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Verification of the properties obtained by using different pseudoatom databases. Joanna M. Bąk[a], Paulina M. Dominiak[a], [a]*Chemistry Department, University of Warsaw, Poland*
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The aim of the current study was to test the quality of structural and electrostatic properties obtained by the use of databases of aspherical pseudoatoms: ELMAM [1], UBDB [2], Invariom [3] and new-ELMAM [4]. For the crystal structures of Ala, HisAla, His, and GlyHis, we performed the transferred aspherical atom model (TAAM) refinements [5] utilizing the databases and we checked deviations of the results from the referential values. The results from theoretical calculations, without the use of multipolar model, were treated as referential.
The structural parameters (bond lengths and angles) obtained from the TAAM refinements and the standard IAM refinements were verified against the corresponding parameters optimized in theoretical periodic calculations. For the root mean square deviations (RMSDs) see the table below.
The electrostatic potentials, dipole moments and the electrostatic energies (Ees) of interactions between dimers, estimated from the databases models, were compared to the theoretical results. Theoretical results were obtained from MP2 calculations for isolated dimers, and from multipolar model fitted to CRYSTAL06 structure factors. For all the studied models we showed correlations and RMSDs of the electrostatic properties, as well as, quantities of the electrostatic potential mapped on the isosurfaces, according to Politzer [6].
The database models were compared to the experimental multipolar high resolution refinement of HisAla and Ala. For these we showed differences in anisotropic displacement parameters (ADPs), and correlations of deformation electron density maps among the models.

RMSDs	UBDB	Invariom	New ELMAM	ELMAM	IAM
Bond lengths [Å]	0,03	0,03	0,02	0,04	0,12
Angles [°]	2	2	2	3	2
Ees [kJ/mole] Ees(MP2) as referential	UBDB	Invariom	New ELMAM	ELMAM	Crystal
	26	35	33	35	28
Dipole moment [D]	2	1	4	2	3
Ees [kJ/mole] Ees(CRYSTAL06) as referential	UBDB	Invariom	New ELMAM	ELMAM	Exp.
	15	28	24	30	31

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Electron density studies of short intermolecular halogen bonds. Ulli Englert[a], Ruimin Wang[a], Thomas Dols[a,b] and Christian W. Lehmann[b], [a]*Institut für Anorganische Chemie, RWTH Aachen University, Germany,* [b]*MPI für Kohlenforschung, Mülheim, Germany*
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Experimental electron density studies help to understand intra- and inter-molecular interactions in coordination compounds of formal composition [M(X)2(py)2] (M = Zn, Cd; X = Cl, Br; py = substituted pyridine) [1,2]. We have recently reported on five coordination polymers [3], and we now wish to communicate our results on three mononuclear compounds of similar composition. Crystals of the pseudo-tetrahedral Zn(II) Complexes ZnCl2(3,4,5-trichloropy)2, 1, ZnCl2(3-chloropy)2, 2 and ZnCl2(4-aminopy)2, 3 were studied by high-resolution X-ray diffraction, and the electron density [4,5] has been analysed by the Atoms In
Molecules approach [6]. 1 and 2 are particularly well-suited to investigate interhalogen bonding [7,8], and 3 allows a direct comparison within the same class of compounds. 1 features shortest Cl···Cl contacts of 3.19 Å, significantly shorter than the sum of the van der Waals radii which amounts to ca 3.5 Å [9,10]. For this interaction, a bond-critical point (bcp) with an electron density of 0.078 eÅ-3 is found; similar electron densities have been encountered for short non-
classical hydrogen bonds [3,11]. In 2, intermolecular Cl···Cl distances are longer and associated with a lower electron density in the bcp. This work was supported by DFG, priority program 1178, Experimental Charge Density as the Key to Understand Chemical Interactions.

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Experimental charge density study and topological analysis for metal barbiturates. Marlena Gryl, Anna Krawczuk-Pantula, Katarzyna Stadnick, *Faculty of Chemistry, Jagiellonian University Cracow, Poland*
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Experimental charge density and its topological properties provide a means for the evaluation of intermolecular interactions in the context of understanding structure-property relationship and controlling the self assembly of the molecular