# First-principles study and design of cobalt carbides and metallofullerenes for magneto-thermal cancer therapy

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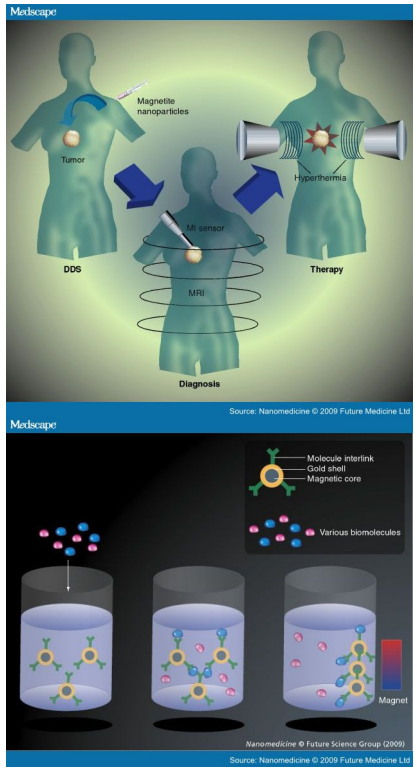
# Magneto-thermal cancer therapy, rules for magnetic particles




$Gd@C_{82}(OH)_{22}$
golden mean of nanotechnology?

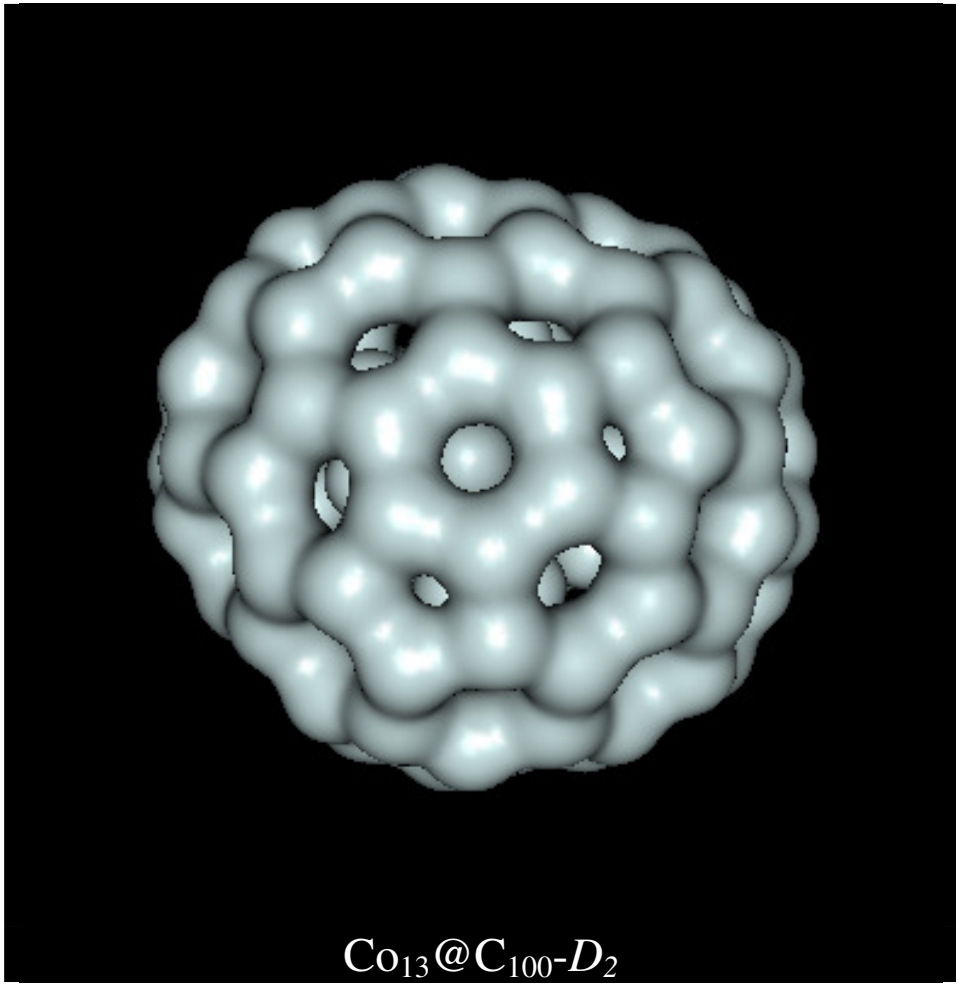
# *Ab initio* approach

**Method**: DFT - density functional theory

GGA-PBE - generalized gradient approximation [Perdew, Burke, Ernzerhof, 1996]

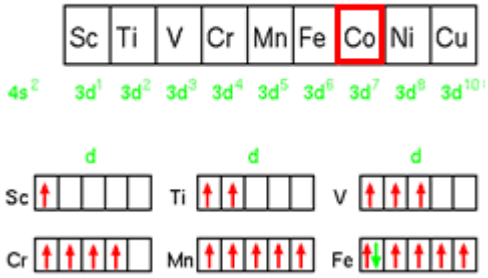
**Calculation**: the total spin magnetic moment, $\mu_B$

**Software**: OpenMX v.3.5 [Ozaki, 2003]

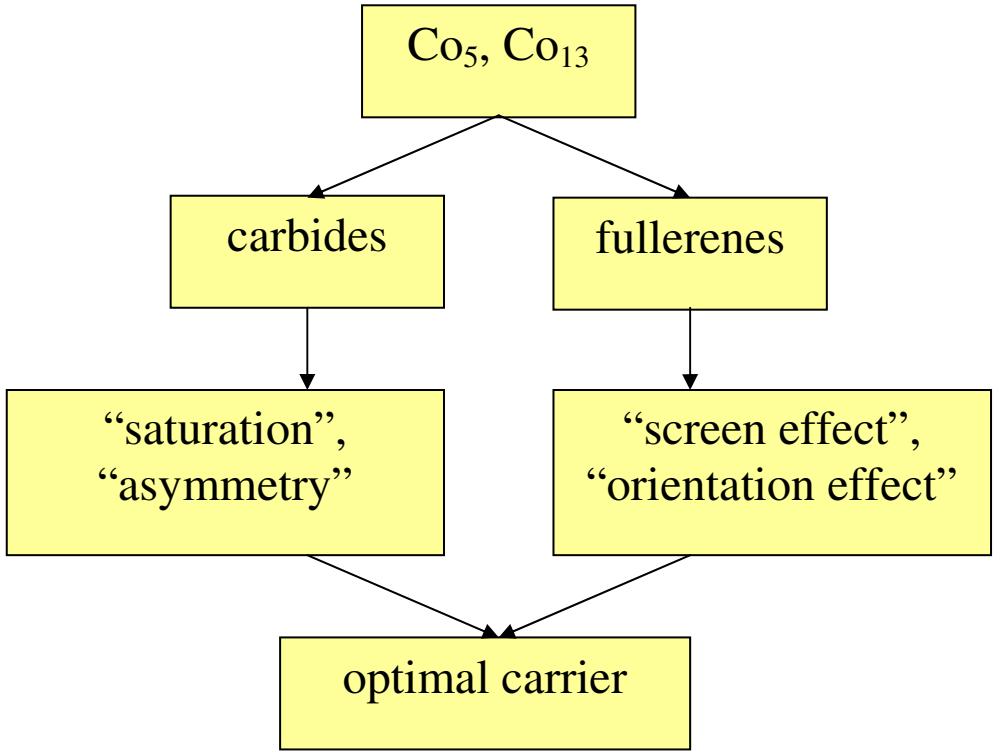


$Co_{13}@C_{100}$-$D_2$

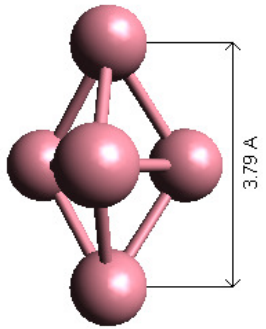
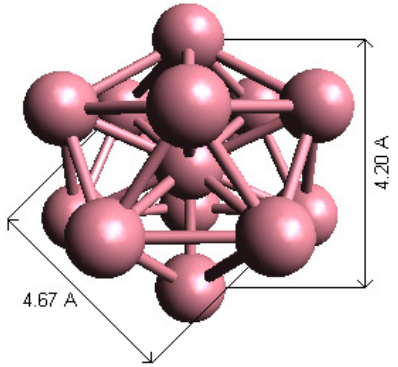
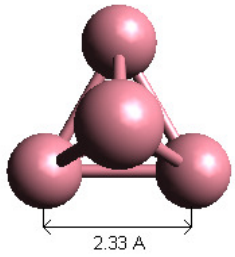
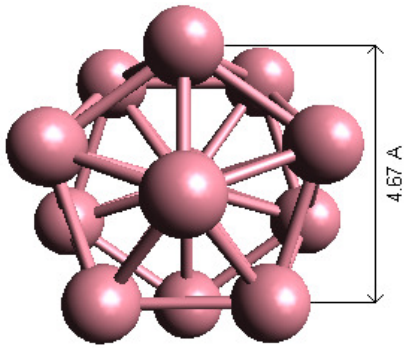
# *d*-Electrons and their spins in transition metals

# Scheme of experiments

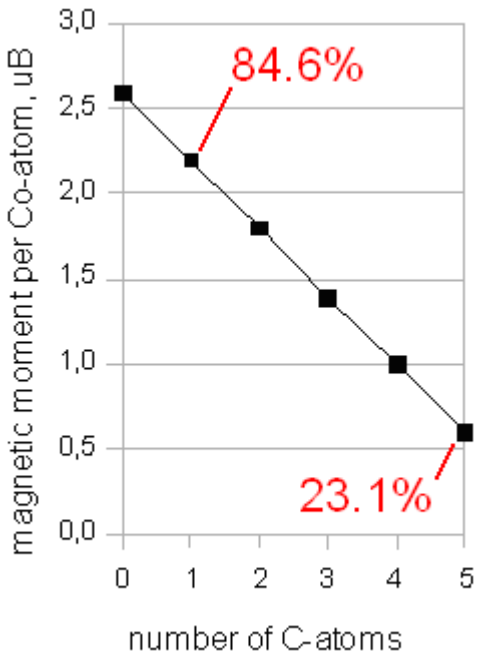


# $Co_5$ and $Co_{13}$ clusters

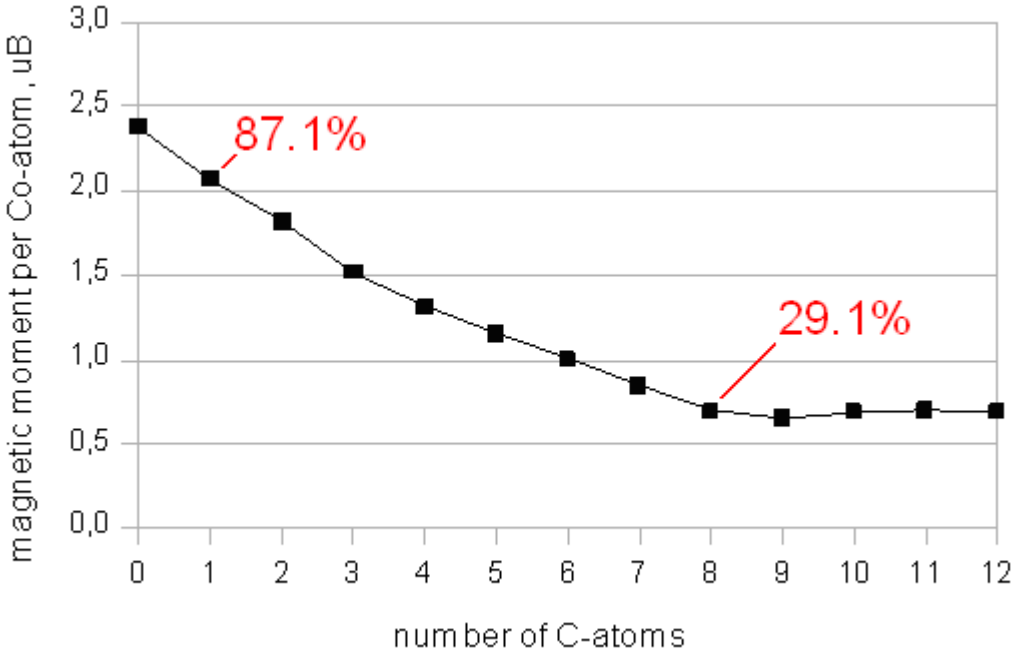
| | $Co_5$-$D_{3h}$ | | $Co_{13}$-$I_h$ |
|---|---|---|---|
| **bottom-up** |   | |   |
| **to an observer** |   | |   |
| **total magnetic moment** | 13.00 $\mu_B$ | < | 31.00 $\mu_B$ |
| **magnetic moment per Co-atom** | 2.60 $\mu_B$ | > | 2.39 $\mu_B$ |

# Magnetic activity of carbides $Co_5C_n$ (a) and $Co_{13}C_n$ (b) depending on the number of carbon atoms

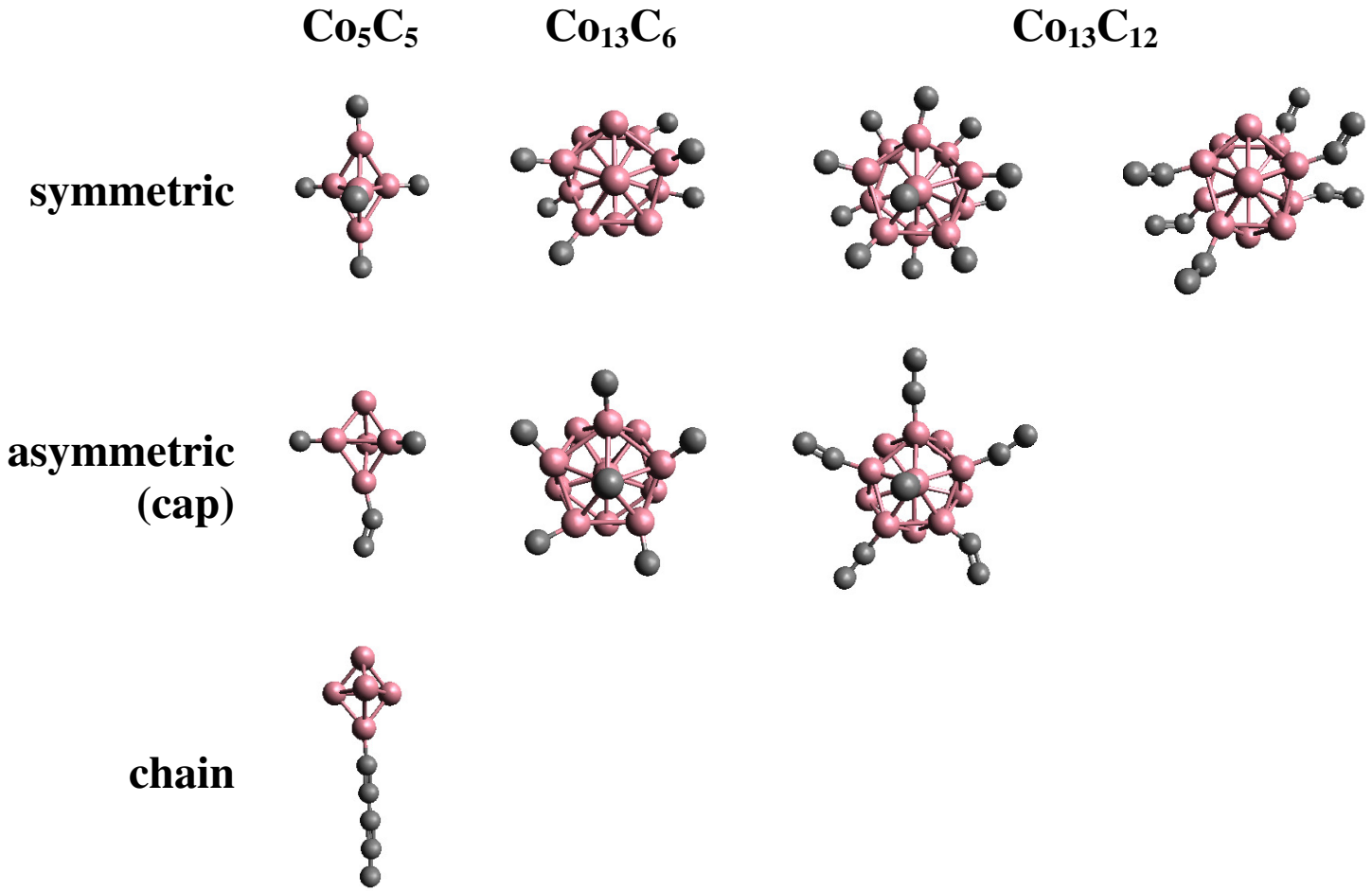
**a**




**b**

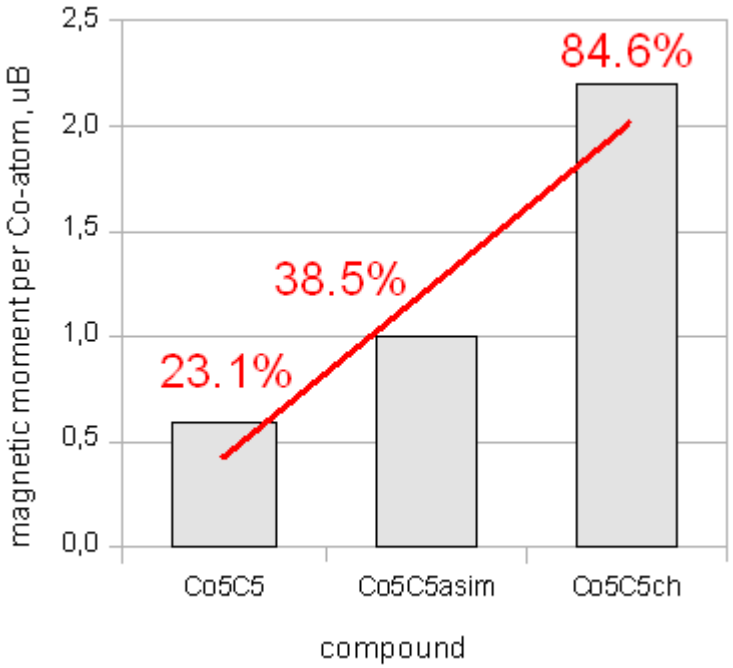


# Isomers of $Co_5C_5$ and $Co_{13}C_{6,12}$ complexes

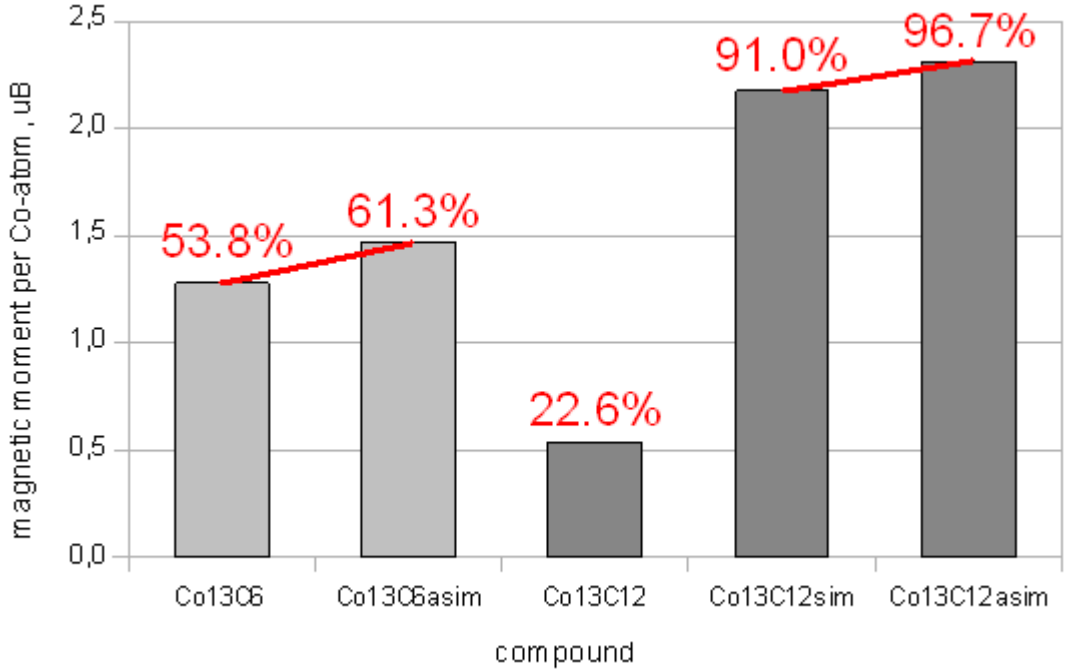


# Magnetism of isomers of $Co_5C_5$ (a) and $Co_{13}C_{6,12}$ (b) complexes

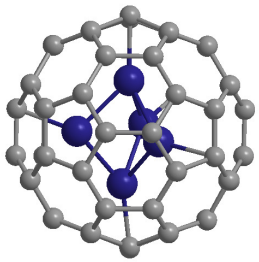
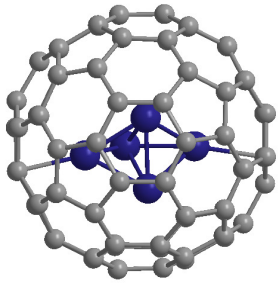
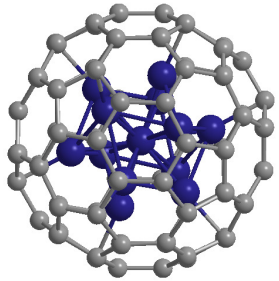
**a**




**b**



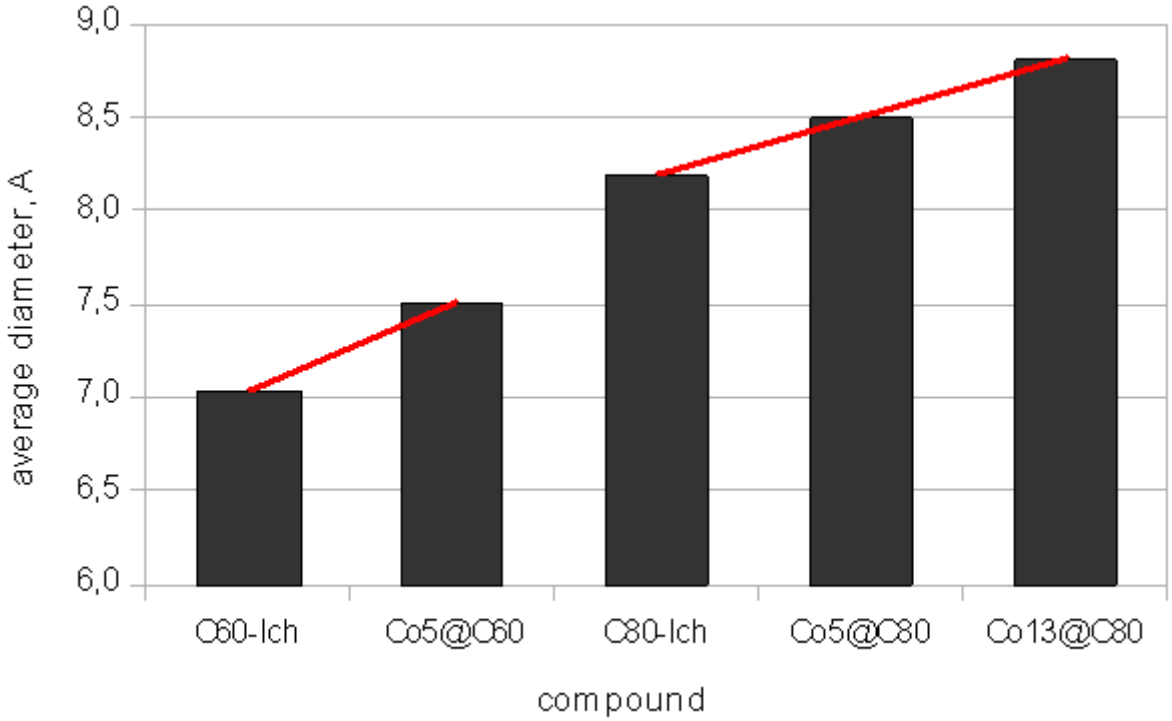
# Endohedral metallofullerenes and their characteristics

| | $Co_5@C_{60}$-$I_h$ | | $Co_5@C_{80}$-$I_h$ | | $Co_{13}@C_{80}$-$I_h$ |
|---|---|---|---|---|---|
| |  | |  | |  |
| **total magnetic moment** | 10.47 $\mu_B$ | < | 11.78 $\mu_B$ | < | 27.00 $\mu_B$ |
| **magnetism per Co-atom** | 2.16 $\mu_B$ | < | 2.39 $\mu_B$ | > | 2.08 $\mu_B$ |
| **related to pure Co cluster** | 80.5 % | < | 90.6 % | > | 87.1 % |
| **length of Co–C bond** | 2.18 Å | < | 2.33 Å | > | 2.09 Å |
| **number of Co–C bonds** | 5 | > | 2 | < | 12 |

$$M \sim \langle L \rangle / N,$$

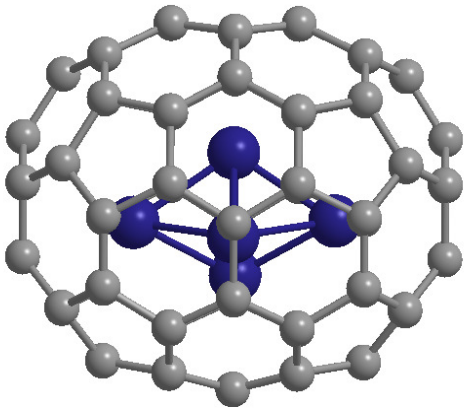
where $M$ is the magnetic moment per Me-atom of given complex ($\mu_B$), $\langle L \rangle$ is the average Me–C bond length in Å, and $N$ is the total number of Me–C bonds in the complex

# The size of fullerene cage depending on the metal cluster insertion



# Along and across oriented $Co_5$ cluster in the $C_{70}$-$D_{5h}$ fullerene

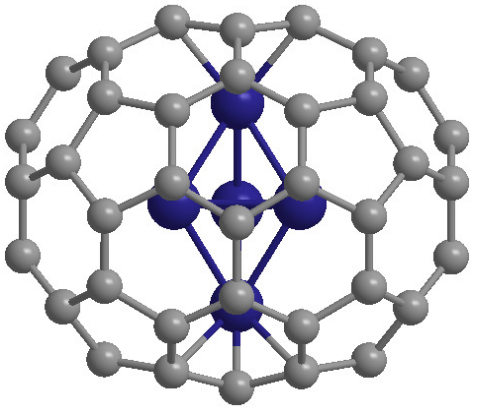
along orientation



2.19 $\mu_B$/Co-atom

>

across orientation



1.80 $\mu_B$/Co-atom

# Conclusion

- Magnetic moment (MM) is strongly correlated to the effective hybridisation between *d*-electrons of core cobalt cluster and *p*- or $\pi$-electrons of carbon shell, which is closely related to the average bond length and the number of bonds

***1a.*** MM of the $Co_mC_n$ complexes is decreased monotonically with the growing number of C-atoms

***1b.*** MM of the $Co_mC_n$ isomers is increased steadily with the decreasing number of Co–C bonds

***1c.*** MM of the Co carbide isomers is improved with the loss of symmetry

***2a.*** MM of the Co clusters embedded into fullerenes is dropped down with the decreasing size of carbon cage

***2b.*** MM of the confined Co cluster is depended on its position in the carbon cage

- Complex $Co_5@C_{80}$ is a good candidate for a cancer treatment

# Publications

*Kuznetsov A*. From carbides to $Co_5$ and $Co_{13}$ metallofullerenes: first-principles study and design // Am. J. Biomed. Eng. (in prep. 2011).

*Kuznetsov A*. Magnetic properties of endohedral complexes $Co_5@C_n$ depending upon the size and symmetry of fullerenes as well as orientation of cobalt cluster // Comp. Mater. Sci. (in press 2011).

*Kuznetsov A*. Magnetic moments of carbides $Co_{13}C_{1\text{-}12}$: a density functional investigation // Actual Problems of Applied Physics 2011, Sevastopol, Ukraine, 18-21 October (2011).

*Tereshchuk P., Kuznetsov A*. Magnetism of $Co_{13}$ cluster embedded into fullerenes of different size and form // 219th ECS Meeting, The Electrochemical Society, Montreal, Canada, 1-6 May 2011.

*Kuznetsov A., Korvink J*. From DNA-structures to a NanoSwarm // DECOI 2006: Design of Collective Intelligence, International Summer School on Collective Intelligence and Evolution, Amsterdam, Holland, 7-11 August (2006).

# Acknowledgements

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