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Formation in aqueous solution of a non-oxido V^{IV} complex with VN_6 coordination. Potentiometric, ESI-MS, spectroscopic and computational characterization.

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Streszczenie

The behaviour of the system formed by $V^{IV}O^{2+}$ ion with all-*cis*-2,4,6-trimethoxycyclohexane-1,3,5-triamine (tmca) was characterized in aqueous solution through the combined application of electron paramagnetic resonance (EPR) and UV-Vis spectroscopy, electrospray ionization mass spectrometry (ESI-MS), pH-potentiometry and DFT methods. The formation of an unusual non-oxido $[V(tmcaH_{-2})_2]$ species with VN_6 coordination, with the ligand in the bianionic form, was demonstrated. The geometry, EPR and UV-Vis spectra and electronic structure of $[V(tmcaH_{-2})_2]$ were simulated with Gaussian 09 and ORCA software and the results were compared with those of similar oxido and non-oxido vanadium(IV) species formed by other polyamine and polyol related ligands, such as 1,3,5-triamino-1,3,5-trideoxy-*cis*-inositol (taci), 1,3,5-trideoxy-1,3,5-tris(dimethylamino)-*cis*-inositol (tdci), *cis*-inositol (ino) and 1,3,5-trideoxy-1,3,5-trimethoxy-*cis*-inositol (tmci). The results indicate that $V^{IV}O^{2+}$ species are formed in acid and weakly basic solution and that $[V(tmcaH_{-2})_2]$ is observed above pH 10. In the non-oxido complex, DFT calculations suggest that the two $–NH_2$ groups are in *trans* position and that the pre-organization of the ligands favours the metal complexation and the formation of the hexa-coordinated species with VN_6 coordination.

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