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Wanda Sawka-dobrowolska<sup>a</sup>; Janusz Kowalik<sup>a</sup>; Tadeusz Glowiak<sup>b</sup>

<sup>a</sup> Institute of Chemistry, University of Wrocław, Wrocław, Poland <sup>b</sup> Institute of Organic and Physical Chemistry, Technical University, Wrocław, Poland

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# Absolute Configuration and Crystal Structure of a Phosphonate Analogue of Tyrosine Produced by Actinomycetes

Wanda Sawka-Dobrowolska,<sup>\*</sup> Janusz Kowalik, Tadeusz Głowiak  
Institute of Chemistry, University of Wrocław, 14 Joliot-Curie,  
50-383 Wrocław, Poland<sup>\*</sup>  
Institute of Organic and Physical Chemistry, Technical University  
50-370 Wrocław, Poland

Levorotatory 1-amino-2-(4-hydroxyphenyl)ethylphosphonic acid (TyrP) of unknown configuration is a part of hypotensive tripeptides produced by Actinomycetes<sup>1</sup> and is the only 1-aminoalkane phosphonate found so far in living organisms. Nitration of enantiomers of PheP followed by reduction of the p-nitro group and diazotization yielded enantiomers of TyrP of specific rotations +67 and -67° (c.0.9; 1n HCl). Single crystal X-ray analysis showed S configuration for dextrorotatory TyrP. Thus, natural levorotatory TyrP has the R configuration and belongs to the L series of aminoacids.

Crystal data for dextrorotatory  $C_7H_{12}NO_4P \cdot 2H_2O$ , space group  $P2_12_1$ ,  $a = 5.851(2)$ ,  $b = 7.672(2)$ ,  $c = 25.145(6)$  Å,  $Z = 4$

The crystal structure has been determined by direct methods and was refined anisotropically to  $R = 0.044$  for 1337 MoK $\alpha$  reflections. The molecule takes a trans-gauche configuration around the central C <sup>$\alpha$</sup> -C <sup>$\beta$</sup>  linkage. One of the interesting aspects of this crystal structure is the hydrogen-bonding pattern. The phosphate protons are located on the 2 rotation axis parallel to  $a$ . The phosphate groups are arranged about the 2 axis and are bound together through the P-O...H...O-P short hydrogen bonds (2.496(4), 2.554(4) Å) to form a dimer.

1 H.Kasa, M.Yamata, T.Koguchi et al., Eur.Pat.Appl.0.061.172(1982)