06.2-12 STRUCTURE/TASTE RELATIONSHIPS OF ARTIFICIAL SWEETENERS. By R. Rudert, J. Buschmann, P. Luger, Institut für Kristallographie der Freien Universität Berlin, D. Gregson, Institut für Kristallographie der Universität Frankfurt, and G. Trummlitz, Dr. K. Thomaß GmbH, Biberach, F.R.G.

Because of the unsufficient taste qualities of saccharin, cyclamate, and aceulfame and the instability of aspartame new synthetic sweeteners are of great interest, especially for diabetics and persons with overweight.

Because little structural variations often change the taste from sweet to bitter it is important for the development of new sweeteners to evaluate parameters for the relation between structure and taste.

Up to now many interesting experiments were undertaken to get structure/taste relationships. However in the class of saccharin analogs no correlation with classical structure-activity parameters as log P, p, E5 or MR could be found.

On the other side it is possible to get information about the sweet/bitter relationship of sulfimid-sweeteners by analyzing the charge distribution using quantum mechanical calculations (CNDO/2). On this basis the sweetener UH-AF 50 NA [(I) (Fig. 1) was modeled and synthesized.

Fig. 1: Neutron Structure of UH-AF 50 NA

The results of the theoretical calculations on CNDO/2 basis suggested that there was a relationship between the charge distribution on the molecular surface and the sweetness of the compound. Therefore we decided to support the theoretical results by experimental investigations. We have investigated the X-ray structures of the sweetener UH-AF 50 NA and of three bitter saccharin derivatives [(II), (III), (IV)]. Moreover, the neutron structures of UH-AF 50 NA and of compound (IV) were determined to obtain X-ray-electron densities of these compounds. The crystal structures and first results of the charge density studies will be presented.