

Electronic Supplementary Information

Theoretical Design of an Ultrafast Supramolecular Rotor Composed of Carbon Nano-rings

Yuhang Jiang,^a Edoardo Jun Mattioli,^b Matteo Calvaresi,^{*b} Zhiyong Wang^{*a}

^a Department of Chemistry, Renmin University of China, Beijing 100872, PR China

^b Dipartimento di Chimica “G. Ciamician”, Alma Mater Studiorum – Università di
Bologna, via F. Selmi 2, 40126 Bologna, Italy.

*E-mails: zhiyongwang@ruc.edu.cn; matteo.calvaresi3@unibo.it.

(1) Theoretical calculation methods and results

Density functional theory (DFT) calculations in this study were performed with the Gaussian 16 software¹. For comparison purpose, the geometrical structures of the [n]CPP ($n = 9 - 14$), cyclo[18]carbon and their host-guest complexes were optimized by using different density functional methods, i.e., ω B97X-D, M06-2X(D3) and CAM-B3LYP(D3). The def2-SVP basis set was used for all the atoms. The exchange-correlation functionals such as ω B97X-D, M06-2X and CAM-B3LYP can well reproduce the bond length alternation character of cyclo[18]carbon. Meanwhile, it is necessary to use dispersion-corrected methods to describe the weak interaction between cyclo[18]carbon and [n]CPP. Vibrational frequency analyses were performed on the optimized structures to ensure that they are local minima on the energy potential surface. The extended basis set def2-TZVP was used for single-point energy calculations to obtain more accurate thermodynamics parameters for the [n]CPP:cyclo[18]carbon complexes, taking into account zero-point energy and basis set superposition error corrections (Table S1).

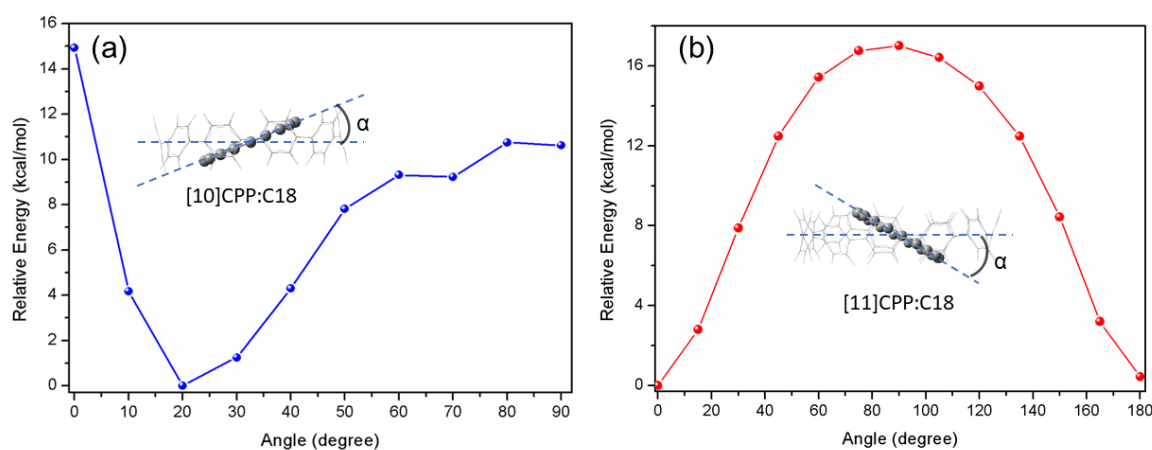


Fig. S1. The relative energy of (a) [10]CPP:C₁₈ and (b) [11]CPP:C₁₈ for scan of out-of-plane angle of C₁₈ in [n]CPP calculated at ω B97X-D/def2-TZVP level. The insert picture shows the reference system used for the calculations.

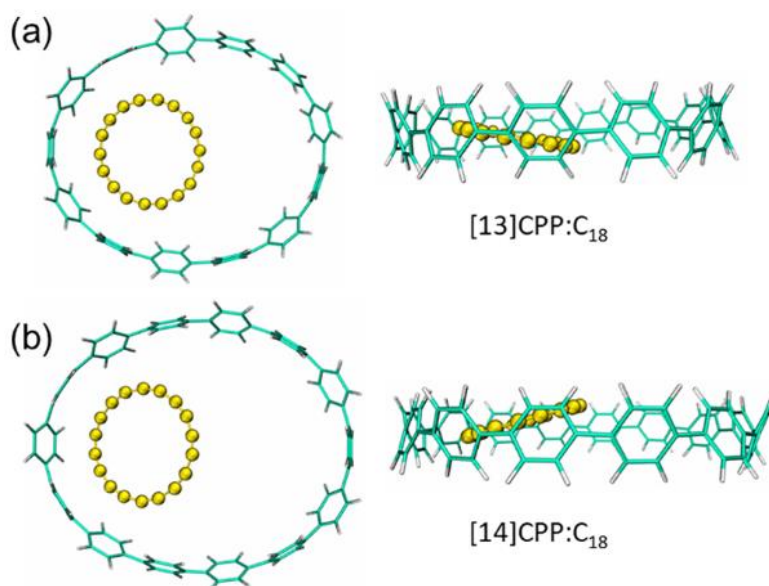


Fig. S2. Top view and side view of the ω B97X-D/def2-SVP optimized structures of (a) [13]CPP:cyclo[18]carbon, (b) [14]CPP:cyclo[18]carbon.

Table S1. The theoretically calculated interaction energies E_{int} (in kcal/mol) ($E_{\text{int}} = E_{\text{complex}} - E_{[n]\text{CPP}} - E_{\text{cyclo}[18]\text{carbon}} + E_{\text{BSSE}}$), the changes in enthalpies ΔH (in kcal/mol), and the Gibbs energies ΔG (in kcal/mol) for the complexation of cyclo[18]carbon and [n]CPP in different methods, taking into account zero-point energy and basis set superposition error corrections ($T = 298.15$ K). The basis set of def2-SVP was used for structural optimization, and the basis set of def2-TZVP was used for single-point energy calculations.

	ω B97X-D			M06-2X(D3)			CAM-B3LYP(D3)		
	E_{int}	ΔH	ΔG	E_{int}	ΔH	ΔG	E_{int}	ΔH	ΔG
[9]CPP : C ₁₈	-16.22	-15.78	-1.66	-16.04	-15.51	-1.45	-11.90	-11.30	1.86
[10]CPP : C ₁₈	-17.19	-17.00	-1.48	-19.58	-19.42	-4.33	-17.82	-17.33	-3.73
[11]CPP : C ₁₈	-20.86	-20.10	-7.87	-18.09	-17.33	-5.08	-21.83	-20.99	-9.67
[12]CPP : C ₁₈	-14.40	-13.71	-1.65	-14.05	-13.36	-1.24	-15.01	-14.18	-3.32
[13]CPP : C ₁₈	-12.63	-11.87	-0.49	-12.23	-11.59	0.93	-12.82	-12.00	-1.22
[14]CPP : C ₁₈	-10.85	-10.16	1.62	-10.46	-9.79	2.20	-11.21	-10.37	0.03

To get a better understanding on the interaction between [n]CPP ($n = 9 - 14$) and cyclo[18]carbon, we carried out independent gradient model (IGM) analysis for the complexes based on promolecular density by using Multiwfn 3.7 software. It is known that intermolecular noncovalent interaction regions can be visualized by IGM analysis without any intramolecular interaction interference.

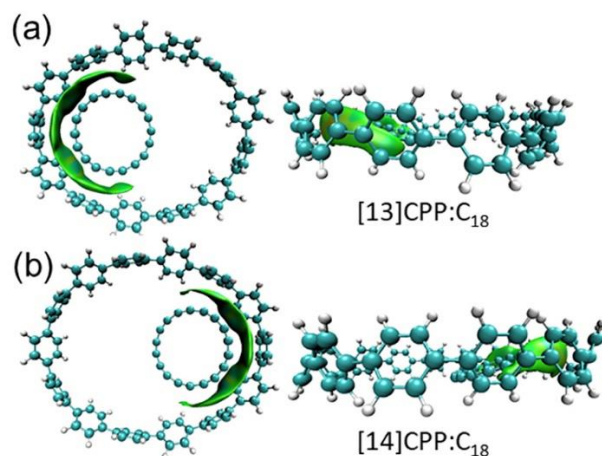


Fig. S3. The visualized weak interaction between [n]CPP and cyclo[18]carbon by IGM analysis based on promolecular density. (isovalue = 0.003)

To provide a dynamical description of the [11]CPP:cyclo[18]carbon system, we carried out molecular dynamics (MD) simulations. Firstly, we developed an ad-hoc force field able to describe the structure of the cyclo[18]carbon at MM level. The conjugation that exist in the alternating “single-like” and “triple-like” bonds impedes the use of common atom types developed to describe single and triple bonds (pure polyynic structure). Starting from the optimized geometry of the cyclo[18]carbon a relaxed scan of the “single-like” and “triple-like” bonds was carried out at the ω B97X-D/def2-SVP level of theory. The calculated parameters for the bond stretching of the “single-like” and “triple-like” bonds in the cyclo[18]carbon are reported in Table S2. For comparison, parameters calculated at the same level of theory for ethane and ethyne, are reported as reference values. Even if the optimized structure is characterized to a 9-fold symmetry with alternating short and long bonds, i.e., a polyynic structure, bond constants calculations revealed the important contribution from the cumulenic resonance structure in the cyclo[18]carbon, that makes the “single-like” bond parameters more short and rigid compared to the ethane reference structure. The opposite happens to the “triple-like” bond parameters in the cyclo[18]carbon compared to the ethyne reference structure. All the remaining MM parameters of the [11]CPP:cyclo[18]carbon system were defined by using parameters form the Generalised Amber Force Field (GAFF). Using the AMBER 16 software package²,

1 μ s MD simulations of the [11]CPP:cyclo[18]carbon system at different temperatures (25, 50, 75, 100, 200, 300, 400 and 500 K) were carried out.

Table S2. Equilibrium length and harmonic constants for “single-like” and “triple-like” bonds in the cyclo[18]carbon with the reference values, calculated at the same level of theory, for ethane and ethyne molecules.

	“Single-like” bond in cyclo[18]carbon	“Triple-like” bond in cyclo[18]carbon
Eq. length (Å)	1.36	1.23
K (kcal mol⁻¹ Å⁻²)	552.69	1045.97
	Ethane	Ethyne
Eq. length (Å)	1.52	1.21
K (kcal mol⁻¹ Å⁻²)	319.17	1290.39

References:

1. Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, O.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian 16, revision A.03. Gaussian, Inc.: Wallingford, CT, 2016.
2. Case, D. A.; Betz, R. M.; Cerutti, D. S.; Cheatham III, T. E.; Darden, T. A.; Duke, R. E.; Giese, T. J.; Gohlke, H.; Goetz, A. W.; Homeyer, N. and Izadi, S.; Janowski, P.; Kaus, J.; Kovalenko, A.; Lee, T. S.; LeGrand, S.; Li, P.; Lin, C.; Luchko, T.; Luo, R.; Madej, B.; Mermelstein, D.; Merz, K. M.; Monard, G.; Nguyen, H.; Nguyen, H. T.; Omelyan, I.; Onufriev, A.; Roe, D. R.; Roitberg, A.; Sagui, C.; Simmeling, C. L.; Botello-Smith, W. M.; Swails, J.; Walker, R. C.; Wang, J.; Wolf, R. M.; Wu, X.; Xiao, L.; Kollman, P. A. (2016) 944 AMBER 2016. University of California, San Francisco.

(2) Cartesian Coordinates (in Angstrom) of DFT-Optimized Structures:

[9]CPP : cyclo[18]carbon

HF = - 2764.6675817 a.u. (in ω B97X-D/def-TZVP// ω B97X-D/def2-SVP level)

C	2.78775700	-5.25750400	0.71899100
C	3.59574300	-5.15395600	1.86372400
C	4.71683100	-4.33143700	1.87921500
C	5.08400200	-3.59240000	0.74377500
C	4.41356200	-3.88107900	-0.45182300
C	3.27982600	-4.68788400	-0.46347600
C	5.86348900	-2.32754200	0.84051300
C	5.57943800	-1.48186000	1.92114900
C	5.86994100	-0.12636900	1.86957300
C	6.46975900	0.45287300	0.74098500
C	6.93210600	-0.42913800	-0.24972900
C	6.62712300	-1.78896900	-0.20679500
C	6.26100000	1.91139100	0.50742600
C	5.90384500	2.77415300	1.55618800
C	5.13012100	3.90464900	1.32354300
C	4.71054700	4.24593800	0.02812700
C	5.31134600	3.54622800	-1.02872600
C	6.05705000	2.39524700	-0.79446600
C	2.62650100	4.73437100	-1.24267100
C	1.30040700	5.14488400	-1.26527900
C	0.75296000	5.88816900	-0.21101600
C	1.63140600	6.32781400	0.79025000
C	2.96501800	5.92565100	0.80483300
C	-0.72723900	5.94601100	-0.08431800

C	-1.32058000	5.62805900	1.14406300
C	-2.65598000	5.24642500	1.21686700
C	-3.45801500	5.17610400	0.06813000
C	-2.91092500	5.67867100	-1.12353000
C	-1.57216100	6.04819900	-1.20013300
C	-4.68143100	4.32752700	0.08913100
C	-4.99095100	3.54030500	-1.02855400
C	-5.76946800	2.39391800	-0.90848900
C	-6.25957700	1.97951000	0.33767100
C	-6.14886700	2.89392100	1.39827300
C	-5.37851200	4.04485600	1.27576100
C	3.47417800	5.05319000	-0.17074300
C	-6.50787100	0.52873000	0.56574800
C	-5.99444500	-0.04176000	1.73961900
C	-5.72185900	-1.40078600	1.82220300
C	-5.94598600	-2.25465700	0.73351800
C	-6.63296900	-1.71751200	-0.36760600
C	-6.91093700	-0.35440600	-0.44817600
C	-5.18356500	-3.53311000	0.68403600
C	-4.52726800	-3.88432600	-0.50264700
C	-3.40551000	-4.70689000	-0.48920500
C	-2.91093000	-5.23432800	0.71116200
C	-3.71236600	-5.07520700	1.85456700
C	-4.82091100	-4.23587900	1.84424400
C	-1.48719900	-5.66107700	0.80135600
C	-0.76114100	-6.15996900	-0.29207200
C	0.63203000	-6.16376700	-0.29238300

C	1.36006400	-5.67146500	0.80219700
C	0.63153400	-5.31981200	1.94740800
C	-0.75670900	-5.31402000	1.94673500
H	3.29881000	-5.66222600	2.78413100
H	5.26977400	-4.20104200	2.81282500
H	4.69105900	-3.35390200	-1.36576700
H	2.69777700	-4.75720200	-1.38549400
H	4.99162100	-1.85837500	2.76054700
H	5.49100900	0.50645100	2.67282500
H	7.46794800	-0.04071900	-1.11890000
H	6.92801800	-2.42757300	-1.04123900
H	6.12665300	2.50133000	2.58942500
H	4.74414500	4.45324100	2.18499600
H	5.09965400	3.82830600	-2.06203800
H	6.36355700	1.79546800	-1.65356100
H	2.96651300	4.04899500	-2.02039800
H	0.64878900	4.77717000	-2.06073100
H	1.25517800	6.95694600	1.60076600
H	3.60352100	6.25457500	1.62786400
H	-0.69851800	5.54758900	2.03842000
H	-3.03782500	4.87348100	2.16916300
H	-3.52183900	5.71853700	-2.02817800
H	-1.16007300	6.36444100	-2.16153600
H	-4.49711800	3.73031100	-1.98326100
H	-5.85274800	1.73021900	-1.77107500
H	-6.60017800	2.66017800	2.36550000
H	-5.25146100	4.68947300	2.14850900

H	-5.66572100	0.60341200	2.55651300
H	-5.19317800	-1.77322800	2.70164700
H	-6.89142700	-2.36173200	-1.21172200
H	-7.37788100	0.03732500	-1.35520300
H	-4.80292600	-3.39457000	-1.43743200
H	-2.83285300	-4.82129500	-1.41235100
H	-3.41986400	-5.55237900	2.79277100
H	-5.36678600	-4.06572800	2.77547900
H	-1.29040200	-6.50032900	-1.18532800
H	1.16063500	-6.50559300	-1.18558600
H	1.15362700	-4.92455400	2.82076700
H	-1.27515400	-4.91359200	2.81976800
C	3.45565200	0.51728600	-0.65850300
C	2.85948200	1.37689900	0.19742700
C	1.94733700	1.97704400	0.76987000
C	0.71118100	2.37123800	1.15480900
C	-0.52219400	2.33998200	1.17417100
C	-1.79594600	1.97302700	0.90036700
C	-2.69205900	1.32536400	0.35342400
C	-3.33326700	0.44759600	-0.45128500
C	-3.51614800	-0.41067900	-1.31678600
C	-3.31774500	-1.32792000	-2.29103500
C	-2.74031600	-2.07576100	-3.08352000
C	-1.76828900	-2.72984700	-3.76218300
C	-0.61935600	-3.03521400	-4.09153900
C	0.73333100	-3.04963200	-4.15416200
C	1.87429000	-2.68948400	-3.85209100

C	2.90543500	-2.04193400	-3.26111700
C	3.44369600	-1.25241600	-2.47997900
C	3.69031400	-0.32580100	-1.52736400

[10]CPP : cyclo[18]carbon

HF = -2995.7389156 a.u. (in ω B97X-D/def-TZVP// ω B97X-D/def2-SVP level)

C	2.82499900	-6.16991500	-0.21210600
C	3.69591200	-6.20623000	0.88919900
C	4.84428800	-5.41911200	0.92921900
C	5.17568900	-4.56118400	-0.13105600
C	4.38207700	-4.63599100	-1.28449900
C	3.23578800	-5.41862300	-1.32297800
C	6.12466500	-3.42223700	0.00574600
C	6.18779300	-2.71508500	1.21414700
C	6.67130500	-1.41170700	1.25958400
C	7.11792600	-0.75780200	0.10209900
C	7.25079900	-1.54250700	-1.05540700
C	6.76154500	-2.84334700	-1.10378500
C	7.12553300	0.73236100	0.05896700
C	6.75530500	1.39454700	-1.12097000
C	6.27756300	2.70137800	-1.09890400
C	6.13959300	3.40117900	0.10653500
C	6.71488700	2.81724700	1.24746700
C	7.20013400	1.51456600	1.22372100
C	5.16928700	4.52658900	0.20598500
C	4.32829600	4.57673100	1.32721900

C	3.18321500	5.36064900	1.33924000
C	2.81570500	6.14051100	0.23236500
C	3.71752000	6.18320800	-0.84275400
C	4.86748600	5.39401700	-0.85579300
C	0.69592600	6.61620600	-1.03037400
C	-0.69849400	6.61717800	-1.03042300
C	-1.42268600	6.65990300	0.16837100
C	-0.69537100	6.94164200	1.33750000
C	0.69316800	6.94021900	1.33759400
C	-2.81894000	6.14472800	0.23215200
C	-3.18777600	5.36636800	1.33968400
C	-4.33210200	4.58146400	1.32684700
C	-5.17090200	4.52854200	0.20405900
C	-4.86875000	5.39562800	-0.85789800
C	-3.71962300	6.18603200	-0.84396400
C	-6.13881700	3.40111200	0.10363300
C	-6.27542600	2.70160700	-1.10213100
C	-6.75173800	1.39423300	-1.12509100
C	-7.12157800	0.73080100	0.05427700
C	-7.19640600	1.51211800	1.21968400
C	-6.71299400	2.81539900	1.24424500
C	1.42009900	6.65737400	0.16851800
C	-7.11638600	-0.75948100	0.09604300
C	-6.67712900	-1.41646400	1.25456600
C	-6.19539200	-2.72064000	1.20903000
C	-6.12713500	-3.42527800	-0.00045500
C	-6.75877300	-2.84369800	-1.11162600

C	-7.24599300	-1.54223900	-1.06323000
C	-5.17720300	-4.56349100	-0.13686200
C	-4.37970100	-4.63371400	-1.28792000
C	-3.23305300	-5.41573900	-1.32547700
C	-2.82589200	-6.17097600	-0.21601000
C	-3.70007200	-6.21138700	0.88251700
C	-4.84881100	-5.42470300	0.92167700
C	-1.42217200	-6.66727200	-0.16430600
C	-0.69377400	-6.93808100	-1.33588800
C	0.69457600	-6.93781300	-1.33494000
C	1.42131800	-6.66673700	-0.16239500
C	0.69514100	-6.62284500	1.03428000
C	-0.69780100	-6.62301700	1.03335800
H	3.44989700	-6.82537400	1.75513300
H	5.46760100	-5.43653000	1.82651100
H	4.59342900	-3.97775500	-2.12948800
H	2.58862800	-5.34707000	-2.19874000
H	5.71942300	-3.13035000	2.10928200
H	6.55886500	-0.85382800	2.19075600
H	7.67729300	-1.10817800	-1.96231600
H	6.81463900	-3.39436300	-2.04573300
H	6.69695000	0.84167300	-2.06027000
H	5.86369400	3.11995900	-2.01870900
H	6.71797700	3.36474300	2.19290100
H	7.57386800	1.07635800	2.15176500
H	4.50713400	3.90336800	2.16739500
H	2.50547700	5.27468200	2.19011700

H	3.49900200	6.81259000	-1.70882100
H	5.51931100	5.42402200	-1.73232400
H	1.21699900	6.43347700	-1.97269200
H	-1.21975000	6.43452000	-1.97269200
H	-1.22328500	7.09392400	2.28155000
H	1.22130300	7.09138700	2.28170600
H	-2.51128600	5.28190500	2.19168700
H	-4.51140800	3.90891900	2.16756000
H	-5.51930800	5.42413600	-1.73541500
H	-3.50039700	6.81457600	-1.71044900
H	-5.86194300	3.12120300	-2.02166600
H	-6.69303700	0.84243600	-2.06496000
H	-7.56978900	1.07305200	2.14744200
H	-6.71703000	3.36223600	2.19003800
H	-6.56815400	-0.86061900	2.18736400
H	-5.73173800	-3.13817600	2.10560100
H	-6.80879400	-3.39310300	-2.05467400
H	-7.66824600	-1.10603300	-1.97119200
H	-4.58840000	-3.97236300	-2.13110400
H	-2.58290500	-5.34089400	-2.19875700
H	-3.45624300	-6.83326000	1.74712400
H	-5.47492400	-5.44517900	1.81696700
H	-1.22073800	-7.08571000	-2.28116800
H	1.22274800	-7.08531100	-2.27955800
H	1.21264800	-6.43562800	1.97758500
H	-1.21683200	-6.43570000	1.97586300
C	-2.84502100	-2.22026700	0.65309300

C	-3.52893900	-1.12415700	0.25720100
C	-3.70803400	0.02935100	-0.14080200
C	-3.47486900	1.29278300	-0.55919700
C	-2.84193100	2.29652800	-0.89223500
C	-1.82366400	3.13780100	-1.17885500
C	-0.65113800	3.49404800	-1.31426200
C	0.69985900	3.50979200	-1.33004000
C	1.84882000	3.08643600	-1.18646000
C	2.89432900	2.27290700	-0.92085900
C	3.47140600	1.23857400	-0.57832200
C	3.73930400	-0.01746200	-0.15886900
C	3.49362400	-1.15725100	0.24350200
C	2.83984400	-2.26658000	0.65398700
C	1.86837500	-2.97484000	0.93046800
C	0.59820400	-3.40255400	1.10098300
C	-0.63455800	-3.37409200	1.09199700
C	-1.91937100	-2.98285800	0.94244800

[11]CPP : cyclo[18]carbon

HF = -3226.8039601 a.u. (in ω B97X-D/def-TZVP// ω B97X-D/def2-SVP level)

C	-1.39484100	-7.24637100	-0.14172900
C	-0.79031900	-7.31573500	1.12199700
C	0.59174300	-7.32737800	1.26195000
C	1.43468600	-7.23747000	0.14523900
C	0.83059500	-7.31190600	-1.11840800
C	-0.55138000	-7.33233200	-1.25833300

C	2.86019000	-6.83839900	0.27298400
C	3.25566600	-6.04760600	1.36070200
C	4.45942000	-5.35718900	1.34796700
C	5.31409700	-5.41863200	0.23994200
C	4.99142600	-6.32078600	-0.78272700
C	3.79105900	-7.02385700	-0.76104600
C	6.33360000	-4.35113300	0.08843100
C	6.36529100	-3.62276400	-1.10718400
C	6.95879600	-2.36750100	-1.16049300
C	7.54673600	-1.80017800	-0.02227300
C	7.66898300	-2.60584900	1.11970000
C	7.06847900	-3.85830700	1.17602500
C	7.74547800	-0.32945000	0.02420600
C	7.32851400	0.36451400	1.16771300
C	7.10569300	1.73434900	1.13134700
C	7.28893900	2.46258700	-0.05096900
C	7.85690100	1.79668400	-1.14675900
C	8.08280500	0.42486500	-1.10926200
C	5.87270700	4.06492200	-1.31281300
C	4.93144500	5.08669300	-1.31307700
C	4.71935400	5.87038300	-0.17166300
C	5.59348100	5.69836200	0.91126300
C	6.53656000	4.67672800	0.91122600
C	3.45160700	6.63282200	-0.05398800
C	2.70482700	6.51529800	1.12576500
C	1.36511900	6.88009500	1.16322600
C	0.72111400	7.37787400	0.02293100

C	1.50598300	7.63195400	-1.11128000
C	2.84685500	7.26496300	-1.14973300
C	-0.76224900	7.37434400	-0.02199000
C	-1.40381600	6.87273200	-1.16195700
C	-2.74173400	6.50145200	-1.12430500
C	-3.48915700	6.61613700	0.05532700
C	-2.88747000	7.25192000	1.15068800
C	-1.54837400	7.62531100	1.11205100
C	-4.75343600	5.84793300	0.17314000
C	-4.96349300	5.06563100	1.31586800
C	-5.89872500	4.03829600	1.31577600
C	-6.65895700	3.75705400	0.17308200
C	-6.56196600	4.64201300	-0.91059400
C	-5.62492800	5.66911800	-0.91083700
C	6.63716000	3.79068100	-0.17120500
C	-7.30141300	2.42438000	0.05307200
C	-7.11256100	1.69711000	-1.12897200
C	-7.32643600	0.32587700	-1.16532500
C	-7.73974200	-0.37058900	-0.02204000
C	-8.08231600	0.38159400	1.11125600
C	-7.86545200	1.75487600	1.14870700
C	-7.53257100	-1.84012900	0.02443200
C	-6.94090100	-2.40403400	1.16242300
C	-6.34159600	-3.65654700	1.10925800
C	-6.30769500	-4.38555600	-0.08592800
C	-7.04543500	-3.89652300	-1.17329400
C	-7.65163900	-2.64679100	-1.11716100

C	-5.28377200	-5.44881000	-0.23736600
C	-4.43000300	-5.38437400	-1.34593600
C	-3.22275200	-6.06862400	-1.35844500
C	-2.82268800	-6.85591800	-0.26987000
C	-3.75233400	-7.04542800	0.76451300
C	-4.95629600	-6.34850900	0.78592900
H	-1.40502200	-7.27330700	2.02299300
H	1.01654900	-7.33600300	2.26751400
H	1.44506500	-7.26668500	-2.01943500
H	-0.97620200	-7.34457000	-2.26385500
H	2.56427000	-5.86801900	2.18525100
H	4.67969600	-4.66048200	2.15967900
H	5.66575500	-6.43487100	-1.63506300
H	3.55291800	-7.68762500	-1.59504600
H	5.80280700	-3.98220300	-1.97179800
H	6.84771100	-1.76894300	-2.06712200
H	8.18464700	-2.21923300	2.00196700
H	7.11502000	-4.43644200	2.10217600
H	7.05236700	-0.19062200	2.06643000
H	6.66126300	2.22090800	2.00208500
H	8.07147100	2.35062000	-2.06389800
H	8.47269800	-0.07788900	-1.99759200
H	5.92482800	3.39246800	-2.17180300
H	4.26549900	5.19252000	-2.17211600
H	5.49499800	6.33764400	1.79193800
H	7.16597200	4.52764100	1.79187100
H	3.14370800	6.02063500	1.99482700

H	0.78292200	6.66265100	2.06106900
H	1.04731800	8.07715700	-1.99737500
H	3.42089600	7.42543900	-2.06551300
H	-0.82053200	6.65746900	-2.05962200
H	-3.17816100	6.00415900	-1.99309900
H	-3.46232500	7.41038000	2.06630600
H	-1.09189900	8.07329800	1.99787700
H	-4.29979800	5.17690900	2.17595500
H	-5.94844700	3.36718300	2.17596100
H	-7.18897700	4.48776200	-1.79205500
H	-5.52864600	6.30736000	-1.79250500
H	-6.67069300	2.18640300	-1.99947400
H	-7.04619800	-0.22758500	-2.06381100
H	-8.46932500	-0.12367700	1.99942100
H	-8.08420400	2.30750400	2.06564600
H	-6.83207100	-1.80451200	2.06869300
H	-5.77684600	-4.01291800	1.97365800
H	-7.08998200	-4.47531400	-2.09913500
H	-8.16973400	-2.26297400	-1.99922700
H	-4.65415200	-4.68960400	-2.15825000
H	-2.53242300	-5.88633400	-2.18329800
H	-3.51042300	-7.70707800	1.59910700
H	-5.62969900	-6.46512100	1.63865400
C	0.62713000	3.64393200	-0.00550900
C	1.90985300	3.20340100	-0.01376900
C	2.84348500	2.39562100	-0.02206400
C	3.54579900	1.23495700	-0.03038700

C	3.73366500	0.01448900	-0.03162600
C	3.51317400	-1.32418200	-0.02853000
C	2.86318400	-2.37414000	-0.02504900
C	1.83112200	-3.25416900	-0.02081900
C	0.66127400	-3.64852800	-0.01215300
C	-0.69479800	-3.66773600	-0.00251600
C	-1.84504400	-3.21938400	0.00685800
C	-2.90091100	-2.36794700	0.01336500
C	-3.50075600	-1.28868200	0.01903600
C	-3.76052900	0.04293800	0.02407700
C	-3.51561300	1.25326200	0.02287600
C	-2.84769700	2.43397200	0.01600300
C	-1.87725700	3.19726600	0.00903000
C	-0.60704900	3.67270400	0.00200400

[12]CPP : cyclo[18]carbon

HF = -3457.8580604 a.u. (in ω B97X-D/def-TZVP// ω B97X-D/def2-SVP level)

C	5.13494600	-6.12457900	0.04911100
C	4.63185300	-6.78660800	-1.08110100
C	3.35560900	-7.33676700	-1.08062400
C	2.53196100	-7.25405800	0.05219100
C	3.08794000	-6.71734900	1.22027100
C	4.36206700	-6.16236700	1.21773700
C	1.07440800	-7.53180000	-0.01258100
C	0.34959400	-7.13993000	-1.14618600
C	-1.04002100	-7.13487900	-1.14340500

C	-1.76199500	-7.51942900	-0.00599100
C	-1.03902500	-8.00751200	1.09200100
C	0.35207600	-8.01437700	1.08842800
C	-3.21517900	-7.22019600	0.06794000
C	-3.73474900	-6.61555900	1.21991800
C	-4.99996400	-6.04038800	1.21785900
C	-5.79710200	-6.04832700	0.06492700
C	-5.32962100	-6.76831500	-1.04420300
C	-4.06191700	-7.34149600	-1.04340600
C	-6.95166200	-5.11606300	-0.01862600
C	-7.11210100	-4.33746600	-1.17244000
C	-7.90927800	-3.19949500	-1.16308700
C	-8.57842000	-2.79452200	0.00001700
C	-8.54849200	-3.66340600	1.10107200
C	-7.74920300	-4.80236700	1.09212300
C	-8.70514100	-0.66120100	1.26559900
C	-8.69154000	0.72820100	1.26528000
C	-8.99830600	1.45329800	0.10598100
C	-9.49154300	0.73643100	-0.99471500
C	-9.50516900	-0.65492500	-0.99440200
C	-8.52501700	2.85862500	-0.00107900
C	-7.85005100	3.25203700	-1.16481100
C	-7.03570600	4.37781100	-1.17578300
C	-6.86296700	5.15505200	-0.02287100
C	-7.66308500	4.85354700	1.08934400
C	-8.47984700	3.72708700	1.09975200
C	-5.69787000	6.07427600	0.05760100

C	-4.89652500	6.05620400	1.20745200
C	-3.62767700	6.62320900	1.20713200
C	-3.10879100	7.23005400	0.05603500
C	-3.95774000	7.35901300	-1.05270600
C	-5.22887200	6.79346700	-1.05135400
C	-1.65509100	7.52604900	-0.01943100
C	-0.93546400	7.14587600	-1.16016900
C	0.45421100	7.14639300	-1.16417800
C	1.18164700	7.52876300	-0.02883200
C	0.46193400	8.01007600	1.07417000
C	-0.92934700	8.00788700	1.07928000
C	-9.02600500	-1.38074800	0.10663500
C	2.63484900	7.23048900	0.03926500
C	3.17653800	6.68199700	1.20931100
C	4.43922500	6.10088600	1.21134000
C	5.21493100	6.04531600	0.04493700
C	4.72850300	6.71636600	-1.08696900
C	3.46386100	7.29464600	-1.09054200
C	6.35907000	5.09990700	-0.02464200
C	6.54418300	4.33355600	-1.18334700
C	7.33063100	3.18815500	-1.16919600
C	7.96554900	2.75981300	0.00460900
C	7.91083200	3.61374400	1.11660300
C	7.12369600	4.76044100	1.10198300
C	8.41181700	1.34608200	0.10414700
C	8.11037600	0.62149700	1.26477300
C	8.10626600	-0.76778300	1.26201700

C	8.40502600	-1.49023500	0.09869400
C	8.87558500	-0.76656300	-1.00770100
C	8.87835500	0.62427600	-1.00502100
C	7.95411600	-2.90254200	-0.00298500
C	7.87972400	-3.74884200	1.11390500
C	7.07052600	-4.87918300	1.10313500
C	6.30283400	-5.20859600	-0.02478600
C	6.51640200	-4.46020000	-1.19011000
C	7.32635800	-3.33140600	-1.17959900
H	5.23179000	-6.83527200	-1.99269700
H	2.97663200	-7.80830300	-1.99035200
H	2.47540600	-6.63176400	2.12044700
H	4.71295400	-5.64963900	2.11558000
H	0.87900100	-6.74306800	-2.01517800
H	-1.57167900	-6.73462600	-2.00945500
H	-1.57464300	-8.36063500	1.97651400
H	0.88773900	-8.37531400	1.96964100
H	-3.10005000	-6.50003400	2.10136000
H	-5.32872400	-5.48159400	2.09671400
H	-5.94996700	-6.84284100	-1.94063100
H	-3.70698500	-7.85895700	-1.93799400
H	-6.50920900	-4.55245600	-2.05731800
H	-7.90931300	-2.54860700	-2.03994600
H	-9.11195700	-3.41293100	2.00322200
H	-7.70035400	-5.42834100	1.98647800
H	-8.33219600	-1.19123800	2.14455100
H	-8.30837800	1.25122300	2.14403300

H	-9.80803100	1.27356200	-1.89219200
H	-9.83199100	-1.18616400	-1.89168200
H	-7.86112400	2.60068300	-2.04125600
H	-6.43083400	4.58367900	-2.06151200
H	-7.60370800	5.47936400	1.98317200
H	-9.04637300	3.48599900	2.00253000
H	-5.22628200	5.49682000	2.08556800
H	-2.99062700	6.50042900	2.08587200
H	-3.60258800	7.87746400	-1.94662600
H	-5.85177400	6.87463600	-1.94543100
H	-1.46955000	6.75252900	-2.02796100
H	0.98119700	6.75006600	-2.03469500
H	0.99918500	8.36419300	1.95717700
H	-1.46273700	8.35870500	1.96603200
H	2.55955800	6.60845000	2.10742700
H	4.77675800	5.58122700	2.11030000
H	5.33090900	6.74956300	-1.99767900
H	3.09767400	7.77187200	-2.00253700
H	5.96588500	4.56061900	-2.08109100
H	7.34551700	2.55036600	-2.05530300
H	8.44883500	3.34864500	2.02982800
H	7.06169300	5.37426100	2.00360800
H	7.74208300	1.14517700	2.14922300
H	7.73607500	-1.29268000	2.14496800
H	9.18725100	-1.29818100	-1.90990900
H	9.19133800	1.15800800	-1.90555400
H	8.41673100	-3.48728500	2.02871400

H	6.99162200	-5.48548100	2.00845800
H	5.94148200	-4.68348900	-2.09107900
H	7.35891700	-2.70145900	-2.07080900
C	-0.46597700	-3.24351800	-0.25001000
C	-1.50395400	-2.37270200	-0.27300800
C	-2.09299300	-1.28814500	-0.27698100
C	-2.36565900	0.03942400	-0.26828100
C	-2.16709600	1.25721300	-0.24474600
C	-1.56891900	2.47294000	-0.20758100
C	-0.64062400	3.28514800	-0.16348100
C	0.60759800	3.80994900	-0.11037300
C	1.84061600	3.77799900	-0.06441400
C	3.11626800	3.32666800	-0.01940900
C	4.03402100	2.50265400	0.01349300
C	4.73565000	1.34518300	0.03328600
C	4.94568900	0.12936500	0.03295200
C	4.77051300	-1.21312900	0.01439600
C	4.17411200	-2.29247700	-0.03081800
C	3.18760500	-3.21774600	-0.10133200
C	2.03579600	-3.65657700	-0.16337300
C	0.68247800	-3.69449800	-0.21643500

[13]CPP : cyclo[18]carbon

HF = -3688.9136548 a.u. (in ω B97X-D/def-TZVP// ω B97X-D/def2-SVP level)

C	-4.42841100	-7.55568700	1.34292900
C	-3.09057900	-7.91143600	1.21255300

C	-7.71549300	-4.68458100	1.45432900
C	-6.68277400	-5.61285800	1.44671800
C	-10.37574500	-1.37183400	1.30865900
C	-9.99793400	-2.70978500	1.35553200
C	-9.14403700	2.83324800	1.27268100
C	-9.57899900	1.51477600	1.32290600
C	-7.08963000	6.57174000	0.98709800
C	-8.15104900	5.67267400	1.01878400
C	-2.78780400	7.53007800	1.14160400
C	-4.13633300	7.19344800	1.12649800
C	1.47589300	8.32048900	1.08224000
C	0.09454700	8.48438600	1.04874800
C	5.29342200	6.09072000	1.33913900
C	4.06112800	6.73329800	1.30100400
C	-5.19832200	-7.20192900	0.22541000
C	-4.60942500	-7.36713700	-1.03669700
C	-3.27831400	-7.74463300	-1.16824200
C	-2.46774900	-7.95232800	-0.04328500
C	-8.59598300	-4.57203100	0.37008900
C	-8.48686100	-5.52135600	-0.65570000
C	-7.45866100	-6.46008700	-0.65609600
C	-6.49066300	-6.47784900	0.36024200
C	-10.16292000	-0.60107400	0.15530800
C	-9.72440500	-1.26870700	-0.99660300
C	-9.35460100	-2.60823200	-0.95276800
C	-9.40266000	-3.32974700	0.24712500
C	-9.22520200	3.57622500	0.08746700

C	-9.90554500	2.99826100	-0.99465400
C	-10.34535300	1.67882200	-0.94244900
C	-10.11672300	0.88506700	0.19182800
C	-6.22312600	6.62866600	-0.11464400
C	-6.54750800	5.85358300	-1.23606800
C	-7.60807300	4.95580000	-1.20475800
C	-8.38676200	4.79599600	-0.05045500
C	-2.14199600	7.97831600	-0.01805500
C	-2.92592200	8.18367100	-1.16262100
C	-4.27635800	7.84915500	-1.17682500
C	-4.89514300	7.29299100	-0.04787100
C	2.15840300	7.71990400	0.01507100
C	1.41517200	7.36900700	-1.12021000
C	0.03519900	7.53167000	-1.15316000
C	-0.65848300	8.05266400	-0.05242900
C	6.10044900	5.99690400	0.19636200
C	5.67355900	6.67855400	-0.95310600
C	4.43784900	7.31487800	-0.99445800
C	3.58078600	7.30529200	0.11563500
C	8.69755100	3.48429100	1.34043800
C	7.92830600	4.64347400	1.31369100
C	8.87879700	-0.90657400	1.40477000
C	8.90228700	0.48296200	1.44149700
C	7.76860200	-5.01197100	1.07725500
C	8.59117100	-3.89230700	1.14707800
C	3.83875500	-6.97803100	1.08182300
C	5.09436500	-6.38088600	1.11149800

C	8.78835200	2.64934600	0.21652600
C	8.20174600	3.10537300	-0.97229100
C	7.43408300	4.26266400	-0.99863800
C	7.21724600	5.01673700	0.16278400
C	9.17597700	-1.60359600	0.22582100
C	9.67833700	-0.86057100	-0.85353600
C	9.70271700	0.52899400	-0.81597700
C	9.22431100	1.23106300	0.30127900
C	7.00657500	-5.28235700	-0.07015600
C	7.23003000	-4.47470900	-1.19373300
C	8.05501900	-3.35972000	-1.12588000
C	8.68965400	-2.99903800	0.07010900
C	3.28118700	-7.42156400	-0.12358600
C	4.07937400	-7.35836100	-1.27468100
C	5.34078700	-6.77624700	-1.24021200
C	5.84802000	-6.21419500	-0.05890000
C	-0.18757800	-8.68232300	0.79355600
C	1.19825200	-8.54866100	0.78263900
C	-0.98753500	-8.03306600	-0.15889700
C	-0.33424700	-7.31637900	-1.17193200
C	1.04907900	-7.19715200	-1.19409500
C	1.84054700	-7.77469900	-0.19314100
H	-4.86262100	-7.49549200	2.34315600
H	-2.50266700	-8.08655400	2.11608900
H	-7.76805500	-3.95732600	2.26746600
H	-5.95151200	-5.58645200	2.25656600
H	-10.78488000	-0.90172300	2.20612900

H	-10.11111800	-3.26685200	2.28888300
H	-8.62167800	3.25023700	2.13639800
H	-9.38369000	0.93118600	2.22483400
H	-6.90307900	7.20947600	1.85453600
H	-8.77836700	5.61663900	1.91176400
H	-2.20570400	7.35096200	2.04834800
H	-4.58241500	6.75360300	2.02109100
H	2.03299900	8.64726100	1.96355100
H	-0.41212500	8.93717700	1.90438200
H	5.58150000	5.56158000	2.24967100
H	3.41861500	6.70136400	2.18369900
H	-5.17594400	-7.11983200	-1.93677500
H	-2.84915100	-7.82379100	-2.16925200
H	-9.19067400	-5.49664600	-1.49141400
H	-7.38347000	-7.16233300	-1.48952200
H	-9.54930200	-0.70456400	-1.91508100
H	-8.90191300	-3.06320900	-1.83673400
H	-10.04484700	3.57236300	-1.91400300
H	-10.82380100	1.24133200	-1.82202700
H	-5.89434300	5.87021600	-2.11124600
H	-7.76082100	4.28719000	-2.05475000
H	-2.46379700	8.58420500	-2.06812600
H	-4.85276500	7.99094900	-2.09416800
H	1.91338000	6.88158700	-1.96114900
H	-0.52267200	7.16951500	-2.01961000
H	6.30124700	6.68033700	-1.84702400
H	4.11881900	7.80419300	-1.91771400

H	9.19492300	3.19784700	2.27006300
H	7.84126100	5.24333400	2.22256000
H	8.49044700	-1.44806200	2.26996300
H	8.53019000	0.98953300	2.33432300
H	7.68067200	-5.65998000	1.95221500
H	9.12461600	-3.68068100	2.07685600
H	3.24052700	-7.01085500	1.99540800
H	5.44640000	-5.94700500	2.04952100
H	8.24091800	2.48294000	-1.86829500
H	6.89650500	4.51191700	-1.91541100
H	9.99495900	-1.37472000	-1.76409100
H	10.03934100	1.07885900	-1.69797900
H	6.65776700	-4.64436700	-2.10759900
H	8.10035500	-2.68861900	-1.98583400
H	3.69226800	-7.74723900	-2.21956000
H	5.92478300	-6.72292400	-2.16151600
H	-0.65594500	-9.28842900	1.57241600
H	1.79242600	-9.04336000	1.55492300
H	-0.91880800	-6.77338400	-1.91682200
H	1.51844300	-6.57298600	-1.95798000
C	0.59178500	-3.28253400	-0.74932100
C	-0.44199500	-2.43010100	-0.95063700
C	-1.04175500	-1.35725100	-1.06048100
C	-1.34054900	-0.03632700	-1.10538600
C	-1.17645400	1.18569700	-1.05688400
C	-0.62650600	2.41780600	-0.93082700
C	0.25668300	3.25867000	-0.74117200

C	1.46116300	3.82708700	-0.49211800
C	2.67099600	3.82639500	-0.24722500
C	3.92957000	3.39581200	0.00288400
C	4.83716900	2.58027500	0.18493400
C	5.54341800	1.43429200	0.32195000
C	5.77449500	0.22324200	0.36323800
C	5.64257000	-1.12342600	0.33126700
C	5.10008700	-2.22463700	0.20908000
C	4.16426600	-3.18012700	-0.00308800
C	3.05068900	-3.65245300	-0.24640800
C	1.72554400	-3.71364400	-0.52157200

[14]CPP : cyclo[18]carbon

HF = -3919.9732402 a.u. (in ω B97X-D/def-TZVP// ω B97X-D/def2-SVP level)

C	10.36272700	0.68897100	-0.91818500
C	10.36015900	-0.70120200	-0.91763800
C	8.06436000	4.40720800	-1.09505400
C	8.83933600	3.25446700	-1.07330500
C	5.12932600	7.53789400	-1.04205700
C	6.34647200	6.86537600	-1.02977400
C	0.74299900	8.01737500	-1.09575500
C	2.10650100	7.74734000	-1.09126700
C	-3.52002100	8.78603900	-1.05102300
C	-2.14076200	8.96729200	-1.05500100
C	-7.22473100	6.39702000	-1.09150200
C	-6.03514900	7.11513900	-1.11079500

C	-10.56475100	3.71494900	-0.92935900
C	-9.85064400	4.90902300	-0.93789800
C	-10.61437100	-0.68630200	-1.06444200
C	-10.61328200	0.70327500	-1.06397700
C	9.92454200	1.41413200	0.20089200
C	9.66594900	0.69117600	1.37322700
C	9.66358100	-0.69923800	1.37378600
C	9.91946700	-1.42395300	0.20199700
C	7.88657000	5.18290500	0.05860100
C	8.63825600	4.83524100	1.19140200
C	9.41573600	3.68177400	1.21251000
C	9.47243200	2.82639300	0.10192700
C	4.29859200	7.55202800	0.08772600
C	4.78231000	6.95319900	1.25823200
C	5.99646500	6.27663900	1.26800800
C	6.77960800	6.17261400	0.11000300
C	0.11540200	8.59207300	0.01777200
C	0.92020500	8.95591800	1.10649700
C	2.28546000	8.68727700	1.11042600
C	2.89845500	8.04347200	0.02636500
C	-4.18029100	8.28319100	0.07948800
C	-3.41871600	8.07149900	1.23702400
C	-2.04085000	8.25670000	1.23461500
C	-1.36779900	8.65775600	0.07318300
C	-8.01356600	6.33320000	0.06523200
C	-7.62590400	7.11872100	1.16042100
C	-6.43517500	7.83857700	1.14057700

C	-5.58497600	7.80049000	0.02553400
C	-10.52344000	2.85636800	0.17926200
C	-9.86144700	3.31179600	1.32760500
C	-9.14936800	4.50539400	1.31972400
C	-9.06939400	5.29155700	0.16256100
C	-10.92459700	-1.40997000	0.09489600
C	-11.38023100	-0.68745200	1.20773500
C	-11.37913400	0.70412100	1.20820300
C	-10.92236900	1.42666000	0.09584300
C	-9.85829400	-4.89337500	-0.94104000
C	-10.57047400	-3.69815200	-0.93180200
C	-6.04647000	-7.10597000	-1.11470700
C	-7.23488700	-6.38591200	-1.09522900
C	-2.15500000	-8.96496400	-1.05860700
C	-3.53396200	-8.78137900	-1.05490100
C	2.09464700	-7.75275400	-1.09396800
C	0.73074800	-8.02083600	-1.09902900
C	-9.07779600	-5.27789500	0.15926000
C	-9.15660500	-4.49232500	1.31690700
C	-9.86675400	-3.29758700	1.32548700
C	-10.52791600	-2.84035800	0.17738300
C	-5.59751200	-7.79246000	0.02141200
C	-6.44789000	-7.82965300	1.13634700
C	-7.63745800	-7.10789900	1.15636000
C	-8.02371000	-6.32126100	0.06147300
C	-1.38170900	-8.65659100	0.06967500
C	-2.05430400	-8.25418400	1.23090800

C	-3.43185300	-8.06670800	1.23307000
C	-4.19359300	-8.27734900	0.07545700
C	2.88545300	-8.04879600	0.02450200
C	2.27091700	-8.69089300	1.10869100
C	0.90530100	-8.95763400	1.10416600
C	0.10162600	-8.59347500	0.01471700
C	6.33506000	-6.87297700	-1.02916900
C	5.11785900	-7.54549200	-1.04212600
C	8.82670400	-3.26048000	-1.07102100
C	8.05082700	-4.41257600	-1.09315100
C	9.46230100	-2.83461000	0.10370800
C	9.40513800	-3.69056500	1.21382200
C	8.62665500	-4.84345200	1.19231000
C	7.87428100	-5.18983200	0.05964300
C	6.76713500	-6.17933400	0.11048500
C	5.98278000	-6.28231300	1.26778700
C	4.76845800	-6.95857300	1.25724600
C	4.28590700	-7.55842700	0.08674600
H	10.65239700	1.21924700	-1.82831500
H	10.64775200	-1.23327100	-1.82738800
H	7.49391100	4.63855500	-1.99672200
H	8.84982600	2.61443200	-1.95760200
H	4.80608100	8.04343300	-1.95506100
H	6.95648300	6.85335800	-1.93586100
H	0.14044100	7.70439000	-1.95138800
H	2.54926400	7.22605100	-1.94297800
H	-4.09150600	9.01228000	-1.95433200

H	-1.65055600	9.33289200	-1.96052600
H	-7.49146700	5.79105000	-1.96008600
H	-5.39693900	7.05749600	-1.99514600
H	-11.12419900	3.42033100	-1.82055500
H	-9.86165500	5.53255300	-1.83518600
H	-10.25407600	-1.21405900	-1.95006700
H	-10.25216000	1.23105900	-1.94925000
H	9.32844900	1.21531300	2.26966600
H	9.32438700	-1.22156700	2.27063100
H	8.57964900	5.45348700	2.09020000
H	9.94856400	3.41688100	2.12873100
H	4.15742000	6.93719500	2.15396100
H	6.29030100	5.73505100	2.16949200
H	0.46693400	9.44403600	1.97262300
H	2.88498700	8.96985700	1.97908600
H	-3.89781400	7.66780700	2.13164600
H	-1.46739200	7.99886200	2.12788400
H	-8.24685500	7.13619600	2.05938900
H	-6.14256900	8.41206500	2.02341600
H	-9.80530600	2.66921200	2.20888000
H	-8.55333300	4.77162500	2.19537600
H	-11.69192000	-1.22184000	2.10847300
H	-11.68997600	1.23839900	2.10929700
H	-9.87022800	-5.51631100	-1.83872800
H	-11.12936200	-3.40206500	-1.82286400
H	-5.40805400	-7.04902500	-1.99895800
H	-7.50056400	-5.77916100	-1.96359300

H	-1.66527500	-9.33155000	-1.96399300
H	-4.10568000	-9.00676800	-1.95827700
H	2.53879700	-7.23307400	-1.94592800
H	0.12915400	-7.70796400	-1.95538700
H	-8.56110000	-4.76006500	2.19245800
H	-9.80966600	-2.65567100	2.20718800
H	-6.15627600	-8.40396600	2.01897900
H	-8.25853500	-7.12475900	2.05525100
H	-1.48059900	-7.99713400	2.12424000
H	-3.91042400	-7.66206600	2.12754400
H	2.86949800	-8.97348400	1.97800000
H	0.45084200	-9.44435800	1.97045200
H	6.94600500	-6.86158800	-1.93464900
H	4.79546100	-8.05166700	-1.95507600
H	8.83688800	-2.61948900	-1.95462700
H	7.47901300	-4.64251100	-1.99432000
H	9.93908100	-3.42695200	2.12977300
H	8.56812800	-5.46238200	2.09065100
H	6.27583800	-5.74000900	2.16908400
H	4.14254800	-6.94155000	2.15224300
C	1.89667300	-3.60289100	-0.79169400
C	0.78456500	-2.89521500	-1.10642600
C	0.08007400	-1.90249000	-1.30903100
C	-0.35118800	-0.62418100	-1.43670100
C	-0.32513400	0.60940000	-1.43626100
C	0.06773800	1.90233900	-1.33379600
C	0.81469100	2.86316900	-1.13005600

C	1.90151300	3.61559600	-0.83114600
C	3.07440600	3.81599200	-0.50245600
C	4.35974500	3.59019500	-0.14088300
C	5.34221600	2.90099000	0.14616000
C	6.15810800	1.84881000	0.38777300
C	6.50657400	0.67027900	0.49311600
C	6.52388800	-0.68264000	0.50538300
C	6.12863000	-1.84590000	0.39871700
C	5.34474400	-2.92740700	0.17939700
C	4.33521900	-3.57546300	-0.10695600
C	3.05888300	-3.85746700	-0.46349200