Title:	Two-Coordinate Cu(I) and Au(I) Complexes Supported by BICAAC and CAAC Ligands
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Abstract:	Two-coordinate Cu(I) and Au(I) complexes supported by bicyclic (alkyl)(amino)carbene, [BICAAC-CuCl] (1), [BICAAC-CuI] (2), [(BICAAC)2Cu]+[PF6]– (3) and [(BICAAC)2Au]+[AuCl2]– (6) have been synthesized. The reaction of cyclic (alkyl)(amino)carbene, CAACcy with CuCl afforded [CAACcy-CuCl] (4) and its further reaction with KPF6 gave [(CAACcy)2Cu]+[PF6]– (5). Complexes 1–6 have been characterized by multinuclear NMR, IR and UV-Vis., spectroscopic method and high-resolution mass spectrometry (HRMS). Single crystal X-ray structure of heteroleptic complexes 1 and 4 and homoleptic complexes [(BICAAC)2Cu]+[CuI2]– (2'), 3 and 6 have also been determined. The crystal structure of these complexes confirmed linear two-coordinate geometry around the metal centers. In the solid- state, complexes 1, 2', 4 and 6 displayed C−H···M (M=Cu, Au) and weak non-covalent C−H···X (X=Cl, I) and C−H···H−C interactions. Computational calculations correlate well to the experimentally observed geometry and help elucidate the absorption characteristics type of transitions and the frontier orbitals involved in them.
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