Capra, leapfrog and other related operations on maps

Mircea V. Diudea

Faculty of Chemistry and Chemical Engineering
Babes-Bolyai University
400084 Cluj, ROMANIA
diudea@chem.ubbcluj.ro

Contents

Relations in a map

* A map *M* is a combinatorial representation of a closed surface.[1] The graph associated to the map is called regular if all its vertices have the same degree.

* Basic relations in *M* :

$$\sum d v_d = 2e$$

$$\sum s f_s = 2e$$

$$v - e + f = \chi(M) = 2(1 - g) \quad \textit{Euler}^{2}$$

T. Pisanski, and M. Randić, in *Geometry at Work*, M. A. A. Notes, **2000**, *53*, 174-194.
L. Euler, *Comment. Acad. Sci. I. Petropolitanae*, **1736**, *8*, 128-140

Basic operations in a map

Stellation[1] *St* (capping, triangulation):

add a new vertex in the center of a face and connect it with each boundary vertex.

$St(M)$:

$$v = v_0 + f_0$$

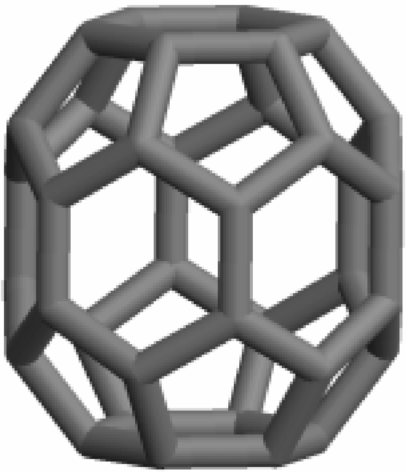
$$e = 3e_0$$

$$f = 2e_0$$

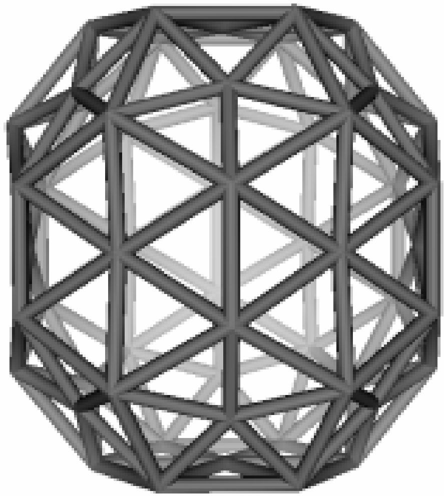
1. T. Pisanski, and M. Randić, in *Geometry at Work*, M. A. A. Notes, **2000**, *53*, 174-194.

Stellation *St*

C_{36}:15 [1] (C_{2h})



St (C_{36}:15)



1. P. W. Fowler and D. E. Manolopolous, *An atlas of fullerenes*, Oxford University Press, Oxford, U.K., 1995.

Basic operations in a map

Dual [1] *Du* (Poincaré *dual*):

locate a point in the center of each face and join two such points if their corresponding faces share a common edge.

$$Du(Du(M)) = M$$

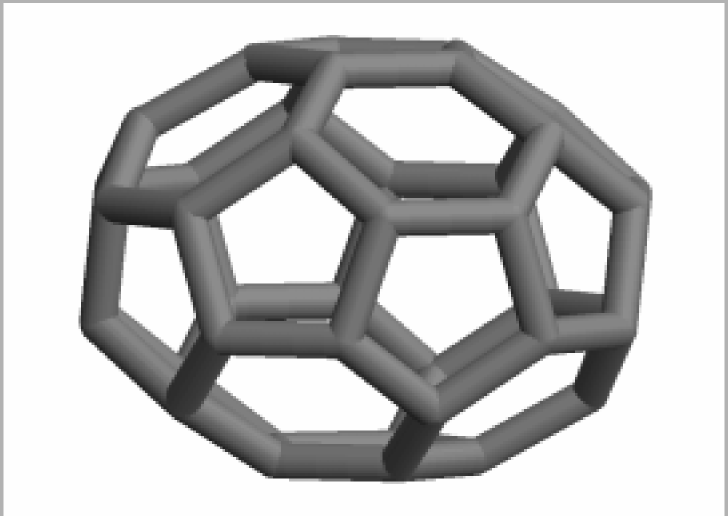
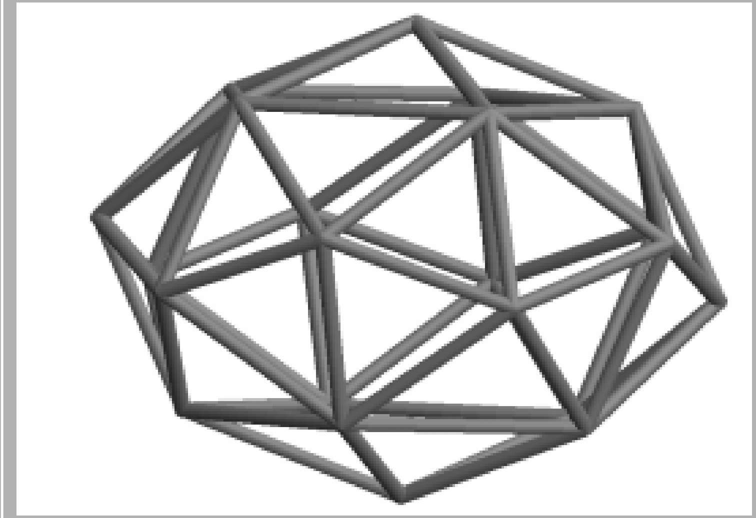
$Du(M)$: $v = f_0$

$e = e_0$

$f = v_0$

1. T. Pisanski, and M. Randić, in *Geometry at Work*, M. A. A. Notes, **2000**, *53*, 174-194.

Dual *Du*

C_{40}:39 [1] (D_{5d})	*Du* (C_{40}:39)
	

1. P. W. Fowler and D. E. Manolopolous, *An atlas of fullerenes*, Oxford University Press, Oxford, U.K., 1995.

Basic operations in a map

Medial [1] *Me* :

put the new vertices as the midpoints of the original edges. Join two vertices if and only if the original edges span an angle.

$Me\,(M) = Me\,(Du\,(M))$ (a 4-valent graph)

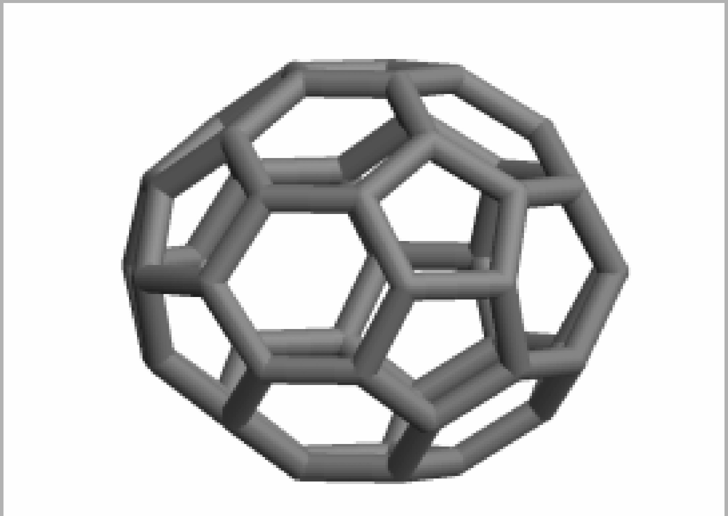
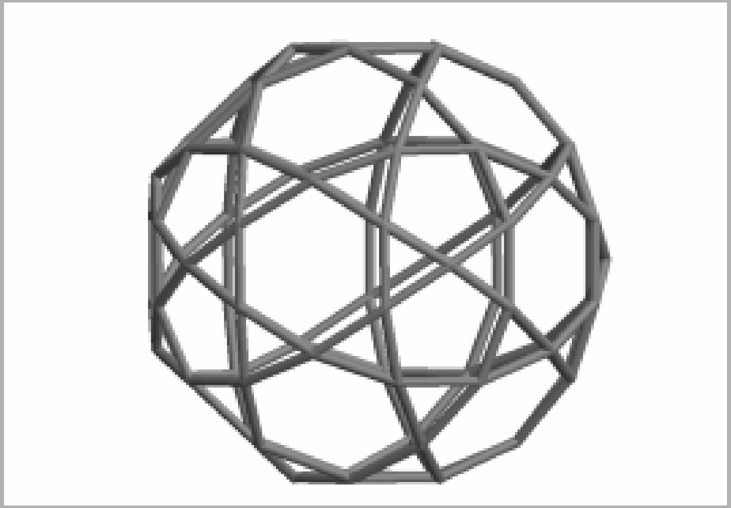
$Me(M)$: $v = e_0$

$e = 2e_0$

$f = f_0 + v_0$

1. T. Pisanski, and M. Randić, in *Geometry at Work*, M. A. A. Notes, **2000**, *53*, 174-194.

Medial *Me*

C_{50}:271 [1] (C_s)	*Me* (C_{50}:271)
	

1. P. W. Fowler and D. E. Manolopolous, *An atlas of fullerenes*, Oxford University Press, Oxford, U.K., 1995.

Basic operations in a map

Truncation [1] *Tr* :

cut of the neighborhood of each vertex by a plane close to the vertex, such that it intersects each edge incident to the vertex.

Truncation is similar to $Me\,(M)$

$Tr\,(M)$:

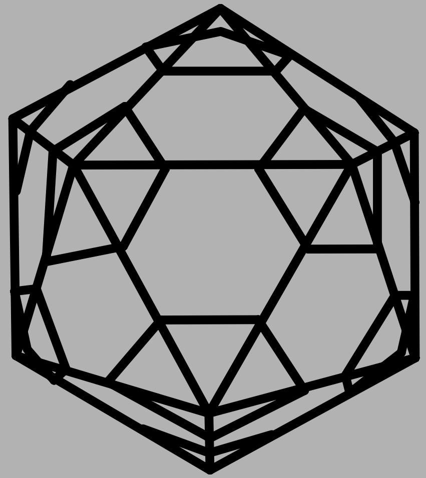
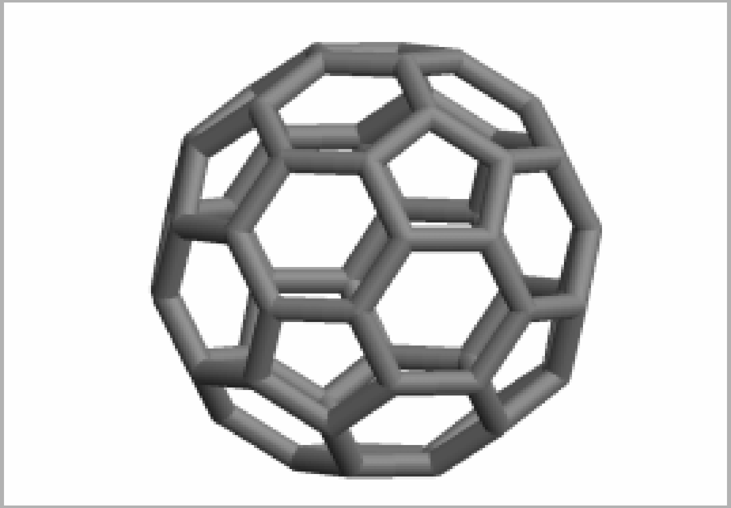
$$v = d_0 v_0$$

$$e = 3e_0$$

$$f = f_0 + v_0$$

1. T. Pisanski, and M. Randić, in *Geometry at Work*, M. A. A. Notes, **2000**, *53*, 174-194.

Truncation *Tr*

Icosahedron (I_h)	*Tr* (Icosahedron) = C_{60} (PC)
	

1. P. W. Fowler and D. E. Manolopolous, *An atlas of fullerenes*, Oxford University Press, Oxford, U.K., 1995.

Composite operations

Leapfrog[1] Le :

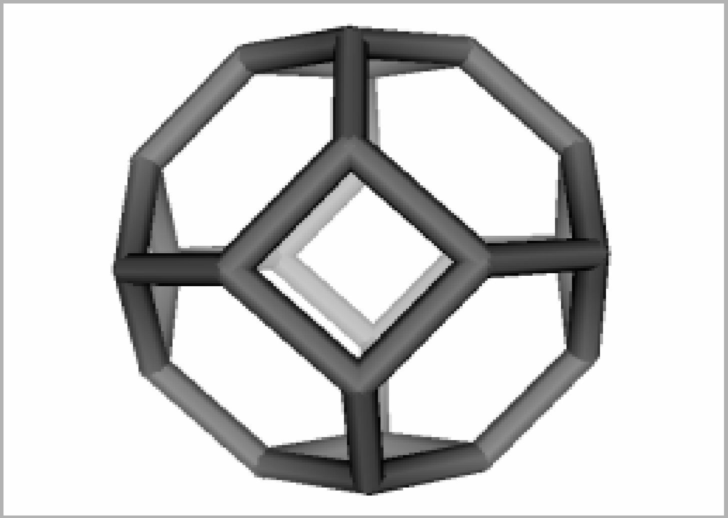
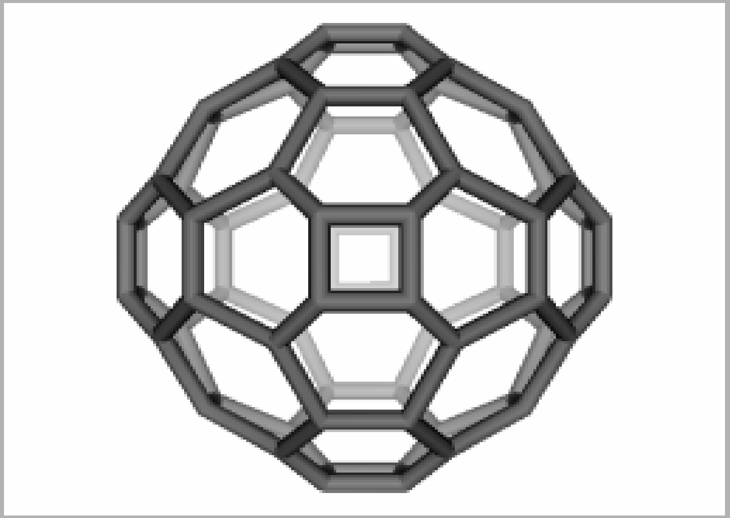
$$Le(M) = Du(St(M)) = Tr(Du(M))$$

$$Le(M): \quad v = d_0 v_0$$
$$e = 3e_0$$
$$f = f_0 + v_0$$

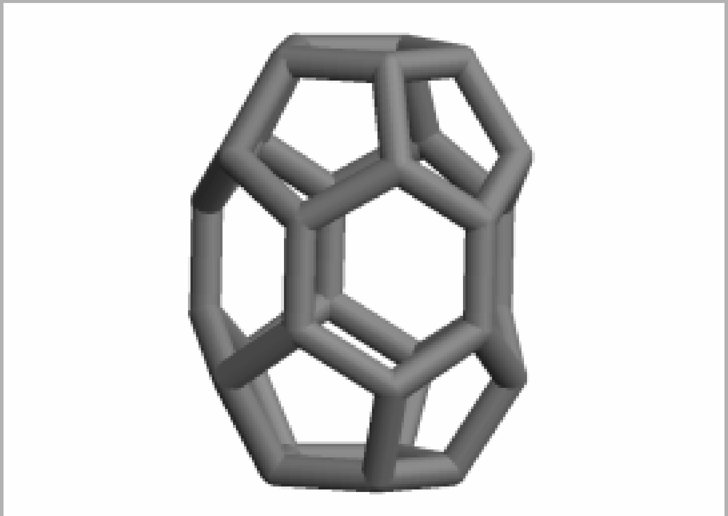
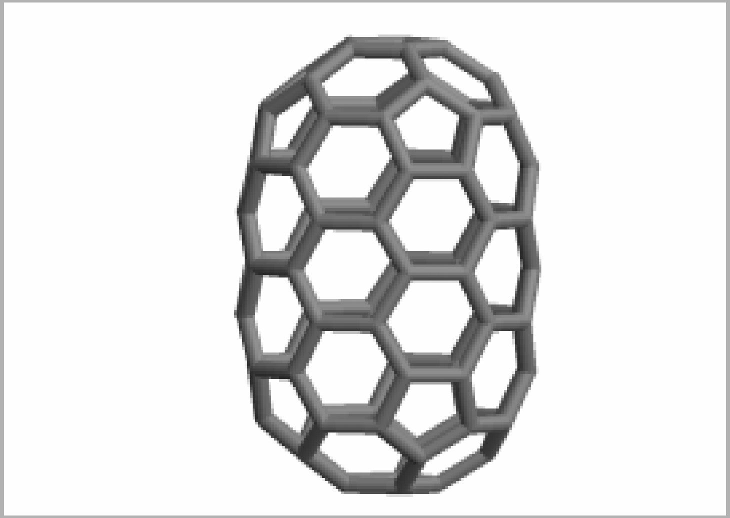
It rotates the parent faces by π / s

1. **P. W. Fowler, *Phys. Lett.*, 1986, *131*, 444.**

Leapfrog Le

Le (Cube)	*Le* (*Le* (Cube))
	

Leapfrog Le

C_{30}:1 (C_s)	*Le* (C_{30}:1) = C_{90}:1 (C_s)
	

Leapfrog *Le - electronic implications*

- In simple Hückel theory,[1] the energy of the i th π -molecular orbital is calculated on the grounds of A(G)

$$E_i = \alpha + \beta\lambda_i$$

$$E_{\text{HOMO}} - E_{\text{LUMO}} = \text{gap}$$

- Study of eigenvalue spectra provided some rules of thumb for the stability of fullerenes.

1. E. Hückel, *Z. Phys.*, 1931, **70**, 204.

π -Electronic Structure

	Relation	GAP	shell	symbol
1	$\lambda_{N/2} > 0 \geq \lambda_{N/2+1}$	$\neq 0$	properly closed	PC
2	$\lambda_{N/2} > \lambda_{N/2+1} > 0$	$\neq 0$	pseudo closed	PSC
3	$0 \geq \lambda_{N/2} > \lambda_{N/2+1}$	$\neq 0$	meta closed	MC
4	$\lambda_{N/2} = \lambda_{N/2+1}$	0	open	OP

Leapfrog Le *- electronic implications*

- ***Leapfrog*** **rule**[1] ***LER*** **:** (PC)

$$N_{Le} = 60 + 6m \; ; \quad (m \neq 1)$$
$$= 3(20 + 2m)$$

In a-tubulenes $C_{12k,k}$**-V[2*k*,*n*]-[6] ;** (PC)

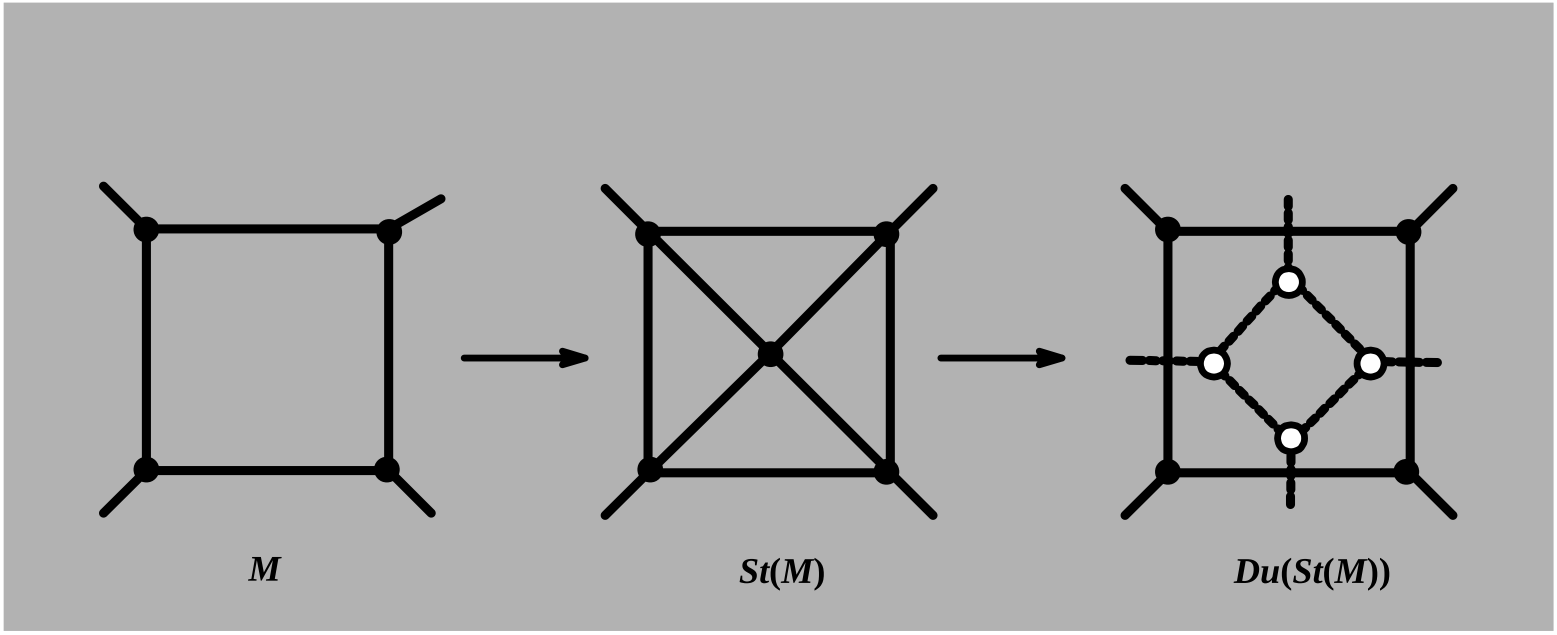
$$N_{Le} = 12k + 2k \cdot 3m$$

$m = 0, 1, 2, \ldots, (k = 4 \text{ to } 7)$

1. P. W. Fowler and J. I. Steer, *J. Chem. Soc.*, *Chem. Commun.*, 1987, 1403-1405.

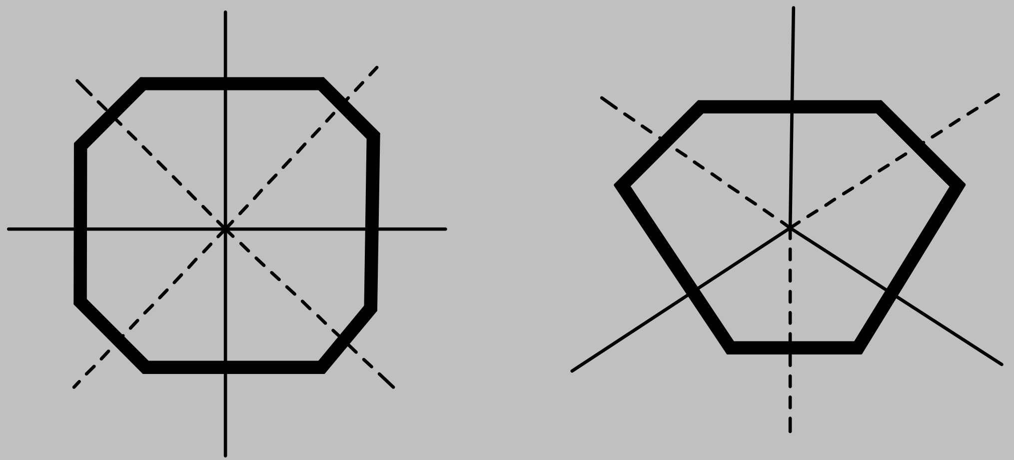
Composite operations

Leapfrog



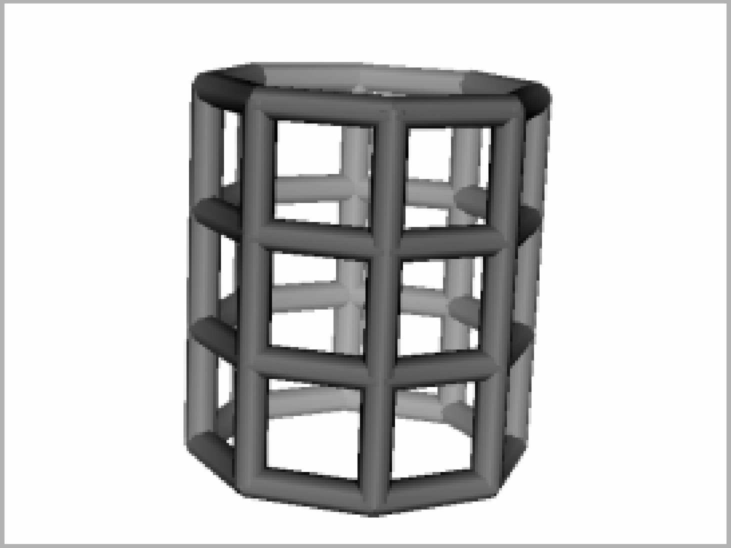
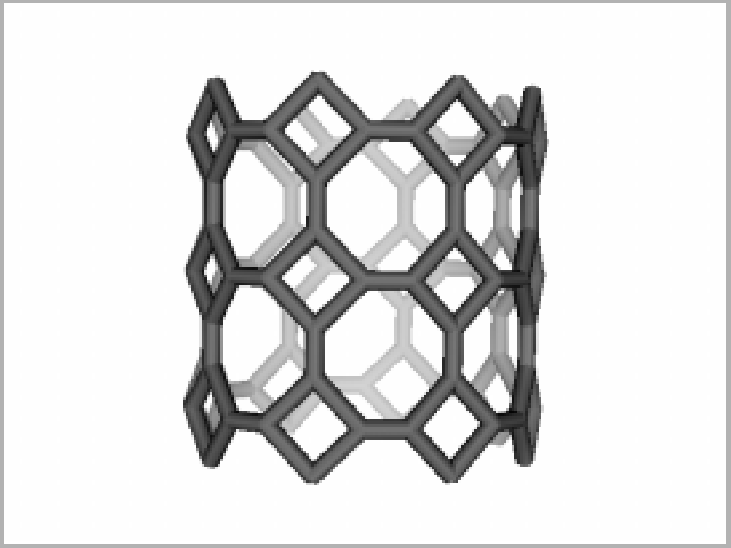
Composite operations

Leapfrog: bounding polygon has $s = 2d_0$



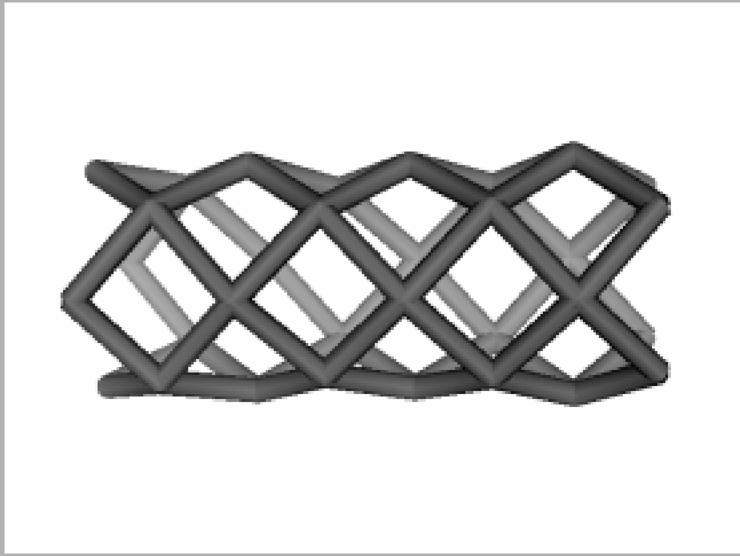
(a) (b)

Leapfrog of a 4-valent net

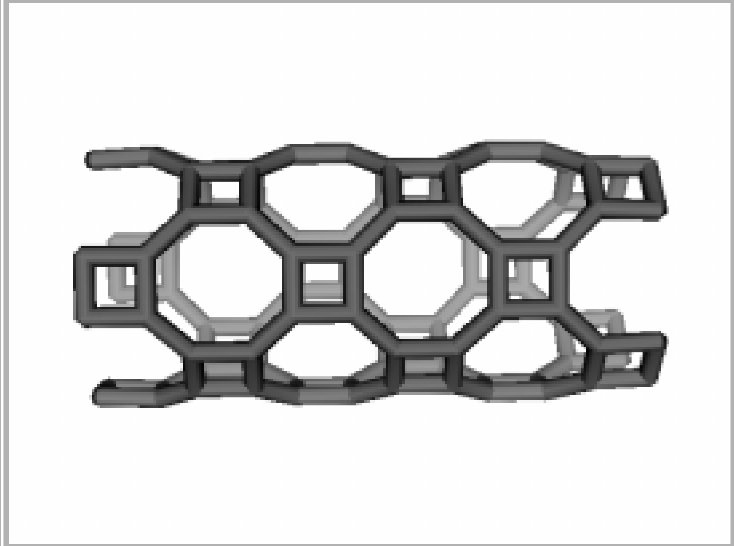
$TUC_4[8,4]$	$TURC_4C_8[8,4]$
	

Leapfrog of a 4-valent net

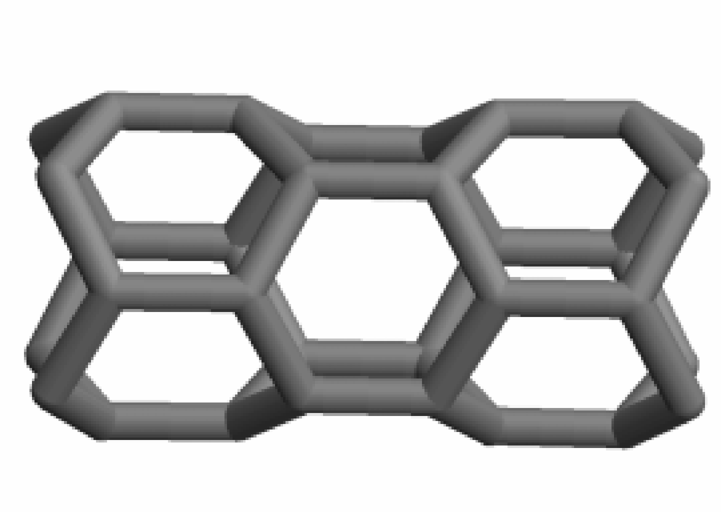
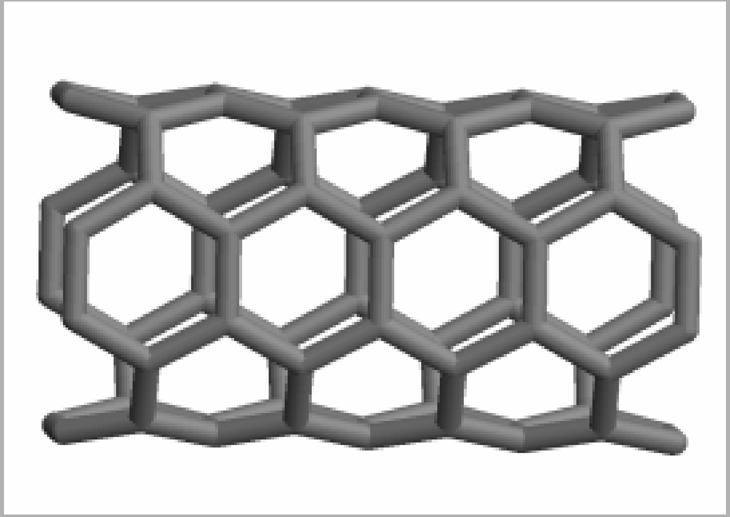
$TUHRC_4[8,4]$ = *Me* ($TUC_4[8,4]$)



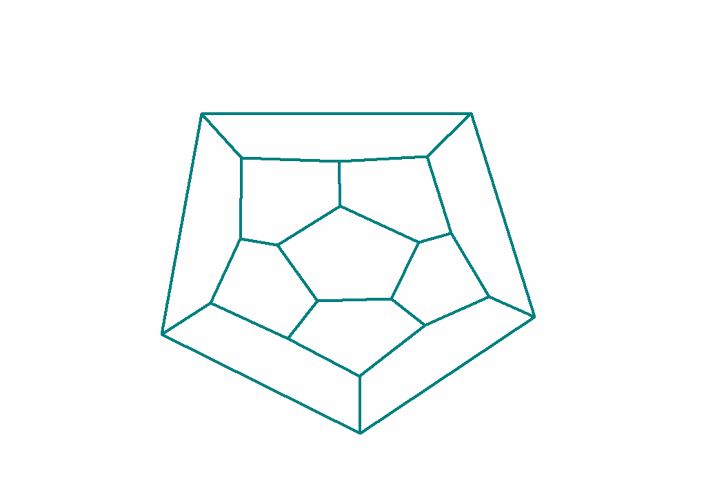
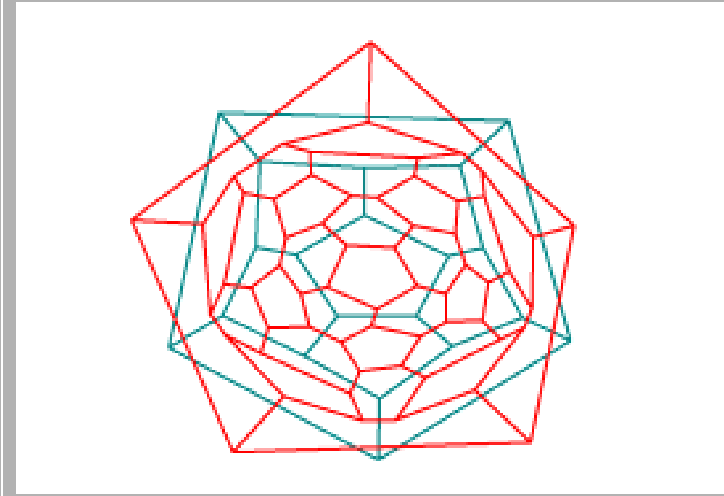
Le ($TUHRC_4[8,4]$)=$TUVSC_4C_8[8,12]$



Leapfrog Le

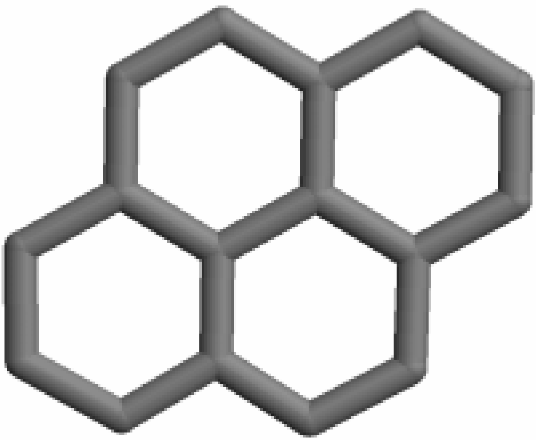
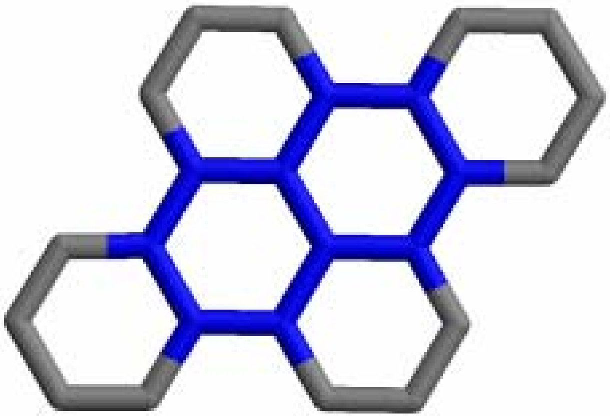
TUZ[8,4]	*Le* (TUZ[8,4]) = TUA[8,9]
	

Schlegel version[1] of *Le* (*M*)

Dodecahedron = C_{20}	***Le*** **(Dodecahedron)= C_{60}**
	

1. J. R. Dias, From benzenoid hydrocarbons to fullerene carbons. *MATCH Commun. Math. Chem. Comput.* 1996, *33*, 57-85.

Leapfrog of planar benzenoids

C_{16}	*Le* (C_{16})
	

Composite operations

Dual of Stellation of Medial = DSM(M) [1]

$$DSM(M) = Du(St(Me(M))) = Le(Me(M))$$

$DSM(M)$:

$$v = 2d_0v_0 = 4e_0 \quad (d_0 = 4;\ s_0 = 4)$$

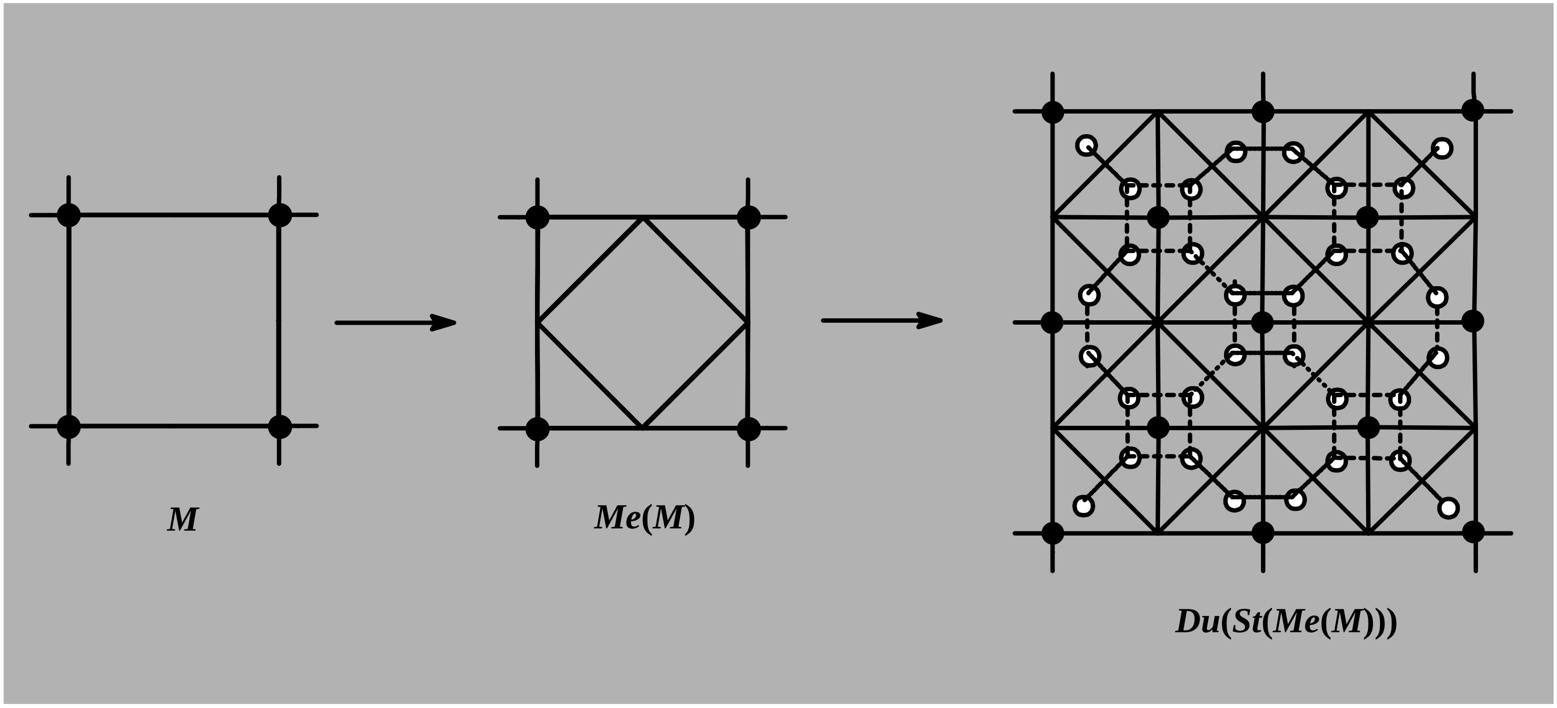
$$e = 6e_0$$

$$f = f_0 + e_0 + v_0$$

It involves two rotations by π/s = no rotation

1. M. V. Diudea, P. E. John, A. Graovac, M. Primorac, and T. Pisanski, *Croat. Chem. Acta*, 2003, *76*, 153-159.

Dual of Stellation of Medial



Composite operations

Quadrupling Q(M) *Chamfering*[1]

$$Q(M) = Du(Str(Me(M)))$$

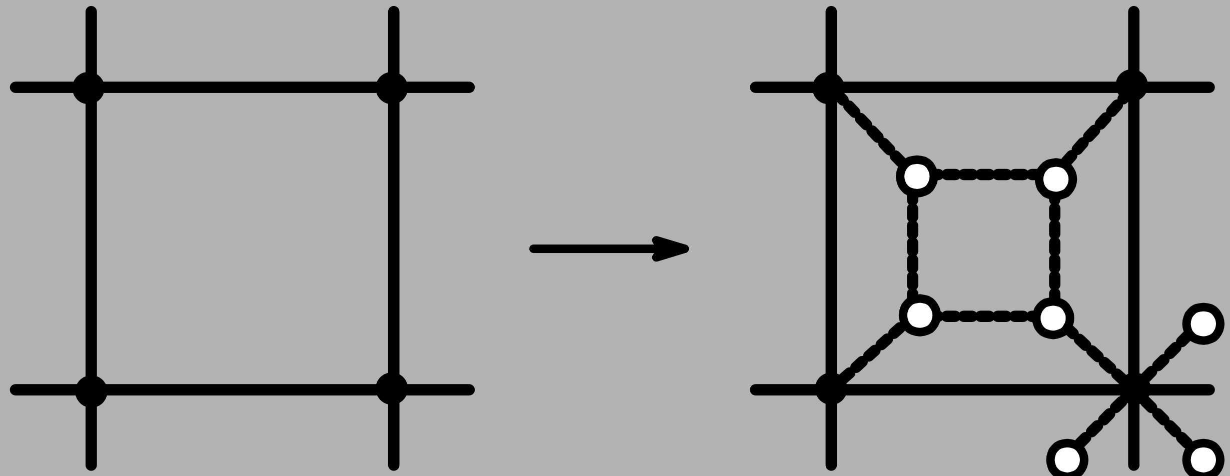
$Q(M)$:

$$v = (d_0+1)v_0$$
$$e = 4e_0$$
$$f = f_0 + e_0$$

It involves two rotations by π/s = no rotation

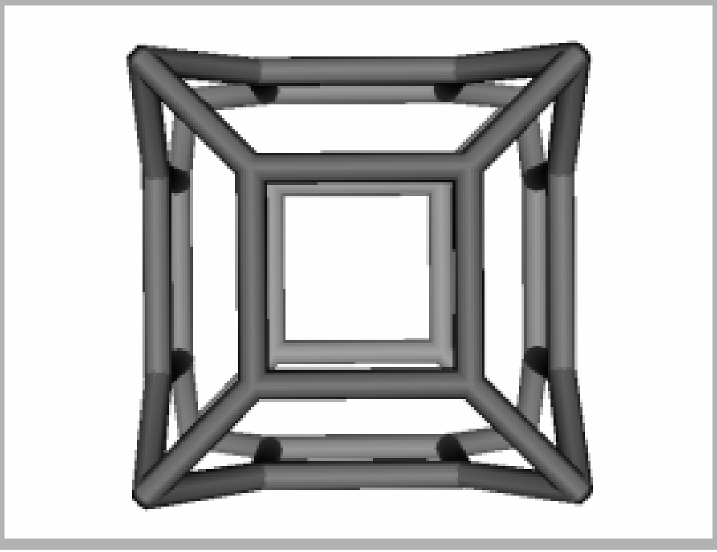
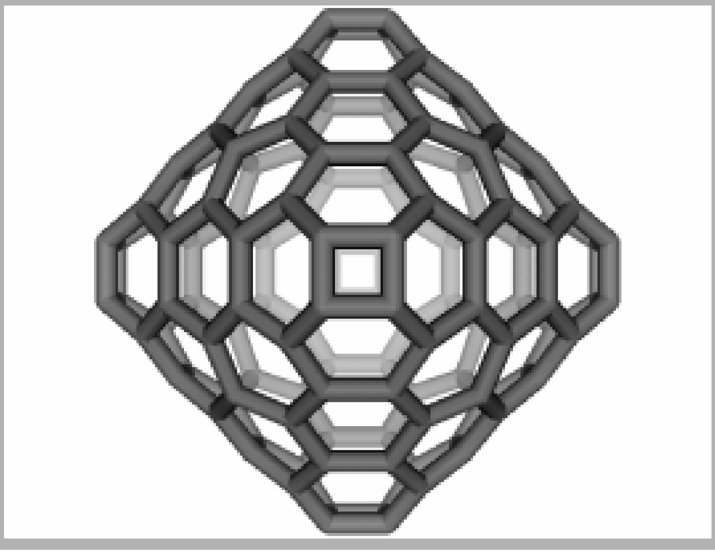
1. A. Deza, M. Deza and V. P. Grishukhin, *Discrete Math.*, 1998, *192*, 41-80.

Quadrupling Q (M)



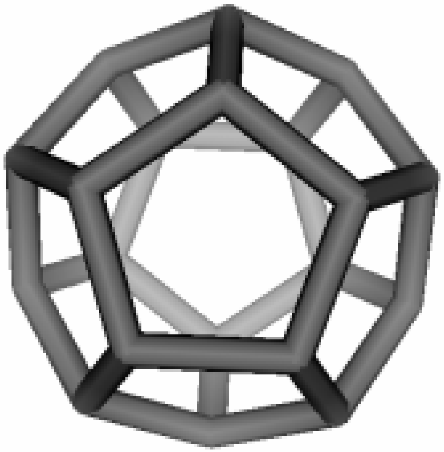
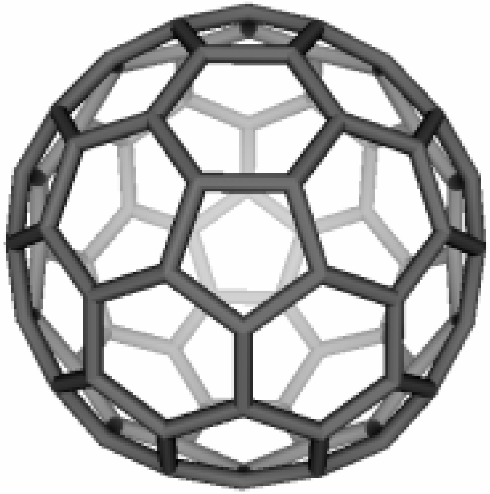
M. V. Diudea, P. E. John, A. Graovac, M. Primorac, and T. Pisanski, *Croat. Chem. Acta*, 2003, *76*, 153-159.

Quadrupling Q (M)

Q (Cube)=Chamfering[1]	*Q* (*Q* (*Cube*))
	

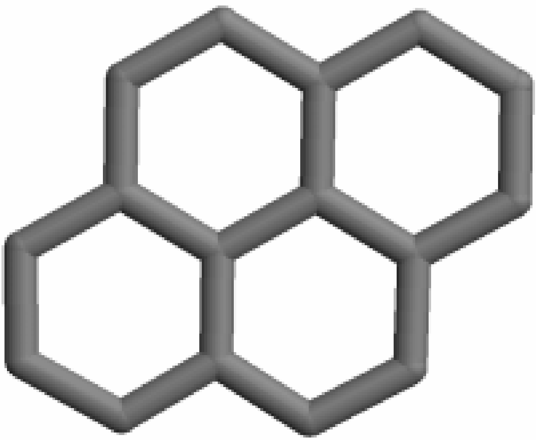
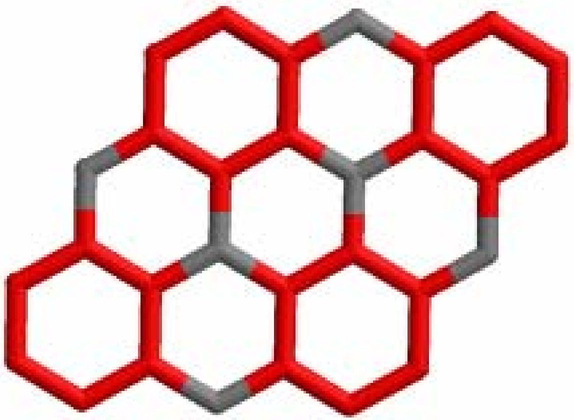
1. M. Goldberg, *Tôhoku Math. J.*, 1934, *40*, 226-236

Quadrupling Q (M)

C_{20}	$Q(C_{20})^1 = C_{80}$ (OP)
	

1. P. W. Fowler, J. E. Cremona, and J. I. Steer, Theor. Chim. Acta, 1988, 73, 1

Quadrupling of planar benzenoids

C_{16}	$\mathit{Q}\,(C_{16})$
	

Capra Ca (M)

Ca **(*M*)[1] – Romanian Leapfrog**

$$Ca\,(M) = Trr\,(Pe\,(E2\,(M)))$$

$Ca(M)$:

$$v = (2d_0+1)v_0 = v_0 + 2e_0 + s_0 f_0$$
$$e = 7e_0 = 3e_0 + 2s_0 f_0$$
$$f = (s_0+1) f_0$$

It involves rotation by $\pi/2s$ of the parent faces

1. **M. V. Diudea, *Studia Univ. Babes-Bolyai*, 2003, 48, 3-21**

Capra *Ca* (M)

$Ca_n\,(M)$; Iterative operation

$$v_n = 8v_{n-1} - 7v_{n-2};\quad n \geq 2$$

$$v_n = 7^n \cdot v_0;\ d_0 = 3$$

$$e_n = 7^n \cdot e_0 = 7^n \cdot 3v_0/2$$

$$f_n = f_0 + (7^n - 1) \cdot v_0/2$$

Capra *Ca* (M)

- Goldberg[1] relation:

$$m = (a^2 + ab + b^2);\quad a \geq b\,;\ a + b > 0$$

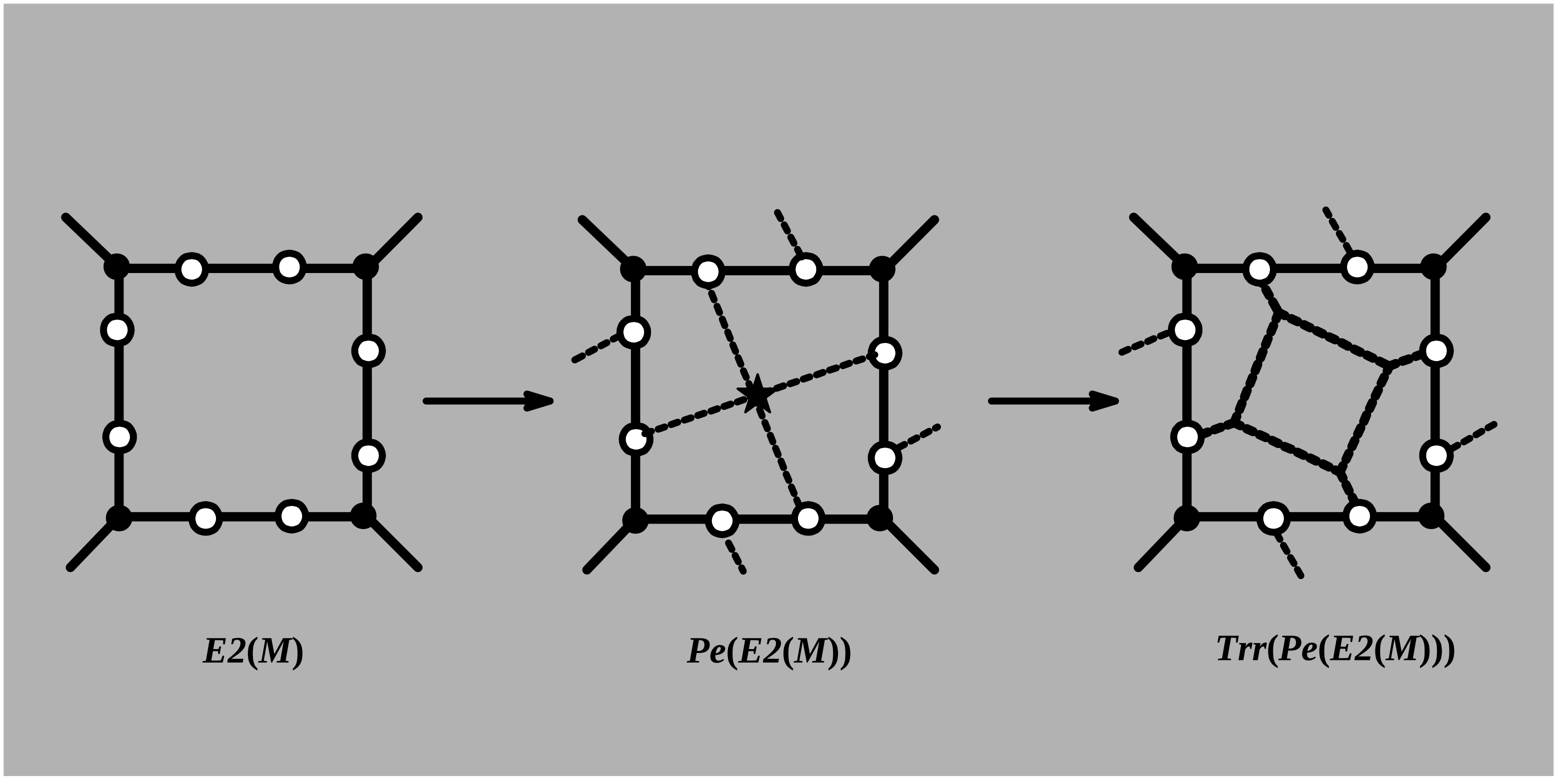
Le : (1, 1); m = 3

Q : (2, 0); m = 4

Ca : (2, 1); m = 7

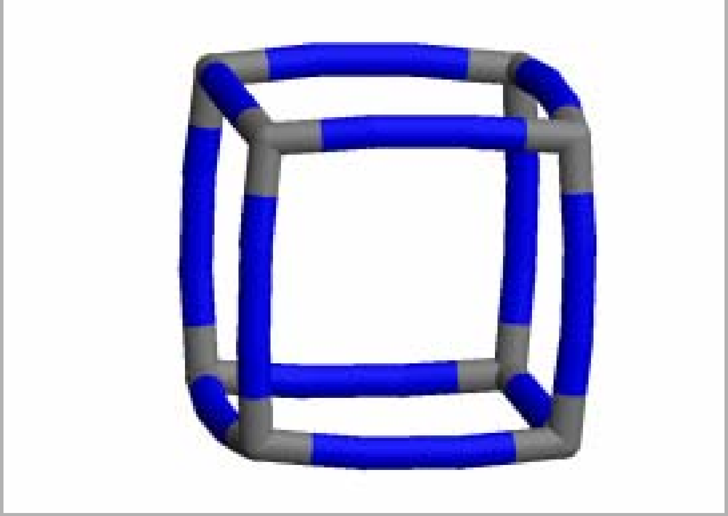
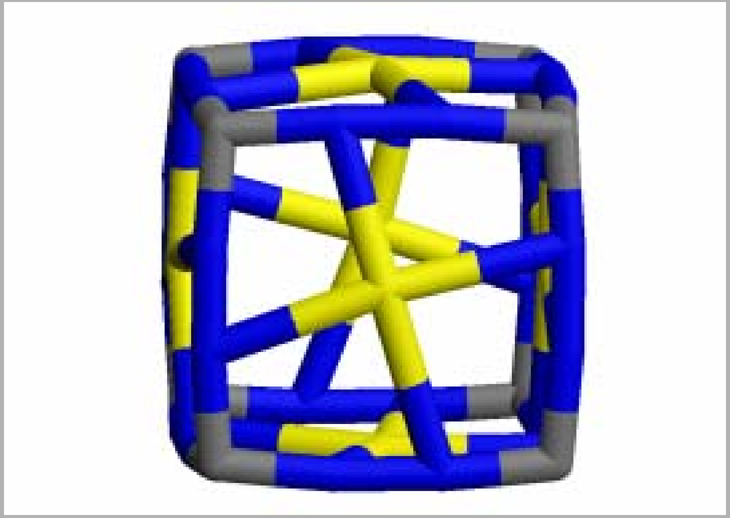
1. M. Goldberg, *Tohoku Math. J.*, 1937, *43*, 104-108.

Capra *Ca* (M)



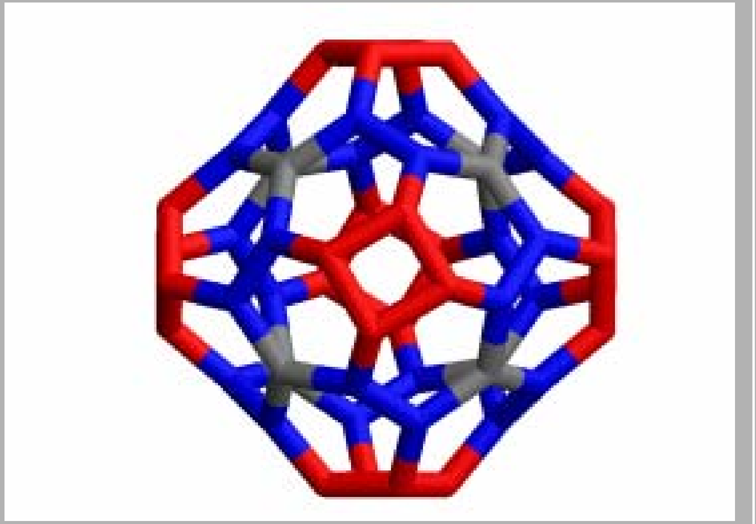
M. V. Diudea, *Studia Univ. Babes-Bolyai*, 2003, 48, 3-21

Capra *Ca* (M)

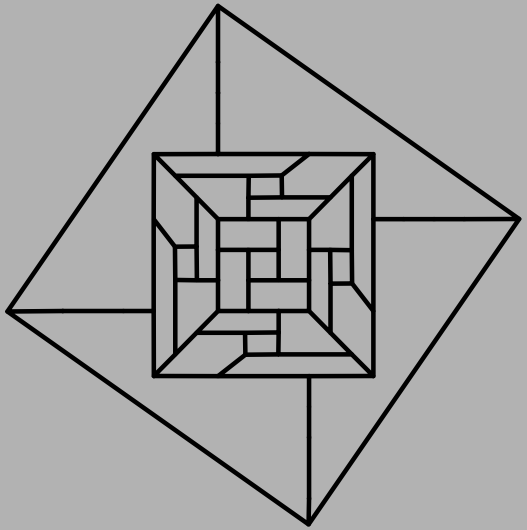
E2 (Cube)	*Pe* (*E2* (Cube))
	

Capra *Ca* (M)

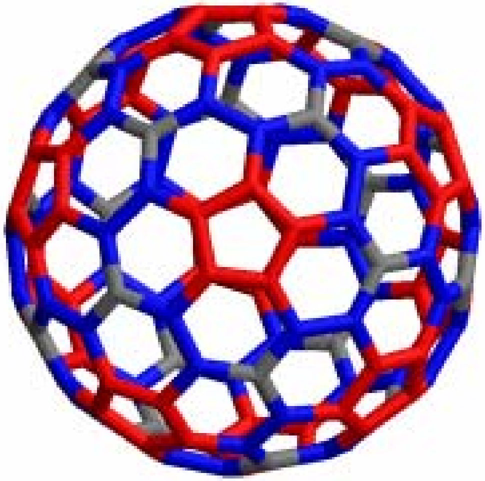
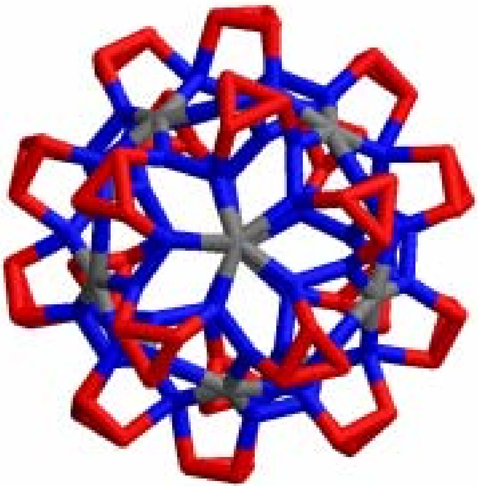
Trr(*Pe*(*E2*(Cube)))



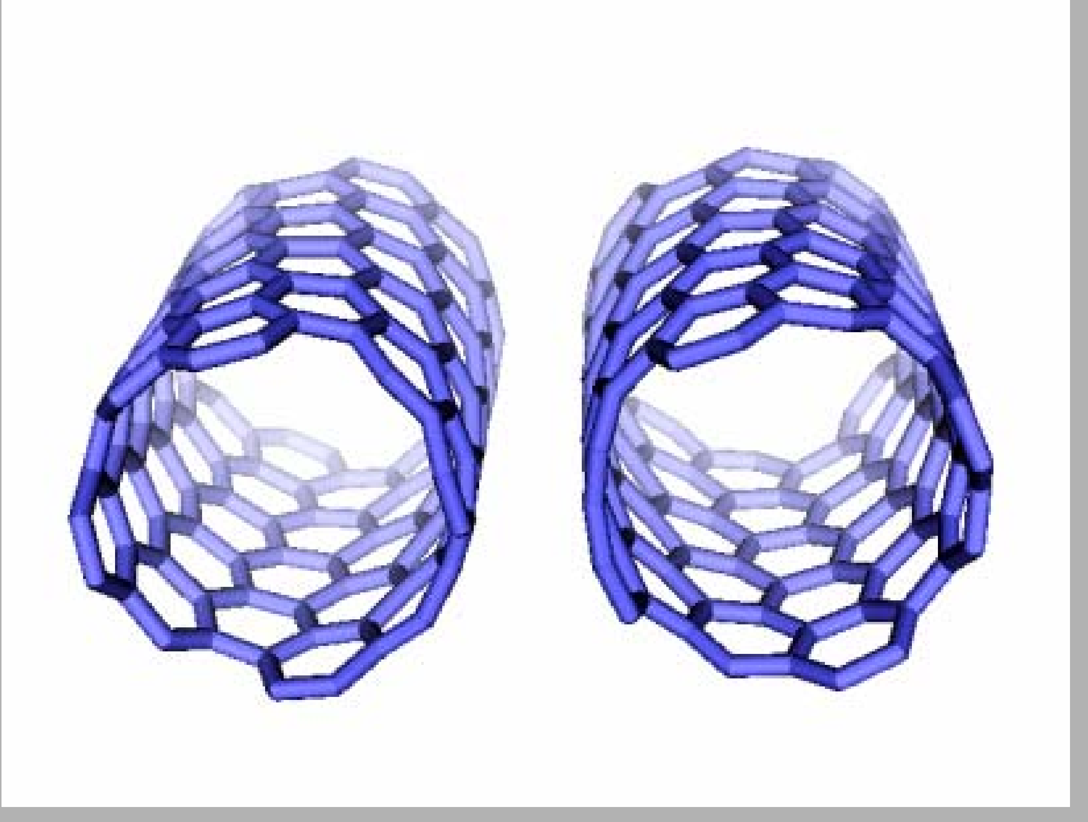
Ca (Cube) – Schlegel project.



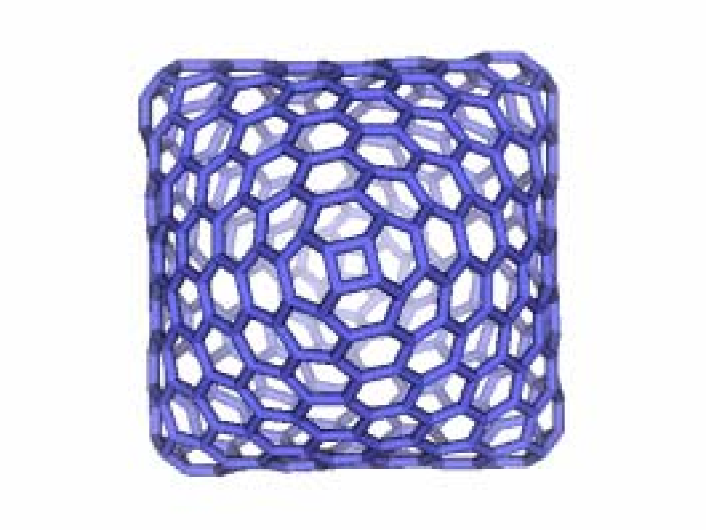
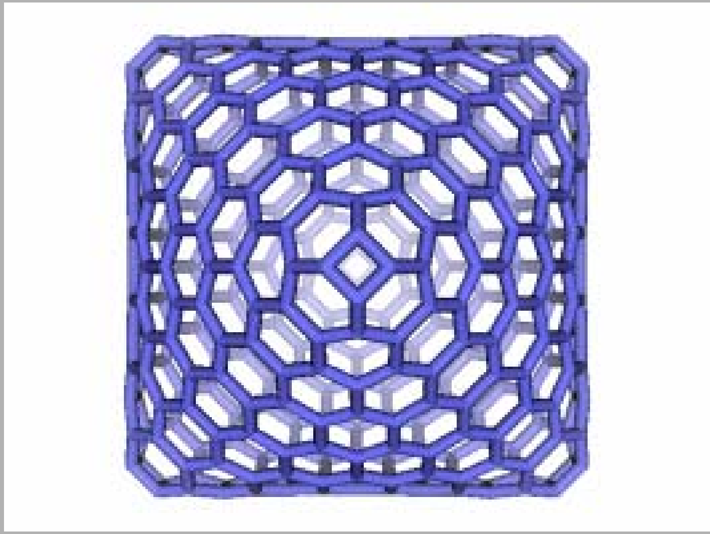
Capra Ca (M)

Ca (Dodecahedron) = C_{140}	*Ca* (Icosahedron) = C_{132}
	

A “racemic” pair of *Ca* -transformed TUZ[8,3]

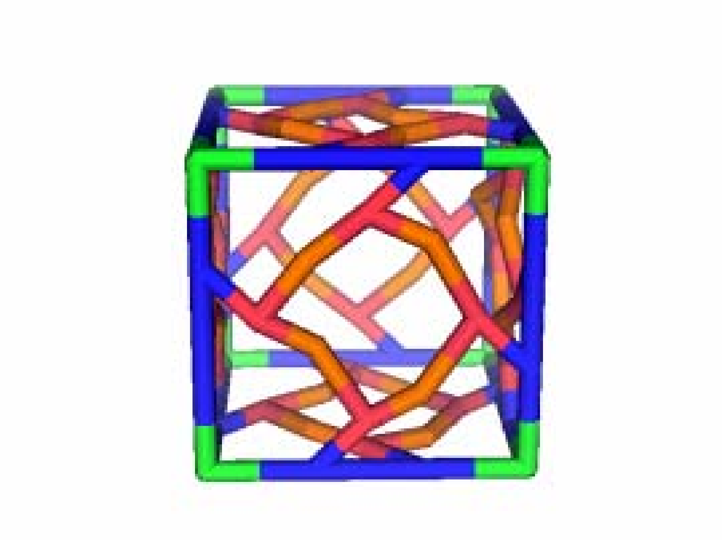


Two successive *Ca-operations*

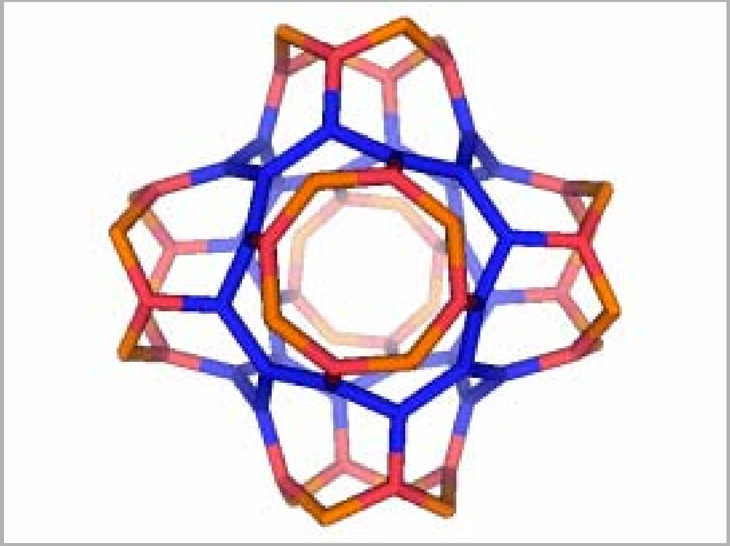
CaS (*CaS* (Cube))	*CaR* (*CaS* (Cube))
	

Capra Ca (M) – Negative curvature lattices

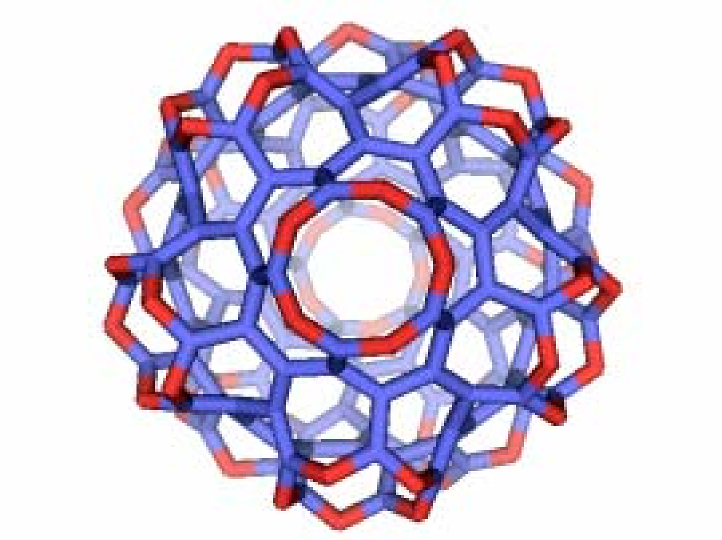
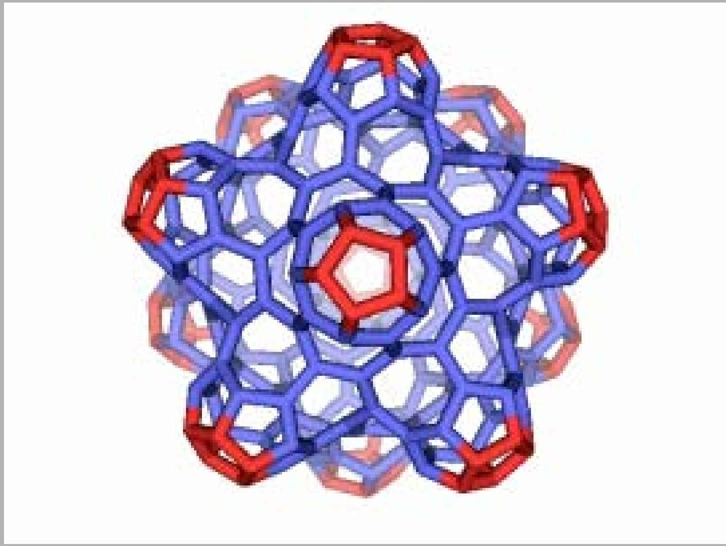
Ca(Cube)$_{[7]}$



Ca(Cube)$_{[7]}$ (optimized)

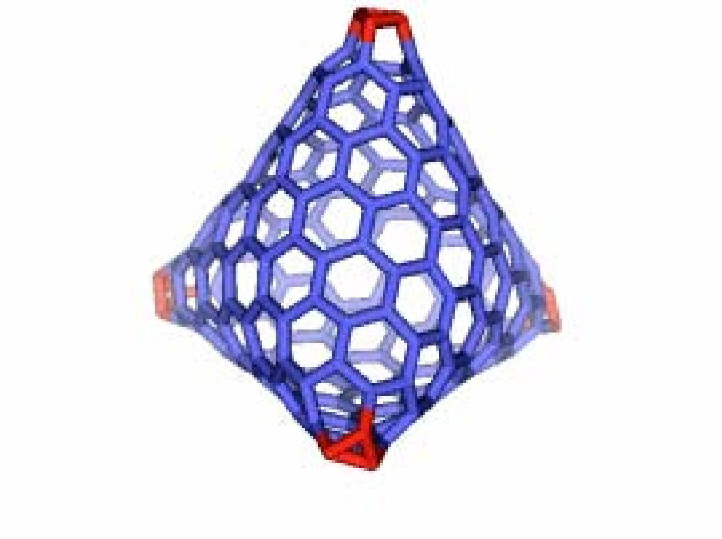
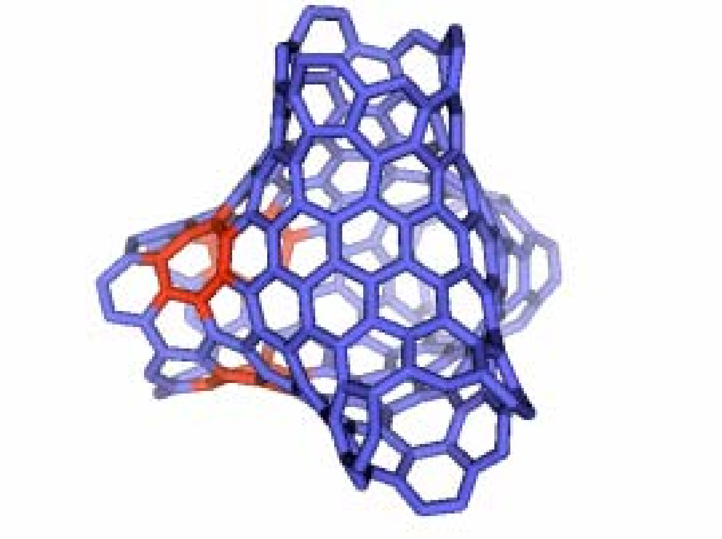


Negative and Positive Curvature Lattices

Ca $(C_{20})_{[7]}$; $N = 200$	$C_{260}(I_h)$ Fowler[1]
	

1. A. Dress and G. Brinkmann, *MATCH- Commun. Math. Comput. Chem.*, 1996, *33*, 87-100.

Positive and Negative Curvature Lattices

Ca (*Ca* (Tetrahedron)); N = 196	*Ca* (*Ca* (Tetrahedron)$_{[7]}$); N = 232
	

POAV – Strain Energy

In the POAV1 theory[1,2] the π-orbital axis vector makes equal angles to the three σ-bonds of the sp^2 carbon:

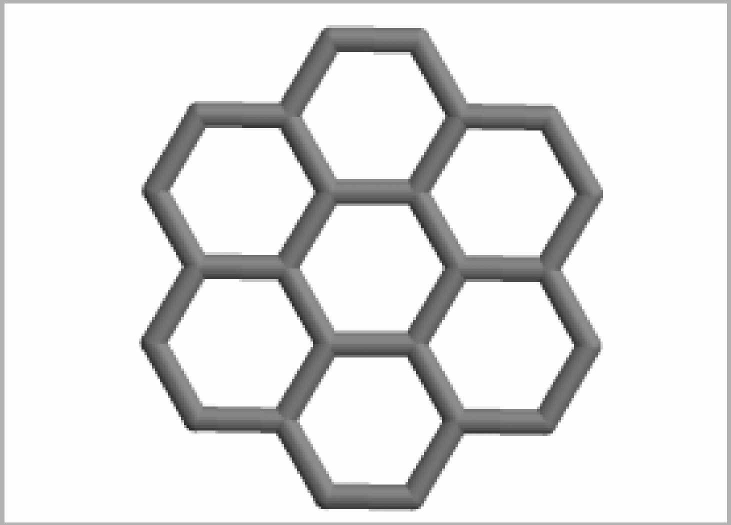
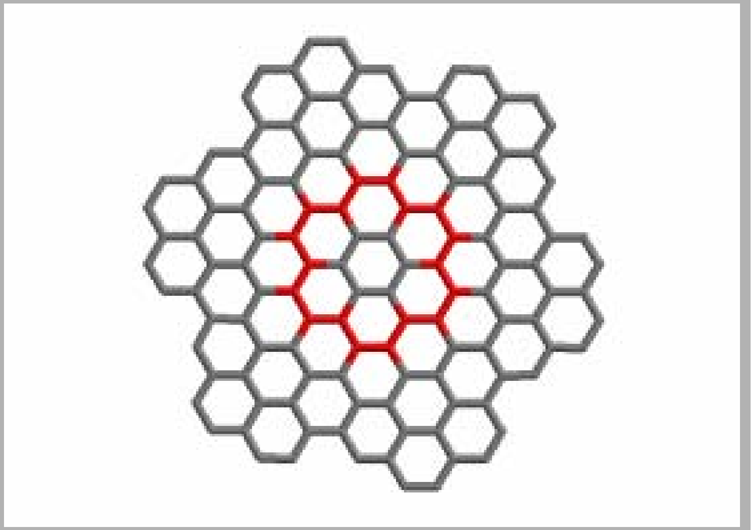
$\theta_p = \theta_{\sigma\pi} - 90^o$	*pyramidalization* angle
$SE = 200(\theta_p)^2$	strain energy
$120 - (1/3)\ \Sigma\theta_{ij}$	deviation to planarity

1. R.C. Haddon, *J. Am. Chem. Soc.*, 112, 3385 (1990).
2. R.C. Haddon, *J. Phys. Chem. A*, 105, 4164 (2001).

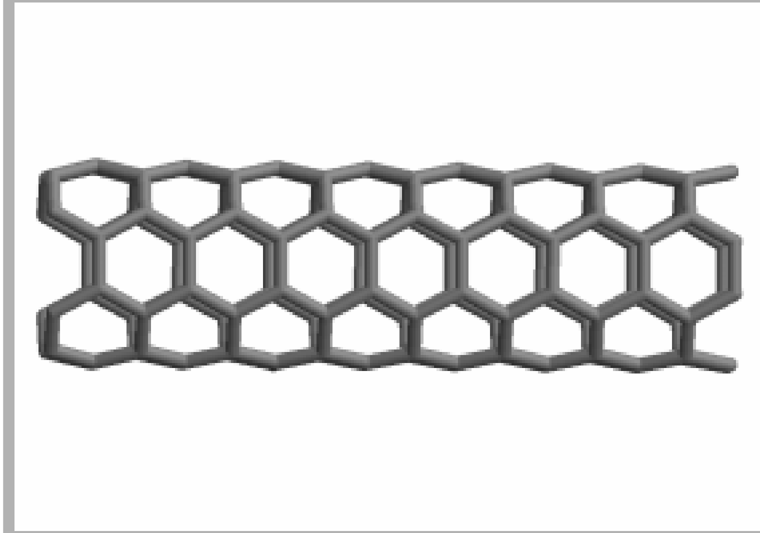
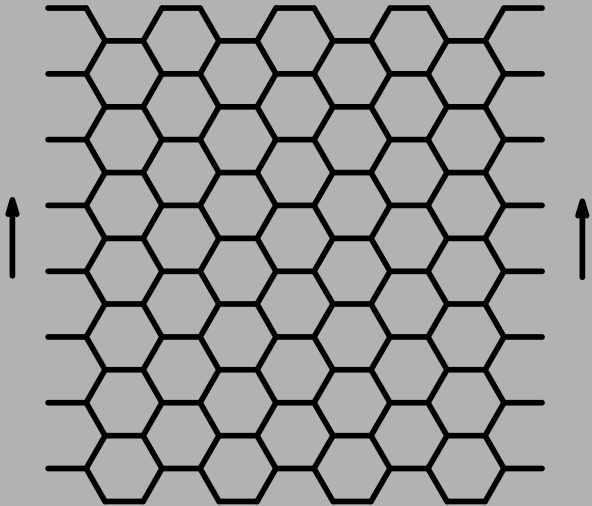
POAV1 – Strain Energy

Angle (deg)			Deviation	θ_p	SE
1	2	3	(deg)	(deg)	(kcal/mol)
$C_{3,6,6}$ *Ca* (*Ca* (Tetrahedron))					
108.017	108.078	60.006	27.967	31.692	61.189
108.090	108.026	60.000	27.961	31.687	61.171
108.071	108.017	59.995	27.972	31.695	61.202
average			**27.967**	**31.691**	**61.188**
$C_{7,6,6}$ *Ca* (*Ca* (Tetrahedron)$_{[7]}$)					
117.475	125.063	114.694	0.923	5.529	1.862
118.227	117.678	120.442	1.218	6.378	2.478
114.883	117.99	126.795	0.111	1.906	0.221
114.105	116.541	129.236	0.039	1.133	0.078
117.824	117.818	122.078	0.760	5.027	1.539
116.736	119.16	123.226	0.293	3.112	0.590
114.422	114.902	130.022	0.218	2.664	0.432
average			**0.509**	**3.678**	**1.029**

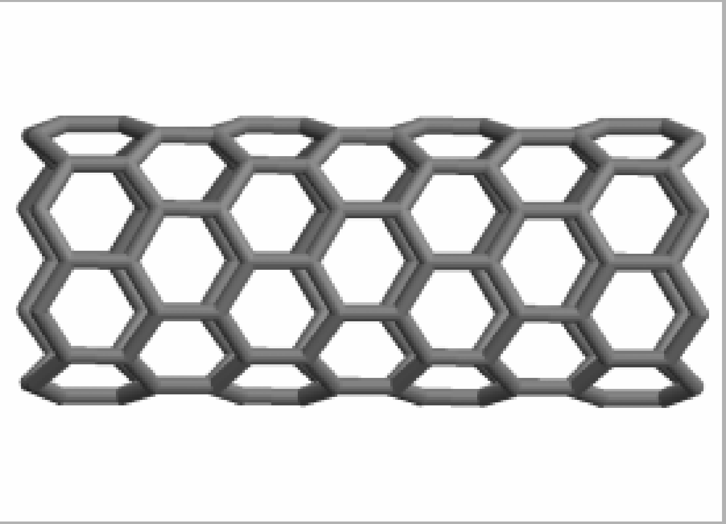
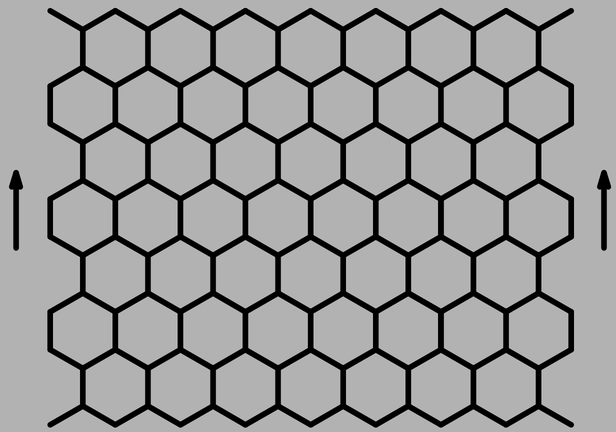
Capra of planar benzenoids

Ca (C_6)	$Ca_2(C_6)$
	

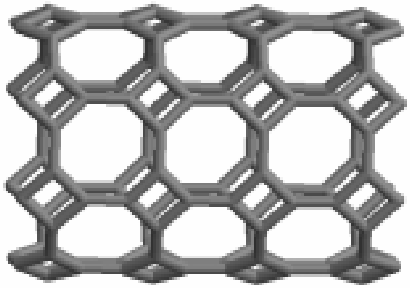
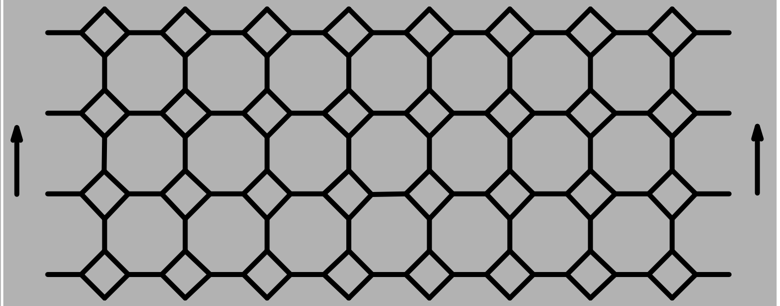
VARIOUS NANOTUBES

$TUAC_6[8,16]V1,2$	Geodesic projection
	

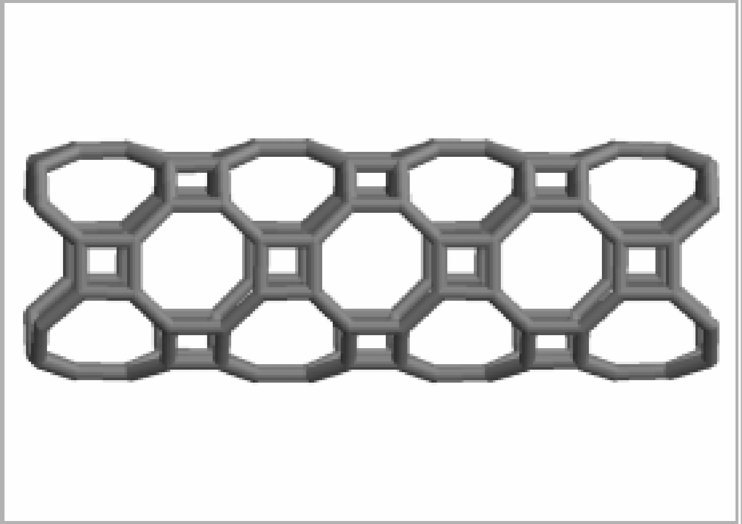
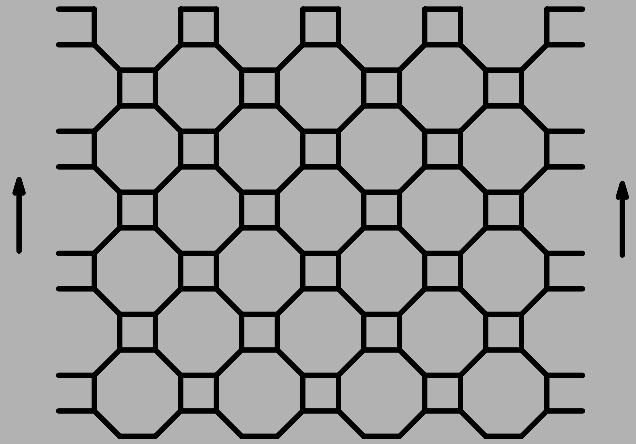
VARIOUS NANOTUBES

$TUZC_6[16,8]H1,2$	Geodesic projection
	

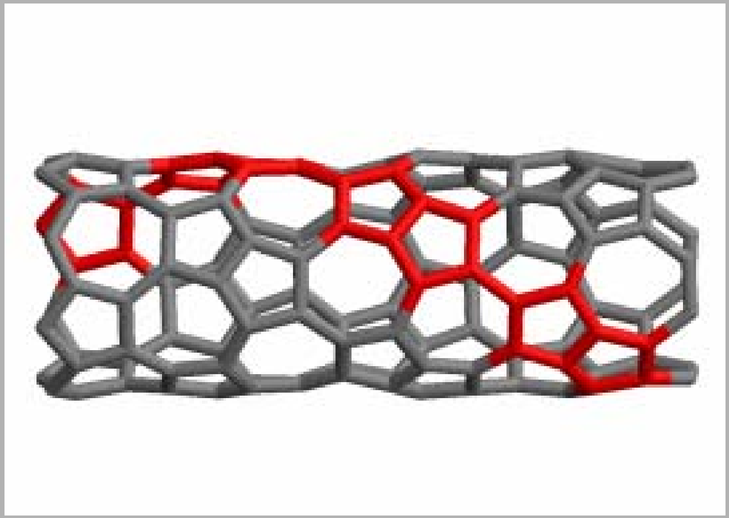
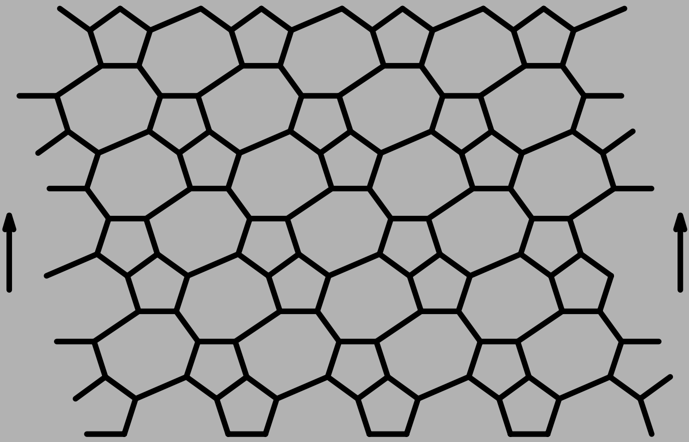
VARIOUS NANOTUBES

$RC_4C_8[16,8]$	Geodesic projection
	

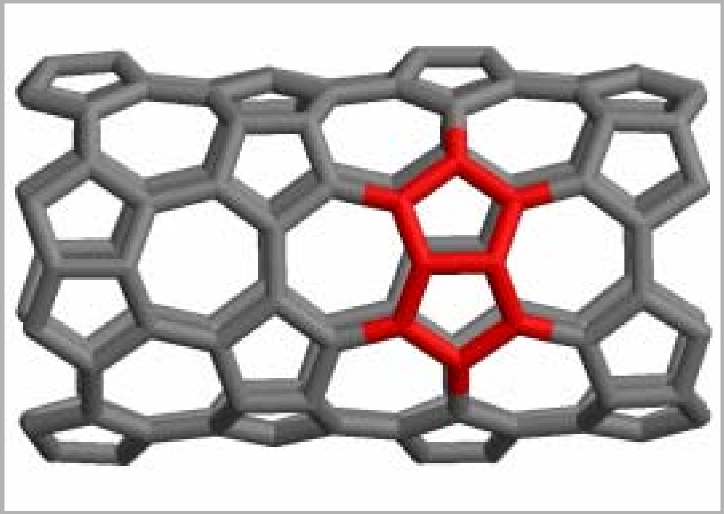
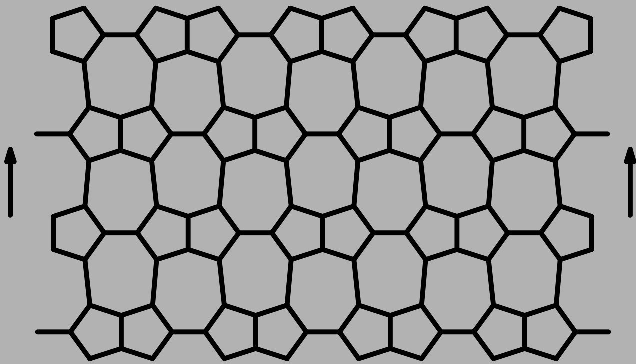
VARIOUS NANOTUBES

$SC_4C_8[16,8]$	Geodesic projection
	

VARIOUS NANOTUBES

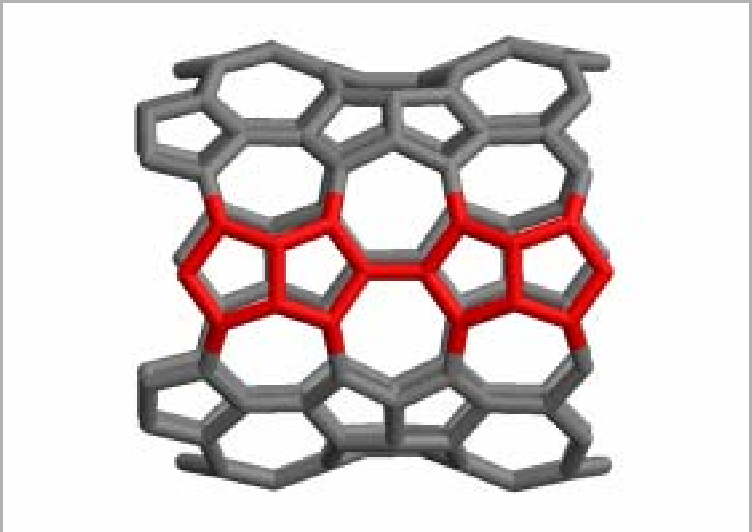
$SC_5C_7[16,8]$	Geodesic projection
	

VARIOUS NANOTUBES

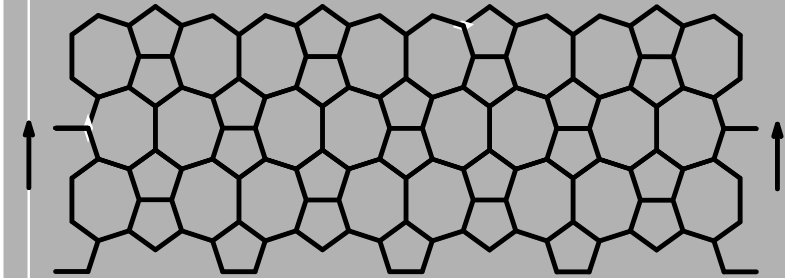
$HC_5C_7[16,8]$	Geodesic projection
	

VARIOUS NANOTUBES

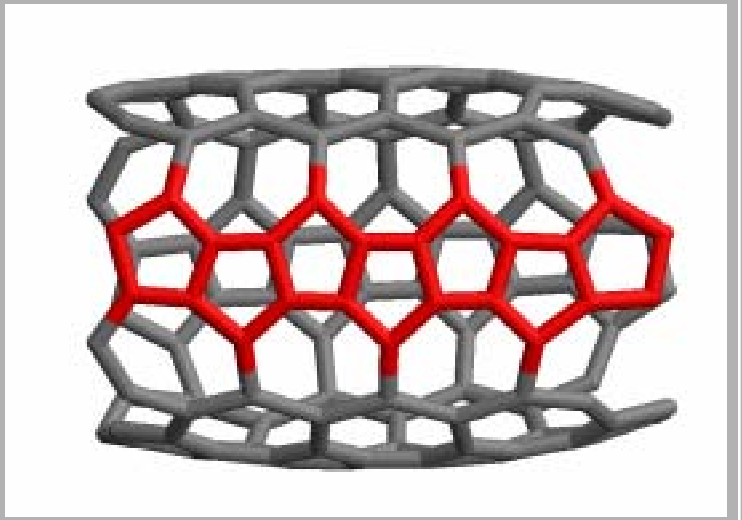
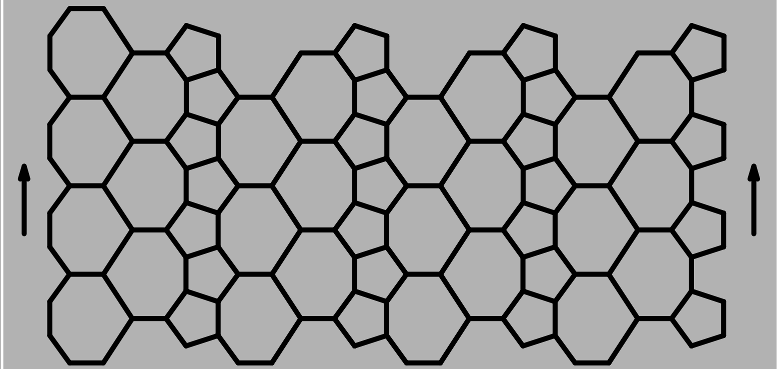
$VC_5C_7[16,8]$



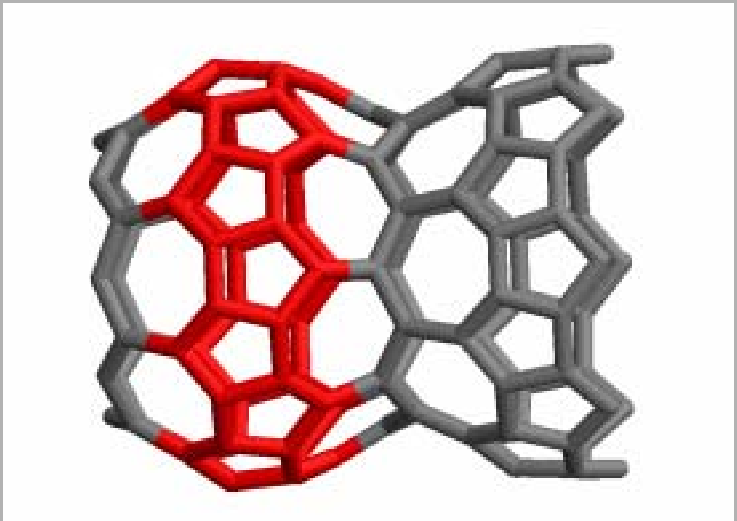
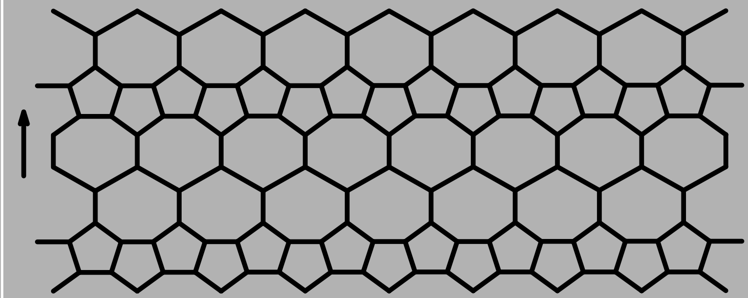
Geodesic projection



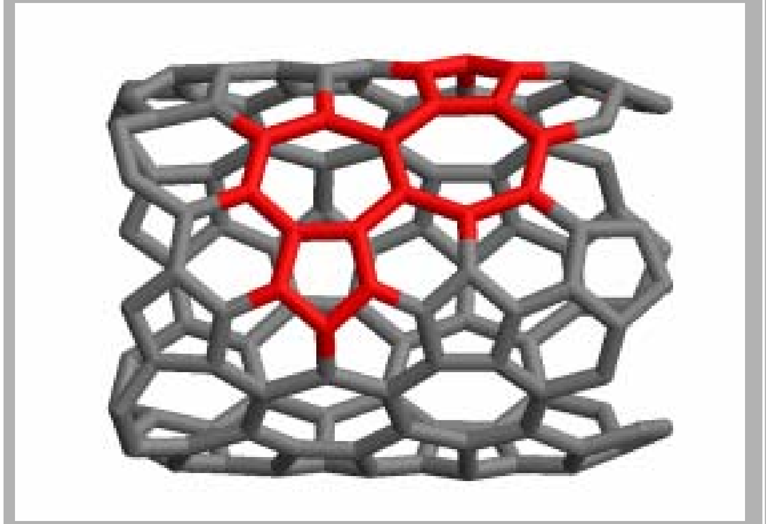
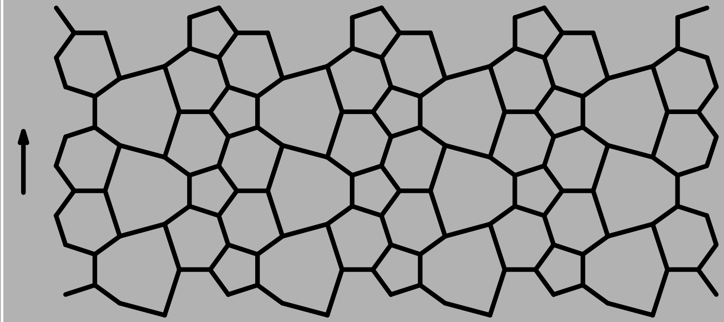
VARIOUS NANOTUBES

$VAC_5C_7[16,8]$	Geodesic projection
	

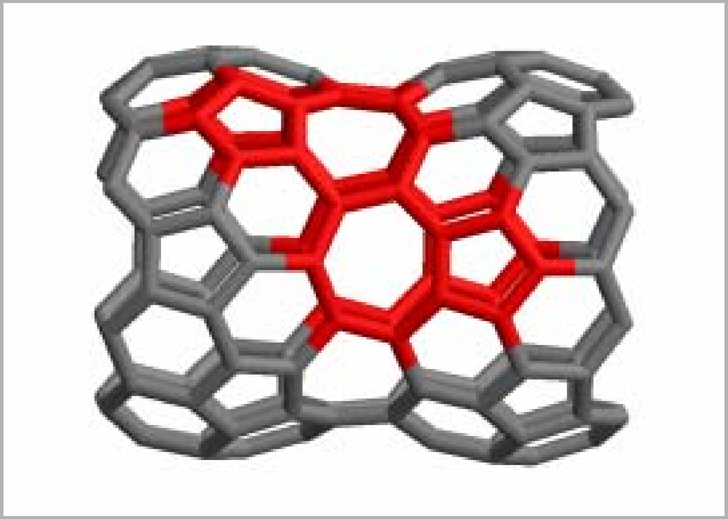
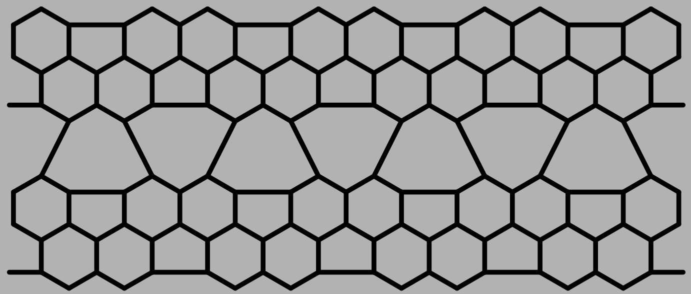
VARIOUS NANOTUBES

$HAC_5C_7[16,8]$	Geodesic projection
	

VARIOUS NANOTUBES

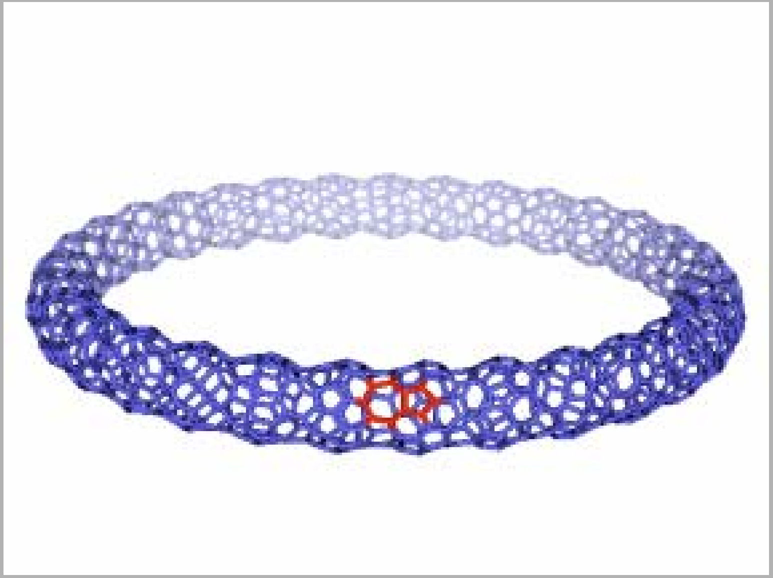
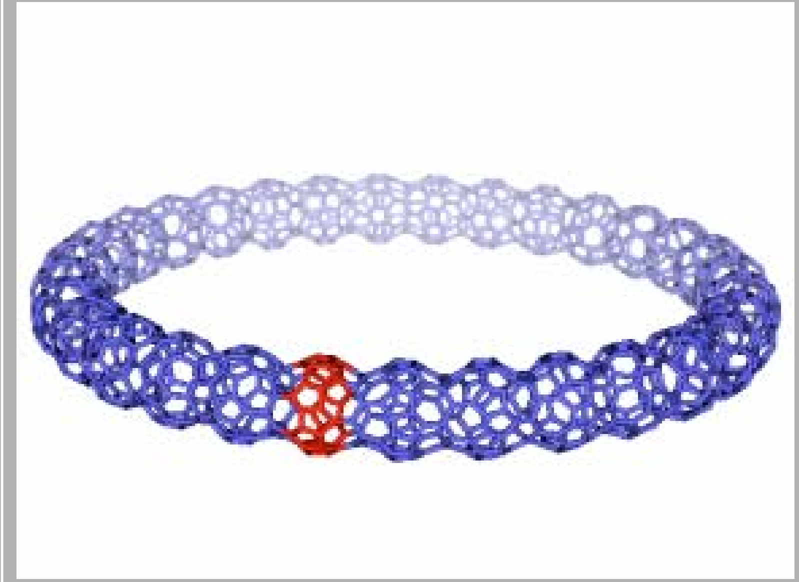
$VAC_5C_6C_7[16,8]$	Geodesic projection
	

VARIOUS NANOTUBES

$HAC_5C_6C_7[16,8]$	Geodesic projection
	

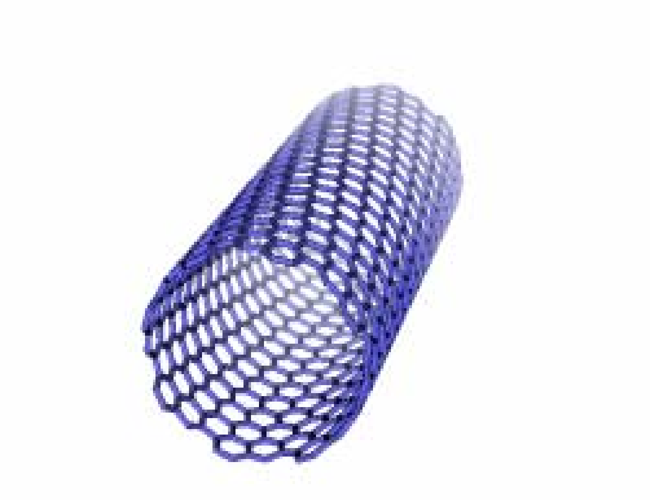
VARIOUS TORI

A C_{60} –like toroidal object

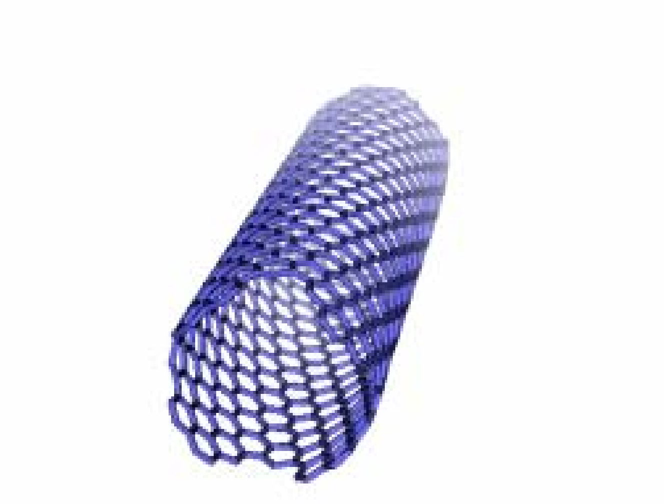
$HAC_5C_6C_7[12,120]$; N=1440	$HAC_5C_7[12,120]$; N=1440
	

Capra of VARIOUS NANOTUBES

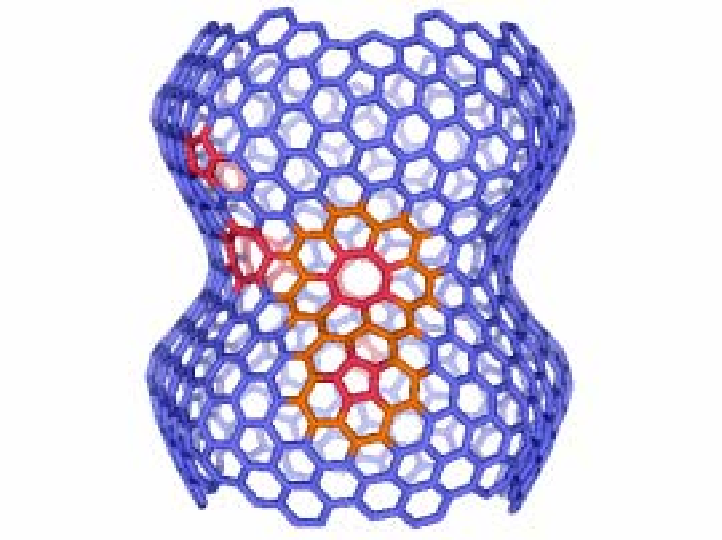
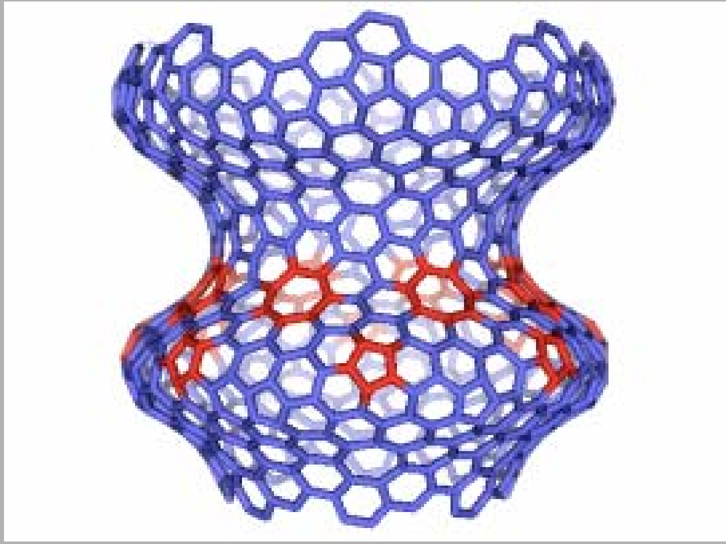
Ca ($ZC_6[16,8]$); N=832



Ca ($AC_6[8,16]$); N=832

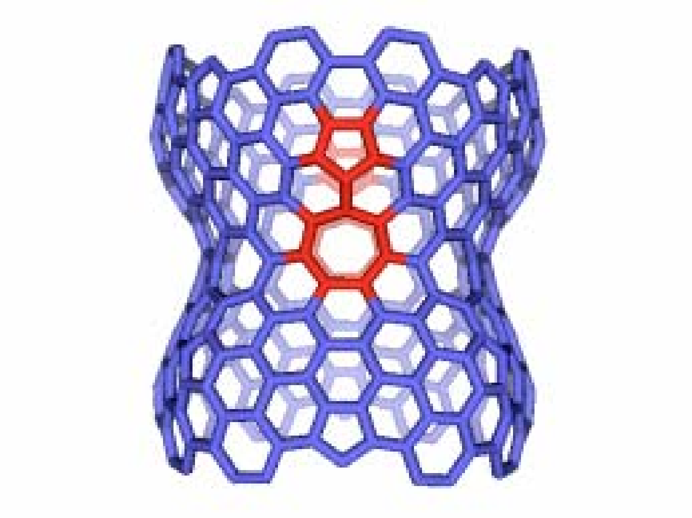


Capra of VARIOUS NANOTUBES

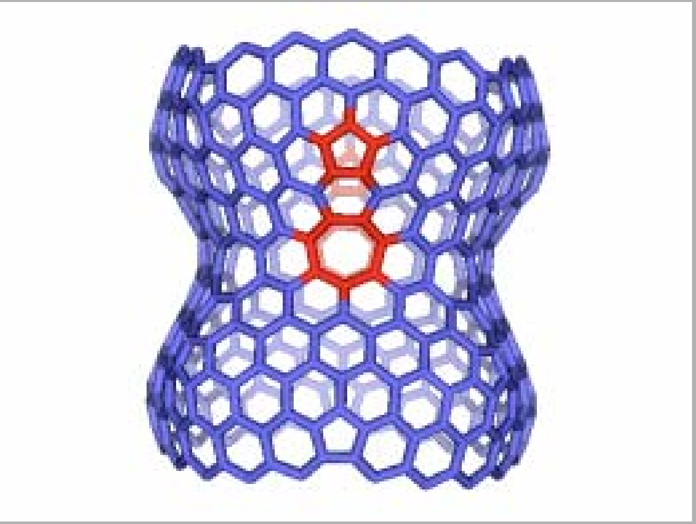
Ca ($HAC_5C_6C_7$[16,8]); N=824	*Ca* (HAC_5C_7[16,8]) ; N=824
	

VARIOUS NANOTUBES

Le ($HAC_5C_6C_7$[16,8]); N=328



Q (HAC_5C_7[16,8]); N=440



Spectral implications of ***Ca*** operation

- *Ca* operation, applied to a finite structure, leaves unchanged its π-electronic shells. There exist exceptions, the most notably being the transformed *Ca* (Tuz/a[*c*,*n*]) of nanotubes, which all have PC shell disregarding the character of their parent shell.

Spectral data of open nanotubes Tuz/a[*c*,*n*] and tori Z/A[*c*,*n*] and their *Ca* -transforms

	STRUCTURE	*N*	$HOMO_{-1}$	HOMO	LUMO	$LUMO_{+1}$	Gap	Shell
1	Tuz[8,4]	32	0.705	0	0	-0.705	0	OP
2	*Ca*(Tuz[8,4])	192	0.273	0.017	-0.017	-0.273	0.034	PC
3	Tuz[10,4]	40	0.095	0.095	-0.095	-0.095	0.190	PC
4	*Ca*(Tuz[10,4])	240	0.064	0.064	-0.064	-0.064	0.129	PC
5	Tua[4,8]	32	0.532	0	0	-0.532	0	OP
6	*Ca*(Tua[4,8])	192	0.265	0.024	-0.024	-0.265	0.048	PC
7	Tua[4,10]	40	0.310	0.169	-0.169	-0.310	0.338	PC
8	*Ca*(Tua[4,10])	248	0.132	0.095	-0.095	-0.132	0.189	PC
9	Z[8,10]	80	0.414	0.414	-0.414	-0.414	0.828	PC
10	*Ca*(Z[8,10])	560	0.169	0.169	-0.169	-0.169	0.337	PC
11	A[8,12]	96	0	0	0	0	0	M
12	*Ca*(A[8,12])	672	0	0	0	0	0	M

Spectral data of various types of open nanotubes

	TUBE	HOMO	LUMO	GAP	E_π	x+	x0	x-	SHELL
1	TUH[16,8]	0	0	0	1.527	63	2	63	OP
2	HC_5C_7[16,8]	0.139	0.139	0	1.490	67	1	60	OP
3	HAC_5C_7[16,8]	0.191	0	0.191	1.487	64	3	61	PSC
4	$HAC_5C_6C_7$[16,8]	0	0	0	1.517	63	2	63	OP
5	RC_4C_8[16,8]	0	0	0	1.425	62	4	62	M
6	SC_4C_8[16,8]	0.063	-0.063	0.126	1.446	64	0	64	PC
7	SC_5C_7[16,8]	0.134	0.068	0.066	1.497	65	1	62	PSC
8	TUV[8,16]	0.109	-0.109	0.217	1.537	64	0	64	PC
9	VC_5C_7[16,8]	0.244	0.153	0.091	1.474	67	1	60	PSC
10	VAC_5C_7[16,8]	0.147	0.128	0.019	1.477	65	1	62	PSC
11	$VAC_5C_6C_7$[16,8]	0.174	0.138	0.036	1.495	65	0	63	PSC

Spectral data of the *Le* transforms of various types of open nanotubes

	TUBE	HOMO	LUMO	GAP	E_π	x+	x_0	x-	SHELL
1	TUH[16,8] *Le*	0.081	-0.081	0.163	1.548	168	0	168	PC
2	HC_5C_7[16,8] *Le*	0.211	0.203	0.009	1.519	168	0	160	PSC
3	HAC_5C_7[16,8] *Le*	0.203	0.158	0.045	1.519	168	0	160	PSC
4	$HAC_5C_6C_7$[16,8] *Le*	0.183	0.170	0.014	1.530	167	0	161	PSC
5	RC_4C_8[16,8] *Le*	0	0	0	1.464	152	16	152	M
6	SC_4C_8[16,8] *Le*	0	0	0	1.464	152	16	152	M
7	SC_5C_7[16,8] *Le*	0.077	0.027	0.050	1.531	169	0	167	PSC
8	TUV[8,16] *Le*	0.108	-0.108	0.217	1.547	168	0	168	PC
9	VC_5C_7[16,8] *Le*	0.256	0.201	0.055	1.507	157	0	151	PSC
10	VAC_5C_7[16,8] *Le*	0.203	0.124	0.079	1.506	156	0	152	PSC
11	$VAC_5C_6C_7$[16,8] *Le*	0.239	0.147	0.092	1.514	156	0	152	PSC

Spectral data of the *Q* transforms of various types of open nanotubes

	TUBE	HOMO	LUMO	GAP	E_π	x+	x0	x-	SHELL
1	TUH[16,8]*Q*	0	0	0	1.547	223	2	223	OP
2	HC_5C_7[16,8]*Q*	0.115	0.115	0	1.528	227	0	213	OP
3	HAC_5C_7[16,8]*Q*	0.099	0.099	0	1.530	223	1	216	OP
4	$HAC_5C_6C_7$[16,8]*Q*	0.003	0.003	0	1.538	221	0	219	OP
5	RC_4C_8[16,8]*Q*	0	0	0	1.486	213	6	213	M
6	SC_4C_8[16,8]*Q*	0	0	0	1.505	221	6	221	M
7	SC_5C_7[16,8]*Q*	0.055	0	0.055	1.536	224	1	223	PSC
8	TUV[8,16]*Q*	0.078	-0.078	0.156	1.553	224	0	224	PC
9	VC_5C_7[16,8]*Q*	0.082	0.082	0	1.517	208	1	203	OP
10	VAC_5C_7[16,8]*Q*	0.130	0.130	0	1.520	208	0	204	OP
11	$VAC_5C_6C_7$[16,8]*Q*	0.078	0.078	0	1.527	208	0	204	OP

Spectral data of the *Ca* transforms of various types of open nanotubes

	TUBE	HOMO	LUMO	GAP	E_{π}	x+	x0	x-	SHELL
1	TUH[16,8]*Ca*	0	0	0	1.557	416	0	416	OP/PC
2	HC_5C_7[16,8]*Ca*	-0.006	-0.016	0.011	1.547	411	0	413	MC
3	HAC_5C_7[16,8]*Ca*	0.075	0.075	0	1.547	416	0	408	OP
4	$HAC_5C_6C_7$[16,8]*Ca*	0.077	0.071	0.007	1.551	416	0	408	PSC
5	RC_4C_8[16,8]*Ca*	0.007	-0.007	0.014	1.528	408	0	408	PC
6	SC_4C_8[16,8]*Ca*	0.009	-0.009	0.017	1.536	416	0	416	PC
7	SC_5C_7[16,8]*Ca*	0.100	-0.012	0.113	1.550	416	0	416	PC
8	TUV[8,16]*Ca*	0.057	-0.057	0.114	1.558	416	0	416	PC
9	VC_5C_7[16,8]*Ca*	0.092	0.092	0	1.539	400	0	396	OP
10	VAC_5C_7[16,8]*Ca*	0.082	0.079	0.003	1.539	400	0	396	PSC
11	$VAC_5C_6C_7$[16,8]*Ca*	0.017	0.017	0	1.543	399	0	397	OP

Spectral data of the Platonic polyhedra and their *Ca* $_{[7]}$ -transforms

	Structure	$HOMO_{-1}$	HOMO	LUMO	$LUMO_{+1}$	Gap	Shell	Ex. *e*
1	*M* = Tetrahedron	3	-1	-1	-1	0	OP	
	$Ca(M)_{[7]}$	0.154	0.154	0.154	-0.614	0	OP	
	$CaS(CaS(M)_{[7]})$	-0.005	-0.005	-0.005	-0.306	0	OP	4
	$CaR(CaS(M)_{[7]})$	-0.010	-0.010	-0.010	-0.325	0	OP	4
2	*M* = Cube	1	1	-1	-1	2	PC	
	$Ca(M)_{[7]}$	0	0	0	-0.188	0	OP	
	$CaS(CaS(M)_{[7]})$	-0.010	-0.010	-0.127	-0.127	0.117	MC	6
	$CaR(CaS(M)_{[7]})$	-0.004	-0.004	-0.141	-0.141	0.137	MC	6
3	*M* = Dodecahedron	1	0	0	0	0	OP	
	$Ca(M)_{[7]}$	0	0	0	-0.165	0	OP	
	$CaS(CaS(M)_{[7]})$	-0.069	-0.069	-0.069	-0.131	0	OP	6
	$CaR(CaS(M)_{[7]})$	-0.070	-0.070	-0.070	-0.138	0	OP	6
4	*M* = Octahedron	0	0	0	-2	0	OP	
	$Ca(M)_{[7]}$	0.222	0	0	0	0	OP	
	$CaS(CaS(M)_{[7]})$	0.008	-0.044	-0.044	-0.044	0	OP	2
	$CaR(CaS(M)_{[7]})$	0.021	-0.058	-0.058	-0.058	0	OP	2
5	*M* = Icosahedron	-1	-1	-1	-1	0	OP	
	$Ca(M)_{[7]}$	0.101	0.101	0.101	0.101	0	OP	
	$CaS(CaS(M)_{[7]})$	-0.022	-0.022	-0.022	-0.022	0	OP	6
	$CaR(CaS(M)_{[7]})$	-0.029	-0.029	-0.029	-0.029	0	OP	6

Negative curvature lattices

- **GAUSS-BONET Theorem - relates the geometric curvature to the topology**

$$\int_S \kappa dA = 2\pi\chi(S)$$

Euler characteristic $$\chi(S) = v - e + f$$

$$v - e + f = 2(1 - g)$$

$$g = (e_0 - v_0 + 2)/2 = f_0/2$$

O. Bonnet, *C. R. Acad. Sci. Paris*, **1853**, *37*, 529-532

Negative curvature lattices

- The genus of *Ca* $(M)_{[7]}$ objects is calculable as:

- $\chi(M)_{[7]} = v_{1[7]} - e_{1[7]} + f_{1[7]} = 2(1 - g) = v_0 - e_0$
- $g = (e_0 - v_0 + 2)/2 = f_0/2$

(spherical character of the parent polyhedron involves: $v_0 - e_0 + f_0 = 2$)

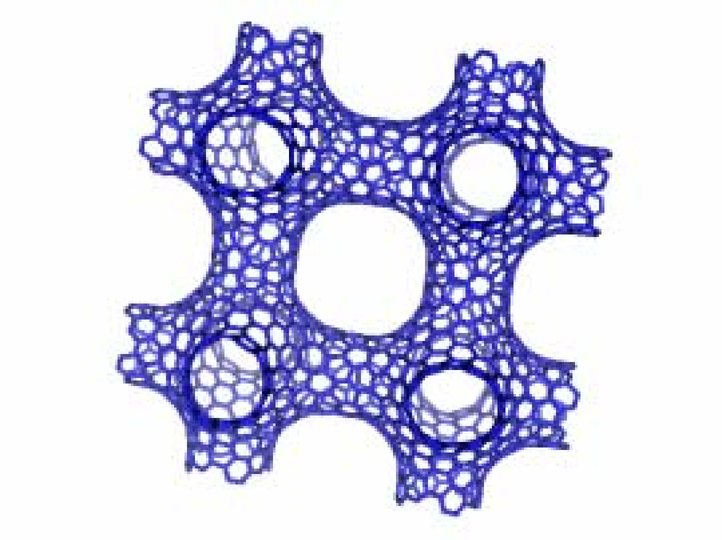
- Lattices with $g > 1$ will have negative $\chi(M)_{[7]}$ and consequently negative curvature.
- For the five **Platonic** solids, the genus of the corresponding *Ca* $(M)_{[7]}$ is:

  2 (Tetrahedron); 3 (Cube); 4 (Octahedron); 6 (Dodecahedron) and

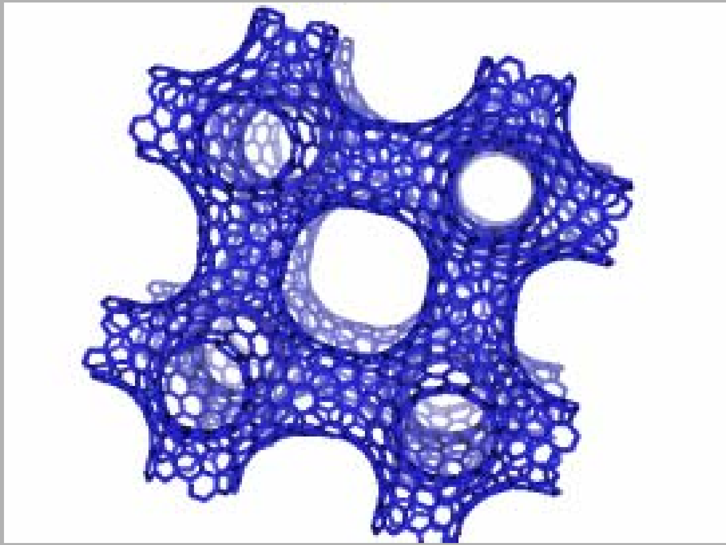
  10 (Icosahedron).

Negative curvature lattices

Ca_2(Cube)$_{[7]}$, P2D; N=1760

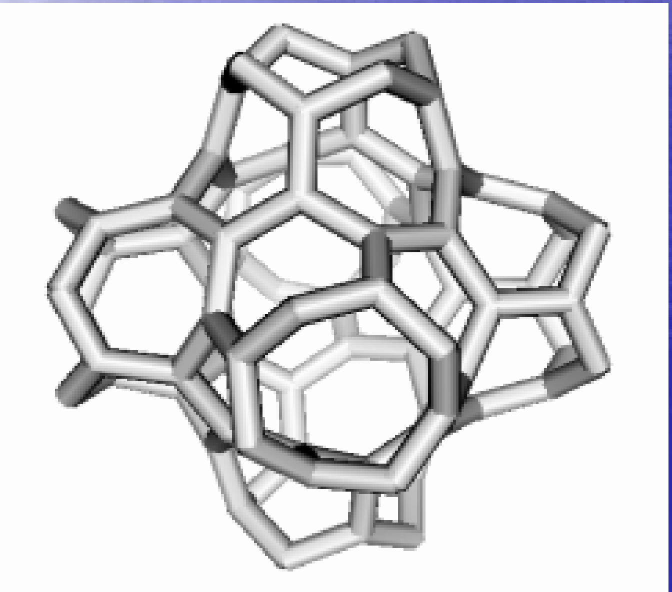
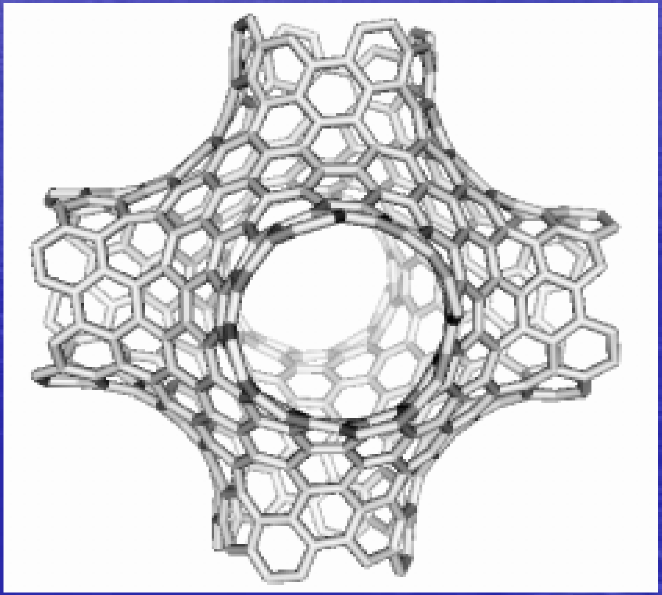


Ca_2(Cube)$_{[7]}$, P3D; N=3424

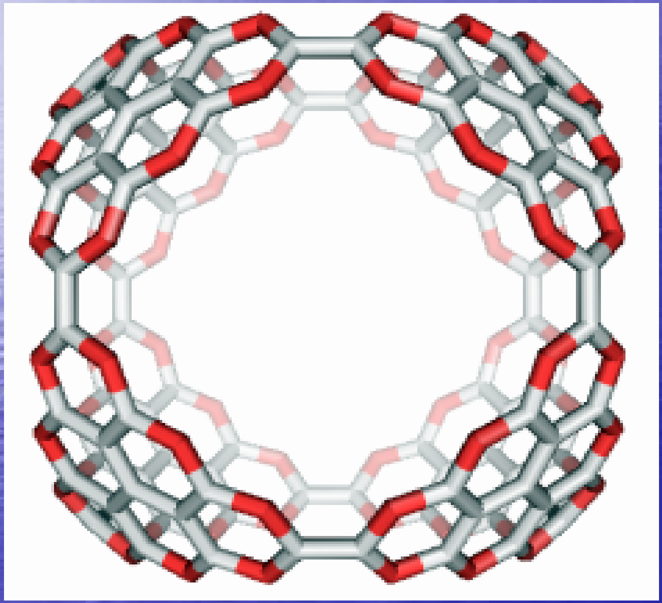
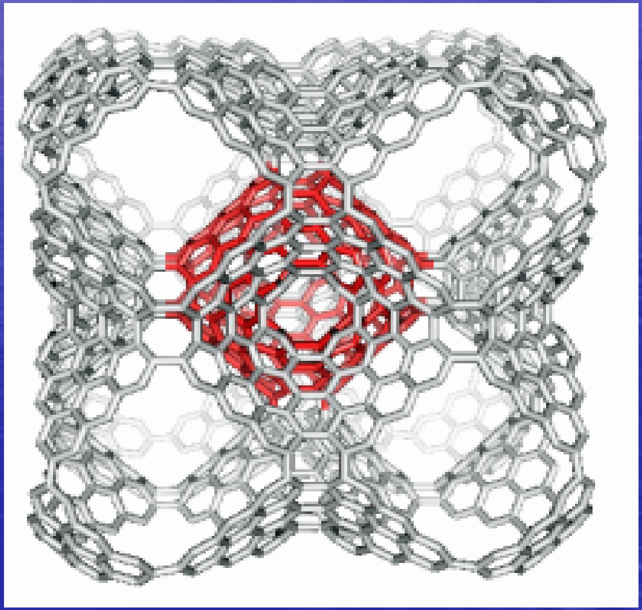


Diudea, M. V., Capra-a leapfrog related operation on maps, *Studia Univ. "Babes-Bolyai"*, **2003,** *48* (2), 3-22

Negative curvature lattices

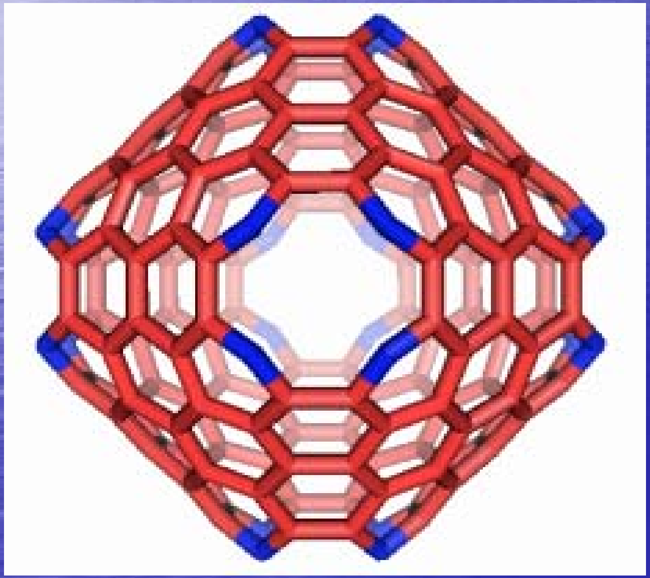
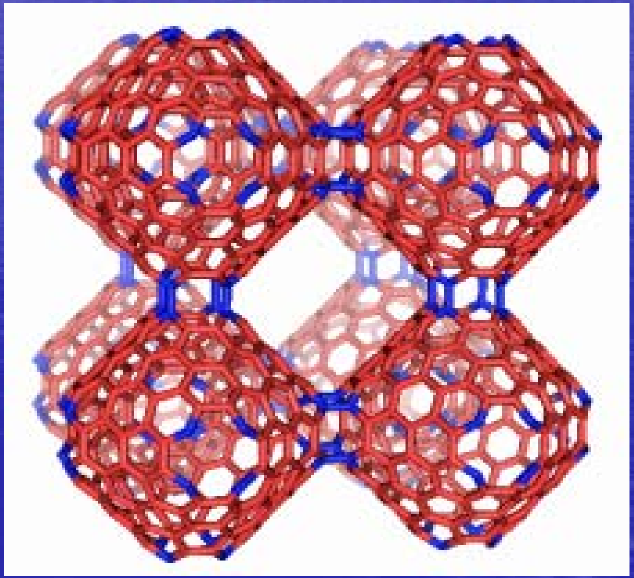
O1CaM(7)	C-Ca1-7-Ca2 = M; N = 464
	

Negative curvature lattices

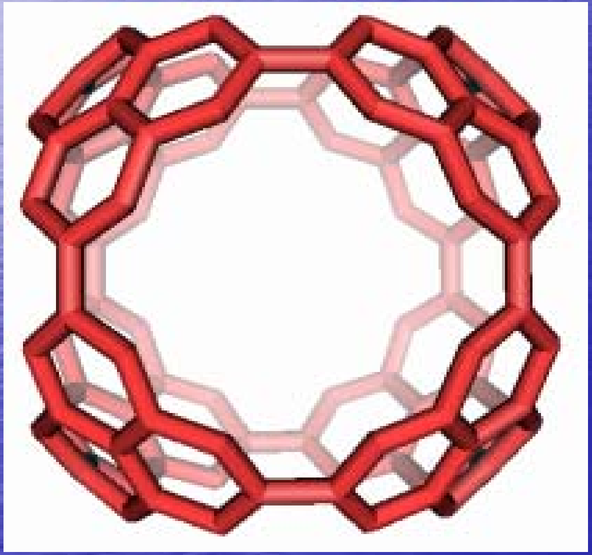
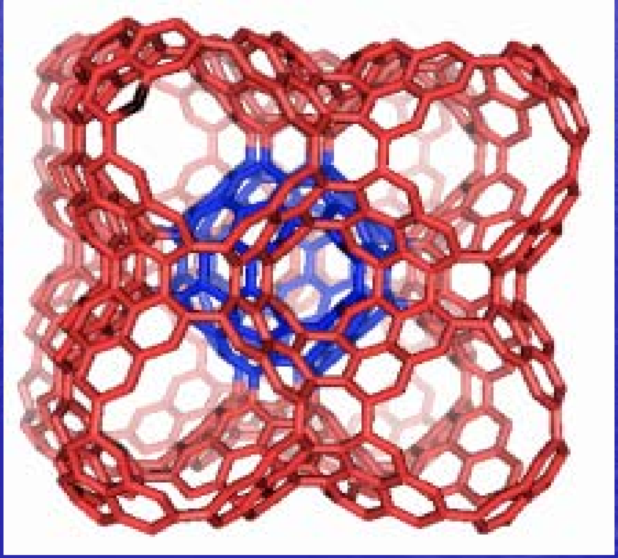
UM; N = 176	LUMj
	

Nagy, Cs. L., Diudea, M. V., Carbon allotropes with negative curvature, *Studia Univ. “Babes-Bolyai”*, **2003,** *48* (2), 35-46

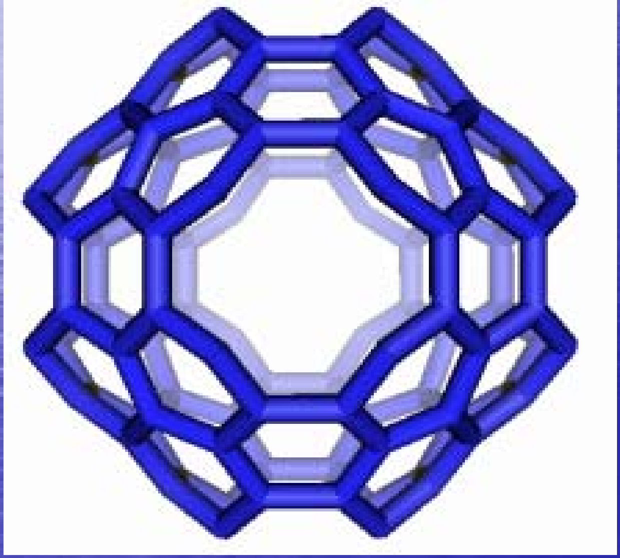
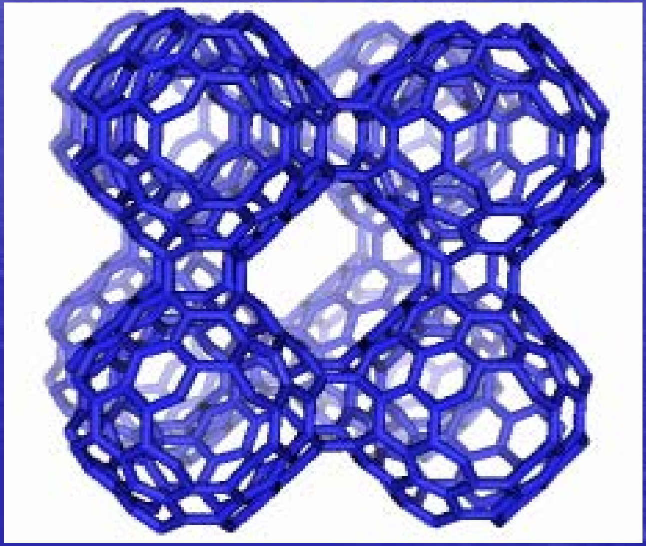
Negative curvature lattices

CUM; N = 176	LCUMj
	

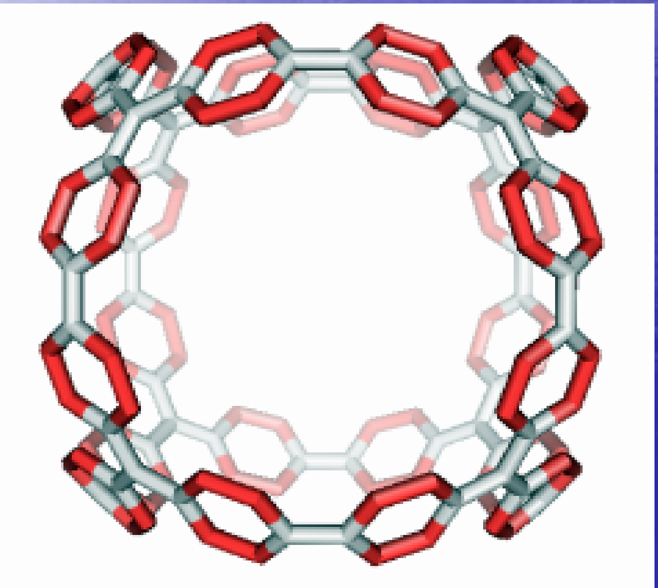
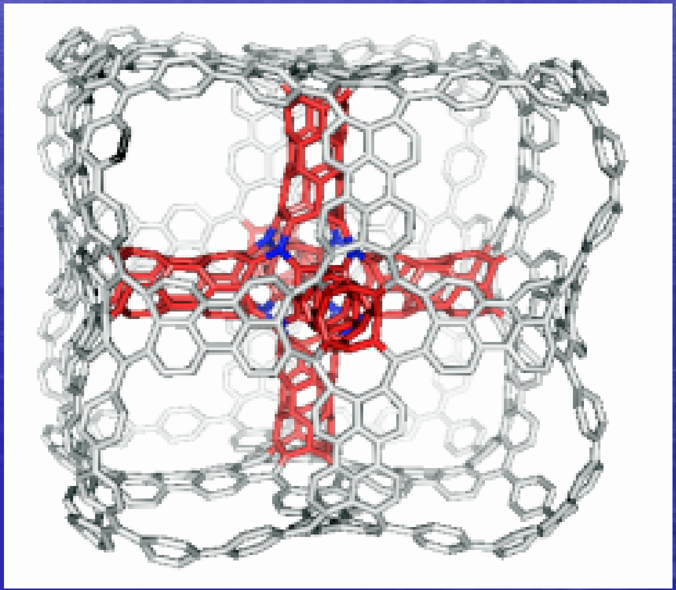
Negative curvature lattices

UCUM; N = 104	LUCUMj
	

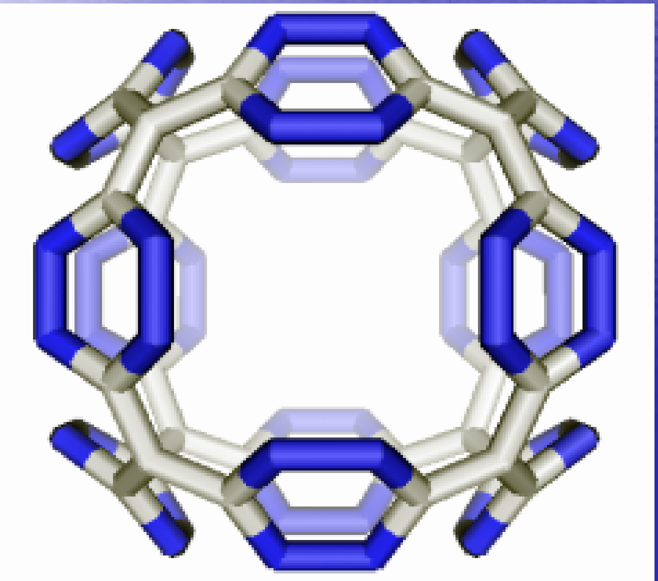
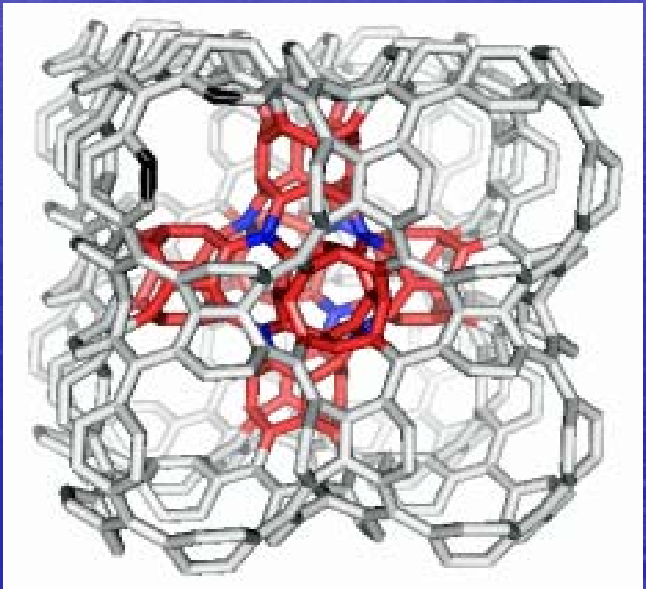
Negative curvature lattices

CUCUM; N = 104	LCUCUMj
	

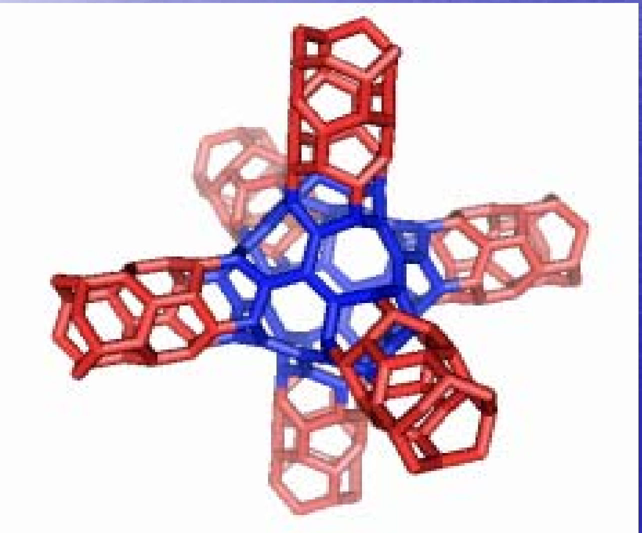
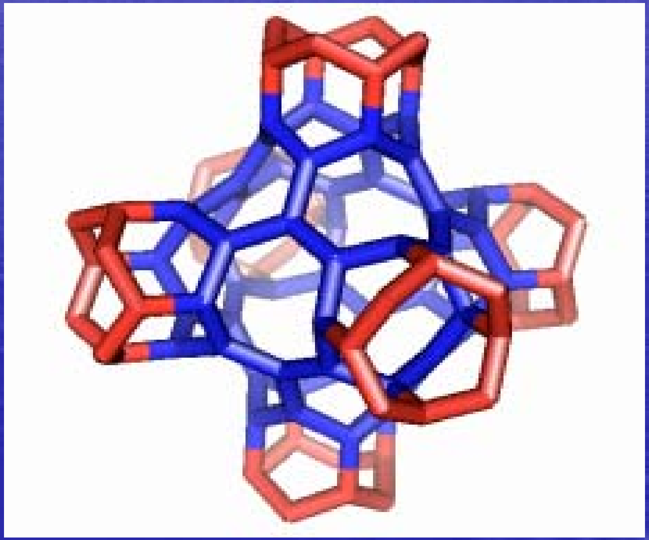
Negative curvature lattices

SUM; N = 152	LSUMi
	

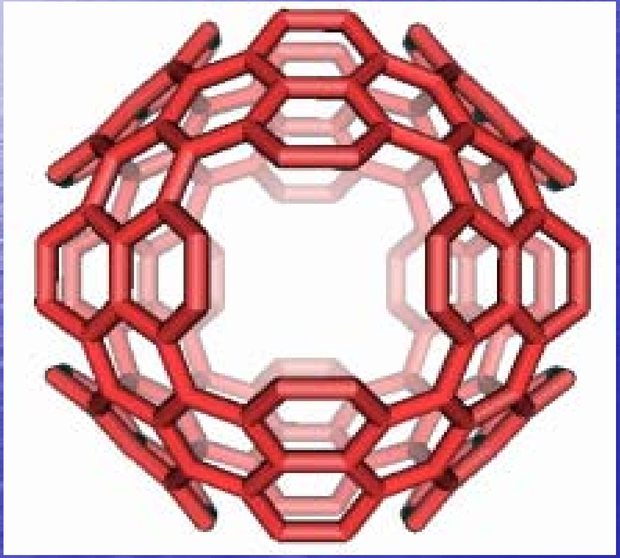
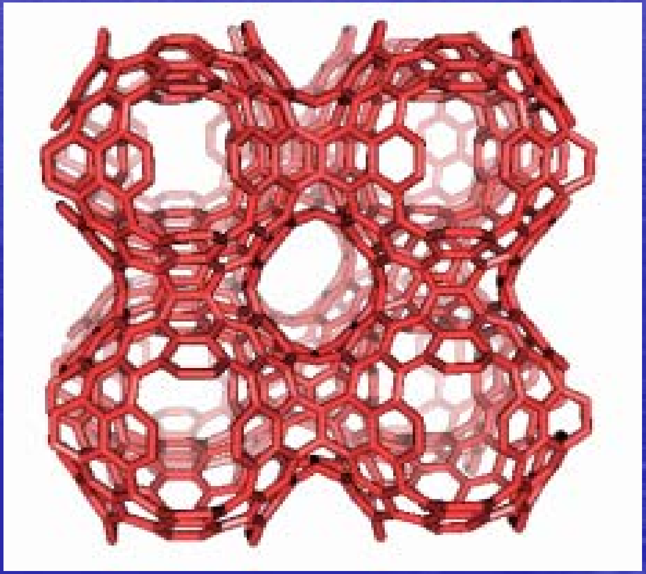
Negative curvature lattices

SCUCUM; N = 80	LSCUCUMi
	

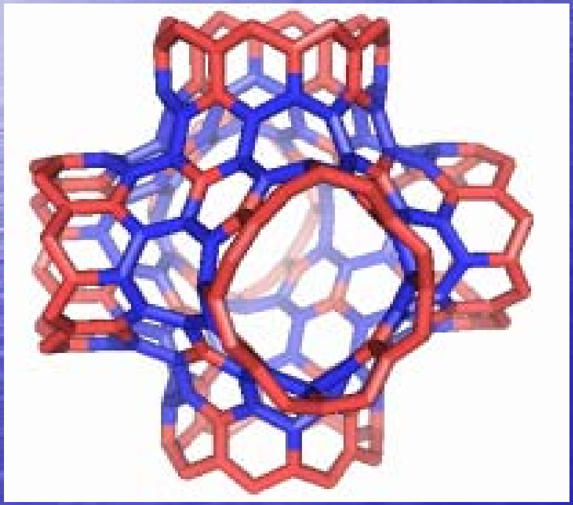
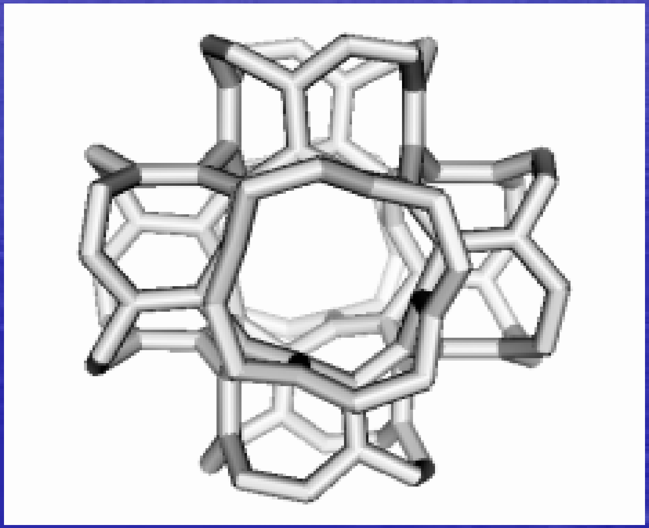
Negative curvature lattices

PLSUM; N = 200	PLSCUCUM; N = 104
	

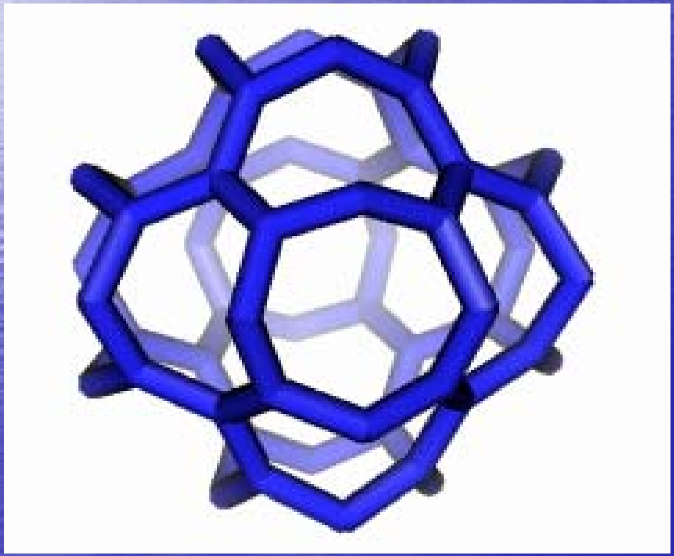
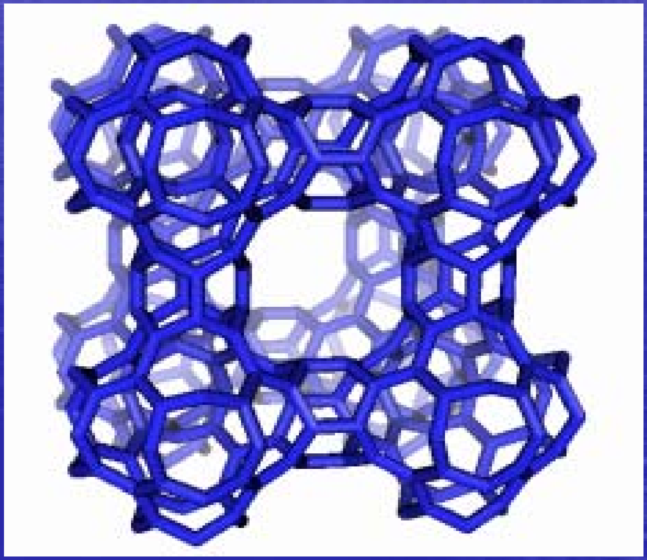
Negative curvature lattices

SCUM; N = 152	LSCUMi
	

Negative curvature lattices

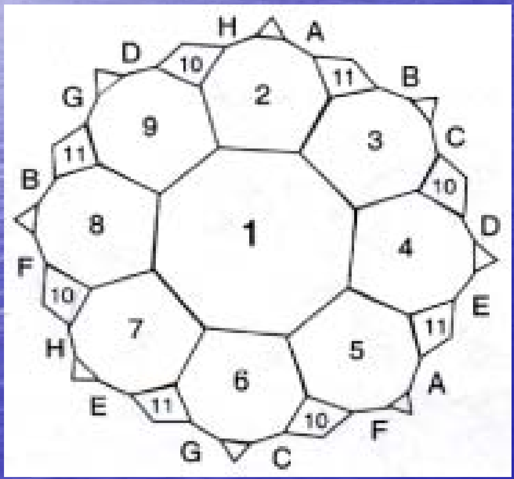
PLSCUM; N = 224	O2CaM(8)
	

Negative curvature lattices

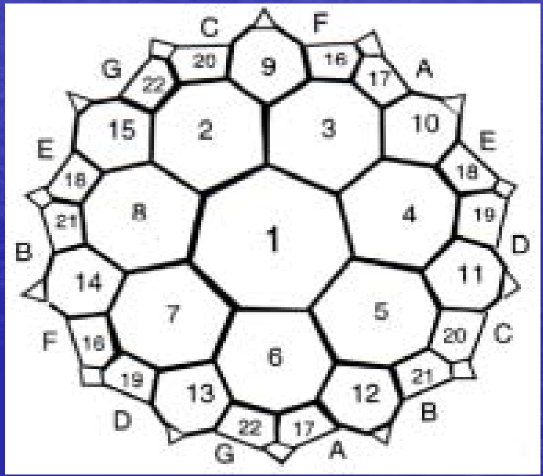
PLSCUMO=O1QM; N = 56 DYCK GRAPH	LPLSCUMOj
	

Negative curvature lattices

DYCK TESSELLATION (8,3)
12 + 6 OCTAGONS

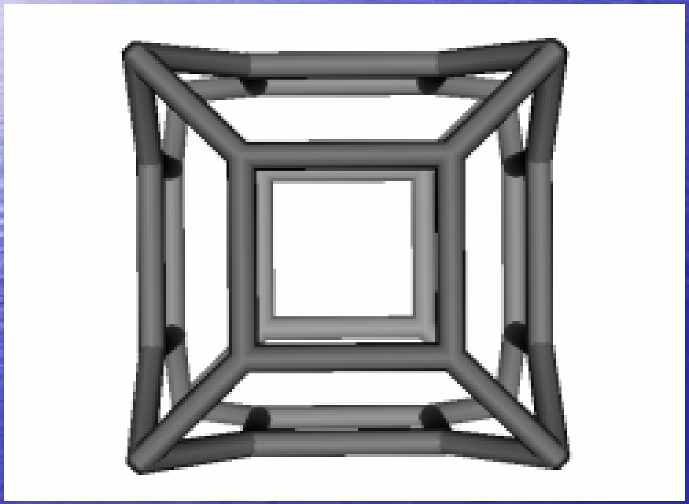


KLEIN TESSELLATION (7,3)
24 HEPTAGONS + 6 OCTAGONS

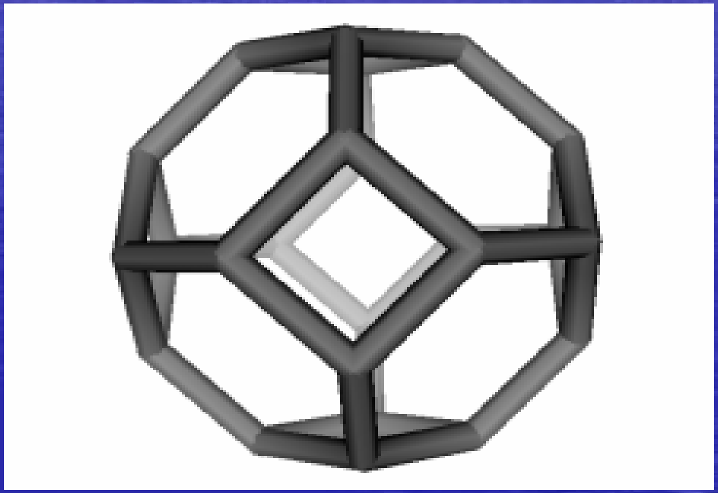


Negative curvature lattices

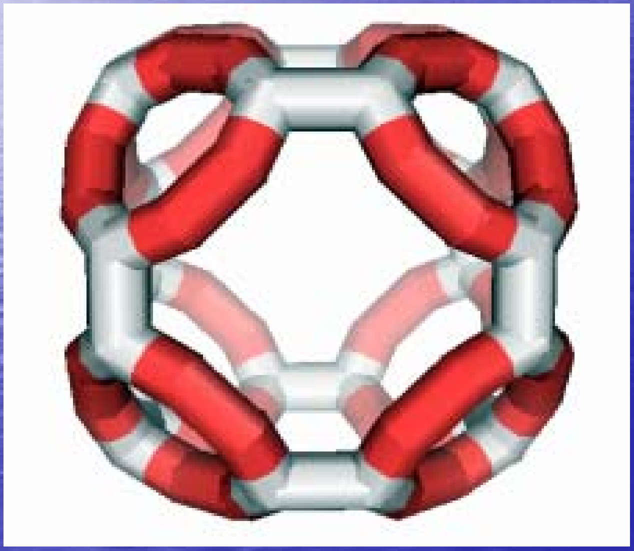
QM; N = 32



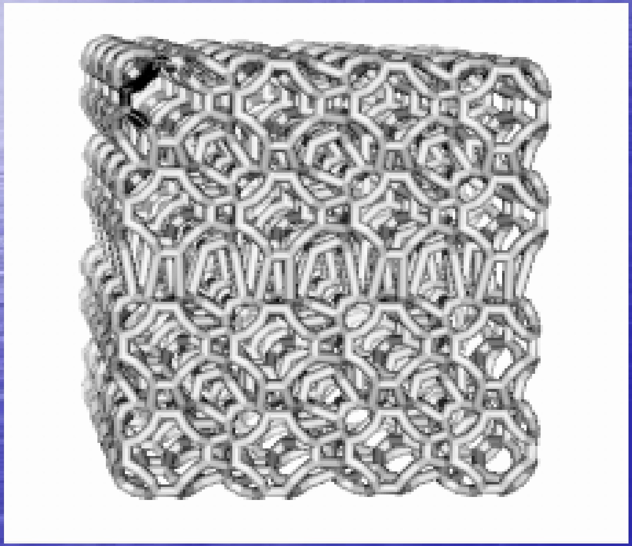
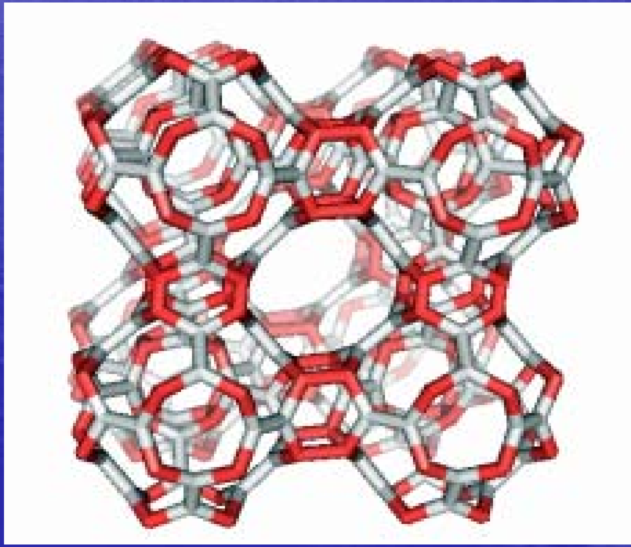
LEM; N = 24



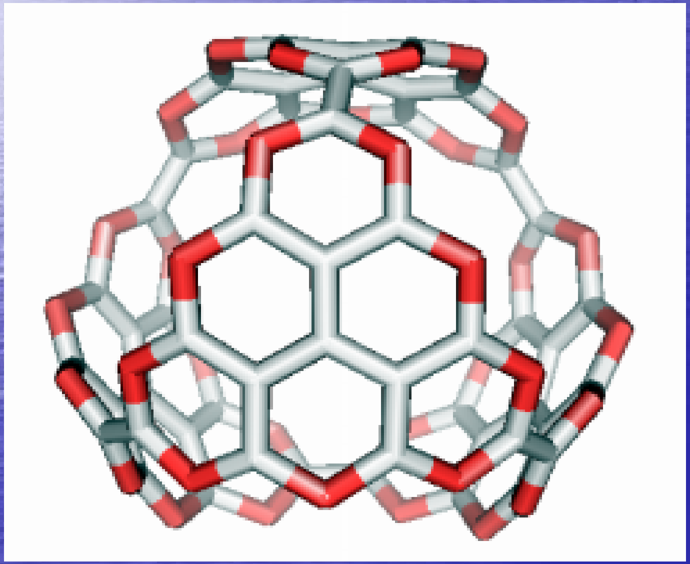
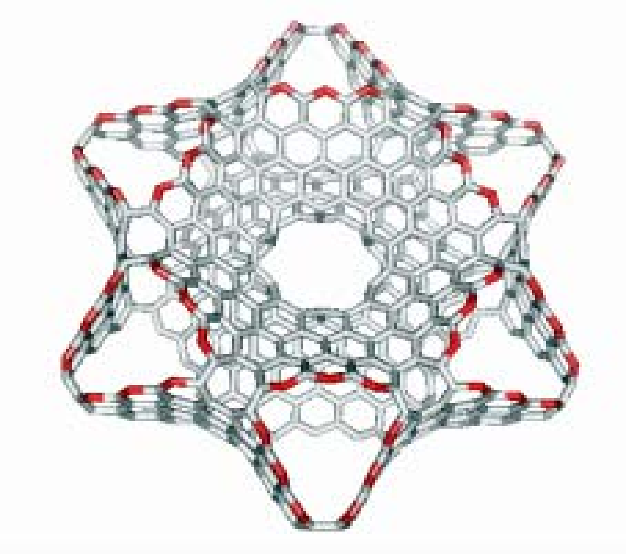
Negative curvature lattices

UO1LEM; N = 72	CUO1LEM; N = 42
	

Negative curvature lattices

LUO1LEMi	LCUO1LEMj
	

Negative curvature lattices

TUM; N = 88	LTUM
	

SOFTWARE

- TOPOCLUJ 2.0 - Calculations in MOLECULAR TOPOLOGY

M. V. Diudea, O. Ursu and Cs. L. Nagy, B-B Univ. 2002

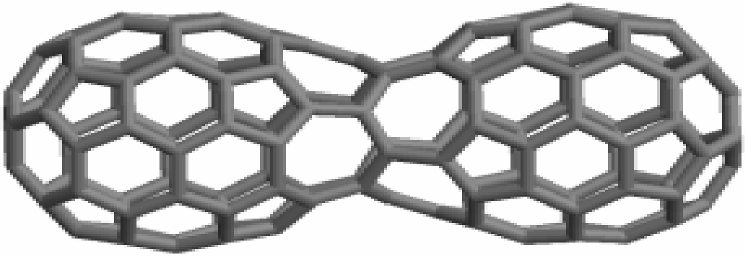
- CageVersatile 1.1

Operations on maps

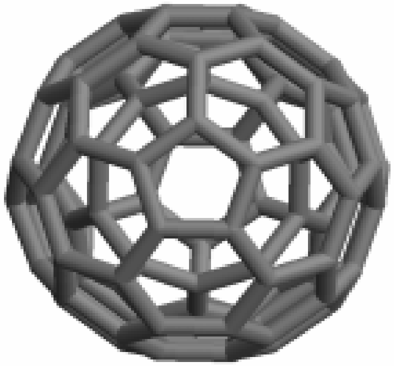
M. Stefu and M. V. Diudea, B-B Univ. 2003

Peanut dimers; topology[1]

$C_{2(70\text{-}5),5\text{-}H[10,1]\text{-}[7]} = C_{140}\ (C_1)$



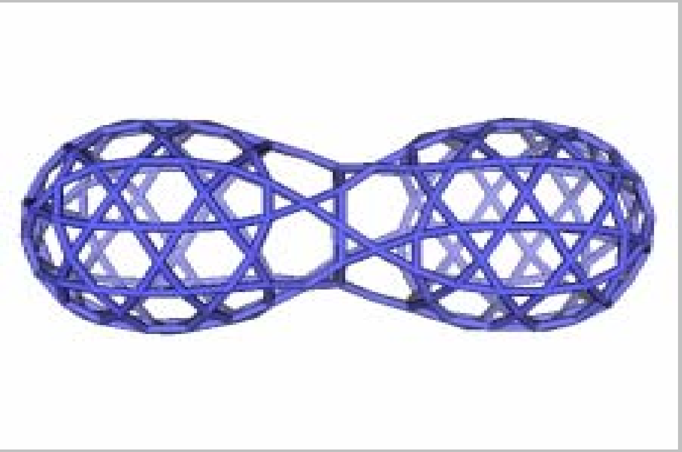
vertex orbits: 4{10}; 5{20}



1. Cs. L. Nagy, M. Stefu; M. V. Diudea and A. Dress, A. Mueler, C_{70} Dimers - energetics and topology, *Croat. Chem. Acta*, 2003 (accepted).

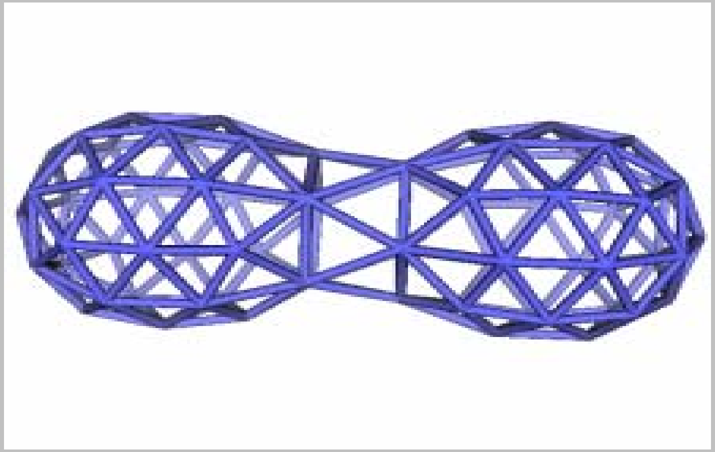
Peanut dimers; topology

Me(C_{140}); **edge orbits: 9{10}; 6{20}**



Du(C_{140}); face orbits:

[5]{2}; 2{10}; [6] 4{10}; [7] {10}



Conclusions

- A new operation on maps, called *Capra Ca*, was proposed and discussed in comparison with the well-known Leapfrog *Le* and Quadrupling *Q* operations.
- *Ca*-operation insulates each parent face by its own hexagons (*i.e.*, coronene-like substructures), in contrast to *Le* and *Q* . The transformed constitutive parameters were given.
- The utility of this operation is in building of large cages that preserve the symmetry and spectral properties of the parent structures and in extremely facile access to several constructions with negative curvature.
- Clearly, many other authors have used such a transformation but no paper, in our best knowledge, has been devoted so far.

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23. **Diudea, M.V.; Ursu, O., Parv, B., Hex tubes from square tubes, *Studia Univ. "Babes-Bolyai"*, 2003, *48*, 11-20.**

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TOPO GROUP CLUJ, ROMANIA

- Mircea V. Diudea
- Gabriel Katona
- Oleg Ursu
- Csaba L. Nagy
- Monica Stefu
- Crina V. Veres
- Mihaela Caprioara
- Cristina D. Moldovan
- Ioana Florea

TOPO GROUP CLUJ, ROMANIA, EUROPE

TOPO GROUP CLUJ, ROMANIA, EUROPE

TOPO GROUP CLUJ, ROMANIA, EUROPE

TOPO GROUP CLUJ, ROMANIA, EUROPE