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David Escobar Martín *

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Abstract: In this work, we will study metallic clusters equivalent to the organic ones intercalated with metals, of solid benzene type, Ba anthracene and K3.45picene; and we will try to calculate its superconducting Tc, for each of these compounds, from electronic correlations at room temperature. We will also study metal hydrides and clusters, totally composed of metals, which adopt forms analogous to molecular organic picene and anthracene; also calculating its T_C.

Keywords: polyciclic aromatic hydrocarbons; materials; superconductors

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Introduction

Solid hydrocarbon superconductors, consisting of benzene rings (C_6H_6), fused together, forming chains. When they form molecular solids, there are usually 2 molecules per unit cell. These solid hydrocarbons, doped with intercalated metals, were discovered in 2010 by Yoshiro Kubozono and his team [1,2]. They studied compounds, such as: $k_3$picene (6.9 - 18ºK), $Rb_{3.8}$ picene, (11ºK), $Ca_{1.5}$ picene (7ºK), Sm picene (4º K), K_3penanthrene (4.95ºK), Rb_3penanthrene (4 75ºK), $Sr_{1.5}$penanthrene (5.6ºK), $Ba_{1.5}$ penanthrene (5.4ºK), Sm penanthrene (4.4 - 5ºK), K3.45 dibenzopentacene (33ºK), Sm chrysene (7.4ºK), K_3 coronero, (3. 5 - 15ºK), Ba anthracene (35ºK), K_3pentacene (4. 5ºK) and K_3tefernilo [3].

These molecular solids have a low superconducting fraction. The π electrons in these molecules are delocalized; Because of this, these types of molecular solids behave like semiconductors. By inserting metals between the molecules, they transfer mobile electrons to said molecules, causing the solid to now behave like a metal, and can superconduct with a Tc higher than that of metal atoms when they form crystals [4].

However, during the last few years, some works that have been developed on the subject question the appearance of a superconducting phase, in this type of compounds, MXHAP. Some authors [5] reported that they have found superconductivity in Ba anthracene (BaC14H10), with a Tc = 22ºK; and in K picene (K3.45C22H14), with a T_C= 22ºK. They attribute this superconductivity to a magnetic anomaly, which they identify with the magnetic susceptibility (χm). In addition, these authors have not found a correlation between the number of benzene rings that form the chains, and the T_C, at which they superconduct; when they form molecular solid crystals doped with metals. The C and H atoms would not intervene in superconductivity in polycyclic aromatic hydrocarbons doped with metals.

Exposition

Relationship between Resistivity and Superconductivity

Minjae Kim, Hong Chul Choi, and other authors conclude in their study that superconductivity in solid polycyclic hydrocarbons doped with metals is of the conventional BCS type, mediated by phonons; instead of other more exotic mechanisms [6]. In this line, a relationship can be established between the electronic resistivity and the superconducting Tc; that relates the interatomic distance and the intensity of the free electron - phonon coupling; this intensifying, at a smaller distance between atoms in the crystal lattice.

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The electronic resistivity is defined by some parameters of previous calculation, for its determination. We first have its mass density:

$$\rho_m = \frac{m}{V} \qquad (1)$$

, where m, is the mass; and V is the volume of the unit cell. Then we have the density, or concentration of free electrons, in the solid [7].

$$n_e = N_A \frac{Z}{A} \rho_m \qquad (2)$$

In this expression, we have N_A, as Avogadro's number (6.02214 x 1023 mol-1); Z is the electronic valence number of the atom; A is the atomic mass number; and ρm , as we have already seen, in its previous expression, is the mass density.

Per unit cell, this equation simplifies to:

$$n_e \sim \frac{Z}{A} n^{o}_A \qquad (3)$$

Being n^{o}_A, the number of atoms that make up the unit cell; which is what we will use here.

The mean free path between collisions of the free electrons with the ions is defined by the equation [7]:

$$\ell = \frac{1}{n^{o}_{ion}\, \pi r^2_{ion}} \qquad (4)$$

Where the number of ions (nºion) is directly proportional to their radius (rion); and inversely proportional to that of the mean free path (ℓ). Finally, we arrive at the final expression, for the electrical resistivity [7]:

$$\rho_e = \frac{m_e}{n_e e^2 \ell} \sqrt{\frac{3K_BT}{m_e}} = \frac{1}{n_e e^2 \ell} \sqrt{3m_eK_BT} \qquad (5)$$

K_B, is the Boltzman constant (8.61733 × 10-5 eV K−1), and the temperature (T), comes in absolute degrees or Kelvin.

The electron´s effective or dynamic máss, came difinited by the math formula [8]:

$$m^* = \frac{\sigma}{e^2 \tau} = \sqrt{n_e} \qquad (6)$$

According to Kittel and G. T. Meaden [9–11], only metals compute electronic resistivity, excluding semi-metallic and non-metallic elements.

Table 1. Electrical resistivity of K and Ba, , not computing non-metallic.

E	ρ_e x 10^{-8} Ωm
H	
C	
K	7.19
Ba	39

For the calculation of the superconducting TC, in the case of having only one metallic element (in this case, dopant metallic atoms), in a molecular solid, as is the case; we have found the relation:

$$T_C = \rho_e \times 0,8975 \qquad (7)$$

, for Ba - anthracene and K - picene, is a fairly good approximation, for superconducting T_C.

Table 2. Intercalated reference compounds for this study. Ba - anthracene (TC = 35ºK) and K - picene (TC = 22ºK), in their experimental record. (TC, calculated with the equation, 7).

C	ρ_e x 10^{-8} Ωm	T_C Cal	T_C Exp
$BaC_{14}H_{10}$	39	35, 0025	35
$K_{3.45}C_{22}H_{14}$	24, 8055	22, 2529	22

High Electrical Resistivity, among Metals

Some of the most resistive elements among the metals in the periodic table are:

Table 3. Some of most resistive metals of the periodic table.

E	ρ_e x 10^{-8} Ωm
Mn	139
Gd	134
Tb	111
Sm	99
Dy	90, 0
Eu	89
Ce	81

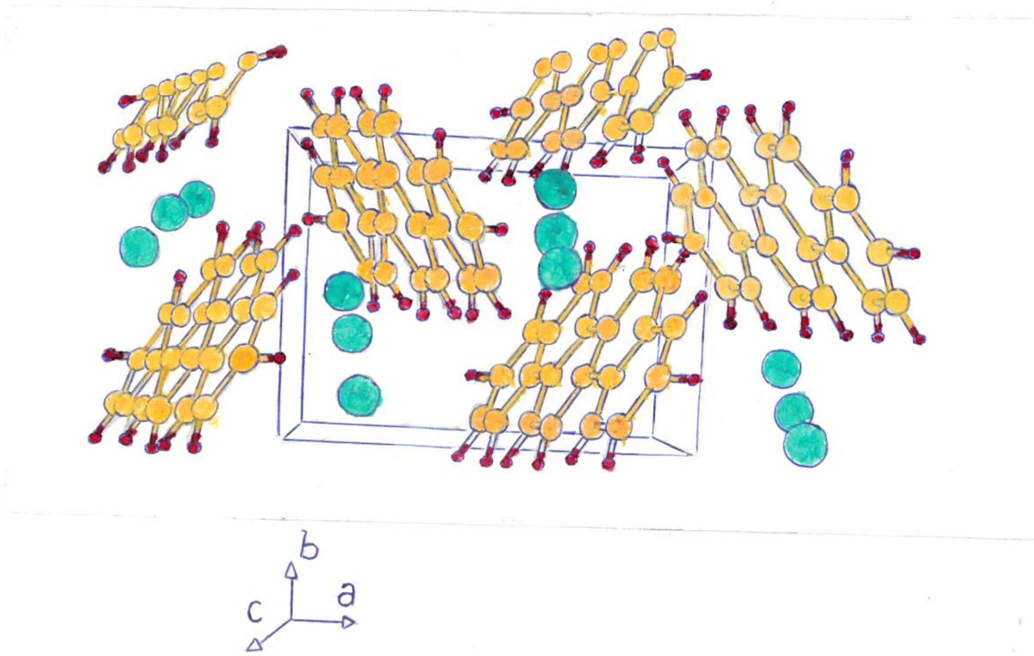

Figure 1. $Mn_3C_{22}H_{14}$, in his unit cell.

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Table 4. Polyciclic Aromatic Hydrocarbons doped with metals, of high resistivity.

C	ρ_e x 10^{-8} Ωm	T_c Cal.
$MnC_{14}H_{10}$	139	124, 7525
$Mn_{3.45}C_{22}H_{14}$	479, 55	430, 3961
$GdC_{14}H_{10}$	134	120, 265
$Gd_{3.45}C_{22}H_{14}$	462, 3	414, 9142
$TbC_{14}H_{10}$	111	99, 6225
$Tb_{3.45}C_{22}H_{14}$	382, 95	343, 6976
$SmC_{14}H_{10}$	99	88, 8525
$Sm_{3.45}C_{22}H_{14}$	345, 55	306, 5411
$DyC_{14}H_{10}$	90, 0	80, 775
$Dy_{3.45}C_{22}H_{14}$	310, 5	278, 6735
$EuC_{14}H_{10}$	89	79, 8775
$Eu_{3.45}C_{22}H_{14}$	307, 05	275, 577
$CeC_{14}H_{10}$	81	75, 6975
$Ce_{3.45}C_{22}H_{14}$	279, 45	250, 8063

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E D	nº$_{Am}$	ρ x 10^{-8} Ω m	T_C ºK Calc. ρ_e x 0, 8975	ρ_e x 0,43
Ti	1	43, 1	38, 68225	18, 533
	1, 5	64, 65	58, 02337	27, 7995
	2	86, 2	77, 3645	33, 2667
	2, 5	107, 75	96, 7056	41, 5834
	3	129, 3	116, 04675	49, 9001
Sc	1	46, 8	42, 003	18, 06129
	1, 5	70, 2	63, 0045	27, 091935
	2	93, 6	84, 006	36, 12258
	2, 5	117	105, 0075	45, 1532
	3	140, 4	126, 009	54, 1838
Y	1	58, 5	52, 50375	22, 5766
	1, 5	87, 75	78, 755625	33, 8649
	2	117	105, 0075	45, 1532
	2, 5	146, 25	131, 25937	56, 4415
	3	175, 5	157, 51125	67, 7298
Ba	1	39	35, 0025	15, 05107
	1, 5	58, 5	52, 50375	22, 57661
	2	78	70, 005	30, 1021
	2, 5	97, 5	87, 50625	37, 6276
	3	117	105, 0075	45, 1532
Hf	1	30, 6	27, 4635	13, 158
	1, 5	45, 9	36, 9727	19, 737
	2	61, 2	54, 927	26, 316
	2, 5	76, 5	68, 65875	32, 895
	3	91, 8	82, 3905	39, 474

Table 4.1 . Proportion dopant elements in superconducting polycyclic aromatic hydrocarbons, and T_c

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C	nº$_{Am}$	ρ x 10^{-8} Ω m	T_C ºK Calc.
$MnC_{14}H_{10}$	1	139	124, 75
$Mn_{1, 5}$	1, 5	208, 5	187, 1287
Mn_2	2	278	249. 505
$Mn_{2,5}$	2, 5	347, 5	311, 881
Mn_3	3	417	374, 257
$VC_{22}H_{14}$	1	19, 9	17, 860
$V_{1,5}$	1, 5	29, 85	26, 790
V_2	2	39, 8	35, 720
$V_{2,5}$	2, 5	49, 65	44, 659
V_3	3	59, 7	53, 580

Table 4. 2. Hydrocarbons with variable metal doping (TC = ρe x 0.8975)

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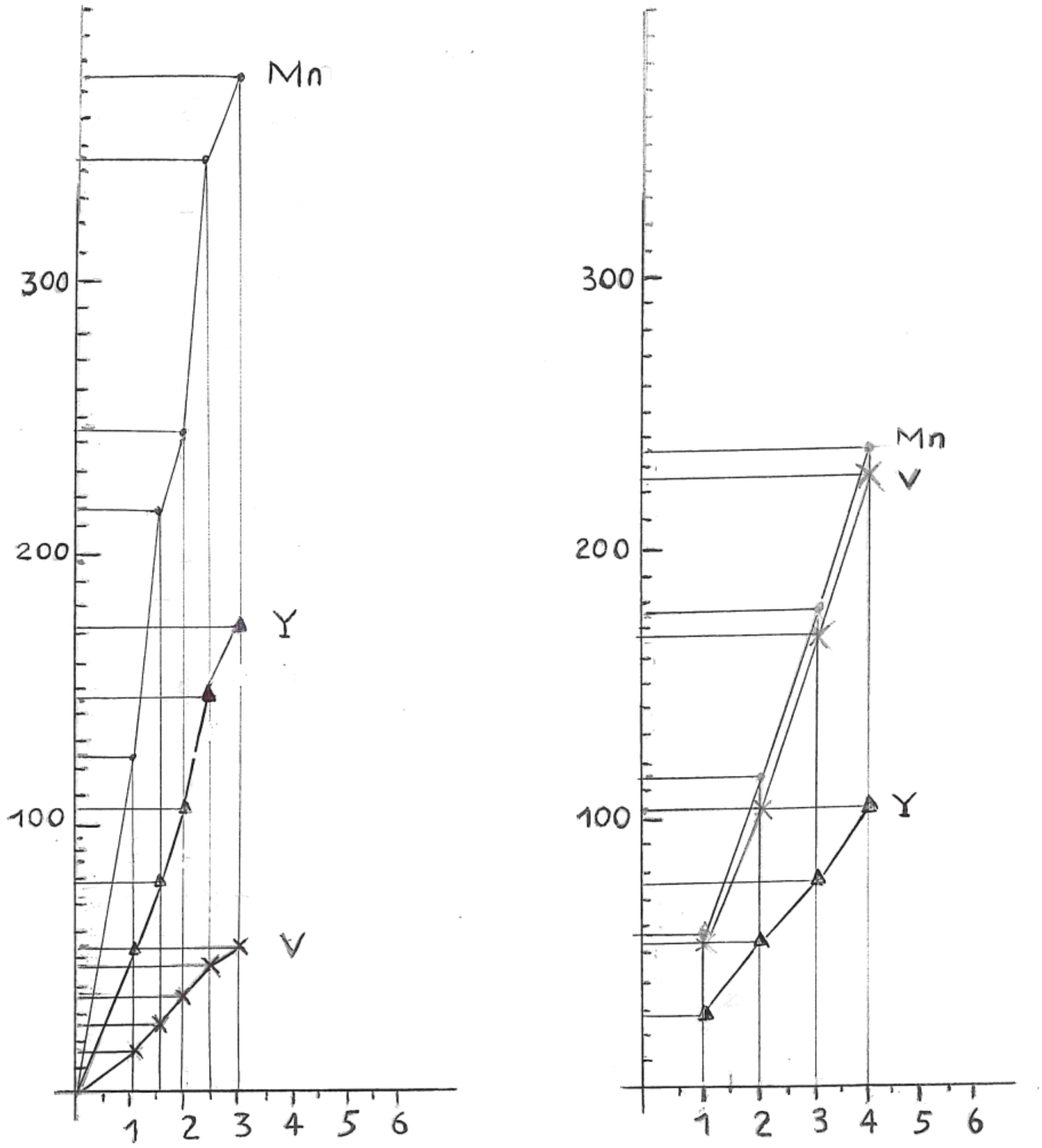

Graphic 1. Relationship, between Tc superconductivity and number of metallic atoms doping component, in polycyclic aromatic hydrocarbons (PAH).

For solids composed of simple or discrete molecules, of the solid benzene type, equation number 7 changes to:

$$T_C = \rho_e \times 0,42 \qquad (8)$$

When we have two components that form the star ring, such as Cr_6V_6, we can use the same equation that we used to calculate the reduced mass [11].

If we have the formula $A_m B_n C_o$ and the resistivities $\rho_{e,m}$; $\rho_{e,n}$ and $\rho_{e,o}$:

$$\rho_e(m) = \frac{m\rho_{e,m} + n\rho_{e,n} + o\rho_{e,o}}{m+n+o} \qquad (9)$$

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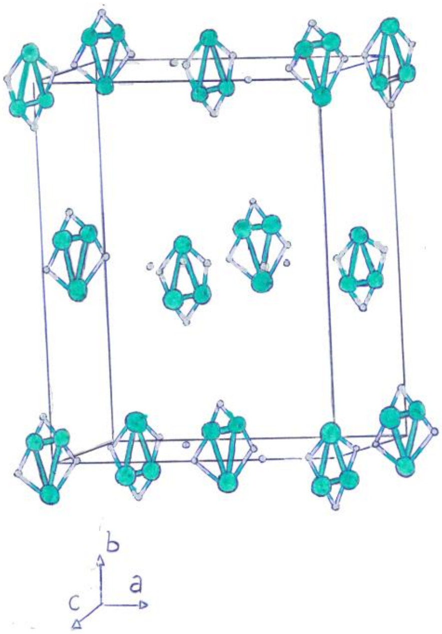

Figure 2. $Mn_3B_3C_6H_3$.

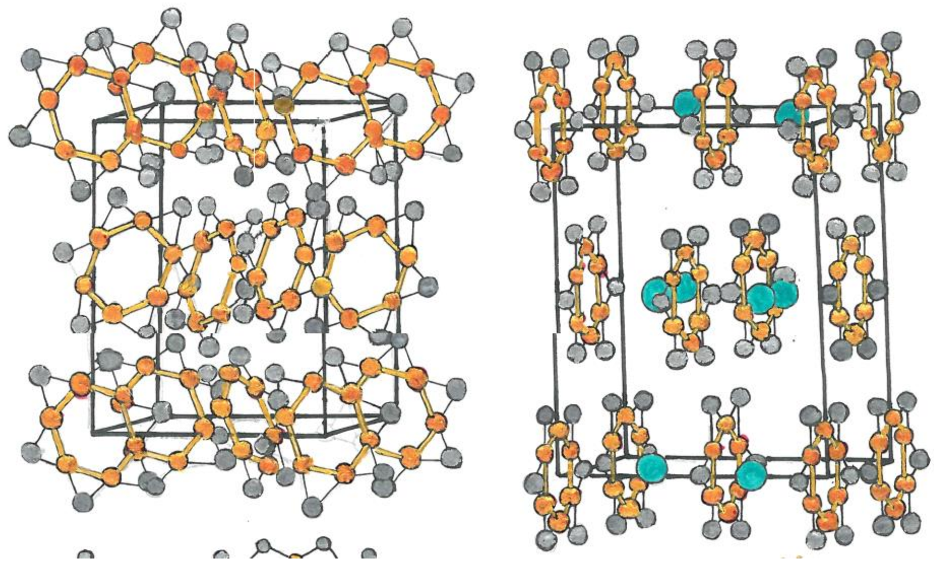

Figure 3. Cr_6V_6 and $K_2Cr_6V_6$.

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Table 5. Aromatic ring hydrocarbon doped whit high resistivity metals.

C	ρ_e x 10^{-8} Ωm	T_C Cal.	T_C Exp. (º K)
$K_2C_6H_6$	14, 38	6, 0396	5 - 7
Mn_2 C_6H_6	278	94, 95	
$Gd_2C_6H_6$	268	112, 56	
$Tb_2C_6H_6$	222	46, 62	
$Sm_2C_6H_6$	198	83, 16	
$Dy_2C_6H_6$	180	75, 6	
$Eu_2C_6H_6$	178	74, 66	
$Ce_2C_6H_6$	162	68, 04	
$Mn_3B_3C_6H_3$	417	175, 14	
$K_2Cr_6V_6$	15, 0842	6, 3354	
$V_6C_2H_6$	119, 4	50, 148	
$Ti_6C_2H_6$	258, 6	111, 198	
$Sc_6C_2H_6$	280, 8	117, 936	

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C	$nº_{Am}$	ρ $\times 10^{-8}\ \Omega$ m	T_C ºK Calc.
$MnB_3C_6H_3$	1	139	25, 7011
Mn_2	2	278	119, 54
Mn_3	3	417	179, 31
Mn_4	4	556	239, 08
GdC_6H_6	1	134	57, 62
Gd_2	2	268	49, 5532
Gd_3	3	402	172, 86
Gd_4	4	536	230, 48

Table 5.2. Solid benzene, of variable metal doping. (TC = ρe x 0.43)

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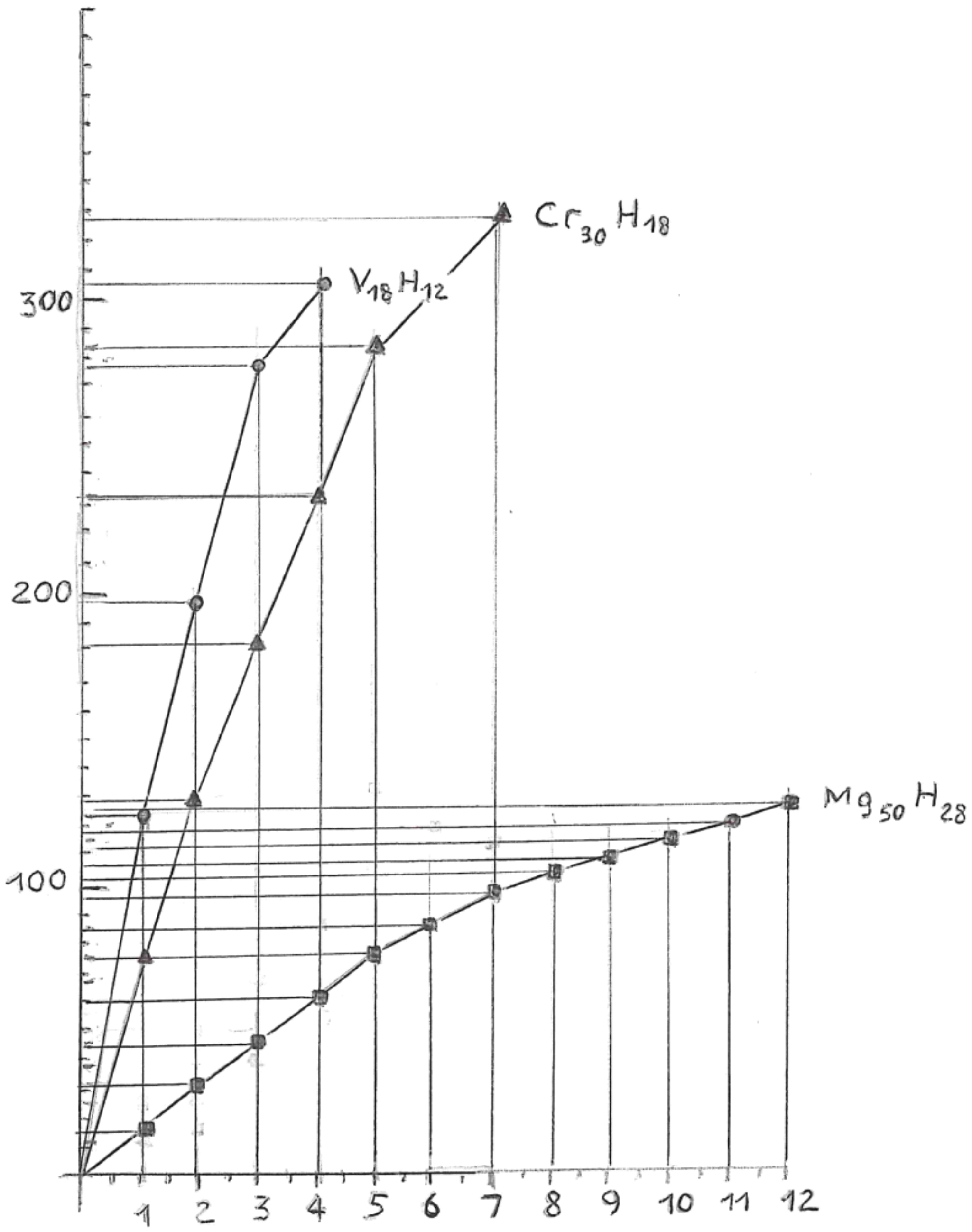

Graphic 2. Critical temperature of three metal doped polyciclic aromatic hydrocarbon.

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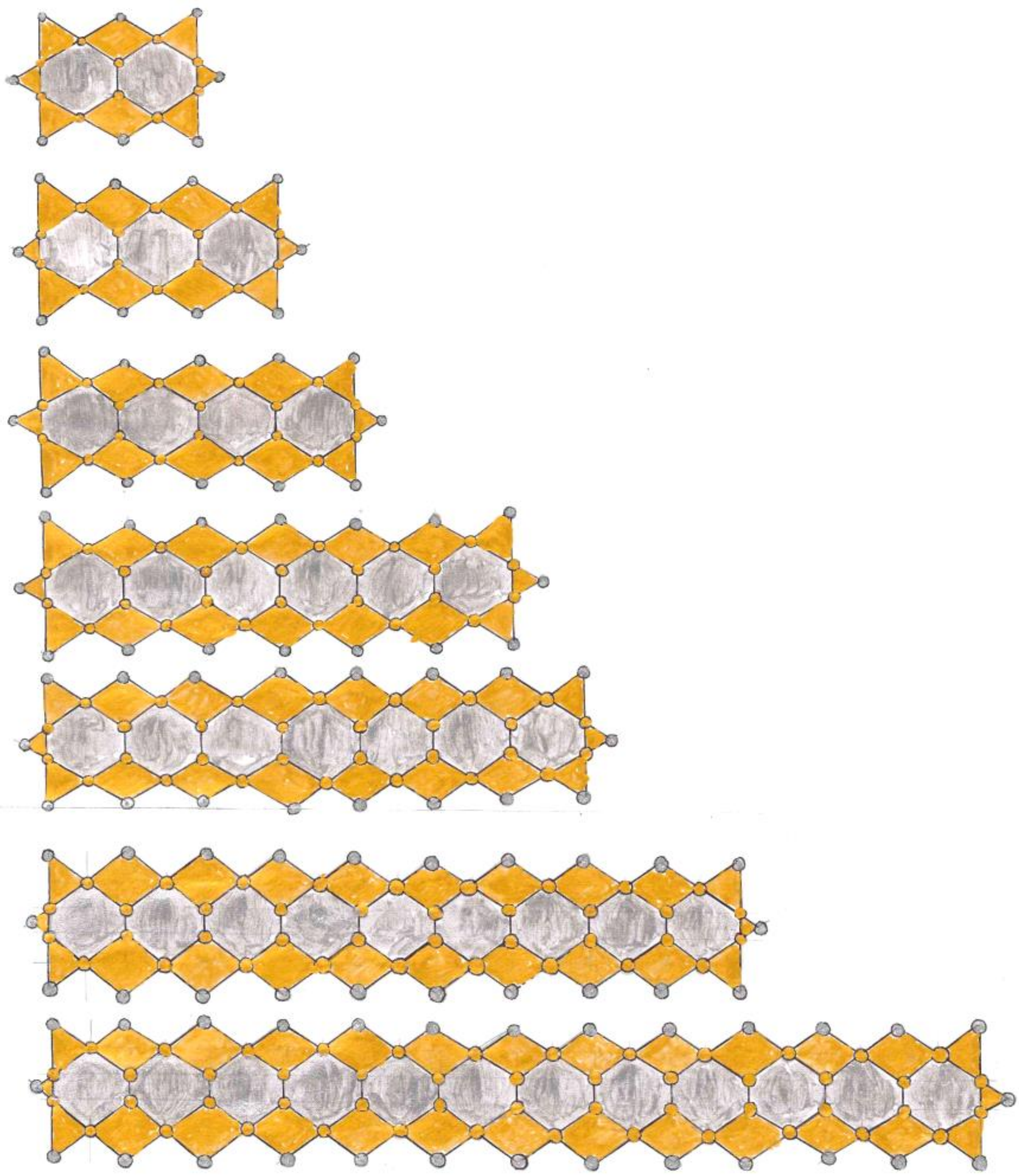

Figure 4. Different lengths of polycyclic aromatic hydrocarbon chains; formed by n cycles (n = 2 to 12).

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Table 6. Electrical resistivity as a function of the number of rings, and its relationship with the T_C, of superconducting.

C	Número de anillos	ρ_e x 10^{-8} Ω m	T_c Cal. (ºK)
$La_{10}H_8$	2	790	331, 8
$Y_{14}H_{10}$	3	819	690, 15
$Sc_{14}H_{10}$	3	655, 2	556, 92
$Ti_{14}H_{10}$	3	603, 4	512, 89
$Zr_{14}H_{10}$	3	420	357
$V_{18}H_{12}$	4	358, 2	304, 47
$Zr_{18}H_{12}$	4	763, 2	684, 972
$Ba_{18}H_{12}$	4	702	630, 045
$Sr_{18}H_{12}$	4	763, 2	684, 972
$Cr_{30}H_{18}$	7	337	328, 95
$V_{30}H_{18}$	7	597	507, 45
$Rb_{30}H_{18}$	7	375	336, 5625
$Cs_{30}H_{18}$	7	600	538, 5
$Sr_{30}H_{18}$	7	645	578, 8875
$Cu_{30}H_{18}$	7	51	45, 7725
$Li_{38}H_{20}$	9	354, 16	317, 8586
$Fe_{38}C_{20}$	9	372, 4	334, 229
$K_{50}H_{28}$	12	359, 5	305, 575
$Cu_{50}H_{28}$	12	85	76, 2875
$Al_{50}H_{28}$	12	137	122, 9575
$Mg_{50}H_{28}$	12	215	192, 9625

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C	nº$_{Am}$	ρ x 10^{-8} Ω m	T_C ºK Calc.
Cr_6H_6	6	77, 4	69, 4665
$Cr_{10}H_8$	10	129	115, 7775
$Cr_{14}H_{10}$	14	180. 6	162, 0885
$Cr_{18}H_{12}$	18	232, 2	208, 3995
$Cr_{22}H_{14}$	22	283, 8	254, 7105
$Cr_{26}H_{16}$	26	335, 4	301, 0215
$Cr_{30}H_{18}$	30	387	347, 33

Table 6. 1. Number of metallic rings - T_C ($T_C = \rho_e$ x 0.8975)

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C	$nº_{Am}$	ρ x 10^{-8} Ω m	T_C ºK Calc.
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$Cr_{10}H_8$	10	129	115, 7775
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$Cr_{18}H_{12}$	18	232, 2	208, 3995
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Table 6. Number of metallic rings - T_C ($T_C = \rho_e$ x 0.8975)

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C	nº$_{Am}$	ρ x 10^{-8} Ω m	T_C ºK Calc.
$MnB_3C_6H_3$	1	139	25, 7011
Mn_2	2	278	119, 54
Mn_3	3	417	179, 31
Mn_4	4	556	239, 08
GdC_6H_6	1	134	57, 62
Gd_2	2	268	49, 5532
Gd_3	3	402	172, 86
Gd_4	4	536	230, 48

Table 7. Solid benzene, of variable metal doping. (TC = ρe x 0.43)

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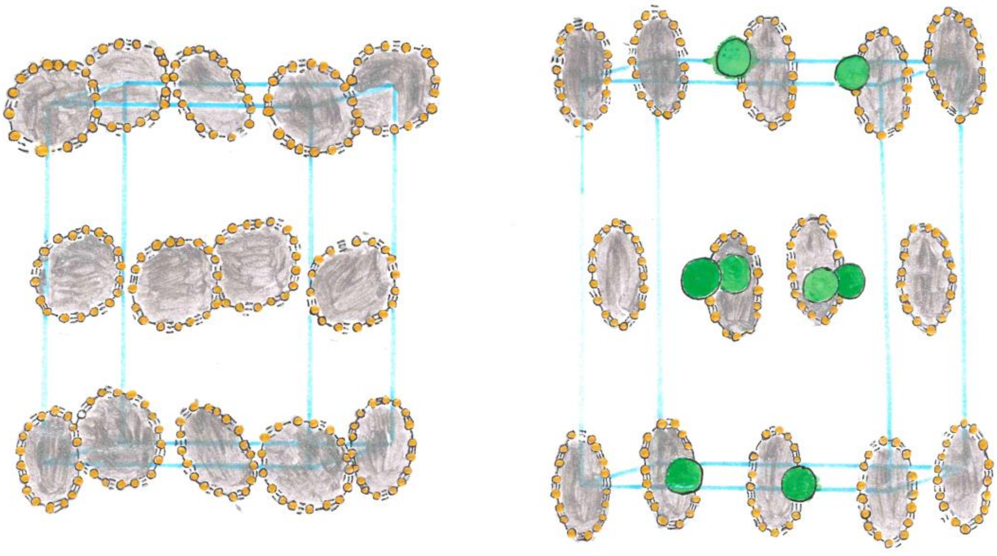

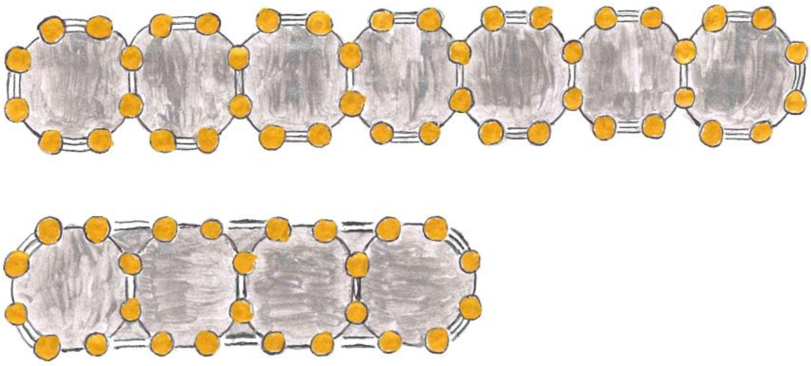

Figure 5. Cyclic hydrocarbons of the benzene type, composed of 18 atoms, with single and triple bonds; in its pure state, undoped (top left), and doped with metal atoms (top right).

Below, different lengths of chains, formed by cycles of 8 atoms, formed by single and triple bonds.

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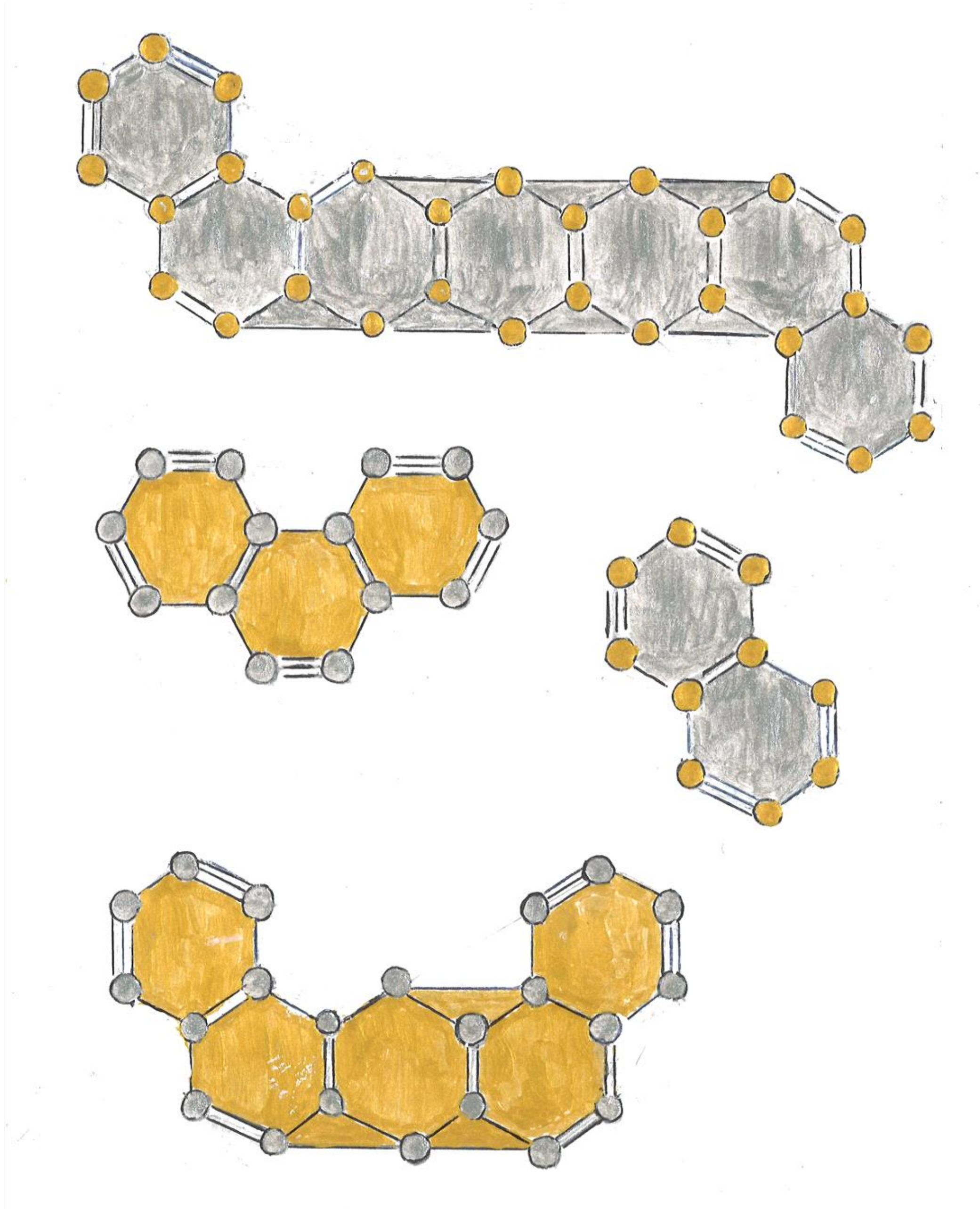

Figure 6. Non-aromatic (non-toxic) polycyclic chains, formed by joined carbon and silicon hexagons.

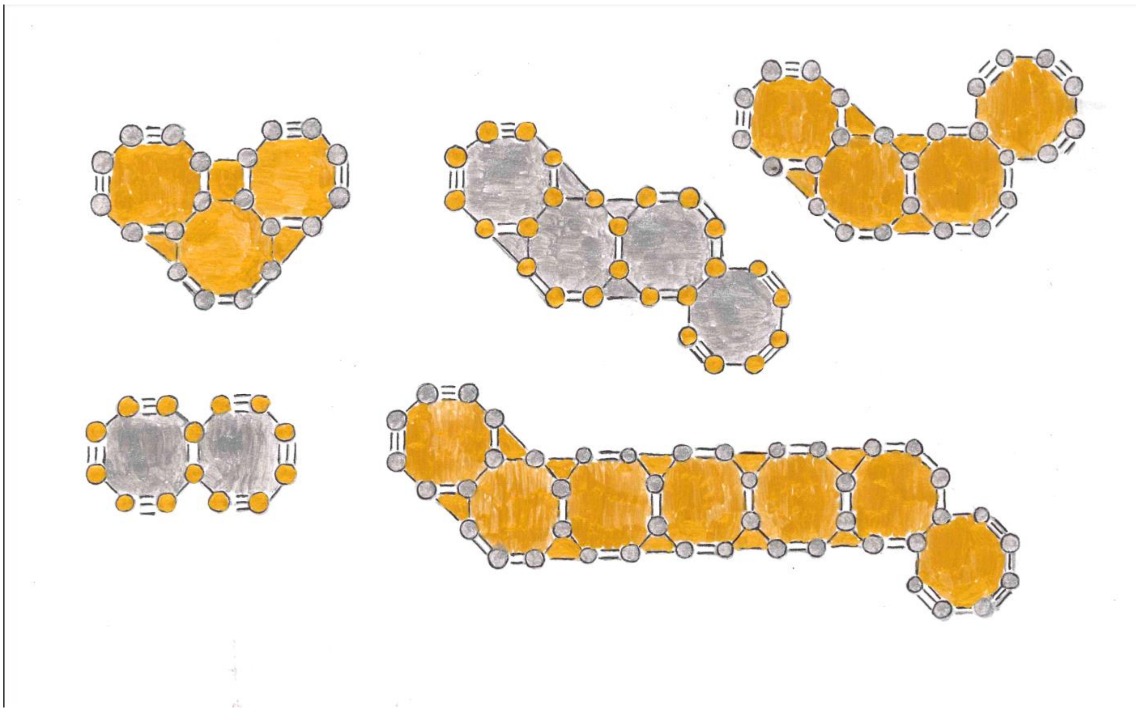

Figure 7. Nonlinear chains, formed by cycles [18] carbon and silicon.

Conclusions

We have seen that when the dopant metals have a high resistivity, the T_C seems to take higher values than when they have a low resistivity; likewise, when the rings are formed by metals with high electronic resistivity, when they are made up of two or three metals, the average resistivity is lower than when these rings are made up of only one kind of metal; the other components being non-metals or semi-metals. In any case, we do not have resistivity values per atom, which would imply not taking into account the collision times. On the other hand, if we could count on the effective mass, since this will depend on the density of electrons per atoms.

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