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Supporting information for article:

Cyclic networks of halogen bonding interactions in molecular self-assemblies: A theoretical N-X...N vs C-X...N investigation

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Table S1 wB97X-D/DGDZVP Total energies and zero-point energies, both in Hartrees.

C-X...N	Monomer		Dimer		Trimer	
	E	ZPVE	E	ZPVE	E	ZPVE
X						
Cl	-3121.062287	0.264581	-6242.127591	0.529520	-9363.192830	0.794719
Br	-11575.353337	0.262158	-23150.716375	0.524826	-34726.079382	0.787598
I	-28960.525573	0.260539	-57921.068711	0.521914	-86881.611835	0.783316

N-X...N	Monomer		Dimer		Trimer	
	E	ZPVE	E	ZPVE	E	ZPVE
X						
Cl	-3120.848133	0.262108	-6241.710753	0.525530	-9362.573383	0.788969
Br	-11575.174244	0.259860	-23150.379121	0.521401	-34725.584019	0.783169
I	-28960.390683	0.258315	-57920.840484	0.519670	-86881.290293	N/A*

* ZPVE calculations of the N-I...N trimer exceeded our computer resources.

Na⁺@N-I...N Complexes

System	E
2Na ⁺ @trimer	-87043.417464
Na ⁺ @trimer	-87205.506421
Na ⁺ @dimer	-58082.967271
Na ⁺	-162.052054

Table S2 w B97X-D/DGDZVP Counterpoise-corrected energies, and basis set superposition errors (BSSE). All in Hartrees**C-X...N**

Dimer			
X	Ecomplex	E (sum of monomers)	BSSE
Cl	-6242.126942	-6242.124531	0.0006496
Br	-23150.71537	-23150.70650	0.001003
I	-57921.06685	-57921.05078	0.001859
Trimer			
X	Ecomplex	E (sum of monomers)	BSSE
Cl	-9363.19153	-9363.18681	0.001296
Br	-34726.07738	-34726.05973	0.002001
I	-86881.60812	-86881.57598	0.003711

Table S3 w B97X-D/DGDZVP Counterpoise-corrected energies, and basis set superposition errors (BSSE). All in Hartrees**N-X...N**

Dimer			
X	Ecomplex	E (sum of monomers)	BSSE
Cl	-6241.709539	-6241.695786	0.001231
Br	-23150.377032	-23150.345495	0.002089
I	-57920.834422	-57920.716572	0.006061
Trimer			
X	Ecomplex	E (sum of monomers)	BSSE
Cl	-9362.570902	-9362.543381	0.002481
Br	-34725.579841	-34725.516727	0.004178
I	-86881.278106	-86881.038775	0.012187

Table S4 Table S4: w B97X-D/DGDZVP Counterpoise-corrected energies, and basis set superposition errors (BSSE). All in Hartrees.**Na⁺@N-I...N complexes**

Dimer			
	Ecomplex	E (sum of monomers)	BSSE
Na ⁺	-58082.969291	-58082.894039	0.001785
Trimer			
	Ecomplex	E (sum of monomers)	BSSE
Na ⁺	-87043.421326	-87043.345086	0.001821
2Na ⁺	-87205.508599	-87205.395284	0.003591

ω B97X-D/DGDZVP optimized cartesian coordinates of the compounds presented in the manuscript.

C-Br...N_Dimer

0	1			
C	11.55365197	-2.15360805	0.00000000	
H	10.78503795	-4.12773705	0.00000000	
C	12.31882800	5.32808994	0.00000000	
H	10.08303300	5.50535095	0.00000000	
C	10.33144697	-1.43103605	0.00000000	
C	9.26285397	-0.85907804	0.00000000	
C	9.95612299	2.74355895	0.00000000	
C	9.00576599	1.99828496	0.00000000	
C	7.86596098	1.14445897	0.00000000	
C	7.98880298	-0.22266803	0.00000000	
C	11.01087200	4.95549095	0.00000000	
N	12.77775097	-1.64712206	0.00000000	
N	13.15057800	4.22293694	0.00000000	
H	12.72301501	6.33003994	0.00000000	
H	13.22372395	-4.93165906	0.00000000	
C	12.90619396	-3.90125006	0.00000000	
C	4.29726899	3.06700999	0.00000000	
H	5.05758300	5.04455498	0.00000000	
C	-4.29726899	-3.06700999	0.00000000	
H	-5.05758300	-5.04455498	0.00000000	
C	3.53112595	-4.40105501	0.00000000	
H	5.76617195	-4.57712602	0.00000000	
C	-3.53112595	4.40105501	0.00000000	
H	-5.76617195	4.57712602	0.00000000	
C	5.89518797	-1.81732002	0.00000000	
C	6.84805097	-1.07571503	0.00000000	
C	5.52204799	2.34956698	0.00000000	
C	6.59221899	1.78005197	0.00000000	
C	-5.52204799	-2.34956698	0.00000000	
C	-6.59221899	-1.78005197	0.00000000	
C	-5.89518797	1.81732002	0.00000000	
C	-6.84805097	1.07571503	0.00000000	
C	4.83838196	-4.02733702	0.00000000	
C	-4.83838196	4.02733702	0.00000000	
N	-3.07527904	-2.55528998	0.00000000	
N	2.70263496	-3.29443900	0.00000000	
N	3.07527904	2.55528998	0.00000000	
N	-2.70263496	3.29443900	0.00000000	
H	2.61633201	5.83504099	0.00000000	
H	-3.12440699	5.40183103	0.00000000	
H	-2.61633201	-5.83504099	0.00000000	
H	3.12440699	-5.40183103	0.00000000	
C	2.93742900	4.80560599	0.00000000	
C	-2.93742900	-4.80560599	0.00000000	
Br	15.47281896	-2.52844707	0.00000000	
Br	12.84628298	1.39052594	0.00000000	
Br	0.36900699	3.42890201	0.00000000	
Br	3.00033597	-0.46225601	0.00000000	
Br	-0.36900699	-3.42890201	0.00000000	
Br	-3.00033597	0.46225601	0.00000000	
C	12.36368299	3.19220594	0.00000000	
C	13.60710096	-2.71982006	0.00000000	
C	2.23538900	3.62275800	0.00000000	
C	-3.48815701	2.26014203	0.00000000	
C	-2.23538900	-3.62275800	0.00000000	
C	3.48815701	-2.26014203	0.00000000	
N	11.02528699	3.56123095	0.00000000	
N	11.59062396	-3.51936505	0.00000000	
N	4.25517900	4.43233099	0.00000000	
N	-4.82362701	2.63324104	0.00000000	
N	-4.25517900	-4.43233099	0.00000000	
N	4.82362701	-2.63324104	0.00000000	
C	-11.55365197	2.15360805	0.00000000	
H	-10.78503795	4.12773705	0.00000000	
C	-12.31882800	-5.32808994	0.00000000	
H	-10.08303300	-5.50535095	0.00000000	
C	-9.95612299	-2.74355895	0.00000000	
C	-9.00576599	-1.99828496	0.00000000	

C	-10.33144697	1.43103605	0.00000000
C	-9.26285397	0.85907804	0.00000000
C	-7.98880298	0.22266803	0.00000000
C	-7.86596098	-1.14445897	0.00000000
C	-11.01087200	-4.95549095	0.00000000
N	-13.15057800	-4.22293694	0.00000000
N	-12.77775097	1.64712206	0.00000000
H	-13.22372395	4.93165906	0.00000000
H	-12.72301501	-6.33003994	0.00000000
C	-12.90619396	3.90125006	0.00000000
Br	-15.47281896	2.52844707	0.00000000
Br	-12.84628298	-1.39052594	0.00000000
C	-13.60710096	2.71982006	0.00000000
C	-12.36368299	-3.19220594	0.00000000
N	-11.59062396	3.51936505	0.00000000
N	-11.02528699	-3.56123095	0.00000000

C-Br...N_Trimer

0 1

C	-19.41095401	-2.33817804	0.00000000
H	-18.57741401	-4.28584304	0.00000000
C	-20.43738000	5.11199196	0.00000000
H	-18.20940400	5.36974296	0.00000000
C	-18.21378701	-1.57483404	0.00000000
C	-17.16644001	-0.96482804	0.00000000
C	-17.98348900	2.61346396	0.00000000
C	-17.00869100	1.90042496	0.00000000
C	-15.84006201	1.08631996	0.00000000
C	-15.91536501	-0.28428804	0.00000000
C	-19.11681700	4.78679096	0.00000000
N	-20.65117501	-1.87257704	0.00000000
N	-21.22879900	3.97762996	0.00000000
H	-20.87729900	6.09878096	0.00000000
H	-20.98823301	-5.16998204	0.00000000
C	-20.70497401	-4.12963504	0.00000000
C	-12.33833800	3.12855996	0.00000000
H	-13.16124000	5.08103596	0.00000000
C	-3.53883901	-2.72948505	0.00000000
H	-2.71367301	-4.68066605	0.00000000
C	-11.31893201	-4.31001604	0.00000000
H	-13.54667601	-4.56247804	0.00000000
C	-4.56107500	4.70792995	0.00000000
H	-2.33329800	4.96087595	0.00000000
C	-13.76961501	-1.80812804	0.00000000
C	-14.74610401	-1.09788004	0.00000000
C	-13.53925000	2.37184396	0.00000000
C	-14.58911400	1.76566396	0.00000000
C	-2.33832201	-1.97184805	0.00000000
C	-1.28858501	-1.36548705	0.00000000
C	-2.10937400	2.20698495	0.00000000
C	-1.13217501	1.49778095	0.00000000
C	-12.63822201	-3.98129604	0.00000000
C	-3.24168100	4.37956995	0.00000000
N	-4.77699001	-2.25848105	0.00000000
N	-10.52874301	-3.17575804	0.00000000
N	-11.10065500	2.65614896	0.00000000
N	-5.35095500	3.57337595	0.00000000
H	-10.74641600	5.94876096	0.00000000
H	-5.00201900	5.69410595	0.00000000
H	-5.12791801	-5.55166905	0.00000000
H	-10.87822301	-5.29629704	0.00000000
C	-11.03457300	4.90962396	0.00000000
C	-4.84097101	-4.51221405	0.00000000
Br	-23.31562601	-2.84241303	0.00000000
Br	-20.82339701	1.15832796	0.00000000
Br	-8.42355100	3.61463896	0.00000000
Br	-10.92268201	-0.35561304	0.00000000
Br	-7.45303601	-3.21939004	0.00000000
Br	-4.95582401	0.75332995	0.00000000
C	-20.40517200	2.97594596	0.00000000
C	-21.44458601	-2.97205504	0.00000000
C	-10.29510300	3.74974796	0.00000000
C	-4.52995600	2.56685195	0.00000000
C	-5.58125501	-3.35320905	0.00000000

C	-11.34914301	-2.16891904	0.00000000
N	-19.08093900	3.39289496	0.00000000
N	-19.40267901	-3.70445004	0.00000000
N	-12.33980300	4.49461196	0.00000000
N	-3.20828800	2.98583795	0.00000000
N	-3.53594501	-4.09548405	0.00000000
N	-12.67117501	-2.58745004	0.00000000
C	3.53883901	2.72948505	0.00000000
H	2.71367301	4.68066605	0.00000000
C	12.33833800	-3.12855996	0.00000000
H	13.16124000	-5.08103596	0.00000000
C	4.56107500	-4.70792995	0.00000000
H	2.33329800	-4.96087595	0.00000000
C	11.31893201	4.31001604	0.00000000
H	13.54667601	4.56247804	0.00000000
C	2.10937400	-2.20698495	0.00000000
C	1.13217501	-1.49778095	0.00000000
C	2.33832201	1.97184805	0.00000000
C	1.28858501	1.36548705	0.00000000
C	13.53925000	-2.37184396	0.00000000
C	14.58911400	-1.76566396	0.00000000
C	13.76961501	1.80812804	0.00000000
C	14.74610401	1.09788004	0.00000000
C	15.91536501	0.28428804	0.00000000
C	15.84006201	-1.08631996	0.00000000
C	0.03801099	0.68526395	0.00000000
C	-0.03801099	-0.68526395	0.00000000
C	3.24168100	-4.37956995	0.00000000
C	12.63822201	3.98129604	0.00000000
N	11.10065500	-2.65614896	0.00000000
N	5.35095500	-3.57337595	0.00000000
N	4.77699001	2.25848105	0.00000000
N	10.52874301	3.17575804	0.00000000
H	5.12791801	5.55166905	0.00000000
H	10.87822301	5.29629704	0.00000000
H	10.74641600	-5.94876096	0.00000000
H	5.00201900	-5.69410595	0.00000000
C	4.84097101	4.51221405	0.00000000
C	11.03457300	-4.90962396	0.00000000
C	19.41095401	2.33817804	0.00000000
H	18.57741401	4.28584304	0.00000000
C	20.43738000	-5.11199196	0.00000000
H	18.20940400	-5.36974296	0.00000000
C	17.98348900	-2.61346396	0.00000000
C	17.00869100	-1.90042496	0.00000000
C	18.21378701	1.57483404	0.00000000
C	17.16644001	0.96482804	0.00000000
C	19.11681700	-4.78679096	0.00000000
N	21.22879900	-3.97762996	0.00000000
N	20.65117501	1.87257704	0.00000000
H	20.98823301	5.16998204	0.00000000
H	20.87729900	-6.09878096	0.00000000
C	20.70497401	4.12963504	0.00000000
Br	7.45303601	3.21939004	0.00000000
Br	4.95582401	-0.75332995	0.00000000
Br	8.42355100	-3.61463896	0.00000000
Br	10.92268201	0.35561304	0.00000000
Br	23.31562601	2.84241303	0.00000000
Br	20.82339701	-1.15832796	0.00000000
C	5.58125501	3.35320905	0.00000000
C	11.34914301	2.16891904	0.00000000
C	10.29510300	-3.74974796	0.00000000
C	4.52995600	-2.56685195	0.00000000
C	21.44458601	2.97205504	0.00000000
C	20.40517200	-2.97594596	0.00000000
N	3.53594501	4.09548405	0.00000000
N	12.67117501	2.58745004	0.00000000
N	12.33980300	-4.49461196	0.00000000
N	3.20828800	-2.98583795	0.00000000
N	19.40267901	3.70445004	0.00000000
N	19.08093900	-3.39289496	0.00000000

C-Br...N_Monomer

C	4.07766400	1.83118400	-0.00002800
H	3.72640600	3.92072100	-0.00004100
C	3.32273100	-5.65240200	0.00001600
H	1.09679600	-5.37867100	0.00002600
C	2.73461300	1.37085200	-0.00001500
C	1.57321600	1.02427400	-0.00000500
C	1.52612000	-2.64643500	0.00000600
C	0.74666900	-1.72385000	0.00000600
C	-0.19708600	-0.65740200	0.00000600
C	0.19708600	0.65740100	0.00000300
C	2.11585400	-5.02550100	0.00001900
N	5.17332600	1.08652900	-0.00003200
N	4.35889700	-4.73623800	0.00000600
C	3.79450100	-3.56882000	0.00000200
N	2.40916100	-3.66221800	0.00000800
H	3.51804500	-6.71500800	0.00002200
H	6.27719700	4.21171600	-0.00006400
C	5.75681500	3.26736000	-0.00005300
C	-4.07766500	-1.83118400	0.00001700
H	-3.72641100	-3.92072200	0.00002200
C	-3.32273300	5.65239900	0.00003400
H	-1.09679800	5.37867000	0.00002300
C	-1.52612000	2.64643300	0.00001200
C	-0.74666800	1.72384900	0.00000700
C	-2.73461300	-1.37085400	0.00001300
C	-1.57321600	-1.02427700	0.00001000
C	-2.11585600	5.02549900	0.00002600
N	-4.35889900	4.73623500	0.00003500
N	-5.17332500	-1.08652700	0.00001600
C	-3.79450200	3.56881700	0.00002700
N	-2.40916100	3.66221600	0.00002000
H	-6.27720300	-4.21171300	0.00002600
H	-3.51804800	6.71500500	0.00004000
C	-5.75681800	-3.26735700	0.00002300
C	-6.20329400	-1.96804400	0.00002000
C	6.20329300	1.96804700	-0.00004700
N	-4.39127800	-3.16102700	0.00002100
N	4.39127400	3.16102800	-0.00004100
Br	-4.62860900	1.90067800	0.00002300
Br	4.62861200	-1.90068200	-0.00001200
Br	7.99101000	1.40156000	-0.00005700
Br	-7.99101000	-1.40155300	0.00002100

C-Cl...N__Dimer

0 1			
C	-11.49835103	-2.38291195	0.00000000
H	-10.70448304	-4.34828695	0.00000000
C	-12.48801599	4.99743506	0.00000000
H	-10.26080999	5.26253505	0.00000000
C	-10.28507003	-1.64587496	0.00000000
C	-9.22481402	-1.05868296	0.00000000
C	-10.02589100	2.50552004	0.00000000
C	-9.04853501	1.79650104	0.00000000
C	-11.16656399	4.67712405	0.00000000
N	-12.72729903	-1.88993794	0.00000000
N	-13.27623200	3.86099706	0.00000000
H	-12.93113798	5.98265406	0.00000000
H	-13.13456504	-5.18124894	0.00000000
C	-12.82768104	-4.14758494	0.00000000
C	-12.44714900	2.86494206	0.00000000
C	-13.54079203	-2.97254694	0.00000000
N	-11.12527200	3.28262705	0.00000000
N	-11.51703204	-3.74946595	0.00000000
C	-4.34339900	2.95516501	0.00000000
H	-5.11971199	4.92798002	0.00000000
C	4.34339900	-2.95516501	0.00000000
H	5.11971199	-4.92798002	0.00000000
C	-3.38183104	-4.42876199	0.00000000
H	-5.61083404	-4.67596198	0.00000000
C	3.38183104	4.42876199	0.00000000
H	5.61083404	4.67596198	0.00000000
C	-5.82565403	-1.91988198	0.00000000
C	-6.80210502	-1.20971297	0.00000000
C	-5.56234901	2.22815602	0.00000000

C	-6.62544301	1.64567102	0.00000000
C	5.56234901	-2.22815602	0.00000000
C	6.62544301	-1.64567102	0.00000000
C	5.82565403	1.91988198	0.00000000
C	6.80210502	1.20971297	0.00000000
C	7.96751599	0.39115894	0.00000000
C	7.88234698	-0.97892006	0.00000000
C	-7.88234698	0.97892006	0.00000000
C	-7.96751599	-0.39115894	0.00000000
C	-4.70044204	-4.09785199	0.00000000
C	4.70044204	4.09785199	0.00000000
N	3.11916397	-2.45096603	0.00000000
N	-2.58631004	-3.29822300	0.00000000
N	-3.11916397	2.45096603	0.00000000
N	2.58631004	3.29822300	0.00000000
H	-2.68286899	5.73650300	0.00000000
H	2.94501201	5.41672597	0.00000000
H	2.68286899	-5.73650300	0.00000000
H	-2.94501201	-5.41672597	0.00000000
C	-2.99852399	4.70539100	0.00000000
C	2.99852399	-4.70539100	0.00000000
C	11.49835103	2.38291195	0.00000000
H	10.70448304	4.34828695	0.00000000
C	12.48801599	-4.99743506	0.00000000
H	10.26080999	-5.26253505	0.00000000
C	10.02589100	-2.50552004	0.00000000
C	9.04853501	-1.79650104	0.00000000
C	10.28507003	1.64587496	0.00000000
C	9.22481402	1.05868296	0.00000000
C	11.16656399	-4.67712405	0.00000000
N	13.27623200	-3.86099706	0.00000000
N	12.72729903	1.88993794	0.00000000
H	13.13456504	5.18124894	0.00000000
H	12.93113798	-5.98265406	0.00000000
C	12.82768104	4.14758494	0.00000000
C	-2.29151900	3.52485500	0.00000000
C	3.40606300	2.29371897	0.00000000
C	2.29151900	-3.52485500	0.00000000
C	-3.40606300	-2.29371897	0.00000000
C	13.54079203	2.97254694	0.00000000
C	12.44714900	-2.86494206	0.00000000
N	-4.31317799	4.32138601	0.00000000
N	4.73049400	2.70300896	0.00000000
N	4.31317799	-4.32138601	0.00000000
N	-4.73049400	-2.70300896	0.00000000
N	11.51703204	3.74946595	0.00000000
N	11.12527200	-3.28262705	0.00000000
Cl	-15.25460003	-2.81804593	0.00000000
Cl	-12.83346801	1.20582906	0.00000000
Cl	0.58154896	-3.35864002	0.00000000
Cl	-3.00475202	-0.64030500	0.00000000
Cl	-0.58154896	3.35864002	0.00000000
Cl	3.00475202	0.64030500	0.00000000
Cl	12.83346801	-1.20582906	0.00000000
Cl	15.25460003	2.81804593	0.00000000

C-Cl...N_Trimer

0 1			
C	19.38828001	2.50213397	0.00000000
H	18.56369901	4.45483897	0.00000000
C	20.50454601	-4.86267004	0.00000000
H	18.28161701	-5.16162004	0.00000000
C	18.18701301	1.74565797	0.00000000
C	17.13710301	1.14015897	0.00000000
C	18.00426901	-2.40927304	0.00000000
C	17.01455001	-1.71765504	0.00000000
C	15.83325401	-0.92204603	0.00000000
C	15.89240801	0.44939297	0.00000000
C	19.17836501	-4.56251504	0.00000000
N	20.62482601	2.02849496	0.00000000
N	21.27536501	-3.71437904	0.00000000
H	20.96263701	-5.84102204	0.00000000
H	20.98047601	5.32576297	0.00000000
C	20.68985001	4.28740997	0.00000000

C	12.33450301	-2.96840003	0.00000000
H	13.15236501	-4.92443103	0.00000000
C	3.52671401	2.73493097	0.00000000
H	2.70516101	4.68903398	0.00000000
C	11.22800701	4.39543797	0.00000000
H	13.45178701	4.68622597	0.00000000
C	4.63897401	-4.62730303	0.00000000
H	2.41516901	-4.91879903	0.00000000
C	13.72061501	1.93520697	0.00000000
C	14.71145401	1.24526297	0.00000000
C	13.53808501	-2.21627603	0.00000000
C	14.58942801	-1.61280703	0.00000000
C	2.32394401	1.98121197	0.00000000
C	1.27280601	1.37744197	0.00000000
C	2.14485901	-2.16838703	0.00000000
C	1.15316401	-1.47978203	0.00000000
C	12.55286401	4.09044097	0.00000000
C	3.31394401	-4.32278303	0.00000000
N	4.76218301	2.25896597	0.00000000
N	10.45476701	3.24962597	0.00000000
N	11.09988001	-2.49015203	0.00000000
N	5.41171101	-3.48114703	0.00000000
H	10.73306801	-5.78415403	0.00000000
H	5.09540001	-5.60637703	0.00000000
H	5.12329701	5.55380997	0.00000000
H	10.77192001	5.37466597	0.00000000
C	11.02697901	-4.74663303	0.00000000
C	4.83134401	4.51575297	0.00000000
C	20.43118101	-2.73107704	0.00000000
C	21.42125401	3.12369396	0.00000000
C	10.29508101	-3.58132303	0.00000000
C	4.57176601	-2.49329303	0.00000000
C	5.56489901	3.35181397	0.00000000
C	11.29389001	2.26134197	0.00000000
N	19.11586401	-3.16884104	0.00000000
N	19.38552801	3.86881697	0.00000000
N	12.33320001	-4.33502903	0.00000000
N	3.25602501	-2.92896603	0.00000000
N	3.52563901	4.10150697	0.00000000
N	12.61018201	2.69641797	0.00000000
C	-3.52671401	-2.73493097	0.00000000
H	-2.70516101	-4.68903398	0.00000000
C	-12.33450301	2.96840003	0.00000000
H	-13.15236501	4.92443103	0.00000000
C	-4.63897401	4.62730303	0.00000000
H	-2.41516901	4.91879903	0.00000000
C	-11.22800701	-4.39543797	0.00000000
H	-13.45178701	-4.68622597	0.00000000
C	-2.14485901	2.16838703	0.00000000
C	-1.15316401	1.47978203	0.00000000
C	-2.32394401	-1.98121197	0.00000000
C	-1.27280601	-1.37744197	0.00000000
C	-13.53808501	2.21627603	0.00000000
C	-14.58942801	1.61280703	0.00000000
C	-13.72061501	-1.93520697	0.00000000
C	-14.71145401	-1.24526297	0.00000000
C	-15.89240801	-0.44939297	0.00000000
C	-15.83325401	0.92204603	0.00000000
C	-0.02927499	-0.68572803	0.00000000
C	0.02927499	0.68572803	0.00000000
C	-3.31394401	4.32278303	0.00000000
C	-12.55286401	-4.09044097	0.00000000
N	-11.09988001	2.49015203	0.00000000
N	-5.41171101	3.48114703	0.00000000
N	-4.76218301	-2.25896597	0.00000000
N	-10.45476701	-3.24962597	0.00000000
H	-5.12329701	-5.55380997	0.00000000
H	-10.77192001	-5.37466597	0.00000000
H	-10.73306801	5.78415403	0.00000000
H	-5.09540001	5.60637703	0.00000000
C	-4.83134401	-4.51575297	0.00000000
C	-11.02697901	4.74663303	0.00000000
C	-19.38828001	-2.50213397	0.00000000
H	-18.56369901	-4.45483897	0.00000000
C	-20.50454601	4.86267004	0.00000000

H	-18.28161701	5.16162004	0.00000000
C	-18.00426901	2.40927304	0.00000000
C	-17.01455001	1.71765504	0.00000000
C	-18.18701301	-1.74565797	0.00000000
C	-17.13710301	-1.14015897	0.00000000
C	-19.17836501	4.56251504	0.00000000
N	-21.27536501	3.71437904	0.00000000
N	-20.62482601	-2.02849496	0.00000000
H	-20.98047601	-5.32576297	0.00000000
H	-20.96263701	5.84102204	0.00000000
C	-20.68985001	-4.28740997	0.00000000
C	-5.56489901	-3.35181397	0.00000000
C	-11.29389001	-2.26134197	0.00000000
C	-10.29508101	3.58132303	0.00000000
C	-4.57176601	2.49329303	0.00000000
C	-21.42125401	-3.12369396	0.00000000
C	-20.43118101	2.73107704	0.00000000
N	-3.52563901	-4.10150697	0.00000000
N	-12.61018201	-2.69641797	0.00000000
N	-12.33320001	4.33502903	0.00000000
N	-3.25602501	2.92896603	0.00000000
N	-19.38552801	-3.86881697	0.00000000
N	-19.11586401	3.16884104	0.00000000
Cl	23.13731101	2.99605896	0.00000000
Cl	20.79159801	-1.06609804	0.00000000
Cl	7.27851301	3.22544197	0.00000000
Cl	10.92482201	0.60039897	0.00000000
Cl	8.58199901	-3.45251603	0.00000000
Cl	4.94016801	-0.83208203	0.00000000
Cl	-8.58199901	3.45251603	0.00000000
Cl	-4.94016801	0.83208203	0.00000000
Cl	-7.27851301	-3.22544197	0.00000000
Cl	-10.92482201	-0.60039897	0.00000000
Cl	-20.79159801	1.06609804	0.00000000
Cl	-23.13731101	-2.99605896	0.00000000

C-Cl...N_Monomer

0 1			
C	4.00519200	1.97028500	-0.00002200
H	3.59683800	4.05069700	-0.00002000
C	3.61264400	-5.46819400	-0.00000700
H	1.37516900	-5.31389400	0.00001400
C	2.67539000	1.47359600	-0.00001200
C	1.52522500	1.09145000	-0.00000400
C	1.65791700	-2.56152300	0.00000400
C	0.82853200	-1.68393300	0.00000800
C	-0.16697800	-0.66572200	0.00001000
C	0.16697800	0.66572400	0.00000500
C	2.37404600	-4.90732300	0.00000400
N	5.11893700	1.25419800	-0.00002900
N	4.59880800	-4.49845600	-0.00001700
C	3.97012700	-3.36540000	-0.00001300
N	2.59336200	-3.52945500	-0.00000200
H	3.86453300	-6.51869600	-0.00000800
H	6.14004800	4.40919900	-0.00003800
C	5.64348000	3.45207000	-0.00003400
C	-4.00519100	-1.97028500	0.00002600
H	-3.59683000	-4.05069500	0.00005400
C	-3.61264000	5.46819800	0.00001600
H	-1.37516500	5.31389300	0.00001300
C	-1.65791900	2.56152300	0.00000800
C	-0.82853300	1.68393500	0.00000700
C	-2.67539100	-1.47359200	0.00002200
C	-1.52522500	-1.09144600	0.00001700
C	-2.37404400	4.90732400	0.00001300
N	-4.59880600	4.49846300	0.00001500
N	-5.11893900	-1.25420100	0.00001600
C	-3.97012800	3.36540500	0.00001200
N	-2.59336300	3.52945700	0.00001100
H	-6.14003800	-4.40920600	0.00005500
H	-3.86452700	6.51870100	0.00001800
C	-5.64347400	-3.45207500	0.00004300
C	-6.12218300	-2.16343800	0.00002600
C	6.12218500	2.16343100	-0.00003700

N	-4.28135500	-3.30885300	0.00004300
N	4.28136000	3.30885200	-0.00002400
Cl	7.77580800	1.68818000	-0.00004900
Cl	4.65798100	-1.80706000	-0.00002200
Cl	-4.65798800	1.80706800	0.00001000
Cl	-7.77580900	-1.68819300	0.00001700

C-I...N_Trimer_2Na

2 1

C	-19.56416303	-2.28028007	0.00000000
H	-18.73811202	-4.23469706	0.00000000
C	-20.35402007	5.40236293	0.00000000
H	-18.11845907	5.54698994	0.00000000
C	-18.36938203	-1.51259906	0.00000000
C	-17.32974203	-0.88784505	0.00000000
C	-18.03873005	2.78204694	0.00000000
C	-17.10878805	2.00837495	0.00000000
C	-15.97357405	1.15430095	0.00000000
C	-16.07596604	-0.21583805	0.00000000
C	-19.05341107	5.00936294	0.00000000
N	-20.80449303	-1.81567007	0.00000000
N	-21.20244006	4.30955393	0.00000000
H	-20.74260307	6.41050893	0.00000000
H	-21.14137801	-5.10839707	0.00000000
C	-20.86015502	-4.06701207	0.00000000
C	-12.49160806	3.24050897	0.00000000
H	-13.31169707	5.18850597	0.00000000
C	-3.55251802	-2.74350998	0.00000000
H	-2.77305001	-4.71150897	0.00000000
C	-11.48054002	-4.28972102	0.00000000
H	-13.69837101	-4.60349403	0.00000000
C	-4.48630707	4.80888802	0.00000000
H	-2.26587507	5.09305303	0.00000000
C	-13.99344603	-1.83154904	0.00000000
C	-14.92365203	-1.06133304	0.00000000
C	-13.68369605	2.46753797	0.00000000
C	-14.71125605	1.82367596	0.00000000
C	-2.34678103	-1.99055497	0.00000000
C	-1.31435703	-1.35404697	0.00000000
C	-2.01306905	2.31676503	0.00000000
C	-1.08807505	1.53947803	0.00000000
C	0.05450896	0.68479204	0.00000000
C	-0.05450896	-0.68479204	0.00000000
C	-12.80931202	-3.99299403	0.00000000
C	-3.16308606	4.49468102	0.00000000
N	-4.78740703	-2.25479599	0.00000000
N	-10.72528402	-3.13083802	0.00000000
N	-11.24675005	2.77595098	0.00000000
N	-5.25900606	3.66043301	0.00000000
H	-10.90987607	6.06853198	0.00000000
H	-4.93850607	5.78965301	0.00000000
H	-5.18912601	-5.53720299	0.00000000
H	-11.01548501	-5.26444502	0.00000000
C	-11.18568807	5.02571898	0.00000000
C	-4.89169501	-4.50015699	0.00000000
C	-20.44284006	3.25886193	0.00000000
C	-21.60847302	-2.91203208	0.00000000
C	-10.43958106	3.87355698	0.00000000
C	-4.42391805	2.66431702	0.00000000
C	-5.61910402	-3.33363599	0.00000000
C	-11.58058803	-2.14760902	0.00000000
N	-19.09025206	3.61366894	0.00000000
N	-19.55893102	-3.64700807	0.00000000
N	-12.48807806	4.60234597	0.00000000
N	-3.10967006	3.10305602	0.00000000
N	-3.58174202	-4.10559498	0.00000000
N	-12.88261903	-2.60534603	0.00000000
I	-8.35319106	3.71314999	0.00000000
I	-4.83168704	0.61902401	0.00000000
I	-7.70562802	-3.14910000	0.00000000
I	-11.21107004	-0.09544802	0.00000000
I	-21.00946405	1.25866193	0.00000000
I	-23.68285002	-2.76043409	0.00000000
C	3.55251802	2.74350998	0.00000000

H	2.77305001	4.71150897	0.00000000
C	12.49160806	-3.24050897	0.00000000
H	13.31169707	-5.18850597	0.00000000
C	4.48630707	-4.80888802	0.00000000
H	2.26587507	-5.09305303	0.00000000
C	11.48054002	4.28972102	0.00000000
H	13.69837101	4.60349403	0.00000000
C	2.01306905	-2.31676503	0.00000000
C	1.08807505	-1.53947803	0.00000000
C	2.34678103	1.99055497	0.00000000
C	1.31435703	1.35404697	0.00000000
C	13.68369605	-2.46753797	0.00000000
C	14.71125605	-1.82367596	0.00000000
C	13.99344603	1.83154904	0.00000000
C	14.92365203	1.06133304	0.00000000
C	16.07596604	0.21583805	0.00000000
C	15.97357405	-1.15430095	0.00000000
C	3.16308606	-4.49468102	0.00000000
C	12.80931202	3.99299403	0.00000000
N	11.24675005	-2.77595098	0.00000000
N	5.25900606	-3.66043301	0.00000000
N	4.78740703	2.25479599	0.00000000
N	10.72528402	3.13083802	0.00000000
H	5.18912601	5.53720299	0.00000000
H	11.01548501	5.26444502	0.00000000
H	10.90987607	-6.06853198	0.00000000
H	4.93850607	-5.78965301	0.00000000
C	4.89169501	4.50015699	0.00000000
C	11.18568807	-5.02571898	0.00000000
C	19.56416303	2.28028007	0.00000000
H	18.73811202	4.23469706	0.00000000
C	20.35402007	-5.40236293	0.00000000
H	18.11845907	-5.54698994	0.00000000
C	18.03873005	-2.78204694	0.00000000
C	17.10878805	-2.00837495	0.00000000
C	18.36938203	1.51259906	0.00000000
C	17.32974203	0.88784505	0.00000000
C	19.05341107	-5.00936294	0.00000000
N	21.20244006	-4.30955393	0.00000000
N	20.80449303	1.81567007	0.00000000
H	21.14137801	5.10839707	0.00000000
H	20.74260307	-6.41050893	0.00000000
C	20.86015502	4.06701207	0.00000000
C	5.61910402	3.33363599	0.00000000
C	11.58058803	2.14760902	0.00000000
C	10.43958106	-3.87355698	0.00000000
C	4.42391805	-2.66431702	0.00000000
C	21.60847302	2.91203208	0.00000000
C	20.44284006	-3.25886193	0.00000000
N	3.58174202	4.10559498	0.00000000
N	12.88261903	2.60534603	0.00000000
N	12.48807806	-4.60234597	0.00000000
N	3.10967006	-3.10305602	0.00000000
N	19.55893102	3.64700807	0.00000000
N	19.09025206	-3.61366894	0.00000000
I	23.68285002	2.76043409	0.00000000
I	21.00946405	-1.25866193	0.00000000
I	7.70562802	3.14910000	0.00000000
I	11.21107004	0.09544802	0.00000000
I	8.35319106	-3.71314999	0.00000000
I	4.83168704	-0.61902401	0.00000000
Na	-8.06512004	0.31140100	0.00000000
Na	8.06512004	-0.31140100	0.00000000

C-I...N__Dimer_Na

1 1			
C	-11.64815420	-2.04543485	0.00000000
H	-10.89590403	-4.02854986	0.00000000
C	-12.10420923	5.66255415	0.00000000
H	-9.86400412	5.70563112	0.00000000
C	-10.42351616	-1.32598887	0.00000000
C	-9.35692312	-0.74892088	0.00000000
C	-9.90740516	2.94174912	0.00000000
C	-9.01024412	2.13078511	0.00000000

C	-7.91115908	1.22961110	0.00000000
C	-8.07343508	-0.13428790	0.00000000
C	-10.82246217	5.21110813	0.00000000
N	-12.86989432	-1.53398784	0.00000000
N	-13.00098228	4.60928416	0.00000000
H	-12.44670023	6.68728815	0.00000000
H	-13.33116016	-4.81218183	0.00000000
C	-13.01099720	-3.78214583	0.00000000
C	-4.33885799	3.15649605	0.00000000
H	-5.07044906	5.13961206	0.00000000
C	4.33885799	-3.15649605	0.00000000
H	5.07044906	-5.13961206	0.00000000
C	-3.67296394	-4.41432495	0.00000000
H	-5.90354001	-4.61955692	0.00000000
C	3.67296394	4.41432495	0.00000000
H	5.90354001	4.61955692	0.00000000
C	-6.06358801	-1.83889892	0.00000000
C	-6.96036404	-1.02997491	0.00000000
C	-5.56521702	2.43895707	0.00000000
C	-6.62137805	1.84329508	0.00000000
C	5.56521702	-2.43895707	0.00000000
C	6.62137805	-1.84329508	0.00000000
C	6.06358801	1.83889892	0.00000000
C	6.96036404	1.02997491	0.00000000
C	8.07343508	0.13428790	0.00000000
C	7.91115908	-1.22961110	0.00000000
C	-4.98555298	-4.05351493	0.00000000
C	4.98555298	4.05351493	0.00000000
N	3.11658608	-2.63660904	0.00000000
N	-2.86224891	-3.29370796	0.00000000
N	-3.11658608	2.63660904	0.00000000
N	2.86224891	3.29370796	0.00000000
H	-2.63079199	5.90904303	0.00000000
H	3.25521030	5.41011896	0.00000000
H	2.63079199	-5.90904303	0.00000000
H	-3.25521030	-5.41011896	0.00000000
C	-2.95399397	4.87990904	0.00000000
C	2.95399397	-4.87990904	0.00000000
C	-12.28836826	3.52549015	0.00000000
C	-13.71441232	-2.59978983	0.00000000
C	-2.25912992	3.69556603	0.00000000
C	3.66695422	2.26963396	0.00000000
C	2.25912992	-3.69556603	0.00000000
C	-3.66695422	-2.26963396	0.00000000
N	-10.92229019	3.81912513	0.00000000
N	-11.69466613	-3.41115385	0.00000000
N	-4.27444101	4.51688605	0.00000000
N	4.99112223	2.66331194	0.00000000
N	4.27444101	-4.51688605	0.00000000
N	-4.99112223	-2.66331194	0.00000000
I	-0.18063983	3.44687600	0.00000000
I	3.19389918	0.23839996	0.00000000
I	0.18063983	-3.44687600	0.00000000
I	-3.19389918	-0.23839996	0.00000000
I	-12.94361532	1.55214816	0.00000000
I	-15.78191347	-2.36987881	0.00000000
C	11.64815420	2.04543485	0.00000000
H	10.89590403	4.02854986	0.00000000
C	12.10420923	-5.66255415	0.00000000
H	9.86400412	-5.70563112	0.00000000
C	9.90740516	-2.94174912	0.00000000
C	9.01024412	-2.13078511	0.00000000
C	10.42351616	1.32598887	0.00000000
C	9.35692312	0.74892088	0.00000000
C	10.82246217	-5.21110813	0.00000000
N	13.00098228	-4.60928416	0.00000000
N	12.86989432	1.53398784	0.00000000
H	13.33116016	4.81218183	0.00000000
H	12.44670023	-6.68728815	0.00000000
C	13.01099720	3.78214583	0.00000000
C	13.71441232	2.59978983	0.00000000
C	12.28836826	-3.52549015	0.00000000
N	11.69466613	3.41115385	0.00000000
N	10.92229019	-3.81912513	0.00000000
I	15.78191347	2.36987881	0.00000000

I	12.94361532	-1.55214816	0.00000000
Na	0.00000000	0.00000000	0.00000000
C-I...N_Dimer			
0 1			
C	11.60013600	-2.00778003	0.00000000
H	10.78501101	-3.96233404	0.00000000
C	12.12904894	5.68809097	0.00000000
H	9.88720994	5.74051096	0.00000000
C	10.39160999	-1.26094504	0.00000000
C	9.32681699	-0.68156905	0.00000000
C	9.90933796	2.98207496	0.00000000
C	8.99940797	2.18710395	0.00000000
C	7.88644097	1.29772594	0.00000000
C	8.04140698	-0.06579106	0.00000000
C	10.84388095	5.24240796	0.00000000
N	12.83682599	-1.53345702	0.00000000
N	13.01928895	4.63086898	0.00000000
H	12.47633894	6.71129998	0.00000000
H	13.19890002	-4.82630002	0.00000000
C	12.91073401	-3.78702102	0.00000000
C	4.32033396	3.22612592	0.00000000
H	5.11012595	5.19090192	0.00000000
C	-4.32033396	-3.22612592	0.00000000
H	-5.11012595	-5.19090192	0.00000000
C	3.78238601	-4.44348409	0.00000000
H	6.02241201	-4.50332807	0.00000000
C	-3.78238601	4.44348409	0.00000000
H	-6.02241201	4.50332807	0.00000000
C	6.01411199	-1.74548607	0.00000000
C	6.92708499	-0.95473606	0.00000000
C	5.53585296	2.49159693	0.00000000
C	6.60150997	1.91328793	0.00000000
C	-5.53585296	-2.49159693	0.00000000
C	-6.60150997	-1.91328793	0.00000000
C	-6.01411199	1.74548607	0.00000000
C	-6.92708499	0.95473606	0.00000000
C	-8.04140698	0.06579106	0.00000000
C	-7.88644097	-1.29772594	0.00000000
C	5.06806201	-4.00109308	0.00000000
C	-5.06806201	4.00109308	0.00000000
N	-3.08917100	-2.73687414	0.00000000
N	2.90126701	-3.37960809	0.00000000
N	3.08917100	2.73687414	0.00000000
N	-2.90126701	3.37960809	0.00000000
H	2.68636194	6.02047991	0.00000000
H	-3.42748206	5.46389086	0.00000000
H	-2.68636194	-6.02047991	0.00000000
H	3.42748206	-5.46389086	0.00000000
C	2.98641795	4.98441591	0.00000000
C	-2.98641795	-4.98441591	0.00000000
C	12.29583496	3.55116898	0.00000000
C	13.64694500	-2.62679701	0.00000000
C	2.25739995	3.81751290	0.00000000
C	-3.62777903	2.29730686	0.00000000
C	-2.25739995	-3.81751290	0.00000000
C	3.62777903	-2.29730686	0.00000000
N	10.93595596	3.85259797	0.00000000
N	11.60546701	-3.37400503	0.00000000
N	4.29796695	4.59151992	0.00000000
N	-4.98107404	2.61140085	0.00000000
N	-4.29796695	-4.59151992	0.00000000
N	4.98107404	-2.61140085	0.00000000
I	0.17807496	3.61907089	0.00000000
I	-2.98928502	0.31812786	0.00000000
I	-0.17807496	-3.61907089	0.00000000
I	2.98928502	-0.31812786	0.00000000
I	12.94087397	1.57340798	0.00000000
I	15.72198200	-2.46046400	0.00000000
C	-11.60013600	2.00778003	0.00000000
H	-10.78501101	3.96233404	0.00000000
C	-12.12904894	-5.68809097	0.00000000
H	-9.88720994	-5.74051096	0.00000000
C	-9.90933796	-2.98207496	0.00000000

C	-8.99940797	-2.18710395	0.00000000
C	-10.39160999	1.26094504	0.00000000
C	-9.32681699	0.68156905	0.00000000
C	-10.84388095	-5.24240796	0.00000000
N	-13.01928895	-4.63086898	0.00000000
N	-12.83682599	1.53345702	0.00000000
H	-13.19890002	4.82630002	0.00000000
H	-12.47633894	-6.71129998	0.00000000
C	-12.91073401	3.78702102	0.00000000
C	-13.64694500	2.62679701	0.00000000
C	-12.29583496	-3.55116898	0.00000000
N	-11.60546701	3.37400503	0.00000000
N	-10.93595596	-3.85259797	0.00000000
I	-15.72198200	2.46046400	0.00000000
I	-12.94087397	-1.57340798	0.00000000

C-I...N_Trimer

0 1

C	-19.48214299	2.23546292	0.00000000
H	-18.58030499	4.15159092	0.00000000
C	-20.35496699	-5.42968408	0.00000000
H	-18.11783099	-5.58398408	0.00000000
C	-18.30840299	1.43505292	0.00000000
C	-17.27115899	0.80767792	0.00000000
C	-18.01464599	-2.82694908	0.00000000
C	-17.07046099	-2.07293308	0.00000000
C	-15.91929799	-1.23346208	0.00000000
C	-16.01423099	0.13557992	0.00000000
C	-19.05085899	-5.04287608	0.00000000
N	-20.73876399	1.81699892	0.00000000
N	-21.19612399	-4.33307408	0.00000000
H	-20.74841499	-6.43603808	0.00000000
H	-20.95328499	5.12264892	0.00000000
C	-20.71188599	4.07152192	0.00000000
C	-12.43952899	-3.31410608	0.00000000
H	-13.30939299	-5.24487508	0.00000000
C	-3.52666199	2.76741793	0.00000000
H	-2.65500399	4.69710393	0.00000000
C	-11.57176699	4.32727692	0.00000000
H	-13.80714699	4.48346592	0.00000000
C	-4.39714399	-4.87275707	0.00000000
H	-2.16171199	-5.02940107	0.00000000
C	-13.91722899	1.72738392	0.00000000
C	-14.86242899	0.97539492	0.00000000
C	-13.62331199	-2.52938108	0.00000000
C	-14.66267099	-1.90497208	0.00000000
C	-2.34319999	1.98189893	0.00000000
C	-1.30411499	1.35703093	0.00000000
C	-2.05094999	-2.27373607	0.00000000
C	-1.10488199	-1.52288907	0.00000000
C	0.04800201	-0.68447607	0.00000000
C	-0.04800201	0.68447607	0.00000000
C	-12.87528699	3.94062992	0.00000000
C	-3.09354699	-4.48650207	0.00000000
N	-4.77722099	2.33043593	0.00000000
N	-10.73732399	3.22650092	0.00000000
N	-11.18929999	-2.87592308	0.00000000
N	-5.23135599	-3.77163107	0.00000000
H	-10.92159099	-6.17310108	0.00000000
H	-4.79595099	-5.87680707	0.00000000
H	-5.04226099	5.62805493	0.00000000
H	-11.17322499	5.33143892	0.00000000
C	-11.17887099	-5.12559308	0.00000000
C	-4.78599799	4.58031293	0.00000000
C	-20.42432999	-3.28737508	0.00000000
C	-21.49920099	2.94541092	0.00000000
C	-10.40247999	-3.98964008	0.00000000
C	-4.45862599	-2.72187907	0.00000000
C	-5.56297199	3.44512893	0.00000000
C	-11.50959599	2.17645692	0.00000000
N	-19.07955599	-3.65029808	0.00000000
N	-19.42626999	3.60057492	0.00000000
N	-12.47336399	-4.67928008	0.00000000
N	-3.12023399	-3.09430807	0.00000000

N	-3.49165999	4.13253293	0.00000000
N	-12.84821999	2.54842292	0.00000000
I	-8.31666599	-3.87743008	0.00000000
I	-5.01101099	-0.71707407	0.00000000
I	-7.64874099	3.33392093	0.00000000
I	-10.95637999	0.17190792	0.00000000
I	-20.97997799	-1.28278108	0.00000000
I	-23.57956199	2.87127091	0.00000000
C	3.52666199	-2.76741793	0.00000000
H	2.65500399	-4.69710393	0.00000000
C	12.43952899	3.31410608	0.00000000
H	13.30939299	5.24487508	0.00000000
C	4.39714399	4.87275707	0.00000000
H	2.16171199	5.02940107	0.00000000
C	11.57176699	-4.32727692	0.00000000
H	13.80714699	-4.48346592	0.00000000
C	2.05094999	2.27373607	0.00000000
C	1.10488199	1.52288907	0.00000000
C	2.34319999	-1.98189893	0.00000000
C	1.30411499	-1.35703093	0.00000000
C	13.62331199	2.52938108	0.00000000
C	14.66267099	1.90497208	0.00000000
C	13.91722899	-1.72738392	0.00000000
C	14.86242899	-0.97539492	0.00000000
C	16.01423099	-0.13557992	0.00000000
C	15.91929799	1.23346208	0.00000000
C	3.09354699	4.48650207	0.00000000
C	12.87528699	-3.94062992	0.00000000
N	11.18929999	2.87592308	0.00000000
N	5.23135599	3.77163107	0.00000000
N	4.77722099	-2.33043593	0.00000000
N	10.73732399	-3.22650092	0.00000000
H	5.04226099	-5.62805493	0.00000000
H	11.17322499	-5.33143892	0.00000000
H	10.92159099	6.17310108	0.00000000
H	4.79595099	5.87680707	0.00000000
C	4.78599799	-4.58031293	0.00000000
C	11.17887099	5.12559308	0.00000000
C	19.48214299	-2.23546292	0.00000000
H	18.58030499	-4.15159092	0.00000000
C	20.35496699	5.42968408	0.00000000
H	18.11783099	5.58398408	0.00000000
C	18.01464599	2.82694908	0.00000000
C	17.07046099	2.07293308	0.00000000
C	18.30840299	-1.43505292	0.00000000
C	17.27115899	-0.80767792	0.00000000
C	19.05085899	5.04287608	0.00000000
N	21.19612399	4.33307408	0.00000000
N	20.73876399	-1.81699892	0.00000000
H	20.95328499	-5.12264892	0.00000000
H	20.74841499	6.43603808	0.00000000
C	20.71188599	-4.07152192	0.00000000
C	5.56297199	-3.44512893	0.00000000
C	11.50959599	-2.17645692	0.00000000
C	10.40247999	3.98964008	0.00000000
C	4.45862599	2.72187907	0.00000000
C	21.49920099	-2.94541092	0.00000000
C	20.42432999	3.28737508	0.00000000
N	3.49165999	-4.13253293	0.00000000
N	12.84821999	-2.54842292	0.00000000
N	12.47336399	4.67928008	0.00000000
N	3.12023399	3.09430807	0.00000000
N	19.42626999	-3.60057492	0.00000000
N	19.07955599	3.65029808	0.00000000
I	23.57956199	-2.87127091	0.00000000
I	20.97997799	1.28278108	0.00000000
I	7.64874099	-3.33392093	0.00000000
I	10.95637999	-0.17190792	0.00000000
I	8.31666599	3.87743008	0.00000000
I	5.01101099	0.71707407	0.00000000

C-I...N_Monomer

0 1			
C	4.12370106	1.76006287	0.00000000

H	3.76131912	3.84678489	0.00000000
C	2.95019582	-5.86428309	0.00000000
H	0.75111983	-5.42606802	0.00000000
C	2.78031704	1.29805892	0.00000000
C	1.61466503	0.96551695	0.00000000
C	1.37552592	-2.73813704	0.00000000
C	0.66378095	-1.76166802	0.00000000
C	-0.22501002	-0.64817399	0.00000000
C	0.22501002	0.64817399	0.00000000
C	1.79339484	-5.14863805	0.00000000
N	5.22479804	1.02382884	0.00000000
N	4.04971284	-5.02701712	0.00000000
I	4.64194894	-2.02692214	0.00000000
I	8.24327704	1.28876274	0.00000000
C	3.57960788	-3.81531011	0.00000000
N	2.18669088	-3.81247606	0.00000000
H	3.06560578	-6.93863909	0.00000000
H	6.30622513	4.15474080	0.00000000
C	5.79520910	3.20498382	0.00000000
C	-4.12370106	-1.76006287	0.00000000
H	-3.76131912	-3.84678489	0.00000000
C	-2.95019582	5.86428309	0.00000000
H	-0.75111983	5.42606802	0.00000000
C	-1.37552592	2.73813704	0.00000000
C	-0.66378095	1.76166802	0.00000000
C	-2.78031704	-1.29805892	0.00000000
C	-1.61466503	-0.96551695	0.00000000
C	-1.79339484	5.14863805	0.00000000
N	-4.04971284	5.02701712	0.00000000
N	-5.22479804	-1.02382884	0.00000000
I	-4.64194894	2.02692214	0.00000000
I	-8.24327704	-1.28876274	0.00000000
C	-3.57960788	3.81531011	0.00000000
N	-2.18669088	3.81247606	0.00000000
H	-6.30622513	-4.15474080	0.00000000
H	-3.06560578	6.93863909	0.00000000
C	-5.79520910	-3.20498382	0.00000000
C	-6.25671906	-1.91052680	0.00000000
C	6.25671906	1.91052680	0.00000000
N	-4.43106910	-3.09124285	0.00000000
N	4.43106910	3.09124285	0.00000000

N-Br...N_Dimer

0 1			
C	8.91387900	-7.44253600	-0.26573200
H	10.18139200	-5.62834100	-0.62344600
C	4.03034300	-12.85439500	0.88927900
H	2.22893300	-11.51466600	0.90641600
C	7.57910400	-6.95061800	-0.18781000
C	6.46007300	-6.49011500	-0.12922100
C	4.13952100	-9.27301100	0.44237100
C	4.09751900	-8.06951200	0.30019600
C	4.03034300	-6.65828400	0.13579000
C	5.16236400	-5.90462000	-0.06782100
C	3.29470100	-11.66097000	0.81758200
N	9.18835300	-8.74806300	-0.13238000
N	5.33930000	-12.64232300	0.73234200
H	3.67435300	-13.86279900	1.04770500
H	12.17899000	-7.53554400	-0.59530900
C	11.11035800	-7.62414900	-0.47261600
C	0.29036300	-5.08989800	0.27672100
H	-0.96519700	-6.88070100	0.75267700
C	-0.29036300	5.08989800	0.27672100
H	0.96519700	6.88070100	0.75267700
C	5.11220200	0.30387700	-0.67535500
H	6.90929200	-1.03128100	-0.73012500
C	-5.11220200	-0.30387700	-0.67535500
H	-6.90929200	1.03128100	-0.73012500
C	5.01225100	-3.28830500	-0.34511600
C	5.08109800	-4.49188400	-0.22261600
C	1.62463200	-5.58527000	0.23003100
C	2.73763500	-6.06282900	0.18902800
C	-1.62463200	5.58527000	0.23003100
C	-2.73763500	6.06282900	0.18902800

C	-5.01225100	3.28830500	-0.34511600
C	-5.08109800	4.49188400	-0.22261600
C	-5.16236400	5.90462000	-0.06782100
C	-4.03034300	6.65828400	0.13579000
C	5.84319500	-0.88908900	-0.64287400
C	-5.84319500	0.88908900	-0.64287400
N	-0.00456100	3.79586600	0.05185100
N	3.80408500	0.07514900	-0.53233300
N	0.00456100	-3.79586600	0.05185100
N	-3.80408500	-0.07514900	-0.53233300
H	-2.97010000	-4.98662300	0.57585200
H	-5.46479800	-1.31917900	-0.79191700
H	2.97010000	4.98662300	0.57585200
H	5.46479800	1.31917900	-0.79191700
C	-1.90093000	-4.89861000	0.45552800
C	1.90093000	4.89861000	0.45552800
C	-8.91387900	7.44253600	-0.26573200
H	-10.18139200	5.62834100	-0.62344600
C	-4.03034300	12.85439500	0.88927900
H	-2.22893300	11.51466600	0.90641600
C	-4.13952100	9.27301100	0.44237100
C	-4.09751900	8.06951200	0.30019600
C	-7.57910400	6.95061800	-0.18781000
C	-6.46007300	6.49011500	-0.12922100
C	-3.29470100	11.66097000	0.81758200
N	-5.33930000	12.64232300	0.73234200
N	-9.18835300	8.74806300	-0.13238000
H	-12.17899000	7.53554400	-0.59530900
H	-3.67435300	13.86279900	1.04770500
C	-11.11035800	7.62414900	-0.47261600
N	5.44974400	-11.32884700	0.56143100
N	10.51274200	-8.82436100	-0.26121200
N	3.68306700	-1.24638300	-0.40517300
N	-1.31924400	-3.71030100	0.16805200
N	-3.68306700	1.24638300	-0.40517300
N	1.31924400	3.71030100	0.16805200
N	-5.44974400	11.32884700	0.56143100
N	-10.51274200	8.82436100	-0.26121200
C	10.09570300	-6.69466700	-0.48195700
C	4.24808100	-10.67423600	0.60199000
C	4.88788300	-1.88349500	-0.46629700
C	-0.88512700	-5.82628600	0.53758500
C	0.88512700	5.82628600	0.53758500
C	-4.88788300	1.88349500	-0.46629700
C	-4.24808100	10.67423600	0.60199000
C	-10.09570300	6.69466700	-0.48195700
Br	-7.09166800	10.50072800	0.29525900
Br	-11.35349500	10.46126100	-0.14624600
Br	-2.03068700	2.10351700	-0.22942400
Br	2.23033700	2.09357400	-0.12907500
Br	2.03068700	-2.10351700	-0.22942400
Br	-2.23033700	-2.09357400	-0.12907500
Br	7.09166800	-10.50072800	0.29525900
Br	11.35349500	-10.46126100	-0.14624600

N-Br...N_Trimer

0 1			
C	19.11912903	2.27770112	-0.25413488
H	18.49632503	4.29530711	-1.00723890
C	20.31479606	-4.60561586	2.12064318
H	18.15315506	-5.21180787	2.11269117
C	17.90632204	1.54224411	-0.12006788
C	16.85318804	0.95174211	-0.02040788
C	17.58702905	-2.44311288	1.16111815
C	16.62178605	-1.77651889	0.85390714
C	15.47854305	-1.00882190	0.49796613
C	15.59164104	0.29685410	0.08149312
C	18.92751706	-4.47805387	1.94798817
N	20.30578004	1.73192713	0.04848613
N	20.96011406	-3.47716686	1.81547017
H	20.88142806	-5.46428385	2.45279819
H	21.22332702	4.71701212	-0.88690489
C	20.62731203	3.84976812	-0.64704389
C	11.93915206	-2.97403091	0.77763413

H	12.55006106	-4.95438290	1.62331215
C	3.57393303	2.69433403	-0.51356796
H	2.91976602	4.83179603	-0.39636798
C	10.70389903	3.88325906	-1.39035593
H	12.86180503	4.48046907	-1.43261793
C	4.90156607	-4.47924396	-0.32131989
H	2.74833507	-5.09311597	-0.36793990
C	13.45436804	1.70406108	-0.54814290
C	14.43784504	1.05585009	-0.26362889
C	13.15166305	-2.23473791	0.67227313
C	14.21286705	-1.65535790	0.59076113
C	2.36462304	1.94252402	-0.48589596
C	1.30660204	1.35171002	-0.47315696
C	2.11616006	-2.18853698	-0.44171692
C	1.12015405	-1.49879098	-0.45938693
C	12.09062603	3.74523707	-1.26198193
C	3.51090707	-4.32963397	-0.36552290
N	4.77689404	2.10130804	-0.60224695
N	10.07324303	2.74513306	-1.08863593
N	10.75733506	-2.45689392	0.39999712
N	5.51741706	-3.29391596	-0.33212490
H	9.83593007	-5.41346492	1.37484814
H	5.49113508	-5.38440996	-0.27895488
H	5.65125702	5.22733004	-0.53745997
H	10.12687403	4.74943106	-1.68281594
C	10.43093906	-4.54396792	1.13971213
C	5.06694402	4.31962104	-0.53633796
Br	22.98609103	2.39396014	0.08171213
Br	20.37344105	-0.88857687	0.91776315
Br	8.05309306	-3.21167994	0.19699211
Br	10.68468005	0.09856507	-0.31034790
Br	7.50009703	2.79326305	-0.79266494
Br	4.87495405	-0.54622496	-0.47096492
C	-3.57393303	-2.69433403	-0.51356796
H	-2.91976602	-4.83179603	-0.39636798
C	-11.93915206	2.97403091	0.77763413
H	-12.55006106	4.95438290	1.62331215
C	-4.90156607	4.47924396	-0.32131989
H	-2.74833507	5.09311597	-0.36793990
C	-10.70389903	-3.88325906	-1.39035593
H	-12.86180503	-4.48046907	-1.43261793
C	-2.11616006	2.18853698	-0.44171692
C	-1.12015405	1.49879098	-0.45938693
C	-2.36462304	-1.94252402	-0.48589596
C	-1.30660204	-1.35171002	-0.47315696
C	-13.15166305	2.23473791	0.67227313
C	-14.21286705	1.65535790	0.59076113
C	-13.45436804	-1.70406108	-0.54814290
C	-14.43784504	-1.05585009	-0.26362889
C	-15.59164104	-0.29685410	0.08149312
C	-15.47854305	1.00882190	0.49796613
C	-0.04823295	-0.68591199	-0.46765594
C	0.04823295	0.68591199	-0.46765594
C	-3.51090707	4.32963397	-0.36552290
C	-12.09062603	-3.74523707	-1.26198193
N	-10.75733506	2.45689392	0.39999712
N	-5.51741706	3.29391596	-0.33212490
N	-4.77689404	-2.10130804	-0.60224695
N	-10.07324303	-2.74513306	-1.08863593
H	-5.65125702	-5.22733004	-0.53745997
H	-10.12687403	-4.74943106	-1.68281594
H	-9.83593007	5.41346492	1.37484814
H	-5.49113508	5.38440996	-0.27895488
C	-5.06694402	-4.31962104	-0.53633796
C	-10.43093906	4.54396792	1.13971213
C	-19.11912903	-2.27770112	-0.25413488
H	-18.49632503	-4.29530711	-1.00723890
C	-20.31479606	4.60561586	2.12064318
H	-18.15315506	5.21180787	2.11269117
C	-17.58702905	2.44311288	1.16111815
C	-16.62178605	1.77651889	0.85390714
C	-17.90632204	-1.54224411	-0.12006788
C	-16.85318804	-0.95174211	-0.02040788
C	-18.92751706	4.47805387	1.94798817
N	-20.96011406	3.47716686	1.81547017

N	-20.30578004	-1.73192713	0.04848613
H	-21.22332702	-4.71701212	-0.88690489
H	-20.88142806	5.46428385	2.45279819
C	-20.62731203	-3.84976812	-0.64704389
Br	-7.50009703	-2.79326305	-0.79266494
Br	-4.87495405	0.54622496	-0.47096492
Br	-8.05309306	3.21167994	0.19699211
Br	-10.68468005	-0.09856507	-0.31034790
Br	-22.98609103	-2.39396014	0.08171213
Br	-20.37344105	0.88857687	0.91776315
N	-21.18937694	-2.69877110	-0.19732302
N	-20.00324698	2.63014692	1.45040394
N	-11.03316394	-1.87837605	-0.76528899
N	-9.86937498	3.42185097	0.63081898
N	-5.65508194	-3.10276802	-0.61199095
N	-4.54423197	2.38437799	-0.37900699
N	4.54423197	-2.38437799	-0.37900699
N	5.65508194	3.10276802	-0.61199095
N	11.03316394	1.87837605	-0.76528899
N	9.86937498	-3.42185097	0.63081898
N	21.18937694	2.69877110	-0.19732302
N	20.00324698	-2.63014692	1.45040394
C	-19.27280593	-3.61273209	-0.69735901
C	-18.74782198	3.17328593	1.50755594
C	-12.27801894	-2.42948006	-0.85410299
C	-11.78131698	4.29330896	1.25345896
C	-3.30512697	2.95510299	-0.40291299
C	-3.70841093	-4.09886501	-0.46831493
C	3.30512697	-2.95510299	-0.40291299
C	3.70841093	4.09886501	-0.46831493
C	12.27801894	2.42948006	-0.85410299
C	11.78131698	-4.29330896	1.25345896
C	18.74782198	-3.17328593	1.50755594
C	19.27280593	3.61273209	-0.69735901

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C	-4.01291896	-1.99073608	0.00000000
H	-3.76889189	-4.21910807	0.00000000
C	-3.90646419	5.38719493	0.00000000
H	-1.66849119	5.56616100	0.00000000
C	-2.68531598	-1.47411904	0.00000000
C	-1.54023199	-1.07878500	0.00000000
C	-1.62934410	2.58417800	0.00000000
C	-0.80546207	1.69440802	0.00000000
C	0.17612996	0.66453605	0.00000000
C	-0.17612996	-0.66453605	0.00000000
C	-2.56667018	4.96747097	0.00000000
N	-5.08024798	-1.17918311	0.00000000
N	-4.75174116	4.35388190	0.00000000
H	-4.30265022	6.39307091	0.00000000
H	-6.52852289	-4.09982116	0.00000000
C	-5.78359592	-3.31882113	0.00000000
C	4.01291896	1.99073608	0.00000000
H	3.76889189	4.21910807	0.00000000
C	3.90646419	-5.38719493	0.00000000
H	1.66849119	-5.56616100	0.00000000
C	1.62934410	-2.58417800	0.00000000
C	0.80546207	-1.69440802	0.00000000
C	2.68531598	1.47411904	0.00000000
C	1.54023199	1.07878500	0.00000000
C	2.56667018	-4.96747097	0.00000000
N	4.75174116	-4.35388190	0.00000000
N	5.08024798	1.17918311	0.00000000
H	6.52852289	4.09982116	0.00000000
H	4.30265022	-6.39307091	0.00000000
C	5.78359592	3.31882113	0.00000000
Br	4.65920303	-1.55363781	0.00000000
Br	-4.65920303	1.55363781	0.00000000
Br	-7.83773098	-1.32027820	0.00000000
Br	7.83773098	1.32027820	0.00000000
N	-3.96941712	3.27890792	0.00000000
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N	6.12587696	2.00526214	0.00000000
C	-2.63411813	3.58022497	0.00000000
C	-4.40795492	-3.34961409	0.00000000
C	2.63411813	-3.58022497	0.00000000
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0 1

C	-0.05828100	11.58005600	-0.12532900
H	-2.22503600	11.43891900	-0.69031400
C	7.05512300	11.24530900	1.55914100
H	7.20284600	9.00934900	1.41899600
C	0.40624500	10.23366900	-0.11129200
C	0.75626500	9.07400500	-0.11282100
C	4.30196000	9.05601400	0.73655100
C	3.43499600	8.25271800	0.46793700
C	2.42338700	7.30328200	0.15380500
C	1.13683700	7.70148600	-0.12310600
C	6.63086300	9.92240800	1.35535800
N	0.75918200	12.60216100	0.16239900
N	6.06117400	12.11980700	1.39232800
H	8.03848700	11.61018500	1.82026400
H	-2.03251900	14.18664800	-0.42928200
C	-1.30073200	13.40375700	-0.30236300
C	3.62266100	3.42726500	0.11846100
H	5.72993900	3.55994100	0.87336600
C	-3.62266100	-3.42726500	0.11846100
H	-5.72993900	-3.55994100	0.87336600
C	-3.49396600	3.71913200	-1.40730300
H	-3.64638600	5.95395600	-1.28967800
C	3.49396600	-3.71913200	-1.40730300
H	3.64638600	-5.95395600	-1.28967800
C	-0.73268000	5.93108000	-0.68130500
C	0.12760600	6.74616400	-0.42902100
C	3.14967700	4.77039000	0.12291400
C	2.80125500	5.93074200	0.13725000
C	-3.14967700	-4.77039000	0.12291400
C	-2.80125500	-5.93074200	0.13725000
C	0.73268000	-5.93108000	-0.68130500
C	-0.12760600	-6.74616400	-0.42902100
C	-1.13683700	-7.70148600	-0.12310600
C	-2.42338700	-7.30328200	0.15380500
C	-3.06901900	5.04408900	-1.23202600
C	3.06901900	-5.04408900	-1.23202600
N	-2.84536500	-2.41187300	-0.28740700
N	-2.48922500	2.85389700	-1.25840300
N	2.84536500	2.41187300	-0.28740700
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H	5.59098800	0.82614700	0.46134800
H	4.48253100	-3.34559500	-1.63461600
H	-5.59098800	-0.82614700	0.46134800
H	-4.48253100	3.34559500	-1.63461600
C	4.86294200	1.60841500	0.31097800
C	-4.86294200	-1.60841500	0.31097800
C	0.05828100	-11.58005600	-0.12532900
H	2.22503600	-11.43891900	-0.69031400
C	-7.05512300	-11.24530900	1.55914100
H	-7.20284600	-9.00934900	1.41899600
C	-4.30196000	-9.05601400	0.73655100
C	-3.43499600	-8.25271800	0.46793700
C	-0.40624500	-10.23366900	-0.11129200
C	-0.75626500	-9.07400500	-0.11282100
C	-6.63086300	-9.92240800	1.35535800
N	-6.06117400	-12.11980700	1.39232800
N	-0.75918200	-12.60216100	0.16239900
H	2.03251900	-14.18664800	-0.42928200
H	-8.03848700	-11.61018500	1.82026400
C	1.30073200	-13.40375700	-0.30236300
N	5.00923700	11.36839900	1.08486800
N	-0.01662400	13.67636500	0.04678300
N	-1.42891600	3.61102100	-0.98664300
N	3.61849300	1.33847900	-0.15758400
N	1.42891600	-3.61102100	-0.98664300
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N	-5.00923700	-11.36839900	1.08486800
N	0.01662400	-13.67636500	0.04678300
C	-1.36584700	12.03513900	-0.42436700
C	5.28168200	10.02716800	1.04441200
C	-1.71066700	4.94835000	-0.95796000
C	4.90431700	2.97029500	0.50580300
C	-4.90431700	-2.97029500	0.50580300
C	1.71066700	-4.94835000	-0.95796000
C	-5.28168200	-10.02716800	1.04441200
C	1.36584700	-12.03513900	-0.42436700
Cl	-0.62797400	-15.21329700	0.32992000
Cl	-3.49396600	-12.06111500	0.77924200
Cl	-0.10349900	-2.92800700	-0.75333700
Cl	3.04383400	-0.19815800	-0.59928300
Cl	0.10349900	2.92800700	-0.75333700
Cl	-3.04383400	0.19815800	-0.59928300
Cl	3.49396600	12.06111500	0.77924200
Cl	0.62797400	15.21329700	0.32992000

N-Cl...N_Trimer

0 1

C	18.98437295	-2.45843797	0.02682701
H	18.37355695	-4.57324396	0.46061505
C	20.18971994	4.63808901	-1.28186813
H	18.04010894	5.25899901	-1.09659014
C	17.77184195	-1.71202097	0.06233199
C	16.71562695	-1.12038397	0.10361898
C	17.45998694	2.38577902	-0.55718709
C	16.48940294	1.70000202	-0.31902607
C	15.34552094	0.90140303	-0.04109406
C	15.45793895	-0.45419797	0.15920397
C	18.80760994	4.50042401	-1.07624113
N	20.15993195	-1.86734197	-0.22686901
N	20.82867994	3.47126301	-1.17843011
H	20.75766194	5.53118901	-1.50126915
H	21.09615695	-4.96935596	0.16751305
C	20.49213995	-4.07777696	0.09824604
C	11.82077894	2.90350603	0.13478591
H	12.40098094	4.97493902	-0.49811413
C	3.58962195	-2.66149299	-0.27097898
H	3.02312295	-4.61259401	-1.22009294
C	10.57616495	-4.18560795	1.25380104
H	12.72493995	-4.80875395	1.09306806
C	4.81865694	4.21511805	1.78693589
H	2.66957794	4.85162605	1.69806588
C	13.32935095	-1.92836296	0.64587800
C	14.30908795	-1.24984696	0.42725899
C	13.02986294	2.15345503	0.07745592
C	14.08735294	1.56469803	0.02157293
C	2.37762695	-1.91529999	-0.22270599
C	1.31809395	-1.32812299	-0.19704400
C	2.07120794	2.05282503	0.88248793
C	1.09141494	1.40943102	0.57593994
C	11.96100695	-4.04663495	1.08156604
C	3.43482394	4.09816204	1.59214489
N	4.74120195	-2.15925098	0.19936301
N	9.94766995	-3.01130096	1.17415002
N	10.66393394	2.33980003	0.51415592
N	5.44921894	3.06129505	1.55938291
H	9.70445794	5.40305902	-0.04192614
H	5.39398894	5.08156106	2.08139587
H	5.71819895	-5.09711300	-0.81458093
H	9.99879595	-5.08191295	1.43198606
C	10.31182394	4.51582102	0.05042588
C	5.10627495	-4.23674900	-0.59109295
C	-3.58962195	2.66149299	0.27097898
H	-3.02312295	4.61259401	1.22009294
C	-11.82077894	-2.90350603	-0.13478591
H	-12.40098094	-4.97493902	0.49811413
C	-4.81865694	-4.21511805	-1.78693589
H	-2.66957794	-4.85162605	-1.69806588
C	-10.57616495	4.18560795	-1.25380104
H	-12.72493995	4.80875395	-1.09306806
C	-2.07120794	-2.05282503	-0.88248793

C	-1.09141494	-1.40943102	-0.57593994
C	-2.37762695	1.91529999	0.22270599
C	-1.31809395	1.32812299	0.19704400
C	-13.02986294	-2.15345503	-0.07745592
C	-14.08735294	-1.56469803	-0.02157293
C	-13.32935095	1.92836296	-0.64587800
C	-14.30908795	1.24984696	-0.42725899
C	-15.45793895	0.45419797	-0.15920397
C	-15.34552094	-0.90140303	0.04109406
C	-0.05644506	0.65438601	0.20570896
C	0.05644506	-0.65438601	-0.20570896
C	-3.43482394	-4.09816204	-1.59214489
C	-11.96100695	4.04663495	-1.08156604
N	-10.66393394	-2.33980003	-0.51415592
N	-5.44921894	-3.06129505	-1.55938291
N	-4.74120195	2.15925098	-0.19936301
N	-9.94766995	3.01130096	-1.17415002
H	-5.71819895	5.09711300	0.81458093
H	-9.99879595	5.08191295	-1.43198606
H	-9.70445794	-5.40305902	0.04192614
H	-5.39398894	-5.08156106	-2.08139587
C	-5.10627495	4.23674900	0.59109295
C	-10.31182394	-4.51582102	-0.05042588
C	-18.98437295	2.45843797	-0.02682701
H	-18.37355695	4.57324396	-0.46061505
C	-20.18971994	-4.63808901	1.28186813
H	-18.04010894	-5.25899901	1.09659014
C	-17.45998694	-2.38577902	0.55718709
C	-16.48940294	-1.70000202	0.31902607
C	-17.77184195	1.71202097	-0.06233199
C	-16.71562695	1.12038397	-0.10361898
C	-18.80760994	-4.50042401	1.07624113
N	-20.82867994	-3.47126301	1.17843011
N	-20.15993195	1.86734197	0.22686901
H	-21.09615695	4.96935596	-0.16751305
H	-20.75766194	-5.53118901	1.50126915
C	-20.49213995	4.07777696	-0.09824604
Cl	22.67863095	-2.55492097	-0.44409199
Cl	20.21853194	0.94963202	-0.69073506
Cl	7.24478995	-2.93585197	0.47538802
Cl	10.57834895	-0.47058996	0.81372297
Cl	8.16050294	3.07600104	0.88733691
Cl	4.82403995	0.58790603	0.87079796
Cl	-8.16050294	-3.07600104	-0.88733691
Cl	-4.82403995	-0.58790603	-0.87079796
Cl	-7.24478995	2.93585197	-0.47538802
Cl	-10.57834895	0.47058996	-0.81372297
Cl	-20.21853194	-0.94963202	0.69073506
Cl	-22.67863095	2.55492097	0.44409199
N	-19.87924905	-2.58447900	0.86312403
N	-21.03793606	2.87520598	0.12747993
N	-10.90901706	2.12465898	-0.93732106
N	-5.62354006	3.12063700	0.04168391
N	4.48445194	2.21060904	1.21831993
N	9.78224594	3.33241603	0.45063090
N	19.87924905	2.58447900	-0.86312403
N	21.03793606	-2.87520598	-0.12747993
N	10.90901706	-2.12465898	0.93732106
N	5.62354006	-3.12063700	-0.04168391
N	-4.48445194	-2.21060904	-1.21831993
C	-18.62955605	-3.13989500	0.79365104
C	-19.13848406	3.85807098	-0.27478609
C	-12.15366306	2.68696398	-0.87880607
C	-11.65677005	-4.27518500	0.17052006
C	-3.76614406	3.96027802	0.81712790
C	-3.23619205	-2.78265102	-1.18363897
C	3.23619205	2.78265102	1.18363897
C	3.76614406	-3.96027802	-0.81712790
C	12.15366306	-2.68696398	0.87880607
C	11.65677005	4.27518500	-0.17052006
C	18.62955605	3.13989500	-0.79365104
C	19.13848406	-3.85807098	0.27478609
N	-9.78224594	-3.33241603	-0.45063090

N-Cl...N_Monomer

0 1			
C	-3.93553300	-2.12893600	-0.00002800
H	-3.61299200	-4.34915000	-0.00003300
C	-4.16530500	5.18438300	-0.00000600
H	-1.93818600	5.46830500	-0.00000400
C	-2.62612300	-1.56873600	-0.00002500
C	-1.49303900	-1.14058200	-0.00002000
C	-1.75488700	2.49336300	-0.00001400
C	-0.88205900	1.65233900	-0.00001300
C	0.14805600	0.67128300	-0.00001100
C	-0.14805600	-0.67128700	-0.00001500
C	-2.80707000	4.82804800	-0.00000700
N	-5.02686100	-1.35125700	-0.00002600
N	-4.96226300	4.11431300	-0.00000900
H	-4.60836000	6.17029900	-0.00000200
H	-6.37979800	-4.32178300	-0.00003400
C	-5.65711100	-3.52037100	-0.00003200
C	3.93553200	2.12893400	0.00002100
H	3.61298500	4.34914700	0.00002800
C	4.16531000	-5.18438300	0.00001300
H	1.93819100	-5.46830800	-0.00000300
C	1.75488800	-2.49336700	-0.00000500
C	0.88205900	-1.65234400	-0.00001000
C	2.62612300	1.56873200	0.00000700
C	1.49303900	1.14057800	-0.00000300
C	2.80707400	-4.82805000	0.00000300
N	4.96226600	-4.11431200	0.00001900
N	5.02686100	1.35125700	0.00002700
H	6.37979100	4.32178800	0.00005400
H	4.60836700	-6.17029800	0.00001600
C	5.65710600	3.52037300	0.00004300
N	-4.12645500	3.08102000	-0.00001300
N	-6.03719000	-2.21610600	-0.00002800
N	4.12645600	-3.08102100	0.00001400
N	6.03718800	2.21610900	0.00004000
C	-2.80507800	3.43959300	-0.00001200
C	-4.28176900	-3.50230700	-0.00003100
C	2.80508000	-3.43959500	0.00000200
C	4.28176400	3.50230600	0.00003000
Cl	7.62962200	1.64861100	0.00005200
Cl	-7.62962200	-1.64860300	-0.00002700
Cl	-4.70087700	1.48748400	-0.00001800
Cl	4.70087700	-1.48748400	0.00002000

N-I...N_Trimer_2Na

2 1			
C	-19.01501600	1.99153300	0.87320900
H	-18.31340000	3.80304400	1.99005300
C	-20.22289800	-4.39246900	-3.01658700
H	-18.05043400	-4.91876500	-3.19488400
C	-17.82520700	1.28917500	0.52075700
C	-16.79118100	0.72208400	0.23997000
C	-17.53231900	-2.41202300	-1.66342300
C	-16.58420100	-1.78487800	-1.23469000
C	-15.45172200	-1.08363100	-0.75308100
C	-15.54539100	0.10049500	-0.05601800
C	-18.83650300	-4.26280600	-2.85245100
N	-20.23017800	1.53517000	0.53358800
N	-20.88365300	-3.37756600	-2.45186700
H	-20.77726600	-5.17341200	-3.51797700
H	-21.02438200	4.26526700	2.11430000
C	-20.46805300	3.45667000	1.66421500
C	-11.89220300	-2.87762200	-1.52695000
H	-12.34985800	-4.65728400	-2.77668300
C	-3.53692400	2.73786400	0.46825800
H	-3.02789200	4.90060200	0.41301300
C	-10.79936100	3.50005800	2.11690700
H	-12.97482100	3.84276400	2.40357700
C	-4.83546500	-4.56873200	0.22466500
H	-2.69052500	-5.09416700	0.48860900
C	-13.40702000	1.38441000	0.80662300
C	-14.37702200	0.77623500	0.40707800
C	-13.13206500	-2.23314700	-1.26877900
C	-14.18275400	-1.68141800	-1.02350800

C	-2.30562600	2.02602500	0.44108800
C	-1.26798000	1.39934700	0.43364600
C	-2.14400800	-2.17751800	0.38844900
C	-1.15767700	-1.47374300	0.42234400
C	0.02507000	-0.67842300	0.44067400
C	-0.02819300	0.69616100	0.43578900
C	-12.15925900	3.26244400	2.00102300
C	-3.47055800	-4.35860400	0.36731900
N	-4.73077100	2.09590600	0.52549300
N	-10.11922200	2.53116700	1.47446400
N	-10.72376100	-2.39455900	-1.03932100
N	-5.46436700	-3.38617900	0.09960100
H	-9.62632900	-4.98044600	-2.59210400
H	-5.39448800	-5.49359400	0.19409500
H	-5.76545900	5.12587600	0.52349600
H	-10.27374500	4.30499000	2.61132500
C	-10.25875800	-4.20558700	-2.18216600
C	-5.14814300	4.23865400	0.50440000
I	-7.64495300	-3.20487100	-0.68739800
I	-4.81641300	-0.16709000	0.29886500
I	-7.92977900	2.68466500	0.96824400
I	-10.68908100	-0.33416500	-0.06484800
I	-20.37024900	-0.83631400	-0.90377500
I	-23.10954000	2.18160800	0.75757800
C	3.53384200	-2.71933100	0.50544600
H	3.02352200	-4.88194900	0.46325800
C	11.89744900	2.88421500	-1.50111000
H	12.35752400	4.66414100	-2.74936800
C	4.83288300	4.58504800	0.21536900
H	2.68675500	5.11161800	0.46573000
C	10.79955700	-3.49244900	2.14244400
H	12.97505600	-3.83883900	2.42413400
C	2.14146400	2.19439000	0.38937600
C	1.15474800	1.49116100	0.42285900
C	2.30277400	-2.00737100	0.47064800
C	1.26506200	-1.38101400	0.45361500
C	13.13652000	2.23763100	-1.24421700
C	14.18657300	1.68358000	-1.00146800
C	13.40830900	-1.38105100	0.82751300
C	14.37927000	-0.77511300	0.42692800
C	15.54774700	-0.10429800	-0.04317300
C	15.45469000	1.08033600	-0.73932500
C	3.46753800	4.37548900	0.35326600
C	12.15954100	-3.25727300	2.02333500
N	10.72825000	2.40257600	-1.01366700
N	5.46260500	3.40169200	0.10261200
N	4.72811100	-2.07781500	0.56063900
N	10.11979500	-2.52227600	1.50156200
H	5.76076300	-5.10831000	0.57973800
H	10.27359100	-4.29623500	2.63838300
H	9.63456000	4.99156200	-2.56360000
H	5.39192700	5.50978500	0.18085000
C	5.14406500	-4.22079400	0.55416800
C	10.26583100	4.21527300	-2.15452400
C	19.01350400	-2.01552000	0.85888400
H	18.30862600	-3.83133300	1.96687400
C	20.22423900	4.36653500	-3.03912400
H	18.05262700	4.90032700	-3.20614000
C	17.53472200	2.40174700	-1.66113000
C	16.58713800	1.77735200	-1.22728100
C	17.82553400	-1.30423700	0.51828600
C	16.79257200	-0.73066000	0.24679100
C	18.83835800	4.24284300	-2.86586100
N	20.88468300	3.35141200	-2.47452400
N	20.22903000	-1.56290400	0.51597400
H	21.01788800	-4.30800300	2.07328700
H	20.77841000	5.14336900	-3.54706600
C	20.46322500	-3.49356200	1.63177700
I	23.10616000	-2.22424000	0.72080900
I	20.37129600	0.81965200	-0.91201100
I	7.92950100	-2.66951600	1.00242400
I	10.69095000	0.34267100	-0.03982600
I	7.64696200	3.21653800	-0.66790400
I	4.81471800	0.18336300	0.32175500
N	-19.94810800	-2.59374800	-1.92569800

N	-21.09006400	2.43554100	1.02114400
N	-11.00313700	1.67727600	0.92506600
N	-9.73187900	-3.20247900	-1.45395900
N	-4.54521800	-2.40983800	0.14240400
N	-5.70556700	3.01563900	0.54005500
N	4.54366800	2.42525900	0.14899500
N	5.70226500	-2.99803200	0.58274500
N	11.00385700	-1.66988800	0.95002900
N	9.73756900	3.21262800	-1.42689400
N	19.94929900	2.57327400	-1.93941500
N	21.08689000	-2.47086100	0.99269000
C	-18.68275400	-3.08112400	-2.13678800
C	-19.11706700	3.20470700	1.58961800
C	-12.25408100	2.09312800	1.23826900
C	-11.63092300	-4.03795400	-2.26323200
C	-3.76697700	4.11560400	0.45331100
C	-3.32196700	-2.97067900	0.31117000
C	3.31961000	2.98704200	0.30830000
C	3.76306500	-4.09722600	0.49989000
C	11.63775500	4.04552200	-2.23627100
C	12.25466200	-2.08807400	1.26030900
C	18.68455800	3.06468000	-2.14453400
C	19.11315100	-3.23429400	1.56621600
Na	7.84998500	0.61859100	1.34407700
Na	-7.85045000	-0.59873200	1.30743300

N-I...N_Dimer_Na

1 1			
C	1.93278200	11.30242900	0.69717600
H	4.00368000	10.63701900	1.23490000
C	-5.29656400	12.36879300	-1.29766500
H	-5.75820000	10.18293600	-1.49899700
C	1.20672200	10.09833000	0.46015500
C	0.62547300	9.05233000	0.26705600
C	-2.91917200	9.72265200	-0.70944700
C	-2.16465300	8.78912700	-0.52435900
C	-1.31944200	7.66946800	-0.31815500
C	0.00000000	7.79058600	0.05502700
C	-5.06998400	10.98482300	-1.27816300
N	1.35616600	12.50798500	0.58105500
N	-4.19903200	13.05382700	-0.96500300
H	-6.20435800	12.90463600	-1.53745600
H	4.38121100	13.35747200	1.42693700
C	3.50238200	12.78490300	1.17063500
I	-1.32318500	12.59722800	-0.16679000
I	1.93089100	15.39957100	0.82876000
C	-3.11174200	4.06379600	-0.84381000
H	-5.16911200	4.48164100	-1.57200600
C	3.11174200	-4.06379600	-0.84381000
H	5.16911200	-4.48164100	-1.57200600
C	4.02892700	3.12043700	0.94508800
H	4.36179100	5.29153900	1.28570400
C	-4.02892700	-3.12043700	0.94508800
H	-4.36179100	-5.29153900	1.28570400
C	1.55606100	5.68838000	0.40817900
C	0.82290300	6.64048900	0.24618300
C	-2.47376500	5.32352600	-0.67941900
C	-1.91821300	6.38775300	-0.51395400
C	2.47376500	-5.32352600	-0.67941900
C	1.91821300	-6.38775300	-0.51395400
C	-1.55606100	-5.68838000	0.40817900
C	-0.82290300	-6.64048900	0.24618300
C	0.00000000	-7.79058600	0.05502700
C	1.31944200	-7.66946800	-0.31815500
C	3.72419100	4.47265000	0.99095200
C	-3.72419100	-4.47265000	0.99095200
N	2.47332200	-2.90065400	-0.56608300
N	2.95256400	2.42968500	0.52700000
N	-2.47332200	2.90065400	-0.56608300
N	-2.95256400	-2.42968500	0.52700000
H	-5.31910200	1.73717300	-1.47543200
H	-4.95260200	-2.60854600	1.17677000
H	5.31910200	-1.73717300	-1.47543200
H	4.95260200	2.60854600	1.17677000

C	-4.49211300	2.39166100	-1.23808000
C	4.49211300	-2.39166100	-1.23808000
C	-1.93278200	-11.30242900	0.69717600
H	-4.00368000	-10.63701900	1.23490000
C	5.29656400	-12.36879300	-1.29766500
H	5.75820000	-10.18293600	-1.49899700
C	2.91917200	-9.72265200	-0.70944700
C	2.16465300	-8.78912700	-0.52435900
C	-1.20672200	-10.09833000	0.46015500
C	-0.62547300	-9.05233000	0.26705600
C	5.06998400	-10.98482300	-1.27816300
N	4.19903200	-13.05382700	-0.96500300
N	-1.35616600	-12.50798500	0.58105500
H	-4.38121100	-13.35747200	1.42693700
H	6.20435800	-12.90463600	-1.53745600
C	-3.50238200	-12.78490300	1.17063500
I	-1.93089100	-15.39957100	0.82876000
I	1.32318500	-12.59722800	-0.16679000
I	-3.05220200	-0.25398900	-0.17188200
I	0.22682400	-2.92933000	-0.16507900
I	3.05220200	0.25398900	-0.17188200
I	-0.22682400	2.92933000	-0.16507900
N	-3.26602900	12.13504300	-0.73082300
N	2.32229800	13.38641700	0.87139500
N	1.95703000	3.30030300	0.28189700
N	-3.31686000	1.88648900	-0.82003400
N	-1.95703000	-3.30030300	0.28189700
N	3.31686000	-1.88648900	-0.82003400
N	3.26602900	-12.13504300	-0.73082300
N	-2.32229800	-13.38641700	0.87139500
C	3.29007200	11.42909600	1.06858800
C	-3.73735700	10.85852300	-0.90524900
C	2.39501600	4.55180100	0.56390900
C	-4.40952600	3.77468500	-1.27657600
C	4.40952600	-3.77468500	-1.27657600
C	-2.39501600	-4.55180100	0.56390900
C	3.73735700	-10.85852300	-0.90524900
C	-3.29007200	-11.42909600	1.06858800
Na	0.00000000	0.00000000	1.04543000

N-I...N_Dimer

0 1			
C	11.33961394	-2.05431884	0.48849213
H	10.62938296	-4.13792885	0.90229415
C	12.47706586	5.29119516	-0.95787194
H	10.29030786	5.78533713	-1.07855495
C	10.14752593	-1.29016386	0.32367412
C	9.10632292	-0.68408087	0.19227511
C	9.81154589	2.90012813	-0.51000792
C	8.86821489	2.14952912	-0.37068292
C	7.73175590	1.30824511	-0.21588991
C	7.84333492	-0.03659489	0.04977810
C	11.09028386	5.07601114	-0.92928894
N	12.55698593	-1.50130083	0.38799113
N	13.15826687	4.16659917	-0.72725693
H	13.01711485	6.21107716	-1.13524695
H	13.34334897	-4.59765682	1.01934716
C	12.78933096	-3.69013782	0.83135815
C	4.13107588	3.15270207	-0.54292493
H	4.58804786	5.28124207	-0.99275295
C	-4.13107588	-3.15270207	-0.54292493
H	-4.58804786	-5.28124207	-0.99275295
C	3.19617296	-4.12875293	0.64280614
H	5.38378596	-4.46815190	0.86590114
C	-3.19617296	4.12875293	0.64280614
H	-5.38378596	4.46815190	0.86590114
C	5.72583993	-1.58821591	0.30579312
C	6.69138693	-0.86402190	0.19236211
C	5.38647889	2.49168408	-0.44836593
C	6.45755890	1.93398410	-0.34559092
C	-5.38647889	-2.49168408	-0.44836593
C	-6.45755890	-1.93398410	-0.34559092
C	-5.72583993	1.58821591	0.30579312
C	-6.69138693	0.86402190	0.19236211

C	-7.84333492	0.03659489	0.04977810
C	-7.73175590	-1.30824511	-0.21588991
C	4.54686796	-3.81343092	0.67851214
C	-4.54686796	3.81343092	0.67851214
N	-2.95684606	-2.50316701	-0.35882389
N	2.48644095	-3.01915194	0.37690312
N	2.95684606	2.50316701	-0.35882389
N	-2.48644095	3.01915194	0.37690312
H	1.83744186	5.45344904	-0.89316596
H	-2.69593014	5.07629501	0.78415903
H	-1.83744186	-5.45344904	-0.89316596
H	2.69593014	-5.07629501	0.78415903
C	2.48353287	4.59759705	-0.75880095
C	-2.48353287	-4.59759705	-0.75880095
I	-0.24584612	3.05322602	-0.05914994
I	-2.90835608	-0.23254200	-0.06267691
I	0.24584612	-3.05322602	-0.05914994
I	2.90835608	0.23254200	-0.06267691
I	12.67704690	1.24084317	-0.15333390
I	15.43380294	-2.16113980	0.54352014
C	-11.33961394	2.05431884	0.48849213
H	-10.62938296	4.13792885	0.90229415
C	-12.47706586	-5.29119516	-0.95787194
H	-10.29030786	-5.78533713	-1.07855495
C	-9.81154589	-2.90012813	-0.51000792
C	-8.86821489	-2.14952912	-0.37068292
C	-10.14752593	1.29016386	0.32367412
C	-9.10632292	0.68408087	0.19227511
C	-11.09028386	-5.07601114	-0.92928894
N	-13.15826687	-4.16659917	-0.72725693
N	-12.55698593	1.50130083	0.38799113
H	-13.34334897	4.59765682	1.01934716
H	-13.01711485	-6.21107716	-1.13524695
C	-12.78933096	3.69013782	0.83135815
I	-15.43380294	2.16113980	0.54352014
I	-12.67704690	-1.24084317	-0.15333390
N	12.22992388	3.22592416	-0.54957092
N	13.41614094	-2.50761782	0.59880414
N	3.32824994	-1.98918393	0.23222812
N	1.96232188	3.38705304	-0.49367794
N	-3.32824994	1.98918393	0.23222812
N	-1.96232188	-3.38705304	-0.49367794
N	-12.22992388	-3.22592416	-0.54957092
N	-13.41614094	2.50761782	0.59880414
C	10.95598388	3.72022914	-0.66108493
C	11.43877295	-3.43700784	0.76814114
C	4.59269494	-2.44116592	0.41088712
C	3.86653887	4.50148106	-0.80385195
C	-3.86653887	-4.50148106	-0.80385195
C	-4.59269494	2.44116592	0.41088712
C	-10.95598388	-3.72022914	-0.66108493
C	-11.43877295	3.43700784	0.76814114

N-I...N_Trimer

0 1			
C	-18.98985997	2.11548712	1.24446580
H	-18.15629696	4.02473712	2.06710678
C	-20.55977999	-4.67115991	-1.71832012
H	-18.40786299	-5.22292793	-2.04287010
C	-17.84643197	1.35509810	0.86173382
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