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Relationship between EHT and CNDO/2 Calculations

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Multiplying EHT atomic charges and dipole moments by 0.3 gives approximate CNDO/2 values.

The widespread use of the EHT [1] and CNDO/2 [2] molecular orbital methods makes any simple relationship between their predictions useful. In the course of other work [3] EHT and CNDO/2 calculations have been carried out for a number of molecules[1]. Some relationships between the atomic charges and dipole moments calculated by the two methods are presented here.

Of the 198 atoms involved, many have the same environment (identical nearest neighbours). In these cases average values were used for the atomic charges. The set was thus reduced to twenty-four atoms, comprising fourteen carbons, four oxygens, three nitrogens and three hydrogens. The average atomic charges ranged from -1.33 to $+1.99$ (EHT method) and -0.34 to $+0.54$ (CNDO/2 method).

Twelve molecules had non-zero dipole moments. Those which have not been published previously [3] are listed in Table 1.

Table 1

Compound	Dipole Moment (Debye)		
	EHT	CNDO/2	Experimental[a]
Toluene	1.16	0.27	0.43
Methanol	4.60	1.98	1.71
Formamide	10.13	3.86	3.48

[a] McLellan, A. L.: Tables of experimental dipole moments. San Francisco and London: W. H. Freeman and Company 1963.

The results of least squares analyses of the calculated atomic charges and dipole moments are given in Table 2.

Extension of the treatment to minor environmental changes (atoms other than nearest neighbours) does not produce significant correlations.

[1] The molecules considered were barbituric acid; 5-ethyl, 5-phenyl barbituric acid; 5,5-diethyl barbituric acid; succinimide; 1-methyl succinimide; 3,5,5-trimethyl oxazolidine-2,4-dione; 3,5-dimethyl, 5-ethyl oxazolidine-2,4-dione; glutarimide; N-methyl glutarimide; β-methyl, β-ethyl glutarimide; α-ethyl, α-phenyl glutarimide; carbon dioxide; methane; formamide; methanol and toluene.

Table 2. $y = mx + c$

y	x	m	c	Average Deviation (y)
CNDO/2 charge (H, C, N, O)	EHT charge (H, C, N, O)	0.283	−0.004	±0.03 (H) ±0.04 (C) −0.03 (O) +0.09 (N)
CNDO/2 charge (C only)	EHT charge (C only)	0.279	0.007	±0.04
CNDO/2 dipole	EHT dipole	0.310	0.437	±0.24
CNDO/2 dipole	expt. dipole	1.25	−0.27	±0.19

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