Synthese und Kristallstruktur neuer 1,1,1,3,3,3-Hexaamino-1λ^5,3λ^5-diphosphazenium-Salze

Synthesis and Crystal Structure of Novel 1,1,1,3,3,3-Hexaamino-1λ^5,3λ^5-diphosphazenium Salts

Kai Landskron und Wolfgang Schnick

Department Chemie der Ludwig-Maximilians-Universität, Lehrstuhl für Anorganische Festkörperchemie, Butenandtstr. 5-13 (Haus D), D-81377 München

Sonderdruckanforderungen an Prof. Dr. W. Schnick. E-mail: wsc@cup.uni-muenchen.de

Z. Naturforsch. **54 b,** 1363–1370 (1999); eingegangen am 13. Juli 1999

Phosphazenes, Ion Exchange, Crystal Structure

1,1,1,3,3,3-Hexaamino-1λ^5,3λ^5-diphosphazenium bromide $[(NH_2)_3PNP(NH_2)_3]Br$, nitrate $[(NH_2)_3PNP(NH_2)_3][NO_3]$, and toluene-4-sulfonate $[(NH_2)_3PNP(NH_2)_3][CH_3C_6H_4SO_3]$ have been prepared by anion exchange in aqueous solution. Single crystals were obtained from acetonitrile solutions in a temperature gradient between 60 °C and room temperature. The crystal structures were determined by single crystal X-ray methods at room temperature. ($[(NH_2)_3PNP(NH_2)_3]Br$: P1, $Z = 2$, $a = 596.2(1)$, $b = 744.5(1)$, $c = 1114.4(1)$ pm, $\alpha = 108.78(1)$, $\beta = 104.18(1)$, $\gamma = 90.64(1)°$, $R1 = 0.048$, $wR2 = 0.104$; $[(NH_2)_3PNP(NH_2)_3][NO_3]$: P1, $Z = 2$, $a = 550.9(1)$, $b = 796.3(1)$, $c = 1115.7(1)$ pm, $\alpha = 94.45(1)$, $\beta = 99.55(1)$, $\gamma = 101.53(1)°$, $R1 = 0.033$, $wR2 = 0.095$; $[(NH_2)_3PNP(NH_2)_3][CH_3C_6H_4SO_3]$: $P2_1/c$, Z = 4, $a = 804.1(1)$, $b = 596.1(1)$, $c = 3218.7(3)$ pm, $\beta = 94.59(1)°$, $R1 = 0.052$, $wR2 = 0.136$). In the solid the three salts consist of discrete $[(NH_2)_3PNP(NH_2)_3]^+$ cations and their corresponding anions. The PN_4 tetrahedra in $[(NH_2)_3PNP(NH_2)_3]Br$ are staggered, while in $[(NH_2)_3PNP(NH_2)_3][NO_3]$ the eclipsed conformation is preferred. The PN_4 tetrahedra of $[(NH_2)_3PNP(NH_2)_3][CH_3C_6H_4SO_3]$ show gauche conformation.