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WEAK [BUT ATTRACTIVE] INTERACTION BETWEEN ALIPHATIC AND AROMATIC GROUPS/ CH... π COMPLEXATION/ ITS IMPLICATION IN CHEMISTRY AND BIOLOGY

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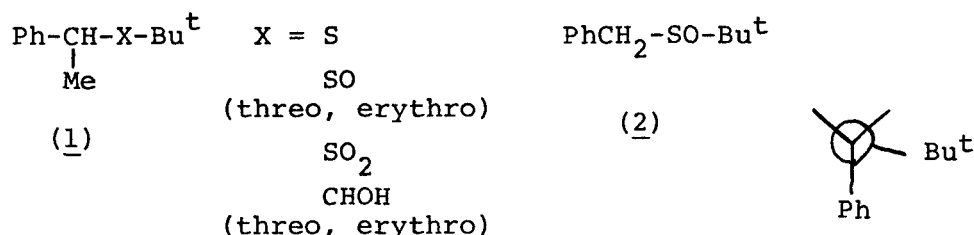
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**WEAK [but attractive] INTERACTION BETWEEN ALIPHATIC AND AROMATIC GROUPS/
CH... π COMPLEXATION/ ITS IMPLICATION IN CHEMISTRY AND BIOLOGY.**

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Evidence has been presented that Bu^t group in 1-phenylethyl t-butyl sul-
phide, sulfoxides, sulphone, carbinols (1) as well as in benzyl t-butyl sul-
phoxide (2) prefers to orient itself anti to Me and gauche to Ph group.



The experimental bases for these conformations are: 1. X-ray crystallo-
graphy, 2. NMR, 3. IR, 4. ORD/CD, 5. dipole moments, and 6. considerations of
the reaction selectivity.

From above result we must seek a possibility that an attractive interac-
tion is present between a t-butyl (alkyl) and a phenyl (π -system) group.
This is supported by a CNDO/2 calculation of a model system and by X-ray data.
The magnitude of the interaction energy is small (3.5kJ/mole), however, we
believe that the weak but attractive interaction of this kind (CH/ π complex)
plays an important role in chemical (e.g. in molecular recognition) and bio-
chemical (e.g. substrate specificity of some biopolymers) systems. Support-
ing data for this suggestion will be presented.

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