s9.m3.p23 **Supramolecular structure of [H(phen)₂][Ni(C₂B₉H₁₁)₂].**

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Keywords: bisphenanthrolinium cation, *commo*-nickelacarboranes, supramolecular interactions.

The metallacarborane sandwich complexes are of considerable interest owing to their possible applications as novel functional materials.

We have carried out single-crystal X-ray analysis of the title compound **1**. Formula **1** is established by x-ray analysis too. It is a first example of a supramolecular assembly with participation of the ions above.

The bis(1,10-phenanthroline)hydrogen(1) cation consists of two phen groups A and B. Both phens are essentially planar. The dihedral angle between these two planes is 25.3°. The two phen rings are held together by three hydrogen-bonding interactions. One of them is N-H...N type with N...N distance of 3.103(1) Å. Two more interactions take place between the two phens of each cation. One ortho hydrogen of each phen (that adjacent to the nitrogen atom interacting with the acidic proton) comes close to the free nitrogen atoms of the counter ligand giving rise to the formation of a hydrogen bond C-H...N. The distances between the carbon and nitrogen atoms are 3.182(1) and 3.285(1) Å. The corresponding H...N distances are 2.356(8) and 2.481(8) Å.

The ring A and the ring B of the neighbouring cations are alternately stacked along the crystallographic *b* axis, forming an infinite columnar stack. The normal to the mean cation plane is parallel to the stacking axis. There are the $\pi..\pi$ interactions between planar aromatic cation fragments of the offset type. In the columns the nearest plane separations are of about 3.45 Å (~1/2 *b*).

The anion has the expected overall geometry in which two {NiC₂B₉} icosahedra are linked *via* a common Ni atom. The carbon atoms are disordered among the two η^5-{C₂B₃} faces binding to the Ni atom. The mean planes defined by the atoms of the two ligating faces are almost parallel, being inclined at 3.1° to each other. The nickel atom is 1.559 and 1.561 Å from the planes of the open carborane faces. The five atoms each of the ligating faces in **1** are, in fact, not exactly coplanar: the faces are folded in an 'envelope' conformation, the dihedral angles being 5.8 and 2.6°. The lower pentagonal belts, in contrast, approach planarity rather more closely.

The anions are packed in the gaps between the cation columns and are connected by them through close B-H...H-C contacts.

Crystal data: C₂₈H₃₉N₄B₁₈Ni, *F.W.* 684.92, monoclinic system, space group *P2₁/n*, a=19.337(3), b=6.997(1), c=25.630(4) Å, β=101.69(1)°, V=3396(1) Å³, Z=4, D_{calc}=1.339 g.cm⁻³, R_F=0.037.

s9.m3.p24 **On the isostructurality of calcium channel antagonist 1,4-dihydropyridines.**

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Keywords: drug design.

Since the early seventies 2,6-dimethyl-4-phenyl-1,4-dihydropyridine-3,5-dicarboxylates have been studied meticulously as calcium channel antagonists with potent cardiovascular/vasodilatory activity. Abundance of 1,4-dihydropyridines archived in CSD enabled us to select several groups with *similar* unit cell parameters and space groups. Naturally, their chemical *formulae* may show[1] only small differences in R, R' and/or X.
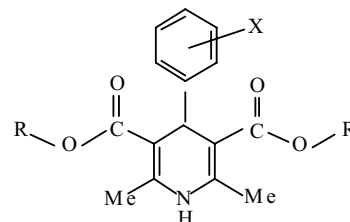
Close packing similarity of FULPEH (R= Me, R'=i-Bu, X=*m*-NO₂) with JEXKUS (nitrendipine, R=Me, R'=Et, X=*m*-NO₂) and FULPOR (R=Me, R'=i-Bu, X=*m*-O-Me), shown by *?* and $I_i(n)$ descriptors of isostructurality[2] suggests that differences either in the phenyl substituents or in the ester groups or in both, permit similar molecular self-complementarity.[3] Similarly, with R,R'=Me the methyl- and nitrophenyl derivatives remain isostructural both in *meta* (BELHAB *vs.* BELHUV, *? = 0.0015*) and *para* forms (BELHEF *vs.* BELHOP, *? = 0.0044*), respectively. The *meta* and *para* isomers differ, however, in their close packing.

FULNUV (R=Me, R'=i-Bu, X=H) and FULPAD (R=Me, R'=i-Bu, X=*o*-NO₂) are homostructural[2] with *?* =0.0017 which can be attributed to the "screened" position[3] of the nitro group. Interestingly, FULPAD and FULPEH (X=*m*-NO₂) exhibit a more relaxed form of packing similarity (unit cells are similar with differently chosen space groups: *P2₁/n vs. P2₁/c*) which deserves special attention. This kind of relationship is also found between TEHXIN (R,R'=n-Bu) and TEHXUZ (R,R'=t-Bu). Finally, isostructurality shown by BETRAM, BETKIU and BETKEQ is presented. Here the terminal trimethylmethane group in R,R'=CH₂CMe₃ is replaced by trimethylsilyl moiety in two steps. It is noteworthy, that in the last five structures X=*m*-NO₂. Descriptors of isostructurality[4] for the related structures are discussed in detail. *Grant: Hung. Research Fund, OTKA T014539.*

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