

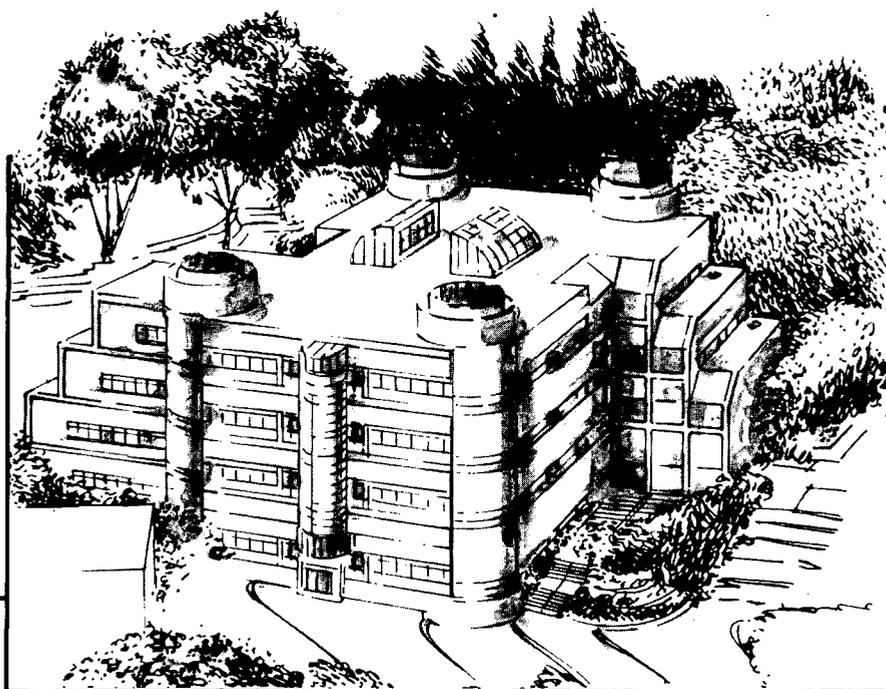
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A correlation between T_c and electronegativity difference in high-temperature superconductors *

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For compound superconductors a correlation is found between superconducting critical temperature, $T_c \geq 10K$ and difference in Pauling's electronegativity, ΔN , between certain elements in the structure. For all the high- T_c oxide layer-structure compounds, T_c increases linearly with ΔN with the T_c corresponding to the extrapolation to $\Delta N=0$ being $\sim 30K$. For all others, the more three-dimensional structures, T_c also appears to be related to ΔN but forms a completely separate correlation curve at lower values of T_c .

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The correlations are illustrated by Fig. 1, the linear relationship for high- T_c layer compounds ($n(\text{CuO}_2)=2$) (a) and the separate correlation curve (b) for conventional more three-dimensional compound superconductors. For all of the compounds ΔN represents $|\sum N(\text{anion}) - \sum N(\text{cation})|$ where N is electronegativity from Pauling's scale. For example the $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$ structure consists of two CuO_2 layers, one CuO layer plus bridging oxygens, O_c , between the CuO_2 and CuO layers. The electronegativities for O and Cu are 3.44 and 1.90 respectively and ΔN is taken as $(3.44 \times 2 - 1.90)3 = 14.94$ as shown in Table I. Since the cations, Y and Ba, are only weakly involved in the layer coupling, their electronegativities are not involved. $\text{Tl}_2(\text{CaBa}_2)\text{Cu}_2\text{O}_{8+\delta}$ has double boundary layers of TlO which, together with O_c , form two units of TlO_2 for the calculation of ΔN . $\text{Bi}_2(\text{CaSr}_2)\text{Cu}_2\text{O}_{8+\delta}$ has a plane of easy cleavage between two layers of BiO . Its coupling unit is thus reduced to two units of $\text{BiO}_{1.5}$. For $\text{Y}_2\text{Ba}_4\text{Cu}_7\text{O}_{15+\delta}$ there are alternate single (CuO) and double ($(\text{CuO})_2$) boundary layers in the stacking sequence, which individually gives CuO_2 and $(\text{CuO})_2$ coupling units, respectively in $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$ and $\text{YBa}_2\text{Cu}_4\text{O}_{8+\delta}$. Together, their coupling to the neighboring CuO_2 layers is in competition due to the stacking sequence of Cu being out-of-phase. Therefore the net coupling for this structure is only the coupling unit difference between $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$ and $\text{YBa}_2\text{Cu}_4\text{O}_{8+\delta}$. Table I shows all the superconducting compounds and the corresponding anion-cation groups that were used for the calculation of ΔN .

An interesting feature of correlation (a) is that it extrapolates at $\Delta N=0$ to $\sim 30\text{K}$ which could be considered the weak coupling limit of the conventional BCS theory for superconductivity. This suggests that either the high- T_c two-dimensional (2-D) superconductors involve an additional mechanism or the BCS electron-phonon mechanism is somehow enhanced in proportion to ΔN . One possibility would be a hybridized mechanism of BCS mechanism and a polaron- or bipolaron-like mechanism. ΔN could be considered as a driving force for the vibration of a dynamically polarized resonating-lattice [18]. Increasing of ΔN would imply an increase of the effective mass of the paired charge carrier to become heavy boson and/or of the electron-phonon coupling parameter λ to the intermediate-strong coupling range, which in turn would yield a higher T_c .

The correlation curve (b) has a linear portion, which contains mainly oxide

superconductors, as well as a non-linear part, which contains the conventional compound superconductors which were selected as the compounds with the highest T_c s in their structural group. For example, PbMo_6S_8 has the highest T_c (15.2K) in all Chevrel phase superconductors and its ΔN , normalized to one unit of anion, is $N(\text{S}) - 1/8 N(\text{Pb}) - 6/8 N(\text{Mo}) = 2.58 - 1/8 \times 2.33 - 6/8 \times 2.16 = 0.67$. Note that all three perovskite-related 214 phases, i.e., $(\text{La}_{1.85}\text{Sr}_{0.15})\text{CuO}_{4-\delta}$ (214-T phase), $[\text{Nd}_{1.3}(\text{Ce}_{0.2}\text{Sr}_{0.5})]\text{CuO}_{4-\delta}$ (214-T* phase) and $(\text{Nd}_{1.85}\text{Ce}_{0.15})\text{CuO}_{4-\delta}$ (214-T' phase), as well as the perovskite 113 phase, i.e., $(\text{Ba}_{0.6}\text{K}_{0.4})\text{BiO}_{3-\delta}$ fit in the linear portion of correlation curve (b) rather than in correlation curve (a) for high-temperature superconductors (HTSC). This may imply that the superconducting mechanism for these materials is more closely related to the conventional BCS phonon mechanism.

Before doping these phases have in common unaltered octahedrons, e.g., CuO_6 and BiO_6 , in their parent structures whereas the HTSC in curve (a) all have 2-D CuO_4 squares in common which share corner oxygens to form CuO_2 layers. This 2-D layer could have a planar breathing mode vibration of oxygen in its sublattice, which could be further stabilized by coupling to that in the boundary layer(s), in the perpendicular direction, through the bridging oxygens. Another common feature of all the HTSCs on curve (a) is the existence of boundary layer(s) with two bridging oxygens on either side. The Macro-Resonance-Cell (MRC) description for the high-temperature oxide superconductors [18] emphasizes the fact that the cations in the boundary layer(s) have two or more possible oxidation states as does Cu in the CuO_2 layers. When oxygen vibrates in a breathing mode in its sublattice, these cations could vary their oxidation states in response (a collective excitation of the ion lattice). Furthermore, a dynamic cooperative Jahn-Teller effect or Peierls distortion could exist in the oxygen sublattice, which in turn could open a gap in the conduction band for superconductivity. This Macro-Resonance-Lattice (MRL) could possibly serve as a host lattice for the condensation of free charge carrier pairs (bosons) at and below T_c . The linear correlation between T_c and ΔN might imply that the stability of the MRL (condensed bosons) is directly related to ΔN . The superconductors lying in curve (b) could also have a MRL. However, since their breathing units would be mostly three-dimensional, e.g. TiO_6 octahedrons in spinel LiTi_2O_4 , PbS_8 cubes in Chevrel PbMo_6S_8 , BiO_6 octahedrons in perovskite $(\text{Ba}_{0.6}\text{K}_{0.4})\text{BiO}_{3-\delta}$, etc., the coupling effect might be less effective or inoperative, therefore, resulting in a less stable MRL and lower T_c s.

Acknowledgment

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Figure Caption

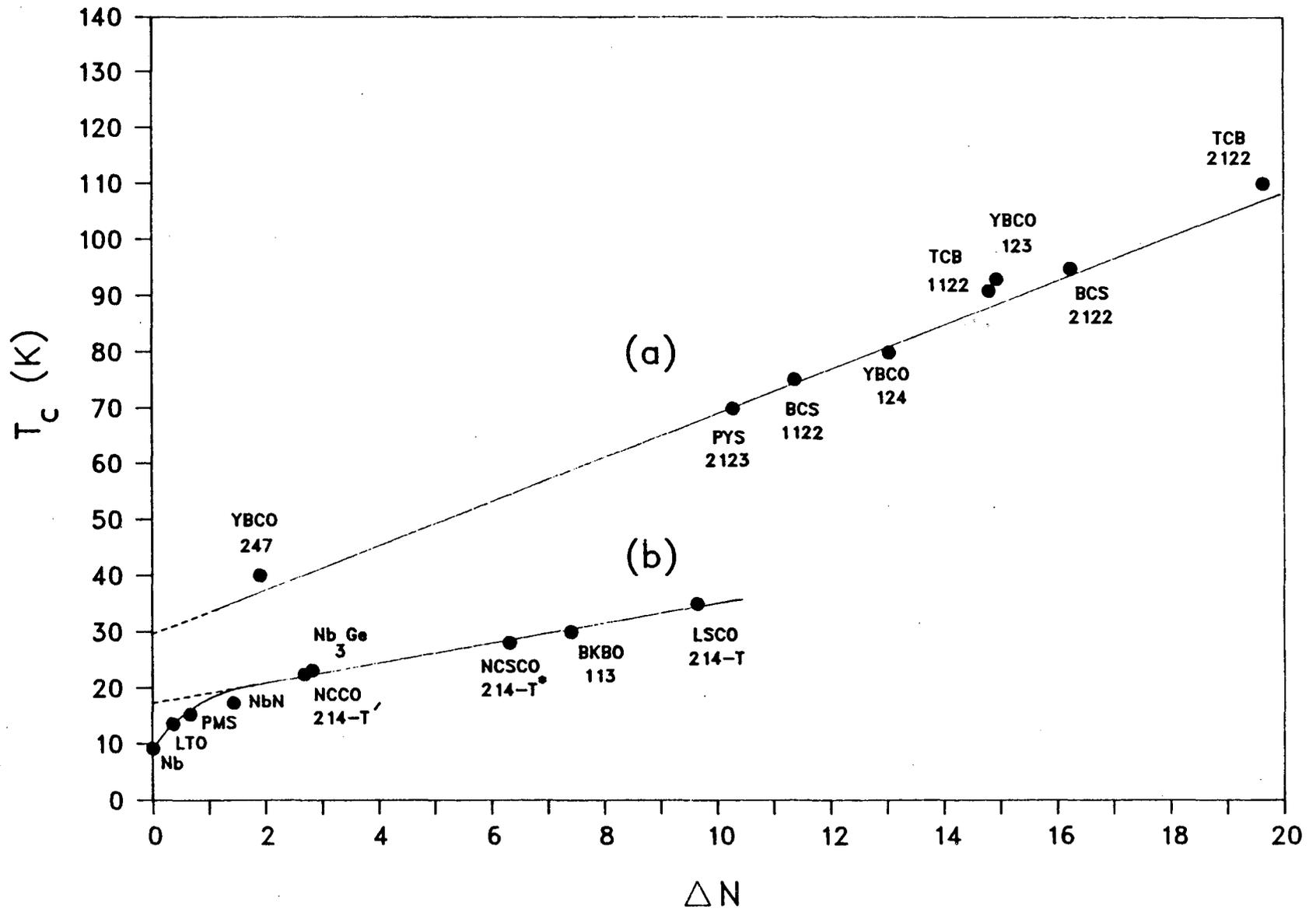
Fig. 1: Correlation between T_c and ΔN , Pauling's electronegativity difference of certain cations and anions in compound superconductors, separates them into two groups: line (a) for high-temperature oxide superconductors with layered structure containing two layers of CuO_2 and boundary layer(s); curve (b) for those conventional compound superconductors ($T_c > 10\text{K}$) having the highest T_c in their own structural group but containing no boundary layer(s) and having three-dimensional characteristics.

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Table I. Compound superconductors ($T_c > 10\text{K}$) with their T_c and elements used for calculating ΔN ($\Delta N = |\Sigma N(\text{anion}) - \Sigma N(\text{cation})|$), where N is the electronegativity in Pauling's scale.

name/ structural group	superconducting material	$T_c(\text{K})$	Ref.	elements used for the calculation of ΔN ($\delta=0$)	ΔN
TCB-2122	$\text{Tl}_2(\text{CaBa}_2)\text{Cu}_2\text{O}_{8+\delta}$	110	1	$\text{CuO}_2 + (\text{TlO}_2 + \text{TlO}_2) + \text{CuO}_2$	19.64
BCS-2122	$\text{Bi}_2(\text{CaSr}_2)\text{Cu}_2\text{O}_{8+\delta}$	95	2	$\text{CuO}_2 + (\text{BiO}_{1.5} + \text{BiO}_{1.5}) + \text{CuO}_2$	16.24
YBCO-123	$\text{Cu}(\text{YBa}_2)\text{Cu}_2\text{O}_{7-\delta}$	93	3	$\text{CuO}_2 + (\text{CuO}_2) + \text{CuO}_2$	14.94
TCB-1122	$\text{Tl}(\text{CaBa}_2)\text{Cu}_2\text{O}_{7-\delta}$	91	4	$\text{CuO}_2 + (\text{TlO}_2) + \text{CuO}_2$	14.80
YBCO-124	$\text{Cu}_2(\text{YBa}_2)\text{Cu}_2\text{O}_{8+\delta}$	80	5	$\text{CuO}_2 + (\text{CuO} + \text{CuO}) + \text{CuO}_2$	13.04
BCS-1122	$\text{Bi}(\text{CaSr}_2)\text{Cu}_2\text{O}_{7-\delta}$	75	6	$\text{CuO}_2 + (\text{BiO}) + \text{CuO}_2$	11.38
PYS-2123	$(\text{Pb}_2\text{Cu})(\text{YSr}_2)\text{Cu}_2\text{O}_{8+\delta}$	70	7	$\text{CuO}_2 + (\text{PbO} + \text{Cu} + \text{PbO}) + \text{CuO}_2$	10.28
YBCO-247	YBCO(123+124)	40	8	YBCO(123) - YBCO(124)	1.90
LSCO-214T	$(\text{La}_{1.85}\text{Sr}_{0.15})\text{CuO}_{4-\delta}$	35	9	$\text{LaO} + \text{CuO}_2 + \text{LaO}$	9.66
BKBO-113	$(\text{Ba}_{0.6}\text{K}_{0.4})\text{BiO}_{3-\delta}$	30	10	BaBiO_3	7.41
NCSCO-214T*	$[\text{Nd}_{1.3}(\text{Ce}_{0.2}\text{Sr}_{0.5})]\text{CuO}_{4-\delta}$	28	11	$\text{Nd} + \text{CuO}_2 + \text{SrO}$	6.33
A15	Nb_3Ge	23.2	12	$\text{Ge}(\text{Nb}_3)$	2.81
NCCO-214T'	$(\text{Nd}_{1.85}\text{Ce}_{0.15})\text{CuO}_{4-\delta}$	22.5	13	$\text{Nd} + \text{CuO}_2 + \text{Nd}$	2.70
B1	NbN	17.3	14	$\text{N}(\text{Nb})$	1.44
Chevrel-PMS	PbMo_6S_8	15.2	15	$\text{S}(\text{Pb}_{1/8}\text{Mo}_{3/4})$	0.67
Spinel-LTO	LiTi_2O_4	13.7	16	$\text{O}(\text{Ti}_2)$	0.36
W	(Nb)	9.2	17	$\text{Nb}(\text{Nb})$	0



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