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Crystallographic data of carboxylic acids and carboxyamides of picoline and pyrazine derivatives.

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Crystal structures of mono-acids and amides of planar six-membered ring compounds have been reported; for example, benzoic acid (Sim, Robertson & Goodwin, 1955), benzamide (Penfold & White, 1959), nicotic acid (Wright & King, 1953), nicotinamide (Wright & King, 1954) and α-pyrazinamide (Takaki, Sasada & Watanabé, 1960). Systematic X-ray examinations on related compounds have been attempted to see relationship among these crystals in molecular arrangement and in hydrogen bond system.

Crystallographic data has been found for picolinic acid, picolinamide, pyrazinic acid and other modifications of pyrazinamide. The lattice constants and the space groups were obtained from oscillation and Weissenberg photographs (Table 1):

Table 1. *Crystallographic data of carboxylic acids and carboxyamides of picoline derivatives*

	Picolinic acid $C_6H_5O_2N$	Pyrazinic acid $C_5H_4O_2N_2$	Picolinamide $C_6H_6ON_2$	β-Pyrazinamide $C_5H_5ON_3$	γ-Pyrazinamide* $C_5H_5ON_3$
M.p. (°C.)	135–137 sub.	213 decomp.	107–108	187–189	185–189
a	13·97 Å	11·37 Å	16·29 Å	10·70 Å	10·84 Å
b	3·84 Å	6·46 Å	7·15 Å	3·73 Å	3·75 Å
c	10·62 Å	7·38 Å	5·22 Å	14·38 Å	7·20 Å
β	107·9°	—	99·8°	101·7°	106·9°
V	542·5 Å^3	541·7 Å^3	599·7 Å^3	561·9 Å^3	280·1 Å^3
Space group	$P2_1/a$	*Pnma* or *Pna*	$P2_1/a$	$P2_1/a$	*Pa*
Z	4	4	4	4	2
D_c (g.cm.$^{-3}$)	1·51	1·52	1·35	1·45	1·46
D_o (g.cm.$^{-3}$)	1·48	1·53	1·4	1·45	1·46

* Takaki *et al.* (1960) named this modification β.

(I) *Picolinic acid*, crystallized in rectangular form by sublimation, showing frequently twinning.

(II) *Picolinamide*, recrystallized from ethanol solution at 0 °C.

(III) *Pyrazinic acid*, crystallized from aqueous solution at room temperature. The crystal turned slightly red by oxidation.

(IV) *Pyrazinamide*, at least four forms. α-form, obtained from alcoholic solution at room temperature (Takaki, Sasada & Watanabé, 1960). β-form, obtained in needle from alcoholic solution at about 0 °C. γ-form, obtained from melt in rectangular shape. δ-form, silvery granule, obtained by pouring hot nitrobenzene solution of this material at 80–140 °C. into tetrachloromethane at room temperature and confirmed by using Debye method. Physicochemical research on these modifications is in progress.

The existence of several modifications of carboxyamides found in the above-mentioned experiments will probably be due to the difference of the possible linking configurations of hydrogen bond systems.

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Kristallstruktur von β′ Cu–12% Al.

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Die Frage der Kristallstruktur der martensitischen β′ Phase der eutektoiden Legierung in dem System Cu–Al bedarf immer noch einer genaueren Klärung (Hunger & Dienst, 1960; Tarora, 1949). Martensitische Phasen entstehen im allgemeinen durch kleine Schubverzerrungen des ursprünglichen Gitters. Aus diesem Grunde sind die Ergebnisse von Hunger & Dienst (1960) zweifelhaft, da die von ihnen gefundenen Gitterkonstanten eine beträchtliche Umordnung erforden würden. Aus den bekannten Gitterkonstanten der β_1 Phase (Tarora, 1949) und den