Cations Form a Ligand-Stabilized \([\text{Ga}^+\]) with an Square-to Clusters that retained the formal oxidation state of \(\text{Ga}^+\). The reaction of \(\text{Ga}^+\) with \(\text{Al}^3\) vs. \(\text{In}^+\) clustering with artention of the was a step ahead and allowed for the elimination of cation–polyether interactions. We discuss the nature of this structure which results from the conversion of the non-bonding 4s lone-pair orbitals into fully Ga-Ga-bonding orbitals and the solid-state arrangement of the ions constituting the lattice as an almost orthogonal AX₅ lattice, possibly the aristotype of any 5:1 salt.

The coordination chemistry of the Group-13-metal monocations \(\text{Ga}^+\) and \(\text{In}^+\) with ligands other than \(\pi\)-coordinating arenes is still rather in its infancy and that of \(\text{Al}^3\) is even unknown. In principle, the mixed-valence salts \(\text{Ga}[\text{AlX}_3]^{-}\) (X = Cl, Br, I)² appeared to be ideal starting materials for such chemistry. Yet, the introduction of neutral \(\sigma\)-donors led to undesired redox chemistry (comproportionation or disproportionation). In this respect, the facile access to an \(\text{In}[\text{SO}_2\text{CF}_3]^{-}\) salt³ was a step ahead and allowed for the characterization of the first \(\text{In}^+\) crown-ether complexes. However, related chemistry with \(\text{Ga}^+\) did not work and the only published compound which seemed likely to be a suitable starting material for coordination chemistry was the \([\text{Ga}_5\text{Cp}^+\text{N}]^{-}\) cluster cation—with the complication of providing one surplus equivalent of neutral \(\text{GaCp}^+\) per used \(\text{Ga}^+\) (Cp\(^+\) = C₅Me₅). The subsequent facile access to arene complexes of \(\text{In}^+\) and \(\text{Ga}^+\) salts⁴ with the non-reactive weakly coordinating anion (WCA)⁵ \([\text{Al(OR})_3]^{-}\) opened a new starting point to interesting coordination chemistry with a variety of \(\sigma\)-donors including phosphines,⁶ carbones,⁷ pyridines,⁸ and also crown ethers.⁹ In all of this, \([\text{Al(OR})_3]^{-}\) was very helpful¹⁰ for the elimination of cation–anion interactions and allowed for a predictable reaction outcome. However, due to its considerable size (diameter 1.25 nm, \(V = 0.76 \text{ nm}^3\)) and the pseudo-gas-phase conditions that the anion provides,¹¹,¹² the overall charge of such coordination compounds was expected to be limited to + 1. However, when changing to bidentate 2,2'-bipyridine (bipy) and phenanthroline (phen) as ligands, unexpectedly, the formation of indium-cluster-cation salts with planar triangles (for example, \([\text{In}_5(bipy)]^{3+}\)) and rhomboids (for example, \([\text{In}_5(phen)]^{3+}\)) that both feature strong In-In bonding was observed.¹³ Gallium, on the contrary, disproportionated in the presence of the same ligands. This was rationalized with the stronger reducing nature of \(\text{Ga}^+\) vs. \(\text{In}^+\) which, in the first case, led to reduced, non-innocent \([\text{bipy}]^3\-) ligands and only for \(\text{In}^+\) to clusters that retained the formal oxidation state of the metal.¹⁴ Concomitantly, Baines et al. reported the formation of strongly Ga-Ga-bonded, polyether-stabilized salts such as \([\text{cryptandGa}_3\text{Cl}_3]^{7+}\) \((\text{SO}_2\text{CF}_3)_2\), A. To shed light on the unclear oxidation states in materials like A, X-ray absorption spectroscopy¹⁶ and Auger-electron kinetic energy¹⁷ measurements were conducted that assigned an intermediate chemical oxidation state of + II in I. Thus, the question remained if \(\text{Ga}^+\) clustering with a retention of the oxidation state + I is also possible, given the fact that an innocent strongly \(\sigma\)-donating ligand is used. This question was recently solved by using \(\text{BuNC}\) as the ligand L, leading to the formation of the salt \([\text{Ga}_5\text{L}_5]^{4+}[\text{Al(OR})_3]^{-}\), with a square-planar central \(\text{Ga}_5\) ring. It represented the first univalent gallium-cluster cation.¹⁸

Here we report on the reaction of the \(\text{Ga}^+\) source \([\text{Ga(PhF)}_3][\text{Al(OR})_3]^{-}\) with the strong \(\sigma\)-donor but weak \(\pi\)-acceptor 4-(N,N-dimethylamino)pyridine (dmap) in ortho-difluorobenzene (oDFB). Reaction in a 2:1 ratio according to Equation (1) and storage for several weeks at −25°C afforded bright orange crystals (Figure S11 in the Supporting Information) suitable for single-crystal X-ray diffraction studies.²⁷ Measurement, structure solution, and refinement revealed the unprecedented 5:1 salt \([\text{Ga}_5\text{dmap}]^{10+}[\text{Al(OR})_3]^{-}\)₃ (Figure 1a). The bright orange color of the solid is in good agreement with the TD-DFT-calculated UV/Vis spectrum of I° (see Supporting Information).

\[
\text{Ga}_5(\text{dmap})^{10+}[\text{Al(OC(CF)}_3]_{15}^{-}\cdot 4\text{oDFB}
\]

\[
\text{Ga}_5(\text{dmap})^{10+}[\text{Al(OC(CF)}_3]_{15}^{-}\cdot 4\text{oDFB}
\]
Crystalline 1 forms reproducibly in good yield but is only stable at temperatures around or below −20 to −25 °C, and is also highly sensitive to air and moisture. In one dedicated reaction, we isolated a yield of 29% orange crystals by always maintaining a cold chain. A powder-X-ray diffractogram of this orange material is in reasonable agreement with the simulation from the single-crystal data. The NMR spectra of oDFB solutions prepared according to Equation (1) detected at −20°C showed 1H-, 13C-, 19F- and 27Al-NMR signals of the intact ligands and anion but no 70Ga resonance, probably due to the unsymmetrical environment of these quadrupolar nuclei. To elucidate possible aggregation reactions in solution, a DOSY-NMR study in o-DFB at −20°C with a stimulated-echo impulse sequence and including the non-reactive salt Nbuc[Al(OH)3] as a reference cation was performed. [Nbuc] (and hypothetic monomeric Ga(dmap)) have similar calculated cation volumes (0.379 vs. 0.376 nm³, see Table S1 in the Supporting Information) and should thus have comparable diffusion constants. A multicomponent analysis involving the reference signal at δ(H) = 3.12 ppm showed two additional dmap-based diffusion coefficients to the [Nbuc] reference velocity of 2.69 × 10⁻¹⁰ m² s⁻¹ (Figure S9), with one of them being higher (1.82 × 10⁻⁹ m² s⁻¹) and the other being lower (6.93 × 10⁻¹⁰ m² s⁻¹) than the reference velocity. One may tentatively assign the first one to a free dmap ligand and the second one to an aggregate. Thus, the formation of the crystals is possibly a stepwise cyclocyclisation of monomeric [Ga(dmap)]⁻¹ units. This conclusion is supported by electrospray-ionization mass spectra of solutions 1 in oDFB, for example, with the isotopic pattern of the signals centered at m/z = 425 for mononuclear [Ga(oDFB)(dmap−H₃)]⁺ as well as of di- and trinuclear complexes such as [Ga₂(oDFB)(dmap−dmap−(dmap−H₃))]⁺ (m/z 837), [(Ga₃(oDFB)₃)(dmap−3H₃)]⁺ (m/z 949), and [Ga₃(PhF)(oDFB)₂(dmap−dmap−H₃)]⁺ (m/z 1139; see Figure S4–S6 and discussion about the energy below).

The main and hitherto unprecedented structural element of the pentacation 1 (hereafter: 1⁺; Figure 1a) is a five-membered Ga₈ ring that includes two dmap ligands attached to each gallium atom. With rather short Ga–Ga distances of 248.75(9)–250.1(1) pm (average: 249.5(6) pm), it forms an essentially planar pentagon. Five dmap ligands are located above the plane of the ring and five below; the average Ga–N separation amounts to 2.033(4) pm (range: 2.012(5) to 2.067(4) pm) and is significantly shorter than other reported Ga–N distances of this kind, for example, in the univalent pyrazine complex Ga(pyrazine)₅[Al(OH)₃]⁻ (average: 233.0 pm). This indicates a heavy involvement of DMAP in the bonding, as indicated by the resonance structures in Figure 1b,c. The neutral digallane(4) (disil)Ga–Ga(disil), (dGa-Ga = 254 pm; disil = –C(H)(SiMe₃)) and the dumbbells of elemental gallium (246 pm) hold similar Ga–Ga distances to 1⁺. Additionally, the recent [Ga(BuNC)₆][(Al(OH)₃)] with a C₃-symmetric square-planar four-membered gallium ring also has an average Ga-Ga-separation of 246 pm.

In agreement with the selected resonance structure shown in Figure 1c, the C–N distances between the pyridine ring and the dimethylamino group are, at dC–N = 133.8(8) pm, about three pm shorter on average than in free dmap.[80] This suggests considerable charge transfer and iminium ion character (Figure 1b,c). The Ga–Ga–Ga angles in the regular and planar pentagon range from 107.05(3) to 108.49(3)° with an average of 107.93(3)°; the N–Ga–N angles are about 96.5(2)° on average. Two pairs of dmap ligands of adjoining gallium atoms are oriented in a π-stacking fashion with an average distance of 370.5(1) pm between the centroids of the pyridine planes, which places the interaction at the limit of the sums of the carbon van-der-Waals radii (340 pm). The cation structure is undistorted and shows only very few weak contacts to the anions as shown by the Hirshfeld plot in Figure S10. The pentacation structure of I is related to the known (SiX₃)₅ pentamers (X = Cl, Br, I), which, in contrast, hold a folded Si₅ ring.[21] However, it was shown that this ring may easily flatten.[22] Related phenomena were observed for the puckered (SiCl₅)₅ hexamer and its planar [SiCl₅Cl]⁺ chloride adduct.[23] The flattening was attributed to the pseudo-Jahn–Teller effect.[24] It is noteworthy that the analogues (GeX₅), directly isoelectronic to I, are unknown.

To our knowledge, an ionic AX₅ lattice constructed from an isolated pentacation A⁺ and five univalent counterions X⁻ is hitherto unknown. Formally, such structures may exist, but as exemplified shown for the compound [P₅N₅(dmap)₅]Cl₅ that contains a formal hexactagon [P₅N₅(dmap)₅]⁻ such formally highly charged system do accommodate many of the counterions in a host–guest assembly; in this example, five out of six chloride ions. So essentially, the ion packing in the [P₅N₅(dmap)₅]Cl₅ salt is that of a 1:1 salt as in [P₅N₅(dmap)₅]Cl. By contrast, I forms a truly ionic lattice. All ions in I are arranged in a hexagonal primitive lattice that is slightly distorted due to the larger size of the pentacation (Figure 2). In every layer, one out of six ions is a pentacation (see Figure 2a). Thus, each pentacation is surrounded by six anions in the plane and one anion each above and below the anions.
structure, describing a hexagonal system with orthorhombic axes in a fixed ratio (≈1:√3), as the archetype of the AX₅ structure of this radius ratio.

It was rather unexpected to observe this pentacation structure with a non-ligand-bridged central Ga₅ ring. Arranging five +1 point charges in the same manner as the formal Ga⁺ cations in the pentagon reveals an enormous Coulomb repulsion energy of 4506 kJ mol⁻¹. BP86-D3(BJ)/TZVP calculations give an overall interaction energy in the naked [Ga₅]⁵⁺ of +3930 kJ mol⁻¹, which is more favorable than the point-charge arrangement by 576 kJ mol⁻¹ (Figure 4). Divided over five Ga–Ga bonds, this suggests a covalent interaction energy of at least 115 kJ mol⁻¹ per bond (Figure 4). Yet, the monocations are still favored by thousands of kJ mol⁻¹. Thus, it appears that the coordination of the dmap ligand lifts the non-bonding 4s² electron pair at Ga⁺ to a level inducing an efficient Ga–Ga bond formation. Additionally, dmap coordination allowed for the delocalization of the unfavorable charge residing on the individual Ga⁺ cations to the ligands (see Figure 1b,c), apparently to a degree so that the Coulomb explosion of 1⁺ into five monocations [Ga(dmap)]⁺ is overcompensated. This was investigated step by step in the next section.

Atoms-in-molecules (AIM) analyses on 1⁺ and free dmap agree with this picture: The AIM charge residing on the Ga₅ basin amounts to +2.90 and that on the ten dmap ligands in 1⁺ to +2.10, indicating heavy charge transfer. Concomitantly, the charge density on the bond critical point ρBCP(CNMe₂) increases from 2.07 e⁻Å⁻³ in free dmap to an average of 2.24 e⁻Å⁻³ in 1⁺. Interestingly, the charge densities ρBCP(Ga–Ga) (average: 0.57 e⁻Å⁻³) and ρBCP(GaGa) (average: 0.44 e⁻Å⁻³) reside on a considerably elliptic bond path with average bond ellipticities ε of 0.07 (GaN) and 0.06 (GaGa). For comparison, ε(CNMe₂) is 0.13 for free, and 0.15, on average, for dmap in 1⁺. Apparently, charge delocalization through hyperconjugation is an important contribution to the bonding in the pentacation. Interestingly, the charge density ρBCP(GaGa) is higher on 1⁺ than that on an isolated Ga₅ unit calculated on the same level: (0.44 (average) vs. 0.30 e⁻Å⁻³). Moreover, we note that, compared to 1⁺, the Si–Si bond in [Si₂Cl₅]⁻ has a slightly higher charge density (0.62 e⁻Å⁻³) but much lower ellipticity (0.01).

The reaction energetics (∆Hᵣ) of the components of 1⁺ were calculated with BP86-D3(BJ)/TZVP starting from five Ga⁺ cations, ten dmap ligands, and four oDFB solvent molecules as the zero point of energy (Figure 4). A first reaction that gives five monomeric complexes [Ga(dmap)]⁺ and four non-bonded oDFB molecules delivers 2272 kJ mol⁻¹. If two of these [Ga(dmap)]⁺ monomers are connected to form a dimer dication [Ga₂(dmap)]²⁺, ∆Hᵣ rises by 74 kJ mol⁻¹. The more monomeric units are connected and the more the charge of the aggregate ions increases, the less favored the complex becomes (stepwise energy changes: +146 to +285 kJ mol⁻¹; Figure 4). Yet, the pentacation arrangement becomes more stable by −265 kJ mol⁻¹ when four solvent molecules oDFB, as observed in the asymmetric unit of the crystal structure of 1, were added. However, from all starting points, five monocations [Ga(dmap)]⁺ (and four non-coordinated oDFB solvent molecules) are the most
favored arrangement on thermodynamic grounds according to these $\Delta_f^\circ$ calculations.

This trend will even be more pronounced if one considers $\Delta_f^G$, which includes entropy loss upon aggregation. Still, one has to be reminded that these calculations are, by definition, performed in the gas phase. Investigations including Gibbs solvation energies calculated at the same level using the COSMO model and a dielectric constant of $\varepsilon_r = 14.26$ for oDFB as the solvent suggest that an aggregation of $n\text{[Ga} 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