

Carbon Allotropes Database

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Nowadays the modeling of new carbon allotropes is very popular. Mistakes in classification and naming of carbon allotropes are almost inevitable due to vast amount of unorganized data. Additionally, a lot of allotropes were re-discovered many times by different research groups. Inspired by this problems we created **SACADA - Samara Carbon Allotrope Database**.

We searched the literature for carbon allotropes with three databases, Web of Science, Scopus and Scifinder, crossing all the references, extracting the coordinates when available, or asking the authors to provide them...or guessing from the figures and the scant data available in the older references. We examined more than 500 papers (most of them published after 2000) collecting geometrical data (as crystallographic coordinates) for more than 600 allotropes. With the help of the suite of programs for topological crystal chemical analysis ToposPro[1] we compared them in order to find duplicates (often called by different names, as mentioned above) finally extracting 281 unique 3-periodic carbon allotropes. They were of 255 distinct topological types, i.e., different underlying nets: an allotrope containing an inserted C≡C triple bond that just extends the length between nodes 3 or 4-coordinated has the same underlying net as the parent with direct single C-C bonds.[2] We assigned a unique name to each, following the same strategy adopted in the analysis of coordination networks: first, if available, we used the three-letter name in RCSR,[3] then other names already in use for coordination networks. For the remaining 125 we adopted a compact name consisting of the list of the inequivalent 3- and/or 4-coordinated nodes, a capital letter "T" for 3-periodic and an ordering number. The maximal space group symmetry of the nets were found using Systre from the Gavrog package.[4]

All the data are collected and organized as a web-table in **SACADA** (Samara Carbon Allotrope Database) at <http://sacada.sctms.ru/>. Almost all carbon allotropes are, of course, hypothetical and predicted on the basis of mathematical (topological) reasoning or quantum mechanical calculations, mostly of the DFT type. Different DFT packages have been used to model allotropes and calculate different properties, leading sometimes to results that are not easily comparable.

To help the researcher, we decided to re-compute all collected allotropes using the same level of approximation to extract the relative energy per atom, with respect to diamond. All computations were performed using the VASP program suite[5], with an energy cutoff of 400 eV, GGA-PBE pseudopotential; the tolerance for ionic relaxation was set at 10^{-6} eV. We allowed full relaxation. The relevant k-mesh was generated automatically, as implemented in VASP. The maximal symmetry of optimized structures (output in space group P1) was found using PLATON.[6] Some calculations in the original papers may be better than ours; the virtue of what we have done is that it is a uniform comparison. Other physical properties have been extracted as well and the coordinates of the nets are downloadable for comparison.

The distribution of coordination numbers in the allotropes in the literature is shown in Figure 1, together with the distribution of allotropes by computed energy, the computation performed as described above.

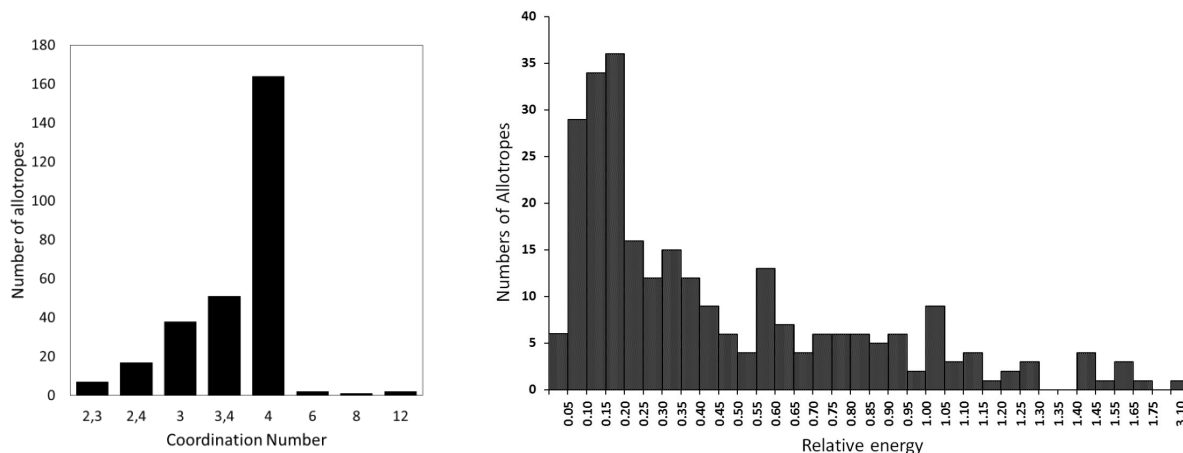


Figure 1 : Distribution of allotropes by coordination numbers (left). Calculated energies (method described in text), eV/C atom relative to diamond (right).

Most of the proposed allotropes are 4-coordinated, while the relative energy plot shows that all but 6 have an energy higher than 0.05 eV/C relative to diamond. These six structures are all polytypes or crossed graphene sheets. The highest energy (3.10 eV) is observed, not surprisingly, for the **nbo** net[3], where all the nodes have square planar geometry.

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