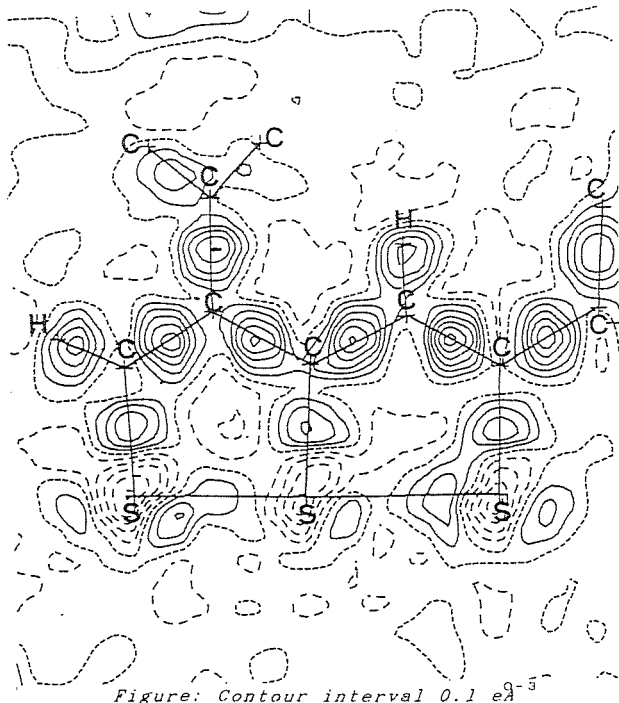


06.2-11 ELECTRON DENSITY DISTRIBUTION STUDIES OF COMPOUNDS CONTAINING SULFUR-SULFUR BOND. By Y. Wang, C.H. Chen, J.H. Liao, Department of Chemistry, National Taiwan University, Taipei, Taiwan ROC

Three sulfur containing compounds : $S_2NH[1]$, $S_2C_2H_2[2]$ and $(Me_2NCS)_2[3]$ were studied by X-ray diffraction both at 100K and 300K. The last one was studied at 143K and 300K, because of a phase transition at lower temperature. All three compounds have sulfur-sulfur bonds. Compound [1] is a cyclic molecule with 2-fold molecular symmetry; it contains many S-S bonds, with lengths 2.055, 2.071 Å. In addition, there is a non-bonding short contact distance of 2.944 Å. Compound [2] has a planar two fused five-membered ring structure with a linear S-S-S part. The two S-S lengths are significantly different, namely 2.213 and 2.509 Å. Compound [3] has a disulfide bridge with two thiouram parts related to each other by a 2-fold symmetry. The S-S distance is 2.005 Å. The X-X deformation density maps of the three molecules present strong positive density accumulations at the midpoints of the C-C and N-C bonds, a somewhat weaker one on the S-C bond and a little accumulation between sulfur atoms. A similar phenomenon was observed with the O-O bond of H_2O_2 (J.M. Savariault and M.S. Lehmann, J. Am. Chem. Soc., 1980, 102, 1298). The deformation density map of the thiothiophene plane in compound [2] is given below as an example where the bond density shows a maximum density of 0.9 and 0.4 eA^{-3} for the C-C and C-S bonds, respectively. There are positive residuals around sulfur atoms on the plane, as well as perpendicular to the plane. All three studies gave similar features around the sulfur atoms. It may indicate that the sulfur atom is no longer spherical in the promolecule.

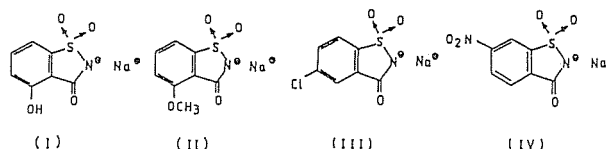


06.2-12 STRUCTURE/TASTE RELATIONSHIPS OF ARTIFICIAL SWEETENERS. By R. Rudert, J. Buschmann, P. Luger, Institut für Kristallographie der Freien Universität Berlin, D. Gregson, Institut für Kristallographie der Universität Frankfurt, and G. Trummli, Dr. K. Thomae GmbH, Biberach, FRG

Because of the insufficient taste qualities of saccharin, cyclamate, and acesulfame 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, σ , E_s or MR could be found.



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

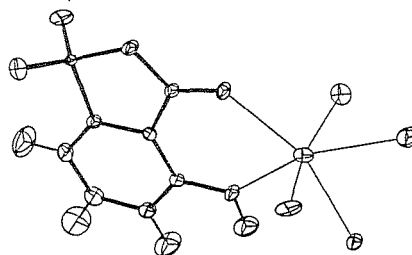


Fig. 1: Neutron Structure of UH-AF 50 NA

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 the 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-N-electron densities of these compounds. The crystal structures and first results of the charge density studies will be presented.