

Use of semiempirical quantum chemical approaches in computation of molecular dipole moments of tropones and tropolones

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Using the MNDO, AM1 and PM3 methods, the dipole moments (m) of 28 tropones and 34 tropolones molecules have been computed. The potentials of the above approaches for the evaluation of m have been revealed. The correlations $m_{\text{exper}} = b m_{\text{theor}}$ have been established.

Keywords: semiempirical quantum chemical method, dipole moment, theory - experimental correlation, tropones, tropolones.

The tropones and tropolones are intriguing series of compounds¹⁻¹³ combining the properties of non-benzenoid aromatic and unsaturated compounds. In some instances tropone manifests itself as a ketone, while tropolone behaves as a vinyllog of a carboxyl. Tropolone derivatives are found in wood and essential oils of the *Cypress* family of plants. They exhibit an antimitotic effect, possess bacteriostatic, bactericidal and antifungal activity, and serve as antibiotics.^{4,6,8,13-16} The tropolones are possible intermediates of alkaloids biogenesis.^{6,8,12,13} Liquid crystals, ionophores, J-aggregated dyes and other advanced materials based on troponoids are known.¹⁷

Molecular recognition and bioactive compound interaction with biosubstrates receptors are preceded by chemical substance selection in accordance with the electrostatic mechanism.¹⁸⁻²¹

An important characteristic of the electric properties of a molecule and a measure of its electrostatic (ion-dipole, dipole-dipole) interaction with other molecular systems is its dipole moment. Along with the elucidation of biological effects, information on the dipole moments is required when considering the mutual influence of atoms, the electronic effects in molecules, intermolecular interactions, hydrogen bonds, tautomeric conversions, solvation and when solving other chemical and physicochemical problems.^{22,23}

The measurement of dipole moments is associated with certain experimental difficulties and is sometimes impossible to realize the relevant methods suffering from essential limitations.^{22,23} This brings up the necessity for theoretical evaluation. Vector-additive schemes are widely applied to the calculation of dipole moments.^{22–24} However, for the determination of absolute values and the direction of bond and group moments, the inclusion of homopolar dipoles and moments of non-binding electron pairs are a fairly complicated challenge.

Dipole moments have been computed by the semiempirical methods of quantum chemistry: MNDO (*Modified Neglect of Differential Overlap*), AM1 (*Austin Model*), PM3 (*Parametric Method*) with absolute errors of 0.30–0.45, 0.24–0.35, 0.38–0.40 D, respectively.^{25–39}

The present work is aimed at computing the molecular dipole moments of tropone, tropolone and their derivatives by the MNDO^{25–32}, AM1^{33–35}, PM3^{36,37} methods, as well as at establishing the correlations between the calculated and experimental values.

Such a problem has previously been solved for 64 acyclic and aromatic compounds CH_3X , $n\text{-C}_5\text{H}_{11}\text{X}$, $\text{C}_6\text{H}_5\text{X}$ with various functional groups,⁴⁰ as well as for 90 mono-, bi-, tri-, poly- and spirocyclic non-aromatic hydrocarbons, 148 three-, five-, six-, and seven-membered N-, O-, S-, Se-, B-containing unsaturated heterocycles.⁴¹

METHODS

The computations were performed using software from the MOPAC package^{42,43} with complete geometry optimization (Broyden-Fletcher-Goldfarb-Shanno function minimizer⁴⁴ involving Thiel’s fast minimization algorithm⁴⁵). The preliminary optimization was realized by the molecular mechanics method (MMX procedure⁴⁶) with software of the PCMODEL complex.⁴⁶ In the quantum chemical computations, the condition of the gradient norm not exceeding 0.02 kcal/mol/Å was preset. In some cases, a sufficient decrease in the gradient norm was achieved when the Thiel’s fast minimization routine was abandoned (the keyword NOTHIEL of the MOPAC package was applied), or under optimization with the Davidon-Fletcher-Powell method (keyword DFP),⁴⁴ or by using combined approaches involving the keywords NOTHIEL and DFP. In calculating the rotational contributions to the thermodynamic functions the symmetry number was taken to be 1.

RESULTS AND DISCUSSION

The obtained results are shown in Table I.

The molecules under study are not so large, and thus *ab initio* treatment is possible. However, the results of non-empirical calculations carried out at a low level of sophistication depend significantly, and not always monotonously, on the selected basis and consideration of the correlation effects.^{53,54} *Ab initio* computations with wide basis sets are too expensive for average size molecules.

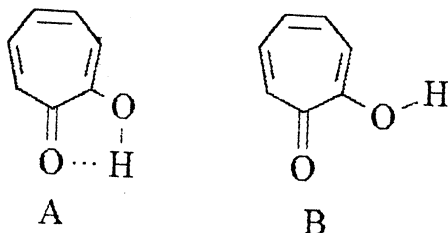
On the other hand, we have established that a correct estimation of the most important thermodynamic and molecular characteristics,^{40,41} as well as of the electronegativity, inductive and mesomeric parameters of atomic groups,⁵⁵ is possible using the MNDO, AM1 and PM3 methods in series of organic compounds belonging to different classes and with various functional groups.

Moreover, a semiempirical approach is preferential from the viewpoint of the simplicity of obtaining predictive relationships.

The correctness of the quantum chemical computations conducted in this work for the molecular electronic structure is attested by the agreement between the experimental and the computed standard gaseous-phase heats of formation for tropolone (kcal/mol):

Experiment ⁵⁶	MNDO	AM1	PM3
-37.23	-39.92	-32.87	-30.99

Also, the presence of an intramolecular hydrogen bond (HB) in the tropolone molecule^{6,8,12,13,17, 56-61} is confirmed by all the used quantum chemical methods. The enthalpy of the HB (ΔH_{HB}) was calculated as the difference between the heats of formation of the planar conformers A and B, distinguished by a 180 °-angle rotation of the O-H bond around the C-O bond.

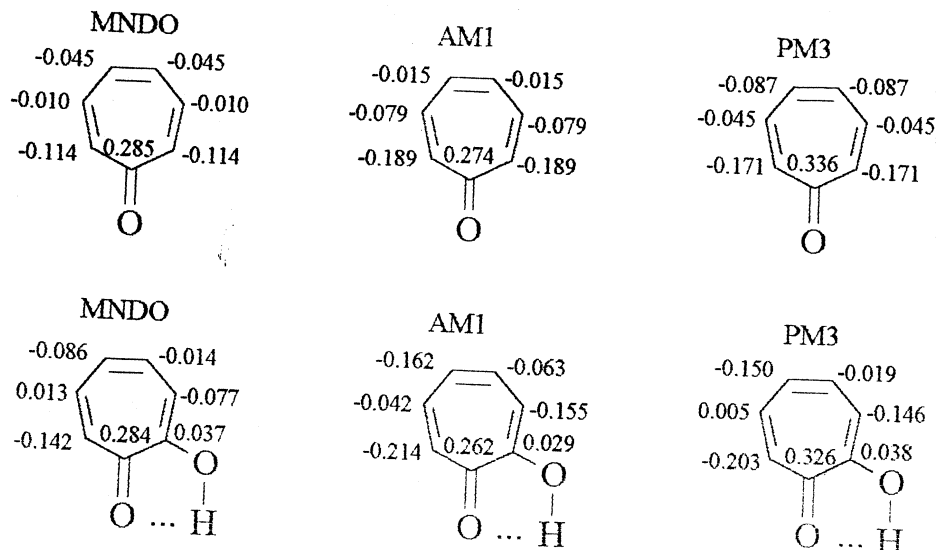


The validity of such an approach for the evaluation of the HB energy was noted in review (Ref. 62). The ΔH_{HB} values obtained are negative which corresponds to the existence of a HB. However, the used semiempirical methods do not estimate the numerical enthalpy value well: the MNDO, AM1 and PM3 methods, give the values -0.696, -4.12, -1.42 kcal/mol, respectively. The AM1 result is the best of the employed methods.

An experimental estimation of the energy of the tropolone molecule HB from IR spectroscopy data gave a value of -7 kcal/mol.⁵⁷ Subsequently⁵⁶ in the context of thermochemical considerations, the value of the HB energy was considered to lie between -5 to -7 kcal/mol, and it was pointed that the value of -7 kcal/mol was an overestimation. On the other hand, the 6-31G and 6-31G* energies of the optimized B conformer are 11.71 and 10.22 kcal/mol, respectively, above the H-bonded A conformer.⁶¹ Probably, the superposition^{63,64} and correlation⁴³ errors are insufficiently considered here in the *ab initio* computations.

A dipole moment is determined by the electron density distribution in a molecule. In the MNDO, AM1 and PM3 methods the Fockian matrix elements are represented by the electron density matrix elements. V_{mn}^B integrals describing the Coulomb interaction of the m and n atomic orbitals of atom A with the core of atom B and by two-electron integrals. The latter are included in the expression of core-core repulsion energy. The resonance integrals, integrals of overlapping and core-core repulsion energy depend (as does the charge distribution) on the internuclear distance. Therefore, reproduction of the heat of formation could serve as an indirect confirmation for the correctness of the dipole moments computations. At the same time, an unsatisfactory HB consideration presents a source of error for the both the energetic characteristics and dipole moments, although the MNDO, AM1, PM3 methods are not parameterized for a description of the HB.

The validity of the electron density distribution (and thus dipole moments) found by means of quantum computations follows also from the fact of the correlation of the regioselectivity of electrophilic substitution reactions in the tropones and tropolones series with atomic charge. The values of the electron density on the carbon atoms of the parent compounds of the two series are given as examples below.



These charges values are in agreement with the occurrence of electrophilic reactions at the 2 and 7 positions of the seven-membered troponone ring and with the processes of azo-coupling, nitrosation, nitration, sulphonation, halogenation, hydroxylation, hydroxymethylation occurring of the 3,5 and 7 positions of the tropolone ring.¹⁻¹³

At the same time, the MNDO, AM1 and PM3 methods generally underestimate the values of the molecular dipole moments for tropones and tropolones as compared to the experimental values; the condition of $m_{\text{theor}} > m_{\text{exper}}$ is met only in 17 out of 186 cases *i.e.*, 9.14% of the total data set from Table I.

Absolute error $m_{\text{theor}} - m_{\text{exper}}$ (D) have the following values:

Compound	MNDO	AM1	PM3
Tropones	from - 3.17 to 0.68	from - 2.74 to 0.58	from - 2.96 to 0.55
Tropolones	from - 3.25 to - 0.48	from - 3.00 to 0.39	from - 2.92 to 0.08

The condition $m_{\text{exper}} > m_{\text{theor}}$ would result from an underestimation of the charge separations in the molecules due to polarization of the C=O bond within the semiempirical treatment. However, the computations show a greater shift of electron density toward the carbonyl oxygen in tropone and tropolone molecules, as compared to other ketones with an exo-cyclic carbonyl group, as expressed in terms of the resonance theory by a noticeable contribution of a bipolar tropylium type structure.⁷⁻¹³



In order to prove this, the molecular electronic structure of two saturated ketones with a seven-membered ring – cycloheptanone (suberone) and its 2-hydroxy substituted product, as well as of compounds analogous to tropone and tropolone in respect to carbonyl groups located in the vicinity of two double bonds have also been computed. Among the latter were 4,5-dihydrotropone and 4,5-dihydrotropolone (differing negligibly in structure from tropone and tropolone, respectively, but having a non-planar structure in contrast to them), fluorone and 2-hydroxy-fluorone (more remote analogs of troponoids featured, however, by the planarity of their molecules). The correctness of the electron characteristic comparisons of the troponoids molecules and their more saturated seven-membered analogs results from the resemblance of the geometric parameters of carbonyl carbon atom (Table II). As the charges on the atoms and the bond orders demonstrate (Table II), the charge polarization between the ring and the carbonyl oxygen is not much stronger expressed in the troponoids than for the other molecules presented. The difference of the electronic structures of the troponoid molecules and the fluorene systems is manifested to a greater extent. This could be related to the essentially different geometry of the carbonyl point.

One of the reasons for the overestimation of the m_{exper} values seems to be the formation of tropones and tropolones donor-acceptor complexes with the solvent in which the dipole moments are measured (mainly benzene). Such a phenomenon has been observed for quinones. The molecules of 1,4-benzoquinone, 2,3,5,6-tetra-

chloro-1,4-benzoquinone, 9,10-anthraquinone are unpolar in themselves. In benzene, mesitylene, 1,4-dioxane, carbon tetrachloride, their polarity is ascribed to complexation with the solvent molecules.⁶⁵

TABLE I. The computed molecular dipole moments of tropones and tropolones and the values measured in benzene by the second Debye method^{6, 8, 12, 13, 24, 47-52}

Compound	m_{exper}/D	Temperature K	MNDO	m_{theor}/D AM1	PM3
Tropones					
Tropone (2,4,6-Cycloheptatrien-1-one)	4.1 [*]	Room	3.58	4.02	3.76
2-Phenyltropone	3.82	298	2.86	2.99	2.90
2- <i>p</i> -Methoxyphenyltropone	3.63	298	1.98	4.14	3.44
2-Aminotropone	3.78	298	2.42	2.34	2.21
4-Hydroxytropone	5.9		2.73	3.16	2.94
2-Methoxytropone	4.72	298	3.62	4.23	3.60
2-Methoxy-3-isopropyltropone	4.11	298	3.50	2.07	4.00
2-Methoxy-6-methyltropone	5.06	298	2.77	4.03	3.60
2-Mercaptotropone	4.36	298	3.39	3.21	2.59
2-Methylmercaptotropone	4.64	298	3.76	2.09	1.73
2-Bromotropone	4.94	303	4.38	4.79	4.34
3-Bromo-2-methoxytropone	3.31	298	3.54	1.76	2.28
4-Bromo-2-phenyltropone	2.73	298	2.36	2.52	2.56
7-Bromo-2-methoxytropone	5.51	298	3.52	4.43	4.43
2,7-Dibromotropone	5.27	298	4.01	4.08	4.67
3,7-Dibromo-2-phenyltropone	3.67	298	2.30	2.39	2.90
2,3-Benzotropone	3.61	298	2.95	3.23	2.98
4,5-Benzotropone	4.70	298	4.17	4.48	4.16
2-Methyl-4,5-benzotropone	4.25	298	4.05	4.04	3.76
2,7-Dimethyl-4,5-benzotropone	3.66	298	3.94	3.61	3.38
2,7-Diethyl-4,5-benzotropone	3.47	298	3.64	3.65	3.26
2,7-Dipropyl-4,5-benzotropone	3.50	298	4.01	3.47	3.34
2,7-Diisopropyl-4,5-benzotropone	3.16	298	3.05	2.78	2.55
2,7-Di- <i>tert</i> -butyl-4,5-benzotropone	2.32	298	3.00	2.49	2.62
2,7-Dihexyl-4,5-benzotroponone	2.08 ^{**}	298	2.88	2.66	2.63
2,7-Pentamethylen-4,5-benzotropone	3.09	298	2.78	3.00	2.85
2,7-Dodecamethylene-4,5-benzotropone	3.46	298	2.96	3.02	2.80
2,7-Diphenyl-4,5-benzotropone	3.69	298	2.68	2.59	2.62
Tropolones					
Tropolone (2-Hydroxy-2,4,6-cycloheptatrien-1-one,Purpurocatechol)	3.53	298	2.12	3.34	3.12
3-Methyltropolone	3.27	298	1.88	3.41	3.21
3-Isopropyltropolone (α -Thujaplicine)	3.37	298	1.84	3.35	3.15

TABLE I. Contd.

Compound	$m_{\text{exper}}/\text{D}$	Temperature K	$m_{\text{theor}}/\text{D}$		
			MNDO	AM1	PM3
4-Methyltropolone	3.88	298	2.31	3.68	3.42
4-Isopropyltropolone (b-Thujaplicine, Hinokitiol)	3.93	298	2.82	3.76	3.45
5-Methyltropolone	3.94	298	2.04	3.69	3.46
7-Isopropyltropolone	3.37	298	1.70	2.96	2.87
3-Nitrohinokitiol	6.19	298	4.85	5.13	4.63
3,5-Dinitrohinokitiol	4.63	293	4.15	3.22	4.01
5,7-Dinitrohinokitiol	4.79	298	5.45	5.96	5.81
3-Chlorohinokitiol	4.74	298	2.27	3.16	2.33
5-Chlorohinokitiol	2.70	298	1.16	2.46	2.42
7-Chlorohinokitiol	4.38	298	2.71	4.26	3.67
3,7-Dichlorohinokitiol	4.46	298	2.07	2.94	2.34
3-Bromotropolone	3.91	298	2.64	3.36	2.86
3-Bromo-4-methyltropolone	4.42	298	2.05	2.90	3.11
3-Bromohinokitiol	4.40	298	1.96	2.86	2.41
3-Bromo-5-methyltropolone	4.51	298	2.11	3.74	3.25
5-Bromotropolone	2.07	298	1.15	1.78	1.74
5-Bromo-3-methyltropolone	1.95	298	1.25	1.92	1.86
5-Bromo-4-methyltropolone	2.68	298	1.39	2.30	2.19
7-Bromo-3-methyltropolone	4.05	303	2.11	3.22	3.53
7-Bromohinokitiol	4.40	298	2.41	4.35	3.68
3,5-Dibromohinokitiol	4.27	306	1.02	1.27	1.35
3,7-Dibromotropolone	3.57	303	1.81	2.53	2.84
3,7-Dibromo-4-methyltropolone	4.19	298	1.80	2.58	3.19
3,7-Dibromohinokitiol	4.27	306	1.78	2.61	2.90
3,7-Dibromo-5-methyltropolone	4.27	298	1.79	2.84	3.25
5,7-Dibromo-3-isopropyltropolone	2.82	298	1.56	2.25	2.36
5,7-Dibromohinokitiol	3.14	293	1.67	3.27	2.66
3,5,7-Tribromotropolone	1.83	298	0.851	1.20	1.67
3,5,7-Tribromo-4-methyl-tropolone	3.02	298	0.681	1.26	1.91
3,5,7-Tribromohinokitiol	3.05	298	0.643	1.24	1.74
3,5'-Ditropolonyl	4.85 ^{***}	298	2.02	4.33	4.60

* Microwave spectroscopy, the "rate-of-growth" method; ** In cyclohexane; *** In dioxane

In support of the afforesaid the following should be pointed out. 1. The molecular dipole moment of 2,7-dihexyl-4,5-benzotropone was measured in cyclohexane, when complexing is impossible; the m_{exper} and m_{theor} values agree well with each other, and $m_{\text{exper}} < m_{\text{theor}}$ for all the methods (Table I). 2. The experimental (in benzene) dipole moments of 2,7-dialkyl-4,5-benzotropones (2.32–3.66 D), and 2,7-diphenyl-4,5-benzo-

tropone (3.69 D) are notably lower than in the case of 4,5-benzotropone (4.70 D) (Table I). Of the mentioned molecules, 2,7-di-*tert*-butyl-4,5-benzotropone possesses the smallest dipole moment (2.32 D). The alkyl and phenyl groups are low-polar, and their electronic effects are poorly expressed.^{55,66,67} Hence, the tendency of dipole moments changes in this series of 4,5-benzotropones is related to steric retardments in respect to complexing with benzene. The electron-donor (even if weak) properties of the alkyl and phenyl substituents^{55,66,67} are also capable of preventing complex formation.

TABLE II. Some molecular electronic structures parameters of troponoids and their analogs

Method	Charge on carbonyl oxygen atom	C= O Bond order	Angle C–CO–C
Tropone			
MNDO	−0.313	1.873	122.46
AM1	−0.320	1.820	122.65
PM3	−0.342	1.840	125.23
Tropolone			
MNDO	−0.302	1.900	118.51
AM1	−0.343	1.782	122.86
PM3	−0.372	1.781	124.34
4,5-Dihydrotropone			
MNDO	−0.288	1.921	118.44
AM1	−0.290	1.880	118.90
PM3	−0.311	1.902	117.89
4,5-Dihydrotropolone			
MNDO	−0.290	1.926	116.06
AM1	−0.305	1.855	121.72
PM3	−0.316	1.894	118.39
Cycloheptanone (Suberone)			
MNDO	−0.291	1.944	121.75
AM1	−0.303	1.901	119.05
PM3	−0.326	1.914	119.67
2-Hydroxysuberone			
MNDO	−0.285	1.951	119.82
AM1	−0.290	1.910	116.27
PM3	−0.303	1.929	116.37
Fluorone			
MNDO	−0.252	1.947	104.43
AM1	−0.237	1.930	104.68
PM3	−0.259	1.940	104.65
2-Hydroxyfluorone			
MNDO	−0.258	1.947	103.86
AM1	−0.244	1.926	103.98
PM3	−0.268	1.937	103.81

However, the increase in the dipole moment due to complexation with solvent would hardly be expected to exceed 1.1 D.⁶⁵ Therefore, it should be noted that the main reason for the error in the computation of the dipole moments of the troponoids is the inadequency of the MNDO, AM1, PM3 approaches as such. It may be connected with the fact that the set of molecular systems applied for the parameterization of the above methods did not involve "non-classical" species including non-benzenoid aromatics, as well as with the aforementioned failure to evaluate the enthalpy of the intramolecular HB.

TABLE III. Coefficients b and correlation coefficients r for the equation $m_{\text{exper}} = b m_{\text{theor}}$ (compounds for which $m_{\text{exper}} - m_{\text{theor}} > 1.8$ D have been excluded)

Computation method	Number of compounds	b	r
Tropones			
MNDO	25	1.1325-0.0866	0.5775
AM1	25	1.1239-0.0771	0.7402
PM3	26	1.1768-0.0696	0.7684
Tropolones			
MNDO	19	1.3502-0.1813	0.8987
AM1	31	1.1566-0.0831	0.7488
PM3	30	1.1731-0.0673	0.8500
Combined sequence			
MNDO	44	1.2010-0.0877	0.7582
AM1	56	1.1415-0.0557	0.7428
PM3	56	1.1749-0.0468	0.8187

In spite of the aforesaid drawbacks, semiempirical quantum chemical methods are suitable for establishing quantitative relationships having a predictive power. As was done previously,^{40,41} the dependences $m_{\text{exper}} = b m_{\text{theor}}$ (Tables III and IV) were studied. Regression analysis was performed at the 0.95 confidence level. The compounds from Table IV, for which the difference $D = m_{\text{exper}} - m_{\text{theor}}$ exceeds 1.8 D in one case⁴⁰ and 1.5 D in another case, were excluded from this correlation.

When $D > 1.5$ D the correlation coefficient r increases, as a rule, compared to $D > 1.8$ D, apart from selected data when the dipole moment of the tropolones were computed by the PM3 method (r value decreases slightly). In the process, diminution of the D criterion for discarding results leads essentially to fewer points in the linear regression (6 in every instance) solely on applying the MNDO and AM1 methods to the results of the computations of the dipole moment of tropolones.

When passing from $D > 1.8$ D to $D > 1.5$ D, the correlation coefficient r increases greatly for the unit of results computed by the AM1 method (tropolones and the combined sequence). For *a priori* evaluation of the dipole moments, equations of the type $m_{\text{exper}} = b m_{\text{theor}}$, presented in Table IV, appear to be the most acceptable in this connection.

TABLE IV. Coefficients b and correlation coefficients r in equations $m_{\text{exper}} = b m_{\text{theor}}$ (compounds for which $m_{\text{exper}} - m_{\text{theor}} > 1.5$ D have been excluded)

Computation method	Number of compounds	b	r
Tropones			
MNDO	24	1.225–0.0816	0.6176
AM1	24	1.1160–0.0719	0.7613
PM3	25	1.1646–0.0638	0.8127
Tropolones			
MNDO	13	1.2492–0.1994	0.9241
AM1	25	1.0923–0.0705	0.8624
PM3	29	1.1610–0.0688	0.8412
Combined sequence			
MNDO	37	1.1574–0.0805	0.7951
AM1	49	1.1041–0.0486	0.8221
PM3	54	1.1627–0.0456	0.8256

TABLE V. Tropones and tropolones whose molecular dipole moments could not be successfully computed by semiempirical quantum chemical methods

Compound	Computation methods
Provided that the compounds for which $m_{\text{exper}} - m_{\text{theor}} > 1.8$ D, are excluded from the correlation series	
4-Hydroxytropone	MNDO, AM1, PM3
2-Methoxy-3-isopropyltropone	AM1
2-Methoxy-6-methyltropone	MNDO
2-Methylmercaptotropone	AM1, PM3
7-Bromo-2-methoxytropone	MNDO
5-Methyltropolone	MNDO
3-Chlorohinokitiol	MNDO, PM3
3,7-Dichlorohinokitiol	MNDO, PM3
3-Bromo-4-methyltropolone	MNDO
3-Bromohinokitiol	MNDO, PM3
3-Bromo-5-methyltropolone	MNDO
7-Bromo-3-methyltropolone	MNDO
7-Bromohinokitiol	MNDO
3,5-Dibromohinokitiol	MNDO, AM1, PM3
3,7-Dibromotropolone	MNDO
3,7-Dibromo-4-methyltropolone	MNDO
3,7-Dibromohinokitiol	MNDO
3,7-Dibromo-5-methyltropolone	MNDO
3,5,7-Tribromo-4-methyltropolone	MNDO, AM1
3,5,7-Tribromohinokitiol	MNDO, AM1
3,5'-Ditropolonyl	MNDO

TABLE V. Contd.

On excluding the cases of $m_{\text{exper}} - m_{\text{theor}} > 1.5$ D dipole moments of the following molecules could in addition not be successfully predicted	
2- <i>p</i> -Methoxyphenyltropone	MNDO
2-Mercaptotropone	PM3
3-Bromo-2-methoxytropone	AM1
3-Isopropyltropolone (a-Thujaplicine)	MNDO
4-Methyltropolone	MNDO
7-Isopropyltropolone	MNDO
3-Nitrohinokitiol	PM3
3-Chlorohinokitiol	AM1
5-Chlorohinokitiol	MNDO
7-Chlorohinokitiol	MNDO
3,7-Dichlorohinokitiol	AM1
3-Bromo-4-methyltropolone	AM1
3-Bromohinokitiol	AM1
3,7-Dibromotropolone	AM1
3,7-Dibromo-4-methyltropolone	AM1
3,7-Dibromohinokitiol	AM1

In the other cases diminution of the D value causes the quantity of r to increase somewhat, and for selected moieties (tropolones, PM3) to decrease slightly. The applicability of m_{exper} vs. m_{theor} correlations from Tables III and IV for quantitative estimations is practically the same with few benefits of the data from Table IV (excluding the PM3 results for tropolones).

The dependences $m_{\text{exper}} = b m_{\text{theor}}$ obtained on the basis of MNDO computations for tropones are characterized by relatively low values of r and can not be recommended for predicting "experimental" dipole moments of the above mentioned series of compounds.

Table V shows the compounds for which the computed dipole moments obtained using one or other of the methods are incorrect. The corresponding values were excluded from the correlation series.

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ИЗВОД

КОРИШЋЕЊЕ ПОЛУЕМПИРИЈСКИХ КВАНТНО-ХЕМИЈСКИХ ПРИСТУПА ЗА ИЗРАЧУНАВАЊЕ ДИПОЛНИХ МОМЕНАТА ТРОПОНА И ТРОПОЛОНА

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Коришћењем метода MNDO, AM1 и PM3 израчунати су диполни моменти (m) за 28 тропона и 34 трополона. Анализиране су потенцијалне могућности поменутих метода за израчунавање m . Утврђене су корелације $m_{\text{exper}} = b m_{\text{theor}}$.

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