10.346407000
H	-4.460977000	8.937192000	9.575593000
C	-7.143387000	7.238089000	8.143308000
H	-7.827808000	7.387411000	7.281067000
H	-7.757621000	7.041010000	9.048694000
H	-6.545005000	6.324665000	7.939520000
C	-5.527814000	8.819064000	7.055769000
C	-5.483489000	10.055678000	6.419478000
H	-5.933019000	10.978566000	6.760054000
C	-4.793003000	9.930390000	5.294148000
H	-4.604983000	10.731430000	4.595449000
C	-4.347451000	8.621766000	5.200022000
C	-3.623147000	8.067232000	4.119866000
C	-3.494914000	8.856962000	2.864809000
C	-2.563965000	9.900698000	2.752065000
C	-2.399995000	10.626517000	1.559997000
C	-3.183733000	10.310564000	0.440976000
C	-4.124363000	9.274682000	0.527854000
C	-4.265712000	8.563550000	1.730871000
C	-3.023331000	6.857111000	4.192358000
C	-2.394773000	6.175935000	3.161059000
H	-2.313191000	6.476437000	2.125005000
C	-1.903897000	5.056875000	3.676262000
H	-1.363524000	4.298477000	3.127027000
C	-2.191255000	5.037248000	5.036307000
C	-1.740485000	3.960541000	6.008694000
C	-2.260339000	4.246836000	7.442590000
H	-1.792017000	5.164518000	7.860458000
H	-2.019806000	3.396469000	8.116994000
H	-3.355877000	4.418285000	7.465149000
C	-0.192602000	4.012139000	6.084488000
H	0.267852000	3.980764000	5.075653000
H	0.199904000	3.168412000	6.691892000
H	0.149160000	4.961662000	6.550810000
C	-2.281322000	2.603307000	5.509904000
C	-3.654031000	2.289384000	5.649188000
H	-4.339664000	2.978216000	6.121204000
C	-4.146603000	1.130654000	5.180351000
H	-5.199150000	0.908792000	5.309435000
C	-3.363657000	0.260413000	4.517969000
H	-3.837096000	-0.632235000	4.136145000
C	-2.048141000	0.525427000	4.295021000
C	-1.505420000	1.717698000	4.835431000
H	-0.468581000	1.933231000	4.636166000
C	-1.162221000	-0.327917000	3.361136000
C	-1.903285000	-1.521485000	2.732987000
H	-2.771615000	-1.181515000	2.127626000
H	-2.243492000	-2.220487000	3.522147000
H	-1.222604000	-2.083650000	2.065367000
C	0.023140000	-0.889827000	4.175076000
H	0.649089000	-1.569040000	3.558342000
H	-0.354444000	-1.473238000	5.042070000
H	0.675657000	-0.075108000	4.552028000
N	-1.486807000	1.501523000	1.659764000
N	-3.495561000	3.058713000	0.408566000
N	-8.799675000	9.397048000	3.113841000
N	-9.226341000	11.379320000	5.132437000
N	-4.823574000	7.916459000	6.343362000
N	-2.853424000	6.091991000	5.376355000
F	-0.644175000	4.062034000	-2.592937000
F	1.289927000	5.744983000	-3.455565000
F	3.013959000	6.880806000	-1.652516000
F	2.793869000	6.281043000	0.996138000
F	0.870994000	4.606883000	1.852438000
F	-5.216288000	11.854552000	2.449945000
F	-4.004752000	13.753499000	0.968773000
F	-5.472927000	15.790482000	-0.119561000
F	-8.173747000	15.890559000	0.310412000
F	-9.378766000	13.989725000	1.799502000
F	-1.800176000	10.219411000	3.791230000
F	-1.502999000	11.604312000	1.489452000
F	-3.033302000	10.982942000	-0.691608000

F	-4.875061000	8.965664000	-0.523103000
F	-5.154567000	7.578536000	1.772123000
H	-9.269617000	9.329961000	4.037524000
H	-2.449835000	1.720289000	1.987284000
H	-4.765022000	6.898784000	6.555031000
C	2.516348000	13.256333000	-4.908155000
C	1.337809000	13.236912000	-4.286007000
H	0.424271000	13.712372000	-4.616249000
C	1.455369000	12.491268000	-3.193791000
H	0.655586000	12.267776000	-2.499546000
C	2.763900000	12.030738000	-3.146397000
C	3.278666000	11.088724000	-2.216430000
C	2.317977000	10.397160000	-1.306603000
C	2.376913000	10.557500000	0.086680000
C	1.513601000	9.869788000	0.957797000
C	0.542421000	9.008353000	0.431042000
C	0.436698000	8.854681000	-0.958145000
C	1.325323000	9.537603000	-1.805045000
C	4.593885000	10.758830000	-2.148602000
C	5.161233000	9.732847000	-1.405552000
H	4.654554000	9.031048000	-0.755812000
C	6.461771000	9.725654000	-1.674551000
H	7.181038000	9.025753000	-1.271782000
C	6.728727000	10.755417000	-2.568237000
C	8.089314000	11.073392000	-3.175222000
C	9.057255000	11.394533000	-2.009616000
H	10.057768000	11.689078000	-2.394150000
H	8.666996000	12.240678000	-1.402716000
H	9.174285000	10.524255000	-1.328753000
C	8.013857000	12.340717000	-4.064173000
H	7.264936000	12.233062000	-4.877132000
H	7.724756000	13.228715000	-3.460808000
H	9.001698000	12.543503000	-4.531603000
C	8.526448000	9.875705000	-4.049161000
C	9.673906000	9.167568000	-3.822129000
H	10.319604000	9.463087000	-3.018150000
C	9.998548000	8.071120000	-4.574232000
C	9.138120000	7.698710000	-5.563965000
H	9.307217000	6.810147000	-6.154863000
C	8.033814000	8.417452000	-5.827461000
H	7.377916000	8.121101000	-6.633962000
C	7.723025000	9.485360000	-5.075829000
H	6.802004000	10.012624000	-5.292639000
C	11.252283000	7.208306000	-4.284482000
C	12.291596000	7.915179000	-3.370933000
H	13.202565000	7.287962000	-3.255908000
H	12.597869000	8.890000000	-3.808909000
H	11.906235000	8.094209000	-2.346170000
C	12.010288000	6.902314000	-5.606493000
H	11.408142000	6.329830000	-6.338098000
H	12.319779000	7.849933000	-6.098292000
H	12.924034000	6.301414000	-5.405860000
C	10.795176000	5.931668000	-3.581518000
C	10.277474000	5.883606000	-2.294257000
H	10.128748000	6.725483000	-1.631154000
C	9.968989000	4.629489000	-2.003365000
H	9.537992000	4.303340000	-1.066541000
C	10.267176000	3.840516000	-3.104167000
C	10.019542000	2.446819000	-3.197227000
C	9.370883000	1.762067000	-2.039635000
C	8.022257000	1.968656000	-1.721005000
C	7.390605000	1.305508000	-0.657559000
C	8.126392000	0.420375000	0.141765000
C	9.479043000	0.193537000	-0.148440000
C	10.080953000	0.862822000	-1.228055000
C	10.334519000	1.707046000	-4.286678000
C	9.946710000	0.395733000	-4.532814000
H	9.341218000	-0.235826000	-3.895010000
C	10.394712000	0.052661000	-5.735058000
H	10.206009000	-0.896415000	-6.218219000
C	11.109465000	1.120436000	-6.263094000
C	11.704125000	1.196217000	-7.661626000
C	12.697197000	2.381743000	-7.762934000
H	13.547331000	2.242099000	-7.060114000
H	13.105120000	2.455865000	-8.794257000
H	12.221502000	3.353285000	-7.514689000
C	12.526101000	-0.093372000	-7.915686000
H	11.888670000	-1.001420000	-7.875757000
H	13.024211000	-0.054422000	-8.908734000
H	13.317272000	-0.208661000	-7.142872000
C	10.546616000	1.413471000	-8.660853000
C	10.259613000	0.529369000	-9.658113000
H	10.848788000	-0.361274000	-9.816694000
C	9.218311000	0.727124000	-10.487793000
H	9.010486000	0.006178000	-11.269177000
C	8.432355000	1.807704000	-10.355187000
H	7.609216000	1.918640000	-11.045338000

C	8.699132000	2.758242000	-9.339717000
C	9.762115000	2.521332000	-8.526312000
H	9.971780000	3.224705000	-7.731214000
C	7.860994000	4.044937000	-9.148280000
C	6.682743000	4.143168000	-10.145114000
H	6.103182000	5.078808000	-9.987799000
H	7.050002000	4.158294000	-11.193985000
H	5.983375000	3.289692000	-10.010166000
C	8.786922000	5.261726000	-9.388099000
H	9.547000000	5.355729000	-8.583318000
H	9.316497000	5.159011000	-10.360131000
H	8.213100000	6.212375000	-9.418133000
C	7.268621000	4.132167000	-7.741262000
C	7.273310000	3.141976000	-6.763483000
H	7.672328000	2.140670000	-6.853185000
C	6.703245000	3.623467000	-5.668254000
H	6.569156000	3.070531000	-4.751963000
C	6.287143000	4.918420000	-5.928393000
C	5.681570000	5.795548000	-5.002297000
C	5.719913000	5.449582000	-3.555396000
C	4.797822000	4.552149000	-2.999270000
C	4.753784000	4.286344000	-1.620501000
C	5.661670000	4.926357000	-0.764561000
C	6.604954000	5.816656000	-1.294021000
C	6.618214000	6.068608000	-2.675283000
C	5.031807000	6.918577000	-5.381948000
C	4.458351000	7.863903000	-4.547211000
H	4.484131000	7.889380000	-3.468221000
C	3.855835000	8.754703000	-5.319969000
H	3.312768000	9.621522000	-4.969016000
C	4.034799000	8.375283000	-6.645077000
C	3.471151000	9.116252000	-7.844595000
C	3.933642000	8.459892000	-9.172930000
H	3.488575000	7.448253000	-9.293893000
H	3.622706000	9.081845000	-10.039979000
H	5.033406000	8.320928000	-9.211308000
C	1.926177000	8.985090000	-7.801668000
H	1.510384000	9.276958000	-6.813882000
H	1.459593000	9.612056000	-8.592043000
H	1.615134000	7.930626000	-7.967670000
C	3.958146000	10.580657000	-7.769966000
C	5.293671000	10.906859000	-8.105698000
H	5.981307000	10.154306000	-8.462775000
C	5.752186000	12.161924000	-7.965825000
H	6.776201000	12.387246000	-8.238048000
C	4.975699000	13.132508000	-7.451490000
H	5.424701000	14.106863000	-7.328598000
C	3.700340000	12.877812000	-7.054765000
C	3.185493000	11.572878000	-7.257951000
H	2.182822000	11.371061000	-6.917378000
C	2.846230000	13.890296000	-6.259320000
C	3.574786000	15.221264000	-5.964920000
H	4.505434000	15.045213000	-5.382483000
H	3.827261000	15.752773000	-6.907826000
H	2.926124000	15.893623000	-5.361847000
C	1.574125000	14.216826000	-7.076106000
H	0.972246000	15.007900000	-6.578962000
H	1.851416000	14.584479000	-8.087761000
H	0.928559000	13.321616000	-7.197335000
N	3.419656000	12.540519000	-4.209425000
N	5.644789000	11.390340000	-2.861830000
N	10.798246000	4.694594000	-4.121505000
N	11.084296000	2.153376000	-5.403496000
N	6.645149000	5.232111000	-7.271269000
N	4.725826000	7.286183000	-6.719028000
F	3.272234000	11.381265000	0.620708000
F	1.617944000	10.032885000	2.271649000
F	-0.265815000	8.332440000	1.237489000
F	-0.499944000	8.061188000	-1.467169000
F	1.215046000	9.335099000	-3.113397000
F	7.299147000	2.819659000	-2.438112000
F	6.102637000	1.511247000	-0.410777000
F	7.538618000	-0.189267000	1.160170000
F	10.188131000	-0.651483000	0.591243000
F	11.366185000	0.628881000	-1.469827000
F	3.929390000	3.944948000	-3.797469000
F	3.852769000	3.446232000	-1.122912000
F	5.626916000	4.705037000	0.539552000
F	7.471205000	6.423281000	-0.490031000
F	7.506627000	6.935553000	-3.139326000
H	11.050320000	4.468076000	-5.103481000
H	4.384041000	12.341119000	-4.543340000
H	6.568795000	6.143211000	-7.769838000
C	14.418167000	4.663219000	6.317862000
C	15.464796000	3.858796000	6.498456000
H	16.348822000	4.068098000	7.085261000
C	15.227585000	2.718688000	5.862383000

H	15.888172000	1.861625000	5.853123000
C	13.971238000	2.822129000	5.279915000
C	13.280405000	1.770416000	4.618145000
C	13.969617000	0.456249000	4.482512000
C	14.455233000	0.013109000	3.242863000
C	15.090090000	-1.231122000	3.092340000
C	15.252341000	-2.066600000	4.206774000
C	14.780145000	-1.646912000	5.458594000
C	14.148525000	-0.397933000	5.581013000
C	12.013954000	1.882888000	4.142899000
C	11.237904000	0.873550000	3.588939000
H	11.514608000	-0.161486000	3.434369000
C	10.053784000	1.401259000	3.301249000
H	9.217981000	0.869728000	2.871019000
C	10.074444000	2.741281000	3.661420000
C	8.927863000	3.725836000	3.486892000
C	8.695065000	3.890251000	1.966106000
H	7.913788000	4.653067000	1.765862000
H	9.628424000	4.226860000	1.464351000
H	8.396790000	2.929757000	1.499182000
C	9.313325000	5.122782000	4.038103000
H	9.613470000	5.075964000	5.106197000
H	10.169135000	5.550434000	3.471416000
H	8.454398000	5.822871000	3.950858000
C	7.697616000	3.205925000	4.265633000
C	6.497038000	2.937648000	3.669384000
H	6.400088000	3.089988000	2.613411000
C	5.426662000	2.470793000	4.386324000
C	5.599297000	2.266047000	5.722592000
H	4.807116000	1.877051000	6.343292000
C	6.768890000	2.546627000	6.321288000
H	6.875601000	2.401327000	7.385923000
C	7.808531000	3.002066000	5.605009000
H	8.741404000	3.195226000	6.119980000
C	4.063947000	2.138325000	3.722010000
C	3.916125000	2.759718000	2.306775000
H	2.912336000	2.548926000	1.893340000
H	4.032294000	3.863567000	2.355960000
H	4.648033000	2.359387000	1.580228000
C	2.888877000	2.740508000	4.539237000
H	2.813298000	2.345283000	5.569931000
H	2.993491000	3.844791000	4.611960000
H	1.919996000	2.512514000	4.043985000
C	3.912031000	0.618393000	3.646279000
C	4.225455000	-0.191278000	2.556109000
H	4.571295000	0.127354000	1.583740000
C	4.056388000	-1.459353000	2.902623000
H	4.220062000	-2.310424000	2.258458000
C	3.629391000	-1.493767000	4.216268000
C	3.402441000	-2.659488000	4.978269000
C	3.980339000	-3.948434000	4.497530000
C	5.367906000	-4.120390000	4.377885000
C	5.941332000	-5.314896000	3.914611000
C	5.112517000	-6.389559000	3.563504000
C	3.722501000	-6.251952000	3.679071000
C	3.176533000	-5.041100000	4.139002000
C	2.682475000	-2.633383000	6.121512000
C	2.501362000	-3.678058000	7.017132000
H	2.948219000	-4.662714000	6.970727000
C	1.687787000	-3.255627000	7.978148000
H	1.380456000	-3.839996000	8.835218000
C	1.318367000	-1.945128000	7.702884000
C	0.456078000	-1.062584000	8.589764000
C	0.149539000	0.289452000	7.896862000
H	-0.465977000	0.132400000	6.986905000
H	-0.415949000	0.956197000	8.583175000
H	1.072388000	0.820677000	7.583775000
C	-0.902097000	-1.777386000	8.800513000
H	-0.772204000	-2.763321000	9.295160000
H	-1.584449000	-1.153601000	9.417670000
H	-1.400338000	-1.960557000	7.823036000
C	1.243500000	-0.803039000	9.889968000
C	0.795594000	-1.201911000	11.113678000
H	-0.160982000	-1.686595000	11.239596000
C	1.538350000	-1.019163000	12.220714000
H	1.161389000	-1.350876000	13.180602000
C	2.745154000	-0.435171000	12.146556000
H	3.301434000	-0.315466000	13.064245000
C	3.244407000	0.007179000	10.896227000
C	2.459259000	-0.191164000	9.805898000
H	2.828284000	0.120967000	8.837327000
C	4.599676000	0.736092000	10.740362000
C	5.365402000	0.853625000	12.079842000
H	6.330287000	1.388693000	11.946928000
H	4.776506000	1.430678000	12.825127000
H	5.594678000	-0.154250000	12.488840000
C	4.315696000	2.169701000	10.231079000

H	3.930522000	2.158409000	9.188992000
H	3.561398000	2.668147000	10.878008000
H	5.232930000	2.796254000	10.241270000
C	5.527413000	0.029211000	9.748392000
C	5.334657000	-1.203889000	9.132092000
H	4.496919000	-1.874268000	9.267582000
C	6.364581000	-1.445435000	8.329601000
H	6.477895000	-2.331586000	7.718117000
C	7.255562000	-0.387082000	8.432331000
C	8.485684000	-0.277032000	7.737898000
C	8.840788000	-1.337871000	6.757758000
C	9.590493000	-2.458088000	7.145897000
C	10.039635000	-3.410973000	6.216870000
C	9.739997000	-3.246079000	4.857051000
C	8.974266000	-2.145698000	4.446129000
C	8.523254000	-1.215024000	5.397725000
C	9.377168000	0.722646000	7.943670000
C	10.598833000	0.884057000	7.308701000
H	11.022882000	0.259652000	6.533530000
C	11.183931000	1.947811000	7.843411000
H	12.160824000	2.318864000	7.570381000
C	10.335953000	2.472897000	8.812597000
C	10.631627000	3.671271000	9.705759000
C	9.379045000	4.022641000	10.556458000
H	9.157023000	3.221179000	11.294560000
H	9.539911000	4.970029000	11.115093000
H	8.469345000	4.121398000	9.927285000
C	11.742518000	3.269909000	10.710591000
H	12.611233000	2.795359000	10.208938000
H	12.094055000	4.159303000	11.276993000
H	11.367047000	2.519220000	11.439568000
C	11.064747000	4.869968000	8.825114000
C	10.130646000	5.828550000	8.360183000
H	9.086099000	5.778932000	8.626497000
C	10.517038000	6.832848000	7.554676000
H	9.784037000	7.555881000	7.217718000
C	11.791054000	6.940151000	7.136642000
H	12.023126000	7.757665000	6.470342000
C	12.733819000	6.037150000	7.513881000
C	12.346487000	4.997127000	8.395119000
H	13.092383000	4.270451000	8.675947000
C	14.172860000	6.031076000	6.951380000
C	14.413255000	7.087774000	5.849282000
H	13.706032000	6.947438000	5.002953000
H	14.300512000	8.117181000	6.252824000
H	15.444826000	6.997334000	5.444069000
C	15.153979000	6.320162000	8.110634000
H	16.199147000	6.392999000	7.739691000
H	14.896972000	7.284614000	8.599888000
H	15.115100000	5.520943000	8.880966000
N	13.498312000	4.059245000	5.541710000
N	11.219567000	3.055811000	4.162561000
N	3.542264000	-0.153645000	4.690140000
N	1.922621000	-1.526453000	6.579250000
N	6.705232000	0.552305000	9.353841000
N	9.258959000	1.764303000	8.897900000
F	14.322146000	0.783233000	2.168144000
F	15.534856000	-1.615798000	1.901165000
F	15.848663000	-3.243387000	4.078170000
F	14.929323000	-2.427706000	6.522964000
F	13.716986000	-0.032898000	6.783506000
F	6.183809000	-3.134072000	4.734640000
F	7.260732000	-5.430303000	3.813187000
F	5.641751000	-7.525300000	3.132835000
F	2.925089000	-7.263387000	3.354154000
F	1.854627000	-4.951337000	4.230060000
F	9.902627000	-2.630459000	8.425923000
F	10.753092000	-4.456263000	6.620488000
F	10.182509000	-4.121074000	3.964982000
F	8.682408000	-1.989710000	3.160527000
F	7.782401000	-0.194667000	4.980873000
H	3.403130000	0.164736000	5.671659000
H	12.592329000	4.497267000	5.284081000
H	7.068177000	1.479707000	9.652366000
C	0.699284000	-0.559648000	-2.197534000
C	-0.520171000	-0.613643000	-1.663761000
H	-1.364565000	0.012665000	-1.913725000
C	-0.546964000	-1.612942000	-0.792596000
H	-1.412815000	-1.926436000	-0.228546000
C	0.711110000	-2.193820000	-0.790182000
C	1.066407000	-3.401241000	-0.138313000
C	-0.030174000	-4.287642000	0.347280000
C	-0.182574000	-4.605954000	1.704619000
C	-1.193577000	-5.468441000	2.164119000
C	-2.079285000	-6.041752000	1.242717000
C	-1.960560000	-5.735798000	-0.119783000
C	-0.947574000	-4.863873000	-0.547733000

C	2.352317000	-3.814645000	-0.018749000
C	2.800603000	-5.049734000	0.426549000
H	2.202209000	-5.882778000	0.770835000
C	4.123344000	-5.056637000	0.297799000
H	4.771418000	-5.892606000	0.525659000
C	4.517914000	-3.825230000	-0.211250000
C	5.937849000	-3.434563000	-0.596643000
C	6.799353000	-3.457752000	0.690000000
H	7.838571000	-3.124500000	0.478807000
H	6.384132000	-2.768815000	1.454589000
H	6.826945000	-4.475009000	1.135483000
C	5.975167000	-1.989298000	-1.150928000
H	5.313231000	-1.867119000	-2.034258000
H	5.633448000	-1.266181000	-0.380044000
H	7.008481000	-1.721318000	-1.459566000
C	6.427385000	-4.397303000	-1.700966000
C	7.551058000	-5.163933000	-1.572195000
H	8.138495000	-5.085697000	-0.677913000
C	7.928511000	-6.045386000	-2.546685000
C	7.148671000	-6.142588000	-3.659903000
H	7.372252000	-6.856527000	-4.441121000
C	6.067452000	-5.360752000	-3.816583000
H	5.477253000	-5.433066000	-4.719052000
C	5.702854000	-4.504935000	-2.848448000
H	4.804838000	-3.917197000	-2.995927000
C	9.161299000	-6.968454000	-2.402997000
C	10.067447000	-6.621362000	-1.191068000
H	10.955624000	-7.289888000	-1.164503000
H	10.430372000	-5.572655000	-1.259113000
H	9.541399000	-6.753096000	-0.222382000
C	10.064685000	-6.831180000	-3.658118000
H	9.550556000	-7.123278000	-4.595345000
H	10.400411000	-5.777890000	-3.774950000
H	10.967447000	-7.473663000	-3.566299000
C	8.656340000	-8.395488000	-2.213158000
C	7.948751000	-8.835948000	-1.104110000
H	7.661898000	-8.238095000	-0.248903000
C	7.668652000	-10.120210000	-1.259285000
H	7.121865000	-10.719316000	-0.543273000
C	8.170748000	-10.531684000	-2.486076000
C	8.020481000	-11.832777000	-3.031838000
C	7.338943000	-12.872296000	-2.205143000
C	5.957892000	-12.848446000	-1.967465000
C	5.311298000	-13.834738000	-1.203201000
C	6.058323000	-14.883504000	-0.649244000
C	7.443185000	-14.931617000	-0.865357000
C	8.062128000	-13.932306000	-1.634249000
C	8.464486000	-12.182647000	-4.263158000
C	8.204623000	-13.377188000	-4.923747000
H	7.619254000	-14.210827000	-4.557356000
C	8.753665000	-13.309505000	-6.131013000
H	8.678596000	-14.078032000	-6.888173000
C	9.405284000	-12.089046000	-6.253483000
C	10.087730000	-11.556711000	-7.505027000
C	11.018310000	-10.369607000	-7.147486000
H	11.826385000	-10.698742000	-6.458390000
H	11.489028000	-9.958324000	-8.066673000
H	10.475393000	-9.542671000	-6.644552000
C	10.998315000	-12.670792000	-8.083262000
H	10.414712000	-13.566407000	-8.382193000
H	11.557217000	-12.301997000	-8.970681000
H	11.742401000	-12.997869000	-7.324432000
C	8.990717000	-11.071516000	-8.477845000
C	8.816554000	-11.610870000	-9.717853000
H	9.455600000	-12.396012000	-10.092781000
C	7.829876000	-11.189110000	-10.530203000
H	7.711648000	-11.638412000	-11.508834000
C	6.990294000	-10.216767000	-10.140188000
H	6.216713000	-9.914187000	-10.830228000
C	7.140638000	-9.619148000	-8.864856000
C	8.147200000	-10.077798000	-8.075064000
H	8.265584000	-9.650040000	-7.088420000
C	6.245744000	-8.459002000	-8.367520000
C	5.153060000	-8.069228000	-9.390534000
H	4.532099000	-7.228336000	-9.011980000
H	5.606827000	-7.734876000	-10.348445000
H	4.472659000	-8.927005000	-9.582815000
C	7.145815000	-7.219777000	-8.142837000
H	7.828945000	-7.367803000	-7.279331000
H	7.761326000	-7.019830000	-9.046746000
H	6.544069000	-6.308438000	-7.939689000
C	5.533864000	-8.808144000	-7.060048000
C	5.488674000	-10.047141000	-6.428563000
H	5.938537000	-10.968692000	-6.772371000
C	4.796942000	-9.926086000	-5.303476000
H	4.608024000	-10.729774000	-4.608074000
C	4.351615000	-8.617729000	-5.204673000

C	3.626380000	-8.067148000	-4.122998000
C	3.494169000	-8.862573000	-2.871849000
C	2.562575000	-9.906549000	-2.766633000
C	2.394402000	-10.637610000	-1.578352000
C	3.175047000	-10.327452000	-0.455533000
C	4.115936000	-9.291194000	-0.534711000
C	4.261192000	-8.574518000	-1.733988000
C	3.028130000	-6.855945000	-4.191133000
C	2.398622000	-6.178329000	-3.157986000
H	2.315314000	-6.482767000	-2.123196000
C	1.909098000	-5.056935000	-3.669527000
H	1.368329000	-4.300387000	-3.118134000
C	2.198210000	-5.032313000	-5.029136000
C	1.748669000	-3.952186000	-5.998298000
C	2.269358000	-4.233888000	-7.432769000
H	1.801533000	-5.150450000	-7.853634000
H	2.028845000	-3.381540000	-8.104699000
H	3.364990000	-4.404690000	-7.455288000
C	0.200819000	-4.002855000	-6.075292000
H	-0.260219000	-3.973456000	-5.066658000
H	-0.190939000	-3.157563000	-6.681088000
H	-0.141014000	-4.951175000	-6.544001000
C	2.290036000	-2.596947000	-5.494964000
C	3.663682000	-2.285086000	-5.629398000
H	4.349563000	-2.974390000	-6.100422000
C	4.156691000	-1.127987000	-5.156989000
H	5.210042000	-0.907710000	-5.282241000
C	3.373058000	-0.257625000	-4.495551000
H	3.846882000	0.633393000	-4.110394000
C	2.056352000	-0.520891000	-4.277244000
C	1.513425000	-1.711252000	-4.821525000
H	0.475685000	-1.925527000	-4.625783000
C	1.169051000	0.331469000	-3.343739000
C	1.909547000	1.523677000	-2.712846000
H	2.775550000	1.182309000	-2.104936000
H	2.253094000	2.222132000	-3.500822000
H	1.227508000	2.086742000	-2.047438000
C	-0.014680000	0.895091000	-4.158825000
H	-0.641912000	1.572978000	-3.542059000
H	0.364635000	1.480494000	-5.023755000
H	-0.666603000	0.081306000	-4.538690000
N	1.488747000	-1.502510000	-1.646446000
N	3.493774000	-3.063621000	-0.395091000
N	8.809881000	-9.405661000	-3.094043000
N	9.234723000	-11.369400000	-5.131271000
N	4.828959000	-7.908196000	-6.344981000
N	2.860318000	-6.086036000	-5.372293000
F	0.634195000	-4.065376000	2.601446000
F	-1.306074000	-5.745427000	3.457952000
F	-3.028138000	-6.875087000	1.648947000
F	-2.799626000	-6.273836000	-0.998229000
F	-0.870383000	-4.603300000	-1.848048000
F	5.217376000	-11.866847000	-2.469496000
F	3.998909000	-13.775444000	-1.006991000
F	5.461438000	-15.820953000	0.073063000
F	8.164319000	-15.918218000	-0.344496000
F	9.376849000	-14.006268000	-1.813138000
F	1.801849000	-10.220307000	-3.809573000
F	1.496332000	-11.614920000	-1.515097000
F	3.021258000	-11.005249000	0.673328000
F	4.863187000	-8.986488000	0.519991000
F	5.149987000	-7.589171000	-1.767285000
H	9.293848000	-9.334579000	-4.010151000
H	2.450810000	-1.724091000	-1.974971000
H	4.770352000	-6.889854000	-6.553290000