Table I. Enthalpies of Solution in MeOH and DMF and Enthalpies of Transfer at 25° [a]

Compound	ΔH_s (MeOH), kcal/mol	ΔH_s (DMF), kcal/mol	$\Delta\Delta H_s$ (MeOH $\rightarrow$DMF), kcal/mol	$\Delta\Delta H_s$ calcd, kcal/mol
Benzene	0.36	0.04	−0.3	
Biphenyl	4.3	3.7	−0.6	−0.6
o-Terphenyl	4.6	3.6	−1.0	−0.9
Naphthalene	4.5	3.9	−0.6	
Acetophenone	1.2	−0.1	−1.3	
Chlorobenzene	0.17	−0.25	−0.4	
o-Dichlorobenzene	0.34	−0.13	−0.5	−0.5
Nitrobenzene	1.0	−0.2	−1.2	
p-Nitrobiphenyl	5.6	4.2	−1.4	−1.4
p,p'-Dinitrobiphenyl	6.1	4.1	−2.0	−2.2
1-Nitronaphthalene	5.3	3.9	−1.4	−1.4
1-Chloronaphthalene	0.55	−0.19	−0.7	−0.7
o-Nitrochlorobenzene	4.7	3.6	−1.1	−1.2
m-Nitrochlorobenzene	5.6	4.4	−1.2	−1.2
p-Nitrochlorobenzene	4.2	3.0	−1.2	−1.2
2,4-Dinitrochlorobenzene	5.5	3.6	−1.9	−2.0
o-Nitroacetophenone	1.7	−0.6	−2.3	−2.1
m-Nitroacetophenone	6.6	4.5	−2.1	−2.1
p-Nitroacetophenone	6.4	4.2	−2.2	−2.1
p-Chloroacetophenone	1.13	−0.25	−1.4	−1.4

[a] All calorimetric values ±0.1 kcal/mol.

From the enthalpies of transfer of the neutral molecules the enthalpy of transfer for the various functional groups may be calculated in the following manner

$$\Delta\Delta H_s\,(\mathrm{NO_2}) = \Delta\Delta H_s\,(\text{nitrobenzene}) - \Delta\Delta H_s\,(\text{benzene})$$

$$\Delta\Delta H_s\,(\mathrm{Cl}) = \Delta\Delta H_s\,(\text{1-chloronaphthalene}) - \Delta\Delta H_s\,(\text{naphthalene})$$

$$\Delta\Delta H_s\,(\mathrm{COCH_3}) = \Delta\Delta H_s\,(\text{acetophenone}) - \Delta\Delta H_s\,(\text{benzene})$$

$$\Delta\Delta H_s\,(\mathrm{C_6H_5}) = \Delta\Delta H_s\,(\text{benzene}) = {}^1\!/_2\Delta\Delta H_s\,(\text{biphenyl}), \text{ etc.}$$

The average values for the functional groups in kcal/g group wt are as follows: $\Delta\Delta H_s$ (NO_2) = −0.8, $\Delta\Delta H_s$ (Cl) = −0.1, $\Delta\Delta H_s$ ($COCH_3$) = −1.0, $\Delta\Delta H_s$ (C_6H_5) = −0.3.

Surprisingly, substituent $\Delta\Delta H_s$ values are not dependent on the overall molecular dipole moment. This is exemplified by the three nitrochlorobenzene isomers which have (within experimental error) the same enthalpy of transfer, but quite different dipole moments. The solvents appear to interact with each functional group individually without interference from ortho substituents, which results in additive values of $\Delta\Delta H_s$.

Group enthalpies of transfer will have a variety of applications when enough data are available, including the following. (1) Calculation of $\Delta\Delta H_s$ values of molecules without resorting to direct calorimetric measurements. Suppose, for example, one wished to calculate $\Delta\Delta H_s$ (2,4-dinitrochlorobenzene)

$$\begin{aligned}\Delta\Delta H_s^{\text{calcd}}\,(\text{2,4-dinitrochlorobenzene}) = {} & -1.6\ (\text{two nitro groups}) + \\ & -0.1\ (\text{chloro group}) + \\ & -0.3\ (\text{phenyl group}) = \\ & -2.0\ \text{kcal/mol}\end{aligned}$$

The observed value of $\Delta\Delta H_s$ (2,4-dinitrochlorobenzene) is −1.9 kcal/mol. Values obtained in this manner would be a convenience in transition-state $\Delta\Delta H$ studies, and would provide an approach to $\Delta\Delta H_s$ values of unstable molecules and molecules which rapidly solvolyze in the solvents of interest. (2) Studies of the interactions between individual functional groups and various types of solvents. (3) Observation of specific interactions between the functional group and the rest of the molecule which alter electron distribution and affect the additivity of $\Delta\Delta H_s$ (for example, a strong direct resonance interaction between $-NH_2$ and $-NO_2$ in *p*-nitroaniline).

We currently are investigating other functional groups using both aromatic and aliphatic models.

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Additions and Corrections

The Proton Magnetic Resonance Spectra of Olefins. V. 3-Chloro- and 3-Methoxypropenes [*J. Amer. Chem. Soc.*, **88,** 2466 (1966)]. By Aksel A.B othner-By,* S. Castellano, S. J. Ebersole, and H. Günther, Mellon Institute, Pittsburgh, Pennsylvania 15213.

Linda Tomsyck and Professor R. Scott Pyron of Furman University have kindly pointed out to us that the values of ΔH, J^g, and J^t given for allyl chloride and allyl methyl ether are incorrect as a result of some computational error. We concur and confirm their findings that the best parameters are as follows (J in Hz and ΔH in cal). $CH_2{=}CHCH_2Cl$: J^g, 2.4; J^t, 11.6; J^{∞}, 5.5; ΔH, 958. $CH_2{=}CHCH_2OCH_3$: J^g, 2.3; J^t, 12.4; J^{∞}, 5.7; ΔH, −160.

Oxygen-17 Nuclear Magnetic Resonance Studies of Aqueous Nickel Ion [*J. Amer. Chem. Soc.*, **94,** 3419 (1972)]. By James W. Neely and Robert E. Connick,* Department of Chemistry, University of California, and the Inorganic Materials Research Division, Lawrence Radiation Laboratory, Berkeley, California 94720.

The rounded off value of $\Delta S^{\ddagger}$ in Table III should be 9 eu. The kinetic parameters obtained in the least-squares fit were 13.88 kcal and 8.7 eu for $\Delta H^{\ddagger}$ and $\Delta S^{\ddagger}$, respectively.

Neopentyl Displacement Reactions without Rearrangements [*J. Amer. Chem. Soc.*, **94,** 4184 (1972)]. By Betty

STEPHENSON, GUY SOLLADIÉ, and HARRY S. MOSHER,* Department of Chemistry, Stanford University, Stanford, California 94305.

On page 4186, footnote 26, the final clause "but the details have not yet been published" should be deleted and replaced by the following. "The details of the reaction of *R*-neopentyl-1-*d* alcohol of 50% enantiomeric purity with triphenylphosphine–carbon tetrachloride and triphenylphosphine–carbon tetrabromide to give (+)-neopentyl-1-*d* chloride and (+)-neopentyl-1-*d* bromide have been published [R. G. Weiss and E. I. Snyder, *J. Org. Chem.*, **36**, 403 (1971)]. These prior results and ours, although differing in some details, are in substantial agreement."

Stereochemistry of the Photochemical Diels–Alder Reaction [*J. Amer. Chem. Soc.*, **94**, 4378 (1972)]. By DOUGLAS A. SEELEY, Department of Chemistry, The Pennsylvania State University, University Park, Pennsylvania 16802.

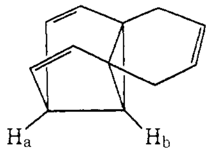
Structures **2** and **3** should be interchanged.

Pyrolytic Conversion of Bicyclo[4.2.0]octatrienes to Cyclooctatetraenes. The Tetracyclo[3.2.0.0^{2,8}.0^{5,7}]octene Pathway of Thermal Bond Reorganization [*J. Amer. Chem. Soc.*, **94**, 4398 (1972)]. By LEO A. PAQUETTE* and ROBERT E. WINGARD, JR., Department of Chemistry, The Ohio State University, Columbus, Ohio 43210.

The name tetracyclo[3.2.0.0^{2,8}.0^{5,7}]octene should be corrected to tetracyclo[4.2.0.0^{2,8}.0^{5,7}]octene in the title and at one point in the text.

Structural Consequences of 2,8 Bridging of the Semibullvalene Nucleus [*J. Amer. Chem. Soc.*, **94**, 4739 (1972)]. By LEO A. PAQUETTE,* ROBERT E. WINGARD, JR., and RONALD K. RUSSELL, Department of Chemistry, The Ohio State University, Columbus, Ohio 43210.

The dominant valence tautomeric form of **9** should be written as



and the equilibrium arrow in Figure 2 should be reversed.

Kinetic Preference between Equatorial and Axial Hydrogens in the Lithiation of Conformationally Fixed 1,3-Dithianes [*J. Amer. Chem. Soc.*, **94**, 4786 (1972). By ERNEST L. ELIEL,* ANTHONY ABATJOGLOU, and ARMANDO A. HARTMANN, Department of Chemistry, University of Notre Dame, Notre Dame, Indiana 46556.

On page 4786, footnote 7, 0.05 should read 6.05.

The Isolation and Characterization of Pure Cyclopropenone [*J. Amer. Chem. Soc.*, **94**, 4787 (1972)]. By RONALD BRESLOW* and MASAJI ODA, Department of Chemistry, Columbia University, New York, New York 10027.

Footnote 6, at the end of the paper, was inadvertently omitted. It should read as follows: (6) For a possible first isolation of crystalline cyclopropenone, see J. T. Groves, Ph.D. Thesis, Columbia University, 1969.

Possible Assignments for the Three Lowest Lying Singlets in Dialkyl Sulfides [*J. Amer. Chem. Soc.*, **94**, 4797 (1972)]. By JOAN SAMOUR ROSENFIELD and ALBERT MOSCOWITZ,* Department of Chemistry, University of Minnesota, Minneapolis, Minnesota 55455.

Equation 8 on page 4801 should read

$$B = -\langle \mathrm{b}_2 | V | \mathrm{b}_1 \rangle / (E_{\mathrm{b}_1 \rightarrow \mathrm{b}_2^*} - E_{\mathrm{b}_2 \rightarrow \mathrm{b}_2^*})$$

In Table IX, all entries under the heading *B* and under the heading Total contribution of states to rotational strength, subheading ($\mathrm{b}_2^{-1}\mathrm{b}_2^*$) only, should have a change of sign. These corrections do not alter the discussion or conclusions of the work in any way.

Preferred Conformations of the Isobutyl, Cyclopropylcarbinyl, and Oxirylcarbinyl Cations, Radicals, and Anions as Determined by Semiempirical Intermediate Neglect of Differential Overlap Calculations [*J. Amer. Chem. Soc.*, **94**, 4835 (1972)]. By WAYNE C. DANEN, Department of Chemistry, Kansas State University, Manhattan, Kansas 66502.

During the editing process the acronym INDO was expanded incorrectly in the title of this work. The title is correct as above with *overlap* having replaced *orbital*.

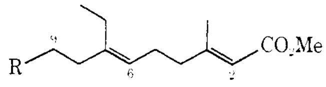
Optically Active Aromatic Chromophores. XI. Circular Dichroism Studies of Some 1-Substituted 2-Phenylcyclohexanes [*J. Amer. Chem. Soc.*, **94**, 5143 (1972)]. By LAWRENCE VERBIT* and HOWARD C. PRICE, Department of Chemistry, State University of New York at Binghamton, Binghamton, New York 13901.

In Chart I, compounds **4** and **5** and their associated data should be moved up directly under compound **3**. Both **4** and **5** are trans compounds.

In Figure 1, compounds **1** and **6** should be interchanged.

Stereoselective Synthesis of the C-18 Cecropia Juvenile Hormone [*J. Amer. Chem. Soc.*, **94**, 5374 (1972)]. By C. A. HENRICK,* F. SCHAUB, and J. B. SIDDALL, Chemical Research Laboratory, Zoecon Corporation, Palo Alto, California 94304.

Structures **10–13** should be



10, R = $-CO_2Me$
11, R = $-CH_2OH$
12, R = $-CHO$
13, R = $EtC(OMe){=}CH-$

Proof of Structure of Steroid Carboxylic Acids in a California Petroleum by Deuterium Labeling, Synthesis, and Mass Spectrometry [*J. Amer. Chem. Soc.*, **94**, 5880 (1972)]. By WOLFGANG K. SEIFERT,* EMILIO J. GAL-