THE FORMATION OF AN ISOMERIDE OF NEOERGOSTEROL BY THE PYROLYSIS OF ERGOPINACONE.

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Ergopinacone (14 g.) prepared from ergosterol (24 g.) according to the directions of H. H. Inhoffen(1) was subjected in portions of 1 g. to decomposition at 190° under the pressure of 0.15–0.25 mm. followed by the immediate distillation at 210–250° under 0.001–0.01 mm. Crystallization of the distillate from ethanol by adding water yielded crude neoergosterol (5.8 g.) melting at 129–134° (corr.). The crude neoergosterol (3 g.) was acetylated with acetic anhydride and the product was fractionally recrystallized from acetone. From the less soluble part pure neoergosteryl acetate (0.66 g.) was obtained in needles melting at 123.5–124° (corr.) (Found: C, 82.49, 81.90; H, 10.41, 10.36. Calculated for $C_{29}H_{42}O_2$: C, 82.41; H, 10.02%). Windaus(2) and Inhoffen(1) give melting point 122–123°. From the more soluble part another substance (0.7 g.) forming fine prisms melting at 108–109° (corr.) was obtained. It gave the same analytical results as neoergosteryl acetate (Found: C, 82.33, 82.24; H, 9.96, 10.35. Calculated for $C_{29}H_{42}O_2$: C, 82.41; H, 10.02%). Its melting point did not rise on further recrystallization. The mixtures of this substance with neoergosteryl acetate melted at 105–108° (corr.) and at 106–115° (corr.) according as the portion of the latter was smaller and greater. Thus it was shown that the new substance is the acetate of an isomeride of neoergosterol, which the authors call "iso-neoergosterol." Hydrolysis of the acetate (100 mg.) melting at 108–109° with alcoholic potash and recrystallization of the product from methanol gave free iso-neoergosterol (58 mg.) in prisms melting at 138–139° (corr.) (Found: C, 84.63, 84.43; H, 10.47, 10.87. Calculated for $C_{27}H_{40}O$: C, 85.19; H, 10.60%).

The crude neoergosterol (1 g.) was then recrystallized from ethanol. From the less soluble part pure neoergosterol (0.4 g.) was obtained, melting point 152–153° (corr.) (Found: C, 84.59, 84.65; H, 10.84, 11.06. Calculated for $C_{27}H_{40}O$: C, 85.19; H, 10.60%). Windaus and Inhoffen give melting point 151–152° (corr.). By the recrystallization of the more soluble part from methanol iso-neoergosterol (0.4) was obtained in prisms melting at 138–139°

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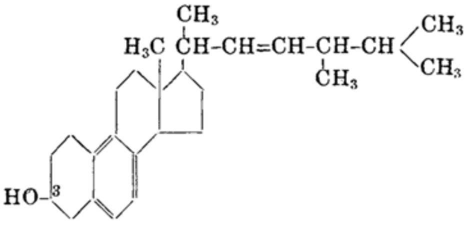
(1) *Ann.*, **497** (1932), 130.

(2) Windaus and Borgeaud, *Ann.*, **460** (1928), 235.

(corr.) alone or in admixture with the specimen from the acetate (Found: C, 84.47; H, 10.99. Calculated for $C_{27}H_{40}O$: C, 85.19; H, 10.60%).

If iso-neoergosterol is demonstrated as the stereoisomeride of neoergosterol with regard to the carbon atom 3, it may be concluded that the carbon atom 3 takes part in the formation and the pyrolytic decomposition of ergopinacone and some light will be thrown on the yet unexplained chemical structure of the dimolecular derivative of ergosterol.



Neoergosterol

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