PARAMETERIZING THE INFLUENCE OF THE ATOM TYPE ON HIGHLY SYMMETRIC STRUCTURES

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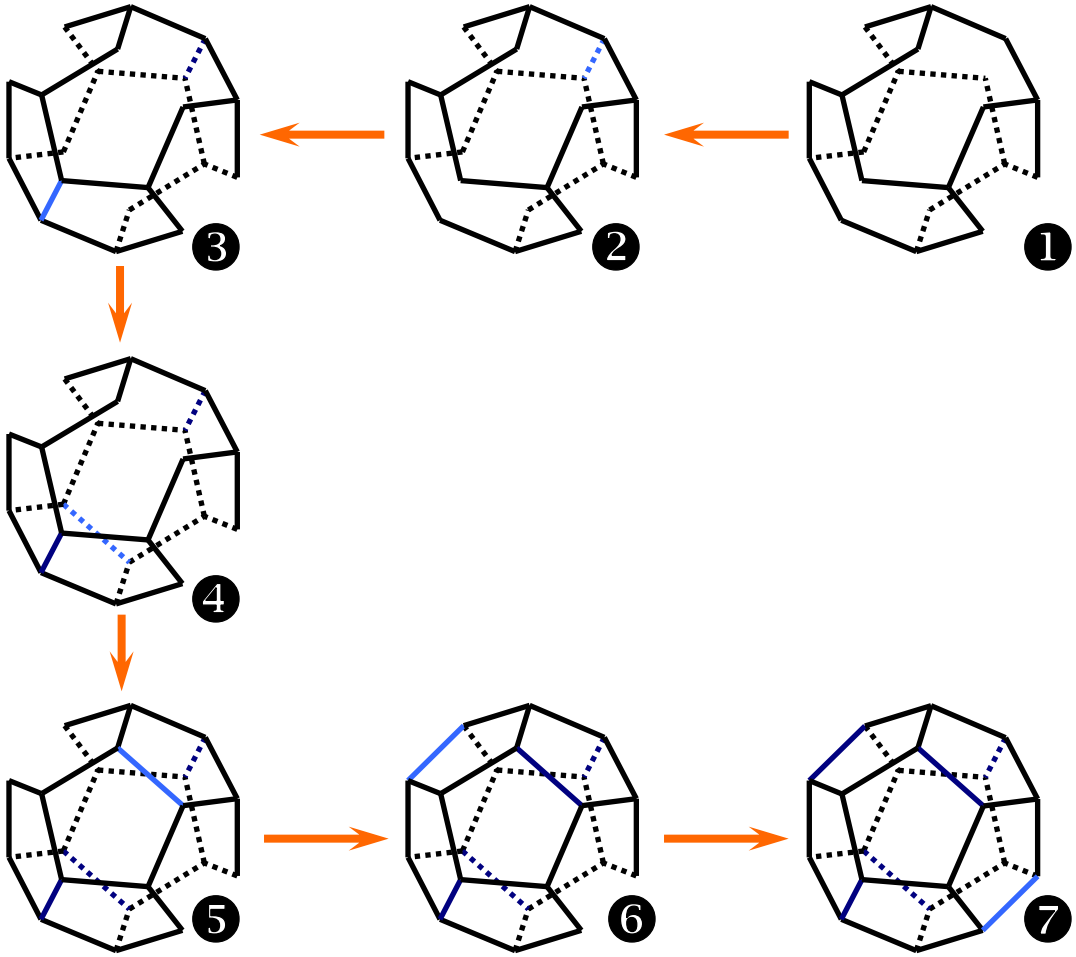
OUTLINE

- Aim
- Material
- Methods
- Results
- Conclusion

Aim

To analyze the influence of three atoms (named carbon, nitrogen and boron) on a set of highly symmetry structure represented by the family of congeners of one-cage pentagonal faced nanostructure.

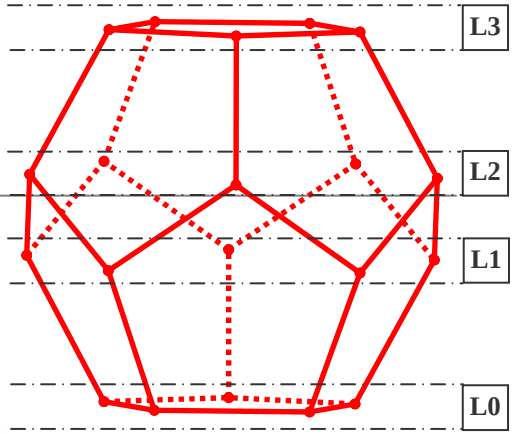
MATERIAL & METHODS



Energy of construction
PM3 estimation

Step	n_C	n_H	SBE
❶	20	32	-5053
❷	20	30	-4963
❸	20	28	-4870
❹	20	26	-4773
❺	20	24	-4666
❻	20	22	-4584
❼	20	20	-4499

MATERIAL



- Layers = 4 & Levels = 3 → 3^4 = 81 structures
- 45 distinct congeners

	L0	L1	L2	L3
01	B	B	B	B
02	B	B	B	N
03	B	B	C	N
04	B	B	N	B
05	B	B	N	N
06	B	C	B	B
07	B	C	B	N
08	B	C	C	B
09	B	C	C	N
10	B	C	N	B
11	B	C	N	N
12	B	N	B	N
13	B	N	C	N
14	B	N	N	B
15	B	N	N	N

	L0	L1	L2	L3
16	C	B	B	B
17	C	B	B	C
18	C	B	B	N
19	C	B	C	B
20	C	B	C	N
21	C	B	N	B
22	C	B	N	C
23	C	B	N	N
24	C	C	B	B
25	C	C	B	C
26	C	C	B	N
27	C	C	C	B
28	C	C	C	C
29	C	C	C	N
30	C	C	N	B

	L0	L1	L2	L3
31	C	C	N	C
32	C	C	N	N
33	C	N	B	B
34	C	N	B	N
35	C	N	C	B
36	C	N	C	N
37	C	N	N	B
38	C	N	N	C
39	C	N	N	N
40	N	B	B	N
41	N	B	N	N
42	N	C	B	N
43	N	C	C	N
44	N	C	N	N
45	N	N	N	N

METHODS

- Structures drawn: HyperChem

- Geometry optimization:
  - Spartan (v. 10)
  - Method: Moller Plesset
  - Basis set: 6-31G*

- Properties calculation (Spartan): volume, surface area, ovality, HOMO and LUMO energies, polarizability, dipole moment, entropy, enthalpy, and total energy

METHODS

Full factorial analysis:

- Properties
- All factors in the model → perfect model ($R^2 = 1$)
- Method: stepwise backward
- Program: home made

- **Szeged Matrix Property Indices (SMPI) Descriptors Family**:
  - pure topological information
  - extended molecular topology
  - information from molecular geometry

C	**B**	**N**
N	**C**	**B**
B	**N**	**C**

Gene	Genome						
Atomic property (A_P)	A	B	C	D	E	F	G
Distance metric (D_M)	T	G	U				
Interaction descriptor (I_D)	E	U	D	Q			
Matrix operation (M_O)	m	M	I	J	E	F	
Linearization operator (L_O)	I	R	L				

RESULTS: FACTORIAL ANALYSIS

Property	Dist	Sym	Zero
DipoleT_C	44	36	
DipoleT_N	44	36	
DipoleT_B	44	36	
EnergyHF_C	44	36	
EnergyHF_N	43	36	
EnergyHF_B	44	36	
HOMO_C	44	36	
HOMO_N	42	37	1
HOMO_B	42	37	1
LUMO_C	44	36	
LUMO_N	43	37	
LUMO_B	44	36	
Volume_C	44	36	
Volume_N	43	37	
Volume_B	41	39	

Property	Dist	Sym	Zero
Ovality_C	44	36	
Ovality_N	41	39	
Ovality_B	22	50	8
Polarizability_C	43	37	
Polarizability_N	44	36	
Polarizability_B	44	36	
SurfaceArea_C	44	36	
SurfaceArea_N	44	36	
SurfaceArea_B	43	37	
TotalsEnth_C	44	36	
TotalsEnth_N	44	36	
TotalsEnth_B	44	36	
TotalsEntr_C	44	36	
TotalsEntr_N	44	36	
TotalsEntr_B	44	36	

RESULTS: FACTORIAL ANALYSIS

Polarizability

F1	F2	F3	F4	r
C4*N2+N3*C1	N4*N2+N3*N1	N4*C1+C4*N1	N4*N1	0.9135
B4+B1	C4+C1	B3+B2	C3+C2	0.9665
N4+N1	B4+B1	B3+B2		0.9615

Energy

F1	F2	F3	r
C4+C1	N4+N1	N3+N2	0.9450
B4+B1	B3+B2	C3+C2	0.9257
N4+N1	B4+B1	N3+N2	0.9450

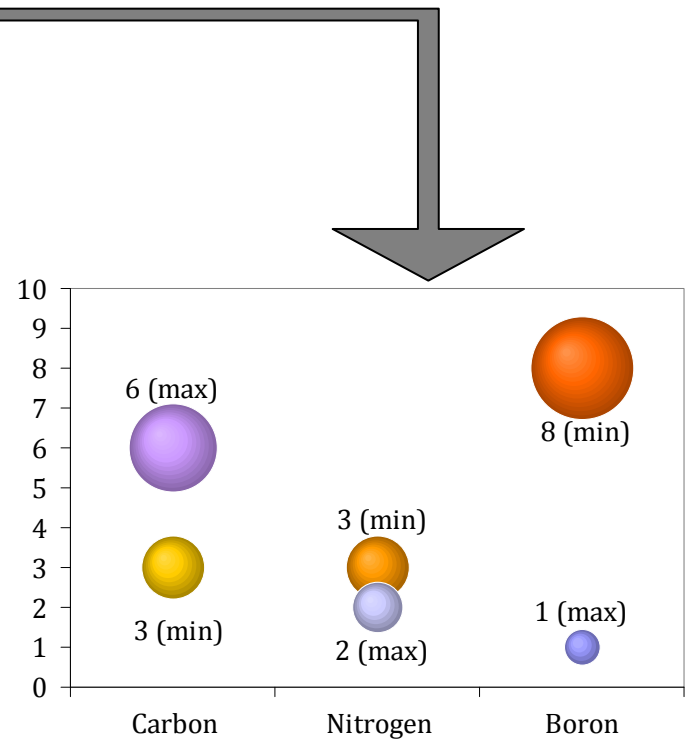
Pol & Eng
r = 0.9366

B4+B1	C4+C1	B3+B2	C3+C2	0.9999
N4+N1	B4+B1	N3+N2	B3+B2	0.9999

RESULTS: FACTORIAL ANALYSIS

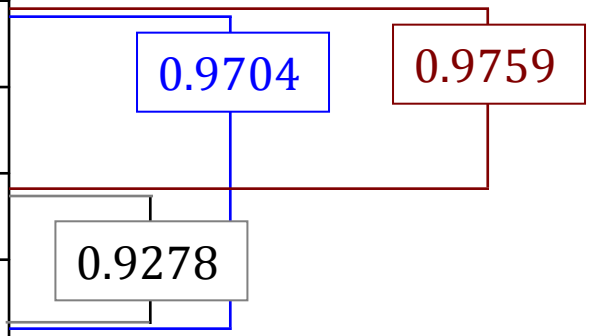
Property	NoF	r
DipoleT_C	19	0.9566
DipoleT_N	14	0.9549
DipoleT_B	15	0.9526
EnergyHF_C	4	0.9999
EnergyHF_N	4	0.9999
EnergyHF_B	4	0.9999
HOMO_C	27	0.9951
HOMO_N	17	0.9522
HOMO_B	12	0.9535
LUMO_C	8	0.9591
LUMO_N	10	0.9504
LUMO_B	8	0.9641
Volume_C	9	0.9548
Volume_N	4	0.9809
Volume_B	3	0.9593

Property	NoF	r
Ovality_C	15	0.9502
Ovality_N	18	0.9508
Ovality_B	7	0.9577
Polarizability_C	8	0.9526
Polarizability_N	4	0.9665
Polarizability_B	3	0.9615
SurfaceArea_C	8	0.9566
SurfaceArea_N	5	0.9536
SurfaceArea_B	3	0.9567
TotalsEnth_C	2	0.9562
TotalsEnth_N	2	0.9562
TotalsEnth_B	9	0.9504
TotalsEntr_C	18	0.9533
TotalsEntr_N	8	0.9622
TotalsEntr_B	7	0.9601



RESULTS: SMPI MODELS

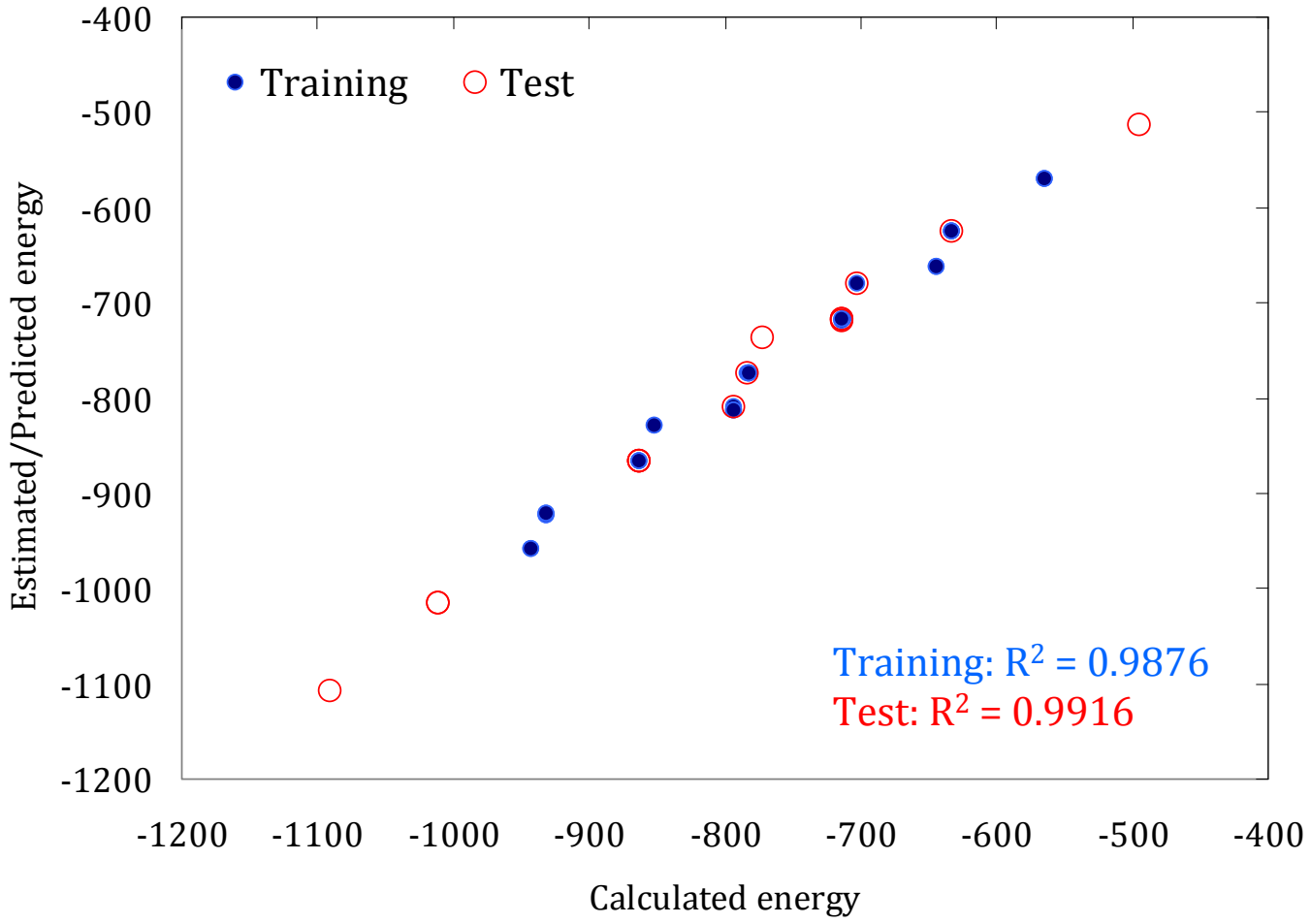
Eq	Model
01	$\hat{Y}_{dipole} = 29.39-292.16\times RMEGE$
02	$\hat{Y}_{energy} = 5939.21-736.49\times LJETE$
03	$\hat{Y}_{HOMO} = -0.122-0.001\times IJUGE$
04	$\hat{Y}_{LUMO} = -3.47+1.10\times LmUTA$
05	$\hat{Y}_{vol} = 346.10-0.64\times IJUGE$
06	$\hat{Y}_{ovality} = 1.43-(2.25\times10^{5})\times RFEGA$
07	$\hat{Y}_{polarizability} = 70.02-0.07\times IJUGE$
08	$\hat{Y}_{surfA} = 267.25-0.35\times IJUGE$
09	$\hat{Y}_{enthalpy} = 172.74+4267.89\times REEGB$
10	$\hat{Y}_{entropy} =-497.32+0.19\times IIEGC$



RESULTS: SMPI MODELS

Eq	Model statistics				LOO statistics		
	R^2	R^2_{adj}	s	$F_{est}(p_{est})$	R^2_{loo}	s_{loo}	$F_{loo}(p_{loo})$
01	0.3341	0.3186	2.80	22 ($3.21 \cdot 10^{-5}$)	0.2809	2.92	17 ($1.99 \cdot 10^{-4}$)
02	0.9895	0.9893	13.39	4062 ($3.30 \cdot 10^{-44}$)	0.9886	13.99	3715 ($3.83 \cdot 10^{-44}$)
03	0.6245	0.6158	0.03	72 ($1.08 \cdot 10^{-10}$)	0.5980	0.04	64 ($4.82 \cdot 10^{-10}$)
04	0.7611	0.7555	0.04	137 ($5.92 \cdot 10^{-15}$)	0.7303	0.05	116 ($8.66 \cdot 10^{-14}$)
05	0.9394	0.9380	6.68	667 ($8.22 \cdot 10^{-28}$)	0.9338	6.98	606 ($2.30 \cdot 10^{-27}$)
06	0.7031	0.6962	0.01	102 ($6.56 \cdot 10^{-13}$)	0.6762	0.01	90 ($4.36 \cdot 10^{-12}$)
07	0.9527	0.9516	0.61	867 ($3.94 \cdot 10^{-30}$)	0.9481	0.64	785 ($1.08 \cdot 10^{-29}$)
08	0.7990	0.7944	7.25	171 ($1.40 \cdot 10^{-16}$)	0.7813	7.57	154 ($8.88 \cdot 10^{-16}$)
09	0.8894	0.8869	64.44	346 ($3.51 \cdot 10^{-22}$)	0.8738	68.87	297 ($3.38 \cdot 10^{-21}$)
10	0.6758	0.6683	18.22	90 ($4.42 \cdot 10^{-12}$)	0.6487	18.97	79 ($2.57 \cdot 10^{-11}$)

RESULTS: SMPI MODELS



REFERENCES

- Monica ŞTEFU, Daniela BUTYKA, Mircea V. DIUDEA, Lorentz JÄNTSCHI, 2005. Bazil PÂRV, Algorithms for basic operations on maps (p. 243-267) In: nanostructures: novel architecture (Mircea V. DIUDEA ed.), Huntington: Nova Science.
- Monica ŞTEFU, Sorana D. BOLBOACĂ, Mugur C. BĂLAN, Lorentz JÄNTSCHI, 2008. Molecular hyperstructures with high symmetry, BUASVM Cluj-Napoca. Horticulture 65(2): 681-686.
- Lorentz JÄNTSCHI, 2012. Structure vs. Property: Algorithms and Models. Habilitation Thesis in Chemistry. Bucharest: CNATDCU, 164 p.