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Computational Studies of Polynitroaromatic Molecules and the Development of Sensitivity Relationships

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A computational study of 48 nitroaromatic molecules has been carried out with the objective of developing an understanding of how chemical structural features are related to the shock/impact sensitivities of these molecules. An ab initio self-consistent-field molecular orbital procedure was used to compute a variety of properties, including atomic charges, electrostatic potentials and ionization potentials. From the results of our computational analyses, it is suggested that the observed high sensitivities of hydroxytrinitroaromatics toward shock and impact may be due to the formation of small but significant quantities of unstable nitronic acid tautomers. When the hydroxynitroaromatics are excluded, the sensitivity is shown to be related to the C-NO_2 linkage with the greatest instability, as measured by the electrostatic potential at the midpoint of the C-NO_2 bond; this is an extension of a relationship discovered earlier. Hydrogen transfer and ring formation reactions of some alkyl- and amine-substituted nitroaromatics have been studied; the energetics of these reactions help to explain the differences in the thermal, shock and impact sensitivities of their larger trinitroaromatic analogues.

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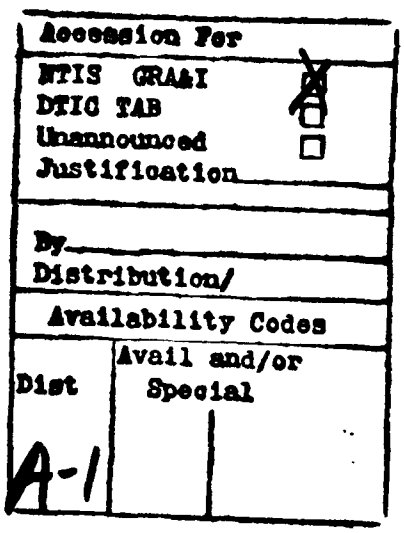
PREFACE

The project was carried out under the direction of Dr. Peter Politzer in the Department of Chemistry, University of New Orleans, New Orleans, Louisiana, 70148. It was supported by Contract No. F08635-87-C-0090, for the period of 15 June 1987 to 15 June 1990. The Project Manager was Dr. Paul R. Bolduc, Air Force Armament Laboratory (MNE), Eglin Air Force Base, Florida, 32542-5434.

The work was carried out by Mrs. Pat Lane, Dr. Jane S. Murray and Dr. Imam Elminyawi. This Final Report has been prepared with the assistance of Ms. Anita Hamel.



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SECTION I
INTRODUCTION

The objective of this project has been to carry out computational studies of certain nitroaromatic molecules in order to develop an understanding of how the sensitivities of these molecules toward shock and impact are related to their chemical structures. This knowledge could then be used to design molecules with desired sensitivity and explosive performance characteristics.

We have investigated 48 substituted trinitroaromatic molecules. All of the molecules examined had been selected for this purpose by the Air Force Armament Laboratory (AFATL). They are listed below, together with the source of each one's crystallographically determined structure (References 1-12).

A. 2,4,6-Trinitro-m-xylene (Reference 1)

B. 2,4,6-Trinitromesitylene (Reference 2)

C. 2,4,6-Trinitroethylbenzene (Reference 3)

D. 3-Chloro-2,4,6-trinitrotoluene (Reference 3)

E. 3-Bromo-2,4,6-trinitrotoluene (Reference 3)

F. Ethyl(2,4,6-trinitrophenyl)carbamate (Reference 4)

G. 3-Amino-2,4,6-trinitrotoluene (Reference 4)

H. 3,5-Diamino-2,4,6-trinitrotoluene (Reference 4)

I. N-Carboethoxy-2,4,6-trinitro-m-toluidine (Reference 2)

J. 3,5-Dibromo-2,4,6-trinitrotoluene (Reference 3)

K. Ethyl picryl sulfide (Reference 3)

L. 1,3-Dimethoxy-2,4,6-trinitrobenzene (Reference 2)

M. 1,3-Dichloro-2,4,6-trinitrobenzene (Reference 5)

N. Methyl 2,4,6-trinitrobenzoate (Reference 2)

O. 3-Chloro-2,4,6-trinitroanisole (Reference 6)

P. Styphnic acid (Reference 7)

Q. 3-Amino-2,4,6-trinitroanisole (Reference 4)

R. 2,4,6-Trinitrophenylethanol (Reference 2)

S. 3,5-Dichloro-2,4,6-trinitroanisole (Reference 2)

T. 3,5-Diamino-2,4,6-trinitrophenol (Reference 8)

U. 2,4,6-Trinitrophloroglucinol (Reference 7)

V. Aminopicric acid (Reference 9)

W. 2,3,4,6-Tetranitroaniline (Reference 10)

X. 1,3,5-Triamino-2,4,6-trinitrobenzene (Reference 11)

Y. 1,3-Diamino-2,4,6-trinitrobenzene (Reference 12)

Z. 2,4,6-Trinitrobenzyl alcohol (Reference 2)

AA. 2,4,6-Trinitrobenzonitrile (Reference 2)

BB. 2,4,6-Trinitroacetophenone (Reference 2)

CC. 3-Amino-2,4,6-trinitroethylbenzene (Reference 3)

DD. 3-(Methylamino)-2,4,6-trinitrotoluene (Reference 3)

EE. N,N-Dimethylpicramide (Reference 3)

FF. N-Methylpicramide (Reference 3)

GG. 3-Trifluoromethyl-2,4,6-trinitroaniline (Reference 2)

HH. 1,3,5-Tribromo-2,4,6-trinitrobenzene (Reference 3)

II. 2,4-Dibromo-1,3,5-trinitrobenzene (Reference 3)

JJ. 3-Trifluoromethyl-2,4,6-trinitrophenol (Reference 6)

KK. N-Ethylpicramide (Reference 6)

LL. 3-Hydroxy-2,4,6-trinitrotoluene (Reference 6)

MM. 3,5-Dimethyl-2,4,6-trinitroanisole (Reference 6)

NN. 2,4,6-Trinitro-3,5-dihydroxyaniline (Reference 6)

OO. 1-Hydroxy-3-isopropyl-2,4,6-trinitrobenzene (Reference 6)

PP. 3-Bromo-2,4,6-trinitroaniline (Reference 6)

QQ. 2,3,4,5-Tetranitrotoluene (Reference 6)

RR. 2,3,5,6-Tetranitrotoluene (Reference 6)

SS. 2,3,4,6-Tetranitrotoluene (Reference 6)

TT. 3-Bromopicric acid (Reference 6)

UU. 3-Bromo-2,4,6-trinitroanisole (Reference 6)

VV. 2,4,6-Trinitro-3-hydroxybenzoic acid (Reference 6)

In the selected substituted trinitroaromatics, the mean plane of each nitro group is generally inclined from the mean plane of the benzene ring by either twisting around the C-N bond or simply bending at the attached carbon atom, or both. The angles of rotation for the nitro groups range from near 0 degrees (coplanar with the benzene ring) to essentially 90 degrees. All of the molecules (except TATB) exhibit some rotation of the nitro groups.

Assuming the van der Waals radii of the O and the H atoms are 1.40 and 1.20 angstroms respectively, the H···O distances between nonbonding atoms which are less than 2.50 angstroms strongly indicate hydrogen bonding. All of the substituted trinitrobenzenes are observed to have some hydrogen bonding.

In Table 1 is given a compilation of some computed and experimental properties for the forty-eight nitroaromatics included in this contract plus the twelve studied in an earlier one-year contract AFATL-88-107. In addition, the following data are presented in Appendices for each of the forty-eight molecules included in this contract:

(a) Z-matrix. This is the format of the input for the GAUSSIAN programs, which we use for our computational analyses. This includes selected bond distances, angles and dihedral angles.

(b) Total molecular energy, in hartrees.

(c) Ionization potential, approximated as the calculated energy of the highest occupied molecular orbital.

(d) Atomic charges, calculated by means of Mulliken's population analysis procedure.

(e) Calculated dipole moment, in Debyes.

(f) Electrostatic potentials, V_{mid}, at the midpoints of the C-NO_2 bonds, as approximated by the formula: $V_{mid} = Q_C/0.5R + Q_N/0.5R$. Q_C and Q_N are the charges on the carbon and nitrogen; R is the C-N bond length, in bohrs (1 bohr = 0.55292 A).

(g) Bond orders of C-NO_2 and N-O bonds, calculated using the formula:

$$\text{Bond Order} = \frac{11.92}{R^3 \nu^2} \qquad (1)$$

R is the actual bond length in Angstroms, and ν is a parameter that is characteristic of given bond types and can be regarded as representing an effective length of the bond. This formula is a modification of our earlier bond order expression (Reference 13) which involved the

TABLE 1. COMPUTED AND EXPERIMENTAL PROPERTIES OF SIXTY NITROAROMATICS[a]

Molecule	$V_{mid,max}$	IP (eV)	Dipole Moment (Debye)	Impact Drop Height[b] (cm) Reference 32	AFATL
2,4,6-Trinitroanisole	0.187	8.44	2.12	192	79.3[c]
α,α,α-Trifluoro-2,4,6-trinitro-toluene	0.237	8.88	0.81	n.a.	101.7[c]
2,4,6-Trinitrophenylhydrazine	0.193	8.13	4.37	n.a.	21.9
2,4,6-Trinitrophenetole	0.258	8.52	2.10	190	n.a.
2,4,6-Trinitrobenzamide	0.206	8.71	2.52	n.a.	62.8[c]
2,4,6-Trinitrobenzoic Acid	0.205	8.79	1.15	109	91.4
2,4,6-Trinitrobenzaldehyde	0.217	8.83	1.24	36	53.5
1,3,5-Trinitro-2-n-propyl-benzene	0.204	8.48	1.73	n.a.	48.1[c]
meta-Dinitrobenzene	0.182	8.15	2.97 (4.10)	n.a.	n.a.
2,4,6-Trinitrochlorobenzene	0.234	8.80	0.85	79	72.5[c]
2,4,6-Trinitrotoluene	0.209	8.57	1.17 (1.37)	160	105.4, 61.7[c]
1,3,5-Trinitrobenzene	0.208	8.71	0.26 (0.00)	100	49.8
2,4,6-Trinitroaniline	0.174	8.24	2.31	177	137.8[c]
2,4,6-Trinitrophenol	0.203	8.40	2.76	87	44.7
2,4,6-Trinitrobenzylchloride	0.214	8.74	1.53	44	79.3
2,4,6-Trinitro-m-xylene	0.204	8.52	1.27	n.a.	75.0
2,4,6-Trinitromesitylene	0.189	8.52	0.11	n.a.	52.6
2,4,6-Trinitroethylbenzene	0.203	8.59	1.13	n.a.	n.a.
3-Chloro-2,4,6-trinitrotoluene	0.205	8.43	2.41	n.a.	79.5
3-Bromo-2,4,6-trinitrotoluene	0.200	8.61	1.25	n.a.	94.7
Ethyl(2,4,6-trinitrophenyl)-carbamate	0.206	8.37	2.92	n.a.	n.a.
3-Amino-2,4,6-trinitrotoluene	0.169	8.23	2.09	n.a.	123.8[c]
3,5-Diamino-2,4,6-trinitro-toluene	0.132	7.82	1.47	n.a.	n.a.
N-Carboethoxy-2,4,6-trinitro-m-toluidine	0.198	8.36	2.51	n.a.	n.a.
3,5-Dibromo-2,4,6-trinitro-toluene	0.209	8.83	1.26	n.a.	n.a.
Ethyl picryl sulfide	0.185	7.91	2.13	n.a.	n.a.

TABLE 1. COMPUTED AND EXPERIMENTAL PROPERTIES OF SIXTY NITROAROMATICS (Continued)[a]

Molecule	$V_{mid,max}$	IP (eV)	Dipole Moment (Debye)	Impact Drop Height[b] (cm)	
				Reference 32	AFATL
1,3-Dimethoxy-2,4,6-trinitro-benzene	0.185	8.66	2.46	251	44.0
1,3-Dichloro-2,4,6-trinitro-benzene	0.219	8.90	1.10	n.a.	85.1
Methyl 2,4,6-trinitrobenzoate	0.223	8.78	1.28	90	93.1[c]
3-Chloro-2,4,6-trinitroanisole	0.202	8.73	2.54	n.a.	151.6
Styphnic acid	0.170	8.10	1.78	43	24.0
3-Amino-2,4,6-trinitroanisole	0.165	8.36	2.19	>325	164.7[c]
2,4,6-Trinitrophenylethanol	0.210	8.22	2.67	68	96.4
3,5-Dichloro-2,4,6-trinitro-anisole	0.202	8.81	2.89	75	94.7
3,5-Diamino-2,4,6-trinitro-phenol	0.125	7.95	2.87	112	n.a.
2,4,6-Trinitrophloroglucinol	0.143	7.86	2.94	27	n.a.
Aminopicric acid	0.151	8.31	0.69	138	n.a.
2,3,4,6-Tetranitroaniline	0.236	8.49	4.85	41	27.7
1,3,5-Triamino-2,4,6-trinitro-benzene	0.105	7.88	0.78	>325	n.a.
1,3-Diamino-2,4,6-trinitro-benzene	0.146	8.09	1.48	320	150.7[c]
2,4,6-Trinitrobenzyl alcohol	0.217	8.50	2.06	52	57.5
2,4,6-Trinitrobenzonitrile	0.213	8.95	2.36	140	72.1
2,4,6-Trinitroacetophenone	0.210	8.66	1.83	79	117.4[c]
3-Amino-2,4,6-trinitroethyl-benzene	0.176	8.20	2.23	n.a.	n.a.
3-(Methylamino)-2,4,6-trinitro-toluene	0.172	7.95	2.82	n.a.	n.a.
N,N-Dimethylpicramide	0.193	8.03	3.63	n.a.	66.7[c]
N-Methylpicramide	0.185	8.08	3.71	n.a.	82.1
3-Trifluoromethyl-2,4,6-trinitroaniline	0.184	8.47	2.99	n.a.	101.7
1,3,5-Tribromo-2,4,6-trinitro-benzene	0.201	8.99	0.03	n.a.	n.a.

TABLE 1. COMPUTED AND EXPERIMENTAL PROPERTIES OF SIXTY NITROAROMATICS (Concluded)[a]

Molecule	$V_{mid,max}$	IP (eV)	Dipole Moment (Debye)	Impact Drop Height[b] (cm)	
				Reference 32	AFATL
2,4-Dibromo-1,3,5-trinitro-benzene	0.213	8.82	0.27	n.a.	n.a.
3-Trifluoromethyl-2,4,6-trinitrophenol	0.195	8.58	2.25	n.a.	121.6[c]
N-Ethylpicramide	0.176	8.01	3.80	n.a.	60.6[c]
3-Hydroxy-2,4,6-trinitro-toluene	0.174	8.26	0.72	191	73.8
3,5-Dimethyl-2,4,6-trinitro-anisole	0.190	8.34	1.34	n.a.	47.0[c]
2,4,6-Trinitro-3,5-dihydroxy-aniline	0.142	7.69	4.40	32	27.8
1-Hydroxy-3-isopropyl-2,4,6-trinitrobenzene	0.182	8.39	0.83	n.a.	96.4
3-Bromo-2,4,6-trinitroaniline	0.183	8.49	1.69	n.a.	n.a.
2,3,4,5-Tetranitrotoluene	0.220	8.83	6.19	n.a.	n.a.
2,3,5,6-Tetranitrotoluene	0.225	8.88	0.93	n.a.	n.a.
2,3,4,6-Tetranitrotoluene	0.223	8.91	3.54	n.a.	n.a.
3-Bromopicric acid	0.185	8.54	1.66	n.a.	n.a.
3-Bromo-2,4,6-trinitroanisole	0.196	8.69	1.79	n.a.	n.a.
2,4,6-Trinitro-3-hydroxy-benzoic acid	0.189	8.48	1.24	n.a.	n.a.

[a]Experimental values for ionization potentials and dipole moments, when available, are given in parentheses.

[b]The impact drop heights were measured with 2.5 kg weights except for those designated with a superscript c. n. a. stands for not available.

[c]Data were measured with 5.0 kg weights.

force constant and the bond length; it was introduced in order to avoid the time and space-consuming computations required to calculate force constants. We have shown that by choosing appropriate values for ν, very good agreement can be obtained with the results of the original formula.

(h) Plots showing calculated molecular electrostatic potential in various planes. This potential is obtained using the exact formula:

$$V(\mathbf{r}) = \sum_{A} \frac{Z_A}{|\mathbf{R}_A - \mathbf{r}|} - \int \frac{\rho(\mathbf{r}')\, d\mathbf{r}'}{|\mathbf{r}' - \mathbf{r}|} \qquad (2)$$

Z_A is the charge on nucleus A, located at $\mathbf{R}_A$, and $\rho(\mathbf{r})$ is the electronic density function, obtained from the computed molecular wave function. The dashed contours represent negative potentials and the solid contours correspond to the zero and positive contours. The zero contour is marked.

SECTION II
DISCUSSION

In the area of nitroaromatics, a number of studies have been carried out which support the idea that C-NO_2 bonds are of key importance in determining impact and shock sensitivities (References 14-19). Some time ago we found a correlation between the shock/impact sensitivities of a group of six nitroaromatics and the quantity V_{mid}, the electrostatic potential at the midpoint of the longest C-NO_2 bond in each system (Reference 17). V_{mid} is approximated from calculated atomic charges, as given in equation (3).

$$V_{mid} = \frac{Q_C}{0.5\ R} + \frac{Q_N}{0.5\ R} \qquad (3)$$

Q_C and Q_N are the charges on the carbon and nitrogen, obtained from the Mulliken population analysis (Reference 20) of the molecular orbital wave function; R is the C-N bond length in A. V_{mid} is almost invariably positive for nitroaromatic C-NO_2 bonds, as a consequence of the calculated charges of the carbon and nitrogen atom forming these bonds usually both being positive. This suggests that the magnitude of V_{mid} reflects a certain degree of instability in these bonds, an interpretation that is supported by Fliszar's formulation of bond energy in terms of atomic charges and the reciprocal of the bond length (References 21 and 22).

During the course of this project we have computed V_{mid} for the C-NO_2 bonds of a large number of nitroaromatics. Table 2 lists the largest value, $V_{mid,max}$, for each of a group of 26 nitroaromatics, along with its measured impact drop height value. It should be noted that a serious problem encountered in seeking to understand and interpret experimentally-determined sensitivity data is the very marked degree to which these depend upon the laboratory at which the measurements were made. This can be seen in Figures 1 and 2, which show the absence of any correlation between impact sensitivities obtained at AFATL and those given in Reference 32. (If the point for 1,3-dimethoxy-2,4,6-trinitrobenzene were removed from Figure 1, the linear correlation coefficient would increase to 0.53, which is a marked improvement but still very poor.)

It is seen in Table 2 that trinitroaromatics with substituents that are strong resonance donors, such as -NH_2, -OH, -OCH_3 and -OC_2H_5, have $V_{mid,max}$ values that are less than that of 1,3,5-trinitrobenzene (I), which can be viewed as a reference molecule (since it has only hydrogens as non-nitro substituents). This is consistent with these groups having a strengthening effect on

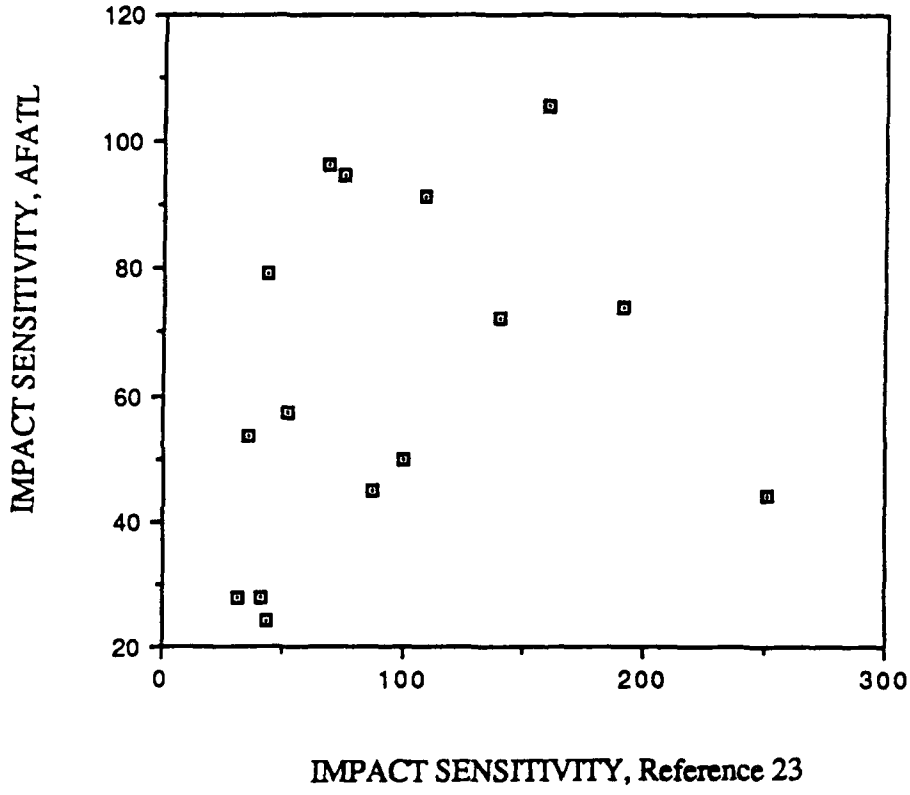


Figure 1. Plot of AFATL impact sensitivities versus those obtained from Reference 32, measured in drop height in cm, for fifteen nitroaromatics. Both sets of data were measured with 2.5 kg weights. The linear correlation coefficient is 0.26.

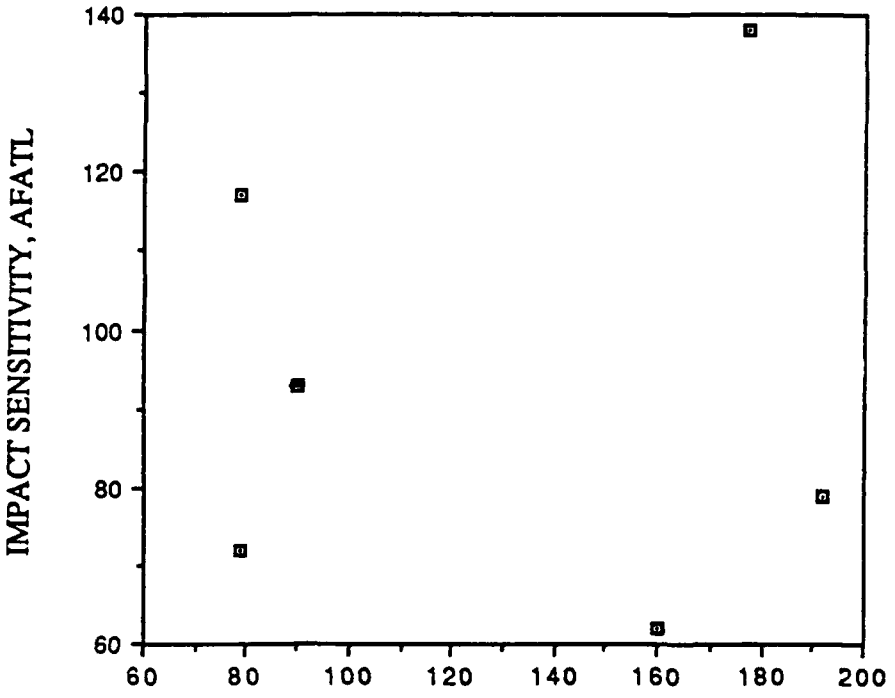
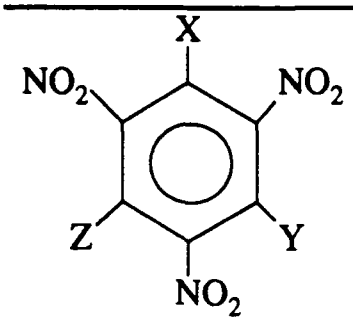


Figure 2. Plot of AFATL impact sensitivities versus those obtained from Reference 32, measured in drop height in cm, for six nitroaromatics. The Navy data were measured using 2.5 kg weights; the AFATL data were obtained with 5.0 kg weights. The linear correlation coefficient is 0.02.

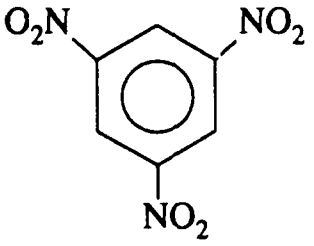
TABLE 2. PROPERTIES OF SOME NITROAROMATICS



XYZ	Impact Drop Height[a] (cm)	$V_{mid,max}$	$\left(\frac{1}{R}\right)_{ave}$, A^{-1}	Reference for Structure
OH, OH, OH	27	.143	.692	Reference 7
NH_2, OH, OH	32	.142	.698	Reference 23
CHO, H, H	36	.217	.675	Reference 23
NH_2, NO_2, H	41	.240	.683	Reference 10
OH, OH, H	43	.170	.685	Reference 7
CH_2Cl, H, H	44	.214	.675	Reference 7
CH_2OH, H, H	52	.217	.679	Reference 7
C_2H_4OH, H, H	68	.210	.678	Reference 7
OCH_3, Cl, Cl	75	.202	.677	Reference 7
Cl, H, H	79	.234	.672	Reference 24
$COCH_3$, H, H	79	.210	.678	Reference 7
OH, H, H	87	.203	.684	Reference 25
$COOCH_3$, H, H	90	.223	.680	Reference 7
H, H, H	100	.208	.675	Reference 26
COOH, H, H	109	.205	.675	Reference 27
OH, NH_2, NH_2	112	.125	.699	Reference 8
OH, NH_2, H	138	.151	.688	Reference 27
CN, H, H	140	.213	.675	Reference 7
CH_3, H, H	160	.209	.678	Reference 28
NH_2, H, H	177	.174	.681	Reference 29
OC_2H_5, H, H	190	.198	.681	Reference 30
OCH_3, H, H	192	.187	.679	Reference 31
OCH_3, OCH_3, H	251	.185	.678	Reference 7
NH_2, NH_2, H	320	.146	.689	Reference 12
OCH_3, NH_2, H	>325	.165	.685	Reference 7
NH_2, NH_2, NH_2	>325	.103	.705	Reference 11

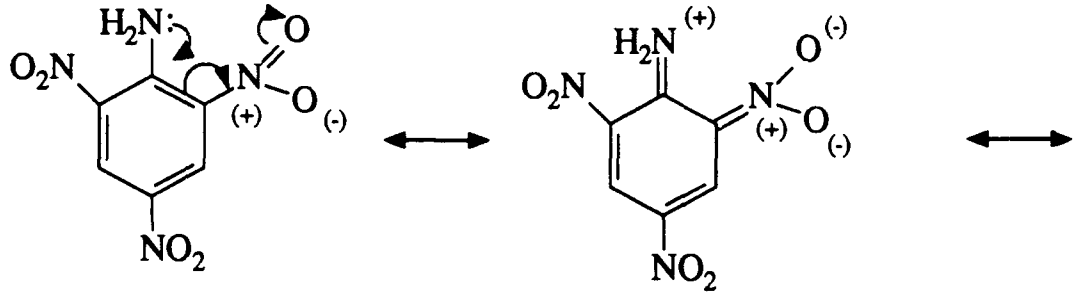
Table 2. Footnote:

[a] Impact sensitivity is measured as the height from which a given weight must be dropped on a compound to produce detonation fifty percent of the time. Thus, the smaller the value given, the more sensitive is the compound toward impact. These data are taken from Reference 32.



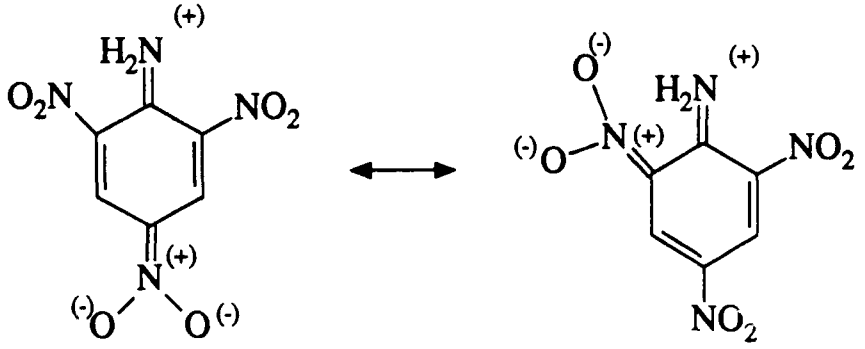
I

C-NO_2 bonds, as indicated by structures IIA - IIC and by the increase in $(1/R)_{ave}$ compared to 1,3,5-trinitrobenzene, I (see Table 2). All of these molecules also have lower $V_{mid,max}$ values than does I.



II IIA

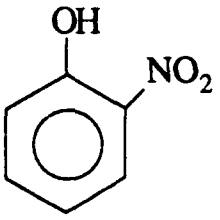
(4)



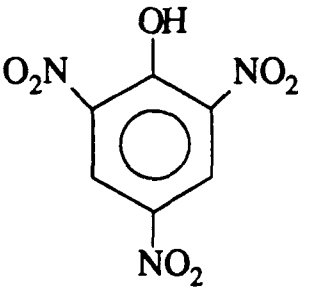
IIB IIC

It has been noted earlier, for nitroaromatics, that a marked decrease in sensitivity accompanies an increase in the number of amine groups (References 16, 32 and 33). It is seen in Table 2 that alkoxy substituents and combinations of -NH_2 and -OR groups have similar effects upon impact sensitivities, as indicated by their large impact drop heights. However hydroxynitroaromatics are found to be very sensitive, despite the fact that -OH has resonance capabilities analogous to -NH_2 and -OR.

This observed sensitizing effect of the hydroxyl group in trinitroaromatics led us to investigate computationally the basis for this behavior, using *o*-nitrophenol (III) as a model for picric acid (IV) (Reference 34). The combined electron-withdrawing power of the three nitro groups in picric acid



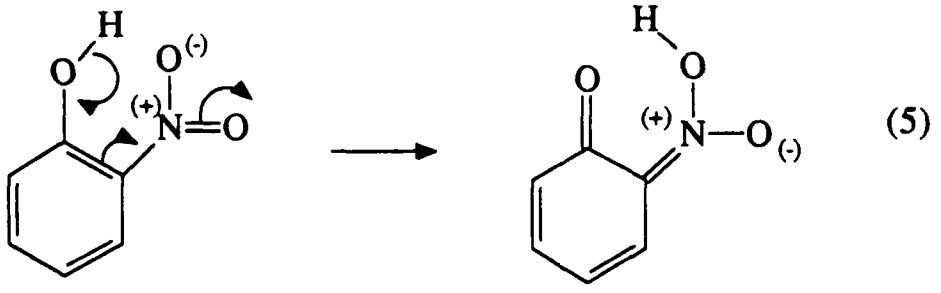
III



IV

makes the hydroxyl hydrogen quite positive in nature. For example, whereas phenol is only weakly acidic, with a pK_a of 9.9, picric acid is a relatively strong acid; its pK_a of 0.38 is comparable to that of trichloroacetic acid (0.70) (Reference 35). In addition, the crystal structure of picric acid indicates significant hydrogen bonding between the hydroxyl and an ortho nitro group (Reference 25). The O···O separation is 2.55 Å, which is near the shorter end of the range that has been identified as typical of O-H···O hydrogen bonds (2.50 - 2.80 Å) (Reference 36). Our optimized 3-21G structure of III shows an O···O separation of 2.55 Å, the same as that found in the crystal structure of picric acid, and an OH···O distance of 1.75 Å (typical of a strong oxygen-hydrogen hydrogen bond (Reference 36)).

The labile nature of the hydroxyl hydrogen in III and its proximity to the nitro oxygen led us to investigate the possibility of hydrogen migration to the nitro oxgyen, as shown in equation (5). V is a nitronic acid; the latter are known to be reactive, unstable systems (Reference 37). Thus, if a

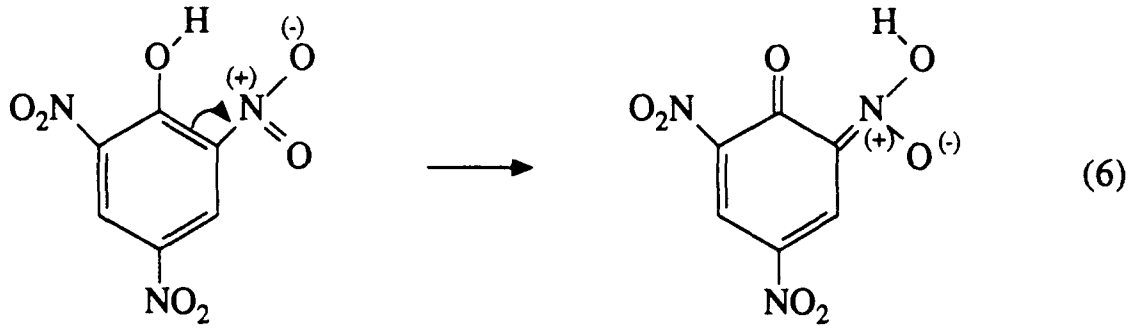


(5)

III V

process analogous to equation (5) were to occur for picric acid (IV), this would represent a decomposition mechanism that could account for its instability, and that of the dihydroxy and

trihydroxy derivatives of trinitrobenzene. At the 3-21G level, the nitronic acid V is 15.4 kcal/mole higher in energy than III. We suggest from these calculated results that the observed high sensitivity of hydroxytrinitroaromatics toward shock and impact may be due to some significant fraction of the molecules being in the form of an unstable nitronic acid, produced through a process



IV VI (6)

such as is shown in equation (6) for picric acid. The proton transfer shown in equation (6) could result, for example, from a vibrational excitation of the O-H bond brought about by the energy input associated with shock or impact. We have shown that there is no similar tendency for nitronic acid formation in aminonitroaromatics (References 34 and 38), revealing a major difference between the amino and hydroxynitroaromatics that may account in part for their contrasting sensitivities.

In light of the anomalous effect of -OH on sensitivity, we have excluded all hydroxytrinitroaromatics in seeking correlations between V_{mid} and impact sensitivity. Figure 3 shows measured impact drop heights plotted against $V_{mid,max}$ values for the molecules in Table 2 that have no hydroxyl groups. The calculated linear correlation coefficient is 0.86. It is noteworthy that nitroaromatics bearing α-CH linkages do not need to be treated separately, as was found to be necessary in establishing the OB_{100} correlations with impact sensitivity (Reference 32). The present relationship suggests that the C-NO_2 linkage with the greatest instability, as indicated by $V_{mid,max}$, may be a key bond involved in initiating decomposition in nitroaromatics subjected to impact.

As part of our continuing study of the relationship between molecular properties and shock, impact and thermal sensitivity, we have investigated the possibilities of hydrogen transfer reactions, analogous to those shown in equations (5) and (6) for *o*-nitrophenol and picric acid, for the model systems *o*-nitroaniline (VII), *o*-nitrotoluene (VIII) and *o*-nitrocumene (IX). VII - IX are

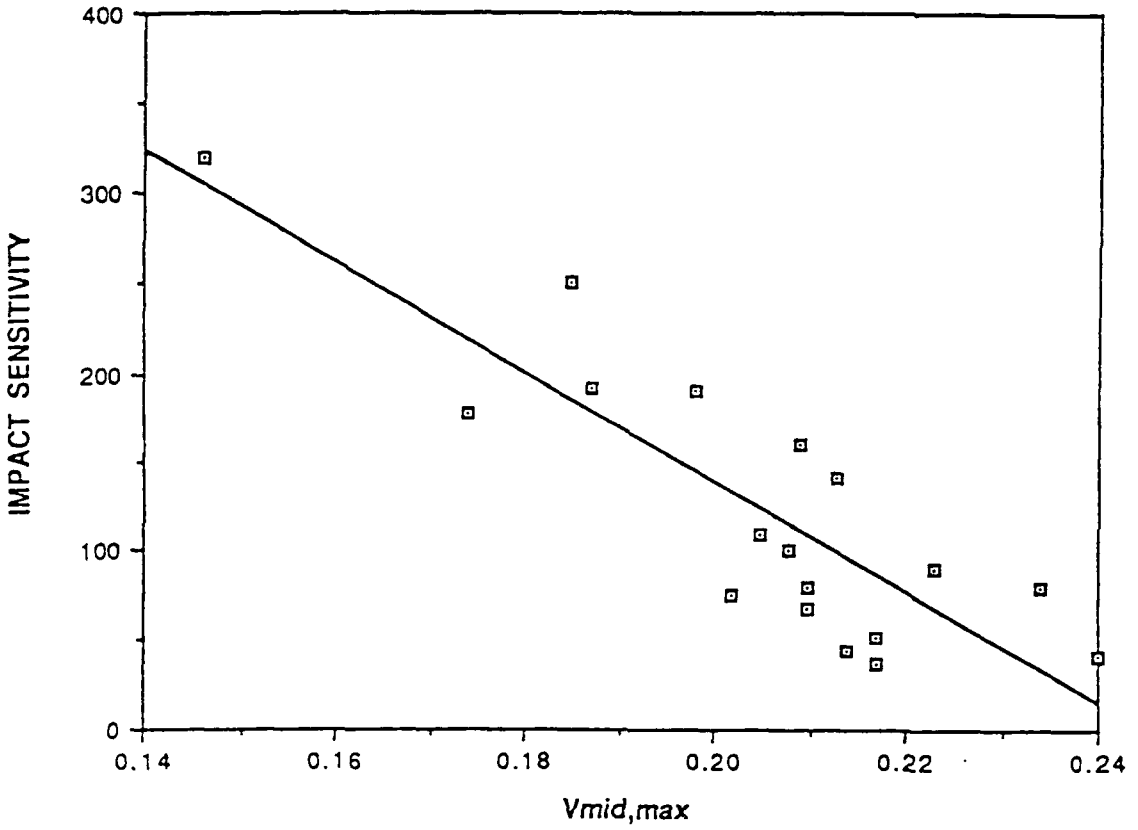
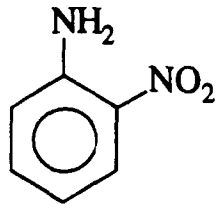
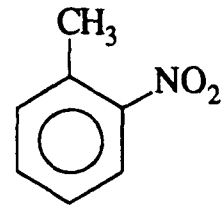


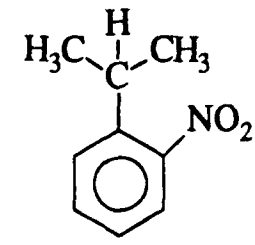
Figure 3. Correlation between impact sensitivity, as measured by impact drop height in cm (Reference 32), and $V_{mid,max}$ for eighteen nitroaromatics. Data are taken from Table 2, excluding hydroxynitroaromatics and molecules for which the impact sensitivities are given as greater than 325 cm. The least squares equation of the line is $y = 755.01 - 3084.27x$, with a correlation coefficient of 0.86.



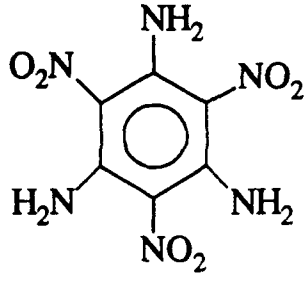
VII



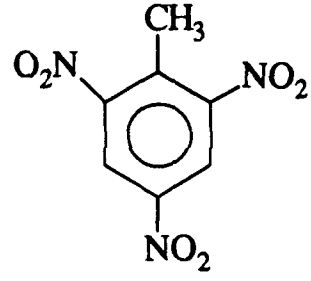
VIII



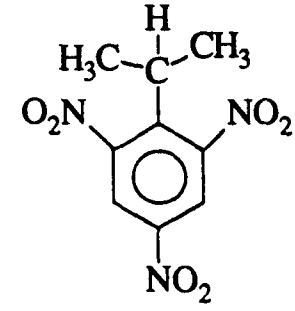
IX



X, TATB



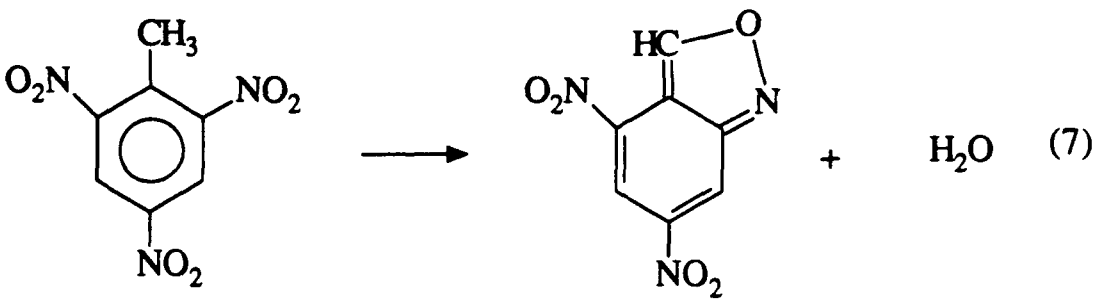
XI, TNT



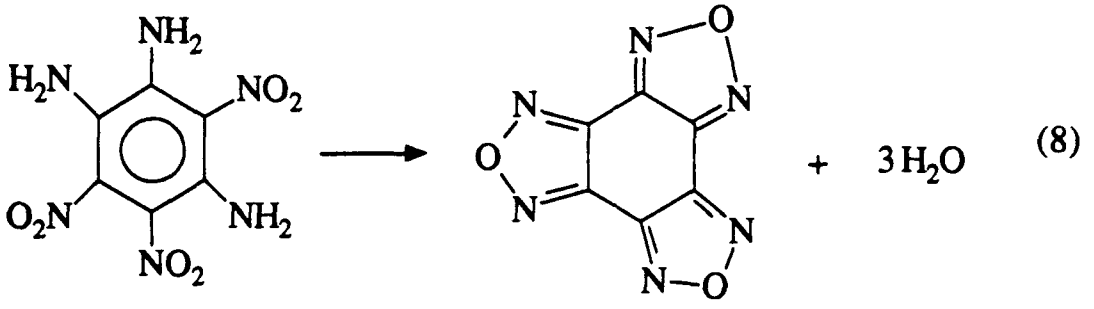
XII

taken as models for the larger trinitroaromatics 1,3,5-triamino-2,4,6-trinitrobenzene (TATB, X), 2,4,6-trinitrotoluene (TNT, XI) and 2,4,6-trinitrocumene (XII). One of our objectives has been to gain insight into factors giving rise to the very different thermal, shock and impact sensitivities of TATB (X) and the alkyltrinitroaromatics XI and XII. TNT (XI), for example, is thermally labile, self-igniting at temperatures between 200 and 210°C (Reference 32), and has intermediate impact and shock sensitivities (References 32 and 39) as does also XII (Reference 40). TATB (X), on the other hand, is stable to temperatures well beyond 300°C (Reference 41) and is so insensitive to impact and shock (References 32 and 39) as to be impractical as an explosive.

The decompositions of TATB and TNT have been studied extensively, using a variety of experimental techniques (References 15,18,19 and 42-51). Most of the studies of TNT point to reactions involving a methyl hydrogen as being involved in the initial steps of its decomposition (References 42-45, 47 and 49), as contrasted to simple C-NO_2 bond rupture (Reference 19). Evidence for the formation of an intramolecular five-membered ring (dinitroanthranil, XIII), as shown in equation (7), has been reported in low temperature studies of TNT (under 300°C) (References 42 and 43). Five-membered ring formation giving furazans has been reported in



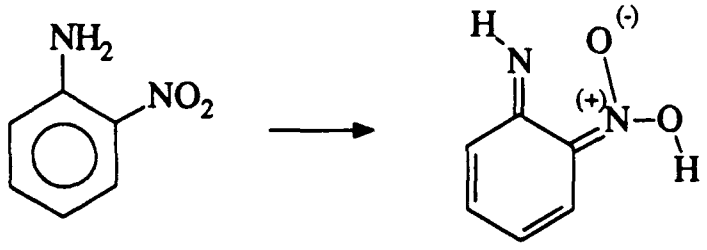
XI XIII



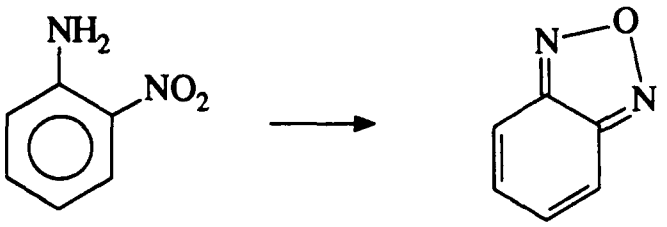
X XIV

thermal decomposition (Reference 48) and underwater shock and impact (Reference 50) studies of TATB [e.g. as given by equation (8)]. These studies led us to investigate analogous intramolecular ring formation processes for our model systems VII and VIII, as well as possible hydrogen transfer reactions for VII - IX.

We will discuss initially our computed results for the hydrogen transfer and intramolecular ring formation reactions of *o*-nitroaniline, VII. The products, XVA and XVI, are shown below in equations (9) and (10). It is important to point out that no local energy minimum was found



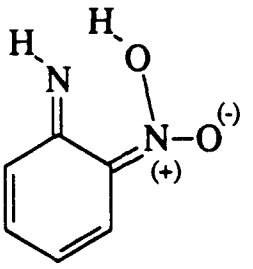
VII XVA



(10)

VII XVI

computationally corresponding to the nitronic acid tautomer XVB of *o*-nitroaniline (Reference 34).



XVB

Our calculated energies for *o*-nitroaniline and the related systems XVA and XVI are given in Table 3. The tautomerization of VII to produce the nitronic acid XVA is calculated to be endothermic by +39.8 kcal/mole at the 3-21G level. For comparison, the energy change associated with the conversion of *o*-nitrophenol to its nitronic acid tautomer V [equation (5)] was found to +15.4 kcal/mole at the same computational level (Reference 34). Our results suggest, therefore, that the formation of XVA is highly unfavored. However the conversion of VII to benzofurazan (XVI) and water has a calculated ΔE of +5.3 kcal/mole. Thus the formation of XVI is calculated to be a nearly neutral thermochemical reaction. This neutral thermochemistry is in accord with earlier speculation concerning the basis for the high thermal stability and very low shock and impact sensitivities of TATB (Reference 52). It has been suggested that its stability reflects the fact that the steps producing furazan derivatives of TATB (e.g. XIV) are thermodynamically nearly neutral (Reference 52), resulting in little or no early release of energy to drive subsequent decomposition steps.

Our findings for *o*-nitrotoluene (VIII) and related reaction products differ considerably from those for *o*-nitroaniline. First, the hydrogen transfer isomer of VIII is not a nitronic acid, but instead contains an intramolecular ring, XVII. It is noteworthy that these computations were begun at several different starting geometries, each involving a methyl hydrogen transferred to a nitro oxygen atom. When the hydrogen was initially placed on the closer oxygen, the parent

TABLE 3. CALCULATED 3-21G ENERGIES

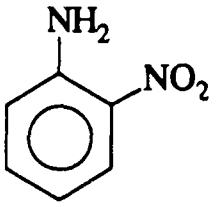
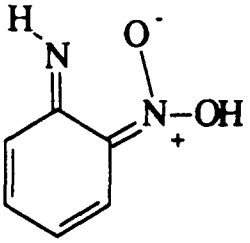
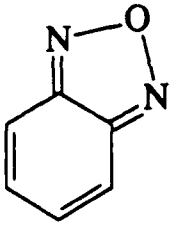
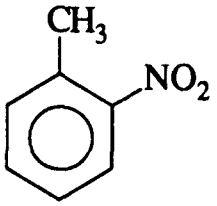
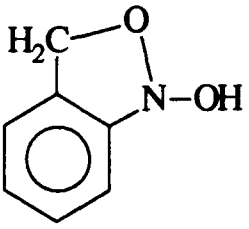
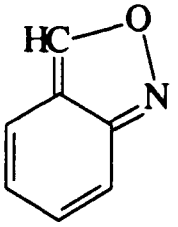
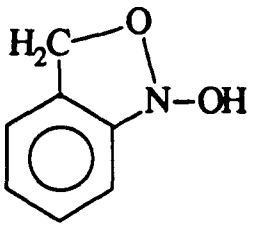
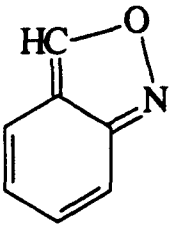
Molecule	Total Energy (hartrees)	Relative Energy (kcal/mole)
1. *o*-Nitroaniline (VII) and related systems:		
VII 	-486.44531	0.0
XVA 	-486.38182	+39.8
XVI 	-410.85083	-----
XVI + H_2O	-486.43679	+5.3

TABLE 3. CALCULATED 3-21G ENERGIES (Concluded).

Molecule		Total Energy (hartrees)	Relative Energy (kcal/mole)
2. o-Nitrotoluene (VIII) and related systems:			
VIII		-470.53030	0.0
XVII		-470.56318	-20.6
XVIII		-394.99237	-----
XVIII + H_2O		-470.57833	-30.1



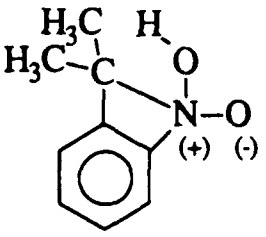
XVII



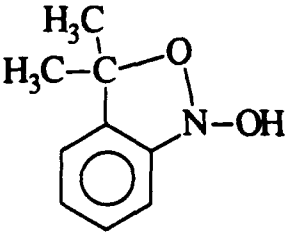
XVIII

molecule, *o*-nitrotoluene, was regenerated computationally. However when the hydrogen was placed on the more distant nitro oxygen, the bicyclic nonplanar XVII was formed. As shown in Table 3, the formation of XVII from VIII is exothermic by -20.6 kcal/mole (at the 3-21G level). The further reaction of XVII to form anthranil (XVIII) and water is also exothermic by -9.5 kcal/mole. From a thermodynamic standpoint, therefore, the formation of both XVII and XVIII from VIII is predicted to be highly favored. Energy released by forming such products could help to stimulate further decomposition steps. This is consistent with experimental evidence indicating that a decay product of the larger trinitroaromatic XI resulting from a methyl hydrogen bond rupture accumulates to a threshold level and then catalytically initiates its continuing exothermic thermochemical decomposition (Reference 44).

In our investigation of *o*-nitrocumene (IX) and its possible α-hydrogen transfer products, we have found local energy minima for a thermodynamically unfavored bicyclic system XIX and a



XIX

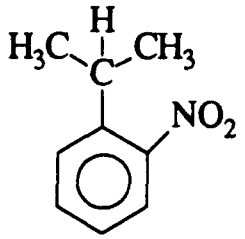
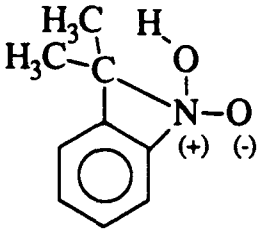
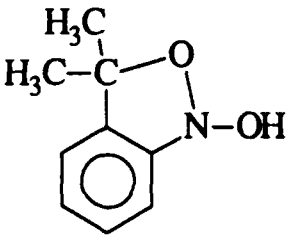


XX

thermodynamically favored bicyclic system XX. Our STO-3G energies for IX, XIX and XX are given in Table 4. As in the case of *o*-nitrotoluene, no local energy minima were found for nitronic acid tautomers of IX.

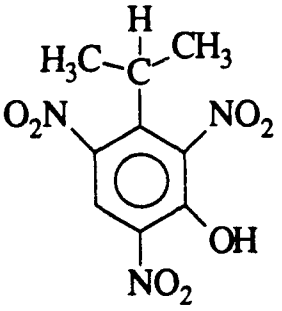
XX is analogous to the hydrogen transfer product XVII, formed from *o*-nitrotoluene. In view of this and the fact that 2,4,6-trinitrocumene and TNT have similar structural features and impact sensitivities (Reference 40), it is conceivable that the decomposition of XII may follow a path initially analogous to that of TNT, involving the rupture of a C-H(α) bond rather than a C-NO_2 bond.

TABLE 4. CALCULATED STO-3G ENERGIES
OF *O*-NITROCUMENE AND RELATED SYSTEMS [a]

	Molecule	Total Energy (hartrees)	Relative Energy (kcal/mole)
IX		-544.33928	0.0
XIX		-544.30219	+23.3
XX		-544.44505	-66.4

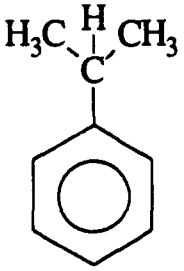
[a]It should be noted that the STO-3G procedure tends to somewhat overestimate the magnitudes of reaction energies.

Our studies relating to 2,4,6-trinitrocumene have also focused on an interesting feature of its x-ray crystal data, which show a planar isopropyl group with relatively short C-CH_3 bond distances (1.418 Å, instead of the typical 1.53 Å) (Reference 53). Gilardi et al have suggested that the apparently planar isopropyl group and shortened C-CH_3 bond distances found in the crystal structure of XII may be a result of turning or flip-flopping by a pyramidal isopropyl group, producing a superpositioning effect in the crystal structure and giving the appearance of a planar isopropyl group with seemingly shortened C-CH_3 distances (References 53 and 54). The crystal structure for a similar molecule, 3-hydroxy-2,4,6-trinitrocumene (XXI), which (unlike XII) has no axis of symmetry, shows a pyramidal isopropyl group with normal C-CH_3 bond distances

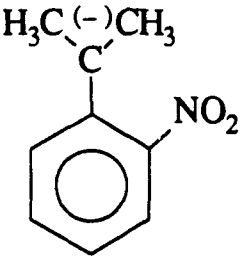


XXI

(Reference 23). In order to clarify the uncertainty concerning the structure of XII, we computed optimized gas phase structures of isopropyl benzene (XXII), 2,4,6-trinitrocumene (XII), *o*-nitrocumene (IX) and the carbanion XXIII of *o*-nitrocumene. All were found to have pyramidal isopropyl groups



XXII



XXIII

with normal C-CH_3 bond lengths. On the basis of our calculations and the other available evidence, we conclude that the isopropyl group of XII in its crystalline form is in fact pyramidal. In this context, it is relevant to point out that both UV (Reference 55) and NMR (Reference 53) studies indicate that the isopropyl group of 2,4,6-trinitrocumene in solution is pyramidal.

SECTION III
CONCLUDING REMARKS

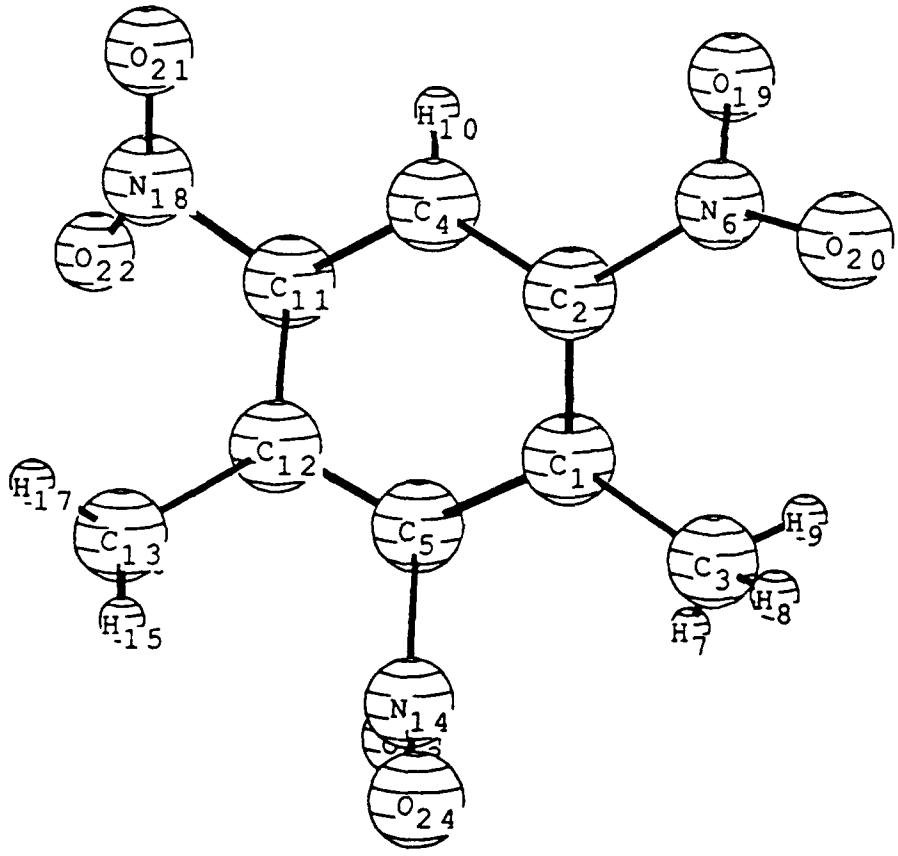
The search for a better understanding of which molecular properties are important in determining the sensitivities of energetic materials to outside stimuli is an important objective of high energy materials research, and reflects a need for the development of less sensitive munitions. In this project, considerable progress has been made in understanding factors which influence sensitivity within separate classes of highly energetic systems. For example, our relationship between $V_{mid,\,max}$ and impact sensitivity for a group of eighteen nitroaromatics suggests that the instability associated with the weakest C-NO_2 linkage in nitroaromatics may be a key factor involved in the initiation of decomposition by impact.

Molecules which do not fit the existing correlations suggest starting points for further investigations aimed at elucidating the basis for their exceptional behavior. This was the driving force for our computational studies relating to hydroxynitroaromatics, which led to our suggestion that the high sensitivities of these compounds may be due to the formation of small quantities of unstable nitronic acid tautomers. We have also investigated possible α-hydrogen transfer and intramolecular ring formation reactions of model systems representing the very insensitive TATB and the alkyl-substituted trinitroaromatics TNT and 2,4,6-trinitrocumene, which have intermediate impact sensitivities but are thermally quite unstable. Our results are consistent with earlier speculation and experimental studies of TATB and TNT.

APPENDIX A
2,4,6-TRINITRO-m-XYLENE

The short distances between non-bonded hydrogens and oxygens are H10-O21 (2.50 Å), H10-O19 (2.50 Å), H17-O22 (2.49 Å), and H9-O20 (2.49 Å).

The N6, N14, and N18 nitro groups are rotated out of the mean plane of the benzene ring by approximately 34°, 36° and 75°, respectively.



Z-MATRIX (ANGSTROMS AND DEGREES)

CD	CENT	ATOM	N1	LENGTH	N2	ALPHA	N3	BETA	J
1	1	C							
2	2	C	1	1.394000 (1)					
3	3	C	1	1.495000 (2)	2	124.600 (24)			
4	4	C	2	1.374000 (3)	1	122.400 (25)	3	174.800 (46)	0
5	5	C	1	1.383000 (4)	2	114.200 (26)	4	-1.700 (47)	0
6	6	N	2	1.474000 (5)	1	120.800 (27)	3	-7.900 (48)	0
7	7	H	3	0.919000 (6)	1	111.800 (28)	2	-137.400 (49)	0
8	8	H	3	1.013000 (7)	1	113.500 (29)	2	85.800 (50)	0
9	9	H	3	0.933000 (8)	1	117.000 (30)	5	151.800 (51)	0
10	10	H	4	0.799000 (9)	2	120.300 (31)	1	-179.100 (52)	0
11	11	C	4	1.374000 (10)	2	119.500 (32)	6	-176.500 (53)	0
12	12	C	5	1.383000 (11)	1	127.200 (33)	3	-175.800 (54)	0
13	13	C	12	1.495000 (12)	5	121.100 (34)	1	-175.800 (55)	0
14	14	N	5	1.480000 (13)	12	116.400 (35)	13	4.200 (56)	0
15	15	H	13	0.919000 (14)	12	111.800 (36)	5	38.800 (57)	0
16	16	H	13	1.013000 (15)	12	113.500 (37)	5	-98.000 (58)	0
17	17	H	13	0.933000 (16)	12	117.000 (38)	11	-24.400 (59)	0
18	18	N	11	1.474000 (17)	4	116.700 (39)	2	-176.500 (60)	0
19	19	O	6	1.220000 (18)	2	116.700 (40)	1	146.400 (61)	0
20	20	O	6	1.223000 (19)	2	118.200 (41)	1	-34.900 (62)	0
21	21	O	18	1.220000 (20)	11	116.700 (42)	4	-36.200 (63)	0
22	22	O	18	1.223000 (21)	11	118.200 (43)	4	142.600 (64)	0
23	23	O	14	1.212000 (22)	5	117.400 (44)	1	-104.400 (65)	0
24	24	O	14	1.212000 (23)	5	117.400 (45)	1	75.600 (66)	0

STOICHIOMETRY C8H7N3O6

E= -915.127510152 **********

EIGENVALUES — -0.31340 -0.31323 0.12593 0.14048 0.18917

Estimated ionization potential: 8.5 ev

TOTAL ATOMIC CHARGES.

		1	Net Charges
1	C	5.928368	+0.07
2	C	5.886401	+0.11
3	C	6.341944	-0.34
4	C	6.122008	-0.12
5	C	5.906374	+0.09
6	N	6.829509	+0.17
7	H	0.868199	+0.13
8	H	0.860808	+0.14
9	H	0.858895	+0.14
10	H	0.851523	+0.15
11	C	5.886519	+0.11
12	C	5.928594	+0.07
13	C	6.341918	-0.34
14	N	6.824424	+0.18
15	H	0.868321	+0.13
16	H	0.860840	+0.14
17	H	0.858946	+0.14
18	N	6.829450	+0.17
19	O	8.186679	-0.19
20	O	8.193803	-0.19
21	O	8.186637	-0.19
22	O	8.193737	-0.19
23	O	8.193052	-0.19
24	O	8.193059	-0.19

DIPOLE MOMENT (DEBYE): X=-0.0464 Y=-0.0094 Z=-1.2699 TOTAL= 1.2707

V_{mid}: C_2-N_6: 0.204
C_{11}-N_{18}: 0.204
C_5-N_{14}: 0.193

Bond Orders: C_2-N_6: 1.24
C_{11}-N_{18}: 1.24
C_5-N_{14}: 1.22
N_6-O_{19}: 2.09
N_6-O_{20}: 2.08
N_{18}-O_{21}: 2.09
N_{18}-O_{22}: 2.08
N_{14}-O_{23}: 2.13
N_{14}-O_{24}: 2.13

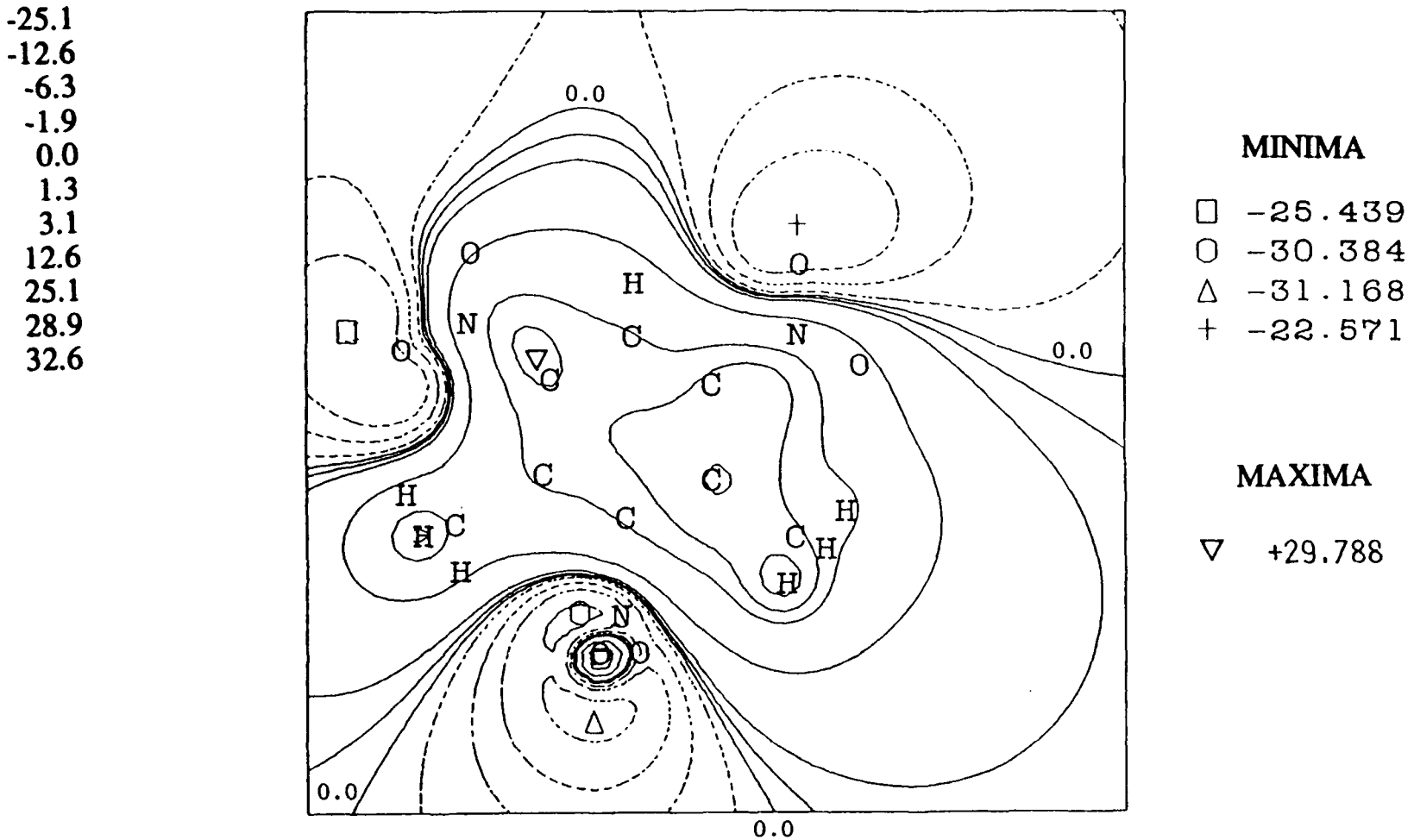
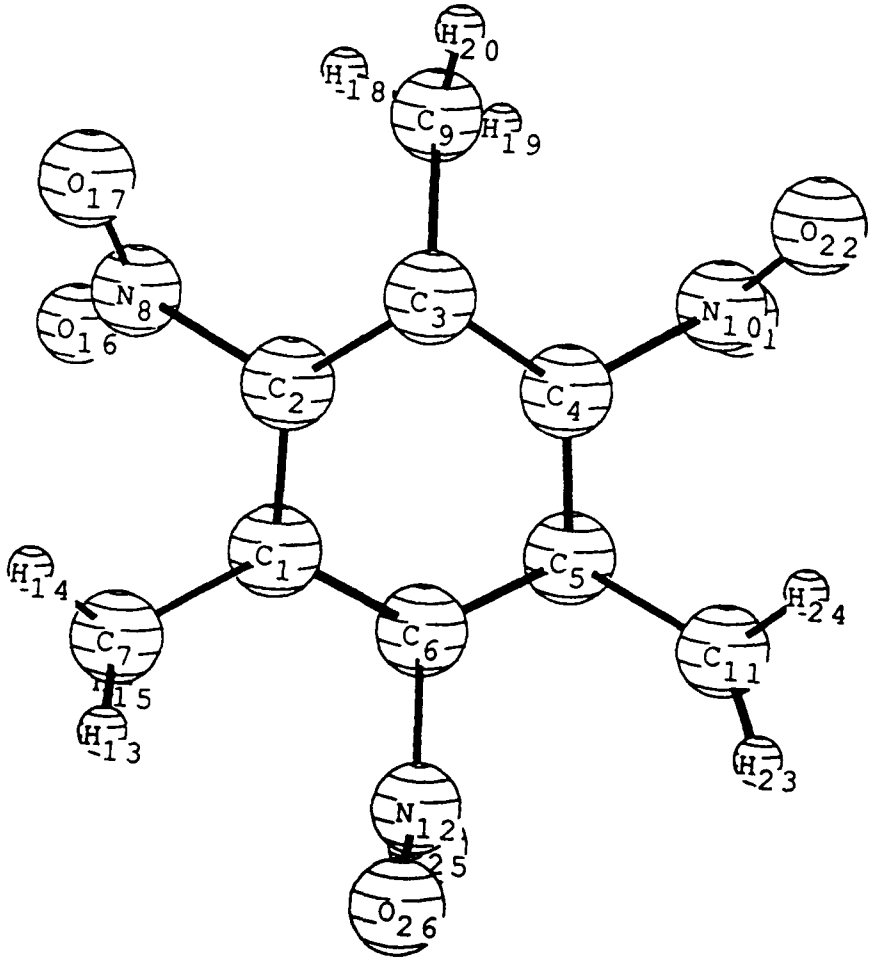


Figure A-1. Calculated electrostatic potential, in kcal/mole, of 2,4,6-trinitro-m-xylene, in the plane 1.75 Å above the aromatic ring. Projected positions of nuclei are shown. The zero contour is indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

APPENDIX B
2,4,6-TRINITROMESITYLENE

The short distances between non-bonded hydrogens and oxygens are H14-O16 (2.54 Å), H13-O27 (2.63 Å) and H18-O17 (2.75 Å). Nitro groups N8, N10 and N12 are rotated out of plane by approximately 68°, 80° and 76° respectively.



Z-MATRIX (ANGSTROMS AND DEGREES)

CD	CENT	ATOM	N1	LENGTH	N2	ALPHA	N3	BETA	J
1	1	C							
2	2	C	1	1.395609 (1)					
3	3	C	2	1.386043 (2)	1	125.260 (27)			
4	4	C	3	1.387340 (3)	2	114.727 (28)	1	0.899 (52)	0
5	5	C	4	1.389094 (4)	3	125.634 (29)	2	-0.110 (53)	0
6	6	C	5	1.386824 (5)	4	114.264 (30)	3	-0.629 (54)	0
7	7	C	1	1.505111 (6)	2	122.513 (31)	3	178.507 (55)	0
8	8	N	2	1.476723 (7)	3	117.487 (32)	4	-178.840 (56)	0
9	9	C	3	1.507730 (8)	2	122.827 (33)	1	179.642 (57)	0
10	10	N	4	1.484054 (9)	3	117.243 (34)	2	179.683 (58)	0
11	11	C	5	1.500910 (10)	4	122.514 (35)	3	-178.694 (59)	0
12	12	N	6	1.481970 (11)	1	117.005 (36)	2	179.542 (60)	0
13	13	H	7	0.897467 (12)	1	109.795 (37)	2	-132.567 (61)	0
14	14	H	7	0.920477 (13)	1	113.329 (38)	2	-6.856 (62)	0
15	15	H	7	0.807418 (14)	1	116.825 (39)	2	116.548 (63)	0
16	16	O	8	1.215072 (15)	2	117.178 (40)	1	-67.545 (64)	0
17	17	O	8	1.210455 (16)	2	118.346 (41)	1	112.427 (65)	0
18	18	H	9	0.985381 (17)	3	110.920 (42)	2	-31.431 (66)	0
19	19	H	9	0.976318 (18)	3	110.997 (43)	2	-144.361 (67)	0
20	20	H	9	0.939811 (19)	3	109.776 (44)	2	93.495 (68)	0
21	21	O	10	1.203774 (20)	4	118.137 (45)	3	80.318 (69)	0
22	22	O	10	1.213591 (21)	4	116.823 (46)	5	-99.956 (70)	0
23	23	H	11	0.939811 (22)	5	110.588 (47)	6	-38.348 (71)	0
24	24	H	11	0.900494 (23)	5	113.224 (48)	6	-160.649 (72)	0
25	25	H	11	0.855687 (24)	5	115.770 (49)	6	81.284 (73)	0
26	26	O	12	1.210209 (25)	6	117.689 (50)	1	104.741 (74)	0
27	27	O	12	1.199151 (26)	6	117.799 (51)	1	-75.967 (75)	0

STOICHIOMETRY C9H9N3O6

SCF DONE: E(RHF) = -953.951944215 A.U. AFTER 22 CYCLES

EIGENVALUES -- -0.31278 0.15650 0.16305 0.19396 0.20529

Estimated ionization potential: 8.52 eV

TOTAL ATOMIC CHARGES.

		1	Net Charge
1	C	5.914823	0.085
2	C	5.912963	0.087
3	C	5.936049	0.064
4	C	5.912801	0.088
5	C	5.922433	0.078
6	C	5.913981	0.086
7	C	6.448136	-0.448
8	N	6.828167	0.172
9	C	6.309673	-0.690
10	N	6.824056	0.176
11	C	6.407643	-0.408
12	N	6.821455	0.179
13	H	0.835545	0.164
14	H	0.846728	0.153
15	H	0.827870	0.172
16	O	8.196955	-0.197
17	O	8.192877	-0.193
18	H	0.877386	0.123
19	H	0.876473	0.124
20	H	0.864341	0.136
21	O	8.194207	-0.194
22	O	8.197069	-0.197
23	H	0.855237	0.145
24	H	0.851193	0.149
25	H	0.837340	0.163
26	O	8.196696	-0.197
27	O	8.197903	-0.198

DIPOLE MOMENT (DEBYE): X= 0.0817 Y=-0.0475 Z= 0.0520 TOTAL= 0.1078

V-mid: N8-C2: 0.186
N10-C4: 0.188
N12-C6: 0.189

Bond Order: N8-C2: 1.22
N10-C4: 1.20
N12-C6: 1.21
O17-N8: 1.96
O18-N8: 1.98
O21-N10: 2.02
O22-N10: 1.97
O26-N12: 1.99
O27-N12: 2.04

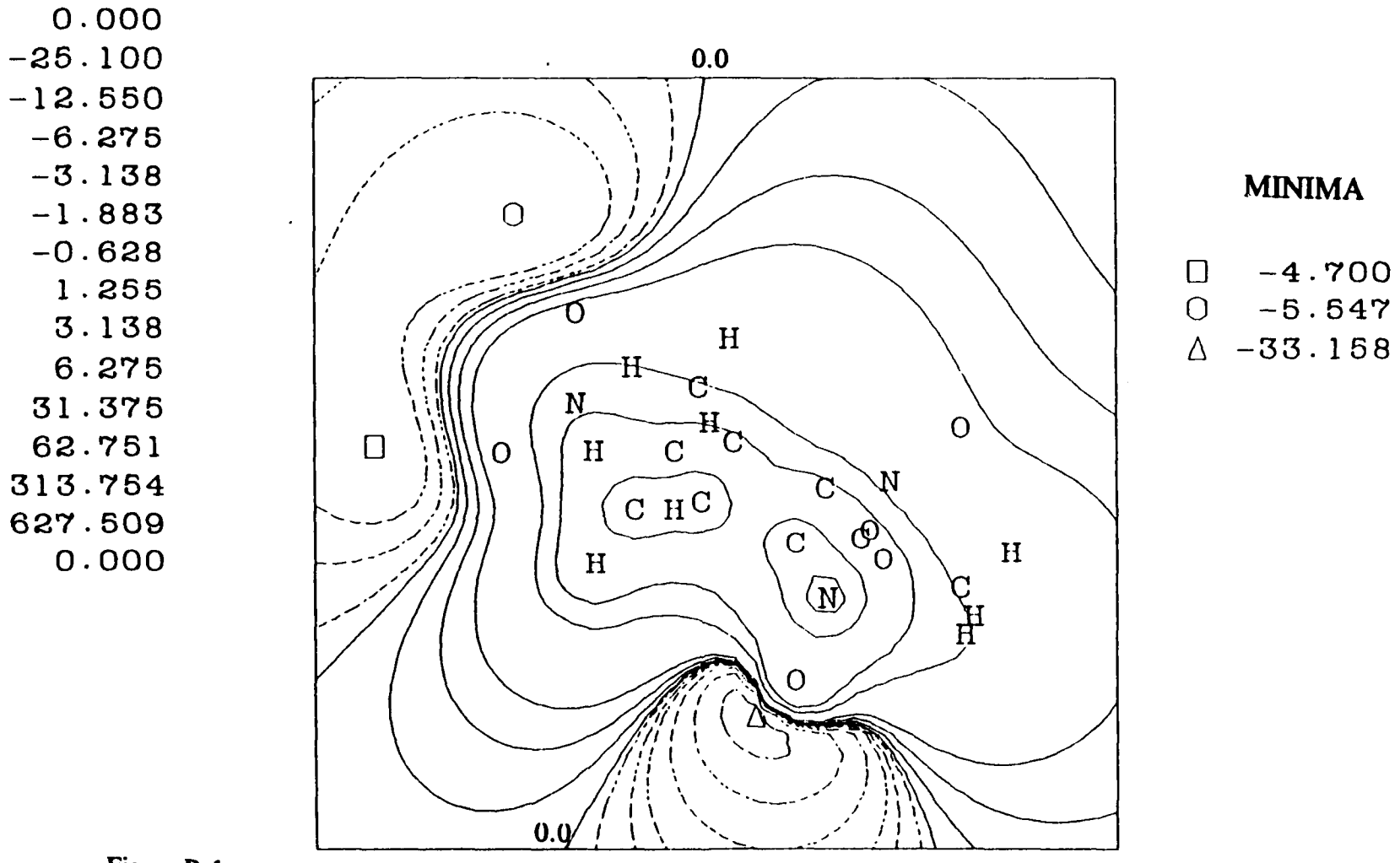


Figure B-1. Calculated electrostatic potential, in kcal/mole, of 2,4,6-trinitromesitylene, in the plane 1.75Å above the N8 nitro group located in the upper left corner. Projected positions of nuclei are shown. The zero contour is indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

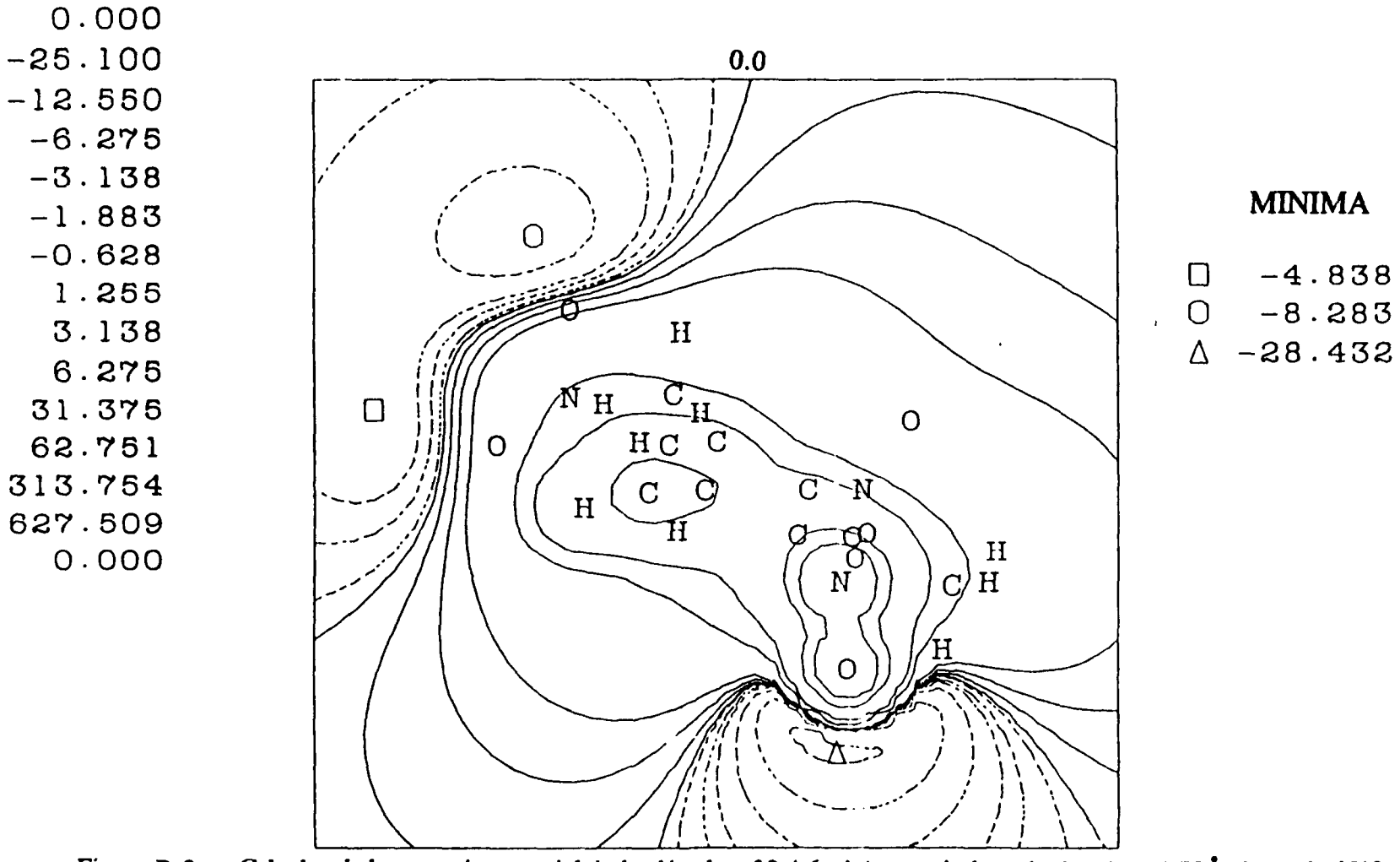
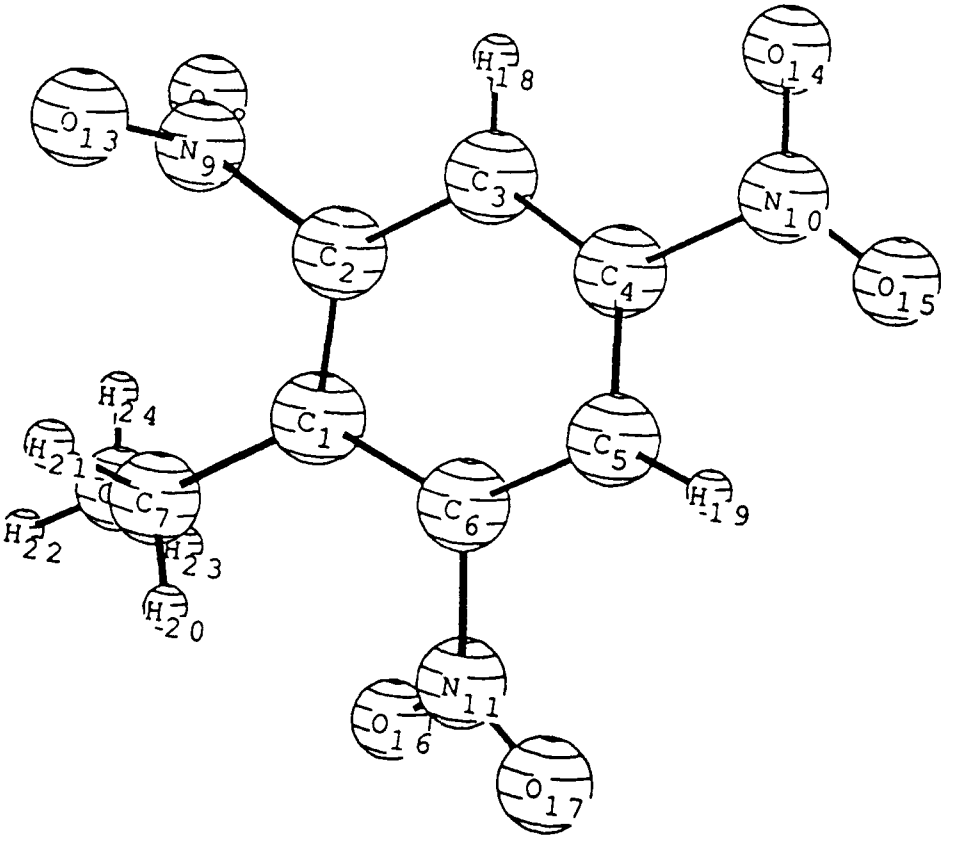


Figure B-2. Calculated electrostatic potential, in kcal/mole, of 2,4,6-trinitromesitylene, in the plane 1.75Å above the N12 nitro group located in the upper left corner. Projected positions of nuclei are shown. The zero contour is indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

APPENDIX C
2,4,6-TRINITROETHYLBENZENE

The short distances between non-bonded hydrogens and oxygens are H18-O14 (2.43 Å), H19-O15 (2.35 Å), H20-O16 (2.43 Å) and H21-O13 (2.50 Å).

The N10 nitro group is rotated by only about 6°, while the other nitro groups are both rotated by more than 50° (N9 ~ 63° and N11 ~ 51°).



Z-MATRIX (ANGSTROMS AND DEGREES)

CD	CENT	ATOM	N1	LENGTH	N2	ALPHA	N3	BETA	J
1	1	C							
2	2	C	1	1.380000 (1)					
3	3	C	2	1.400036 (2)	1	124.138 (24)			
4	4	C	3	1.346180 (3)	2	117.570 (25)	1	-3.060 (46)	0
5	5	C	4	1.397462 (4)	3	123.258 (26)	2	0.463 (47)	0
6	6	C	5	1.367845 (5)	4	115.552 (27)	3	3.213 (48)	0
7	7	C	1	1.505557 (6)	2	123.639 (28)	3	-177.818 (49)	0
8	8	C	7	1.531437 (7)	1	112.348 (29)	2	76.921 (50)	0
9	9	N	2	1.458938 (8)	3	115.966 (30)	4	177.472 (51)	0
10	10	N	4	1.491610 (9)	5	116.888 (31)	6	-178.171 (52)	0
11	11	N	6	1.479831 (10)	5	113.743 (32)	4	176.560 (53)	0
12	12	O	9	1.215648 (11)	2	118.028 (33)	3	62.726 (54)	0
13	13	O	9	1.214990 (12)	2	118.662 (34)	3	-115.532 (55)	0
14	14	O	10	1.233005 (13)	4	114.830 (35)	5	172.910 (56)	0
15	15	O	10	1.196704 (14)	4	119.125 (36)	5	-5.044 (57)	0
16	16	O	11	1.214990 (15)	6	118.365 (37)	5	-129.708 (58)	0
17	17	O	11	1.215648 (16)	6	117.347 (38)	5	50.922 (59)	0
18	18	H	3	0.999000 (17)	2	118.732 (39)	1	177.032 (60)	0
19	19	H	5	0.943875 (18)	4	115.541 (40)	3	-165.104 (61)	0
20	20	H	7	0.958645 (19)	1	108.895 (41)	2	-162.317 (62)	0
21	21	H	7	0.958645 (20)	1	109.240 (42)	2	-43.190 (63)	0
22	22	H	8	0.956504 (21)	7	115.751 (43)	1	-177.865 (64)	0
23	23	H	8	0.961509 (22)	7	103.014 (44)	1	63.451 (65)	0
24	24	H	8	0.951525 (23)	7	108.837 (45)	1	-52.805 (66)	0

STOICHIOMETRY C8H7N3O6

SCF DONE: E(RHF) = -915.264040980

EIGENVALUES -- -0.31648 -0.31536 0.12440 0.13591 0.18671

Estimated ionization potential: 8.59 ev

TOTAL ATOMIC CHARGES.

		1	Net Charge
1	C	5.940839	0.059
2	C	5.897024	0.103
3	C	6.054537	-0.055
4	C	5.893531	0.106
5	C	6.071561	-0.072
6	C	5.895058	0.105
7	C	6.174044	-0.174
8	C	6.295210	-0.295
9	N	6.831461	0.169
10	N	6.819867	0.180
11	N	6.827034	0.173
12	O	8.189978	-0.190
13	O	8.192139	-0.192
14	O	8.198018	-0.198
15	O	8.186915	-0.187
16	O	8.195772	-0.196
17	O	8.190246	-0.190
18	H	0.860837	0.139
19	H	0.852713	0.147
20	H	0.886131	0.114
21	H	0.881087	0.119
22	H	0.885397	0.115
23	H	0.885462	0.115
24	H	0.895142	0.105

DIPOLE MOMENT (DEBYE): X=-0.9287 Y= 0.0689 Z=-0.6332 TOTAL= 1.1262

Bond Order:		V-mid:	
C2-N9:	1.27	C2-N9:	0.197
C4-N10:	1.18	C4-N10:	0.203
C6-N11:	1.21	C6-N11:	0.199
N9-O12:	1.96		
N9-O13:	1.96		
N10-O14:	1.88		
N10-O15:	2.05		
N11-O16:	1.96		
N11-O17:	1.96		

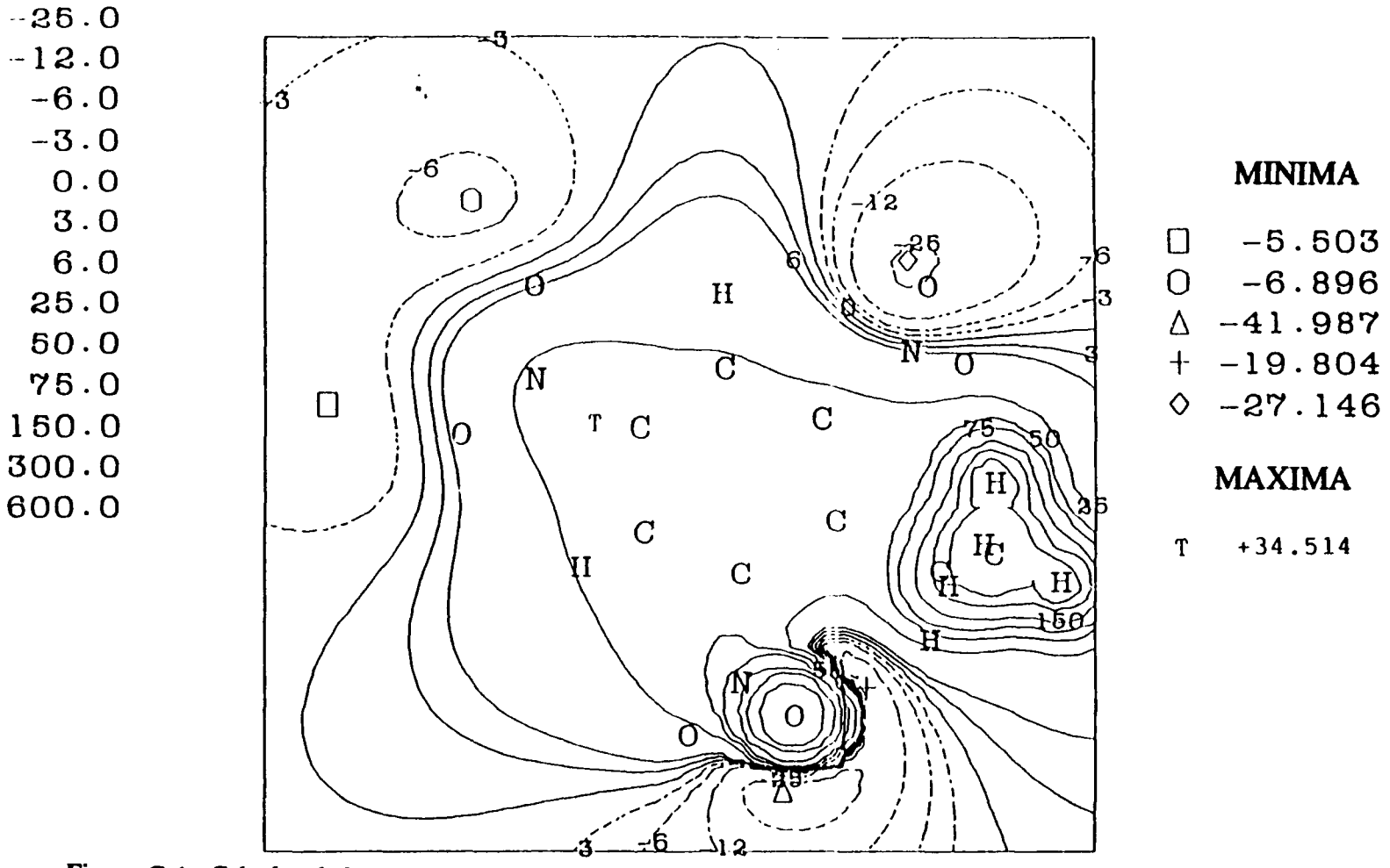


Figure C-1. Calculated electrostatic potential, in kcal/mole, of 2,4,6-trinitroethylbenzene, in the plane 1.75Å above the N10 nitro group located in the upper left corner. Projected positions of nuclei are shown. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

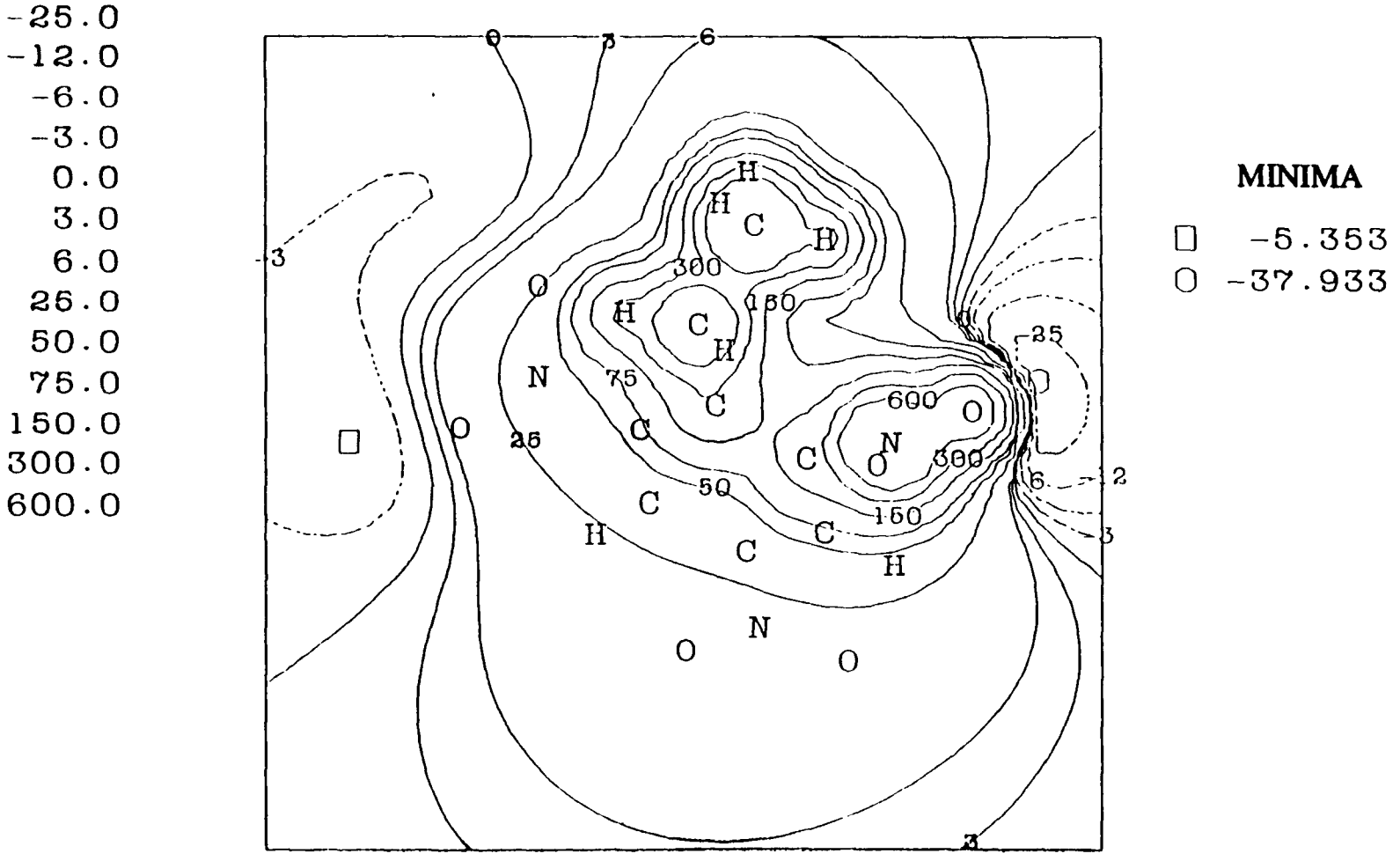
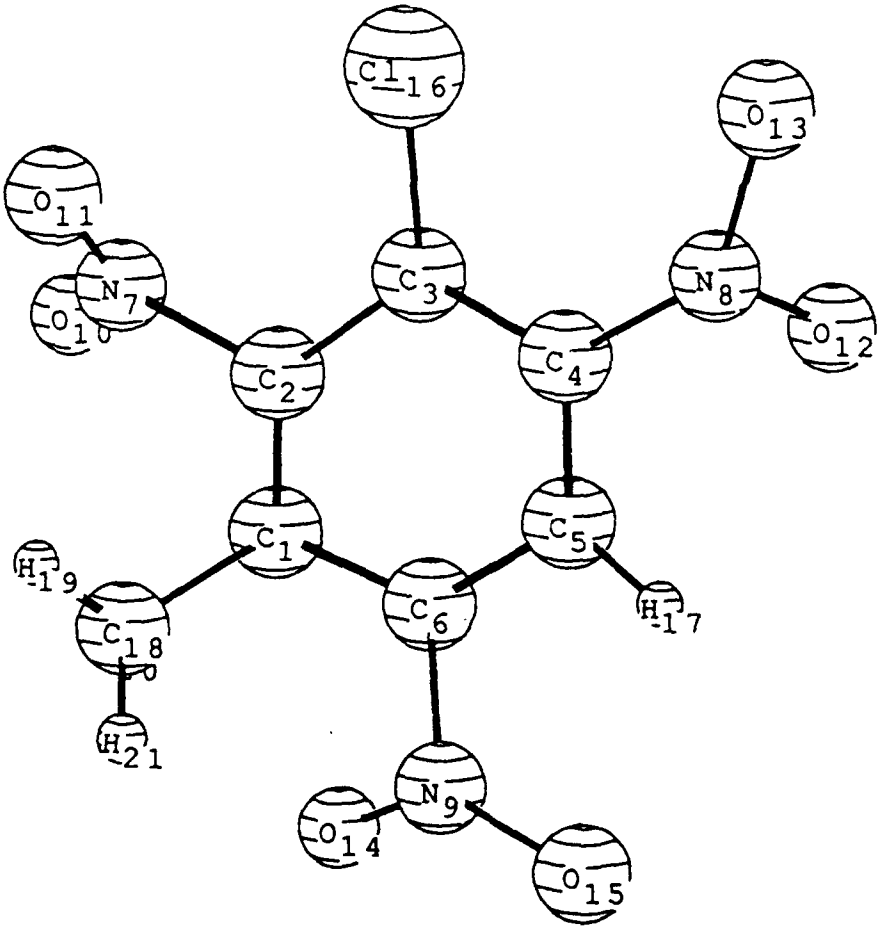


Figure C-2. Calculated electrostatic potential, in kcal/mole, of 2,4,6-trinitroethylbenzene, in the plane 1.75Å above the N11 nitro group located in the upper left corner. Projected positions of nuclei are shown. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

APPENDIX D
3-CHLORO-2,4,6-TRINITROTOLUENE

The short distances between non-bonded hydrogens and oxygens are H21-O14 (2.41 Å) and H17-O15 (2.23 Å).

The N8 and N9 nitro groups are both rotated by approximately 35°,while the N7 nitro group is rotated by more than 80°.



Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.338000(1)					
3	3	C	2	1.431227(2)	1	125.709(21)			
4	4	C	3	1.392368(3)	2	115.670(22)	1	-4.255(40)	0
5	5	C	4	1.397305(4)	3	120.647(23)	2	5.006(41)	0
6	6	C	5	1.352392(5)	4	119.011(24)	3	-4.079(42)	0
7	7	N	2	1.493255(6)	3	115.308(25)	4	-178.749(43)	0
8	8	N	4	1.422590(7)	5	115.670(26)	6	175.975(44)	0
9	9	N	6	1.523058(8)	5	117.187(27)	4	-178.672(45)	0
10	10	O	7	1.269114(9)	2	118.481(28)	3	104.866(46)	0
11	11	O	7	1.177459(10)	2	114.795(29)	3	-80.214(47)	0
12	12	O	9	1.177940(11)	4	121.200(30)	3	-144.258(48)	0
13	13	O	[illegible]	1.243590(12)	4	118.718(31)	3	35.657(49)	0
14	14	O	9	1.199396(13)	6	117.118(32)	5	-141.221(50)	0
15	15	O	9	1.259951(14)	6	113.854(33)	5	34.945(51)	0
16	16	Cl	3	1.7[illegible]3444(15)	4	123.246(34)	5	179.843(52)	0
17	17	H	5	1.0[illegible]2224(16)	4	133.416(35)	3	-174.849(53)	0
18	18	C	1	1.499997(17)	2	123.104(36)	3	179.209(54)	0
19	19	H	18	0.960230(18)	1	109.426(37)	2	-20.452(55)	0
20	20	H	18	0.959922(19)	1	109.476(38)	2	99.587(56)	0
21	21	H	18	0.959896(20)	1	109.444(39)	2	-140.413(57)	0

STOICHIOMETRY C7H4ClN3O6

SCF DONE: E(RHF) = -1333.56294463 A.U. AFTER 23 CYCLES

Alpha eigenvalues — -0.30955 0.10873 0.13643 0.17527 0.19758

Estimated ionization potential: 8.43 ev

Total atomic charges:

		1
1	C	0.066131
2	C	0.095898
3	C	0.061032
4	C	0.105802
5	C	-0.051140
6	C	0.097191
7	N	0.171478
8	N	0.169550
9	N	0.170954
10	O	-0.199021
11	O	-0.160216
12	O	-0.180358
13	O	-0.195691
14	O	-0.169041
15	O	-0.196948
16	Cl	-0.088883
17	H	0.149857
18	C	-0.310376
19	H	0.124371
20	H	0.141483
21	H	0.128727

Dipole moment (Debye):

X= 2.2897 Y= 0.7259 Z= -0.1213 Tot= 2.4050

V-mid: C2-N7: 0.189
C4-N8: 0.205
C6-N9: 0.186

Bond Order: C2-N7: 1.18
C4-N8: 1.36
C6-N9: 1.11
N7-O10: 1.72
N7-O11: 2.16
N8-O12: 2.15
N8-O13: 1.83
N9-O14: 2.04
N9-O15: 1.76

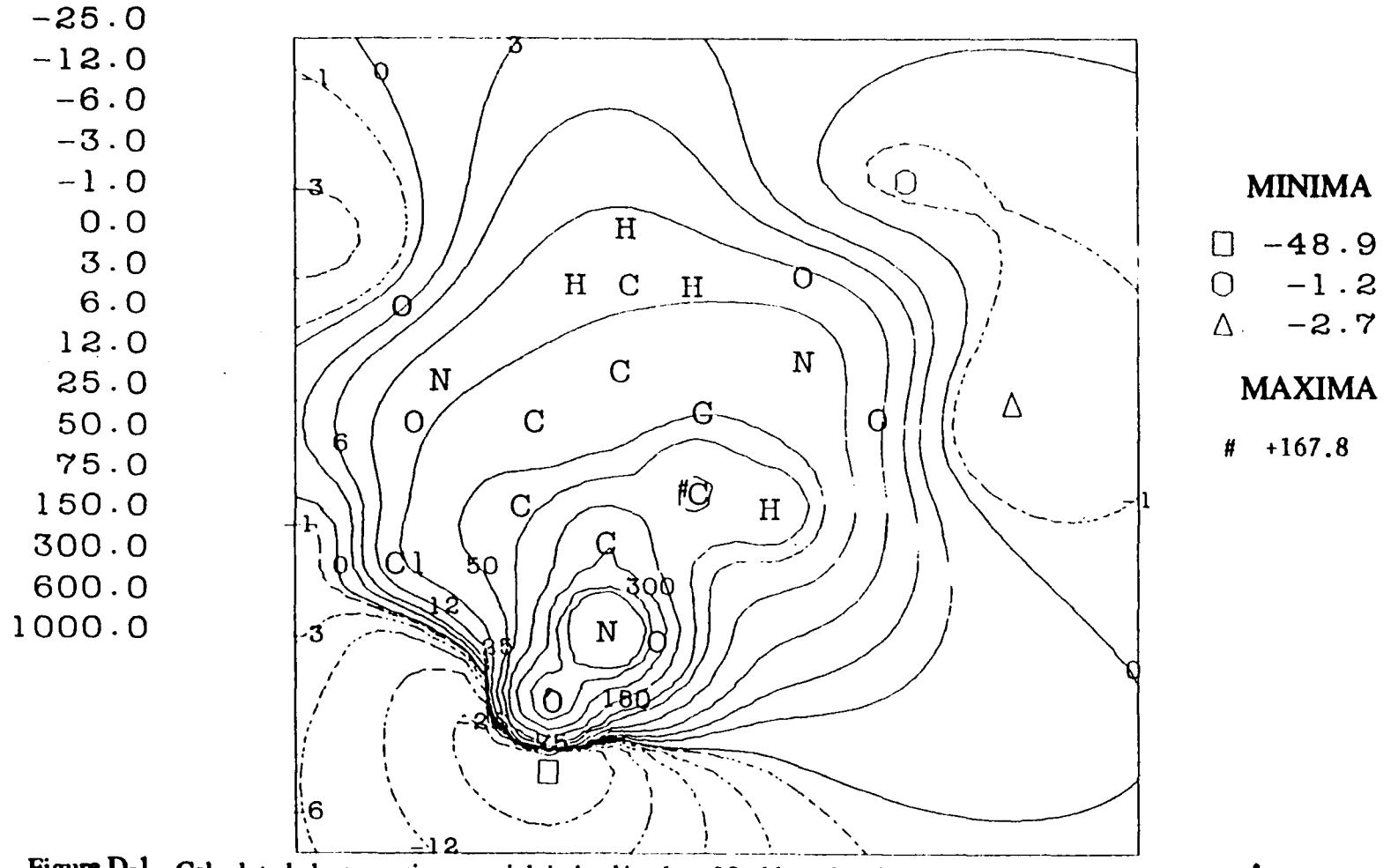


Figure D-1. Calculated electrostatic potential, in kcal/mole, of 3-chloro-2,4,6-trinitrotoluene, in the plane 1.75Å above the N9 nitro group located in the upper right corner. Projected positions of nuclei are shown. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

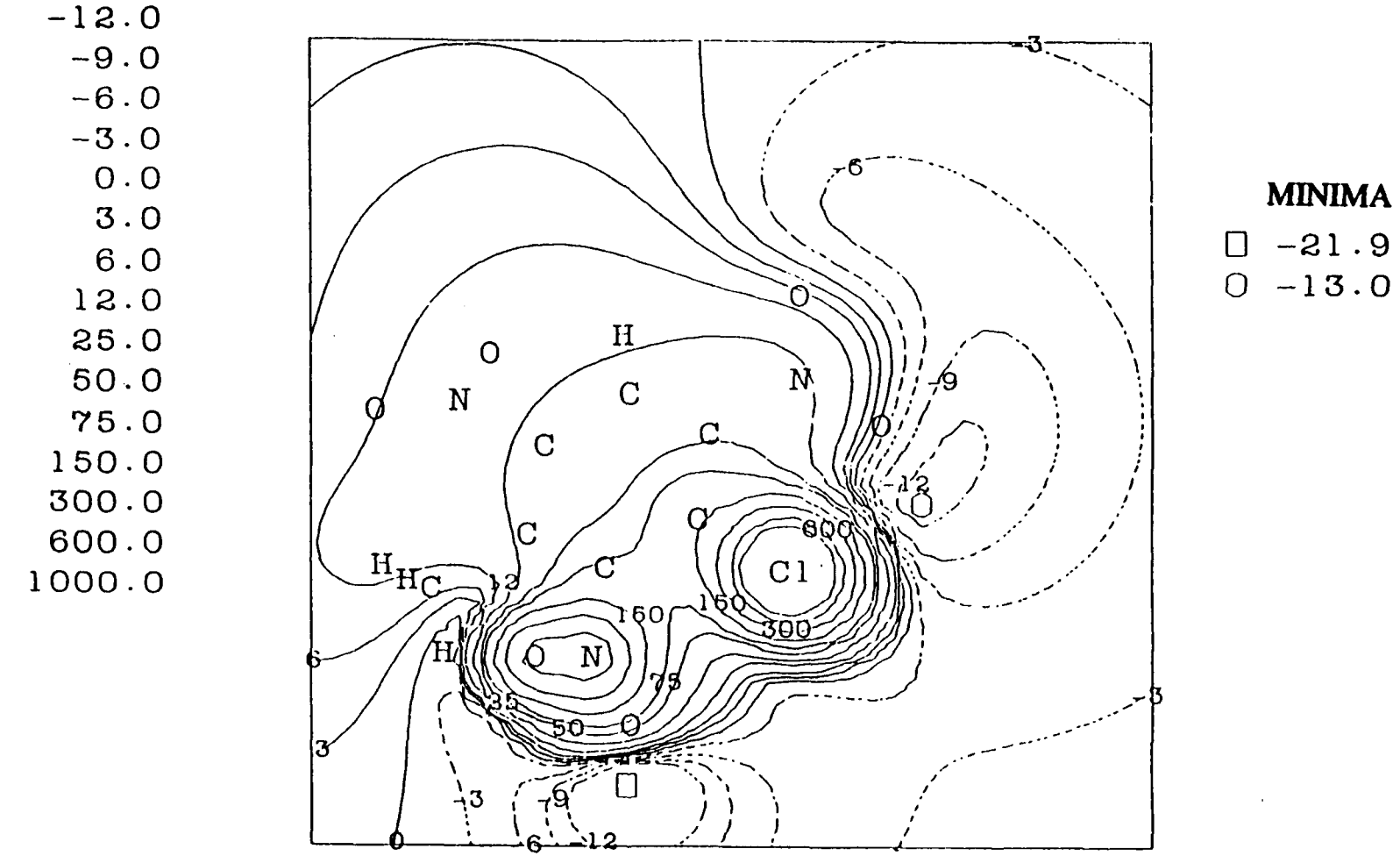
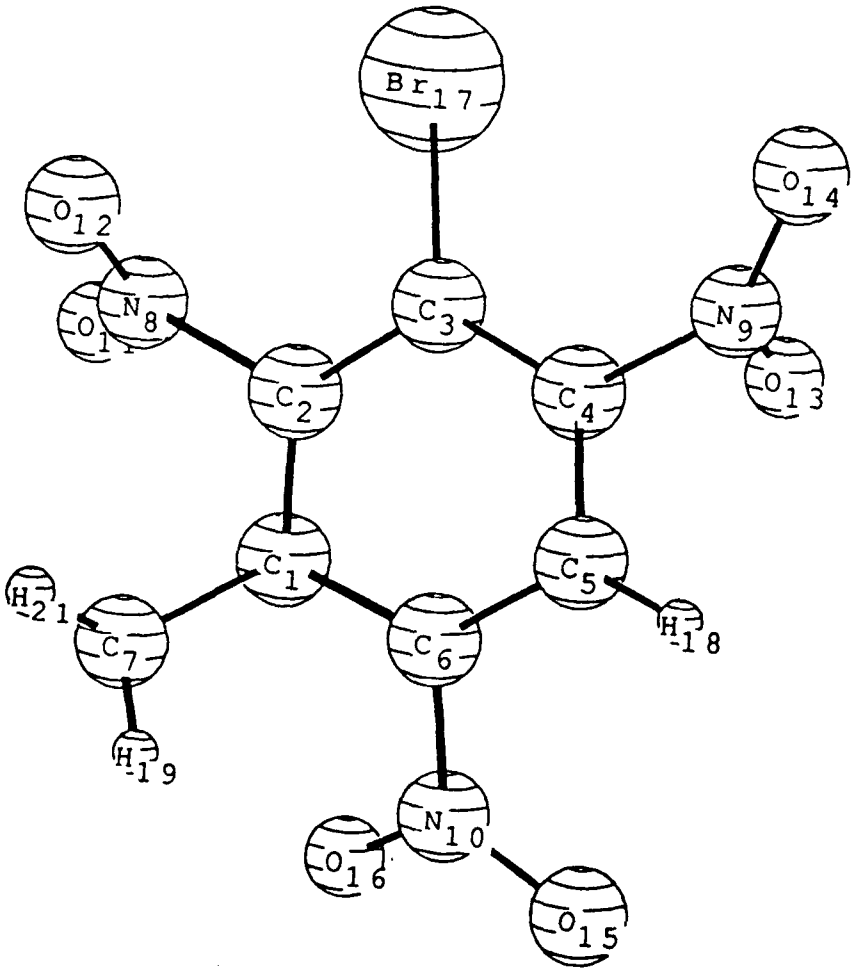


Figure D-2 Calculated electrostatic potential, in kcal/mole, of 3-chloro-2,4,6-trinitrotoluene, in the plane 1.75Å above the N8 nitro group located in the upper right corner. Projected positions of nuclei are shown. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

APPENDIX E
3-BROMO-2,4,6-TRINITROTOLUENE

The short distances between non-bonded hydrogens and oxygens are H18-O15 (2.47 Å) and H19-O16 (2.34 Å).

The N8 nitro group is rotated out of the mean plane of the benzene ring by almost 80°, while the N9 and N1 nitro groups are rotated by about 50° and 37°, respectively.



Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.391000(1)					
3	3	C	2	1.386831(2)	1	124.752(21)			
4	4	C	3	1.367699(3)	2	117.830(22)	1	-2.954(40)	0
5	5	C	4	1.405916(4)	3	122.057(23)	2	2.925(41)	0
6	6	C	5	1.379891(5)	4	117.088(24)	3	-1.195(42)	0
7	7	C	1	1.501066(6)	2	120.867(25)	3	178.765(43)	0
8	8	N	2	1.455638(7)	3	118.921(26)	4	179.894(44)	0
9	9	N	4	1.474076(8)	5	115.988(27)	6	176.831(45)	0
10	10	N	6	1.465537(9)	5	114.783(28)	4	178.164(46)	0
11	11	O	8	1.237110(10)	2	116.781(29)	3	100.573(47)	0
12	12	O	8	1.212164(11)	2	119.976(30)	3	-77.726(48)	0
13	13	O	9	1.227232(12)	4	116.041(31)	3	-131.017(49)	0
14	14	O	9	1.192896(13)	4	118.673(32)	3	50.430(50)	0
15	15	O	10	1.228251(14)	6	118.145(33)	1	-145.222(51)	0
16	16	O	10	1.213507(15)	6	118.555(34)	1	39.369(52)	0
17	17	Br	3	1.866842(16)	4	123.075(35)	5	-177.475(53)	0
18	18	H	5	0.962237(17)	4	121.577(36)	3	178.812(54)	0
19	19	H	7	0.960260(18)	1	109.064(37)	6	13.932(55)	0
20	20	H	7	0.966540(19)	1	108.844(38)	6	-105.062(56)	0
21	21	H	7	0.952576(20)	1	109.759(39)	6	134.493(57)	0

STOICHIOMETRY C7H4BrN3O6

SCF DONE: E(RHF) = -3434.62662133

Alpha eigenvalues -- -0.34376 -0.31921 -0.31638 -0.31605 0.12262

Estimated ionization potential: 8.61 ev

Total atomic charges:

		1
1	C	0.081237
2	C	0.092632
3	C	-0.033527
4	C	0.100238
5	C	-0.050166
6	C	0.096820
7	C	-0.317159
8	N	0.159052
9	N	0.179317
10	N	0.166279
11	O	-0.189477
12	O	-0.176590
13	O	-0.195644
14	O	-0.178994
15	O	-0.194100
16	O	-0.189239
17	Br	0.105347
18	H	0.142476
19	H	0.133943
20	H	0.139252
21	H	0.128303

Dipole moment (Debye):

X= 0.7450 Y= -0.9522 Z= 0.3259 Tot= 1.2522

Bond Order:	C2–N8:	1.28	V–mid: C2–N8:	0.183
	C4–N9:	1.23	C4–N9:	0.200
	C6–N10:	1.25	C6–N10:	0.190
	N8–O11:	1.86		
	N8–O12:	1.98		
	N9–O13:	1.91		
	N9–O14:	2.07		
	N10–O15:	1.90		
	N10–O16:	1.97		

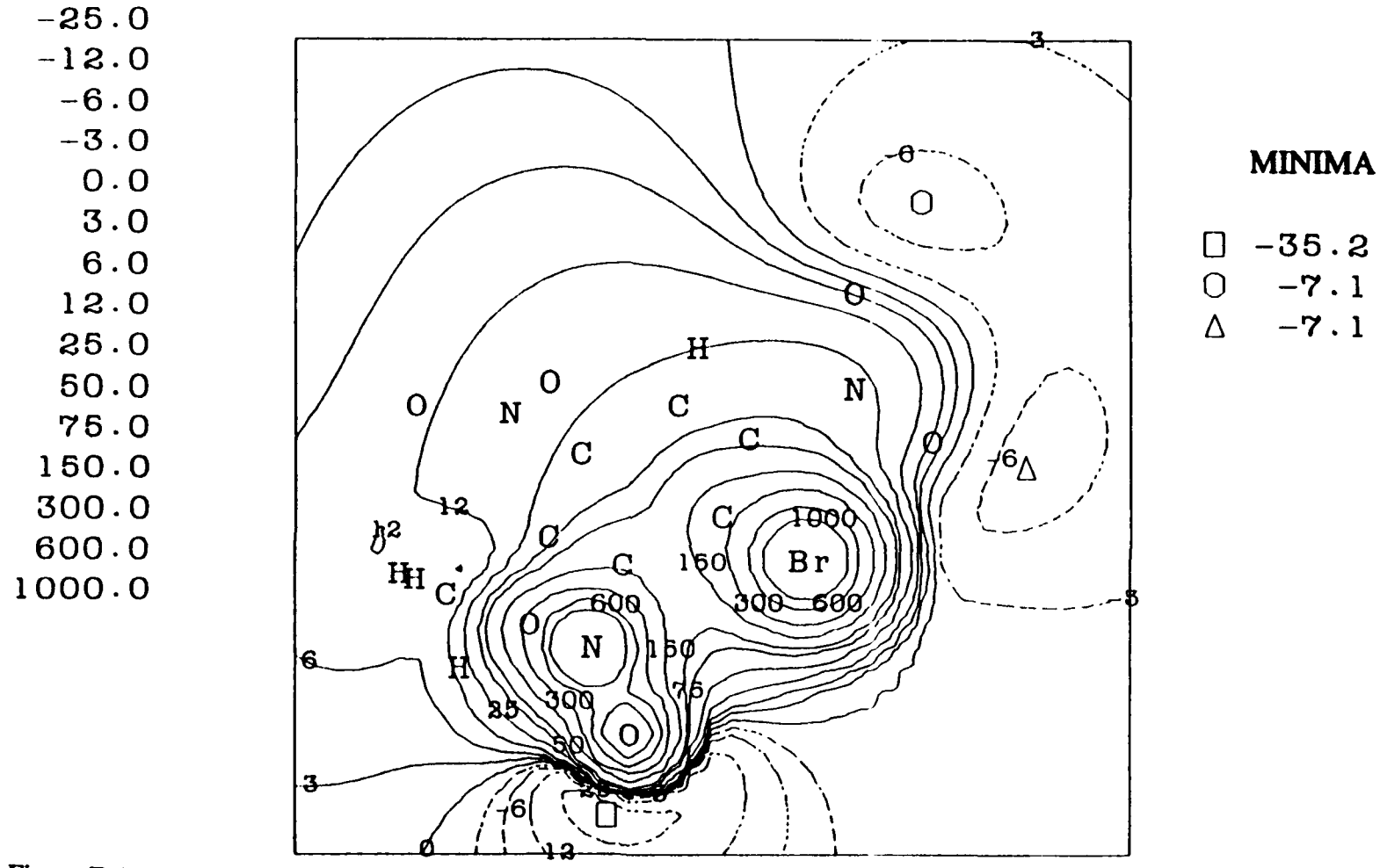


Figure E-1. Calculated electrostatic potential, in kcal/mole, of 3-bromo-2,4,6-trinitrotoluene, in the plane 1.75Å above the N9 nitro group located in the upper right corner. Projected positions of nuclei are shown. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

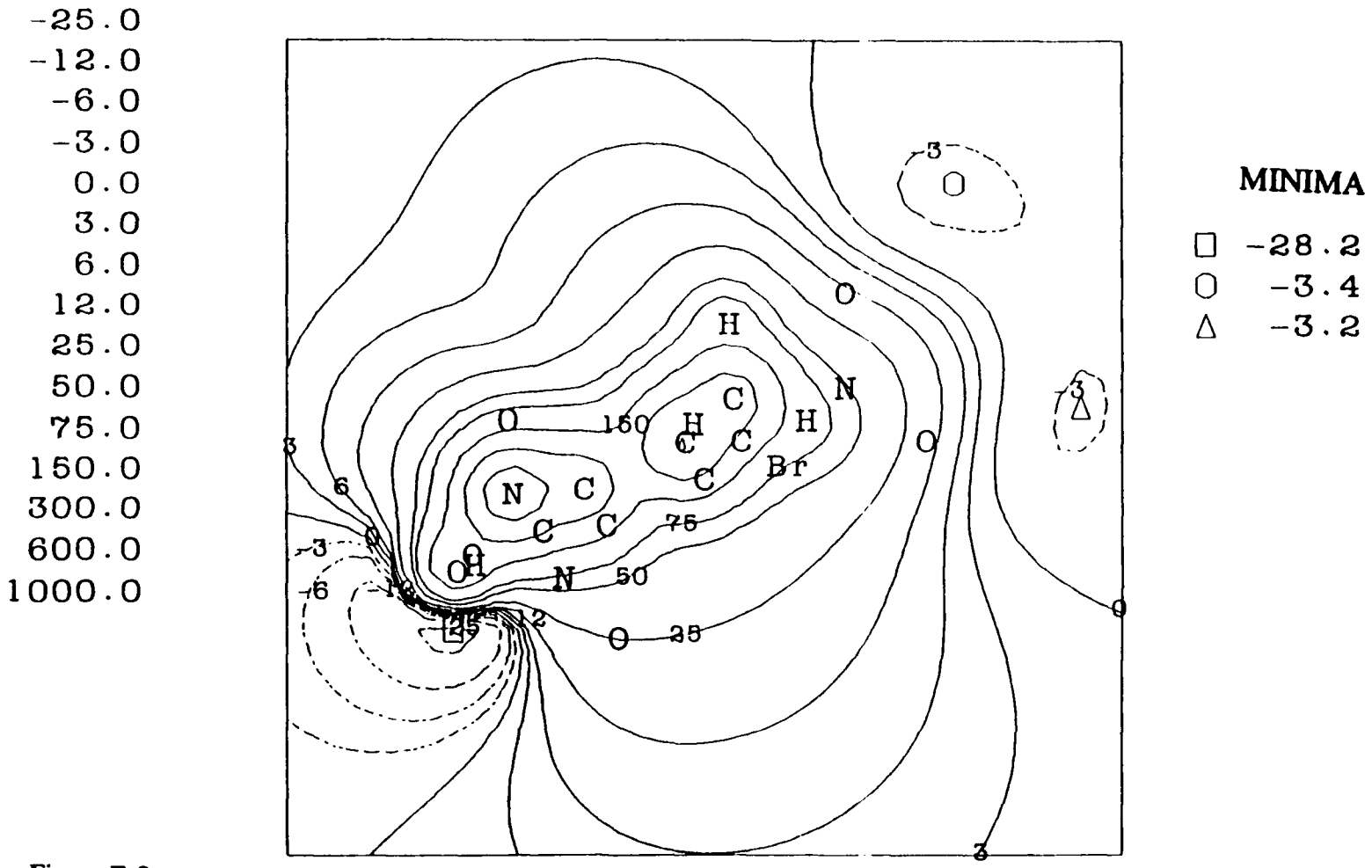
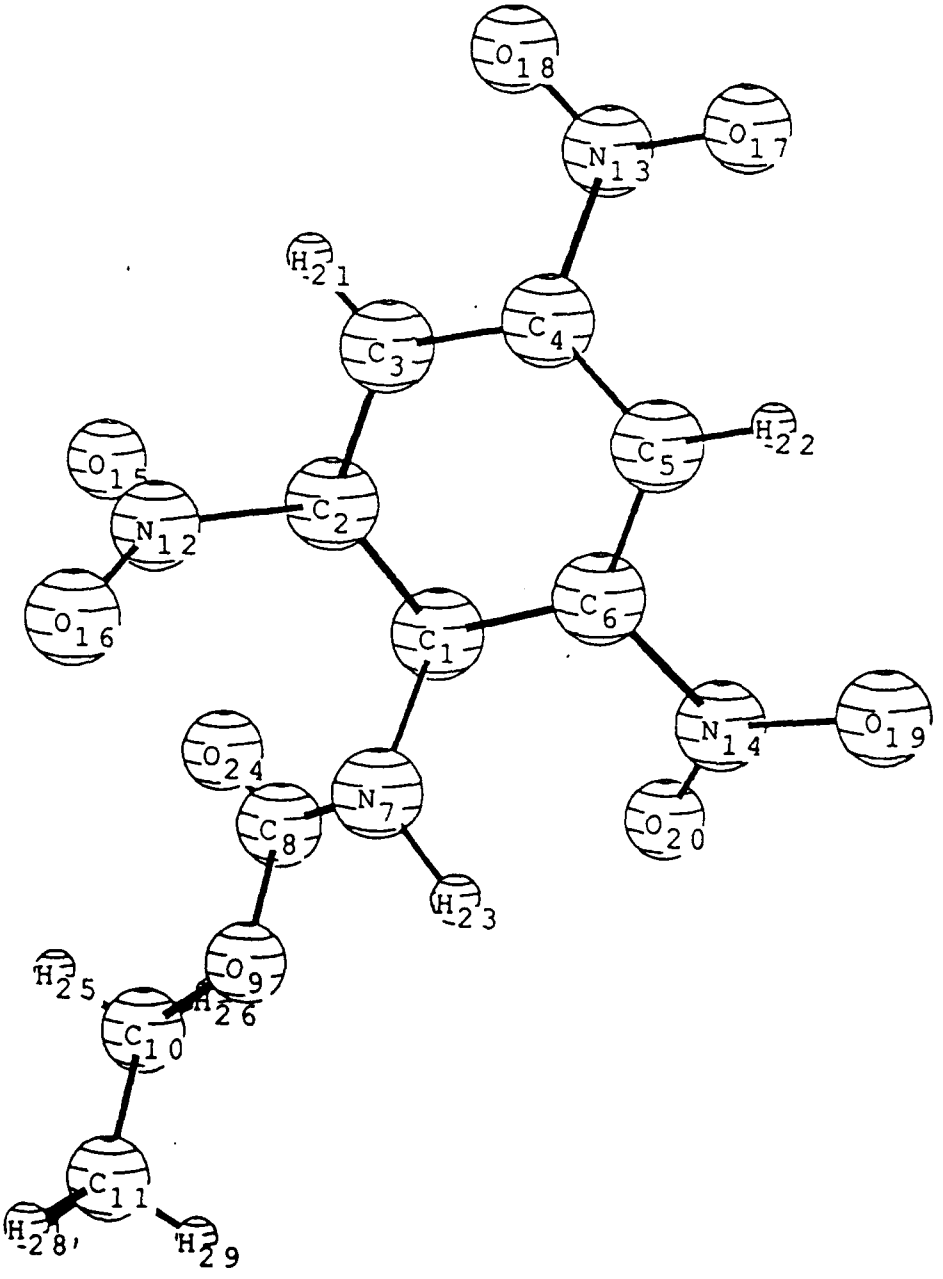


Figure E-2. Calculated electrostatic potential, in kcal/mole, of 3-bromo-2,4,6-trinitrotoluene, in the plane 1.75Å above the N8 nitro group located in the upper right corner. Projected positions of nuclei are shown. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

APPENDIX F
ETHYL(2,4,6-TRINITROPHENYL)CARBAMATE

The short distances between non-bonded hydrogens and oxygens are H21-O18 (2.41 Å), H22-O17 (2.47 Å), H22-O19 (2.49 Å) and H23-O20 (2.47 Å).

The N13 nitro group is rotated out of the mean plane of the benzene ring by approximately 17°, while the N12 and N14 nitro groups are rotated by about 47° and 38°, respectively.



Total atomic charges:

		1
1	C	0.163779
2	C	0.102747
3	C	-0.049115
4	C	0.097327
5	C	-0.045397
6	C	0.084142
7	N	-0.347840
8	C	0.453964
9	O	-0.266240
10	C	-0.017669
11	C	-0.265862
12	N	0.183854
13	N	0.177201
14	N	0.162719
15	O	-0.190126
16	O	-0.188573
17	O	-0.195429
18	O	-0.187207
19	O	-0.180792
20	O	-0.193106
21	H	0.144867
22	H	0.144513
23	H	0.234194
24	O	-0.323841
25	H	0.105095
26	H	0.097999
27	H	0.098282
28	H	0.100922
29	H	0.099590

Dipole moment (Debye):

X= -1.4823 Y= -1.0772 Z= -2.2757 Tot= 2.9217

V-mid:

C2-N12:	0.206
C4-N13:	0.196
C6-N14:	0.178

Bond Order:

C2-N12:	1.22
C4-N13:	1.20
C6-N14:	1.23
N12-O15:	1.86
N12-O16:	2.08
N13-O17:	1.91
N13-O18:	1.99
N14-O19:	1.94
N14-O20:	1.86

Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.399800(1)					
3	3	C	2	1.393593(2)	1	122.211(29)			
4	4	C	3	1.356650(3)	2	117.976(30)	1	-2.034(56)	0
5	5	C	4	1.392623(4)	3	122.722(31)	2	-0.698(57)	0
6	6	C	5	1.371787(5)	4	117.297(32)	3	4.441(58)	0
7	7	N	1	1.417745(6)	6	122.775(33)	5	-175.318(59)	0
8	8	C	7	1.335253(7)	1	123.100(34)	6	-132.616(60)	0
9	9	O	8	1.326876(8)	7	110.646(35)	1	-177.780(61)	0
10	10	C	9	1.455369(9)	8	115.561(36)	7	-175.735(62)	0
11	11	C	10	1.510133(10)	9	106.304(37)	8	-172.991(63)	0
12	12	N	2	1.477193(11)	3	116.070(38)	4	173.007(64)	0
13	13	N	4	1.485025(12)	5	118.794(39)	6	-175.858(65)	0
14	14	N	6	1.473533(13)	5	115.792(40)	4	172.441(66)	0
15	15	O	12	1.237979(14)	2	116.782(41)	3	45.589(67)	0
16	16	O	12	1.191493(15)	2	118.935(42)	3	-131.685(68)	0
17	17	O	13	1.227110(16)	4	117.538(43)	5	-15.869(69)	0
18	18	O	13	1.210411(17)	4	115.965(44)	5	162.675(70)	0
19	19	O	14	1.218843(18)	6	117.626(45)	5	36.970(71)	0
20	20	O	14	1.237588(19)	6	117.526(46)	5	-140.997(72)	0
21	21	H	3	0.990490(20)	4	121.382(47)	5	-179.820(73)	0
22	22	H	5	0.991278(21)	4	121.110(48)	3	-175.253(74)	0
23	23	H	7	1.103857(22)	1	112.322(49)	2	-144.341(75)	0
24	24	O	8	1.240796(23)	7	124.869(50)	1	2.065(76)	0
25	25	H	10	0.988518(24)	9	110.438(51)	8	-53.410(77)	0
26	26	H	10	0.991278(25)	9	110.198(52)	8	67.654(78)	0
27	27	H	11	0.993518(26)	10	109.272(53)	9	179.887(79)	0
28	28	H	11	0.991666(27)	10	109.485(54)	9	60.027(80)	0
29	29	H	11	0.990416(28)	10	109.612(55)	9	-60.207(81)	0

STOICHIOMETRY C9H8N4O8

SCF DONE: E(RHF) = -1156.89781294

EIGENVALUES — -0.31594 -0.30710 0.12151 0.12545 0.18009

Esimated ionization potential: 8.37 ev

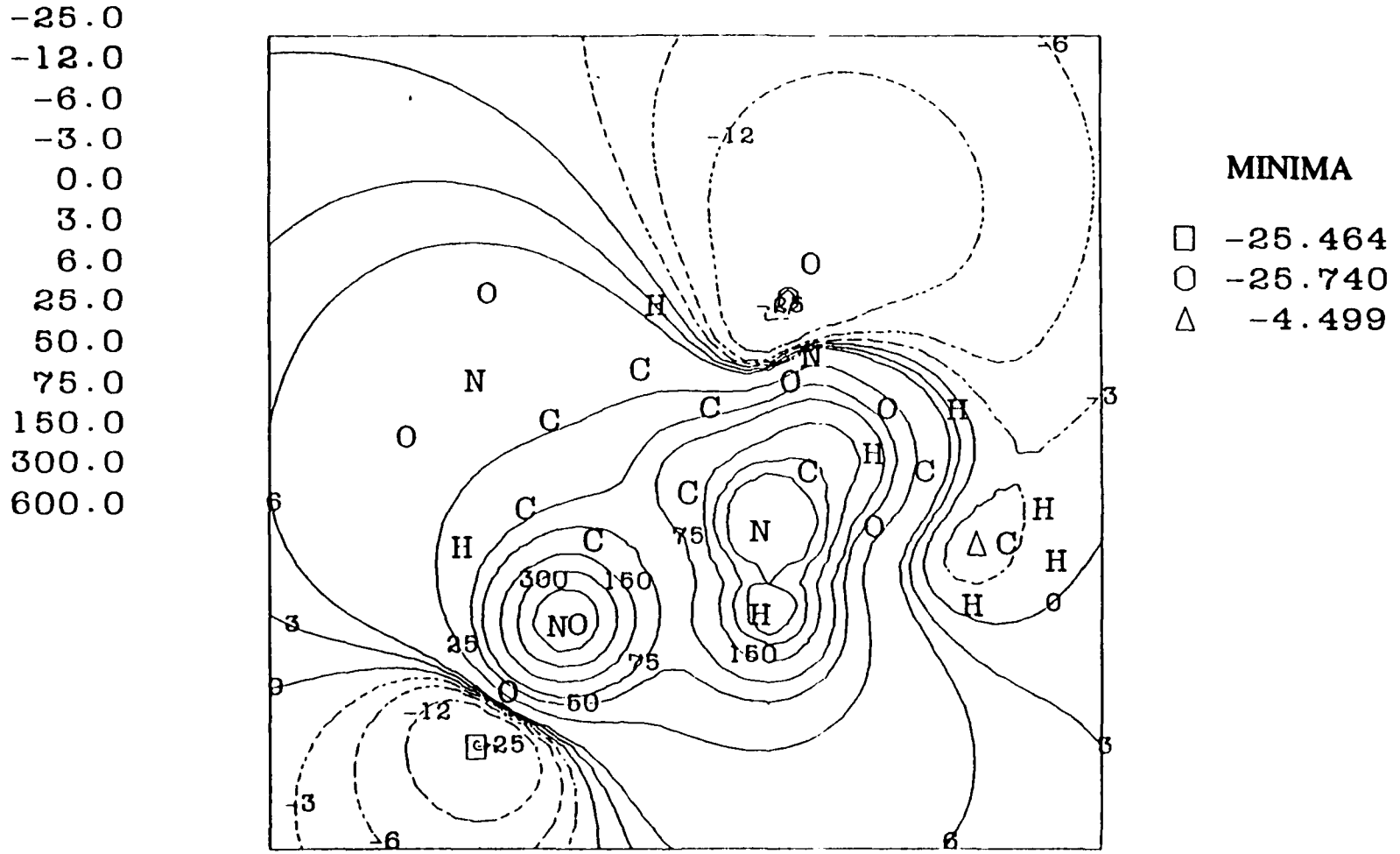


Figure F-1. Calculated electrostatic potential, in kcal/mole, of ethyl(2,4,6-trinitrophenyl)carbamate, in the plane 1.75Å above the N12 nitro group located in the upper right corner. Projected positions of nuclei are shown. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

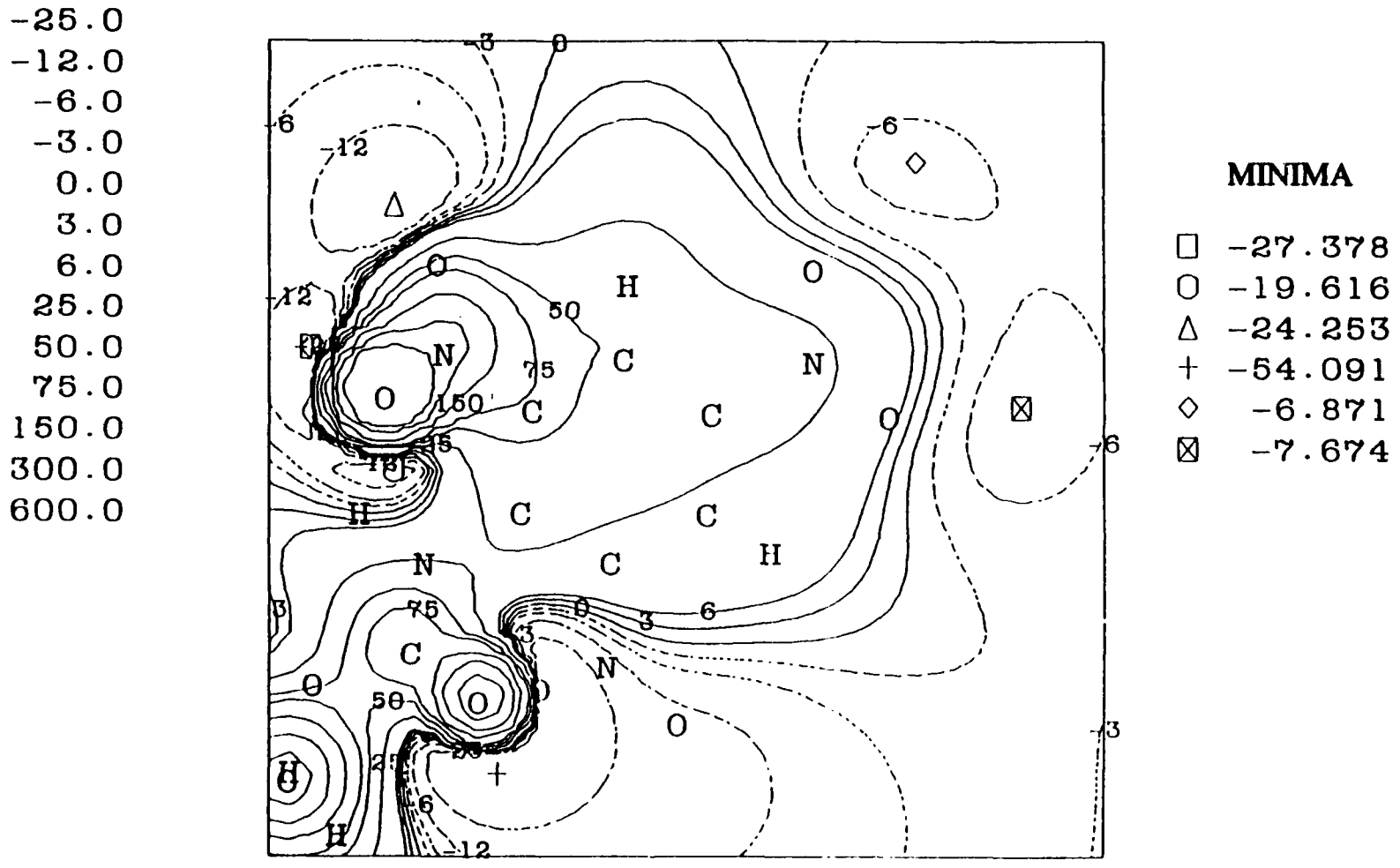
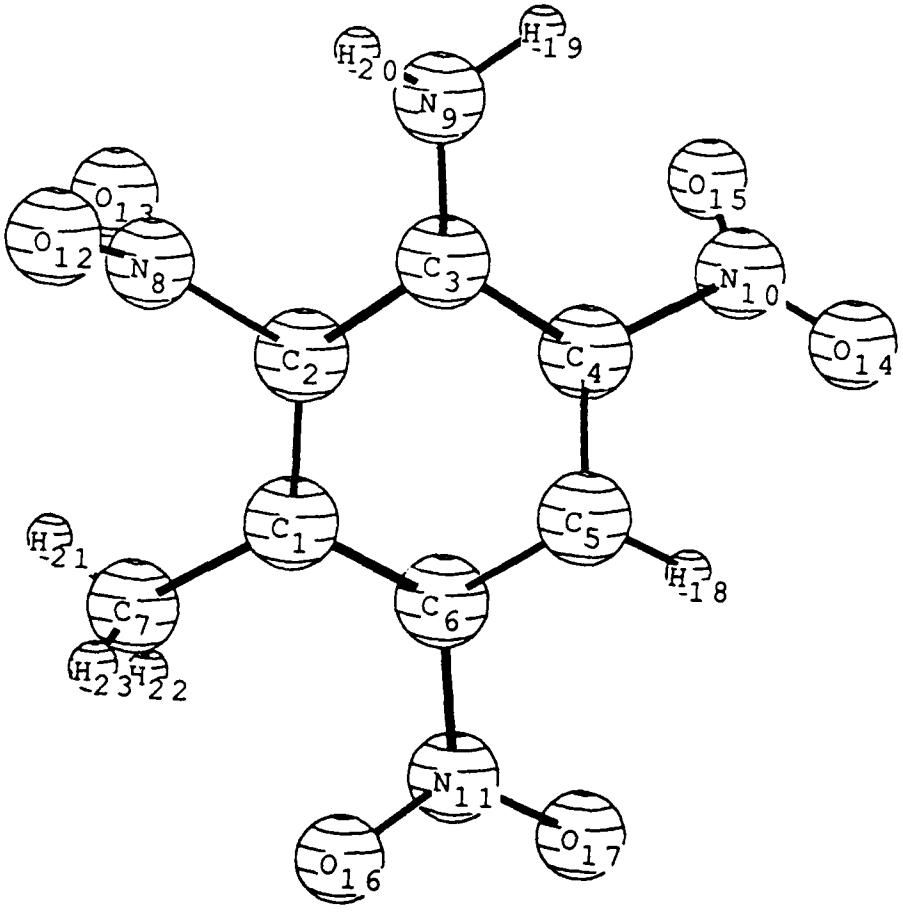


Figure F-2. Calculated electrostatic potential, in kcal/mole, of ethyl(2,4,6-trinitrophenyl)carbamate, in the plane 1.75Å above the N13 nitro group located in the upper right corner. Projected positions of nuclei are shown. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

APPENDIX G
3-AMINO-2,4,6-TRINITROTOLUENE

The short distances between non-bonded hydrogens and oxygens (suggesting hydrogen bonding) are between H18-O14 (2.38 Å), H19-O15 (2.04 Å), H18-O17 (2.40 Å) and H22-O16 (2.45 Å).

The N8 nitro group is rotated out of the mean plane of the benzene ring by 72°, and the N10 and N11 nitro groups are rotated by 28° and 20°, respectively. The amine group (N9) is rotated by only a few degrees.



Z-MATRIX (ANGSTROMS AND DEGREES)

CD	CENT	ATOM	N1	LENGTN		N2	ALPHA		N3	BETA		J
1	1	C										
2	2	C	1	1.395000	(1)							
3	3	C	2	1.410838	(2)	1	126.701	(23)				
4	4	C	3	1.402150	(3)	2	114.129	(24)	1	0.979	(44)	0
5	5	C	4	1.378505	(4)	3	122.224	(25)	2	-1.093	(45)	0
6	6	C	5	1.368058	(5)	4	120.320	(26)	3	1.406	(46)	0
7	7	C	1	1.486318	(6)	2	120.905	(27)	3	-179.014	(47)	0
8	8	N	2	1.478266	(7)	3	115.412	(28)	4	-179.582	(48)	0
9	9	N	3	1.356293	(8)	4	124.097	(29)	5	177.944	(49)	0
10	10	N	4	1.452784	(9)	5	116.851	(30)	6	-179.171	(50)	0
11	11	N	6	1.462607	(10)	5	116.091	(31)	4	179.333	(51)	0
12	12	O	8	1.219979	(11)	2	117.040	(32)	1	72.354	(52)	0
13	13	O	8	1.211423	(12)	2	117.381	(33)	1	-108.844	(53)	0
14	14	O	10	1.226476	(13)	4	118.336	(34)	5	-27.908	(54)	0
15	15	O	10	1.225006	(14)	4	119.166	(35)	5	151.840	(55)	0
16	16	O	11	1.218859	(15)	6	119.900	(36)	5	159.673	(56)	0
17	17	O	11	1.227529	(16)	6	117.202	(37)	5	-20.424	(57)	0
18	18	H	5	0.980143	(17)	4	116.582	(38)	3	-179.380	(58)	0
19	19	H	9	0.978715	(18)	3	118.485	(39)	4	3.497	(59)	0
20	20	H	9	0.802824	(19)	3	121.840	(40)	4	-170.689	(60)	0
21	21	H	7	0.950830	(20)	1	112.366	(41)	2	16.885	(61)	0
22	22	H	7	0.915332	(21)	1	110.477	(42)	2	132.601	(62)	0
23	23	H	7	0.949603	(22)	1	110.427	(43)	2	-107.239	(63)	0

STOICHIOMETRY C7H6N4O6

SCF DONE: E(RHF) = -931.120205284 A.U. AFTER 28 CYCLES

EIGENVALUES -- -0.31333 -0.30205 0.13151 0.14777 0.18649

ESTIMATED IONIZATION POTENTIAL: 8.23 ev

TOTAL ATOMIC CHARGES.

		1	Net Charge
1	C	5.906196	0.014
2	C	5.939706	0.060
3	C	5.797575	0.202
4	C	5.938181	0.062
5	C	6.042300	-0.042
6	C	5.932520	0.067
7	C	6.345575	-0.346
8	N	6.835111	0.165
9	N	7.534281	-0.534
10	N	6.834702	0.165
11	N	6.833735	0.166
12	O	8.195482	-0.195
13	O	8.194229	-0.194
14	O	8.186153	-0.186
15	O	8.214415	-0.214
16	O	8.200247	-0.200
17	O	8.201892	-0.202
18	H	0.854103	0.146
19	H	0.724753	0.275
20	H	0.708393	0.292
21	H	0.870675	0.129
22	H	0.855647	0.144
23	H	0.854132	0.146

DIPOLE MOMENT (DEBYE): X=-1.1727 Y=-0.2785 Z= 1.7132 TOTAL= 2.0947

Vmid: N8-C2: 0.161
N10-C4: 0.165
N11-C6: 0.169

BOND ORDER: N8-C2: 1.22
N10-C4: 1.28
N11-C6: 1.26
O12-N8: 1.94
O13-N8: 1.98
O14-N10: 1.91
O15-N10: 1.91
O16-N11: 1.94
O17-N11: 1.92

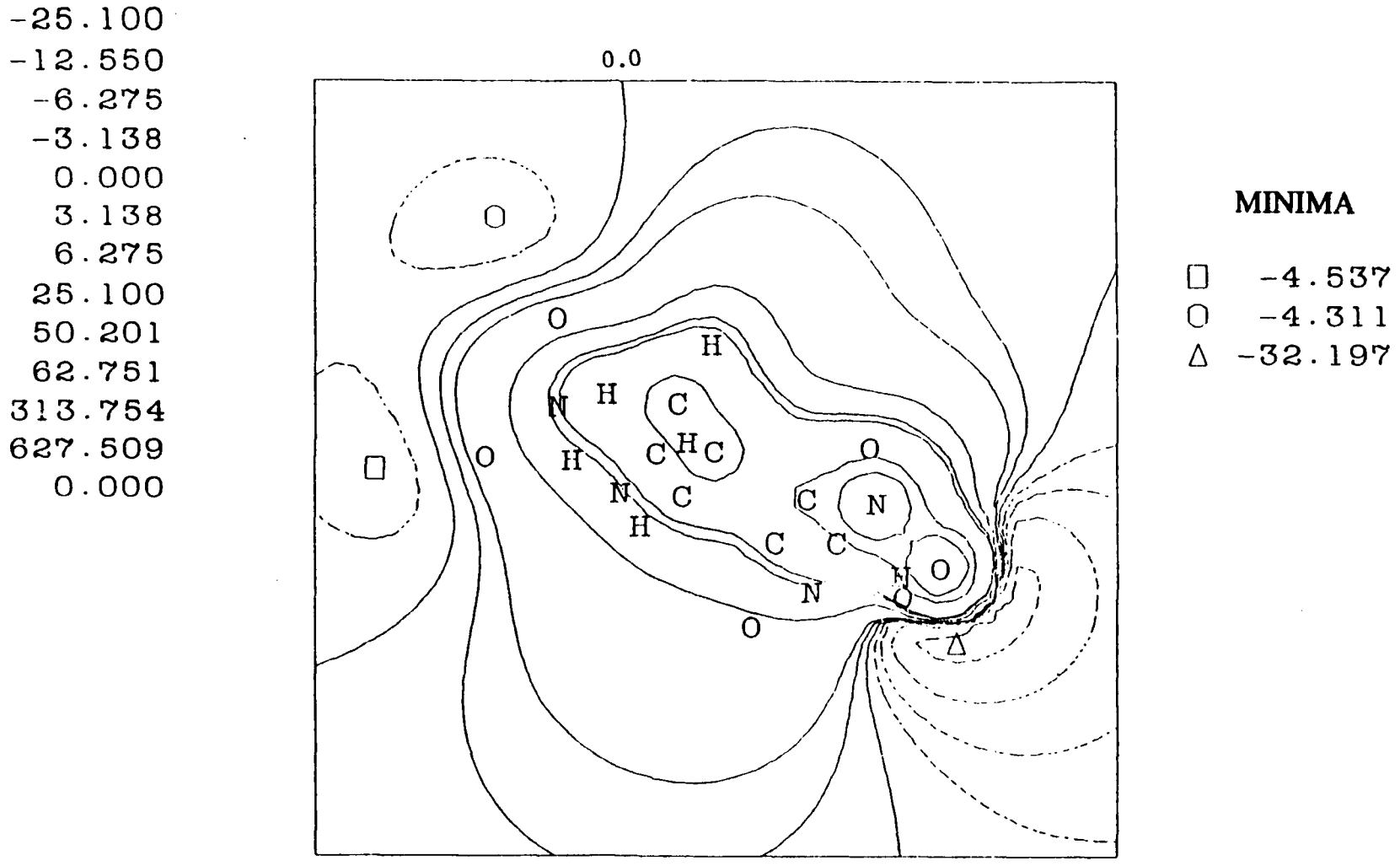


Figure G-1. Calculated electrostatic potential, in kcal/mole, of 3-amino-2,4,6-trinitrotoluene, in the plane 1.75Å above the N8 nitro group located in the upper left corner. Projected positions of nuclei are shown. The zero contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

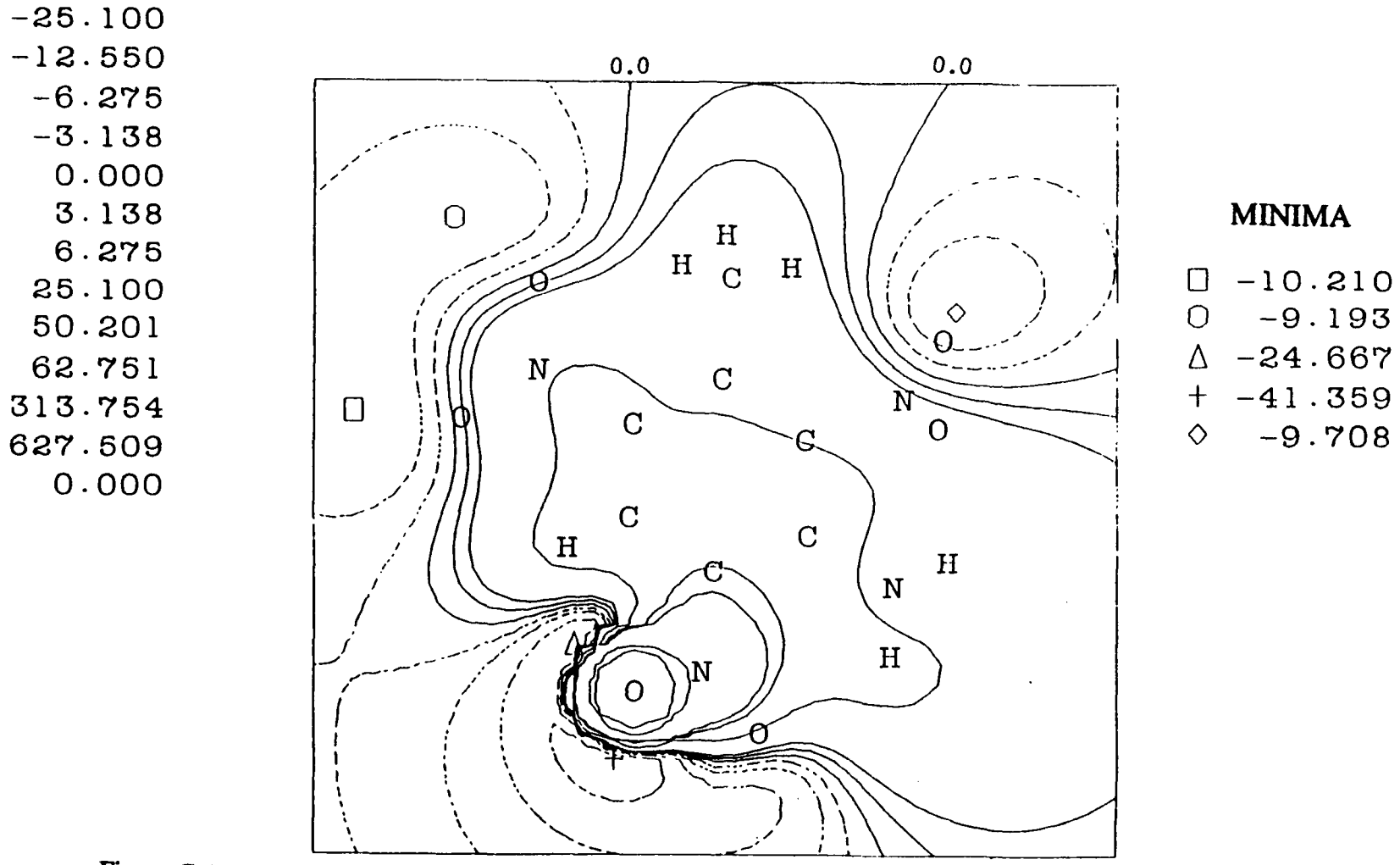
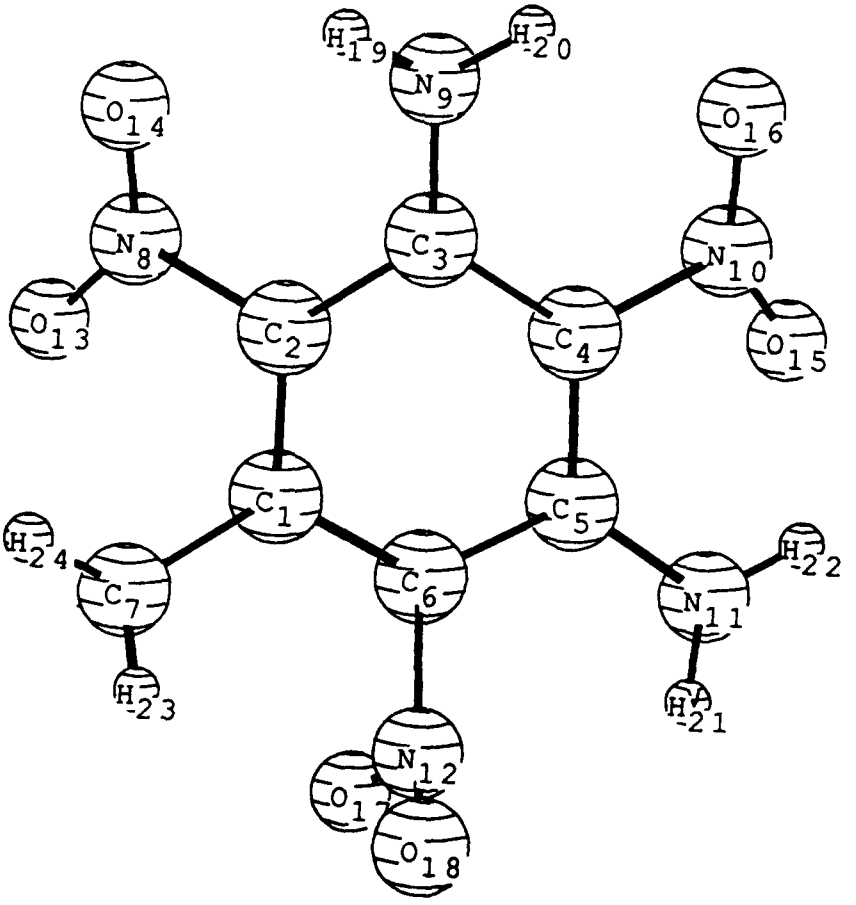


Figure G-2. Calculated electrostatic potential, in kcal/mole, of 3,-amino-2,4,6-trinitrotoluene, in the plane 1.75Å above the N11 nitro group located in the upper left corner. Projected positions of nuclei are shown. The zero contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

APPENDIX H
3,5-DIAMINO-2,4,6-TRINITROTOLUENE

The short distances between non-bonded hydrogens and oxygens (suggesting hydrogen bonding) are between H19-O14 (1.97 Å), H22-O15 (1.91 Å), H24-O13 (2.36 Å) and H20-O16 (1.89 Å).

The N8 and N10 nitro groups are rotated out of the mean plane of the benzene ring by approximately 34° and 22 °, respectively. The N12 nitro group is almost perpendicular to the plane, being rotated by about 80°. The amine groups are approximately planar.



Z-MATRIX (ANGSTROMS AND DEGREES)

CD	CENT	ATOM	N1	LENGTH		N2	ALPHA		N3	BETA		J
1	1	C										
2	2	C	1	1.399500	(1)							
3	3	C	2	1.424227	(2)	1	123.518	(25)				
4	4	C	3	1.436338	(3)	2	116.441	(26)	1	5.613	(48)	0
5	5	C	4	1.415313	(4)	3	121.832	(27)	2	-3.717	(49)	0
6	6	C	5	1.408478	(5)	4	116.129	(28)	3	-1.141	(50)	0
7	7	C	1	1.488618	(6)	2	124.037	(29)	3	173.936	(51)	0
8	8	N	2	1.445386	(7)	3	118.672	(30)	4	-171.743	(52)	0
9	9	N	3	1.326379	(8)	4	121.753	(31)	5	179.278	(53)	0
10	10	N	4	1.434609	(9)	3	119.131	(32)	2	177.627	(54)	0
11	11	N	5	1.348888	(10)	4	124.060	(33)	3	-179.926	(55)	0
12	12	N	6	1.467081	(11)	5	116.345	(34)	4	-176.867	(56)	0
13	13	O	8	1.228633	(12)	2	118.018	(35)	3	144.720	(57)	0
14	14	O	8	1.232337	(13)	2	120.086	(36)	3	-34.210	(58)	0
15	15	O	10	1.241579	(14)	4	118.724	(37)	3	-159.360	(59)	0
16	16	O	10	1.230972	(15)	4	120.728	(38)	3	21.819	(60)	0
17	17	O	12	1.273003	(16)	6	116.635	(39)	5	-110.475	(61)	0
18	18	O	12	1.306374	(17)	6	114.235	(40)	5	98.241	(62)	0
19	19	H	9	0.852295	(18)	3	116.430	(41)	4	-177.948	(63)	0
20	20	H	9	0.910176	(19)	3	118.244	(42)	4	-6.893	(64)	0
21	21	H	11	0.892919	(20)	5	115.418	(43)	4	172.211	(65)	0
22	22	H	11	0.920404	(21)	5	117.933	(44)	4	0.104	(66)	0
23	23	H	7	0.915330	(22)	1	114.609	(45)	2	-153.018	(67)	0
24	24	H	7	0.922669	(23)	1	110.973	(46)	2	-29.739	(68)	0
25	25	H	7	0.882767	(24)	1	112.314	(47)	2	85.590	(69)	0

STOICHIOMETRY C7H7N5O6

SCF DONE: E(RHF) = -985.905123075 A.U. AFTER 44 CYCLES

EIGENVALUES -- -0.28717 0.13494 0.15325 0.16704 0.22261

Estimated ionization potential: 7.82 ev

TOTAL ATOMIC CHARGES.

		1	Net Charge
1	C	5.888064	0.112
2	C	5.978831	0.022
3	C	5.775979	0.224
4	C	5.987531	0.012
5	C	5.788101	0.212
6	C	5.967760	0.032
7	C	6.393238	-0.393
8	N	6.842391	0.158
9	N	7.543006	-0.543
10	N	6.840932	0.159
11	N	7.508429	-0.508
12	N	6.903556	0.096
13	O	8.193744	-0.194
14	O	8.225308	-0.225
15	O	8.216013	-0.216
16	O	8.211316	-0.211
17	O	8.160196	-0.160
18	O	8.180407	-0.180
19	H	0.699784	0.300
20	H	0.705469	0.295
21	H	0.734572	0.265
22	H	0.708944	0.291
23	H	0.855701	0.144
24	H	0.852741	0.147
25	H	0.837985	0.162

DIPOLE MOMENT (DEBYE): X= 1.4423 Y=-0.2507 Z= 0.1758 TOTAL= 1.4745

V-mid: N8-C2: 0.132
N10-C4: 0.126
N12-C6: 0.092

BOND ORDER: N8-C2: 1.30
N10-C4: 1.33
N12-C6: 1.25
O13-N8: 1.90
O14-N8: 1.88
O15-N10: 1.84
O16-N10: 1.89
O17-N12: 1.71
O18-N12: 1.52

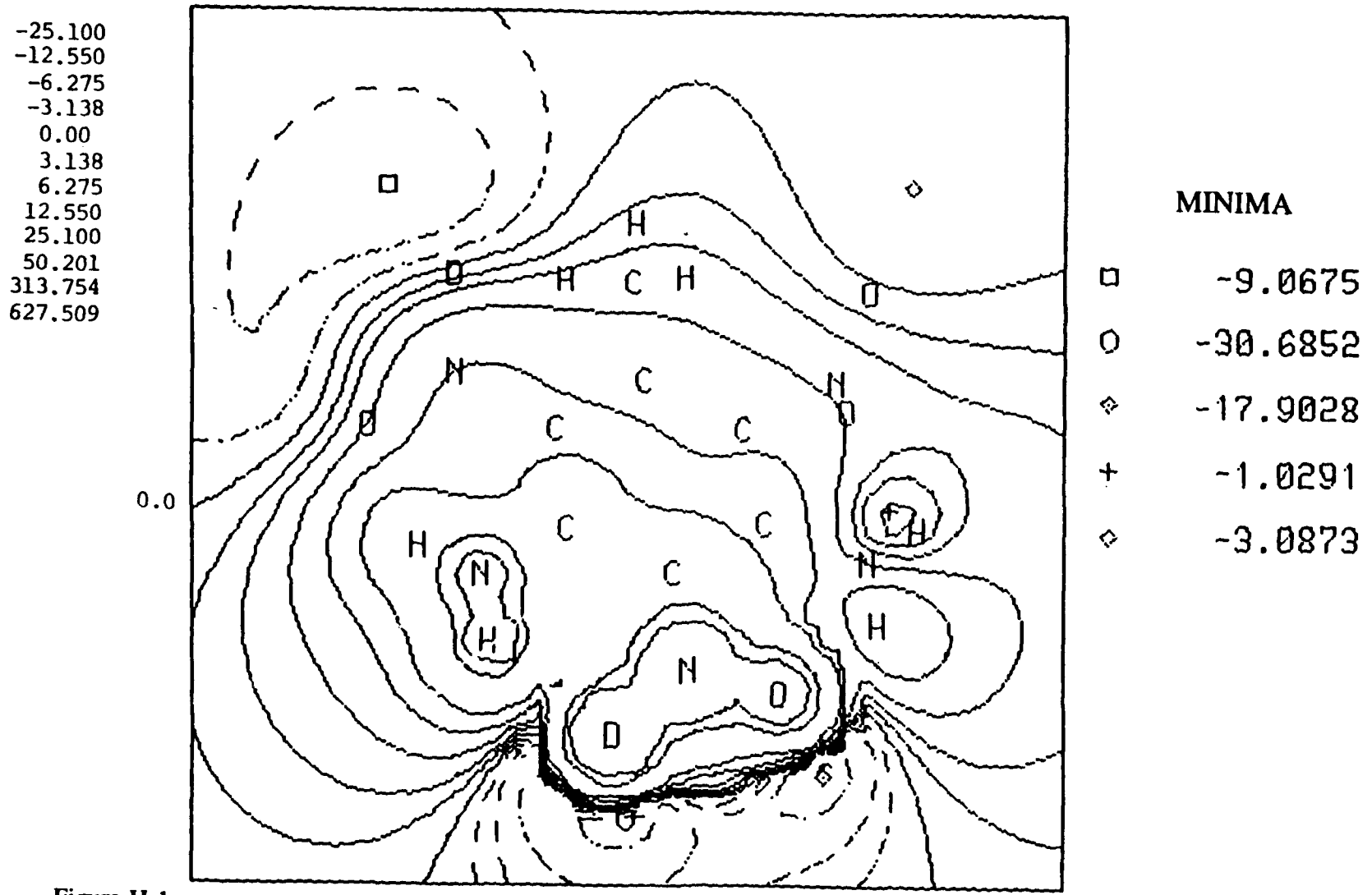


Figure H-1. Calculated electrostatic potential, in kcal/mole, of 3,5-diamino-2,4,6-trinitrotoluene, in the plane 1.75Å above the N8 nitro group located in the upper left corner. Projected positions of nuclei are shown. The zero contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

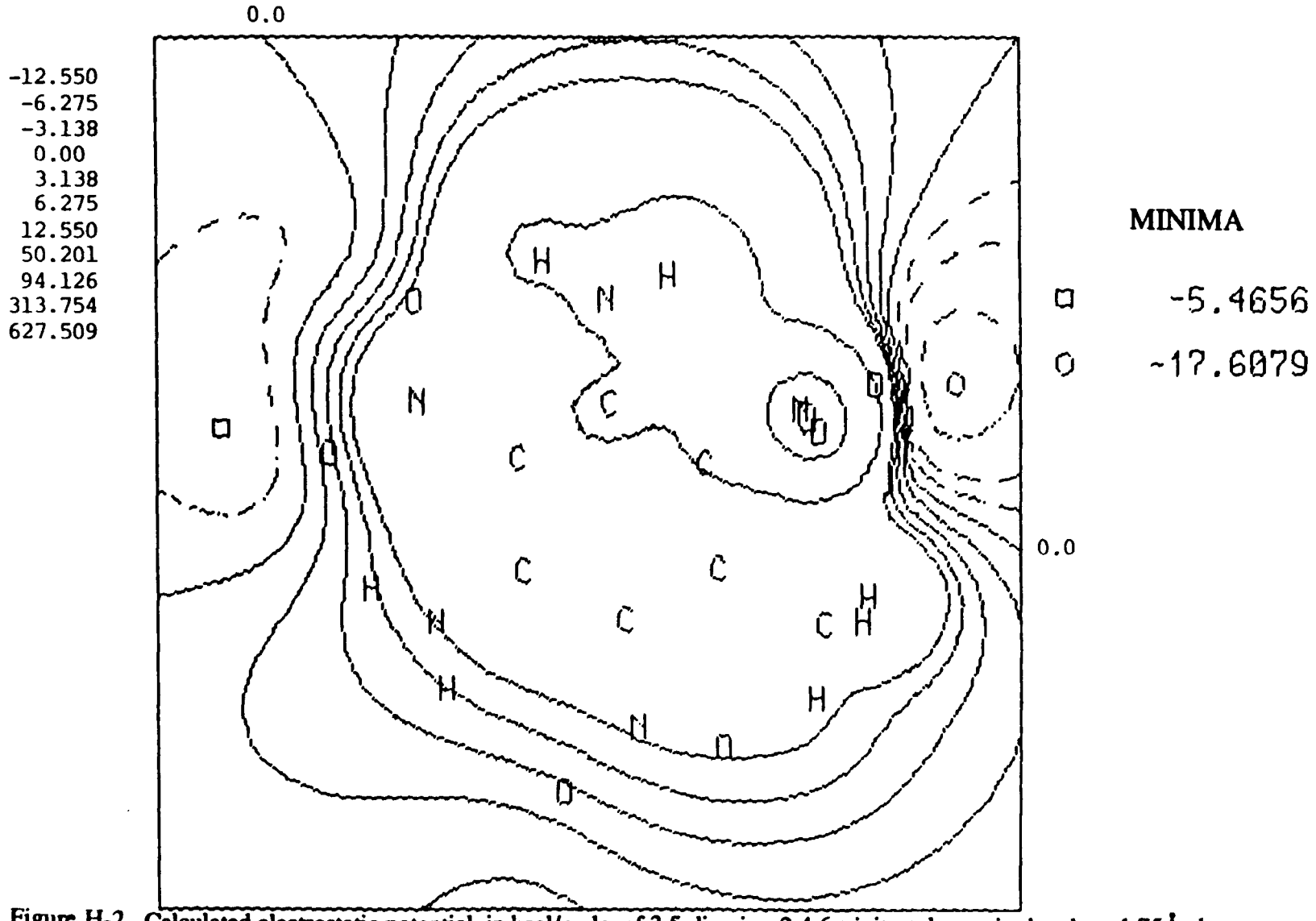
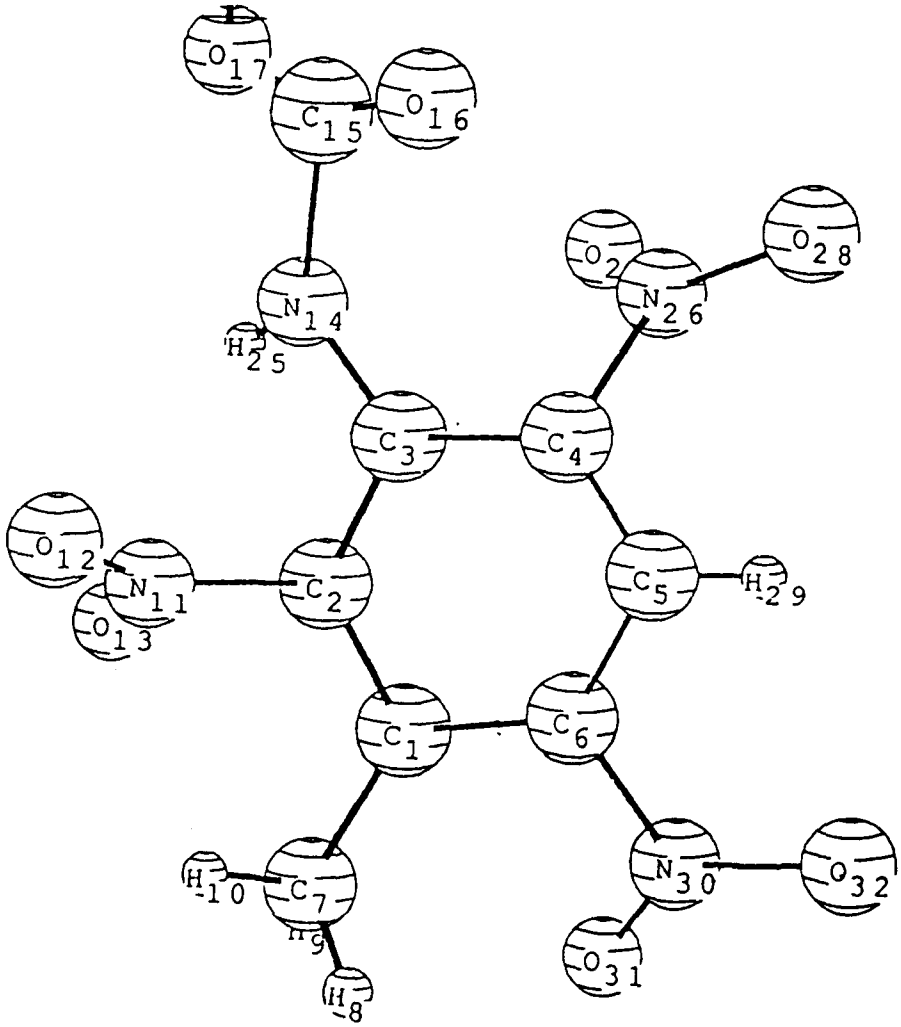


Figure H-2. Calculated electrostatic potential, in kcal/mole, of 3,5-diamino-2,4,6-trinitrotoluene, in the plane 1.75Å above the N10 nitro group located in the upper left corner. Projected positions of nuclei are shown. The zero contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

APPENDIX I
N-CARBOETHOXY-2,4,6-TRINITRO-m-TOLUIDINE

The short distances between non-bonded hydrogens and oxygens are H19-O17 (1.93 Å), H20-O17 (1.91 Å), H25-O17 (2.33 Å) and H29-O32 (2.39 Å).

The N30 nitro group is rotated by approximately 26°, the N26 nitro group is rotated by approximately 43°, and the N11 nitro group is rotated by almost 80°.



The ethyl group bonded to O_{17} is not shown for reasons of clarity.

Z-MATRIX (ANGSTROMS AND DEGREES)

CD	CENT	ATOM	N1	LENGTH	N2	ALPHA	N3	BETA	J
1	1	C							
2	2	C	1	1.390250(1)					
3	3	C	2	1.391064(2)	1	126.771(32)			
4	4	C	3	1.390742(3)	2	115.503(33)	1	-4.433(62)	0
5	5	C	4	1.381592(4)	3	121.733(34)	2	0.756(63)	0
6	6	C	5	1.384425(5)	4	119.005(35)	3	3.511(64)	0
7	7	C	1	1.493449(6)	2	121.586(36)	3	-179.832(65)	0
8	8	H	7	0.967633(7)	1	115.478(37)	2	-139.662(66)	0
9	9	H	7	1.061986(8)	1	116.455(38)	2	101.196(67)	0
10	10	H	7	0.916674(9)	1	114.154(39)	2	-16.427(68)	0
11	11	N	2	1.482241(10)	3	115.743(40)	4	174.575(69)	0
12	12	O	11	1.212032(11)	2	117.007(41)	3	-77.802(70)	0
13	13	O	11	1.215249(12)	2	117.878(42)	3	102.172(71)	0
14	14	N	3	1.397079(13)	4	125.060(43)	5	-178.132(72)	0
15	15	C	14	1.361248(14)	3	122.077(44)	4	-44.150(73)	0
16	16	O	15	1.198292(15)	14	125.748(45)	3	-6.572(74)	0
17	17	O	15	1.346414(16)	14	105.923(46)	3	176.088(75)	0
18	18	C	17	1.447102(17)	15	116.375(47)	14	-177.238(76)	0
19	19	H	18	1.038544(18)	17	100.570(48)	15	-159.541(77)	0
20	20	H	18	0.924146(19)	17	109.974(49)	15	-55.325(78)	0
21	21	C	18	1.473267(20)	17	111.564(50)	15	80.220(79)	0
22	22	H	21	0.959974(21)	18	107.067(51)	17	53.634(80)	0
23	23	H	21	0.959906(22)	18	109.910(52)	17	-65.220(81)	0
24	24	H	21	0.959585(23)	18	111.414(53)	17	173.257(82)	0
25	25	H	14	0.945386(24)	3	116.967(54)	2	-50.333(83)	0
26	26	N	4	1.471524(25)	3	122.678(55)	2	176.140(84)	0
27	27	O	26	1.224059(26)	4	117.245(56)	3	-43.294(85)	0
28	28	O	26	1.226059(27)	4	117.577(57)	3	138.035(86)	0
29	29	H	5	0.929382(28)	4	121.749(58)	3	175.122(87)	0
30	30	N	6	1.485920(29)	1	121.348(59)	2	-177.203(88)	0
31	31	O	30	1.219037(30)	6	118.064(60)	1	27.472(89)	0
32	32	O	30	1.232587(31)	6	117.339(61)	1	-154.539(90)	0

STOICHIOMETRY C10H10N4O8

SCF DONE: E(RHF) = -1195.73406407

EIGENVALUES — -0.30684 0.12465 0.14400 0.18828 0.20432

Estimated ionization potential: 8.36 eV

Total atomic charges:

		1
1	C	0.071515
2	C	0.085263
3	C	0.166048
4	C	0.102347
5	C	-0.066300
6	C	0.096009
7	C	-0.302283
8	H	0.129093
9	H	0.127210
10	H	0.125939
11	N	0.173171
12	C	-0.184355
13	C	-0.196279
14	N	0.406348
15	C	0.473059
16	C	-0.319455
17	C	-0.269170
18	C	-0.028449
19	H	0.096931
20	H	0.111969
21	C	-0.313272
22	H	0.114663
23	H	0.118637
24	H	0.113212
25	H	0.262822
26	N	0.175031
27	O	-0.198244
28	O	-0.176578
29	H	0.143709
30	N	0.167351
31	O	-0.190433
32	O	-0.193413

Sum of Mulliken charges= 0.00000

Dipole moment (Debye):

X= -1.6558 Y= 1.1414 Z= 1.5154 Tot= 2.5182

V-mid: N11-C2: 0.184
N26-C4: 0.198
N30-C6: 0.187

Bond Order: N11-C2: 1.21
N26-C4: 1.24
N30-C6: 1.20
O12-N11: 1.98
O13-N11: 1.96
O27-N26: 1.92
O28-N26: 1.91
O31-N30: 1.94
O32-N30: 1.88

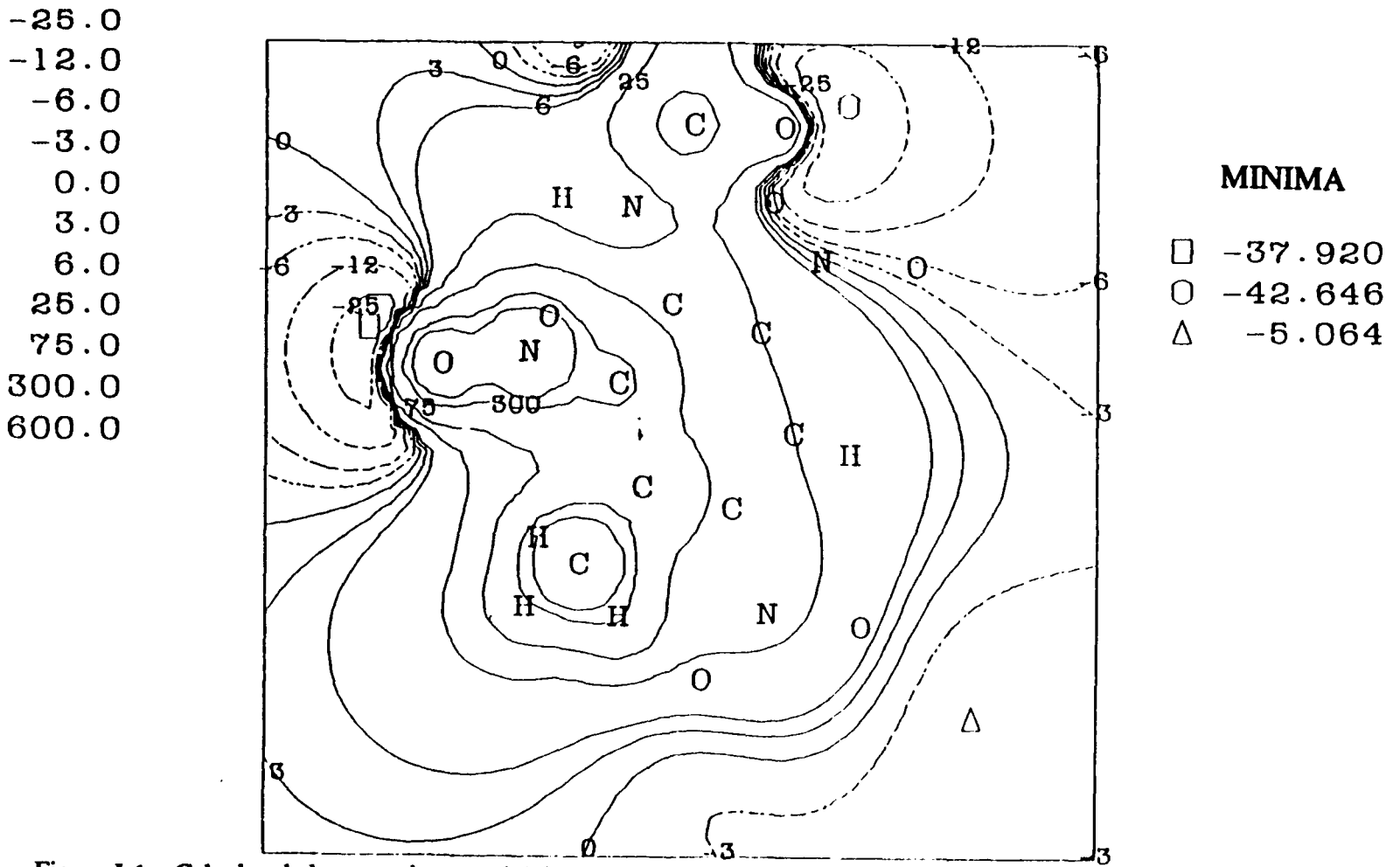


Figure I-1. Calculated electrostatic potential, in kcal/mole, of N-carboethoxy-2,4,6-trinitro-m-toluidine, in the plane 1.75Å above the N30 nitro group located in the lower right corner. Projected positions of nuclei are shown. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

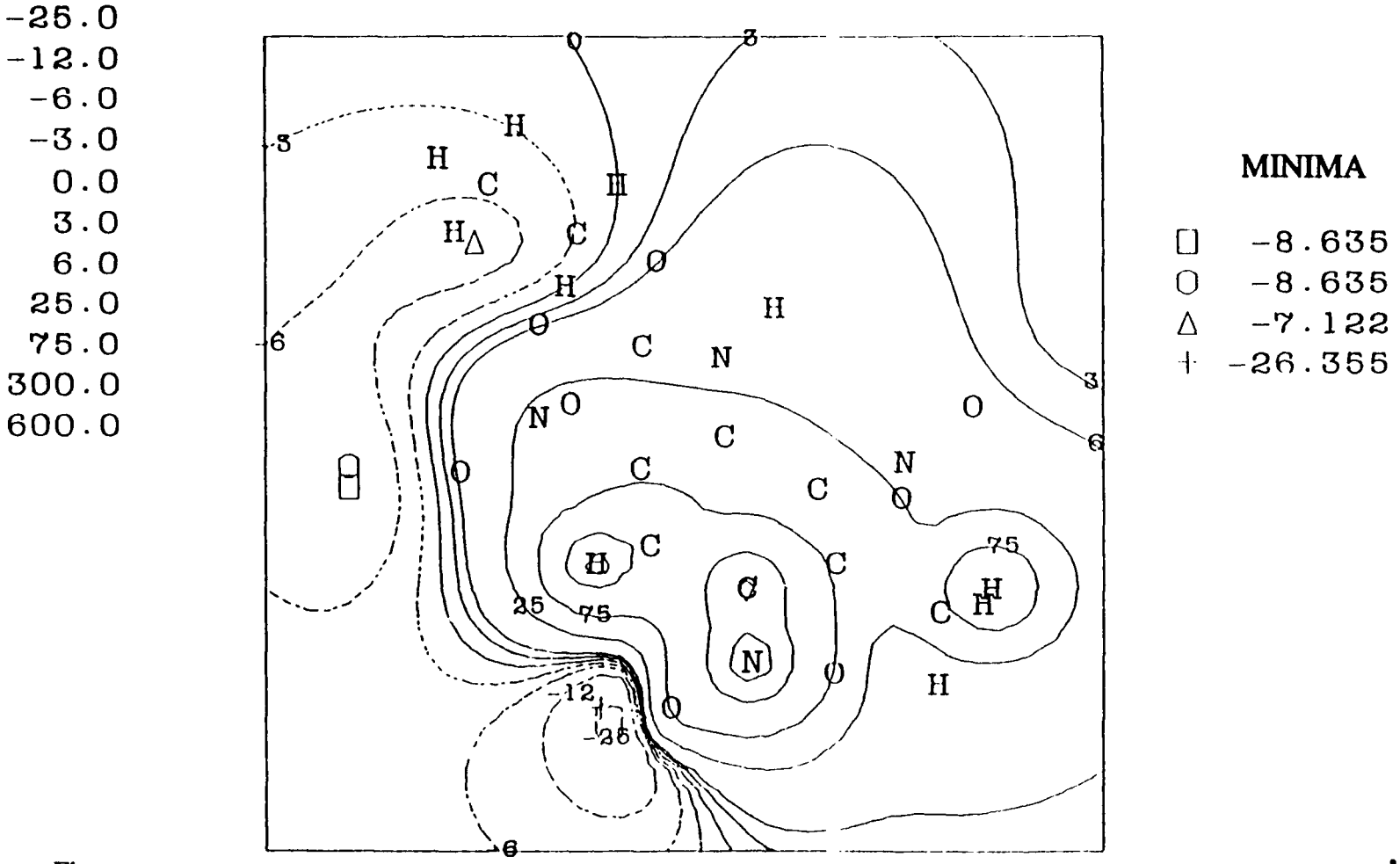
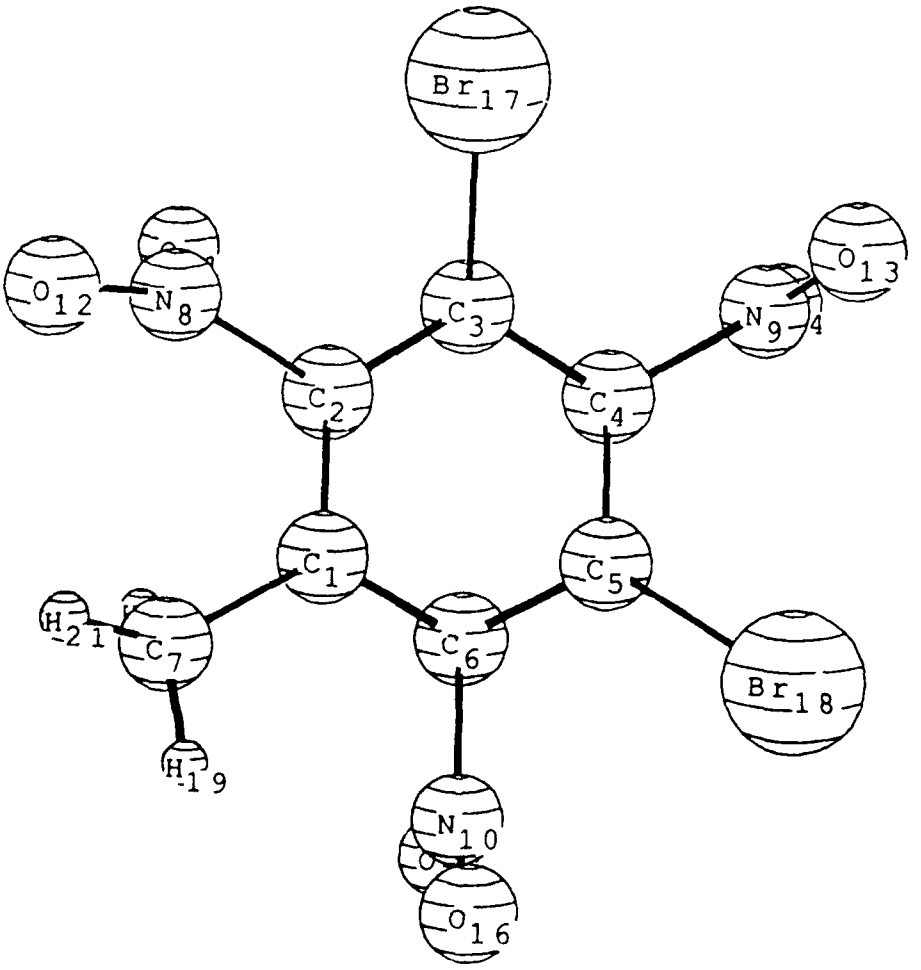


Figure I-2. Calculated electrostatic potential, in kcal/mole, of N-carboethoxy-2,4,6-trinitro-m-toluidine, in the plane 1.75Å above the N26 nitro group located in the upper left corner. Projected positions of nuclei are shown. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

APPENDIX J
3,5-DIBROMO-2,4,6-TRINITROTOLUENE, #18

The only noticeable short distance between non-bonded hydrogens and oxygens is H21-O12 (2.50 Å).

The N8 and N10 nitro groups are rotated by approximately 62° and 80°, respectively. The N9 nitro group is roughly perpendicular to the mean plane of the benzene ring.



Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.370000(1)					
3	3	C	2	1.366230(2)	1	122.557(21)			
4	4	C	3	1.391364(3)	2	116.727(22)	1	1.580(40)	0
5	5	C	4	1.384690(4)	3	121.696(23)	2	-2.381(41)	0
6	6	C	5	1.356721(5)	4	117.881(24)	3	3.198(42)	0
7	7	C	1	1.499745(6)	2	120.350(25)	3	179.066(43)	0
8	8	N	2	1.507550(7)	3	116.858(26)	4	177.670(44)	0
9	9	N	4	1.497292(8)	5	118.760(27)	6	-178.324(45)	0
10	10	N	6	1.498023(9)	5	118.516(28)	4	-179.612(46)	0
11	11	O	8	1.215329(10)	2	116.760(29)	1	-116.703(47)	0
12	12	O	8	1.207687(11)	2	117.680(30)	1	60.430(48)	0
13	13	O	9	1.169336(12)	4	117.809(31)	3	90.462(49)	0
14	14	O	9	1.196739(13)	4	116.397(32)	3	-86.695(50)	0
15	15	O	10	1.212542(14)	6	116.156(33)	5	-101.694(51)	0
16	16	O	10	1.154568(15)	6	118.205(34)	5	81.236(52)	0
17	17	Br	3	1.868548(16)	4	119.748(35)	5	177.402(53)	0
18	18	Br	5	1.865427(17)	4	121.248(36)	3	-177.609(54)	0
19	19	H	7	0.999707(18)	1	109.529(37)	2	179.714(55)	0
20	20	H	7	0.992240(19)	1	109.952(38)	2	59.233(56)	0
21	21	H	7	1.010376(20)	1	109.447(39)	2	-60.330(57)	0

STOICHIOMETRY C7H3Br2N3O6

SCF DONE: E(RHF) = -5992.86404190

Alpha eigenvalues -- -0.33079 -0.32411 0.14114 0.15325 0.19239

Estimated ionization potential: 8.83 ev

Total atomic charges:

		1
1	C	0.062394
2	C	0.085894
3	C	-0.030675
4	C	0.092229
5	C	-0.032007
6	C	0.083762
7	C	-0.272475
8	N	0.181223
9	N	0.203254
10	N	0.204171
11	O	-0.182988
12	O	-0.187541
13	O	-0.185329
14	O	-0.194150
15	O	-0.204145
16	O	-0.182049
17	Br	0.104333
18	Br	0.098127
19	H	0.112404
20	H	0.118445
21	H	0.125125

Dipole moment (Debye):

X= 0.0680 Y= 1.2263 Z= -0.2630 Tot= 1.2560

Bond Order:		V-mid:	
C2–N8:	1.15	C2–N8:	0.187
C4–N9:	1.17	C4–N9:	0.209
C6–N10:	1.17	C6–N10:	0.203
N8–O11:	1.96		
N8–O12:	2.00		
N9–O13:	2.20		
N9–O14:	2.05		
N10–O15:	1.97		
N10–O16:	2.28		

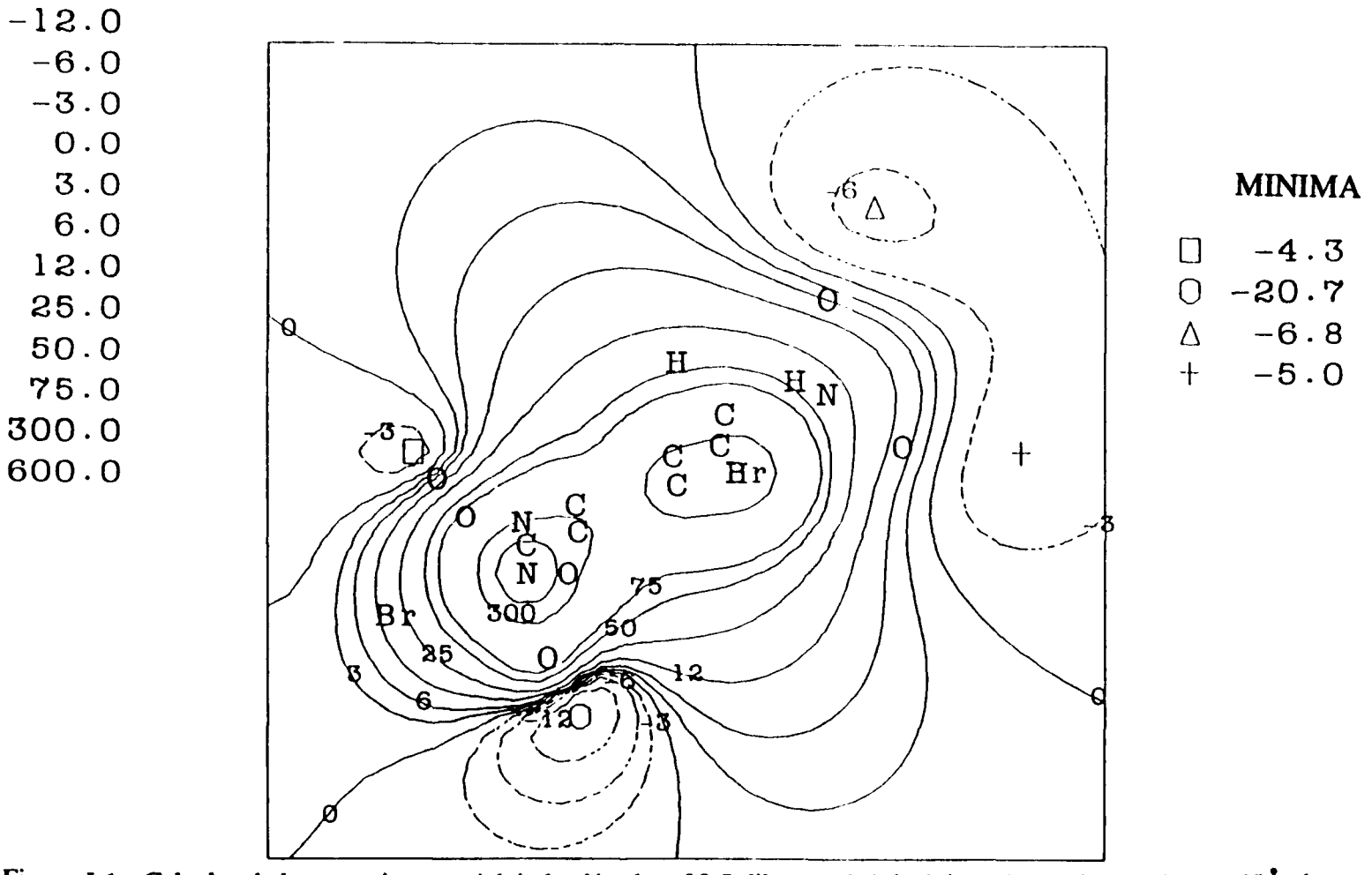


Figure J-1. Calculated electrostatic potential, in kcal/mole, of 3,5-dibromo-2,4,6-trinitrotoluene, in the plane 1.75Å above the N10 nitro group located in the upper right corner. Projected positions of nuclei are shown. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

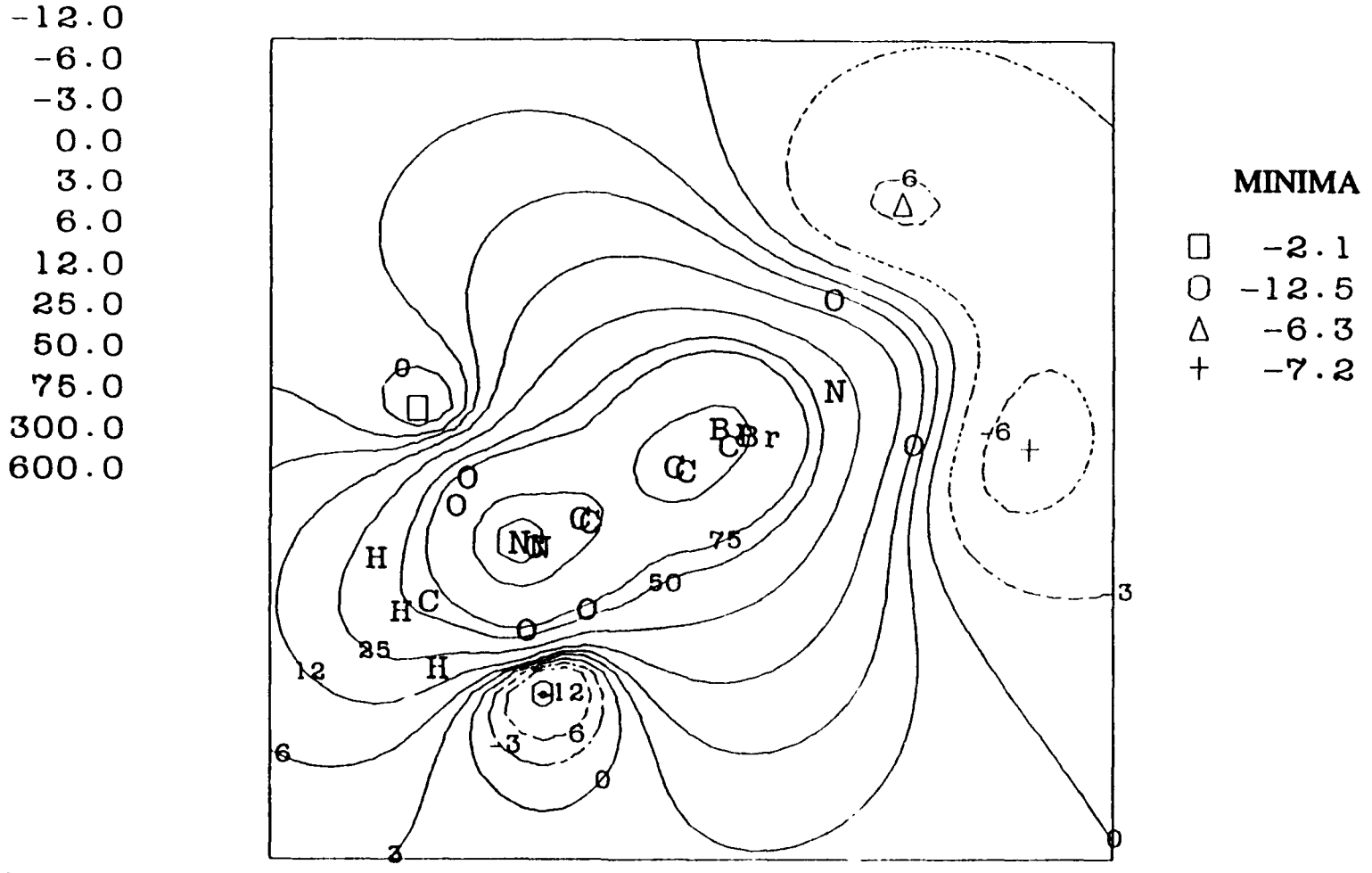
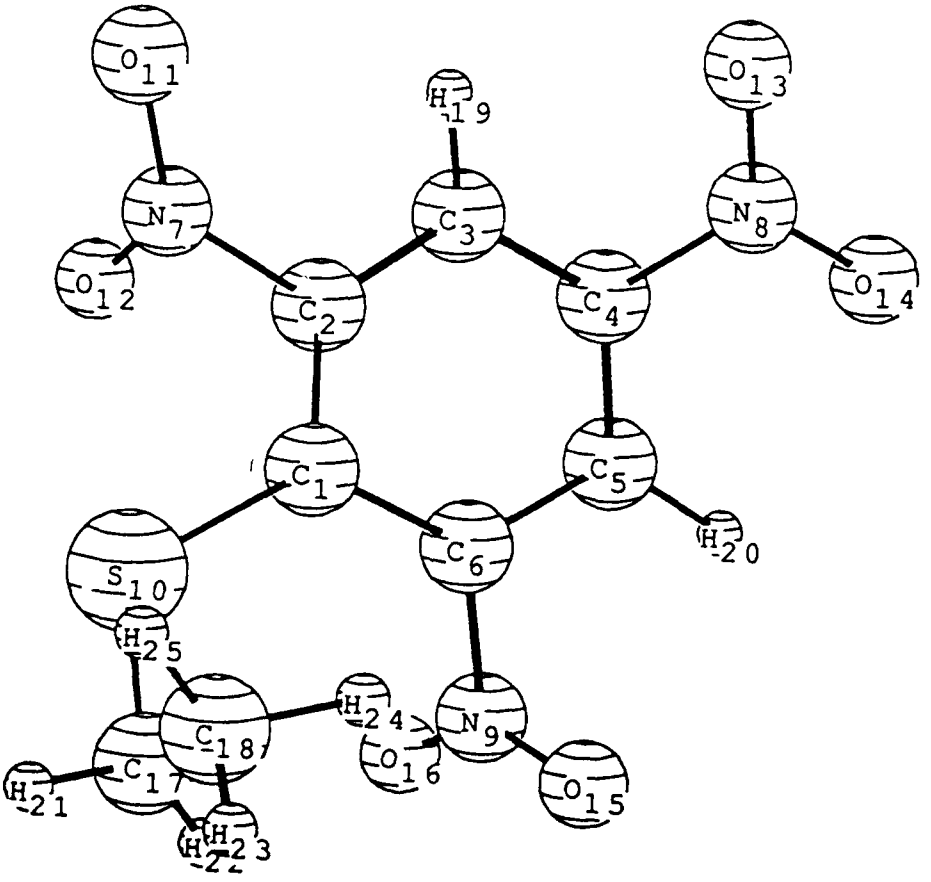


Figure J-2. Calculated electrostatic potential, in kcal/mole, of 3,5-dibromo-2,4,6-trinitrotoluene, in the plane 1.75Å above the N9 nitro group located in the upper right corner. Projected positions of nuclei are shown. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

APPENDIX K
ETHYL PICRYL SULFIDE

The short distances between non-bonded hydrogens and oxygens are H20-O14 (2.50 Å), H20-O15 (2.46 Å), H19-O11 (2.44 Å) and H19-O13 (2.51 Å).

The N7, N8 and N9 nitro groups are rotated out of the mean plane of the benzene ring by approximately 38°, 18°, and 45°, respectively.



Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C		1.375900(1)					
3	3	C	2	1.376557(2)	1	124.918(25)			
4	4	C	3	1.382829(3)	2	118.200(26)	1	2.681(48)	0
5	5	C	4	1.398791(4)	3	121.456(27)	2	-0.590(49)	0
6	6	C	5	1.380410(5)	4	117.821(28)	3	0.481(50)	0
7	7	N	2	1.489709(6)	3	115.593(29)	4	178.934(51)	0
8	8	N	4	1.457060(7)	5	118.259(30)	6	177.848(52)	0
9	9	N	6	1.454312(8)	5	114.988(31)	4	175.943(53)	0
10	10	S	1	1.768547(9)	2	120.736(32)	3	172.875(54)	0
11	11	O	7	1.204119(10)	2	117.786(33)	3	-37.560(55)	0
12	12	O	7	1.217904(11)	2	116.236(34)	3	139.586(56)	0
13	13	O	8	1.222714(12)	4	117.912(35)	5	-164.154(57)	0
14	14	O	8	1.230870(13)	4	117.508(36)	5	18.345(58)	0
15	15	O	9	1.217474(14)	6	117.764(37)	5	44.712(59)	0
16	16	O	9	1.227813(15)	6	117.917(38)	5	-131.235(60)	0
17	17	C	10	1.835985(16)	1	104.995(39)	2	-139.082(61)	0
18	18	C	17	1.504611(17)	10	112.827(40)	1	52.836(62)	0
19	19	H	3	1.035447(18)	4	123.308(41)	5	171.276(63)	0
20	20	H	5	1.094535(19)	4	124.362(42)	3	-177.750(64)	0
21	21	H	17	0.932937(20)	10	97.287(43)	1	161.355(65)	0
22	22	H	17	1.002419(21)	10	98.658(44)	1	-76.501(66)	0
23	23	H	18	0.820296(22)	17	103.954(45)	10	-179.864(67)	0
24	24	H	18	1.070622(23)	17	107.139(46)	10	-75.941(68)	0
25	25	H	18	0.903100(24)	17	103.590(47)	10	49.199(69)	0

STOICHIOMETRY C8H7N3O6S

SCF DONE: E(RHF) = -1311.18935285 A.U. AFTER 22 CYCLES

Alpha eigenvalues — -0.31944 -0.31341 -0.30798 -0.29044 0.11847

Estimated ionization potential: 7.91 ev

Total atomic charges:

		1
1	C	-0.062009
2	C	0.081244
3	C	-0.037111
4	C	0.087693
5	C	-0.021925
6	C	0.078326
7	N	0.178837
8	N	0.165323
9	N	0.159745
10	S	0.245111
11	O	-0.196161
12	O	-0.192559
13	O	-0.190670
14	O	-0.195923
15	O	-0.190331
16	O	-0.195321
17	C	-0.230302
18	C	-0.347789
19	H	0.140349
20	H	0.134270
21	H	0.114158
22	H	0.111445
23	H	0.141620
24	H	0.097764
25	H	0.124216

Dipole moment (Debye):

X= -1.7950 Y= -0.5715 Z= 0.9981 Tot= 2.1319

V-mid: C2-N7: 0.185
C4-N8: 0.164
C6-N9: 0.173

Bond Order: C2-N7: 1.19
C4-N8: 1.27
C6-N9: 1.28
N7-O11: 2.02
N7-O12: 1.95
N8-O13: 1.92
N8-O14: 1.89
N9-O15: 1.95
N9-O16: 1.90

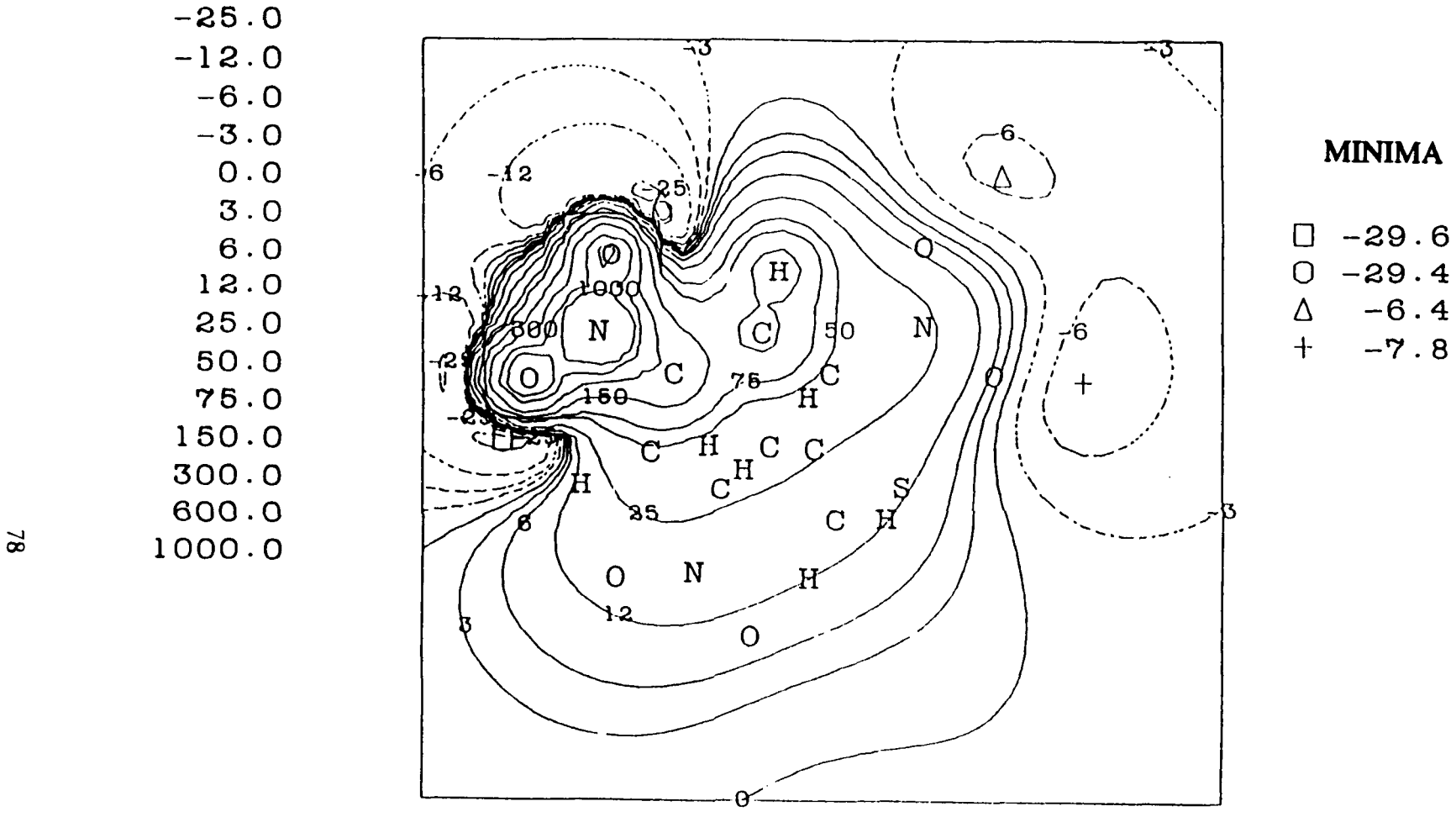


Figure K-1. Calculated electrostatic potential, in kcal/mole, of ethyl picryl sulfide, in the plane 1.75Å above the N7 nitro group located in the upper right corner. Projected positions of nuclei are shown. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

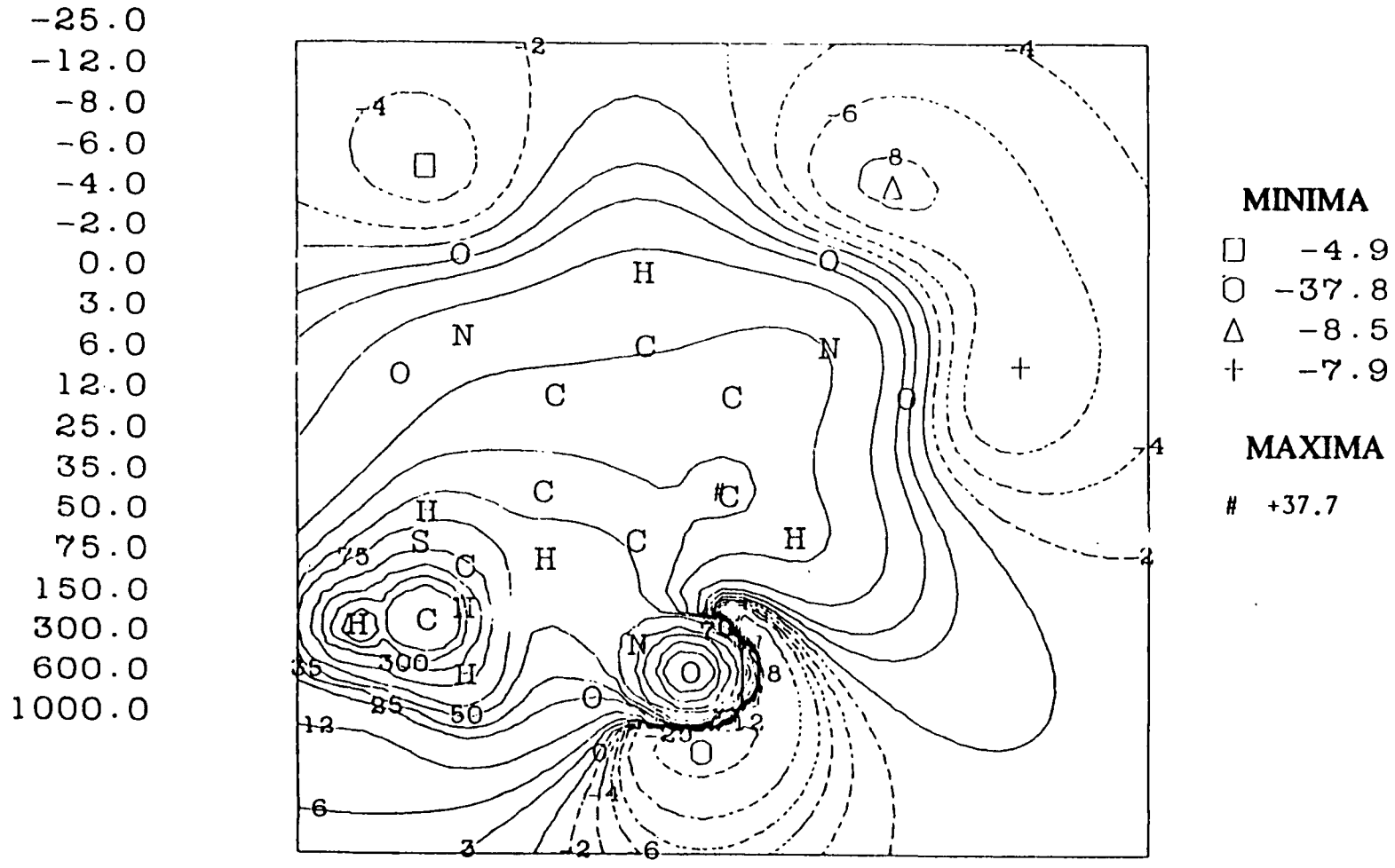
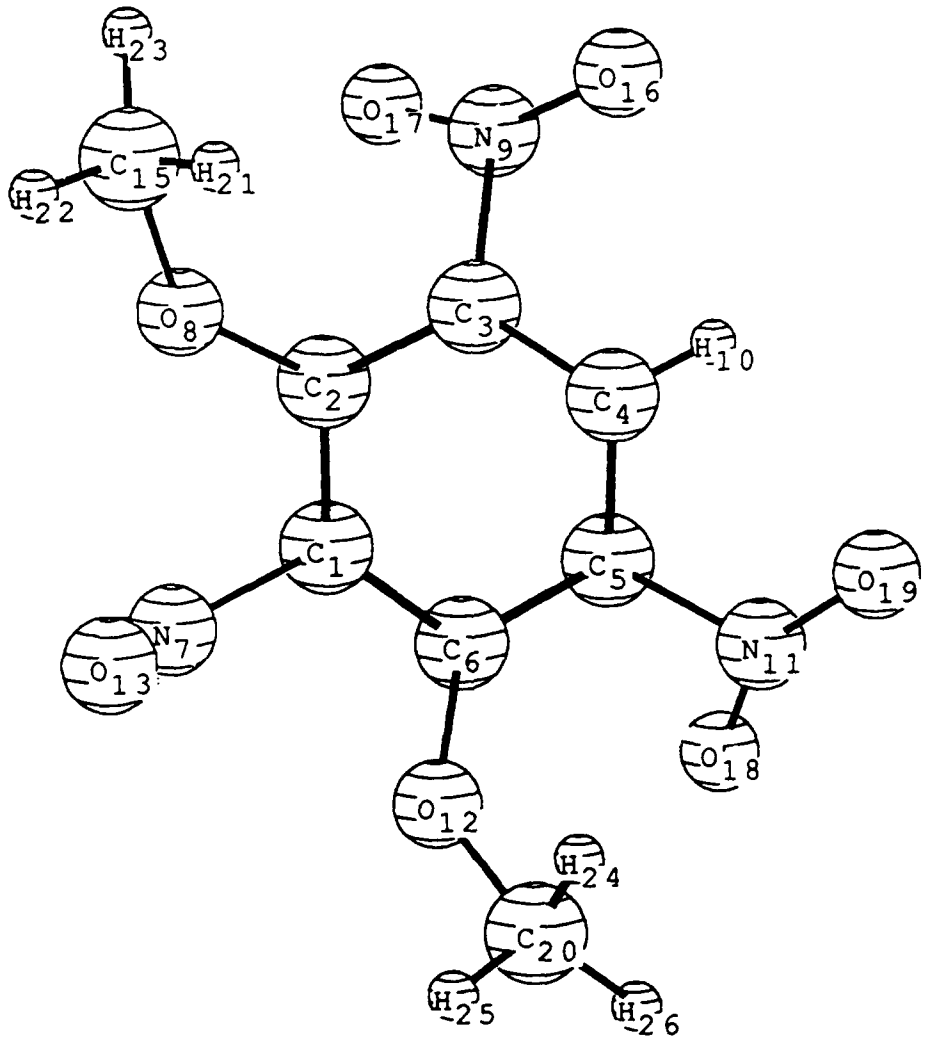


Figure K-2. Calculated electrostatic potential, in kcal/mole, of ethyl picryl sulfide, in the plane 1.75Å above the N8 nitro group located in the upper right corner. Projected positions of nuclei are shown. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

APPENDIX L
1,3-DIMETHOXY-2,4,6-TRINITROBENZENE

The short distances between non-bonded hydrogens and oxygens are H10-O16 (2.40 Å), H10-O19 (2.40 Å), H23-O17 (2.40 Å) and H16-O18 (2.40 Å). Nitro groups N7, N9 and N11 are rotated out of the plane by approximately 87°, 28° and 24 °, respectively.



Z-MATRIX (ANGSTROMS AND DEGREES)

CD	CENT	ATOM	N1	LENGTH	N2	ALPHA	N3	BETA	J
1	1	C							
2	2	C	1	1.380400 (1)					
3	3	C	2	1.396859 (2)	1	115.604 (26)			
4	4	C	3	1.374392 (3)	2	120.903 (27)	1	-0.300 (50)	0
5	5	C	4	1.374392 (4)	3	120.965 (28)	2	1.583 (51)	0
6	6	C	5	1.396707 (5)	4	120.903 (29)	3	-1.577 (52)	0
7	7	N	1	1.477729 (6)	2	116.814 (30)	3	171.627 (53)	0
8	8	O	2	1.348742 (7)	3	127.817 (31)	4	177.893 (54)	0
9	9	N	3	1.472888 (8)	4	116.550 (32)	5	-173.595 (55)	0
10	10	H	4	0.957800 (9)	5	119.491 (33)	6	-178.910 (56)	0
11	11	N	5	1.472798 (10)	6	122.351 (34)	1	-174.561 (57)	0
12	12	O	6	1.348835 (11)	1	116 545 (35)	2	179.456 (58)	0
13	13	O	7	1.201446 (12)	1	117.779 (36)	2	-86.685 (59)	0
14	14	O	7	1.196814 (13)	1	118.545 (37)	2	93.320 (60)	0
15	15	C	8	1.453946 (14)	2	118.793 (38)	3	-52.068 (61)	0
16	16	O	9	1.218047 (15)	3	116.743 (39)	4	-27.682 (62)	0
17	17	O	9	1.208641 (16)	3	118.554 (40)	4	150.656 (63)	0
18	18	O	11	1.208165 (17)	5	118.594 (41)	6	24.374 (64)	0
19	19	O	11	1.219471 (18)	5	116.707 (42)	6	-157.172 (65)	0
20	20	C	12	1.454637 (19)	6	118.815 (43)	1	-126.127 (66)	0
21	21	H	15	0.959584 (20)	8	110.128 (44)	2	-15.097 (67)	0
22	22	H	15	0.835747 (21)	8	102.071 (45)	2	-131.703 (68)	0
23	23	H	15	1.068769 (22)	8	106.925 (46)	2	107.973 (69)	0
24	24	H	20	0.959585 (23)	12	110.102 (47)	6	15.120 (70)	0
25	25	H	20	0.835635 (24)	12	102.070 (48)	6	131.718 (71)	0
26	26	H	20	1.068860 (25)	12	106.978 (49)	6	-107.899 (72)	0

STOICHIOMETRY C8H7N3O8

SCF DONE: E(RHF) = -1064.13065218 A.U. AFTER 27 CYCLES

EIGENVALUES -0.31717 0.12601 0.14363 0.20984 0.21092 0.24237

Estimated ionization potential: 8.66 ev

TOTAL ATOMIC CHARGES.

		1	Net charge
1	C	5.940192	0.060
2	C	5.809986	0.110
3	C	5.939638	0.060
4	C	6.051206	-0.051
5	C	5.939640	0.060
6	C	5.810025	0.190
7	N	6.801851	0.198
8	O	8.225877	-0.226
9	N	6.822849	0.177
10	H	0.852770	0.147
11	N	6.823226	0.177
12	O	8.225815	-0.226
13	O	8.208906	-0.209
14	O	8.183193	-0.183
15	C	6.187587	-0.188
16	O	8.197942	-0.198
17	O	8.196408	-0.196
18	O	8.195929	-0.196
19	O	8.198151	-0.198
20	C	6.187626	-0.188
21	H	0.881395	0.119
22	H	0.853922	0.146
23	H	0.865290	0.135
24	H	0.881356	0.119
25	H	0.853904	0.146
26	H	0.865314	0.135

DIPOLE MOMENT (DEBYE): X= 0.2854 Y=-2.4370 Z= 0.1182 TOTAL= 2.4565

V-mid: N7-C1: 0.185
N9-C3: 0.170
N11-C5: 0.170

Bond Order: N7-C1: 1.22
N9-C3: 1.23
N11-C5: 1.23
O13-N7: 2.03
O14-N7: 2.05
O16-N9: 1.95
O17-N9: 1.99
O18-N11: 2.00
O19-N11: 1.94

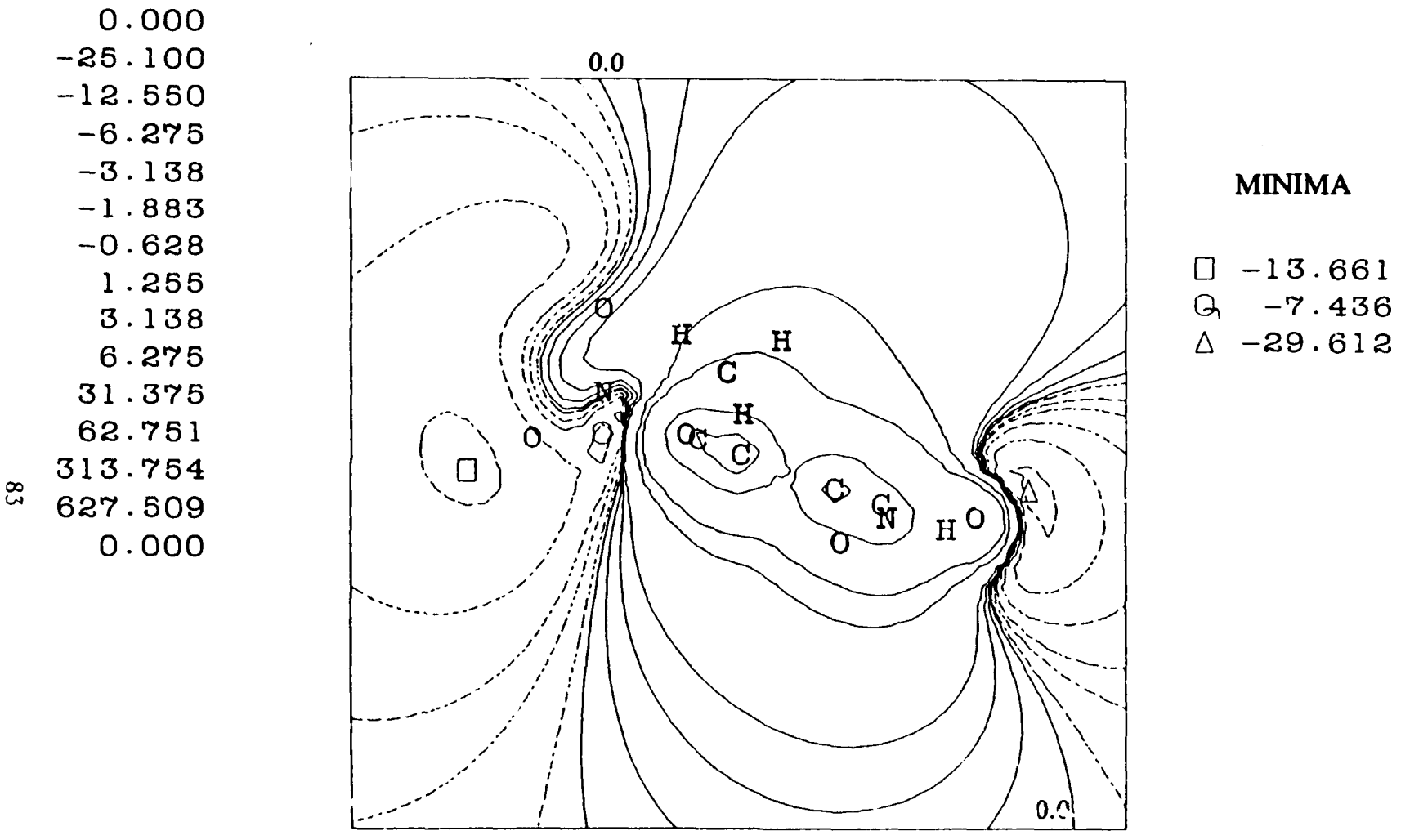


Figure L-1. Calculated electrostatic potential, in kcal/mole, of 1,3-dimethoxy-2,4,6-trinitrobenzene, in the plane 1.75Å above the N7 nitro group located in the upper left corner. Projected positions of nuclei are shown. The zero contour is indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

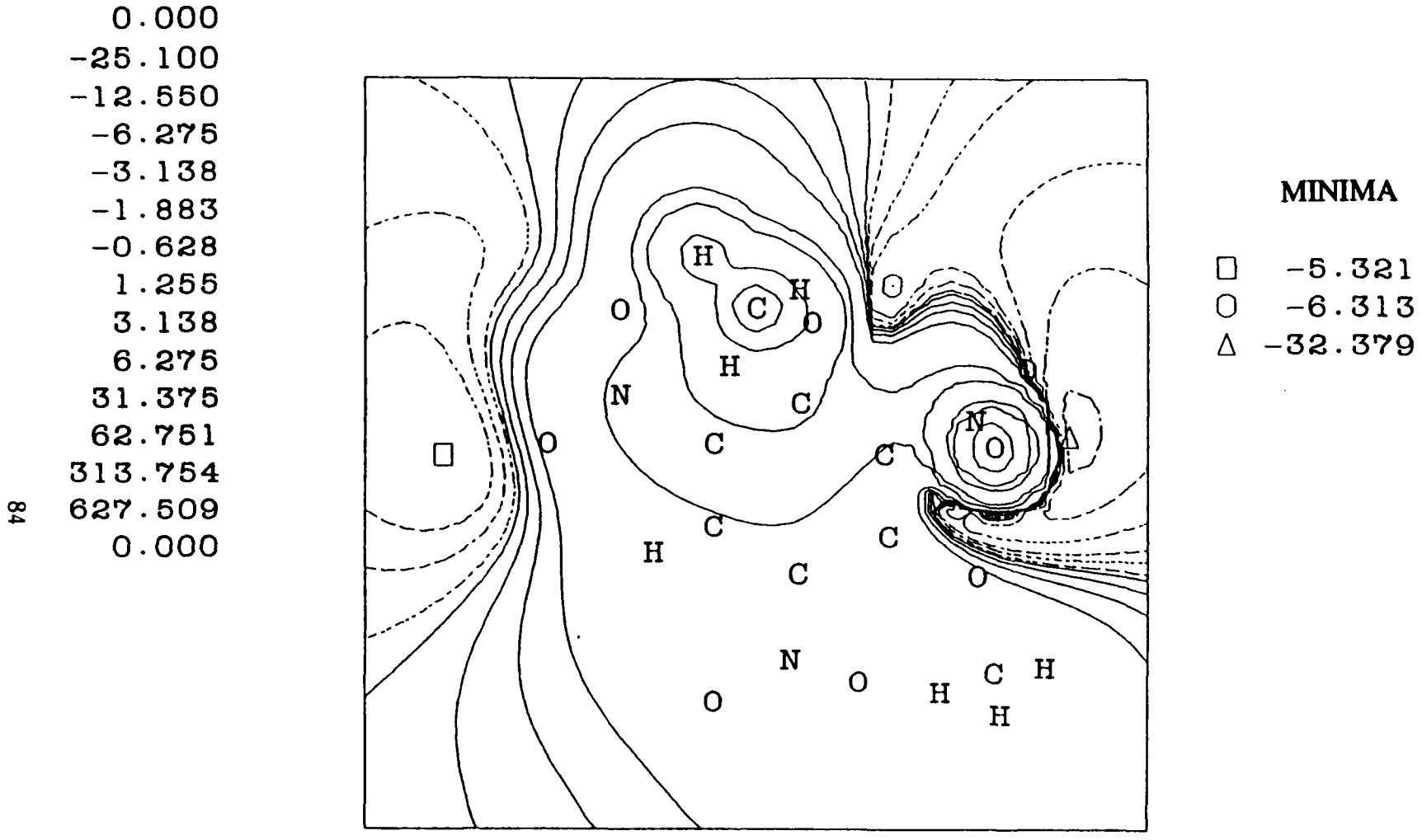
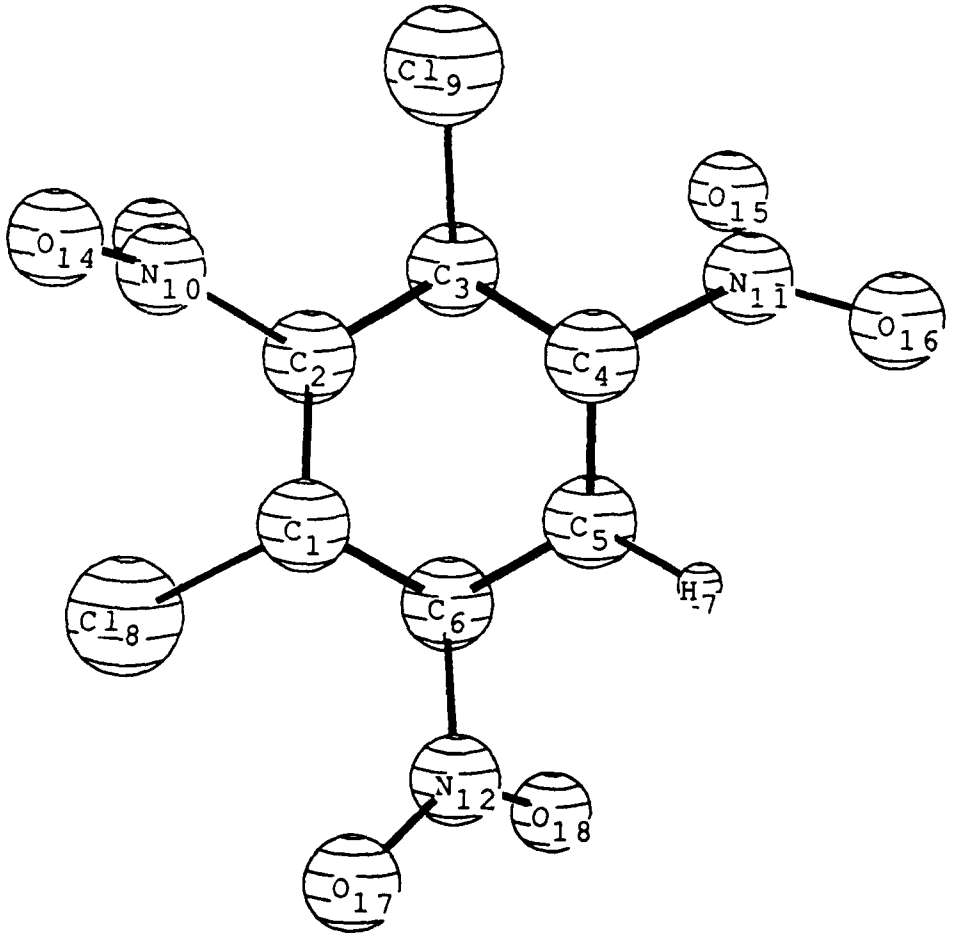


Figure L-2. Calculated electrostatic potential, in kcal/mole, of 1,3-dimethoxy-2,4,6-trinitrobenzene, in the plane 1.75Å above the N11 nitro group located in the upper left corner. Projected positions of nuclei are shown. The zero contour is indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

APPENDIX M
1,3-DICHLORO-2,4,6-TRINITROBENZENE

The short distances between non-bonded hydrogens and oxygens are O18-H7 (2.48 Å) and O16-H7 (2.50 Å).

The N11 and N12 nitro groups are rotated out of the plane by about 37°, while the N10 nitro group is rotated by approximately 75°.



Z-MATRIX (ANGSTROMS AND DEGREES)

CD	CENT	ATOM	N1	LENGTH	N2	ALPHA	N3	BETA	J
1	1	C							
2	2	C	1	1.407000 (1)					
3	3	C	2	1.407000 (2)	1	122.700 (18)			
4	4	C	3	1.371000 (3)	2	116.900 (19)	1	-0.100 (34)	0
5	5	C	4	1.378000 (4)	3	121.600 (20)	2	0.200 (35)	0
6	6	C	5	1.378000 (5)	4	120.200 (21)	3	-0.100 (36)	0
7	7	H	5	1.059000 (6)	4	119.900 (22)	3	179.900 (37)	0
8	8	Cl	1	1.690000 (7)	2	118.300 (23)	3	-177.800 (38)	0
9	9	Cl	3	1.690000 (8)	4	124.800 (24)	5	177.700 (39)	0
10	10	N	2	1.447000 (9)	3	118.600 (25)	9	2.200 (40)	0
11	11	N	4	1.467000 (10)	5	116.900 (26)	7	2.200 (41)	0
12	12	N	6	1.467000 (11)	5	116.900 (27)	4	-177.800 (42)	0
13	13	O	10	1.206000 (12)	2	117.300 (28)	3	74.800 (43)	0
14	14	O	10	1.206000 (13)	2	117.300 (29)	3	-105.200 (44)	0
15	15	O	11	1.224000 (14)	4	117.900 (30)	3	-35.300 (45)	0
16	16	O	11	1.217000 (15)	4	117.200 (31)	5	-37.800 (46)	0
17	17	O	12	1.224000 (16)	6	117.900 (32)	1	-37.800 (47)	0
18	18	O	12	1.217000 (17)	6	117.200 (33)	5	-35.300 (48)	0

STOICHIOMETRY C6HCL2N3O6

E= -1751.88563620 •••••••••

EIGENVALUES — -0.38138 -0.38065 -0.32917 -0.32775 -0.32741

Estimated ionization potential: 8.9 ev

TOTAL ATOMIC CHARGES.

		1	Net Charges
1	C	5.945256	+0.05
2	C	5.881767	+0.12
3	C	5.945048	+0.05
4	C	5.897801	+0.10
5	C	6.021674	-0.02
6	C	5.897935	+0.10
7	H	0.853928	+0.15
8	Cl	17.012369	-0.01
9	Cl	17.011478	-0.01
10	N	6.818918	+0.18
11	N	6.825640	+0.17
12	N	6.825625	+0.17
13	O	8.175416	-0.18
14	O	8.175321	-0.18
15	O	8.172938	-0.17
16	O	8.182942	-0.18
17	O	8.172556	-0.17
18	O	8.183389	-0.18

DIPOLE MOMENT (DEBYE): X= 0.9514 Y= 0.0777 Z=-0.5464 TOTAL= 1.0999

V_{mid}: C_2-N_{10}: 0.219
C_4-N_{11}: 0.200
C_6-N_{12}: 0.199

Bond Orders: C_2-N_{10}: 1.31
C_4-N_{11}: 1.25
C_6-N_{12}: 1.25
N_{10}-O_{13}: 2.17
N_{10}-O_{14}: 2.17
N_{11}-O_{15}: 2.07
N_{11}-O_{16}: 2.11
N_{12}-O_{17}: 2.07
N_{12}-O_{18}: 2.11

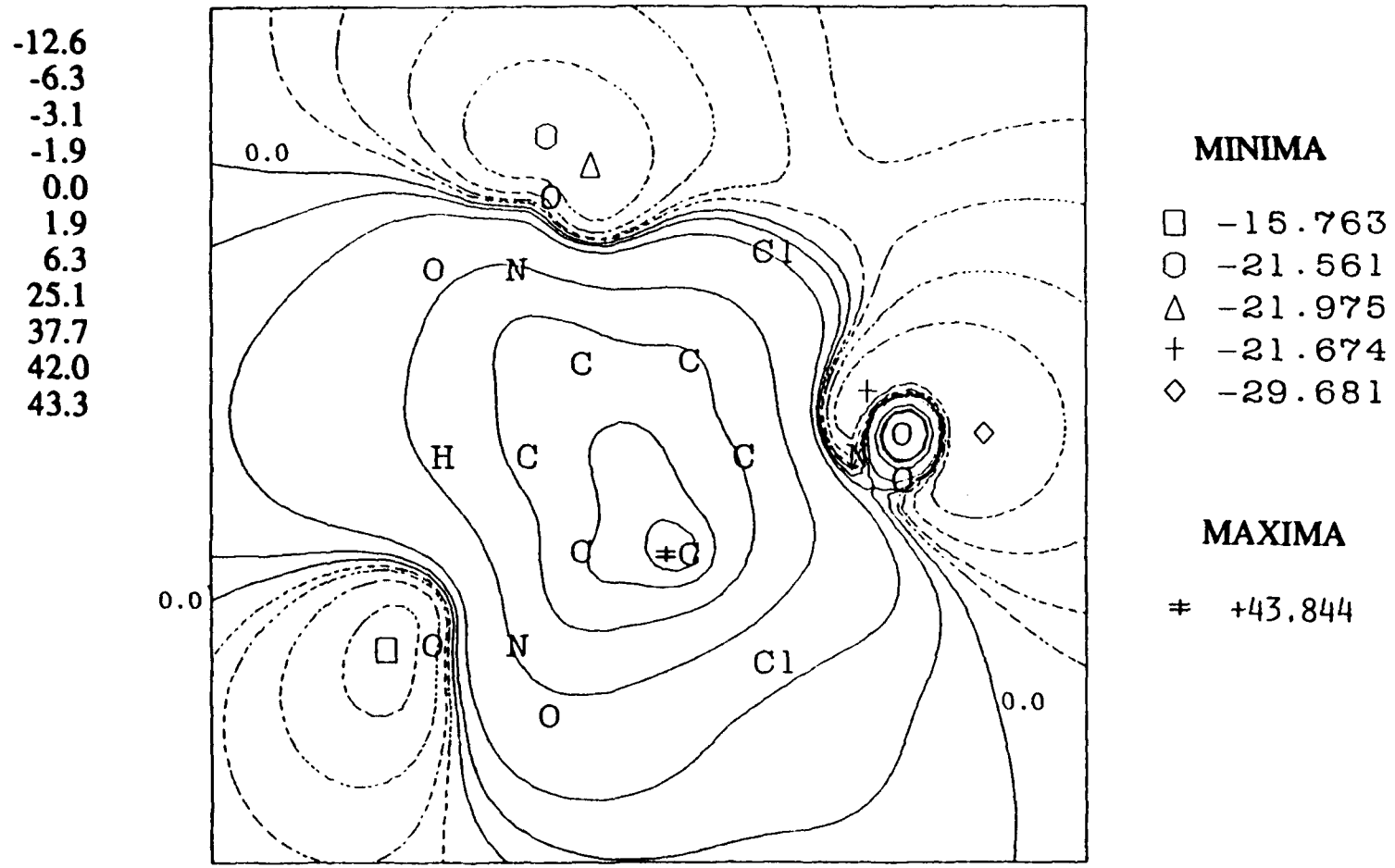
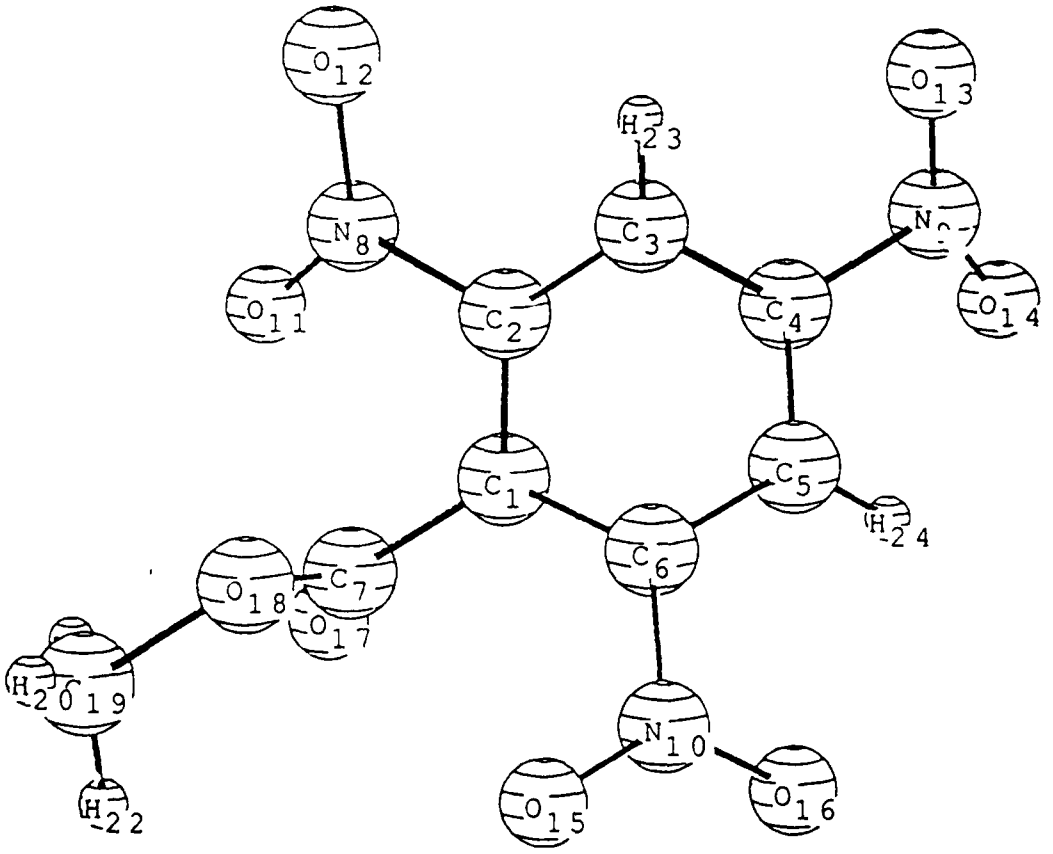


Figure M-1. Calculated electrostatic potential, in kcal/mole, of 1,3-dichloro-2,4,6-trinitrobenzene, in the plane 1.75 Å above the aromatic ring. Projected positions of nuclei are shown. The zero contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

APPENDIX N
METHYL 2,4,6-TRINITROBENZOATE

The short distances between non-bonded hydrogens and oxygens are H24-O16 (2.39 Å), H24-O14 (2.49 Å), H23-O12 (2.51 Å), and H23-O13 (2.46 Å).

The N8, N9 and N10 nitro groups are rotated out of the mean plane of the benzene ring by about 30°,19° and 11°, respectively.



Z-MATRIX (ANGSTROMS AND DEGREES)

CD	CENT	ATOM	N1	LENGTH	N2	ALPHA	N3	BETA	J
1	1	C							
2	2	C	1	1.399000 (1)					
3	3	C	2	1.369201 (2)	1	123.039 (24)			
4	4	C	3	1.367792 (3)	2	118.034 (25)	1	3.951 (46)	0
5	5	C	4	1.381531 (4)	3	122.096 (26)	2	-5.419 (47)	0
6	6	C	5	1.373809 (5)	4	117.508 (27)	3	2.053 (48)	0
7	7	C	1	1.506101 (6)	2	121.789 (28)	3	-174.205 (49)	0
8	8	N	2	1.473057 (7)	3	117.045 (29)	4	-175.495 (50)	0
9	9	N	4	1.468854 (8)	3	119.287 (30)	2	176.619 (51)	0
10	10	N	6	1.469922 (9)	5	116.809 (31)	4	-174.204 (52)	0
11	11	O	8	1.219024 (10)	2	117.687 (32)	3	146.477 (53)	0
12	12	O	8	1.200891 (11)	2	118.570 (33)	3	-30.182 (54)	0
13	13	O	9	1.204490 (12)	4	117.840 (34)	3	18.816 (55)	0
14	14	O	9	1.212250 (13)	4	117.908 (35)	3	-160.143 (56)	0
15	15	O	10	1.215152 (14)	6	118.306 (36)	5	167.609 (57)	0
16	16	O	10	1.202680 (15)	6	118.492 (37)	5	-10.559 (58)	0
17	17	O	7	1.196264 (16)	1	122.533 (38)	2	102.052 (59)	0
18	18	O	7	1.322560 (17)	1	111.245 (39)	2	-77.254 (60)	0
19	19	C	18	1.440833 (18)	7	115.907 (40)	1	-179.604 (61)	0
20	20	H	19	0.934096 (19)	18	110.296 (41)	7	178.879 (62)	0
21	21	H	19	0.792386 (20)	18	109.029 (42)	7	-47.307 (63)	0
22	22	H	19	0.928466 (21)	18	110.944 (43)	7	80.900 (64)	0
23	23	H	3	0.887293 (22)	4	119.957 (44)	5	176.795 (65)	0
24	24	H	5	0.901565 (23)	4	121.367 (45)	3	-178.313 (66)	0

STOICHIOMETRY C8H5N3O8

SCF DONE: E(RHF) = -1062.92339579

EIGENVALUES -- -0.37469 -0.32483 -0.32381 -0.32239 0.10480

Estimated ionization potential: 8.78 ev

TOTAL ATOMIC CHARGES.

		1	Net Charge
1	C	5.975266	0.025
2	C	5.880043	0.120
3	C	6.086838	-0.087
4	C	5.872820	0.127
5	C	6.076690	-0.077
6	C	5.886064	0.114
7	C	5.615164	0.385
8	N	6.818939	0.181
9	N	6.818394	0.182
10	N	6.817896	0.182
11	O	8.195753	-0.196
12	O	8.181190	-0.181
13	O	8.188783	-0.189
14	O	8.190735	-0.191
15	O	8.197226	-0.197
16	O	8.183581	-0.184
17	O	8.260313	-0.260
18	O	8.240812	-0.241
19	C	6.278682	-0.279
20	H	0.852278	0.148
21	H	0.840594	0.159
22	H	0.848691	0.151
23	H	0.847549	0.152
24	H	0.845699	0.154

DIPOLE MOMENT (DEBYE): X=-0.7273 Y=-0.9971 Z=-0.3363 TOTAL= 1.2792

V-mid: C2-N8: 0.216
C4-N9: 0.223
C6-N10: 0.213

Bond Order: C2-N8: 1.23
C4-N9: 1.24
C6-N10: 1.24
N8-O11: 1.95
N8-O12: 2.03
N9-O13: 2.02
N9-O14: 1.98
N10-O15: 1.96
N10-O16: 2.02

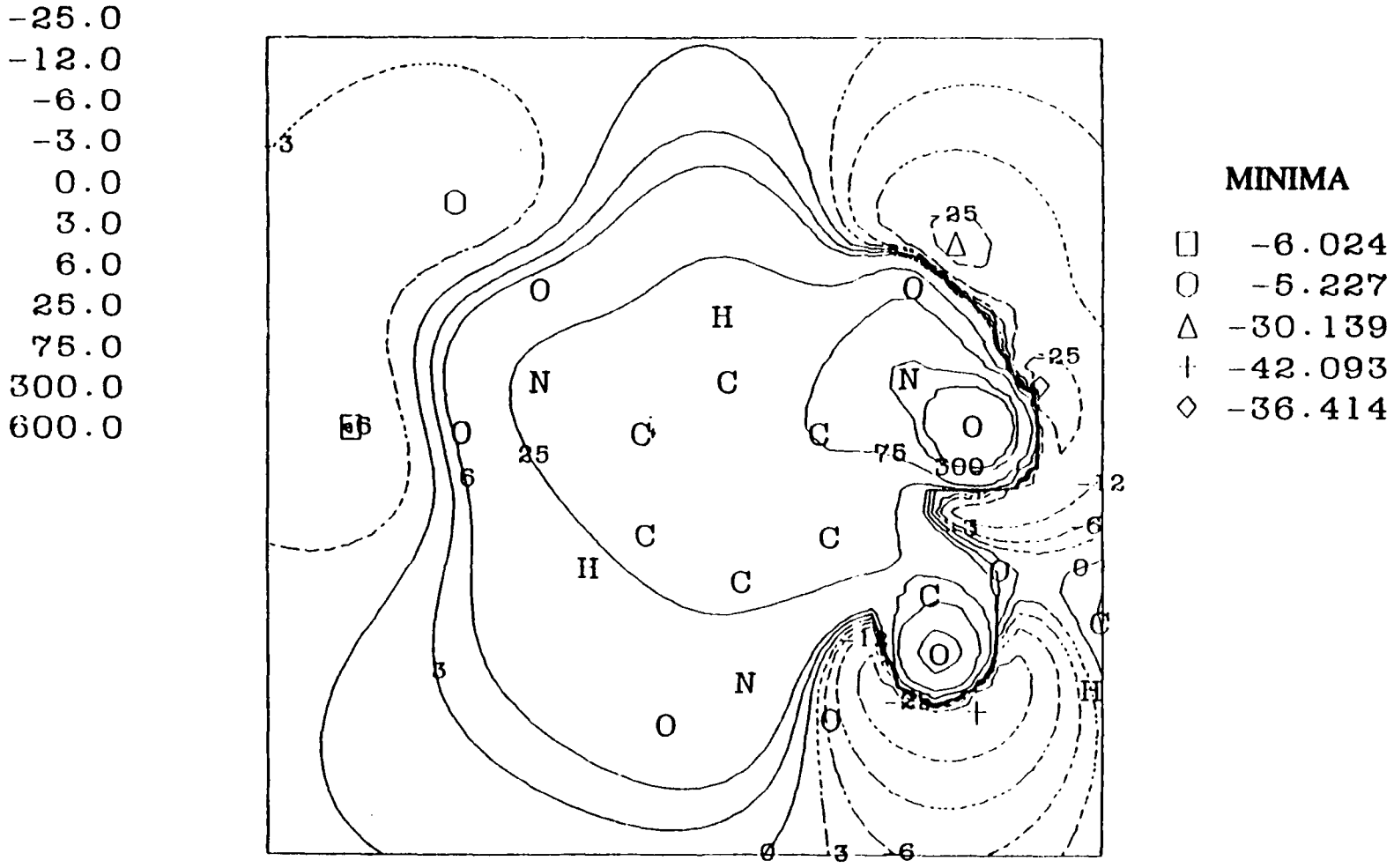


Figure N-1. Calculated electrostatic potential, in kcal/mole, of methyl-2,4,6-trinitrobenzoate, in the plane 1.75Å above the N9 nitro group located in the upper left corner. Projected positions of nuclei are shown. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

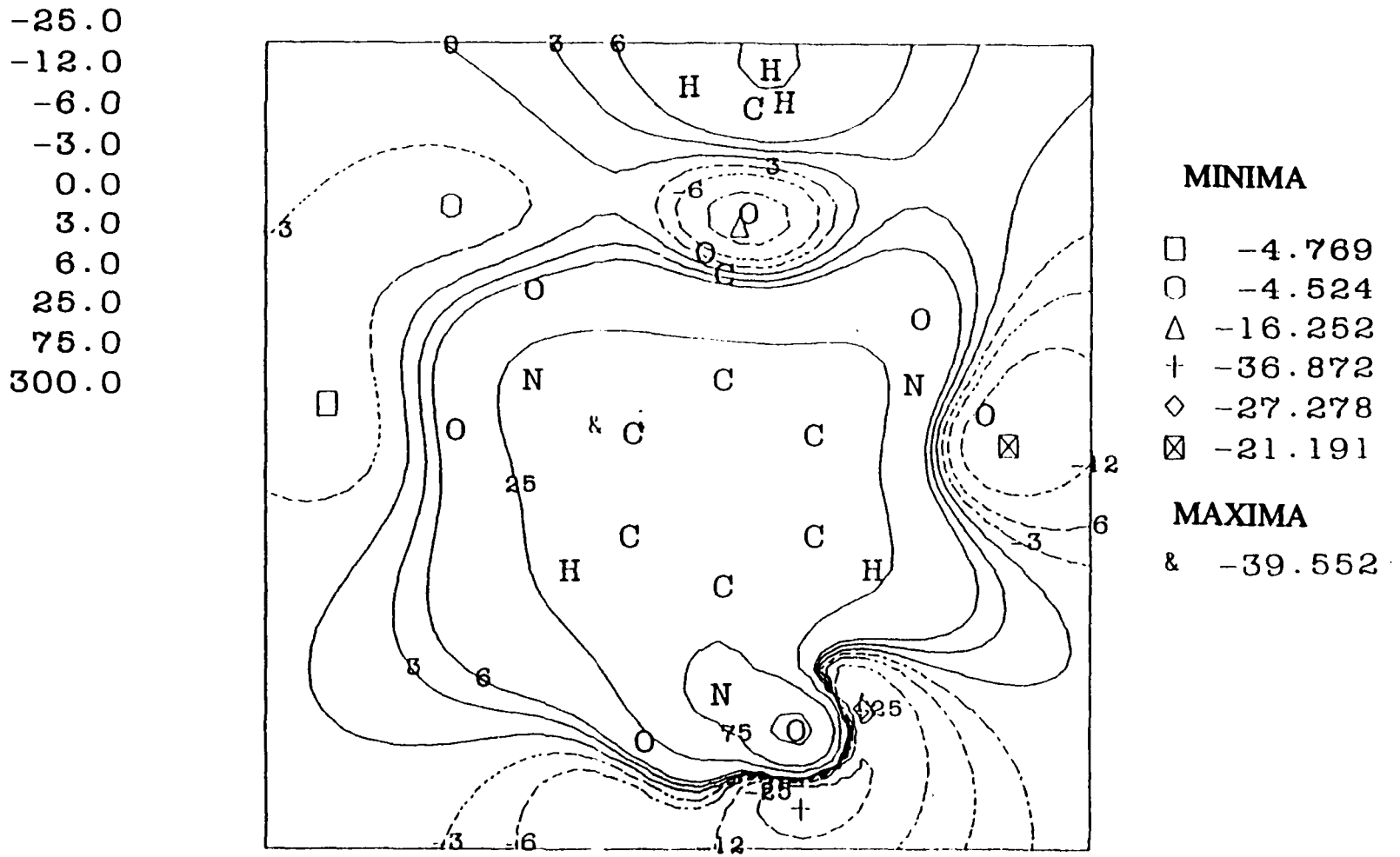
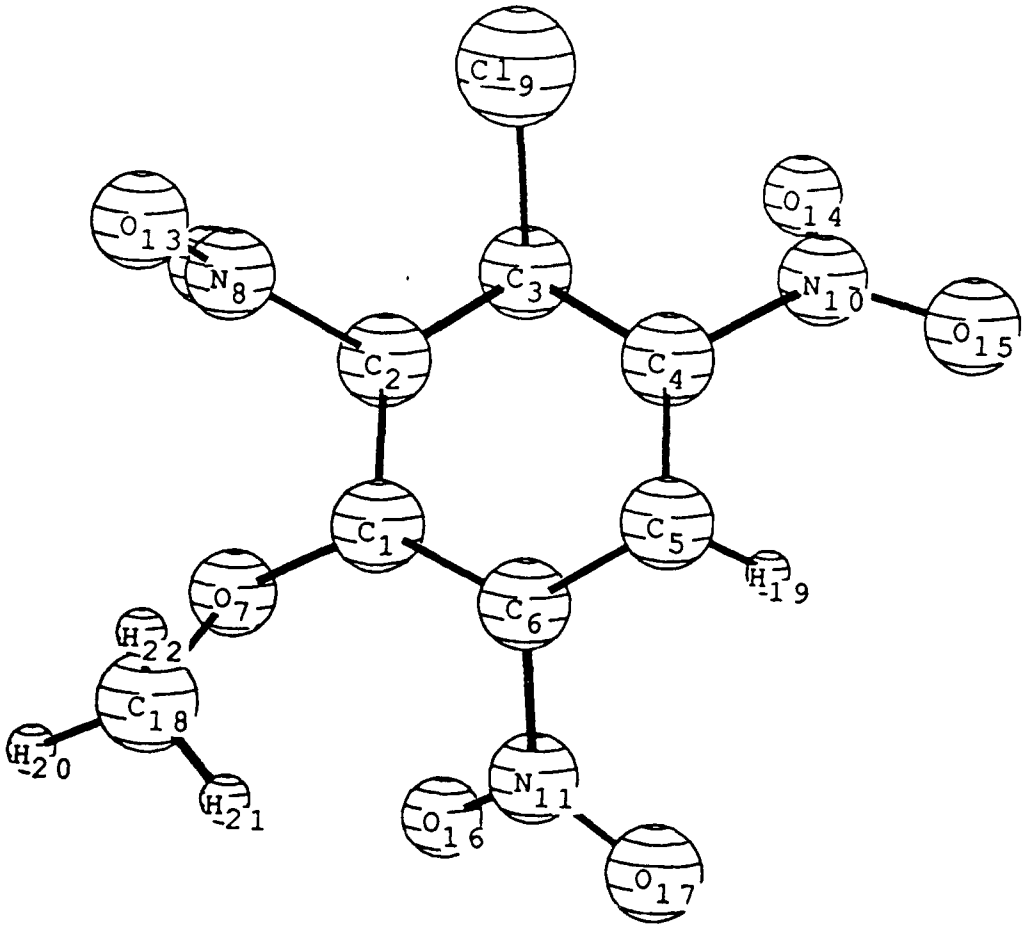


Figure N-2. Calculated electrostatic potential, in kcal/mole, of methyl-2,4,6-trinitrobenzoate, in the plane 1.75Å above the N10 nitro group located in the upper left corner. Projected positions of nuclei are shown. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

APPENDIX O
3-CHLORO-2,4,6-TRINITROANISOLE

The short distances between non-bonded hydrogens and oxygens are H19-O15 (2.40 Å), and H21-O16 (2.49 Å).

The N10 and N11 nitro groups are both rotated out of the mean plane of the benzene ring by about 34°, while the N8 nitro groups is essentially perpendicular to the ring.



Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.393000(1)					
3	3	C	2	1.379882(2)	1	124.169(22)			
4	4	C	3	1.397787(3)	2	117.131(23)	1	-1.982(42)	0
5	5	C	4	1.375273(4)	3	120.917(24)	2	-1.185(43)	0
6	6	C	5	1.379063(5)	4	119.743(25)	3	3.635(44)	0
7	7	O	1	1.337936(6)	2	117.416(26)	3	-175.920(45)	0
8	8	N	2	1.475404(7)	3	119.302(27)	4	176.836(46)	0
9	9	Cl	3	1.708597(8)	4	123.881(28)	5	176.182(47)	0
10	10	N	4	1.467148(9)	5	116.929(29)	6	-175.679(48)	0
11	11	N	6	1.470114(10)	5	116.868(30)	4	175.101(49)	0
12	12	O	8	1.206072(11)	2	116.279(31)	1	-93.668(50)	0
13	13	O	8	1.209100(12)	2	117.012(32)	1	87.023(51)	0
14	14	O	10	1.210823(13)	4	117.965(33)	5	145.702(52)	0
15	15	O	10	1.217797(14)	4	116.529(34)	5	-33.103(53)	0
16	16	O	11	1.213555(15)	6	117.798(35)	5	-143.428(54)	0
17	17	O	11	1.213311(16)	6	117.378(36)	5	34.636(55)	0
18	18	C	7	1.436348(17)	1	117.841(37)	2	-116.169(56)	0
19	19	H	5	0.954598(18)	4	115.499(38)	3	176.687(57)	0
20	20	H	18	0.973907(19)	7	110.200(39)	1	179.977(58)	0
21	21	H	18	0.963601(20)	7	110.585(40)	1	-60.623(59)	0
22	22	H	18	0.961951(21)	7	110.815(41)	1	60.344(60)	0

STOICHIOMETRY C7H4ClN3O7

SCF DONE: E(RHF) = -1408.06215783

Alpha eigenvalues — -0.35582 -0.32435 -0.32228 -0.32083 0.10979

Estimated ionization potential: 8.73 ev

Total atomic charges:

		1
1	C	0.192606
2	C	0.089377
3	C	0.057532
4	C	0.101570
5	C	-0.053390
6	C	0.080864
7	O	-0.231147
8	N	0.190374
9	Cl	-0.028886
10	N	0.178105
11	N	0.175684
12	O	-0.173706
13	O	-0.189534
14	O	-0.176087
15	O	-0.192282
16	O	-0.187936
17	O	-0.189789
18	C	-0.165813
19	H	0.147707
20	H	0.136505
21	H	0.118657
22	H	0.119587

Dipole moment (Debye):

X= -2.1747 Y= -0.2494 Z= 1.2918 Tot= 2.5418

Bond Order		V-mid	
C2-N8:	1.23	C2-N8:	0.201
C4-N10:	1.25	C4-N10:	0.202
C6-N11:	1.24	C6-N11:	0.185
N8-O12:	2.01		
N8-O13:	2.00		
N10-O14:	1.98		
N10-O15:	1.95		
N11-O16:	1.97		
N11-O17:	1.97		

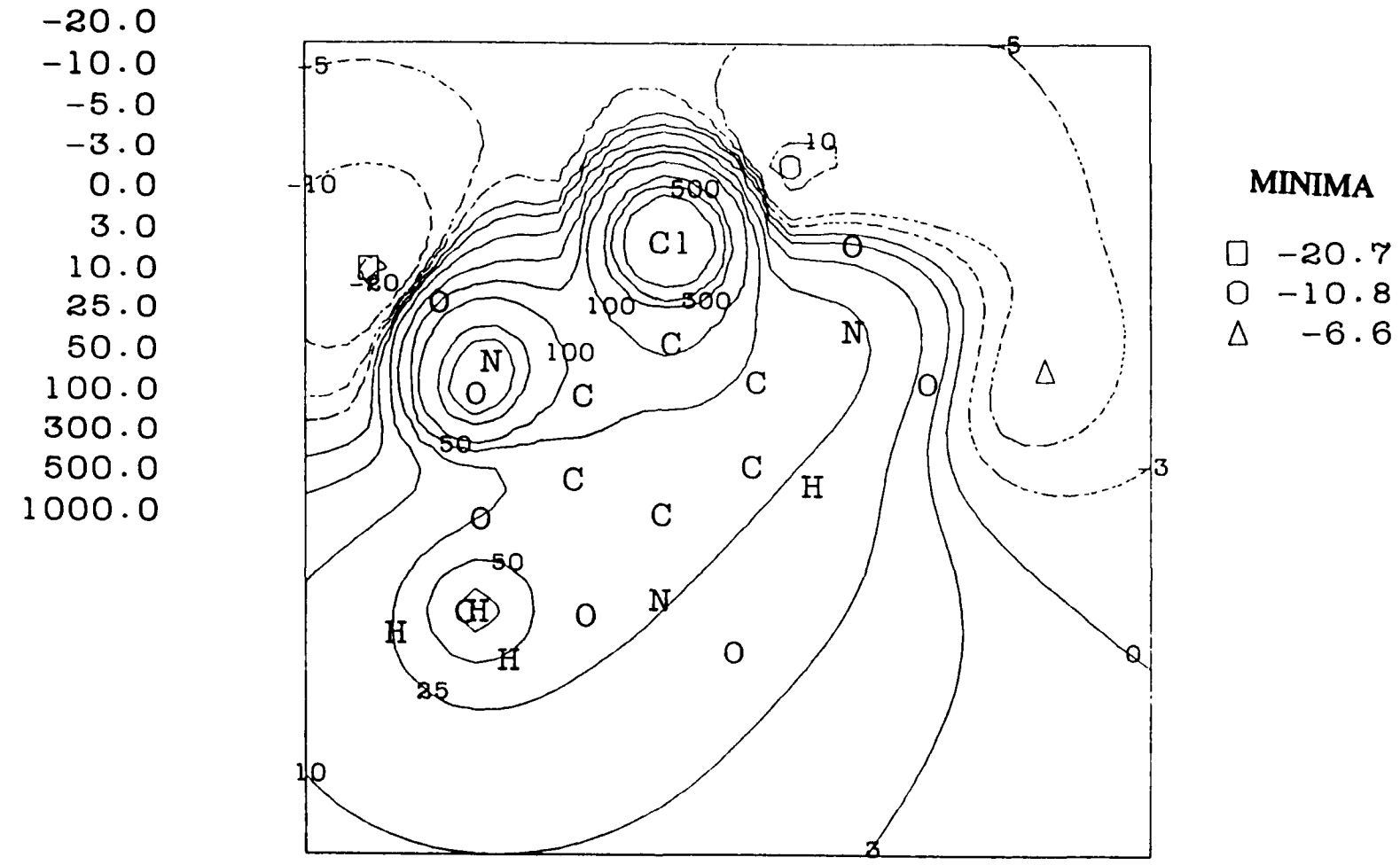


Figure O-1. Calculated electrostatic potential, in kcal/mole, of 3-chloro-2,4,6-trinitroanisole, in the plane 1.75Å above the N10 nitro group located in the upper right corner. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

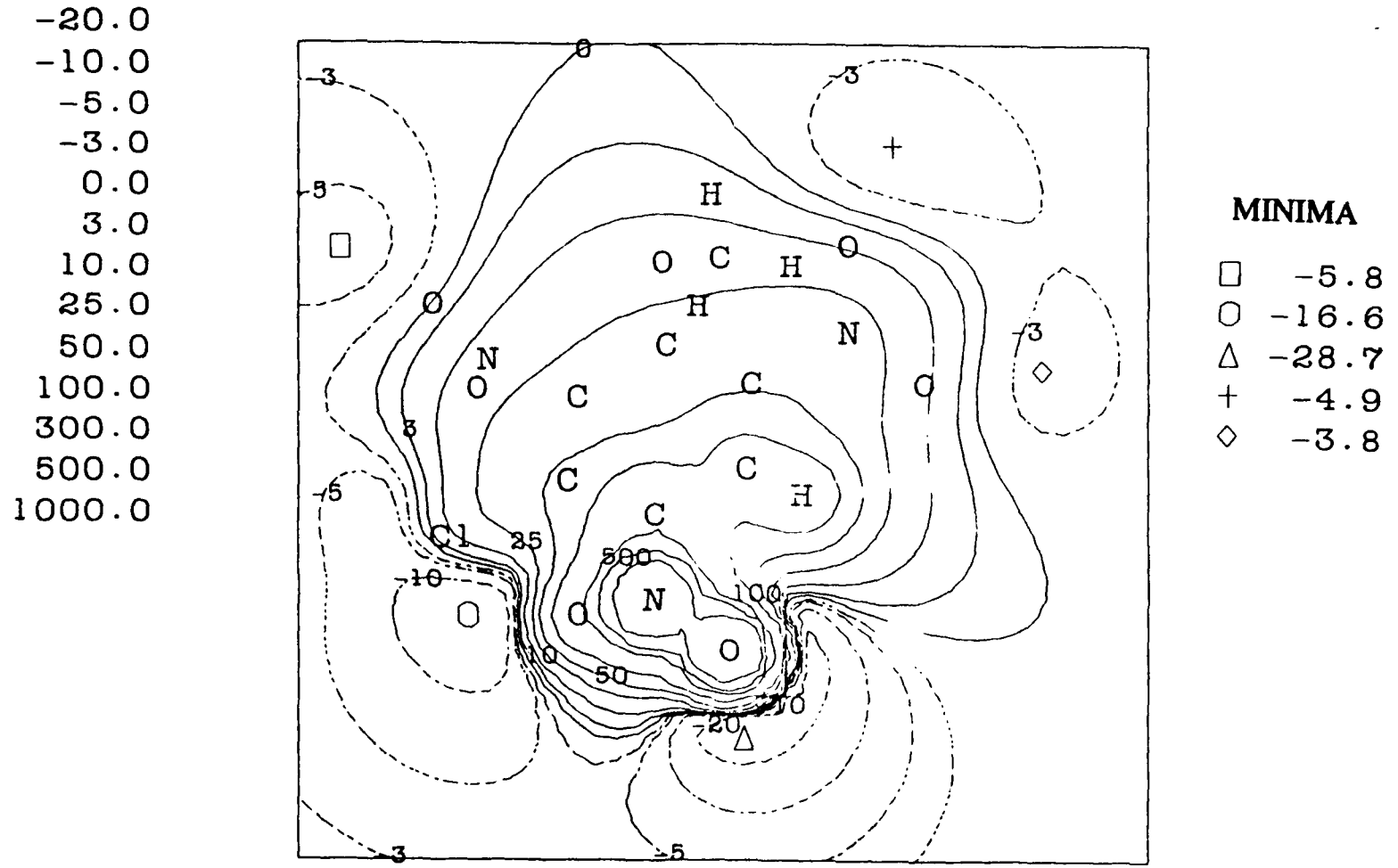
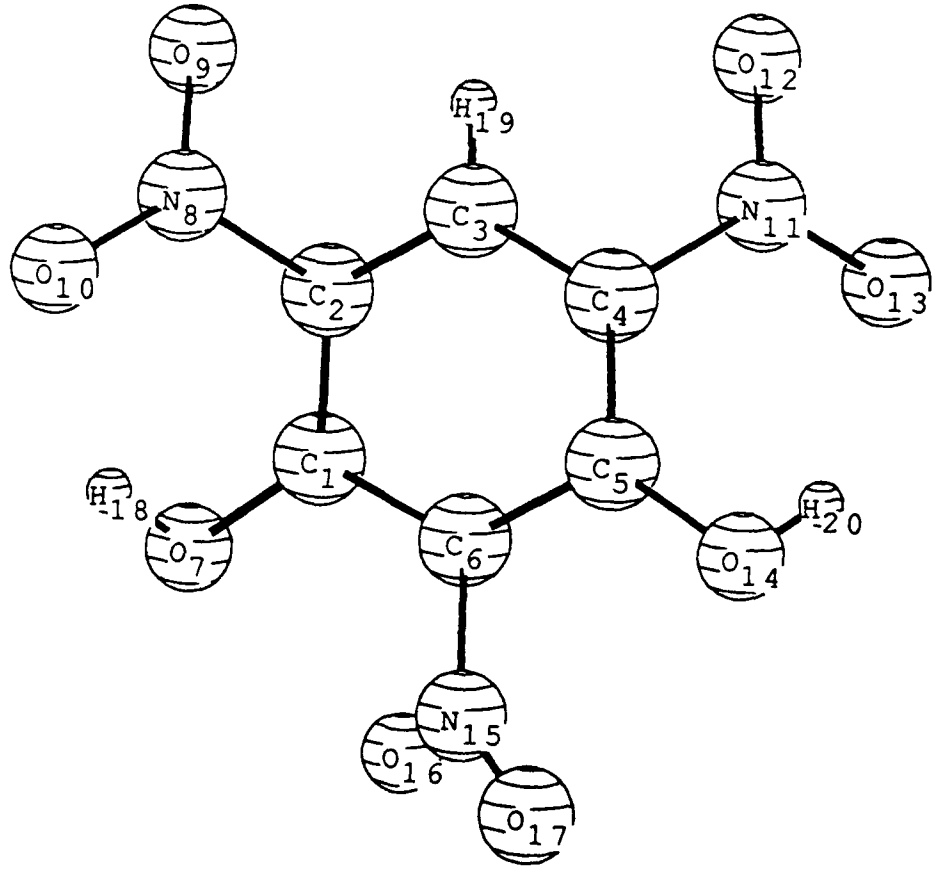


Figure O-2. Calculated electrostatic potential, in kcal/mole, of 3-chloro-2,4,6-trinitroanisole, in the plane 1.75Å above the N11 nitro group located in the upper right corner. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

APPENDIX P
STYPHNIC ACID

The short distances between non-bonded hydrogens and oxygens are H19-O12 (2.40 Å), H20-O13 (1.91 Å), H9-O9 (2.40 Å), and H18-O10 (1.91 Å).

The N8 and N11 nitro groups are essentially co-planar with the mean plane of the benzene ring, while the N15 nitro group is rotated by about 66°.



Z-MATRIX (ANGSTROMS AND DEGREES)

CD	CENT	ATOM	N1	LENGTH	N2	ALPHA	N3	BETA	J
1	1	C							
2	2	C	1	1.402080 (1)					
3	3	C	2	1.369661 (2)	1	121.310 (20)			
4	4	C	3	1.369663 (3)	2	120.570 (21)	1	-1.095 (38)	0
5	5	C	4	1.402073 (4)	3	121.310 (22)	2	-1.094 (39)	0
6	6	C	5	1.392829 (5)	4	116.460 (23)	3	2.086 (40)	0
7	7	O	1	1.326033 (6)	6	116.970 (24)	5	179.558 (41)	0
8	8	N	2	1.455679 (7)	3	118.669 (25)	4	177.595 (42)	0
9	9	O	8	1.216943 (8)	2	118.685 (26)	3	2.789 (43)	0
10	10	O	8	1.235027 (9)	2	118.272 (27)	3	-176.579 (44)	0
11	11	N	4	1.455678 (10)	5	120.009 (28)	6	-176.587 (45)	0
12	12	O	11	1.216944 (11)	4	118.685 (29)	5	-178.504 (46)	0
13	13	O	11	1.235036 (12)	4	118.273 (30)	5	2.129 (47)	0
14	14	O	5	1.326028 (13)	6	116.969 (31)	1	179.558 (48)	0
15	15	N	6	1.467534 (14)	1	118.079 (32)	2	178.989 (49)	0
16	16	O	15	1.217419 (15)	6	117.777 (33)	1	66.121 (50)	0
17	17	O	15	1.217422 (16)	6	117.776 (34)	1	-113.879 (51)	0
18	18	H	7	0.838803 (17)	1	110.127 (35)	2	-14.286 (52)	0
19	19	H	3	0.895145 (18)	4	119.715 (36)	5	178.906 (53)	0
20	20	H	14	0.838806 (19)	5	110.128 (37)	6	165.079 (54)	0

STOICHIOMETRY: C6H3N3O8

E= -986.441730465 ••••••••••••

EIGENVALUES — -0.33180 -0.29774 0.11913 0.11944 0.18924

Estimated ionization potential: 8.10 ev

TOTAL ATOMIC CHARGES.

		1	Net Charges
1	C	5.784320	+0.22
2	C	5.951153	+0.05
3	C	6.060130	-0.06
4	C	5.951145	+0.05
5	C	5.784320	+0.22
6	C	5.947836	+0.05
7	O	8.352258	-0.35
8	N	6 829713	+0.17
9	O	8.169836	-0.17
10	O	8 228012	-0.23
11	N	6.829721	+0.17
12	O	8 169836	-0.17
13	O	8.228023	-0.23
14	O	8.352260	-0.35
15	N	6.816398	+0.18
16	O	8.186697	-0.19
17	O	8.186698	-0.19
18	H	0.663593	+0.34
19	H	0.844464	+0.16
20	H	0.663588	+0.34

DIPOLE MOMENT (DEBYE): X=-0.0496 Y= 0.0296 Z= 1.7812 TOTAL= 1.7821

V_{mid}: C_2-N_8: 0.159
C_4-N_{11}: 0.159
C_6-N_{15}: 0.170

Bond Orders: C_2-N_8: 1.28
C_4-N_{11}: 1.28
C_6-N_{15}: 1.25
N_8-O_9: 2.11
N_8-O_{10}: 2.02
N_{11}-O_{12}: 2.11
N_{11}-O_{13}: 2.02
N_{15}-O_{16}: 2.11
N_{15}-O_{17}: 2.11

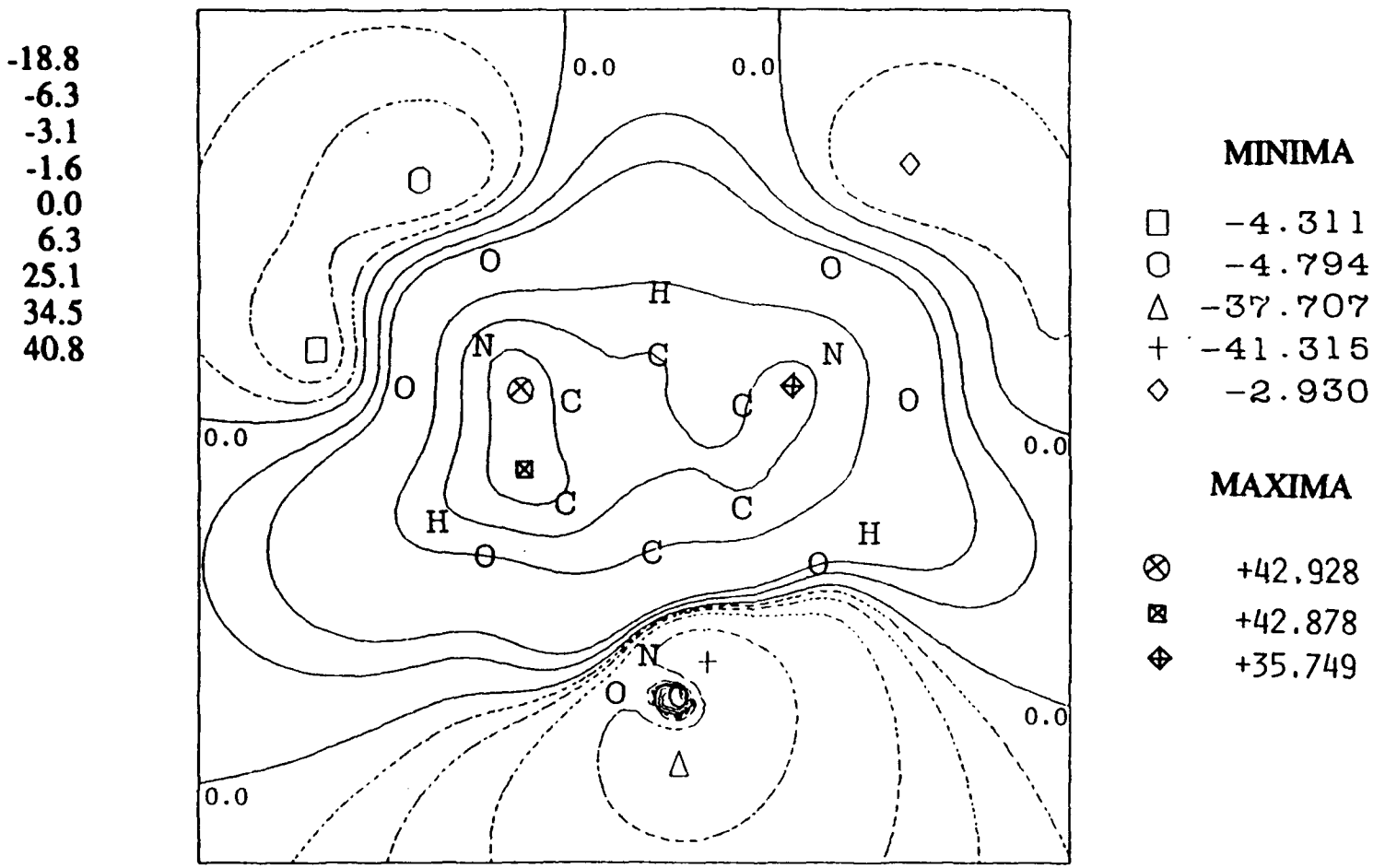
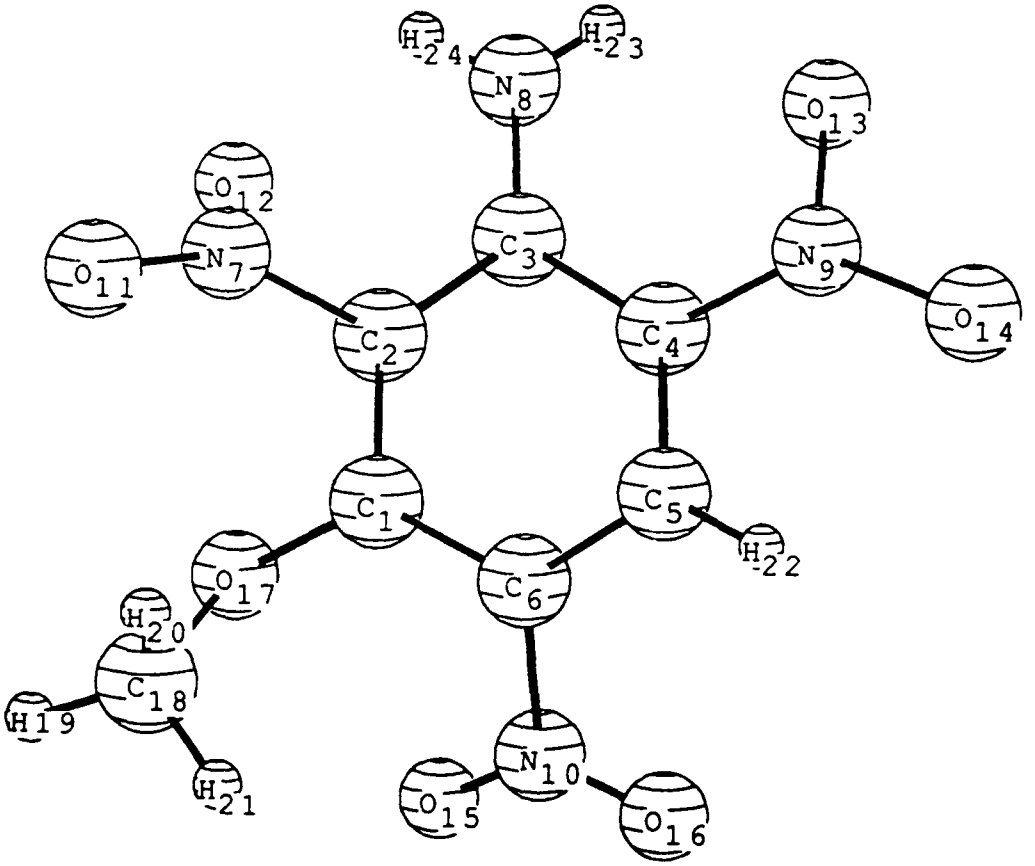


Figure P-1. Calculated electrostatic potential, in kcal/mole, of styphnic acid, in the plane 1.75 Å above the aromatic ring. Projected positions of nuclei are shown. The zero contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

APPENDIX Q
3-AMINO-2,4,6-TRINITROANISOLE

The short distances between non-bonded hydrogens and oxygens (suggesting hydrogen bonding) are between H24-O12 (2.15 Å), H23-O13 (2.01 Å), H22-O14 (2.35 Å) and H21-O15 (2.37 Å).

The N7 is rotated out of the mean plane of the benzene ring by more than 50°, and the N9 and N10 nitro groups are rotated by approximately 10° and 20°, respectively. The amine group (N8) is almost planar with respect to the mean plane of the benzene ring.



Z-MATRIX (ANGSTROMS AND DEGREES)

CD	CENT	ATOM	N1	LENGTH		N2	ALPHA		N3	BETA		J
1	1	C										
2	2	C	1	1.390000	(1)							
3	3	C	2	1.410000	(2)	1	125.700	(24)				
4	4	C	3	1.430000	(3)	2	113.400	(25)	1	-7.800	(46)	0
5	5	C	4	1.380000	(4)	3	122.100	(26)	2	6.750	(47)	0
6	6	C	5	1.380000	(5)	4	121.000	(27)	3	-1.300	(48)	0
7	7	N	2	1.460000	(6)	3	117.300	(28)	4	170.800	(49)	0
8	8	N	3	1.320000	(7)	4	123.600	(29)	5	-177.200	(50)	0
9	9	N	4	1.460000	(8)	5	115.800	(30)	6	179.300	(51)	0
10	10	N	6	1.460000	(9)	5	116.800	(31)	4	173.000	(52)	0
11	11	O	7	1.210000	(10)	2	119.200	(32)	3	-127.100	(53)	0
12	12	O	7	1.240000	(11)	2	116.800	(33)	3	51.100	(54)	0
13	13	O	9	1.230000	(12)	4	118.700	(34)	5	171.400	(55)	0
14	14	O	9	1.210000	(13)	4	119.100	(35)	5	-9.800	(56)	0
15	15	O	10	1.200000	(14)	6	119.100	(36)	5	-158.400	(57)	0
16	16	O	10	1.210000	(15)	6	118.100	(37)	5	17.990	(58)	0
17	17	O	1	1.330000	(16)	2	118.100	(38)	3	-173.700	(59)	0
18	18	C	17	1.430000	(17)	1	117.500	(39)	2	-113.800	(60)	0
19	19	H	18	0.950000	(18)	17	106.100	(40)	1	173.050	(61)	0
20	20	H	18	0.960000	(19)	17	112.000	(41)	1	53.300	(62)	0
21	21	H	18	0.960000	(20)	17	109.500	(42)	1	-68.850	(63)	0
22	22	H	5	0.930000	(21)	4	119.100	(43)	3	171.600	(64)	0
23	23	H	8	0.850000	(22)	3	118.810	(44)	2	-177.700	(65)	0
24	24	H	8	0.870000	(23)	3	117.380	(45)	2	3.240	(66)	0

STOICHIOMETRY C7H6N4O7

E(RHF)= -1005.60972021 A.U.

EIGENVALUES -- -0.30696 0.12681 0.14417 0.18365 0.23639

Estimated ionization potential: 8.36 ev

TOTAL ATOMIC CHARGES.

		1	Net Charge
1	C	5.792603	0.217
2	C	5.961544	0.038
3	C	5.778044	0.222
4	C	5.945189	0.055
5	C	6.050720	-0.051
6	C	5.952368	0.048
7	N	6.833561	0.166
8	N	7.554206	-0.554
9	N	6.827607	0.172
10	N	6.819568	0.180
11	O	8.181589	-0.182
12	O	8.212943	-0.213
13	O	8.225226	-0.225
14	O	8.186964	-0.187
15	O	8.202570	-0.203
16	O	8.208008	-0.208
17	O	8.234741	-0.235
18	C	6.171876	-0.172
19	H	0.862767	0.137
20	H	0.878724	0.121
21	H	0.876168	0.124
22	H	0.849407	0.151
23	H	0.686439	0.324
24	H	0.707169	0.293

DIPOLE MOMENT (DEBYE): X=-1.1358 Y=-1.3317 Z= 1.3143 TOTAL= 2.1888

V-mid: N7-C2: 0.148
N9-C4: 0.165
N10-C6: 0.165

BOND ORDER: N7-C2: 1.27
N9-C4: 1.27
N10-C6: 1.27
O11-N7: 1.99
O12-N7: 1.85
O13-N9: 1.89
O14-N9: 1.99
O15-N10: 2.04
O16-N11: 1.99

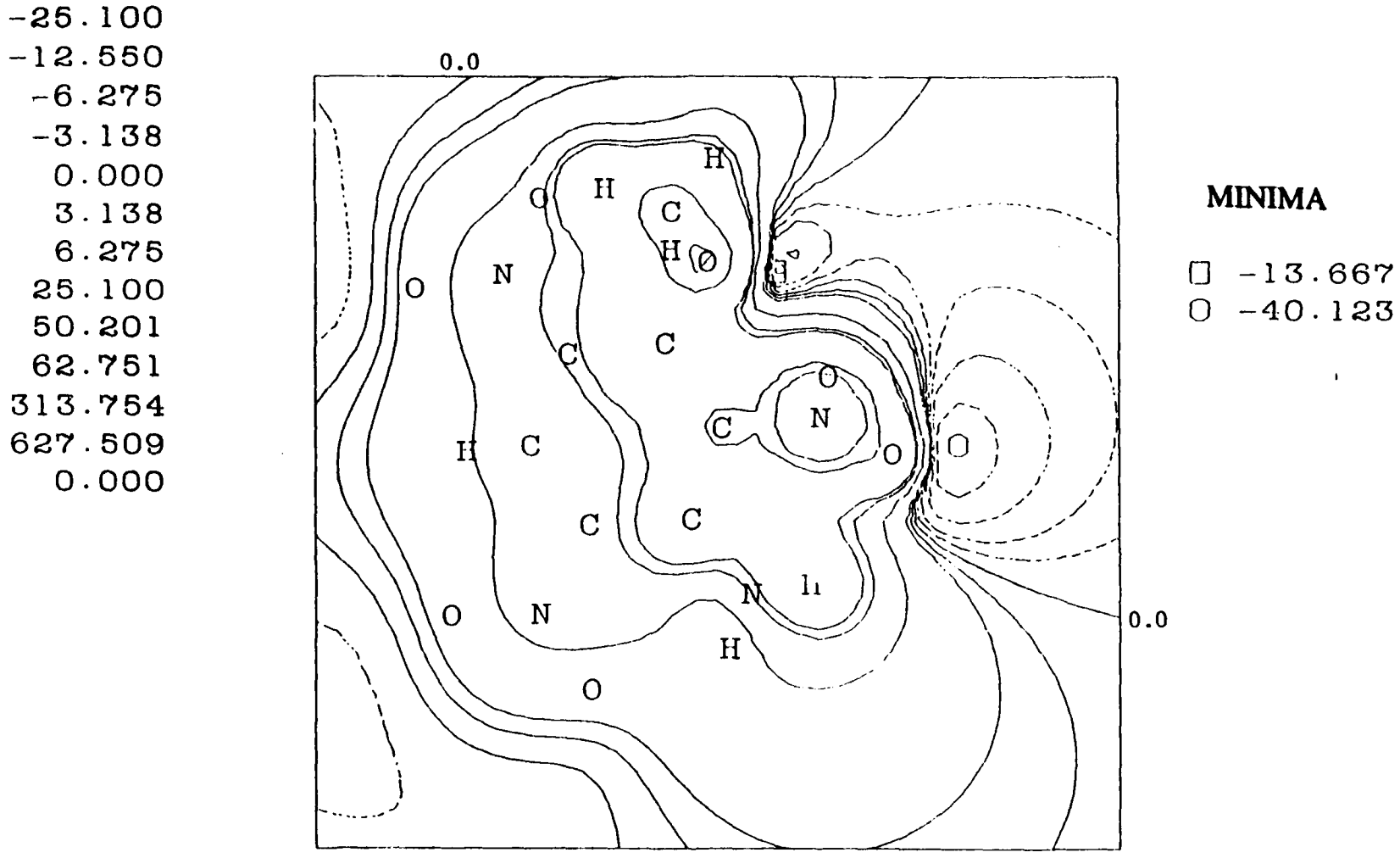


Figure Q-1. Calculated electrostatic potential, in kcal/mole, of 3-amino-2,4,6-trinitroanisole, in the plane 1.75Å above the N10 nitro group located in the upper left corner. The zero contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

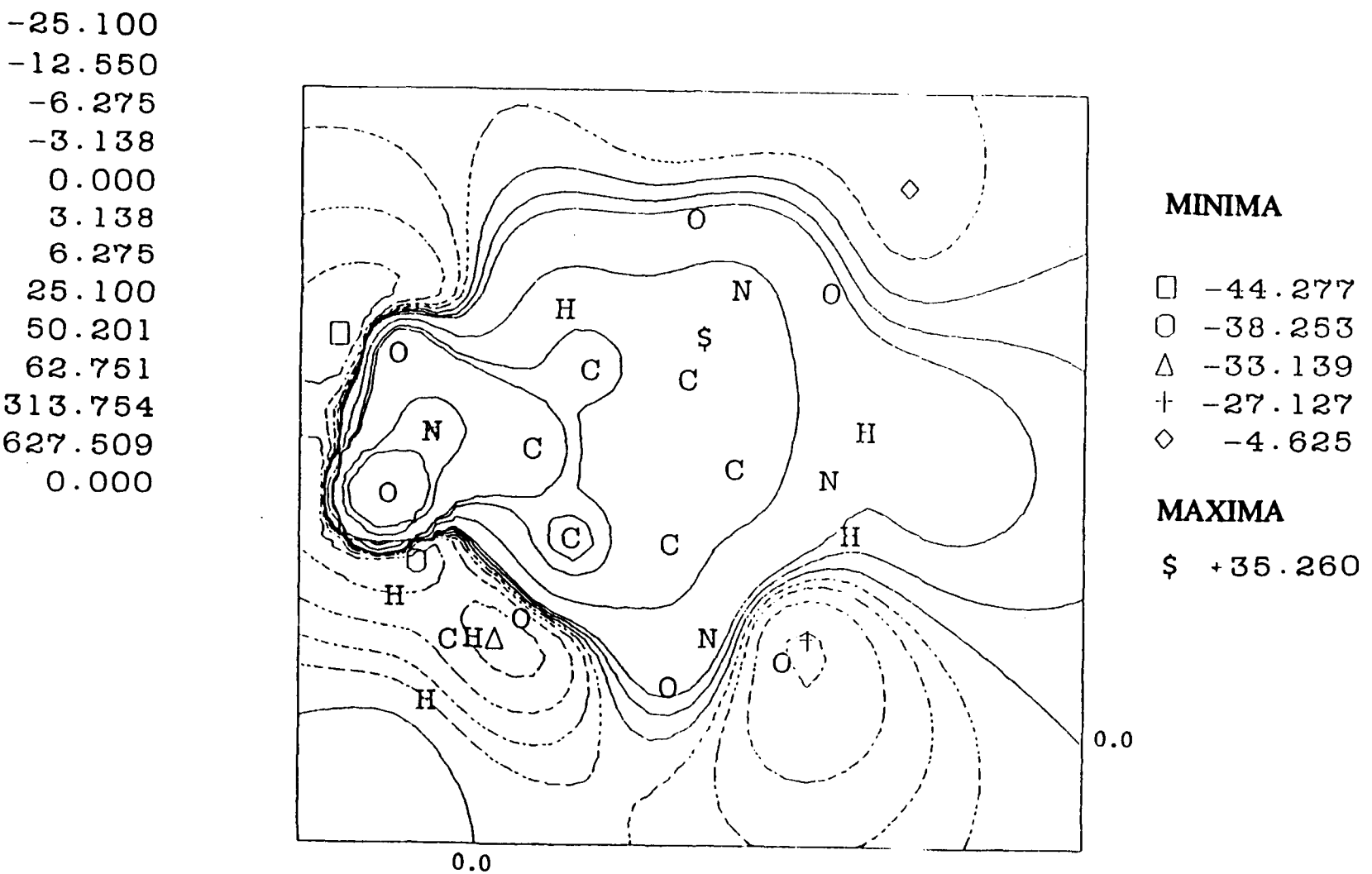
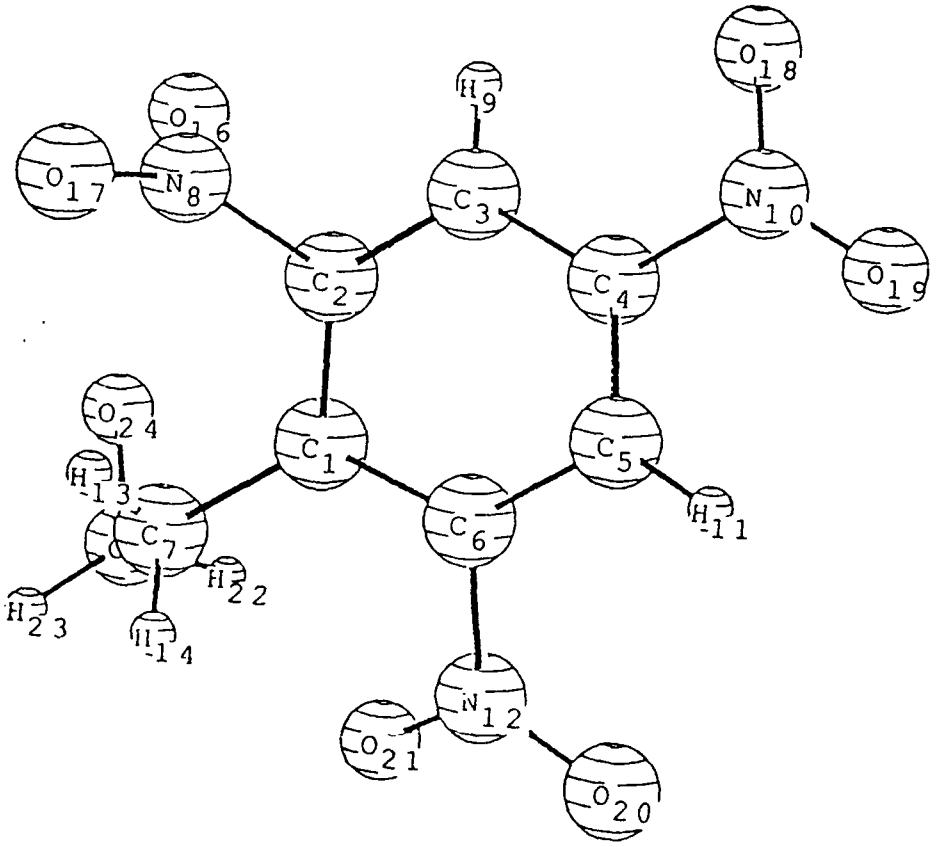


Figure Q-2. Calculated electrostatic potential, in kcal/mole, of 3-amino-2,4,6-trinitroanisole, in the plane 1.75Å above the N9 nitro group located in the upper right corner. The zero contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

APPENDIX R
2,4,6-TRINITROPHENYLETHANOL

The short distances between non-bonded hydrogens and oxygens are H9-O18 (2.36 Å), H11-O19 (2.51 Å) and H11-O20 (2.40 Å).

The N10 nitro group is essentially planar, while the N8 and N12 nitro groups are rotated by about 53° and 38°, respectively.



Z-MATRIX (ANGSTROMS AND DEGREES)

CD	CENT	ATOM	N1	LENGTH	N2	ALPHA	N3	BETA	J
1	1	C							
2	2	C	1	1.405790 (1)					
3	3	C	2	1.385454 (2)	1	124.441 (25)			
4	4	C	3	1.375723 (3)	2	117.275 (26)	1	-3.639 (48)	0
5	5	C	4	1.375494 (4)	3	122.596 (27)	2	1.748 (49)	0
6	6	C	5	1.387018 (5)	4	117.247 (28)	3	1.633 (50)	0
7	7	C	1	1.511773 (6)	2	122.283 (29)	3	-177.102 (51)	0
8	8	N	2	1.473278 (7)	3	114.345 (30)	4	176.070 (52)	0
9	9	H	3	0.935064 (8)	4	118.949 (31)	5	-179.191 (53)	0
10	10	N	4	1.474252 (9)	5	119.211 (32)	6	-178.828 (54)	0
11	11	H	5	0.969896 (10)	6	117.339 (33)	1	177.776 (55)	0
12	12	N	6	1.479221 (11)	1	120.688 (34)	2	-179.154 (56)	0
13	13	H	7	0.892075 (12)	1	107.604 (35)	2	-35.424 (57)	0
14	14	H	7	1.020122 (13)	1	116.186 (36)	2	-144.018 (58)	0
15	15	C	7	1.516479 (14)	1	111.660 (37)	2	86.695 (59)	0
16	16	O	8	1.226461 (15)	2	117.448 (38)	3	52.840 (60)	0
17	17	O	8	1.214653 (16)	2	118.009 (39)	3	-123.320 (61)	0
18	18	O	10	1.221396 (17)	4	117.365 (40)	5	178.357 (62)	0
19	19	O	10	1.226018 (18)	4	117.880 (41)	5	-1.925 (63)	0
20	20	O	12	1.222992 (19)	6	116.957 (42)	1	-142.921 (64)	0
21	21	O	12	1.223812 (20)	6	118.327 (43)	1	38.341 (65)	0
22	22	H	15	1.113303 (21)	7	111.293 (44)	1	49.750 (66)	0
23	23	H	15	1.101230 (22)	7	105.243 (45)	1	176.128 (67)	0
24	24	O	15	1.437708 (23)	7	108.002 (46)	1	-66.161 (68)	0
25	25	H	24	0.667343 (24)	15	116.108 (47)	7	173.061 (69)	0

STOICHIOMETRY C8H7N3O7

SCF DONE: E(RHF) = -989.592181678

EIGENVALUES — -0.30175 0.12168 0.13401 0.18800 0.22444

Estimated ionization potential: 8.22 eV

TOTAL ATOMIC CHARGES.

		1	Net Charge
1	C	5.933057	0.067
2	C	5.886905	0.114
3	C	6.070620	-0.071
4	C	5.892277	0.108
5	C	6.060411	-0.060
6	C	5.903170	0.097
7	C	6.206240	-0.206
8	N	6.821298	0.178
9	H	0.854565	0.145
10	N	6.830005	0.170
11	H	0.856326	0.144
12	N	6.832640	0.167
13	H	0.860920	0.139
14	H	0.884685	0.115
15	C	5.943004	0.057
16	O	8.186415	-0.186
17	O	8.193307	-0.193
18	O	8.191137	-0.191
19	O	8.190719	-0.191
20	O	8.189065	-0.189
21	O	8.197190	-0.197
22	H	0.926404	0.074
23	H	0.927182	0.073
24	O	8.530079	-0.530
25	H	0.632393	0.368

DIPOLE MOMENT (DEBYE): X=-1.2233 Y= 1.1284 Z=-2.0872 TOTAL= 2.6695

V-mid: N8-C2: 0.210
N10-C4: 0.200
N12-C6: 0.189

Bond Order: N8-C2: 1.23
N10-C4: 1.23
N12-C6: 1.22
O16-N8: 1.91
O17-N8: 1.96
O18-N10: 1.93
O19-N10: 1.91
O20-N12: 1.92
O21-N12: 1.92

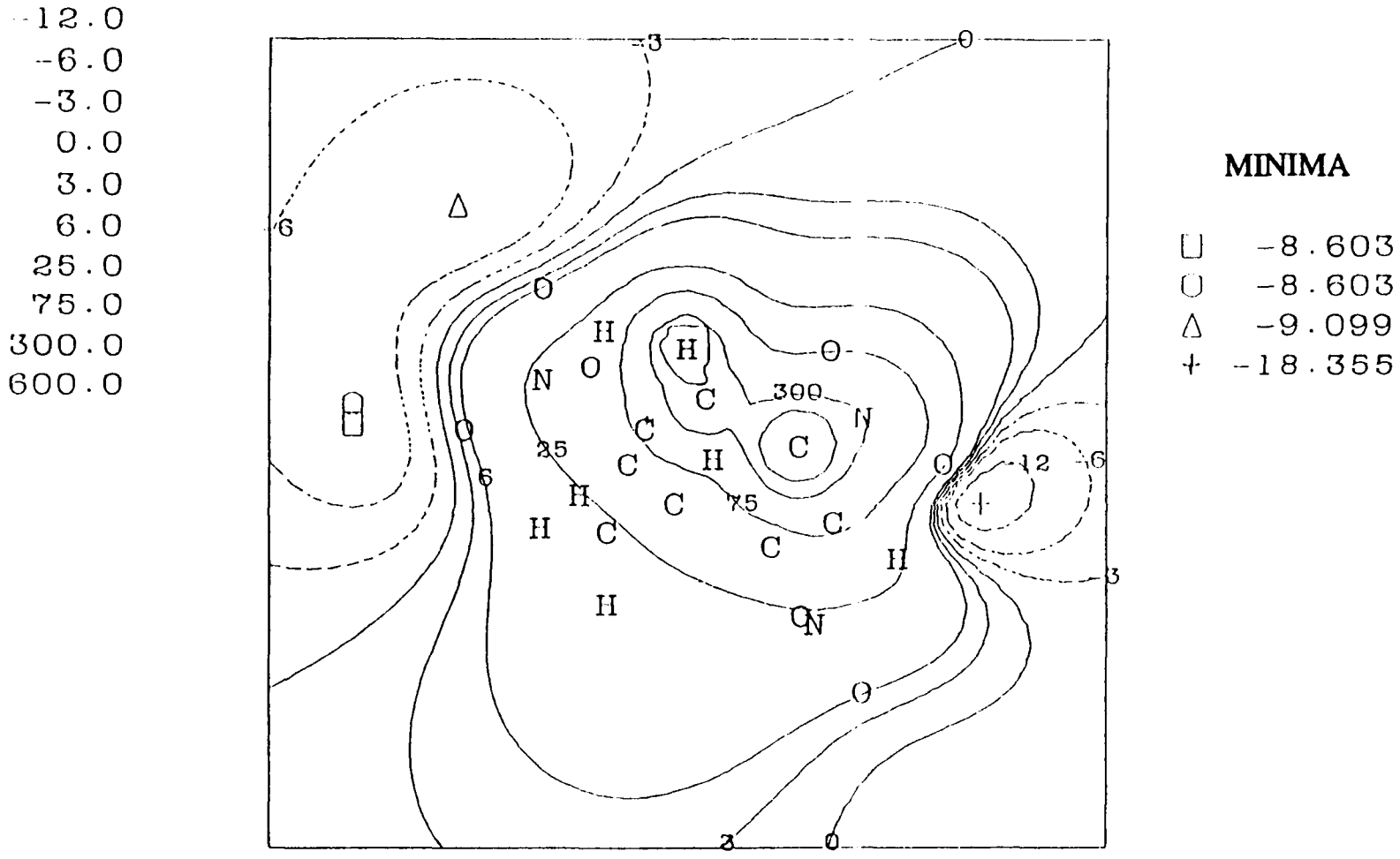


Figure R-1. Calculated electrostatic potential, in kcal/mole, of 2,4,6-trinitrophenylethanol, in the plane 1.75Å above the N8 nitro group located in the upper left corner. Projected positions of nuclei are shown. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

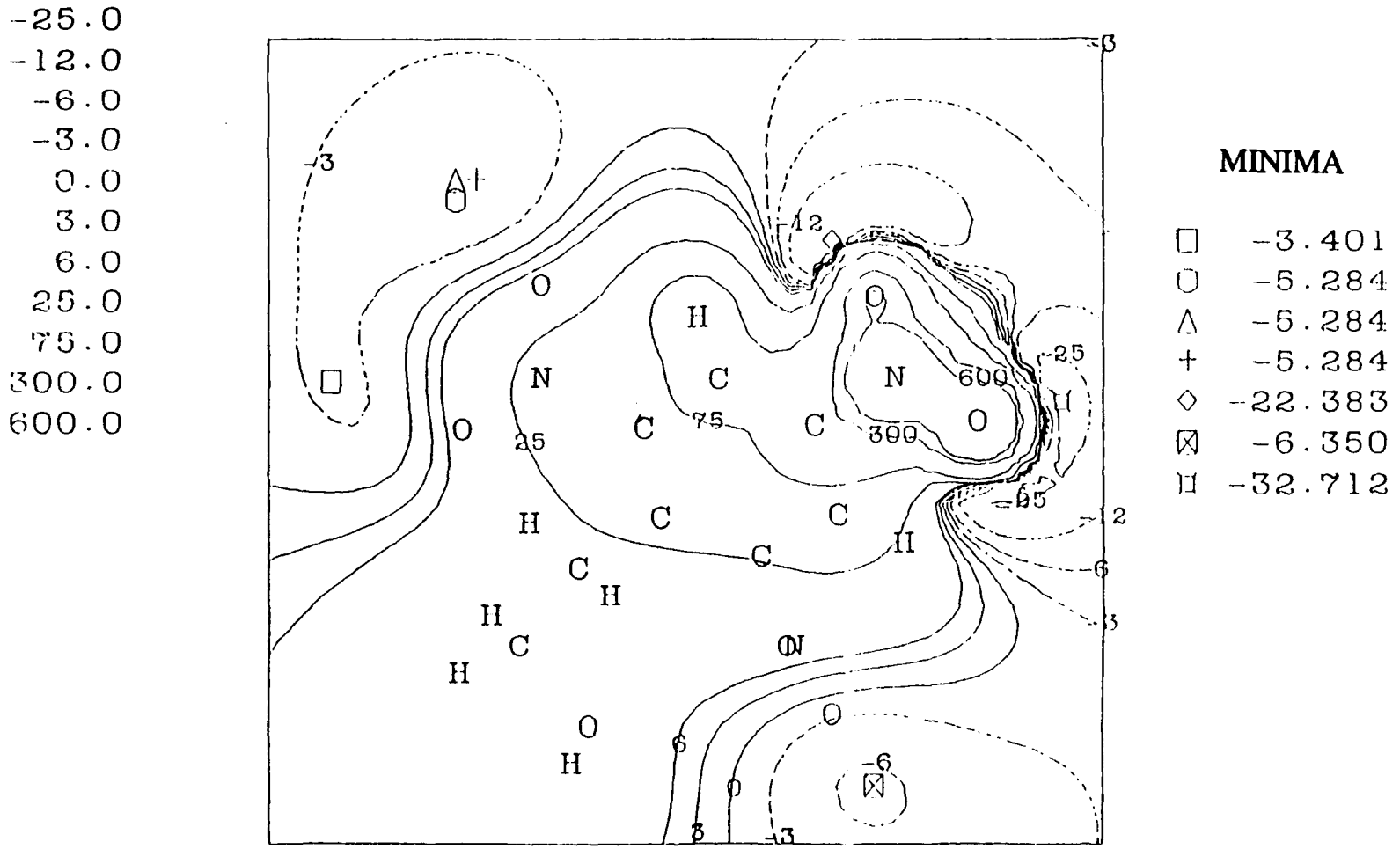
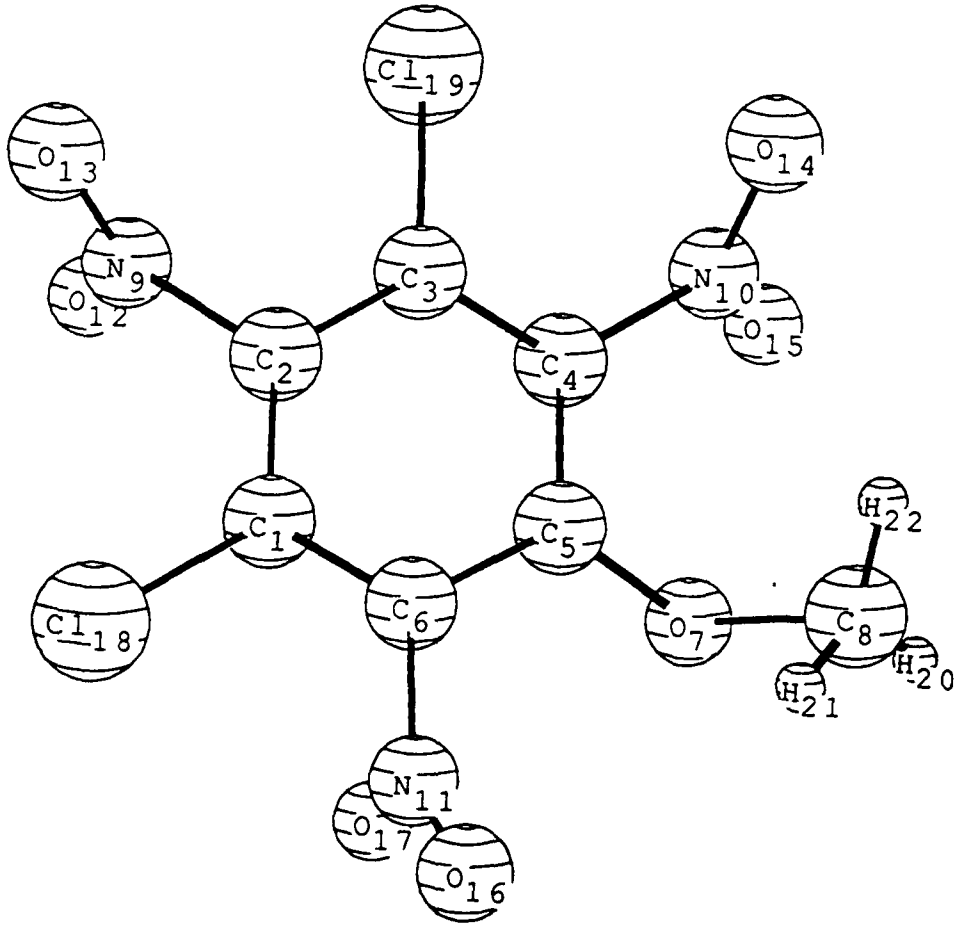


Figure R-2. Calculated electrostatic potential, in kcal/mole, of 2,4,6-trinitrophenylethanol, in the plane 1.75Å above the N12 nitro group located in the upper left corner. Projected positions of nuclei are shown. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

APPENDIX S
3,5-DICHLORO-2,4,6-TRINITROANISOLE

Nitro grous N9, N10 and N11 are rotated out of the plane by approximately 67°, 57° and 69°, respectively.



Z-MATRIX (ANGSTROMS AND DEGREES)

CD	CENT	ATOM	N1	LENGTH		N2	ALPHA		N3	BETA		J
1	1	C										
2	2	C	1	1.391000	(1)							
3	3	C	2	1.389206	(2)	1	121.473	(22)				
4	4	C	3	1.389143	(3)	2	118.999	(23)	1	1.346	(42)	0
5	5	C	4	1.395511	(4)	3	121.461	(24)	2	-1.551	(43)	0
6	6	C	5	1.395780	(5)	4	116.885	(25)	3	-0.898	(44)	0
7	7	O	5	1.340606	(6)	4	125.525	(26)	3	175.299	(45)	0
8	8	C	7	1.415489	(7)	5	121.652	(27)	4	56.587	(46)	0
9	9	N	2	1.476436	(8)	3	119.419	(28)	4	-177.119	(47)	0
10	10	N	4	1.474114	(9)	3	119.067	(29)	2	176.644	(48)	0
11	11	N	6	1.477912	(10)	5	115.855	(30)	4	-177.593	(49)	0
12	12	O	9	1.208747	(11)	2	117.506	(31)	1	-67.457	(50)	0
13	13	O	9	1.211470	(12)	2	117.410	(32)	1	111.862	(51)	0
14	14	O	10	1.212815	(13)	4	117.714	(33)	5	-122.340	(52)	0
15	15	O	10	1.221423	(14)	4	117.033	(34)	5	57.408	(53)	0
16	16	O	11	1.211646	(15)	6	117.282	(35)	5	68.605	(54)	0
17	17	O	11	1.218011	(16)	6	117.087	(36)	5	-111.539	(55)	0
18	18	Cl	1	1.710555	(17)	2	121.070	(37)	3	178.901	(56)	0
19	19	Cl	3	1.718514	(18)	4	120.773	(38)	5	-177.618	(57)	0
20	20	H	8	0.960422	(19)	7	115.442	(39)	5	-164.767	(58)	0
21	21	H	8	0.960380	(20)	7	93.642	(40)	5	81.700	(59)	0
22	22	H	8	0.959845	(21)	7	117.939	(41)	5	-32.636	(60)	0

STOICHIOMETRY C7H3CL2N3O7
SCF DONE: E(RHF) = -1865.25178442 A.U. AFTER 25 CYCLES

EIGENVALUES -- -0.33048 -0.32444 -0.32325 0.11187 0.12706

Estimated ionization potential:8.81eV

TOTAL ATOMIC CHARGES.

		1	Net Charge
1	C	5.938767	0.061
2	C	5.901758	0.098
3	C	5.935152	0.065
4	C	5.924995	0.075
5	C	5.798703	0.201
6	C	5.914277	0.086
7	O	8.235248	-0.235
8	C	6.173128	-0.173
9	N	6.815860	0.184
10	N	6.826736	0.173
11	N	6.814434	0.186
12	O	8.174657	-0.175
13	O	8.176198	-0.176
14	O	8.175399	-0.175
15	O	8.179620	-0.180
16	O	8.184689	-0.185
17	O	8.173291	-0.173
18	Cl	17.024555	-0.025
19	Cl	17.029947	-0.030
20	H	0.858413	0.162
21	H	0.865099	0.135
22	H	0.879074	0.121

DIPOLE MOMENT (DEBYE): X= 2.5338 Y=-1.2750 Z=-0.5635 TOTAL= 2.8919

V-mid: N9-C2: 0.202
N10-C4: 0.178
N11-C6: 0.194

Bond Order: N9-C2: 1.22
N10-C4: 1.23
N11-C6: 1.22
O12-N9: 1.99
O13-N9: 1.98
O14-N10: 1.97
O15-N10: 1.93
O16-N11: 1.98
O17-N11: 1.95

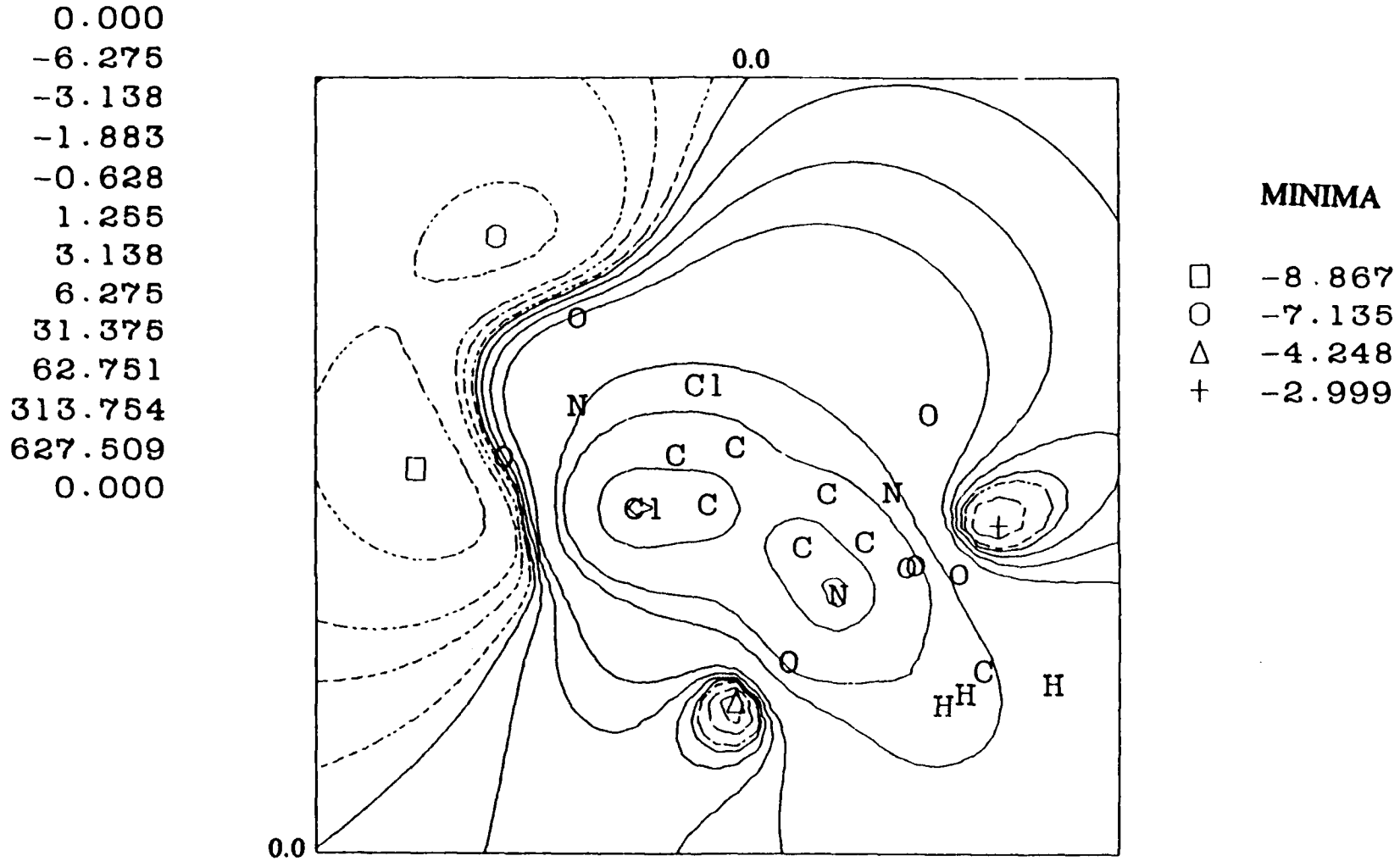


Figure S-1. Calculated electrostatic potential, in kcal/mole, of 3,5-dichloro-2,4,6-trinitroanisole, in the plane 1.75Å above the N9 nitro group located in the upper left corner. Projected positions of nuclei are shown. The zero contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

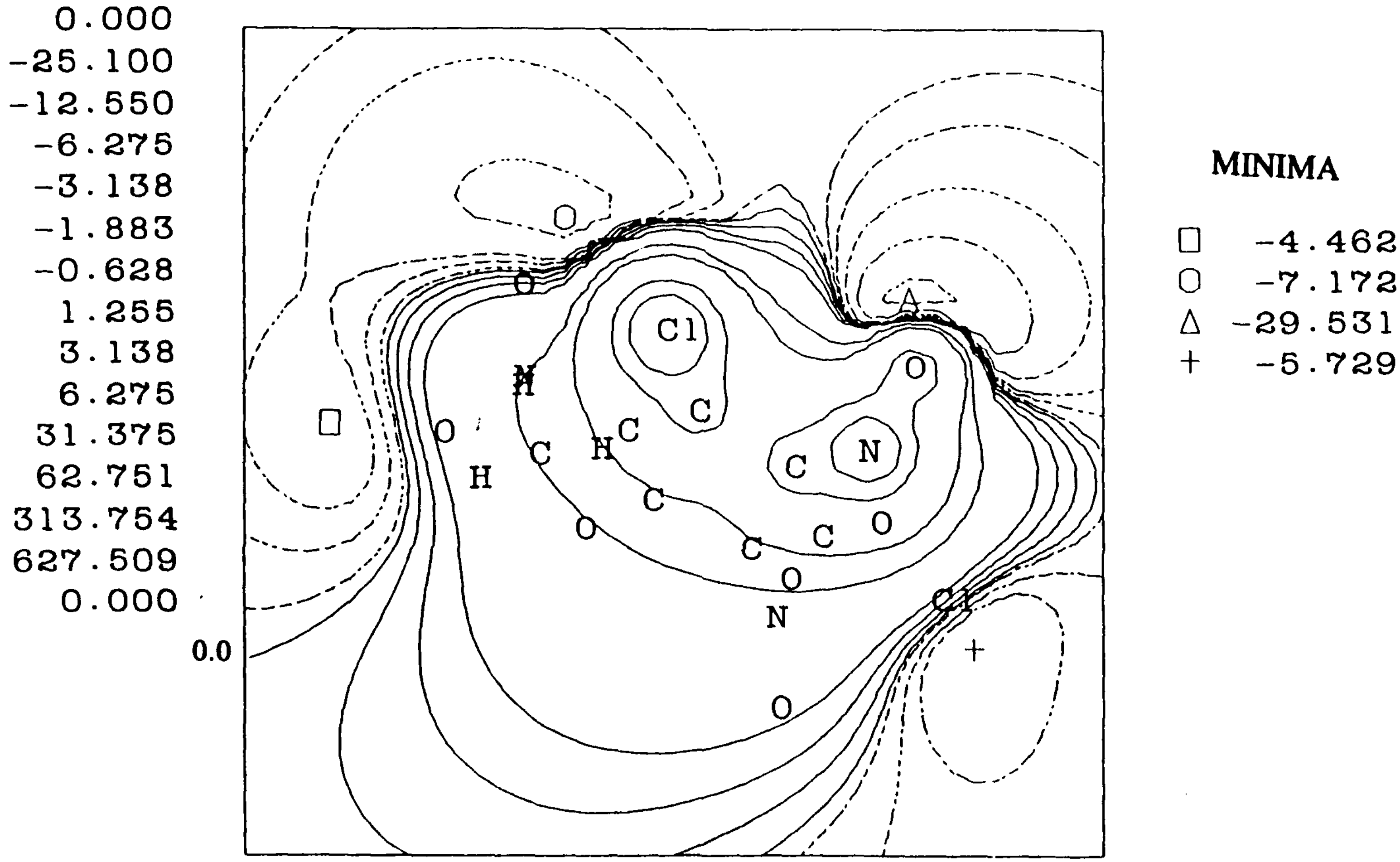
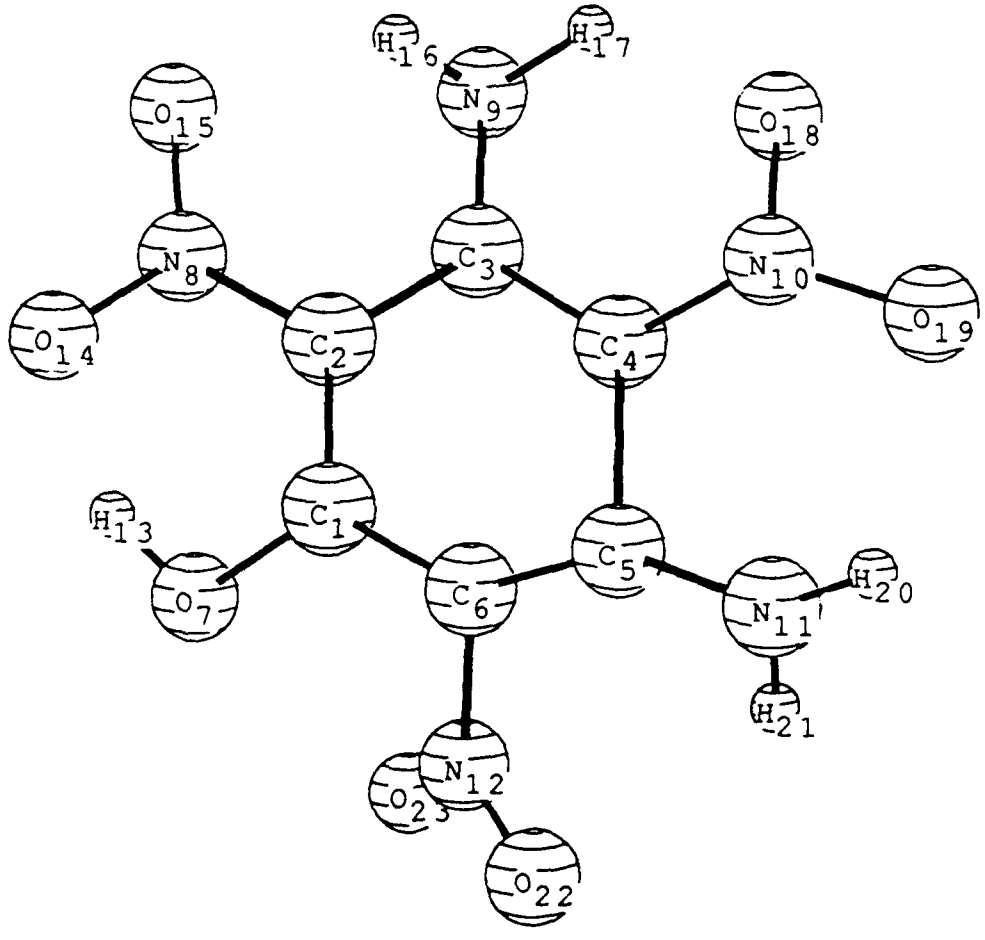


Figure S-2. Calculated electrostatic potential, in kcal/mole, of 3,5-dichloro-2,4,6-trinitroanisole, in the plane 1.75Å above the N10 nitro group located in the upper left corner. Projected positions of nuclei are shown. The zero contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

APPENDIX T
3,5-DIAMINO-2,4,6-TRINITROPHENOL

The short distances between non-bonded hydrogens and oxygens (suggesting hydrogen bonding) are between H13-O14 (1.60 Å), H16-O15 (1.95 Å), H17-O18 (1.76 Å) and H20-O19 (2.05 Å).

The N8 nitro group is rotated by about 5°, the N10 nitro group is rotated by about 13°, and the N12 nitro group is out of the plane by almost 55°. Both the amine groups are rotated by approximately 16°.



Z-MATRIX (ANGSTROMS AND DEGREES)

CO	CENT	ATOM	N1	LENGTH	N2	ALPHA	N3	BETA	J
1	1	C							
2	2	C	1	1.413954 (1)					
3	3	C	2	1.443178 (2)	1	120.438 (23)			
4	4	C	3	1.434645 (3)	2	117.374 (24)	1	-8.553 (44)	0
5	5	C	4	1.436577 (4)	3	121.930 (25)	2	1.239 (45)	0
6	6	C	5	1.421232 (5)	4	115.788 (26)	3	8.545 (46)	0
7	7	O	1	1.332665 (6)	2	123.188 (27)	3	-177.912 (47)	0
8	8	N	2	1.408724 (7)	3	120.150 (28)	4	173.575 (48)	0
9	9	N	3	1.320210 (8)	4	120.822 (29)	5	179.712 (49)	0
10	10	N	4	1.423957 (9)	5	118.620 (30)	6	-172.299 (50)	0
11	11	N	5	1.313367 (10)	6	120.493 (31)	1	169.219 (51)	0
12	12	N	6	1.462077 (11)	1	116.831 (32)	2	-175.794 (52)	0
13	13	H	7	1.016321 (12)	1	102.680 (33)	2	12.438 (53)	0
14	14	O	8	1.277081 (13)	2	119.021 (34)	3	-174.636 (54)	0
15	15	O	8	1.239608 (14)	2	123.042 (35)	3	3.770 (55)	0
16	16	H	9	0.868088 (15)	3	119.640 (36)	4	-162.508 (56)	0
17	17	H	9	1.100023 (16)	3	118.634 (37)	4	-15.787 (57)	0
18	18	O	10	1.247178 (17)	4	120.094 (38)	5	167.570 (58)	0
19	19	O	10	1.247503 (18)	4	120.066 (39)	5	-12.472 (59)	0
20	20	H	11	0.863344 (19)	5	130.140 (40)	6	-167.718 (60)	0
21	21	H	11	0.772446 (20)	5	121.659 (41)	6	16.534 (61)	0
22	22	O	12	1.236374 (21)	6	117.596 (42)	1	-128.339 (62)	0
23	23	O	12	1.208878 (22)	6	118.298 (43)	1	54.347 (63)	0

STOICHIOMETRY C6H5N5O7

EIGENVALUES — -0.29164 0.12482 0.14899 0.18960 0.24369

Estimated ionization potential: 7.95 ev

TOTAL ATOMIC CHARGES.

		1
1	C	5.787545
2	C	6.018021
3	C	5.775208
4	C	5.997978
5	C	5.745618
6	C	5.997326
7	O	8.291952
8	N	6.854899
9	N	7.471661
10	N	6.848168
11	N	7.609589
12	N	6.830704
13	H	0.714630
14	O	8.236545
15	O	8.179622
16	H	0.715319
17	H	0.729[illegible]
18	O	8.226[illegible]
19	O	8.2[illegible]6
20	H	0.681906
21	H	0.675475
22	O	8.221878
23	O	8.183565

Net Charges

C1	+0.212
C2	-0.018
C3	0.225
C4	0.002
C5	0.254
C6	0.003
O7	-0.292
N8	0.145
N9	-0.472
N10	0.152
N11	-0.610
N12	0.169
H13	0.285
O14	-0.237
O15	-0.180
H16	0.295
H17	0.270
O18	-0.226
O19	-0.207
H20	0.318
H21	0.325
O22	-0.222
O23	-0.184

DIPOLE MOMENT (DEBYE): X= 1.4000 Y=-0.6843 Z= 2.4128 TOTAL= 2.8723

V-mid: N8-C2: 0.095
V-mid: N10-C4: 0.114
V-mid: N12-C6: 0.125

Bond Order: N8-C2: 1.41
Bond Order: N10-C4: 1.36
Bond Order: N12-C6: 1.26
Bond Order: O14-N8: 1.69
Bond Order: O15-N8: 1.85
Bond Order: O18-N10: 1.82
Bond Order: O19-N10: 1.82
Bond Order: O22-N12: 1.86
Bond Order: O23-N12: 1.99

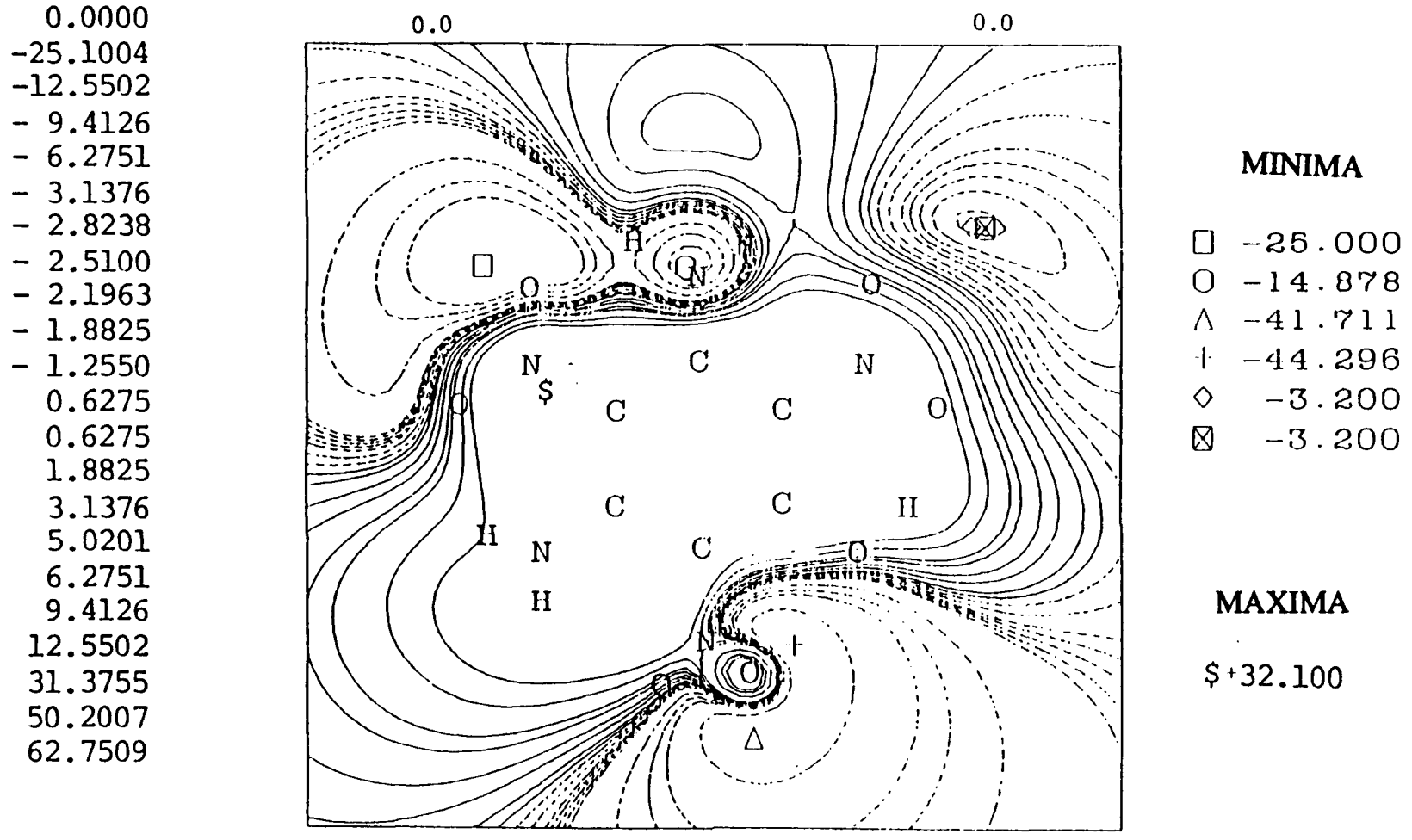
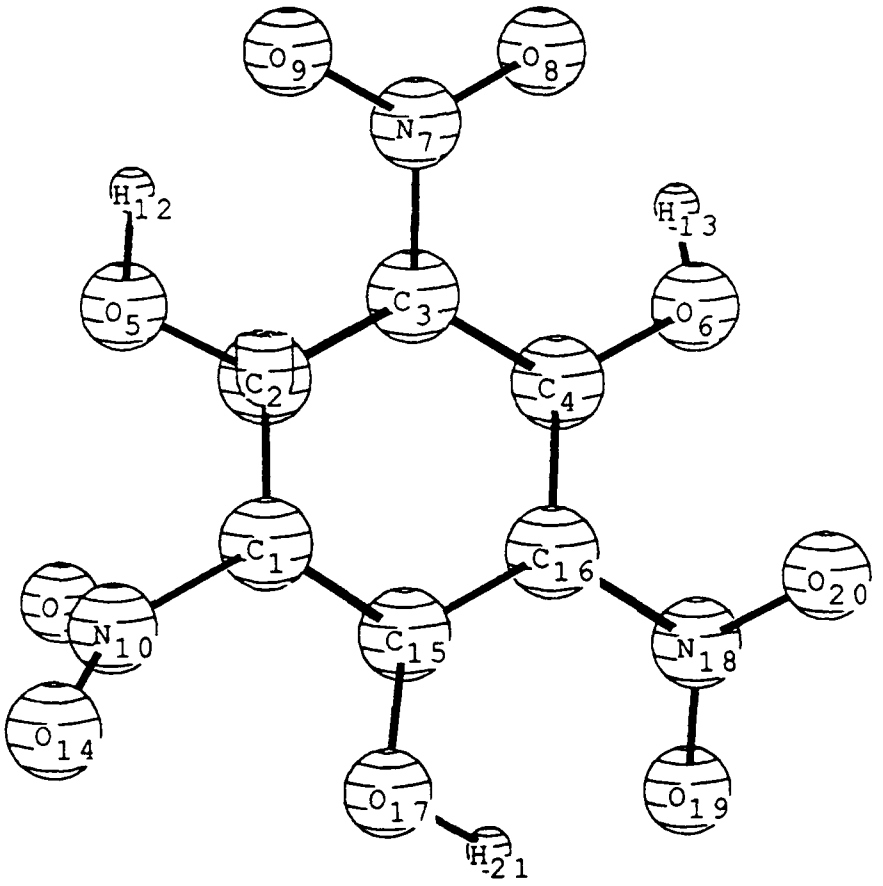


Figure T-1. Calculated electrostatic potential, in kcal/mole, of 3,5-diamino-2,4,6-trinitrophenol, in the plane 1.75 Å above the aromatic ring. Projected positions of nuclei are shown. The zero contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

APPENDIX U
2,4,6-TRINITROPHLOROGLUCINOL

The short distances between non-bonded hydrogens and oxygens are H13-O8 (1.73 Å), H12-O9 (1.73 Å), and H21-O19 (1.74 Å).

The N7 and N18 nitro groups are rotated out of the plane of the benzene ring by only a few degrees, while the N10 nitro group is rotated by approximately 63°.



Z-MATRIX (ANGSTROMS AND DEGREES)

CD	CENT	ATOM	N1	LENGTH	N2	ALPHA	N3	BETA	J
1	1	C							
2	2	C	1	1.386018 (1)					
3	3	C	2	1.410857 (2)	1	118.233 (21)			
4	4	C	3	1.415998 (3)	2	120.706 (22)	1	2.096 (40)	0
5	5	O	2	1.326719 (4)	3	124.750 (23)	4	-178.414 (41)	0
6	6	O	4	1.310592 (5)	3	120.643 (24)	2	178.934 (42)	0
7	7	N	3	1.436206 (6)	2	119.229 (25)	1	-175.048 (43)	0
8	8	O	7	1.227657 (7)	3	120.519 (26)	2	-176.095 (44)	0
9	9	O	7	1.240487 (8)	3	118.609 (27)	2	4.684 (45)	0
10	10	N	1	1.466242 (9)	2	118.321 (28)	3	178.961 (46)	0
11	11	O	10	1.221284 (10)	1	117.732 (29)	2	62.714 (47)	0
12	12	H	5	0.991694 (11)	2	112.087 (30)	3	-14.216 (48)	0
13	13	H	4	1.767937 (12)	3	93.388 (31)	2	178.073 (49)	0
14	14	O	10	1.221284 (13)	1	117.732 (32)	2	-117.286 (50)	0
15	15	C	1	1.386018 (14)	10	118.321 (33)	14	62.714 (51)	0
16	16	C	15	1.410857 (15)	1	118.233 (34)	10	-178.961 (52)	0
17	17	O	15	1.326719 (16)	16	124.750 (35)	4	-178.414 (53)	0
18	18	N	16	1.436206 (17)	15	119.229 (36)	1	-175.048 (54)	0
19	19	O	18	1.240487 (18)	16	118.609 (37)	15	4.684 (55)	0
20	20	O	18	1.227657 (19)	16	120.519 (38)	15	-176.095 (56)	0
21	21	H	17	0.991694 (20)	15	112.087 (39)	16	-14.216 (57)	0

STOICHIOMETRY C6H3N3O9

E=-1061.04187210

EIGENVALUES — -0.28887 0.10982 0.13449 0.19142 0.23070

Estimated ionization potential: 7.9 ev

TOTAL ATOMIC CHARGES.

		1	Net Charges
1	C	5.980876	+0.02
2	C	5.776130	+0.22
3	C	6.021020	-0.02
4	C	5.762782	+0.24
5	O	8.295881	-0.30
6	O	8.342514	-0.34
7	N	6.829723	+0.17
8	O	8.203208	-0.20
9	O	8.209679	-0.21
10	N	6.820550	+0.18
11	O	8.191891	-0.19
12	H	0.705208	+0.29
13	H	0.665175	+0.33
14	O	8.190493	-0.19
15	C	5.775829	+0.22
16	C	5.998390	0.00
17	O	8.295988	-0.30
18	N	6.834414	+0.17
19	O	8.246792	-0.25
20	O	8.152027	-0.15
21	H	0.701428	+0.30

DIPOLE MOMENT (DEBYE): X= 1.4101 Y=-0.0146 Z= 2.5837 TOTAL= 2.9435

V_{mid}: C_1-N_{10}: 0.143
C_3-N_7: 0.110
C_{16}-N_{18}: 0.123

Bond Orders:

C_1-N_{10}:	1.26	N_7-O_9:	1.99
C_3-N_7:	1.34	N_{18}-O_{19}:	1.99
C_{16}-N_{18}:	1.34	N_{18}-O_{20}:	2.05
N_{10}-O_{11}:	2.09		
N_{10}-O_{14}:	2.09		
N_7-O_8:	2.05		

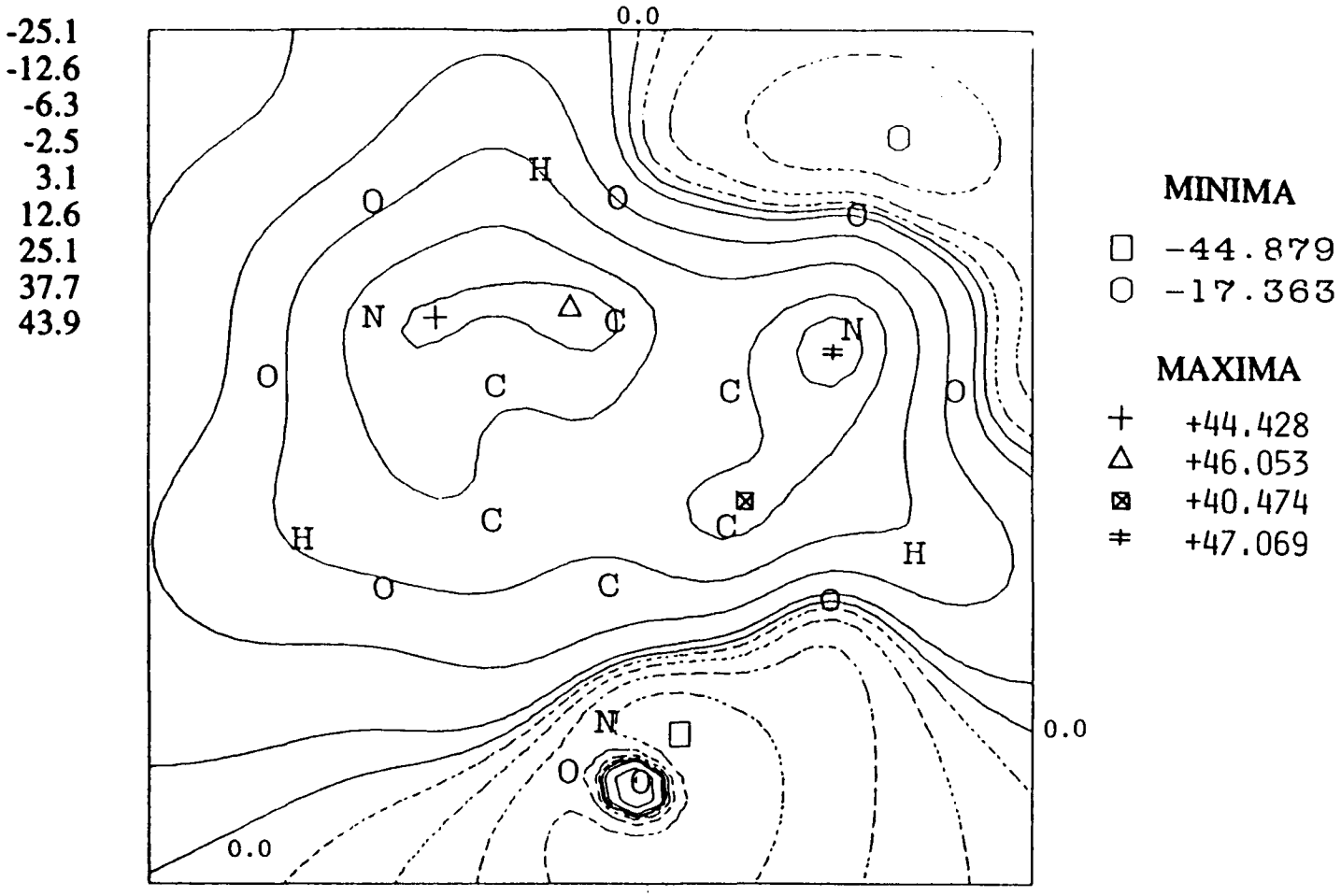
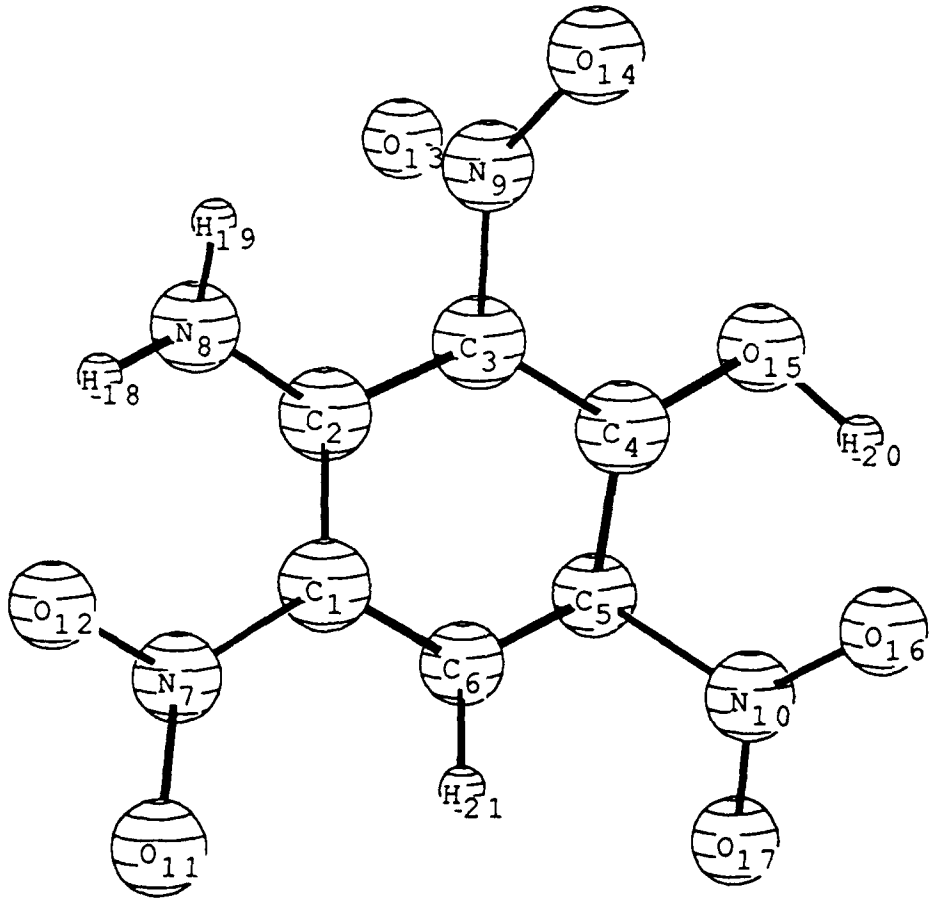


Figure U-1. Calculated electrostatic potential, in kcal/mole, of 2,4,6-trinitrophloroglucinol, in the plane 1.75Å above the N18 nitro group located in the upper right corner. Projected positions of nuclei are shown. The zero contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

APPENDIX V
AMINOPICRIC ACID

The short distances between non-bonded hydrogens and oxygens strongly suggest hydrogen bonding within the molecule. These are between H21-O17 (2.33 Å), H18-O12 (1.96 Å), H19-O13 (2.02 Å), H21-O11 (2.35 Å), and H20-O16 (1.65 Å).

The N7 nitro group is almost planar with the mean plane of the benzene ring, but the N9 nitro group is out of the plane by about 43° and the N10 nitro group is out of the plane by about 4°. The amine group (N8) is essentially planar.



Z-MATRIX (ANGSTROMS AND DEGREES)

CD	CENT	ATOM	N1	LENGTH	N2	ALPHA	N3	BETA	J
1	1	C							
2	2	C	1	1.425800 (1)					
3	3	C	2	1.416065 (2)	1	114.909 (21)			
4	4	C	3	1.394424 (3)	2	124.307 (22)	1	0.780 (40)	0
5	5	C	4	1.411584 (4)	3	116.911 (23)	2	2.197 (41)	0
6	6	C	5	1.374855 (5)	4	120.888 (24)	3	-3.555 (42)	0
7	7	N	1	1.457838 (6)	2	121.380 (25)	3	176.949 (43)	0
8	8	N	2	1.315976 (7)	3	121.291 (26)	4	179.606 (44)	0
9	9	N	3	1.466324 (8)	4	118.004 (27)	5	179.897 (45)	0
10	10	N	5	1.439569 (9)	6	117.313 (28)	1	179.668 (46)	0
11	11	O	7	1.221251 (10)	1	118.353 (29)	2	-178.866 (47)	0
12	12	O	7	1.226672 (11)	1	119.170 (30)	2	0.351 (48)	0
13	13	O	9	1.227247 (12)	3	117.678 (31)	4	136.705 (49)	0
14	14	O	9	1.213759 (13)	3	119.079 (32)	4	-43.446 (50)	0
15	15	O	4	1.336226 (14)	5	123.609 (33)	6	178.929 (51)	0
16	16	O	10	1.244771 (15)	5	118.211 (34)	6	-175.804 (52)	0
17	17	O	10	1.209722 (16)	5	118.526 (35)	6	4.846 (53)	0
18	18	H	8	0.900000 (17)	2	119.800 (36)	3	-178.200 (54)	0
19	19	H	8	0.900000 (18)	2	113.100 (37)	3	-3.540 (55)	0
20	20	H	15	1.150000 (19)	4	108.200 (38)	5	-16.100 (56)	0
21	21	H	6	0.970000 (20)	5	118.000 (39)	4	186.000 (57)	0

STOICHIOMETRY C6H4N4O7

SCF DONE: E(RHF) = -966.795803082 A.U. AFTER 29 CYCLES

EIGENVALUES — -0.30622 -0.30542 0.12645 0.14052 0.18294

Estimated ionization potential: 8.31 ev

TOTAL ATOMIC CHARGES

		1	Net Charges
1	C	5.962634	+0.04
2	C	5.776352	+0.22
3	C	5.982033	+0.02
4	C	5.795539	+0.20
5	C	5.979536	+0.02
6	C	6.030805	-0.03
7	N	6.829224	+0.17
8	N	7.515466	-0.52
9	N	6.831797	+0.17
10	N	6.824527	+0.18
11	O	8.192717	-0.19
12	O	8.226350	-0.23
13	O	8.224539	-0.22
14	O	8.174667	-0.17
15	O	8.268007	-0.27
16	O	8.238083	-0.24
17	O	8.156888	-0.16
18	H	0.697097	+0.30
19	H	0.714770	+0.29
20	H	0.727397	+0.27
21	H	0.851573	+0.15

DIPOLE MOMENT (DEBYE): X=-0.3363 Y=-0.5848 Z=-0.1270 TOTAL= 0 6864

V-mid N7-C1: 0.151
N9-C3: 0.134
N10-C5: 0.143

Bond Orders:

C1-N7:	1.27
C2-N8:	1.71
C3-N9:	1.25
C5-N10:	1.32
N7-O11:	1.95
N7-O12:	1.90
N9-O13:	1.90
N9-O14:	2.00
N10-O16:	1.86
N10-O17:	2.00

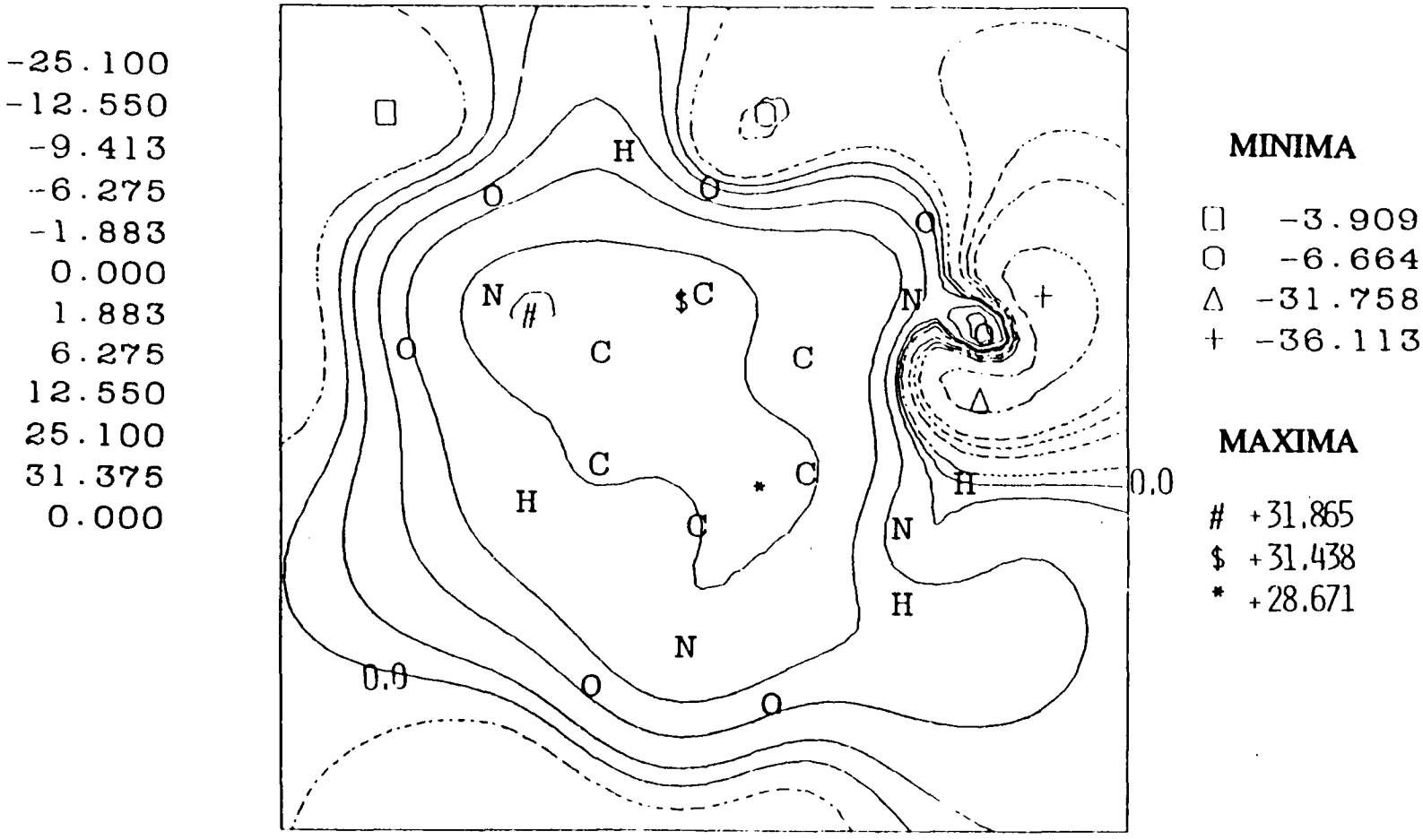


Figure V-1. Calculated electrostatic potential, in kcal/mole, of aminopicric acid, in the plane 1.75Å above the N10 nitro group located in the upper left corner. Projected positions of nuclei are shown. The zero contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

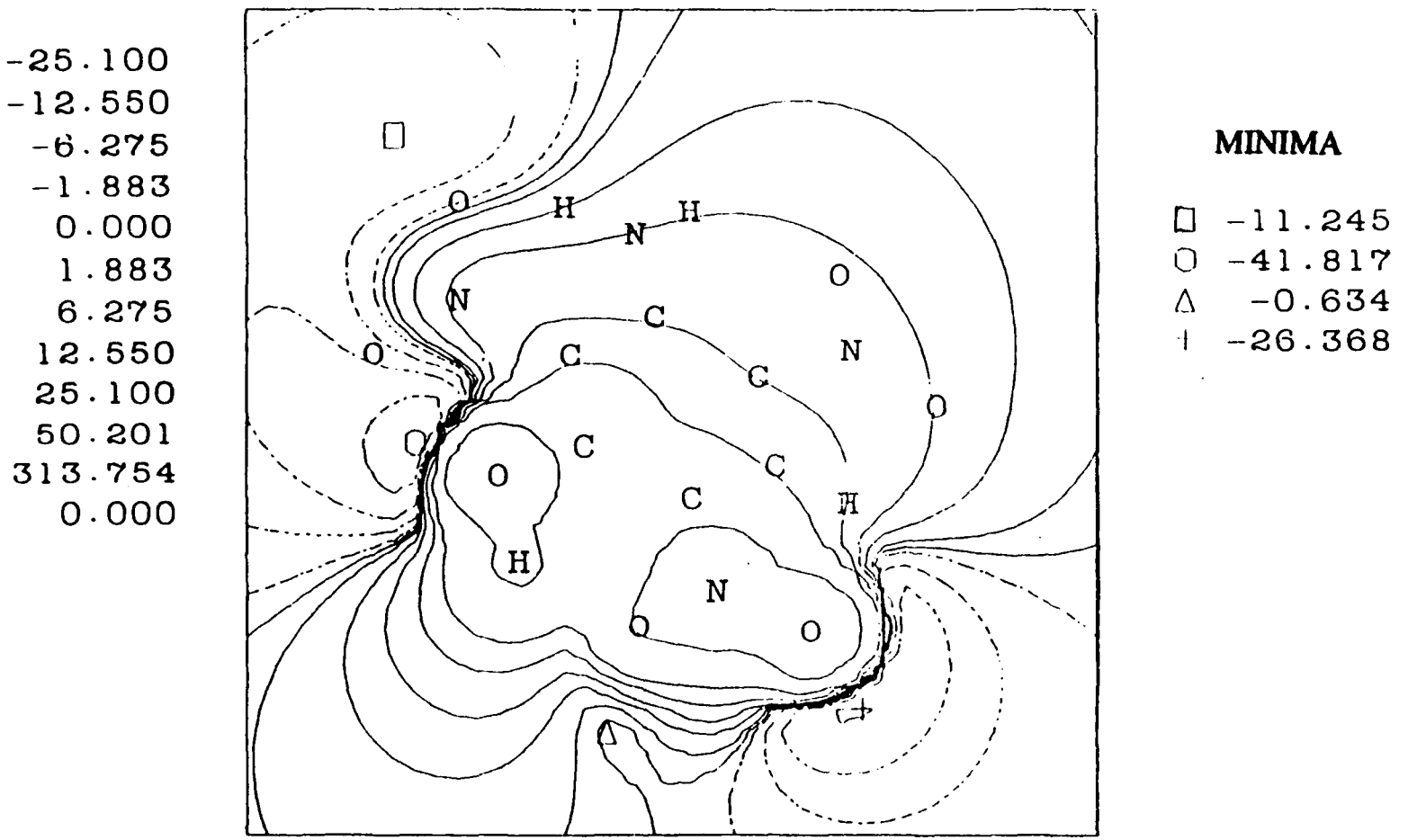
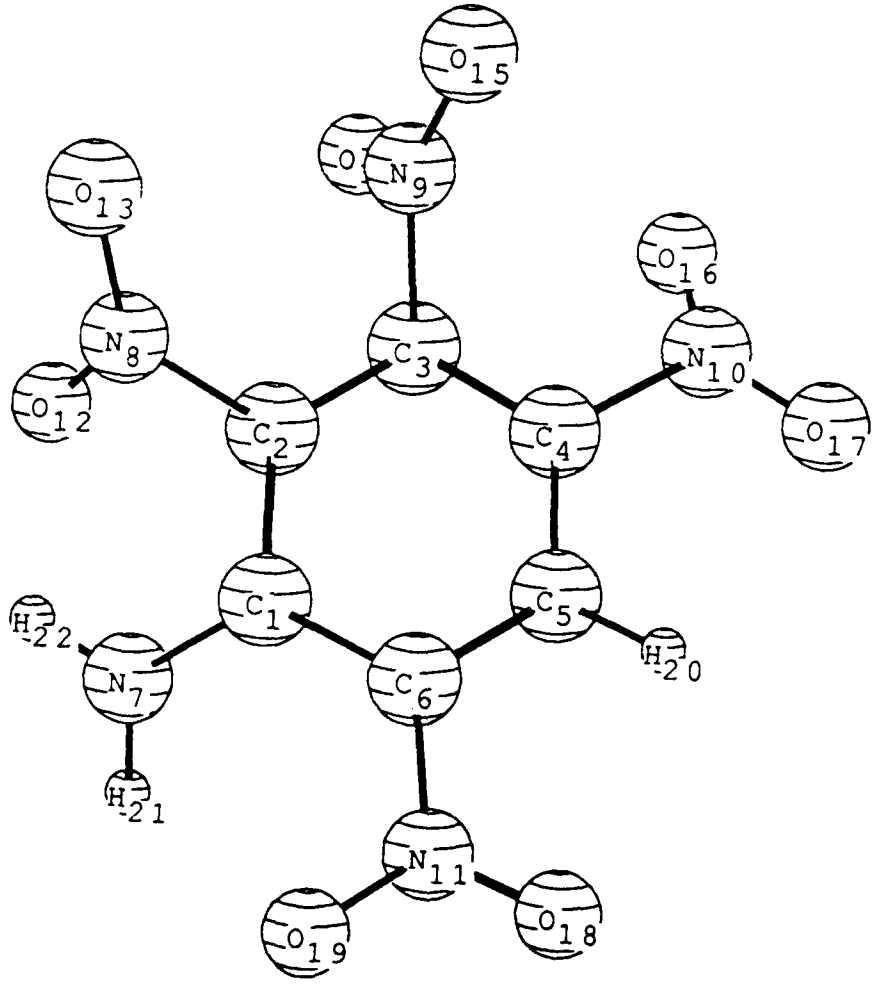


Figure V-2. Calculated electrostatic potential, in kcal/mole, of aminopicric acid, in the plane 1.75Å above the N9 nitro group located in the upper left corner. Projected positions of nuclei are shown. The zero contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

APPENDIX W
2,3,4,6-TETRANITROANILINE

The short distances between non-bonded hydrogens and oxygens are between H22-O12 (2.03Å), H20-O17 (2.32 Å), H20-O18 (2.36Å) and H21-O19 (1.95Å).

The N11 nitro group is approximately coplanar with the ring. The nitro groups N8, N9, N10 are rotated approximately, 45°, 65°, and 14° respectively. The amine group is almost planar.



Z-MATRIX (ANGSTROMS AND DEGREES)

CD	CENT	ATOM	N1	LENGTH	N2	ALPHA	N3	BETA	J
1	1	C							
2	2	C	1	1.434000 (1)					
3	3	C	2	1.361000 (2)	1	122.000 (22)			
4	4	C	3	1.384000 (3)	2	120.000 (23)	1	-0.950 (42)	0
5	5	C	4	1.377000 (4)	3	120.750 (24)	2	-2.930 (43)	0
6	6	C	1	1.428000 (5)	2	115.000 (25)	3	4.790 (44)	0
7	7	N	1	1.312000 (6)	2	122.000 (26)	3	-176.000 (45)	0
8	8	N	2	1.467000 (7)	3	119.000 (27)	4	174.000 (46)	0
9	9	N	3	1.487000 (8)	2	118.000 (28)	1	-179.000 (47)	0
10	10	N	4	1.447000 (9)	3	122.000 (29)	2	172.000 (48)	0
11	11	N	6	1.461000 (10)	1	122.000 (30)	2	177.000 (49)	0
12	12	O	8	1.218000 (11)	2	118.000 (31)	1	-45.000 (0)	0
13	13	O	8	1.218000 (12)	2	117.000 (32)	1	133.000 (51)	0
14	14	O	9	1.211000 (13)	3	116.000 (33)	2	-65.000 (52)	0
15	15	O	9	1.207000 (14)	3	116.000 (34)	2	114.980 (53)	0
16	16	O	10	1.221000 (15)	4	118.000 (35)	3	-14.000 (54)	0
17	17	O	10	1.227000 (16)	4	118.000 (36)	3	165.000 (55)	0
18	18	O	11	1.215000 (17)	6	119.000 (37)	1	-179.000 (56)	0
19	19	O	11	1.222000 (18)	6	118.000 (38)	1	-10.000 (57)	0
20	20	H	5	1.020000 (19)	4	117.000 (39)	3	-179.000 (58)	0
21	21	H	7	0.950000 (20)	1	120.000 (40)	2	177.000 (59)	0
22	22	H	7	0.970000 (21)	1	119.000 (41)	2	5.640 (60)	0

STOICHIOMETRY C6H3N5O8

SCF DONE: E(RHF) = -1094.81498704 A.U. AFTER 36 CYCLES

EIGENVALUES — -0.33140 -0.32703 -0.32170 -0.31199 0.09964

Estimated ionization potential: 8.49 ev

TOTAL ATOMIC CHARGES:

		1	Net Charges
1	C	5.781556	+0.22
2	C	5.940497	+0.06
3	C	5.863175	+0.14
4	C	5.932056	+0.07
5	C	6.020843	-0.02
6	C	5.944619	+0.06
7	N	7.466881	-0.47
8	N	6.822964	+0.18
9	N	6.796636	+0.20
10	N	6.830082	+0.17
11	N	6.824287	+0.18
12	O	8.203361	-0.20
13	O	8.171323	-0.17
14	O	8.177237	-0.17
15	O	8.162989	-0.16
16	O	8.189204	-0.19
17	O	8.194223	-0.19
18	O	8.180426	-0.18
19	O	8.219833	-0.22
20	H	0.843741	+0.16
21	H	0.709041	+0.29
22	H	0.725024	+0.27

DIPOLE MOMENT (DEBYE): X=-2.4264 Y= 0.5727 Z=-4.1587 TOTAL= 4.8487

V-mid:

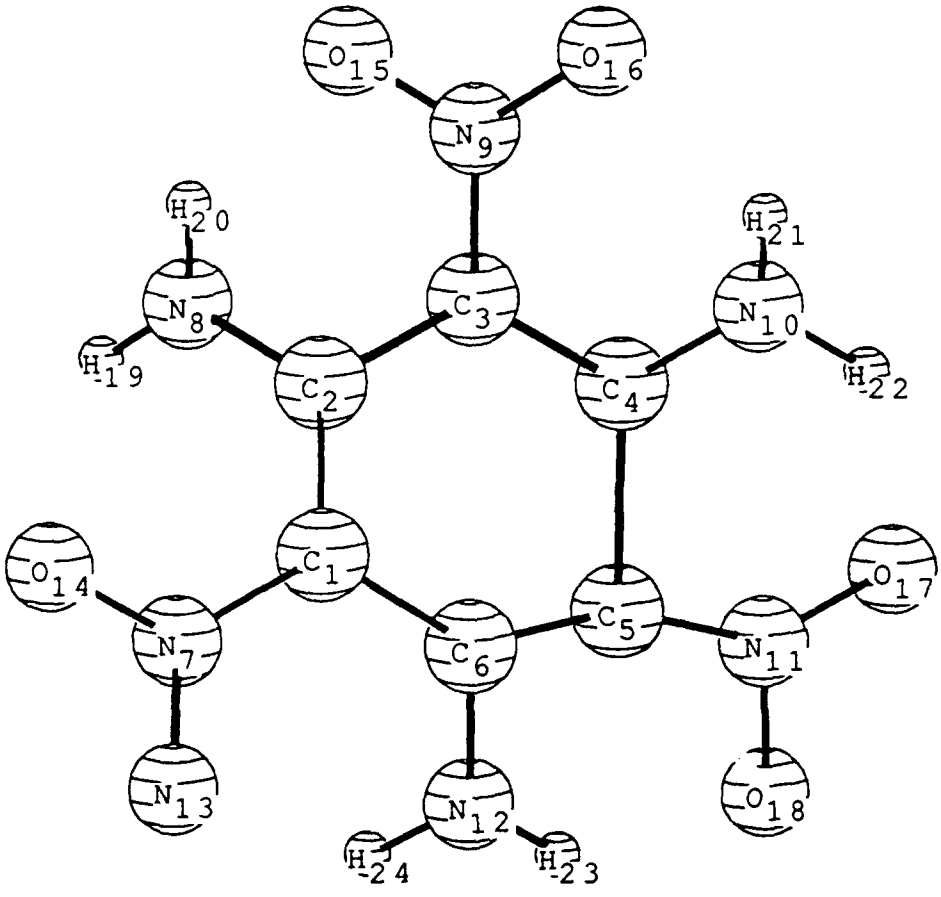
N8-C2:	0.172
N9-C3:	0.236
N10-C4:	0.174
N11-C6:	0.170

Bond Orders:

C1-N7:	1.74
C2-N8:	1.24
C3-N9:	1.20
C4-N10:	1.30
C6-N11:	1.26
N8-O12:	1.96
N8-O13:	1.96
N9-O14:	2.00
N9-O15:	2.02
N10-O16:	1.95
N10-O17:	1.92
N11-O18:	1.98
N11-O19:	1.94

APPENDIX X
1,3,5-TRIAMINO-2,4,6-TRINITROBENZENE

The short distances between non-bonded hydrogens and oxygens are between H21-O16 (1.95Å), H22-O18 (1.69Å), H23-O19 (1.82Å), H19-O14 (1.80Å), H20-O15 (1.84Å), and H24-O13 (1.77Å). All nitro groups are essentially coplanar.



Z-MATRIX (ANGSTROMS AND DEGREES)

CD	CENT	ATOM	N1	LENGTH	N2	ALPHA	N3	BETA	J
1	1	C							
2	2	C	1	1.435000 (1)					
3	3	C	2	1.447835 (2)	1	117.958 (24)			
4	4	C	3	1.436690 (3)	2	121.823 (25)	1	1.563 (46)	0
5	5	C	4	1.445519 (4)	3	117.995 (26)	2	2.699 (47)	0
6	6	C	5	1.435637 (5)	4	122.258 (27)	3	-5.062 (48)	0
7	7	N	1	1.416866 (6)	2	119.178 (28)	3	176.375 (49)	0
8	8	N	2	1.308986 (7)	3	120.727 (29)	4	-177.599 (50)	0
9	9	N	3	1.416524 (8)	4	119.045 (30)	5	-177.489 (51)	0
10	10	N	4	1.318790 (9)	5	120.543 (31)	6	175.500 (52)	0
11	11	N	5	1.422453 (10)	6	119.115 (32)	1	-178.785 (53)	0
12	12	N	6	1.310130 (11)	1	121.122 (33)	2	-177.498 (54)	0
13	13	O	7	1.235980 (12)	1	121.326 (34)	2	-178.209 (55)	0
14	14	O	7	1.242231 (13)	1	120.766 (35)	2	3.156 (56)	0
15	15	O	9	1.245843 (14)	3	120.644 (36)	4	177.655 (57)	0
16	16	O	9	1.238782 (15)	3	121.489 (37)	4	-1.816 (58)	0
17	17	O	11	1.243651 (16)	5	121.325 (38)	6	-179.192 (59)	0
18	18	O	11	1.251906 (17)	5	121.000 (39)	6	-1.683 (60)	0
19	19	H	8	0.864445 (18)	2	117.278 (40)	3	179.362 (61)	0
20	20	H	8	0.848948 (19)	2	119.427 (41)	3	-13.477 (62)	0
21	21	H	10	0.756530 (20)	4	123.058 (42)	5	175.709 (63)	0
22	22	H	10	1.054022 (21)	4	120.725 (43)	5	1.598 (64)	0
23	23	H	12	0.868277 (22)	6	119.010 (44)	1	177.745 (65)	0
24	24	H	12	0.954518 (23)	6	116.561 (45)	1	13.077 (66)	0

STOICHIOMETRY C6H6N6O6

****

SCF DONE: E(RHF) = -1001.76753338 A.U. AFTER 29 CYCLES

****

EIGENVALUES — -0.28957 0.14706 0.15303 0.17304 0.26932

Estimated ionization potential: 7.9 ev

TOTAL ATOMIC CHARGES.

		1	Net Charge
1	C	6.016830	-0.02
2	C	5.752293	+0.25
3	C	6.014397	-0.01
4	C	5.755384	+0.24
5	C	6.015664	-0.02
6	C	5.761298	+0.24
7	N	6.843190	+0.16
8	N	7.567198	-0.57
9	N	6.849386	+0.15
10	N	7.558835	-0.56
11	N	6.849656	+0.15
12	N	7.519123	-0.52
13	O	8.226725	-0.23
14	O	8.225928	-0.23
15	O	8.233159	-0.23
16	O	8.220555	-0.22
17	O	8.227047	-0.23
18	O	8.218506	-0.22
19	H	0.687027	+0.31
20	H	0.683115	+0.32
21	H	0.672935	+0.33
22	H	0.705543	+0.29
23	H	0.694585	+0.31
24	H	0.706062	+0.29

DIPOLE MOMENT (DEBYE): X= 0.3195 Y= 0.2801 Z=-0.6508 TOTAL= 0.7773

V-mid: N7-C1: 0.105
N9-C3: 0.102
N11-C5: 0.103

Bond Orders: N7-C1: 1.38
N8-C2: 1.76
N9-C3: 1.38
N10-C4: 1.72
N11-C5: 1.37
N12-C6: 1.75
N7-O13: 1.86
N7-O14: 1.84
N9-O15: 1.82
N9-O16: 1.85
N11-O17: 1.83
N11-O18: 1.79

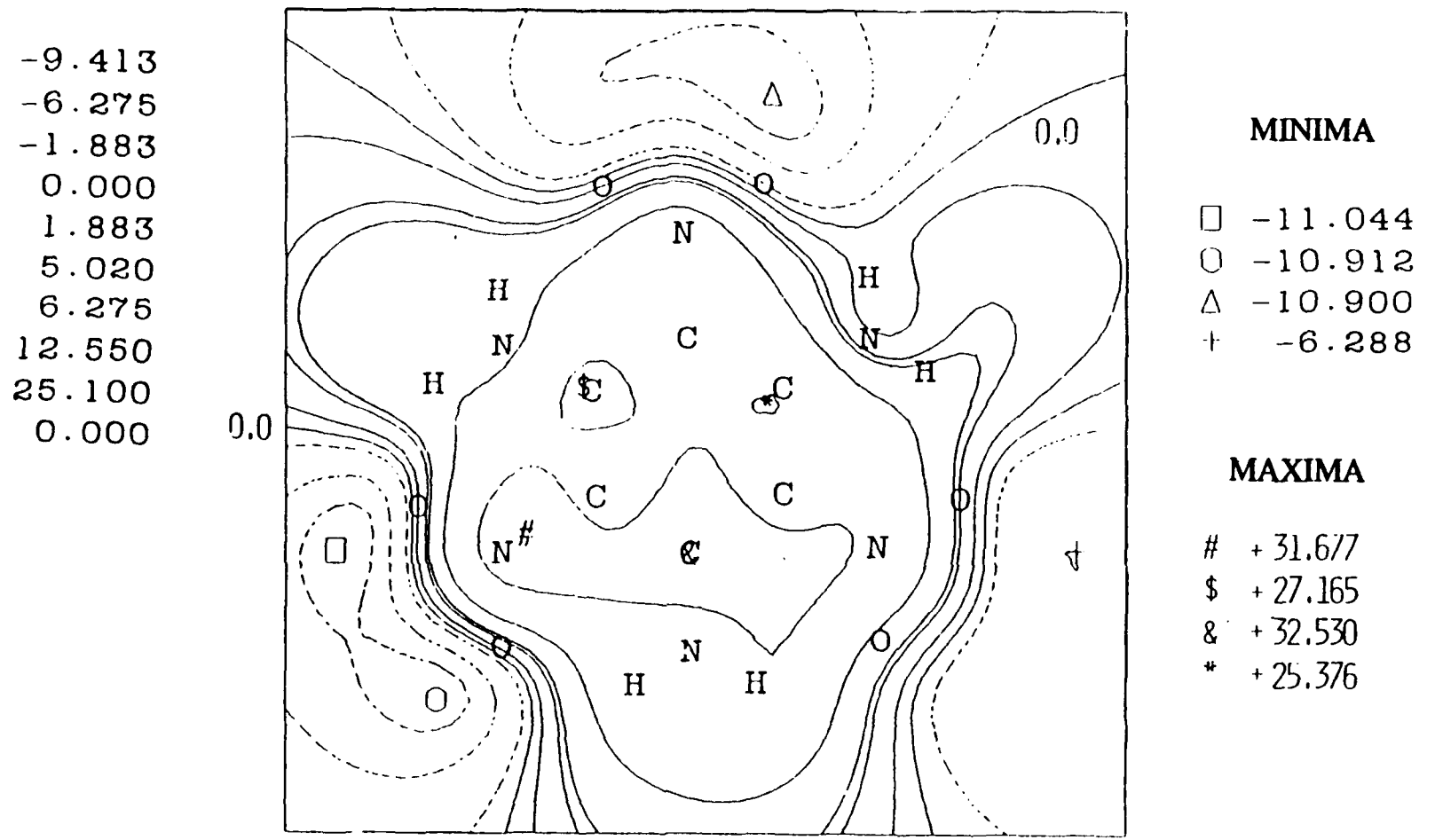
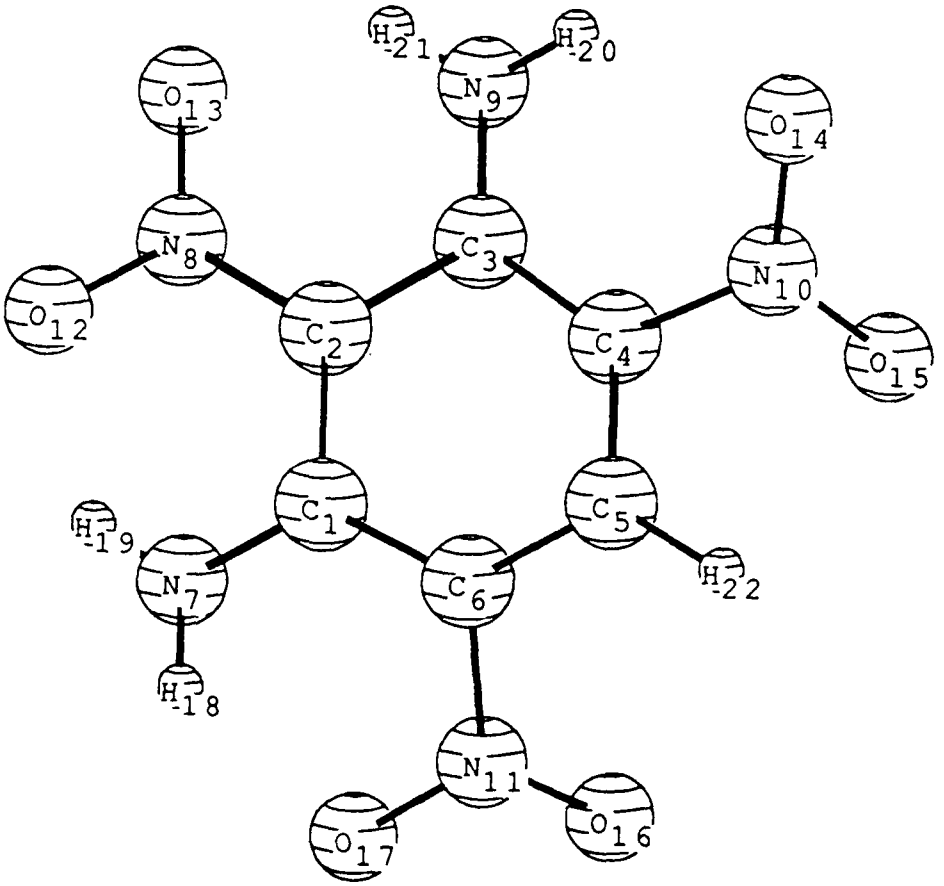


Figure X-1. Calculated electrostatic potential, in kcal/mole, of 1,3,5-triamino-2,4,6-trinitrobenzene, in the plane 1.75 Å above the aromatic ring. Projected positions of nuclei are shown. The zero contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

APPENDIX Y
1,3-DIAMINO-2,4,6-TRINITROBENZENE

The short distances between non-bonded hydrogens and oxygens are H21-O16 (1.95 Å), H22-O18 (1.69 Å), H23-O19 (1.82 Å), H19-O14 (1.80 Å), H20-O15 (1.84 Å) and H24 - O13 (1.77 Å).

All nitro groups and amine groups are essentially coplanar.



Z-Matrix (Angstroms and Degrees)

Cent	Atom	N1	Length	N2	Alpha	N3	Beta
1	C						
2	C	1	1.4664356				
3	C	2	1.4723277	1	120.5247574		
4	C	3	1.3918228	2	115.8793259	1	-4.2251754
5	C	4	1.3789175	3	123.8528214	2	4.0671515
6	C	5	1.3739673	4	119.2582703	3	-3.1503119
7	N	1	1.3228761	6	124.0092850	5	179.7978668
8	N	2	1.4151319	1	119.6532745	6	-178.1909485
9	N	3	1.3177489	2	120.1124573	1	177.7904205
10	N	4	1.4318832	3	122.4196014	2	-179.6103363
11	N	6	1.5139433	1	121.9566345	2	-177.3157349
12	O	8	1.2621572	2	121.7608109	3	-178.2516937
13	O	8	1.2413824	2	120.8816833	3	-1.2636397
14	O	10	1.2597437	4	118.7223892	5	-174.9521942
15	O	10	1.2230211	4	121.2245178	5	1.6063229
16	O	11	1.1772938	6	117.8368988	1	173.3712616
17	O	11	1.2357228	6	115.5550537	1	-8.5564947
18	H	7	0.8897375	1	119.3610306	2	-179.9651947
19	H	7	0.8905061	1	119.2657166	2	0.0104214
20	H	9	0.8902898	3	119.2623444	4	2.1553166
21	H	9	0.8901286	3	119.3083496	4	-177.8555298
22	H	5	1.0802929	6	120.2810669	1	-177.6110077

Stoichiometry: C6H5N5O6

SCF DONE: E(RHF) = -947.084610

EIGENVALUES -- -0.29970 -.29735 0.12008 .15933 0.18091

Estimated ionization potential: 8.09 ev

TOTAL ATOMIC CHARGES.

		1
1	C	5.775821
2	C	5.958405
3	C	5.770389
4	C	5.982352
5	C	5.996443
6	C	5.985343
7	N	7.533139
8	N	6.854927
9	N	7.532075
10	N	6.846354
11	N	6.805783
12	O	8.220766
13	O	8.212966
14	O	8.231972
15	O	8.190286
16	O	8.188858
17	O	8.236980
18	H	0.703012
19	H	0.696854
20	H	0.701672
21	H	0.695836
22	H	0.849761

Net Charges

1	C	+ 0.22
2	C	+ 0.01
3	C	+ 0.23
4	C	+ 0.02
5	C	0.00
6	C	+ 0.01
7	N	- 0.53
8	N	+ 0.15
9	N	- 0.53
10	N	+ 0.15
11	N	+ 0.19
12	O	- 0.22
13	O	- 0.21
14	O	- 0.23
15	O	- 0.19
16	O	- 0.18
17	O	- 0.24
18	H	+ 0.30
19	H	+ 0.30
20	H	+ 0.30
21	H	+ 0.30
22	H	+ 0.15

DIPOLE MOMENT (DEBYE): X = 0.4617 Y = 0.9115 Z = 1.0664 TOTAL = 1.4769

V-mid N8-C2: 0.118
N10-C4: 0.127
N11-C6: 0.146

Bond Orders:

C1-N7: 1.70
C2-N8: 1.39
C3-N9: 1.72
C4-N10: 1.34
C6-N11: 1.13
N8-O12: 1.76
N8-O13: 1.86
N10-O14: 1.77
N10-O15: 1.94
N11-O16: 2.17
N12-O17: 1.88

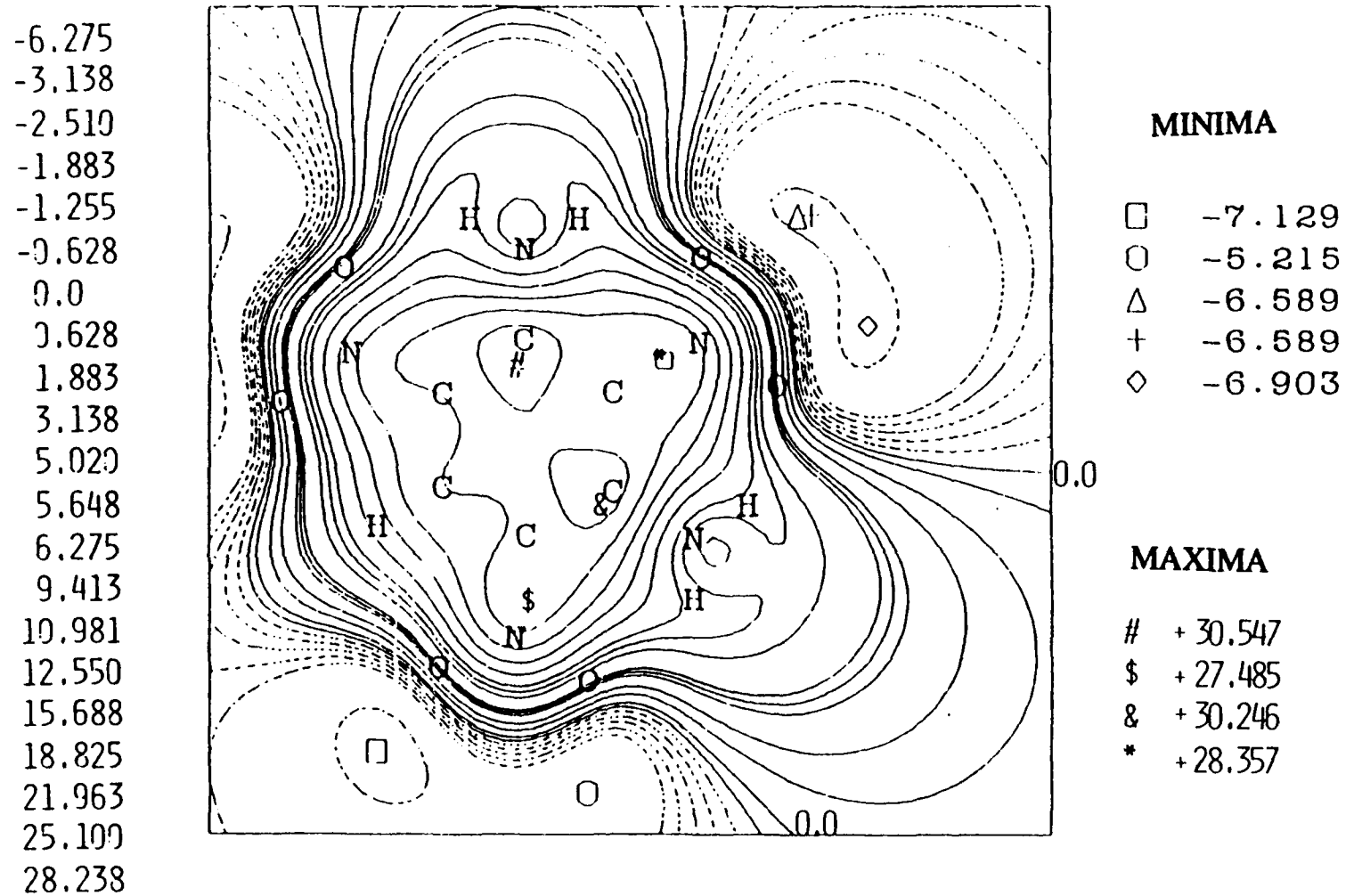
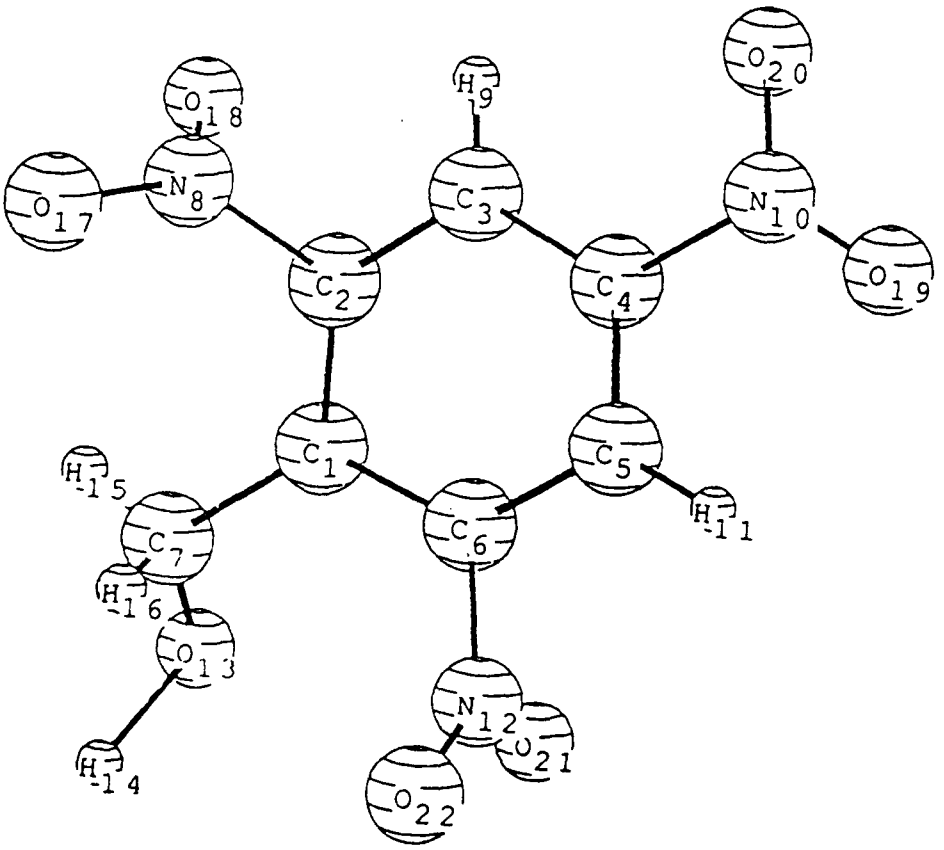


Figure Y-1. Calculated electrostatic potential, in kcal/mole, of 1,3-diamino-2,4,6-trinitrobenzene, in the plane 1.75 Å above the aromatic ring. Projected positions of nuclei are shown. The zero contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

APPENDIX Z
2,4,6-TRINITROBENZYL ALCOHOL

The short distances between non-bonded hydrogens and oxygens are H9-O18 (2.50 Å), H9-O20 (2.45 Å), H11-O19 (2.46 Å) and H15-O17 (2.30 Å).

The N10 nitro group is rotated out of the mean plane of the benzene ring by about 10°, while the N8 and N12 nitro groups are rotated by about 40° and 54°, respectively.



Z-MATRIX (ANGSTROMS AND DEGREES)

CD	CENT	ATOM	N1	LENGTH	N2	ALPHA	N3	BETA	J
1	1	C							
2	2	C	1	1.387619 (1)					
3	3	C	2	1.372534 (2)	1	125.219 (22)			
4	4	C	3	1.377346 (3)	2	117.473 (23)	1	-0.942 (42)	0
5	5	C	4	1.386211 (4)	3	121.410 (24)	2	0.645 (43)	0
6	6	C	5	1.383131 (5)	4	117.678 (25)	3	-0.679 (44)	0
7	7	C	1	1.499325 (6)	2	124.289 (26)	3	-176.777 (45)	0
8	8	N	2	1.482795 (7)	3	115.382 (27)	4	178.228 (46)	0
9	9	H	3	0.960036 (8)	4	121.412 (28)	5	-179.306 (47)	0
10	10	N	4	1.458971 (9)	5	118.640 (29)	6	175.741 (48)	0
11	11	H	5	0.959774 (10)	6	121.176 (30)	1	179.636 (49)	0
12	12	N	6	1.479611 (11)	1	119.555 (31)	2	176.110 (50)	0
13	13	O	7	1.415276 (12)	1	110.270 (32)	2	138.299 (51)	0
14	14	H	13	1.134622 (13)	7	102.775 (33)	1	146.977 (52)	0
15	15	H	7	0.959596 (14)	1	109.227 (34)	2	18.341 (53)	0
16	16	H	7	0.959905 (15)	1	109.405 (35)	2	-101.570 (54)	0
17	17	O	8	1.196034 (16)	2	118.887 (36)	3	-139.745 (55)	0
18	18	O	8	1.233533 (17)	2	116.414 (37)	3	39.673 (56)	0
19	19	O	10	1.175433 (18)	4	119.343 (38)	5	-9.451 (57)	0
20	20	O	10	1.223853 (19)	4	116.632 (39)	5	168.713 (58)	0
21	21	O	12	1.205410 (20)	6	119.000 (40)	5	-53.936 (59)	0
22	22	O	12	1.230981 (21)	6	116.231 (41)	1	-55.129 (60)	0

STOICHIOMETRY C7H5N3O7

SCF DONE: E(RHF) = -950.841755357

EIGENVALUES — -0.31779 -0.31181 0.11651 0.13601 0.18553

Estimated ionization potetial: 8.50 eV

TOTAL ATOMIC CHARGES.

		1	Net Charge
1	C	5.942688	0.057
2	C	5.898740	0.101
3	C	6.061611	-0.062
4	C	5.887629	0.112
5	C	6.065386	-0.107
6	C	5.888654	0.111
7	C	6.082517	-0.083
8	N	6.825415	0.175
9	H	0.852752	0.147
10	N	6.812835	0.187
11	H	0.859317	0.141
12	N	6.819559	0.180
13	O	8.240289	-0.240
14	H	0.837348	0.163
15	H	0.882923	0.117
16	H	0.87624	0.124
17	O	8.190826	-0.190
18	O	8.195151	-0.195
19	O	8.189585	-0.190
20	O	8.205442	-0.205
21	O	8.179062	-0.179
22	O	8.205824	-0.206

DIPOLE MOMENT (DEBYE): X=-1.6231 Y=-0.7876 Z=-0.9997 TOTAL= 2.0626

V-mid: N8-C2: 0.197
N10-C4: 0.217
N12-C6: 0.208

Bond Order: N8-C2: 1.21
N10-C4: 1.27
N12-C6: 1.22
O17-N8: 2.06
O18-N8: 1.85
O19-N10: 2.17
O20-N10: 1.92
O21-N12: 2.01
O22-N12: 1.89

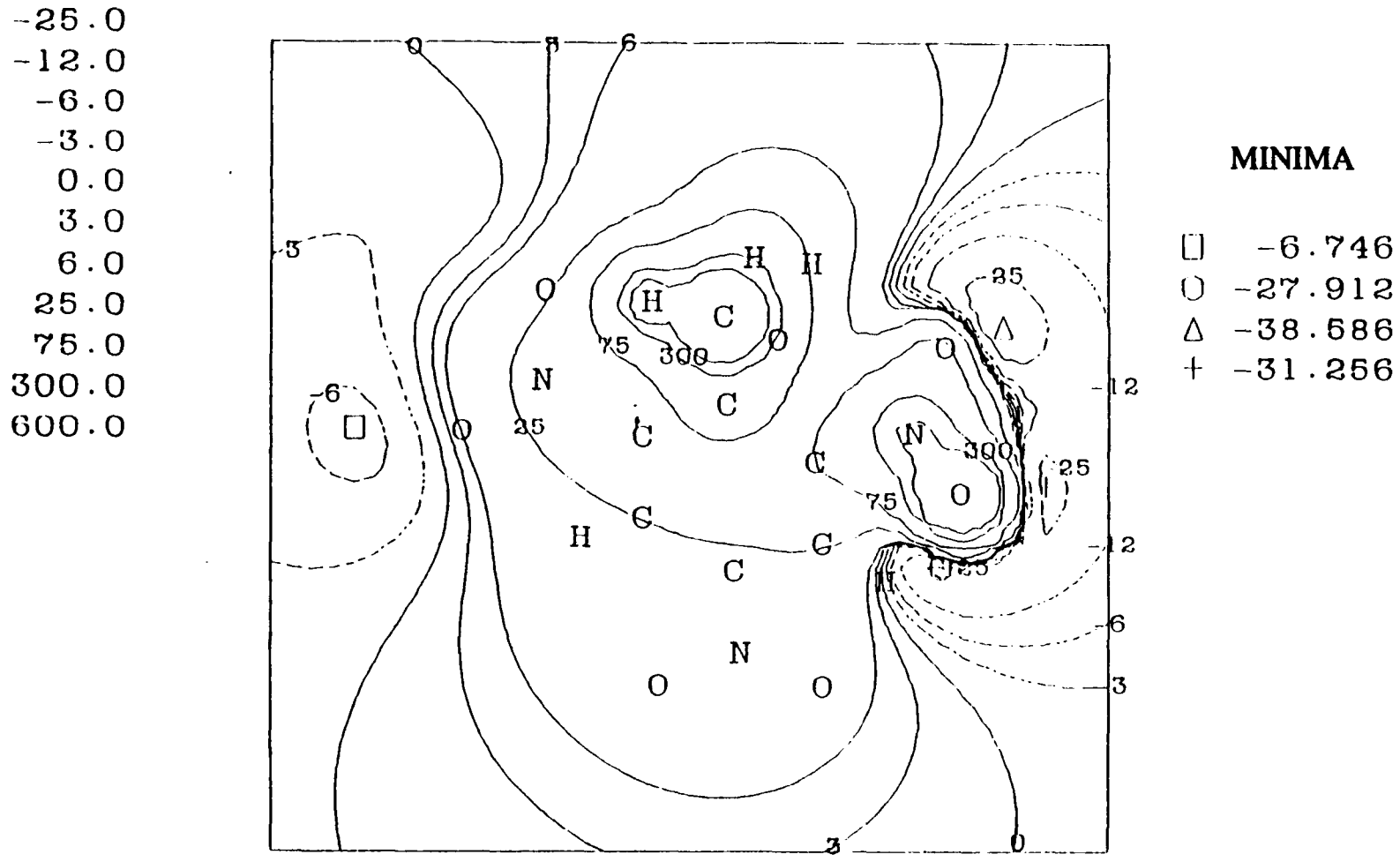


Figure Z-1. Calculated electrostatic potential, in kcal/mole, of 2,4,6-trinitrobenzyl alcohol, in the plane 1.75Å above the N8 nitro group located in the upper left corner. Projected positions of nuclei are shown. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

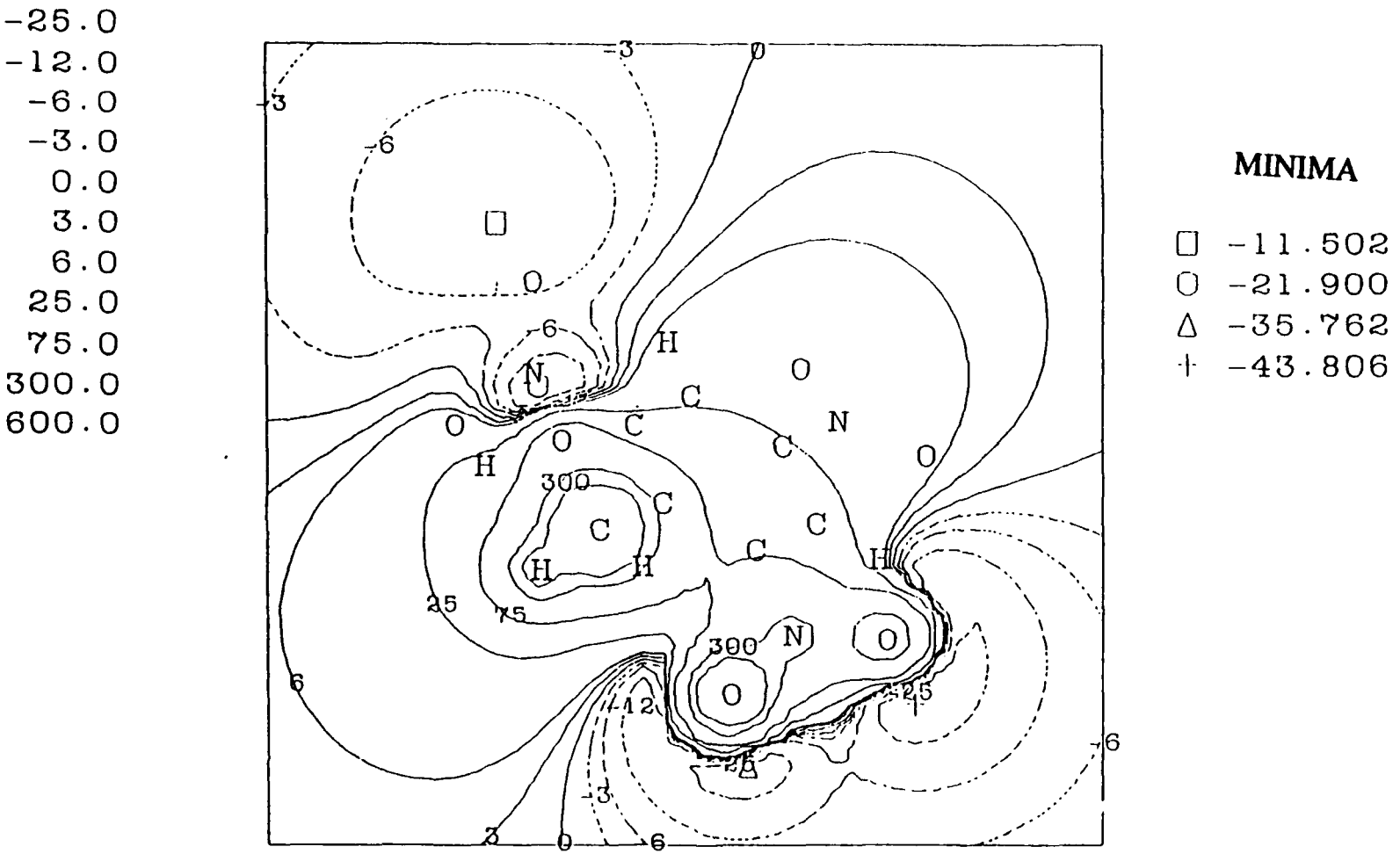
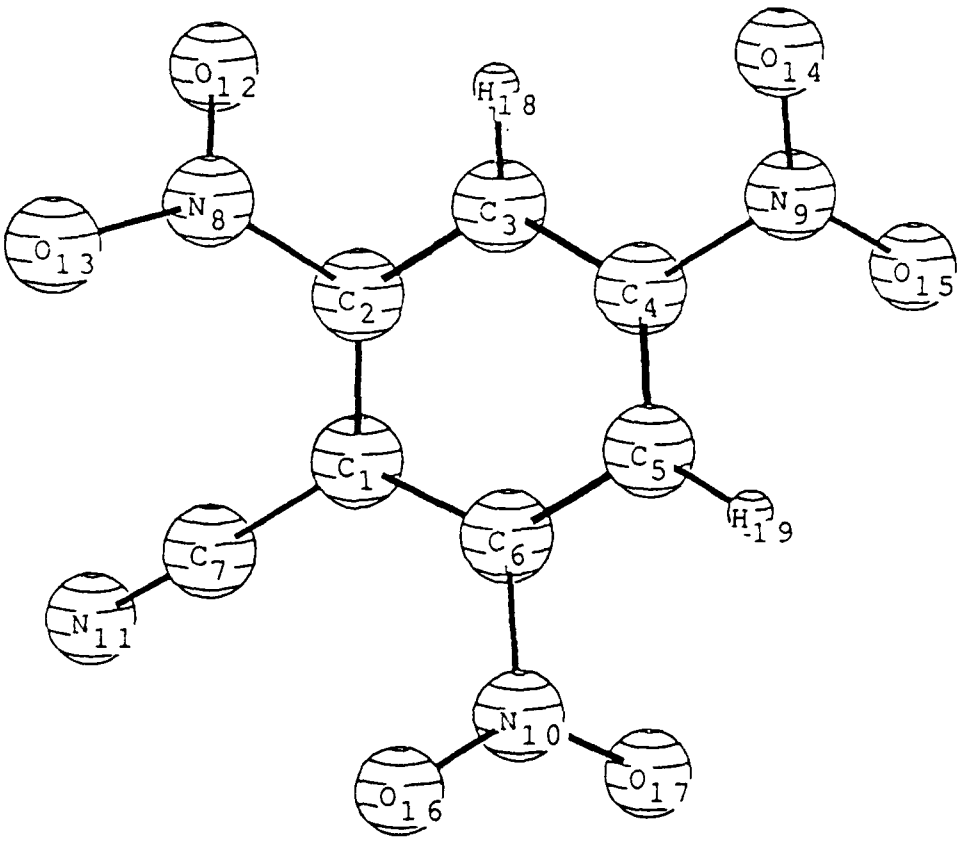


Figure Z-2. Calculated electrostatic potential, in kcal/mole, of 2,4,6-trinitrobenzyl alcohol, in the plane 1.75Å above the N12 nitro group located in the upper left corner. Projected positions of nuclei are shown. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

APPENDIX AA
2,4,6-TRINITROBENZONITRILE

The short distances between non-bonded hydrogens and oxygens are H18-O12 (2.39 Å), H18-O14 (2.42 Å), H19-O15 (2.49 Å) and H19-O17 (2.34 Å).

The N8, N9 and N10 nitro groups are rotated out of the mean plane of the benzene ring by approximately 26°, 12° and 16°, respectively.



Z-MATRIX (ANGSTROMS AND DEGREES)

CD	CENT	ATOM	N1	LENGTH	N2	ALPHA	N3	BETA	J
1	1	C							
2	2	C	1	1.391000 (1)					
3	3	C	2	1.381306 (2)	1	122.868 (19)			
4	4	C	3	1.371322 (3)	2	117.367 (20)	1	-0.952 (36)	0
5	5	C	4	1.358455 (4)	3	123.149 (21)	2	0.610 (37)	0
6	6	C	5	1.384016 (5)	4	117.805 (22)	3	-0.401 (38)	0
7	7	C	1	1.444437 (6)	2	121.382 (23)	3	-174.982 (39)	0
8	8	N	2	1.480487 (7)	3	115.568 (24)	4	177.937 (40)	0
9	9	N	4	1.480034 (8)	3	117.601 (25)	2	-177.192 (41)	0
10	10	N	6	1.485060 (9)	5	116.647 (26)	4	-178.335 (42)	0
11	11	N	7	1.138000 (10)	1	176.811 (27)	2	51.689 (43)	0
12	12	O	8	1.205197 (11)	2	117.195 (28)	1	-154.716 (44)	0
13	13	O	8	1.219426 (12)	2	117.333 (29)	1	26.202 (45)	0
14	14	O	9	1.218041 (13)	4	117.247 (30)	3	12.521 (46)	0
15	15	O	9	1.215971 (14)	4	117.039 (31)	3	-167.466 (47)	0
16	16	O	10	1.208056 (15)	6	117.349 (32)	5	161.878 (48)	0
17	17	O	10	1.214249 (16)	6	116.401 (33)	5	-16.022 (49)	0
18	18	H	3	1.000000 (17)	4	122.543 (34)	5	179.414 (50)	0
19	19	H	5	1.000000 (18)	4	123.385 (35)	3	-172.430 (51)	0

STOICHIOMETRY C7H2N4O6

SCF DONE: E(RHF) = -928.874944710

EIGENVALUES -- -0.38909 -0.38680 -0.33299 -0.32951 -0.32856 0.08269

Estimated ionization potential: 8.95 ev

TOTAL ATOMIC CHARGES.

		1	Net Charge
1	C	5.959718	0.040
2	C	5.884293	0.116
3	C	6.047682	-0.048
4	C	5.889990	0.110
5	C	6.050620	-0.051
6	C	5.884619	0.115
7	C	5.896436	0.104
8	N	6.818527	0.181
9	N	6.821234	0.179
10	N	6.815834	0.184
11	N	7.138529	-0.139
12	O	8.184625	-0.185
13	O	8.179035	-0.179
14	O	8.187497	-0.187
15	O	8.184231	-0.184
16	O	8.175735	-0.176
17	O	8.187217	-0.187
18	H	0.847320	0.153
19	H	0.846857	0.153

DIPOLE MOMENT (DEBYE): X= 2.0748 Y=-0.0299 Z= 1.1260 TOTAL= 2.3609

Bond Order:		V-mid:	
C2-N8:	1.21	C2-N8:	0.213
C4-N9:	1.21	C4-N9:	0.207
C6-N10:	1.20	C6-N10:	0.213
N8-O12:	2.01		
N8-O13:	1.94		
N9-O14:	1.95		
N9-O15:	1.96		
N10-O16:	2.00		
N10-O17:	1.97		

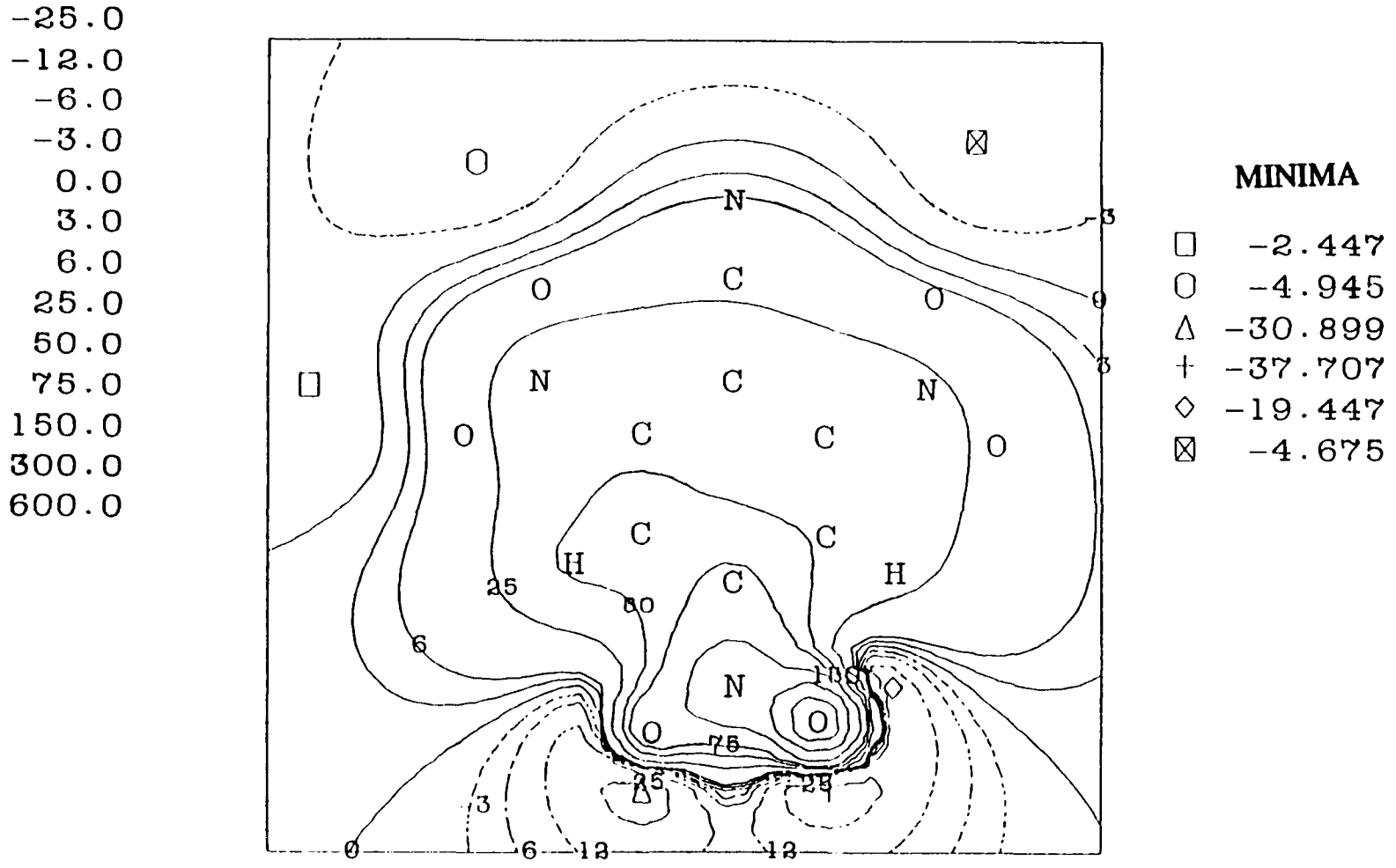


Figure AA-1. Calculated electrostatic potential, in kcal/mole, of 2,4,6-trinitrobenzonitrile, in the plane 1.75Å above the N10 nitro group located in the upper left corner. Projected positions of nuclei are shown. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

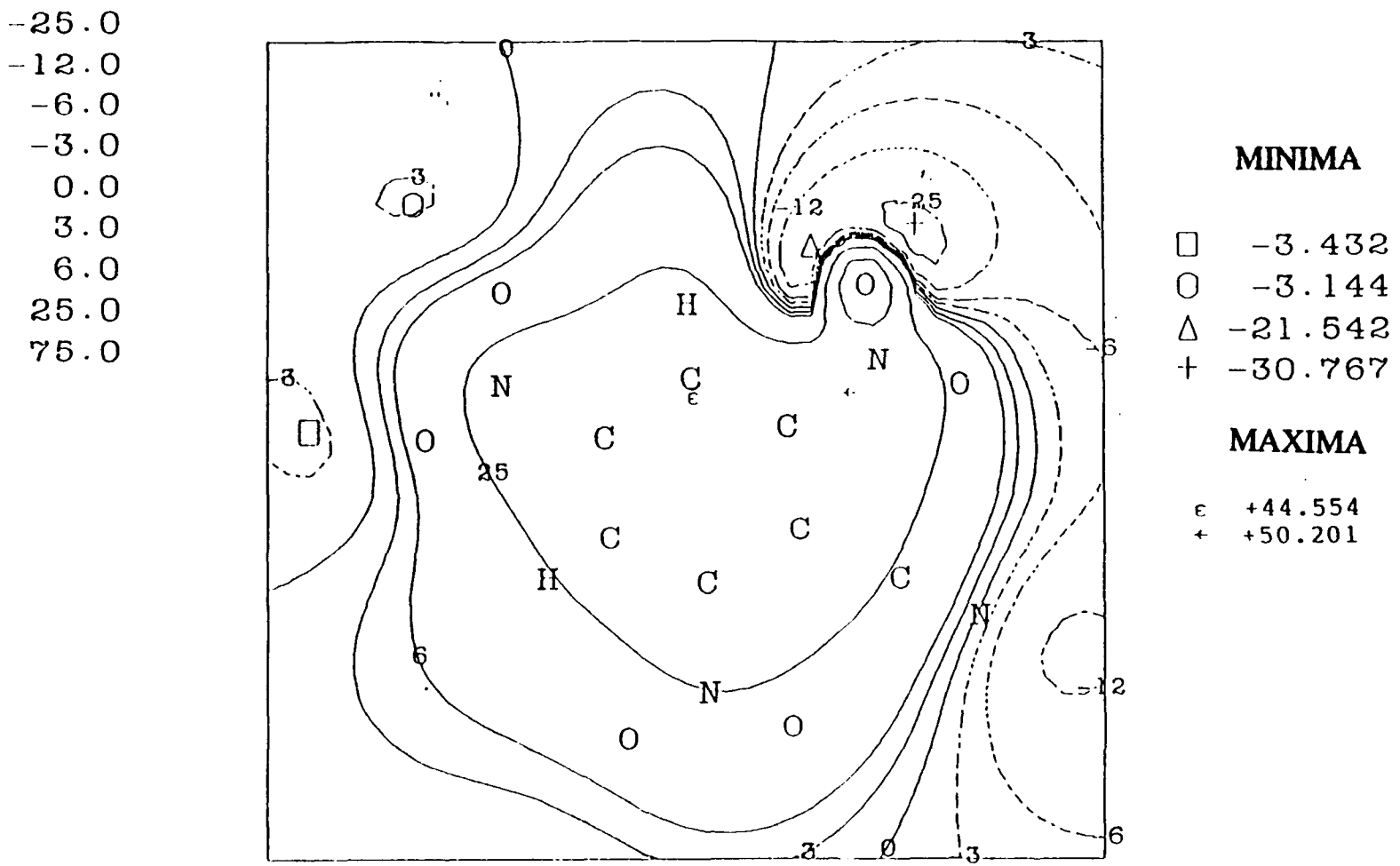
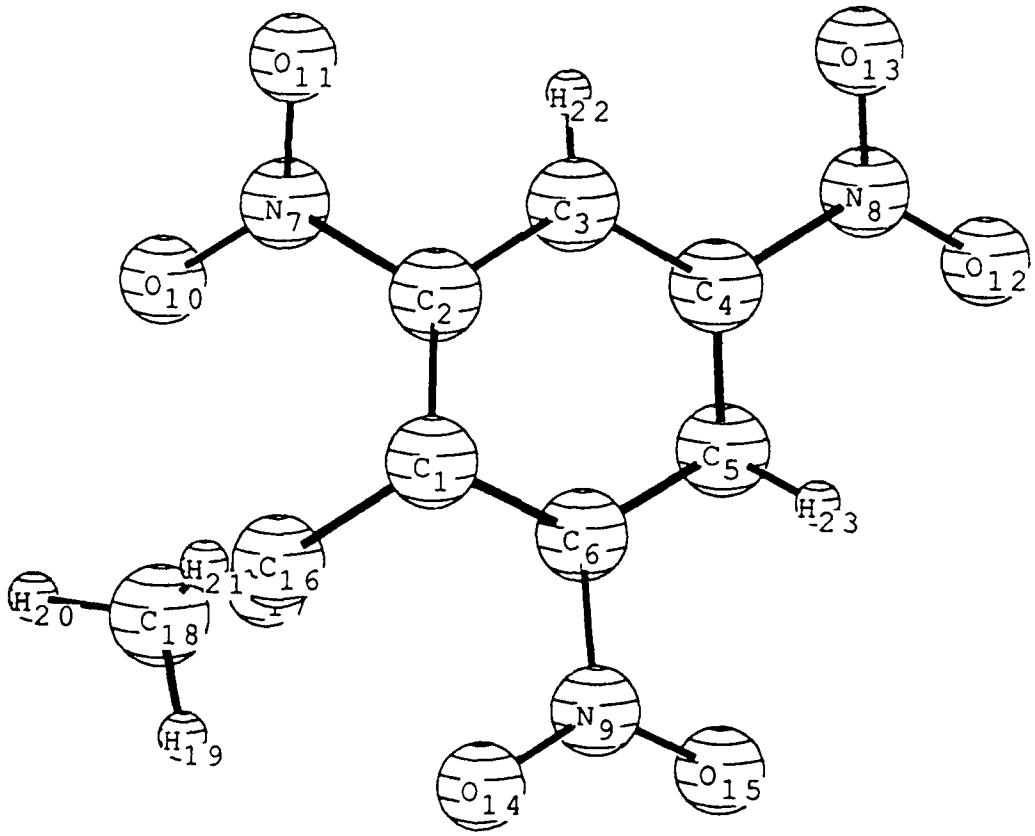


Figure AA-2. Calculated electrostatic potential, in kcal/mole, of 2,4,6-trinitrobenzonitrile, in the plane 1.75Å above the N9 nitro group located in the upper left corner. Projected positions of nuclei are shown. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

APPENDIX BB
2,4,6-TRINITROACETOPHENONE

The short distances between non-bonded hydrogens and oxygens are H19-O14 (2.50 Å), H22-O11 (2.34 Å), H22-O13 (2.47 Å), H23-O12 (2.48 Å), and H23-O15 (2.40 Å). Nitro groups N7, N8 and N9 are rotated out of the plane by approximately 4°, 18° and 20°, respectively.



Z-MATRIX (ANGSTROMS AND DEGREES)

CD	CENT	ATOM	N1	LENGTH		N2	ALPHA		N3	BETA		J
1	1	C										
2	2	C	1	1.392000	(1)							
3	3	C	2	1.376431	(2)	1	124.036	(23)				
4	4	C	3	1.378529	(3)	2	117.369	(24)	1	2.057	(44)	0
5	5	C	4	1.369033	(4)	3	122.420	(25)	2	-1.476	(45)	0
6	6	C	5	1.374375	(5)	4	117.646	(26)	3	-0.430	(46)	0
7	7	N	2	1.482075	(6)	3	116.031	(27)	4	-177.045	(47)	0
8	8	N	4	1.467600	(7)	3	118.482	(28)	2	177.754	(48)	0
9	9	N	6	1.476630	(8)	5	116.075	(29)	4	-178.568	(49)	0
10	10	O	7	1.217664	(9)	2	117.865	(30)	3	175.152	(50)	0
11	11	O	7	1.211071	(10)	2	117.785	(31)	3	-4.138	(51)	0
12	12	O	8	1.223031	(11)	4	117.572	(32)	3	-162.894	(52)	0
13	13	O	8	1.215320	(12)	4	117.940	(33)	3	17.721	(53)	0
14	14	O	9	1.221059	(13)	6	117.270	(34)	5	160.112	(54)	0
15	15	O	9	1.220414	(14)	6	118.112	(35)	5	-20.335	(55)	0
16	16	C	1	1.536863	(15)	2	123.236	(36)	3	-176.449	(56)	0
17	17	O	16	1.202061	(16)	1	117.552	(37)	2	91.705	(57)	0
18	18	C	16	1.488976	(17)	1	117.877	(38)	2	-88.268	(58)	0
19	19	H	18	0.945258	(18)	16	105.483	(39)	1	-105.217	(59)	0
20	20	H	18	0.984491	(19)	16	108.722	(40)	1	136.333	(60)	0
21	21	H	18	0.880823	(20)	16	114.232	(41)	1	6.666	(61)	0
22	22	H	3	0.932775	(21)	2	120.931	(42)	1	179.643	(62)	0
23	23	H	5	0.905621	(22)	4	122.221	(43)	3	-177.399	(63)	0

STOICHIOMETRY C8H5N3O7

SCF DONE: E(RHF) = -988.555699827 A.U. AFTER 41 CYCLES

EIGENVALUES -- -0.38134 -0.37535 -0.32540 -0.32376 -0.31771 0.10850

Estimated ionization potential: 8.66 eV

TOTAL ATOMIC CHARGES.

		1	Net Charge
1	C	5.977507	0.022
2	C	5.899033	0.101
3	C	6.067820	-0.068
4	C	5.882452	0.118
5	C	6.077950	-0.078
6	C	5.894200	0.106
7	N	6.821736	0.178
8	N	6.827279	0.173
9	N	6.827353	0.173
10	O	8.196196	-0.196
11	O	8.185658	-0.186
12	O	8.189231	-0.189
13	O	8.187950	-0.188
14	O	8.198360	-0.198
15	O	8.180660	-0.181
16	C	5.715981	0.284
17	O	8.212960	-0.213
18	C	6.369110	-0.369
19	H	0.855457	0.145
20	H	0.865263	0.135
21	H	0.874293	0.126
22	H	0.846495	0.154
23	H	0.847056	0.153

DIPOLE MOMENT (DEBYE): X=-0.2659 Y=-1.8122 Z=-0.0756 TOTAL= 1.8332

V-mid: N7-C2: 0.199
N8-C4: 0.210
N9-C6: 0.200

Bond Order: N7-C2: 1.21
N8-C4: 1.25
N9-C6: 1.22
O10-N7: 1.95
O11-N7: 1.98
O12-N8: 1.92
O13-N8: 1.96
O14-N9: 1.93
O15-N9: 1.94

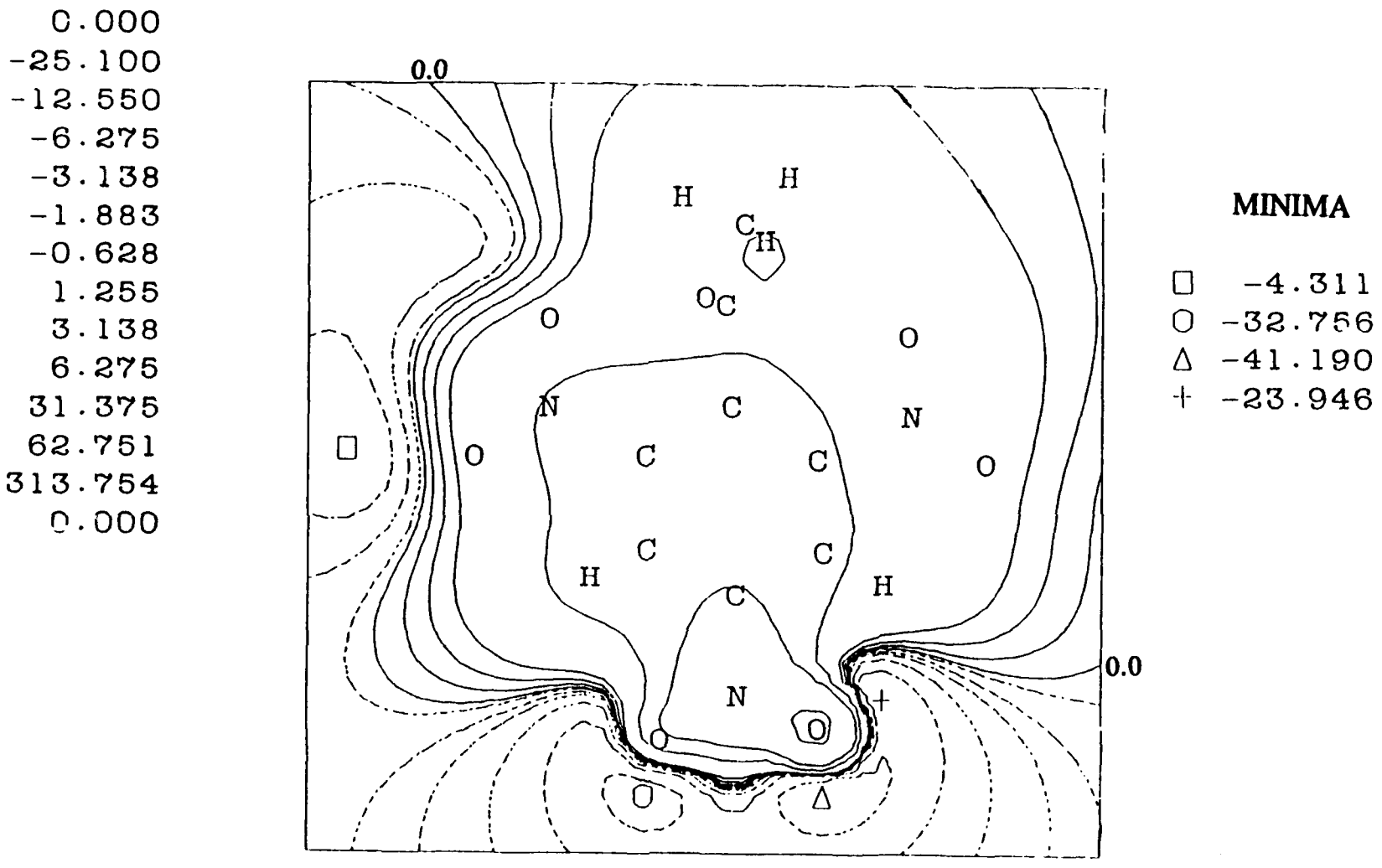
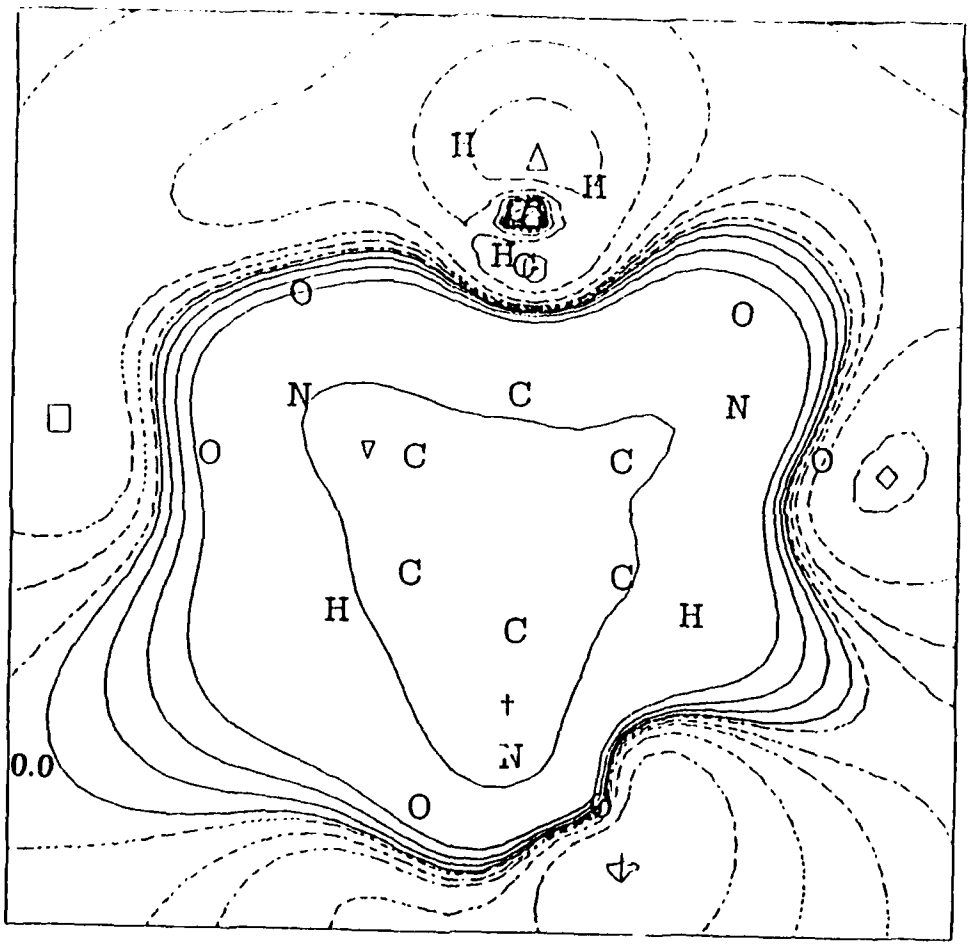


Figure BB-1. Calculated electrostatic potential, in kcal/mole, of 2,4,6-trinitroacetophenone in the plane 1.75Å above the N9 nitro group located in the upper left corner. Projected positions of nuclei are shown. The zero contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

0.000
-25.100
-12.550
-6.275
-3.138
-1.883
-0.628
1.255
3.138
6.275
31.375
0.000



MINIMA

□ -5.196
○ -25.653
△ -39.577
+ -25.985
◇ -13.862

MAXIMA

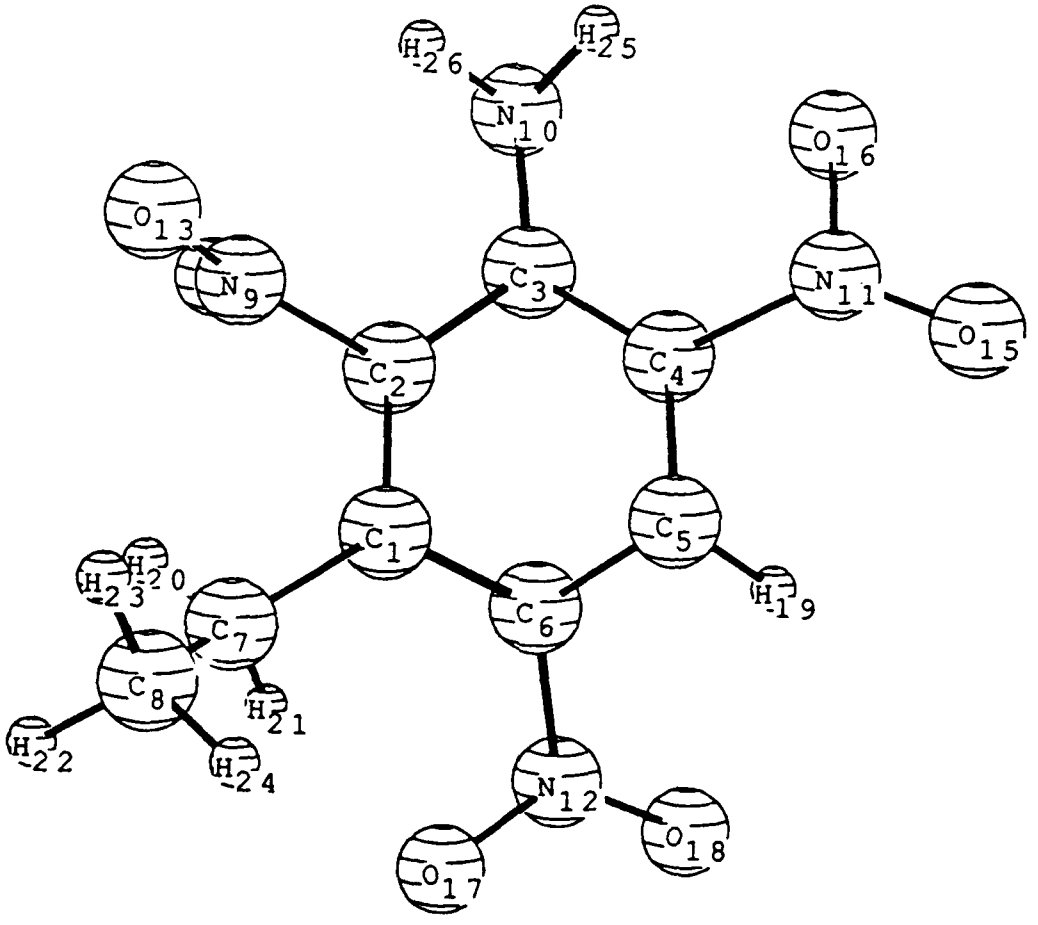
▽ 36.057
† 45.915

Figure BB-2. Calculated electrostatic potential, in kcal/mole, of 2,4,6-trinitroacetophenone in the plane 1.75Å above the N7 nitro group located in the upper left corner. Projected positions of nuclei are shown. The zero contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

APPENDIX CC
3-AMINO-2,4,6-TRINITROETHYLBENZENE

The short distances between non-bonded hydrogens and oxygens are H19-O18 (2.22 Å), H19-O15 (2.51 Å) and H25-O16 (2.19 Å).

The N11 and N12 nitro groups are rotated out of the mean plane of the benzene ring by approximately 27° and 16°. The N9 nitro group is essentially perpendicular to the ring.



Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.386000(1)					
3	3	C	2	1.422212(2)	1	126.283(26)			
4	4	C	3	1.391275(3)	2	114.113(27)	1	-2.941(50)	0
5	5	C	4	1.389812(4)	3	123.198(28)	2	2.752(51)	0
6	6	C	5	1.384322(5)	4	119.091(29)	3	0.643(52)	0
7	7	C	1	1.501938(6)	2	122.276(30)	3	178.570(53)	0
8	8	C	7	1.520060(7)	1	112.660(31)	2	-93.121(54)	0
9	9	N	2	1.459146(8)	3	114.752(32)	4	177.008(55)	0
10	10	N	3	1.346982(9)	4	125.719(33)	5	-176.846(56)	0
11	11	N	4	1.561775(10)	5	114.391(34)	6	-178.704(57)	0
12	12	N	6	1.481676(11)	5	114.336(35)	4	174.042(58)	0
13	13	O	9	1.200006(12)	2	118.610(36)	1	92.920(59)	0
14	14	O	9	1.201423(13)	2	117.837(37)	1	-89.338(60)	0
15	15	O	11	1.177512(14)	4	114.655(38)	5	-27.223(61)	0
16	16	O	11	1.213044(15)	4	113.581(39)	5	162.132(62)	0
17	17	O	12	1.235447(16)	6	118.156(40)	5	165.583(63)	0
18	18	O	12	1.209812(17)	6	118.461(41)	5	-16.250(64)	0
19	19	H	5	1.003240(18)	4	126.191(42)	3	173.591(65)	0
20	20	H	7	1.000000(19)	1	109.900(43)	2	28.400(66)	0
21	21	H	7	1.000000(20)	1	110.300(44)	2	144.100(67)	0
22	22	H	8	1.000000(21)	7	108.900(45)	1	176.600(68)	0
23	23	H	8	1.000000(22)	7	110.700(46)	1	57.100(69)	0
24	24	H	8	1.000000(23)	7	110.300(47)	1	-64.000(70)	0
25	25	H	10	0.953232(24)	3	130.456(48)	4	-2.515(71)	0
26	26	H	10	0.996377(25)	3	127.439(49)	4	-159.940(72)	0

STOICHIOMETRY C8H8N4O6

CF DONE: E(RHF) = -970.119859474

Alpha eigenvalues -- -0.30137 0.14867 0.15733 0.20240 0.22068

Estimated ionization potential: 8.20 ev

Total atomic charges:

		1
1	C	0.069481
2	C	0.061105
3	C	0.190756
4	C	0.051414
5	C	-0.044100
6	C	0.061606
7	C	-0.153866
8	C	-0.250476
9	N	0.175508
10	N	-0.460750
11	N	0.207898
12	N	0.168658
13	O	-0.208019
14	O	-0.198304
15	O	-0.187484
16	O	-0.221248
17	O	-0.207781
18	O	-0.198601
19	H	0.141595
20	H	0.095855
21	H	0.118446
22	H	0.098428
23	H	0.092596
24	H	0.098893
25	H	0.264199
26	H	0.234191

Dipole moment (Debye):

X= 0.7115 Y= 2.0184 Z= 0.6089 Tot= 2.2250

Bond Order:		V-mid:	
C2-N9:	1.27	C2-N9:	0.172
C4-N11:	1.03	C4-N11:	0.176
C6-N12:	1.21	C6-N12:	0.165
N9-O13:	2.04		
N9-O14:	2.03		
N11-O15:	2.15		
N11-O16:	1.97		
N12-O17:	1.87		
N12-O18:	1.99		

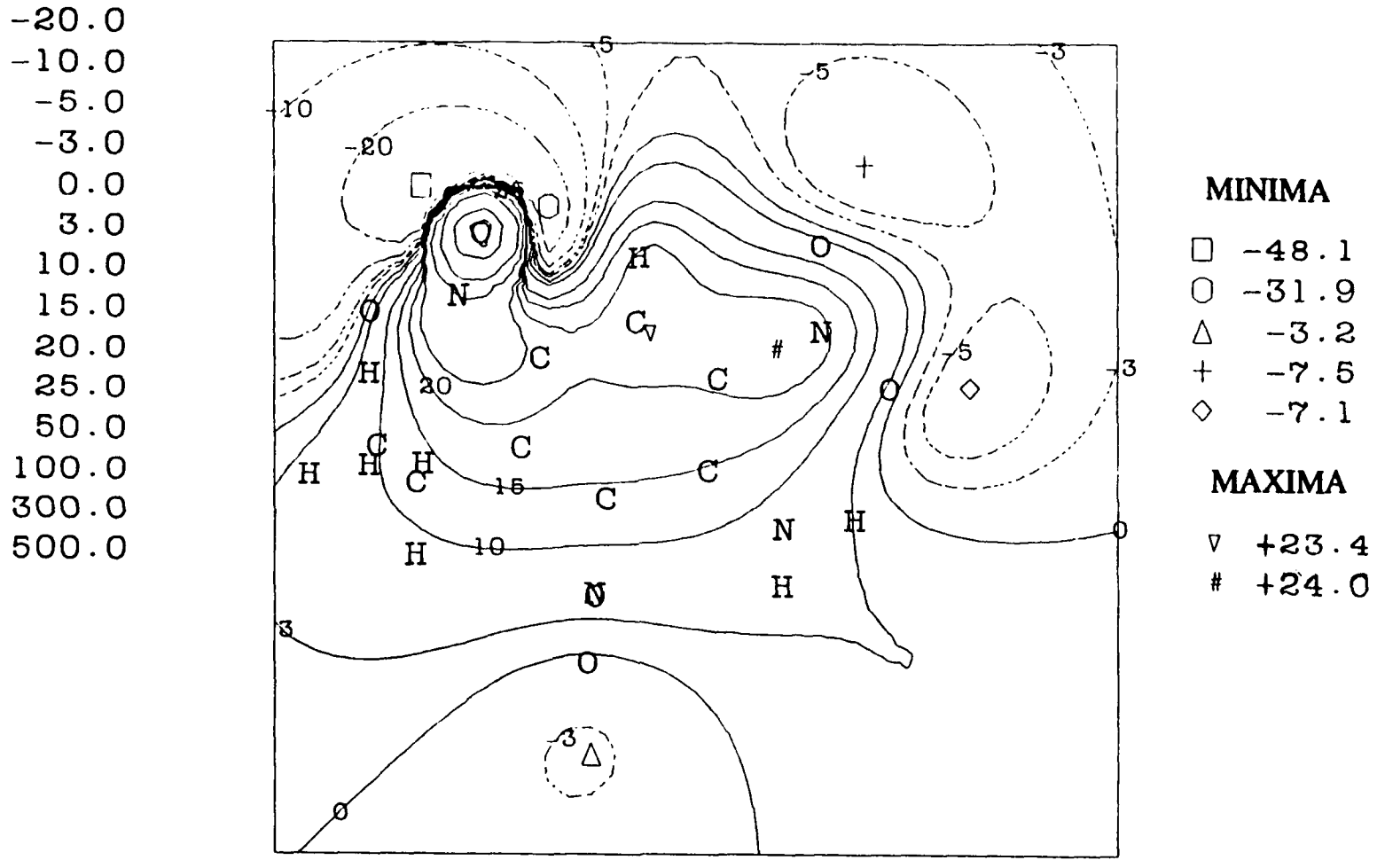


Figure CC-1. Calculated electrostatic potential, in kcal/mole, of 3-amino-2,4,6-trinitroethylbenzene, in the plane 1.75Å above the N11 nitro group located in the upper right corner. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

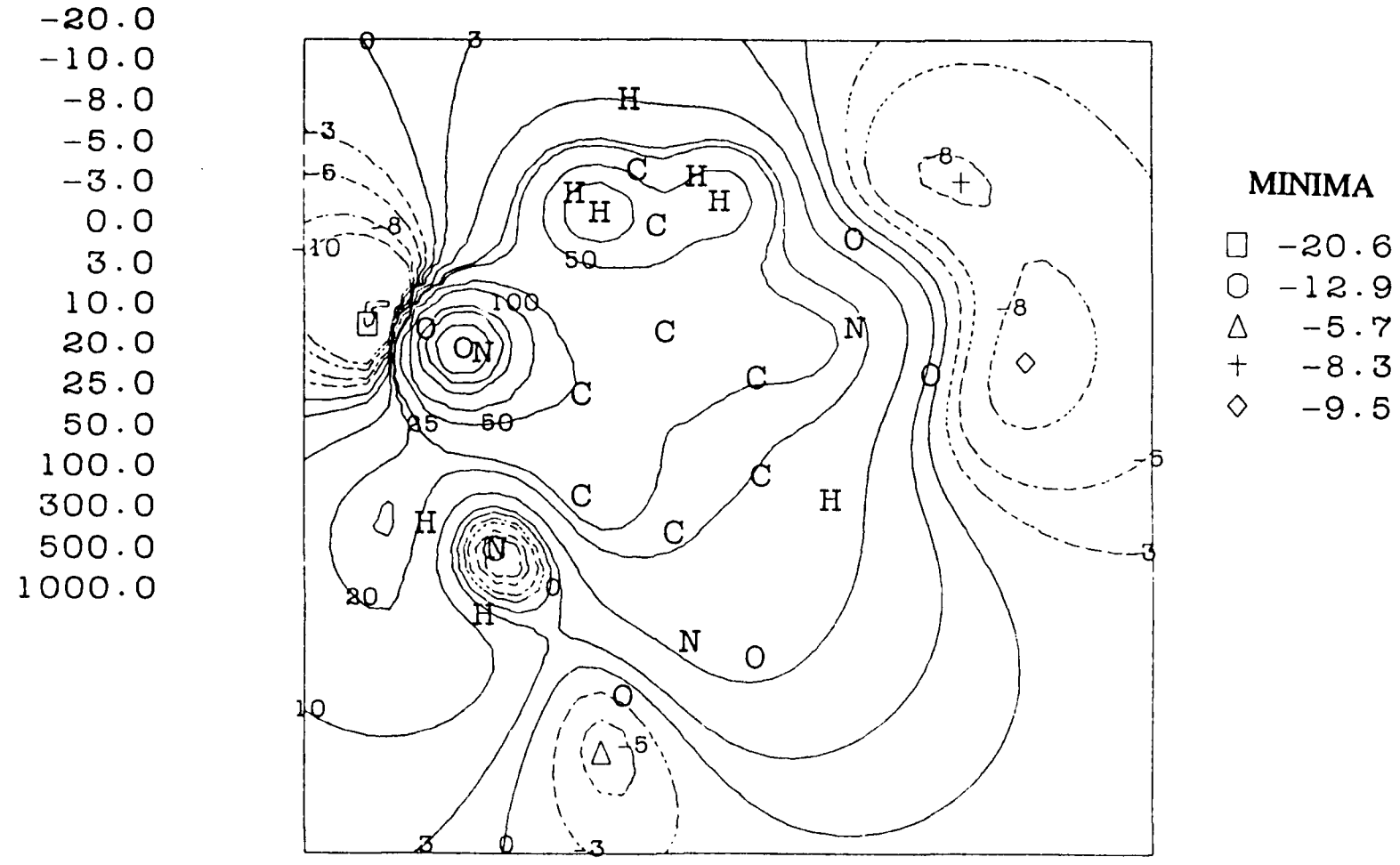
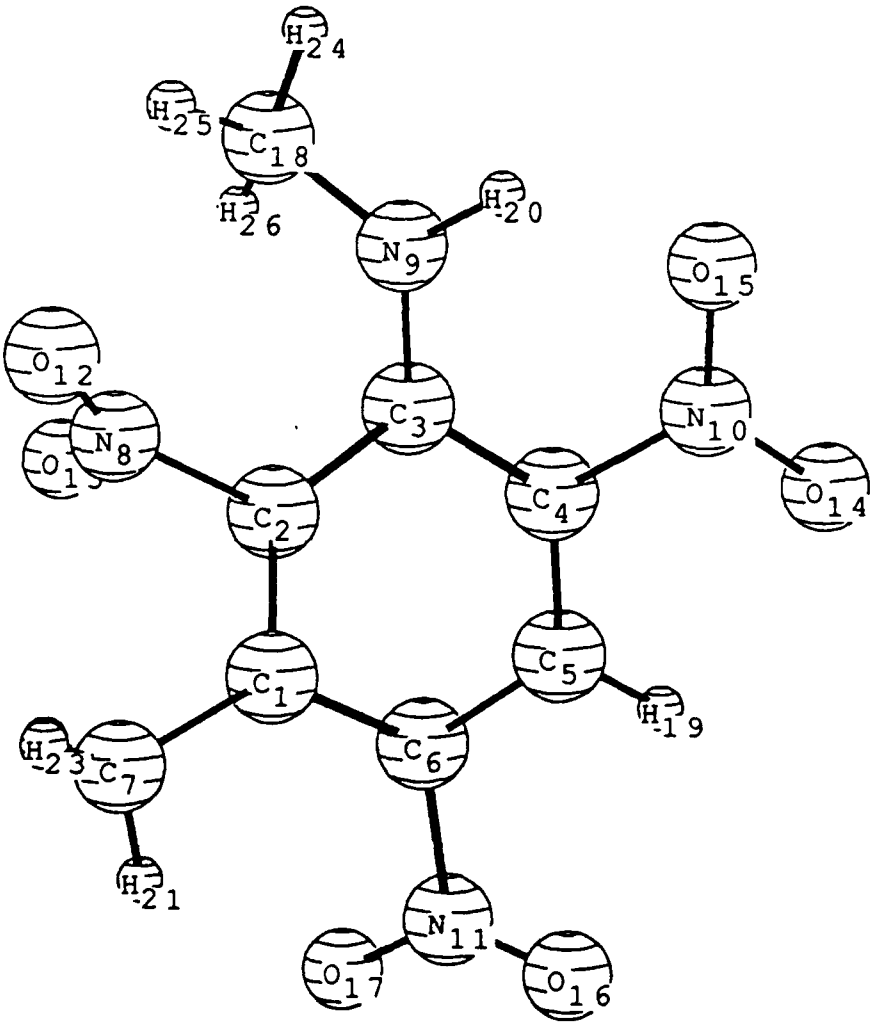


Figure CC-2. Calculated electrostatic potential, in kcal/mole, of 3-amino-2,4,6-trinitroethylbenzene, in the plane 1.75Å above the N12 nitro group located in the upper right corner. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

APPENDIX DD
3-(METHYLAMINO)-2,4,6-TRINITROTOLUENE

The short distances between non-bonded hydrogens and oxygens are H20-O15 (1.86 Å), H19-O14 (2.30 Å), H21-O17 (2.12 Å), H19-O16 (2.39 Å) and H25-O12 (2.26 Å).

The N10 nitro group is rotated by only a few degrees, while the N8 and N11 nitro groups are rotated by about 70° and 28°, respectively.



Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.387000(1)					
3	3	C	2	1.423402(2)	1	127.514(26)			
4	4	C	3	1.414310(3)	2	112.226(27)	1	2.928(50)	0
5	5	C	4	1.361095(4)	3	123.213(28)	2	-0.621(51)	0
6	6	C	5	1.369364(5)	4	119.928(29)	3	1.216(52)	0
7	7	C	1	1.504085(6)	2	120.357(30)	3	170.734(53)	0
8	8	N	2	1.499699(7)	3	117.269(31)	4	172.945(54)	0
9	9	N	3	1.349787(8)	4	122.693(32)	5	-178.451(55)	0
10	10	N	4	1.457821(9)	3	121.264(33)	2	-178.502(56)	0
11	11	N	6	1.488813(10)	1	122.291(34)	2	-177.188(57)	0
12	12	O	8	1.220013(11)	2	119.017(35)	3	-70.735(58)	0
13	13	O	8	1.226737(12)	2	115.633(36)	3	110.924(59)	0
14	14	O	10	1.197185(13)	4	118.962(37)	3	-174.738(60)	0
15	15	O	10	1.216527(14)	4	120.361(38)	3	3.579(61)	0
16	16	O	11	1.194307(15)	6	118.935(39)	1	-150.067(62)	0
17	17	O	11	1.235850(16)	6	116.752(40)	1	27.060(63)	0
18	18	C	9	1.457548(17)	3	130.576(41)	4	167.728(64)	0
19	19	H	5	0.960345(18)	4	120.147(42)	3	-178.965(65)	0
20	20	H	9	0.960046(19)	3	114.694(43)	2	170.062(66)	0
21	21	H	7	0.959826(20)	1	109.497(44)	2	-179.929(67)	0
22	22	H	7	0.959953(21)	1	109.504(45)	2	59.960(68)	0
23	23	H	7	0.959828(22)	1	109.307(46)	2	-59.986(69)	0
24	24	H	18	0.960065(23)	9	109.439(47)	3	179.924(70)	0
25	25	H	18	0.960356(24)	9	109.528(48)	3	59.925(71)	0
26	26	H	18	0.959395(25)	9	109.456(49)	3	-60.081(72)	0

STOICHIOMETRY C8H8N4O6

SCF DONE: E(RHF) = -970.075763639

Alpha eigenvalues — -0.29218 0.13740 0.15765 0.19042 0.22757

Estimated ionization potential: 7.95 ev

Total atomic charges:

		1
1	C	0.085271
2	C	0.053151
3	C	0.188005
4	C	0.054806
5	C	-0.054473
6	C	0.063076
7	C	-0.322866
8	N	0.163997
9	N	-0.368273
10	N	0.182207
11	N	0.176478
12	O	-0.199149
13	O	-0.195273
14	O	-0.188983
15	O	-0.232787
16	O	-0.193338
17	O	-0.214760
18	C	-0.198122
19	H	0.147237
20	H	0.271281
21	H	0.143786
22	H	0.133790
23	H	0.124860
24	H	0.127866
25	H	0.130127
26	H	0.122087

Dipole moment (Debye):

X= -2.7288 Y= -0.7028 Z= -0.0840 Tot= 2.8191

Bond Order		V-mid	
C2–N8:	1.17	C2–N8:	0.153
C4–N10:	1.27	C4–N10:	0.172
C6–N11:	1.19	C6–N11:	0.170
N8–O12:	1.94		
N8–O13:	1.89		
N10–O14:	2.05		
N10–O15:	1.96		
N11–O16:	2.07		
N11–O17:	1.86		

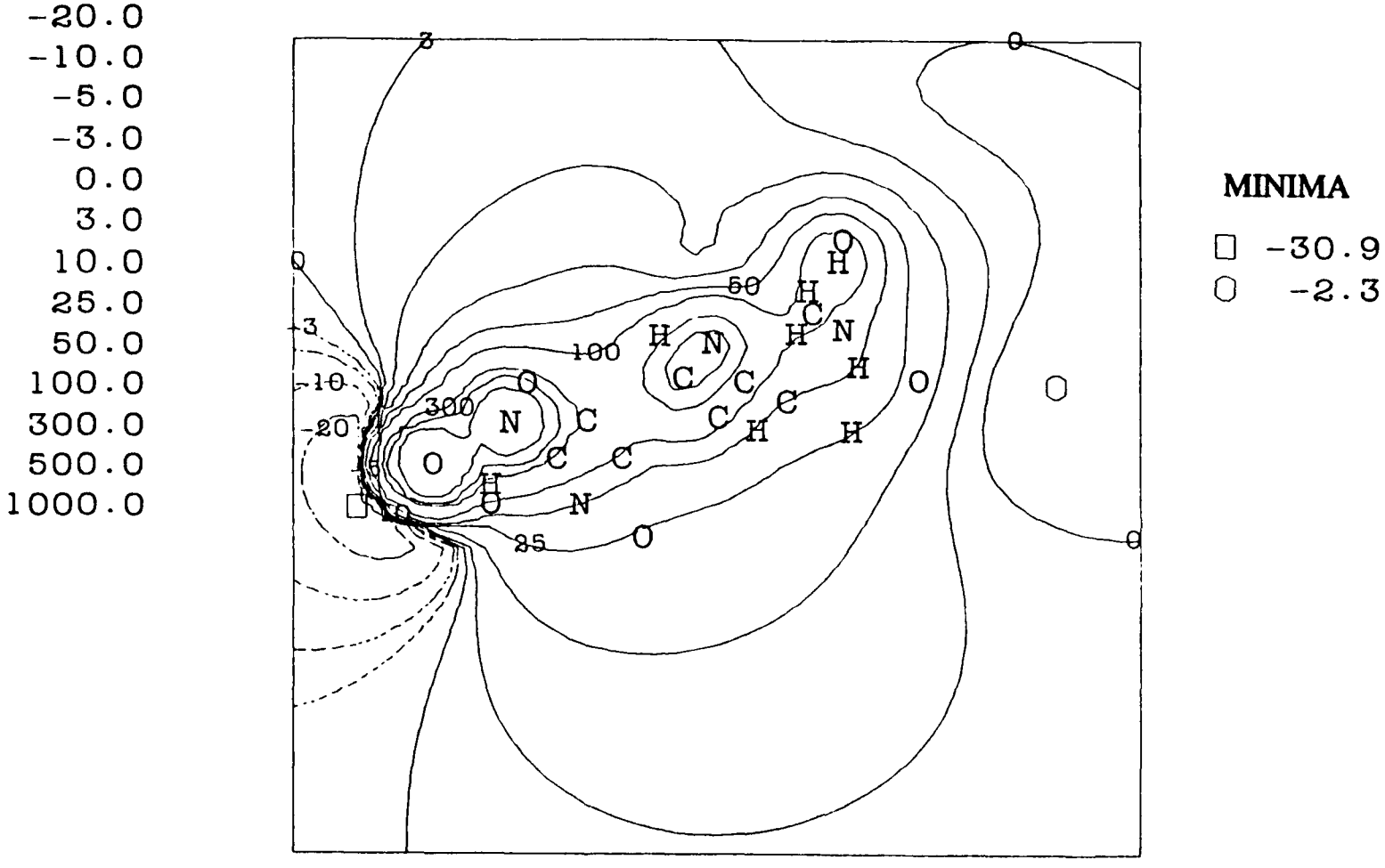


Figure DD-1. Calculated electrostatic potential, in kcal/mole, of 3-(methylamino)-2,4,6-trinitrotoluene, in the plane 1.75Å above the N8 nitro group located in the upper right corner. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

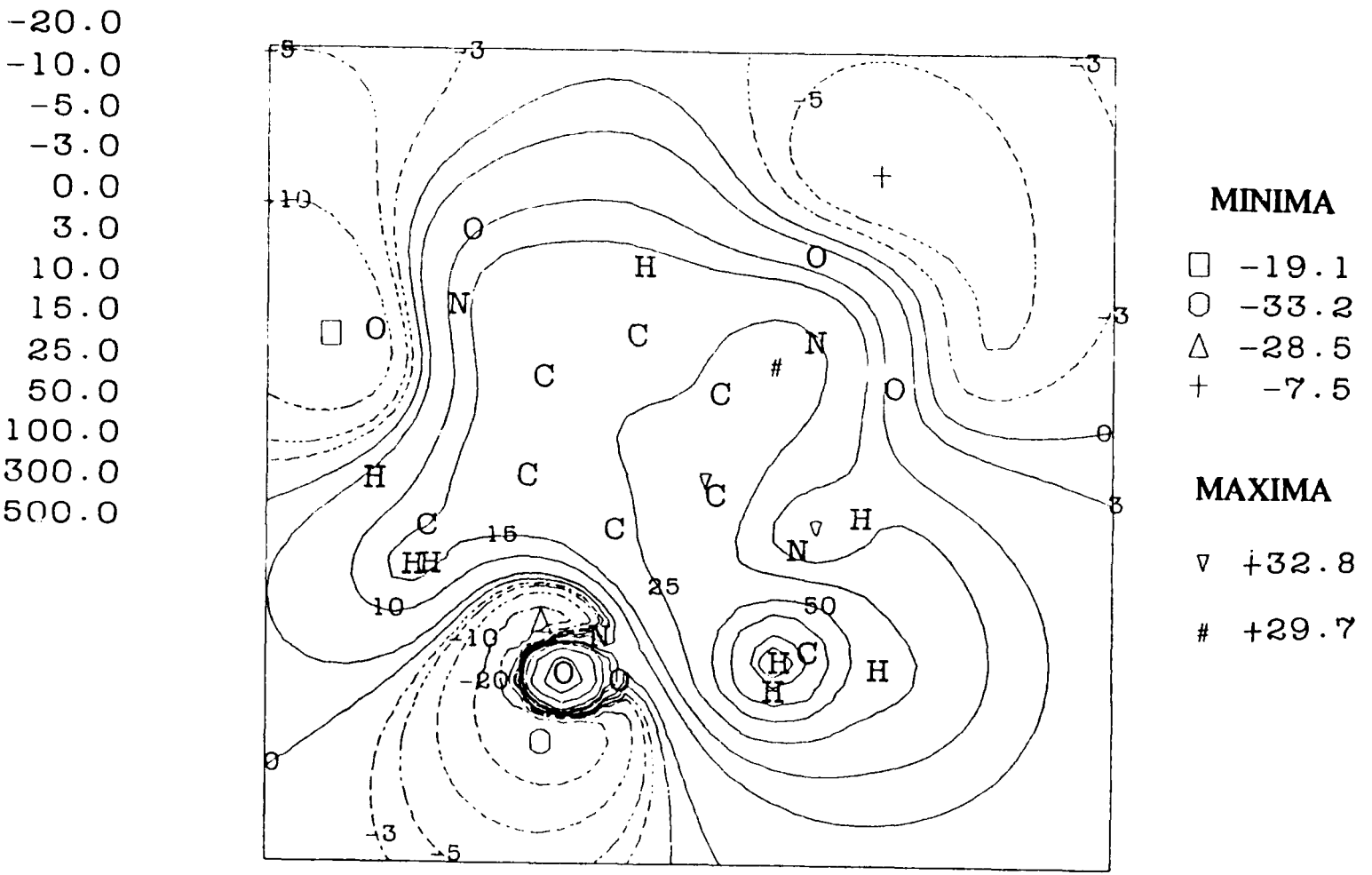
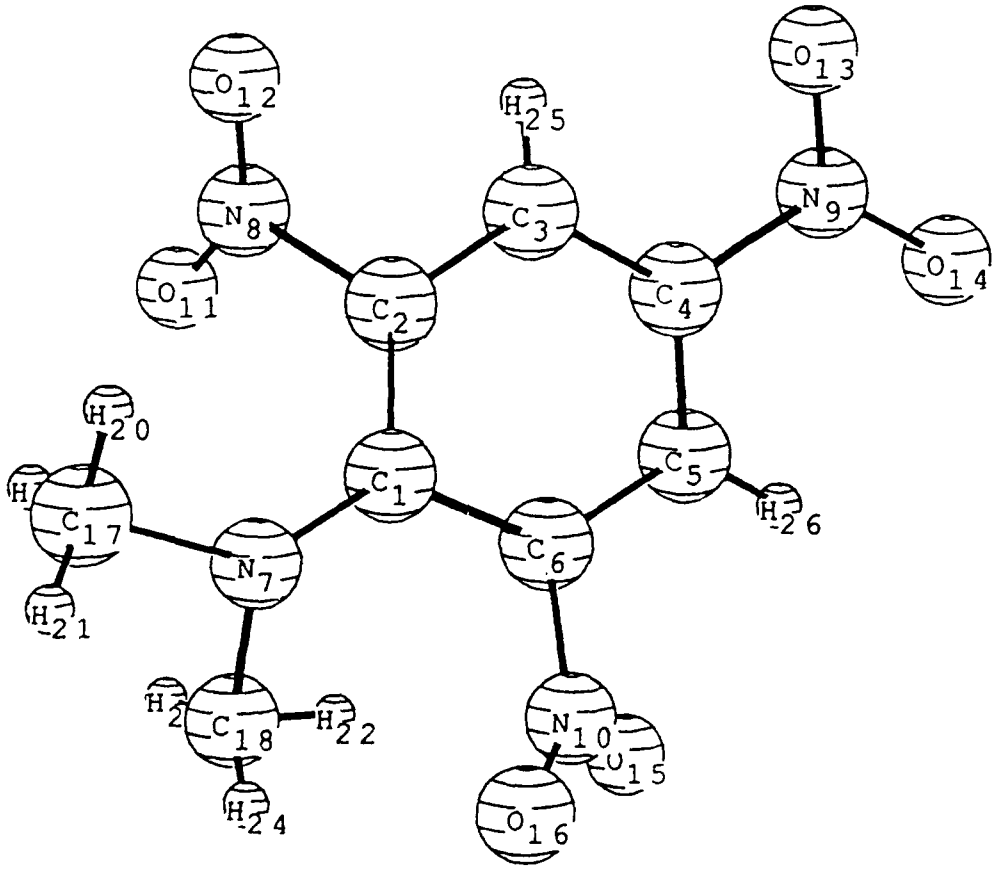


Figure DD-2. Calculated electrostatic potential, in kcal/mole, of 3-(methylamino)-2,4,6-trinitrotoluene, in the plane 1.75Å above the N10 nitro group located in the upper right corner. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

APPENDIX EE
N,N-DIMETHYLPICRAMIDE

The short distances between non-bonded hydrogens and oxygens are H19-O11 (2.45 Å), H25-O12 (2.44 Å), H25-O13 (2.47 Å) and H26-O14 (2.46 Å).

The N8 and N10 nitro groups are rotated out of the mean plane of the benzene ring by about 40° and 60°, respectively an the N9 nitro group is only rotated by about 12°.



Z-MATRIX (ANGSTROMS AND DEGREES)

CD	CENT	ATOM	N1	LENGTH	N2	ALPHA	N3	BETA	J
1	1	C							
2	2	C	1	1.423000 (1)					
3	3	C	2	1.374045 (2)	1	123.619 (26)			
4	4	C	3	1.370644 (3)	2	119.225 (27)	1	5.404 (50)	0
5	5	C	4	1.376151 (4)	3	120.869 (28)	2	-0.276 (51)	0
6	6	C	5	1.372077 (5)	4	118.960 (29)	3	-3.120 (52)	0
7	7	N	1	1.349478 (6)	2	123.521 (30)	3	173.695 (53)	0
8	8	N	2	1.464762 (7)	3	114.848 (31)	4	-167.543 (54)	0
9	9	N	4	1.463054 (8)	3	119.319 (32)	2	-179.969 (55)	0
10	10	N	6	1.472506 (9)	5	114.518 (33)	4	-170.478 (56)	0
11	11	O	8	1.221450 (10)	2	117.933 (34)	3	137.037 (57)	0
12	12	O	8	1.223656 (11)	2	117.859 (35)	3	-38.607 (58)	0
13	13	O	9	1.218935 (12)	4	118.151 (36)	3	12.204 (59)	0
14	14	O	9	1.216440 (13)	4	117.945 (37)	3	-167.562 (60)	0
15	15	O	10	1.217251 (14)	6	117.309 (38)	5	-61.719 (61)	0
16	16	O	10	1.218075 (15)	6	117.586 (39)	5	116.650 (62)	0
17	17	C	7	1.455934 (16)	1	122.585 (40)	2	-34.804 (63)	0
18	18	C	7	1.461052 (17)	1	123.541 (41)	2	146.862 (64)	0
19	19	H	17	0.958692 (18)	7	110.528 (42)	1	111.392 (65)	0
20	20	H	17	0.990708 (19)	7	112.964 (43)	1	-8.518 (66)	0
21	21	H	17	0.959269 (20)	7	108.882 (44)	1	-128.428 (67)	0
22	22	H	18	1.030678 (21)	7	111.441 (45)	1	-15.326 (68)	0
23	23	H	18	0.946545 (22)	7	108.101 (46)	1	-134.306 (69)	0
24	24	H	18	0.945969 (23)	7	110.604 (47)	1	102.403 (70)	0
25	25	H	3	0.919951 (24)	2	119.186 (48)	1	179.212 (71)	0
26	26	H	5	0.901762 (25)	4	120.486 (49)	3	179.569 (72)	0

STOICHIOMETRY C8H8N4O6

SCF DONE: E(RHF) = -970.023626858

EIGENVALUES — -0.29462 0.13090 0.14078 0.18718 0.22142

Estimated ionization potential: 8.03 ev

TOTAL ATOMIC CHARGES.

		1	Net Charge
1	C	5.816149	0.184
2	C	5.923220	0.077
3	C	6.066100	-0.066
4	C	5.905775	0.094
5	C	6.071256	-0.071
6	C	5.919412	0.081
7	N	7.257770	-0.258
8	N	6.834545	0.165
9	N	6.827066	0.173
10	N	6.830101	0.170
11	O	8.197192	-0.197
12	O	8.194999	-0.195
13	O	8.198365	-0.199
14	O	8.198555	-0.199
15	O	8.192531	-0.193
16	O	8.195733	-0.196
17	C	6.187701	-0.188
18	C	6.185064	-0.185
19	H	0.874728	0.125
20	H	0.887417	0.113
21	H	0.880816	0.119
22	H	0.889906	0.110
23	H	0.877204	0.123
24	H	0.875449	0.125
25	H	0.854898	0.145
26	H	0.858047	0.142

DIPOLE MOMENT (DEBYE): X=-2.9260 Y=-0.4301 Z=-2.0966 TOTAL= 3.6252

Bond Order:		V-mid:	
C2-N8:	1.25	C2-N8:	0.175
C4-N9:	1.26	C4-N9:	0.193
C6-N10:	1.23	C6-N10:	0.180
N8-O11:	1.93		
N8-O12:	1.92		
N9-O13:	1.94		
N9-O14:	1.96		
N10-O15:	1.95		
N10-O16:	1.95		

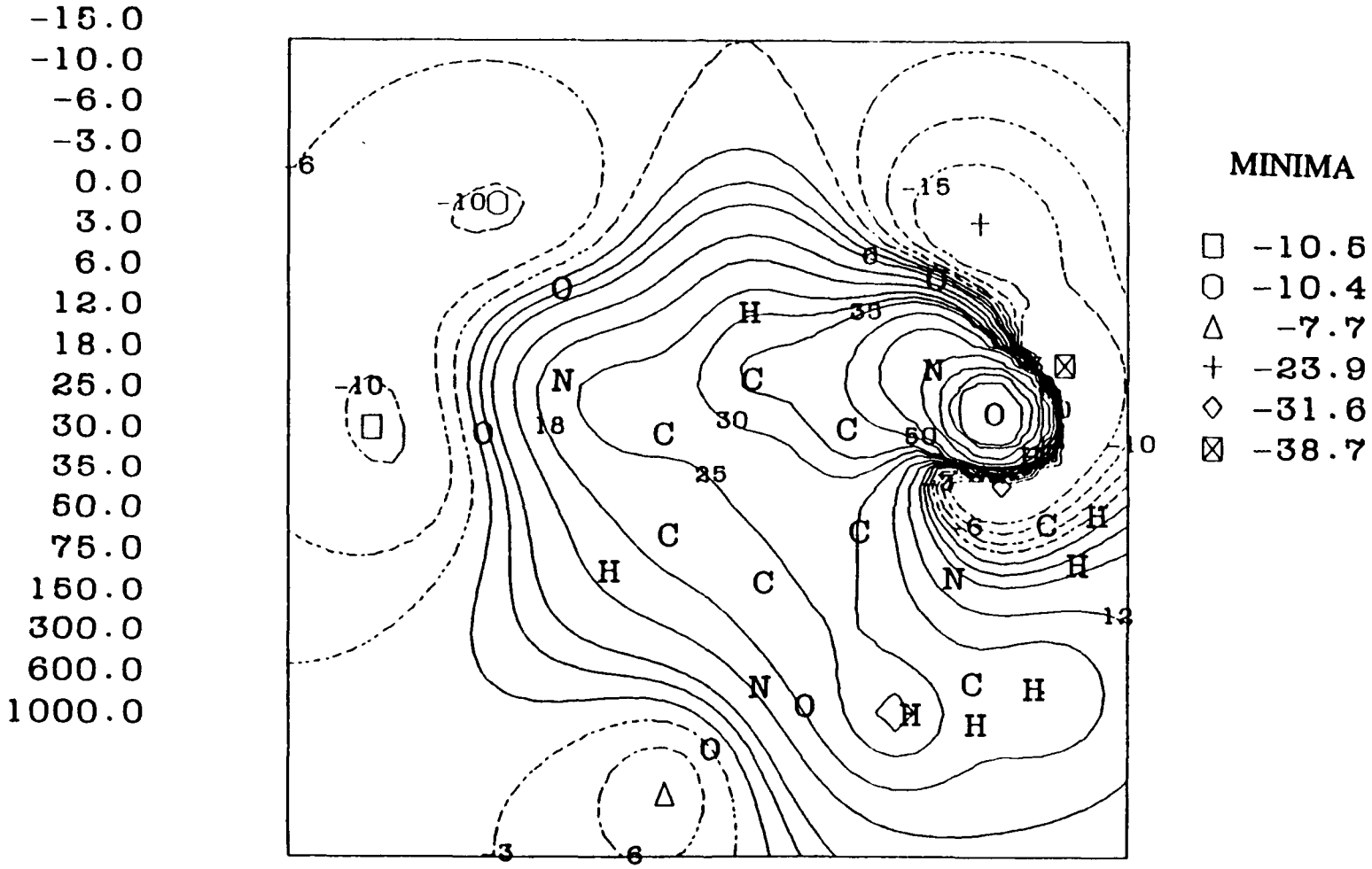


Figure EE-1. Calculated electrostatic potential, in kcal/mole, of N,N-dimethylpicramide, in the plane 1.75Å above the N9 nitro group located in the upper left corner. Projected positions of nuclei are shown. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

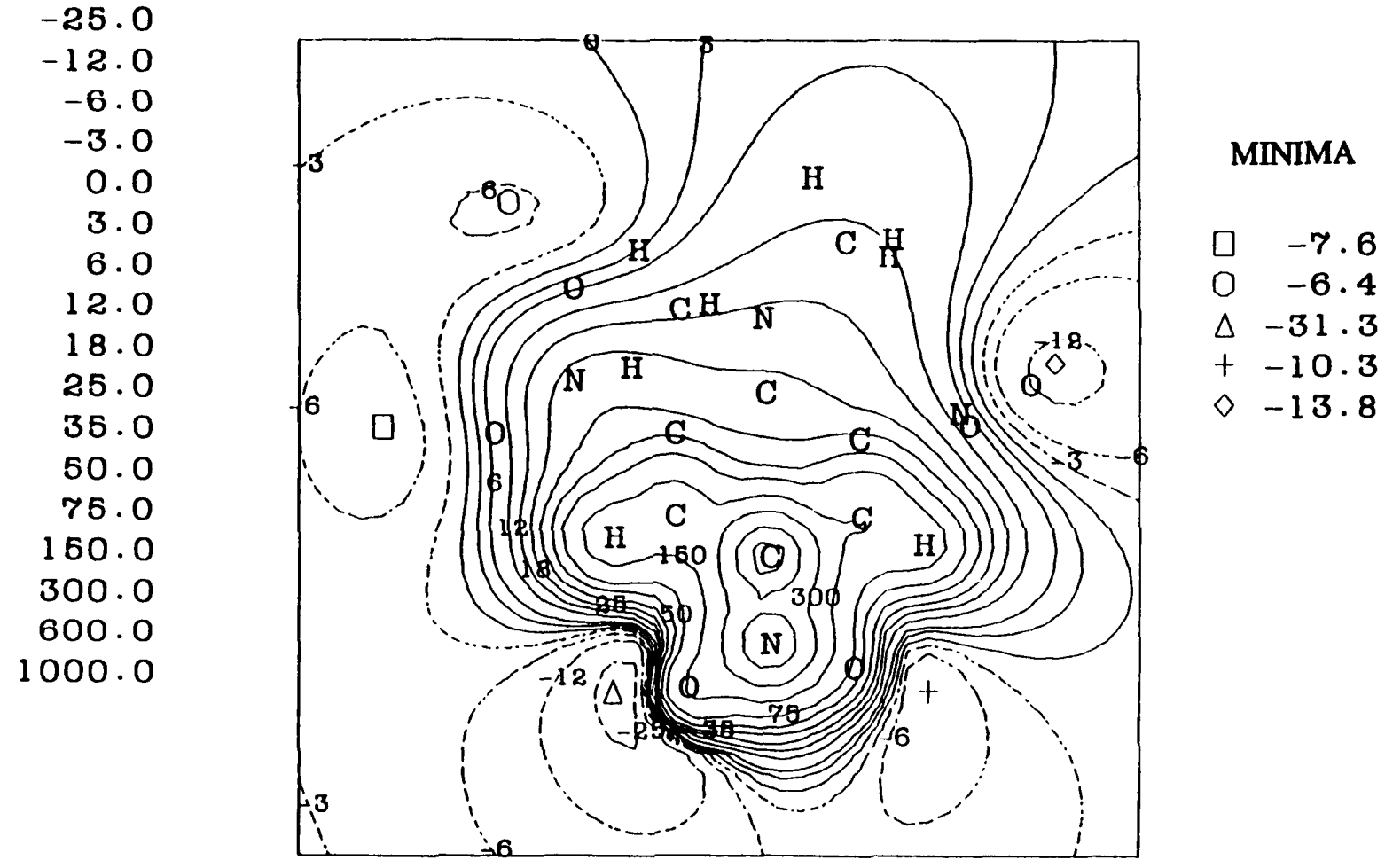
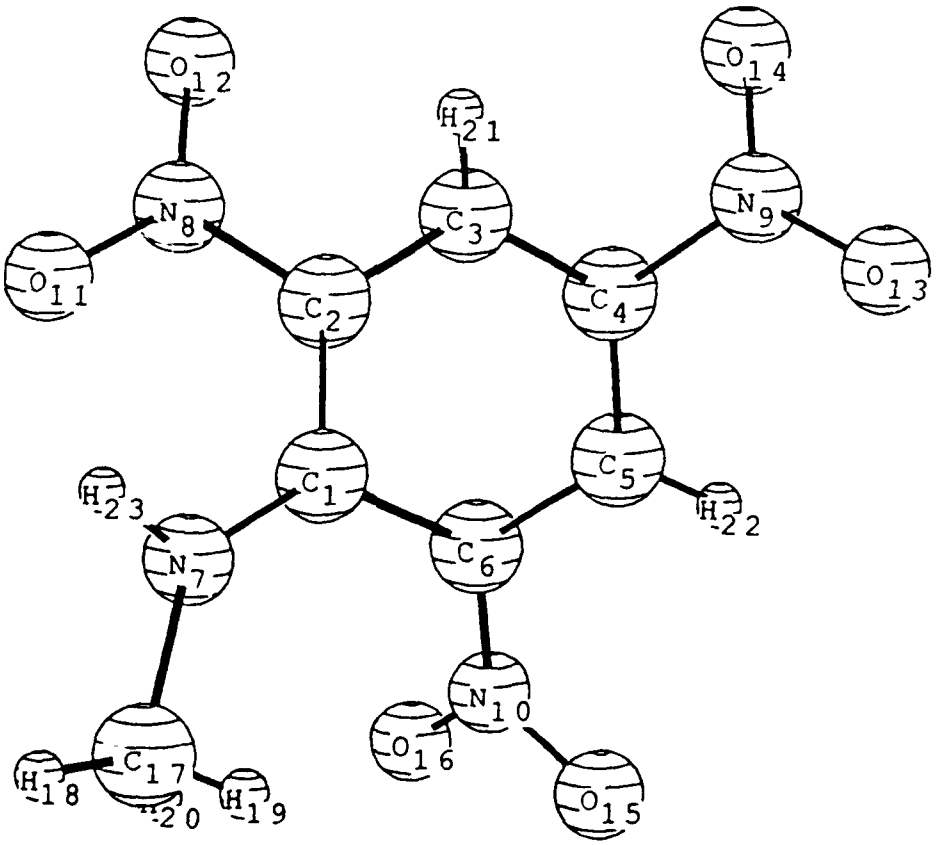


Figure EE-2. Calculated electrostatic potential, in kcal/mole, of N,N-dimethylpicramide, in the plane 1.75Å above the N8 nitro group located in the upper left corner. Projected positions of nuclei are shown. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

APPENDIX FF
N-METHYLPICRAMIDE

The short distances between non-bonded hydrogens and oxygens are H21-O12 (2.31 Å), H23-O11 (1.84 Å), H22-O13 (2.40 Å), H21-O14 (2.44 Å) and H20-O16 (2.38 Å).

The N10 nitro group is rotated out of the mean plane of the benzene ring by approximately 50°, while the N8 and N9 nitro groups are only rotated by about 6° and 9°, respectively.



Z-MATRIX (ANGSTROMS AND DEGREES)

CD	CENT	ATOM	N1	LENGTH	N2	ALPHA	N3	BETA	J
1	1	C							
2	2	C	1	1.436000 (1)					
3	3	C	2	1.365763 (2)	1	122.514 (23)			
4	4	C	3	1.370295 (3)	2	120.392 (24)	1	0.531 (44)	0
5	5	C	4	1.373754 (4)	3	120.663 (25)	2	5.753 (45)	0
6	6	C	5	1.377130 (5)	4	118.833 (26)	3	-3.536 (46)	0
7	7	N	1	1.333529 (6)	2	122.351 (27)	3	168.686 (47)	0
8	8	N	2	1.454798 (7)	3	115.942 (28)	4	-179.970 (48)	0
9	9	N	4	1.456627 (8)	5	120.414 (29)	6	179.874 (49)	0
10	10	N	6	1.458624 (9)	5	114.713 (30)	4	169.974 (50)	0
11	11	O	8	1.230412 (10)	2	119.737 (31)	1	5.834 (51)	0
12	12	O	8	1.216932 (11)	2	118.158 (32)	1	-173.058 (52)	0
13	13	O	9	1.228128 (12)	4	117.256 (33)	5	-9.410 (53)	0
14	14	O	9	1.215386 (13)	4	118.915 (34)	5	171.468 (54)	0
15	15	O	10	1.229009 (14)	6	118.424 (35)	5	47.843 (55)	0
16	16	O	10	1.228699 (15)	6	117.185 (36)	5	-130.096 (56)	0
17	17	C	7	1.460684 (16)	1	128.292 (37)	2	-166.565 (57)	0
18	18	H	17	0.921158 (17)	7	109.960 (38)	1	156.284 (58)	0
19	19	H	17	0.999417 (18)	7	109.668 (39)	1	36.580 (59)	0
20	20	H	17	1.000129 (19)	7	112.597 (40)	1	-89.764 (60)	0
21	21	H	3	0.860628 (20)	4	120.806 (41)	5	-177.546 (61)	0
22	22	H	5	0.942765 (21)	6	124.091 (42)	1	178.406 (62)	0
23	23	H	7	0.925832 (22)	1	110.218 (43)	2	0.512 (63)	0

STOICHIOMETRY C7H6N4O6

SCF DONE: E(RHF) = -931.127125257

EIGENVALUES -- -0.30129 -0.29658 0.12069 0.13943 0.18019

Estimated ionization potential: 8.08 ev

TOTAL ATOMIC CHARGES.

		1	Net Charge
1	C	5.799379	0.211
2	C	5.933513	0.066
3	C	6.081523	-0.082
4	C	5.915315	0.085
5	C	6.049286	-0.049
6	C	5.934450	0.066
7	N	7.374809	-0.375
8	N	6.829976	0.170
9	N	6.830918	0.169
10	N	6.839770	0.160
11	O	8.225055	-0.225
12	O	8.175589	-0.176
13	O	8.203996	-0.204
14	O	8.195592	-0.196
15	O	8.192980	-0.193
16	O	8.197565	-0.198
17	C	6.180449	-0.180
18	H	0.868422	0.132
19	H	0.884976	0.115
20	H	0.868150	0.132
21	H	0.845906	0.154
22	H	0.855156	0.145
23	H	0.717221	0.283

DIPOLE MOMENT (DEBYE): X=-2.7735 Y=-1.2510 Z=-2.1210 TOTAL= 3.7089

Bond Order:		V-mid:	
C2-N8:	1.28	C2-N8:	0.172
C4-N9:	1.27	C4-N9:	0.185
C6-N10:	1.27	C6-N10:	0.164
N8-O11:	1.89		
N8-O12:	1.95		
N9-O13:	1.90		
N9-O14:	1.96		
N10-O15:	1.89		
N10-O16:	1.89		

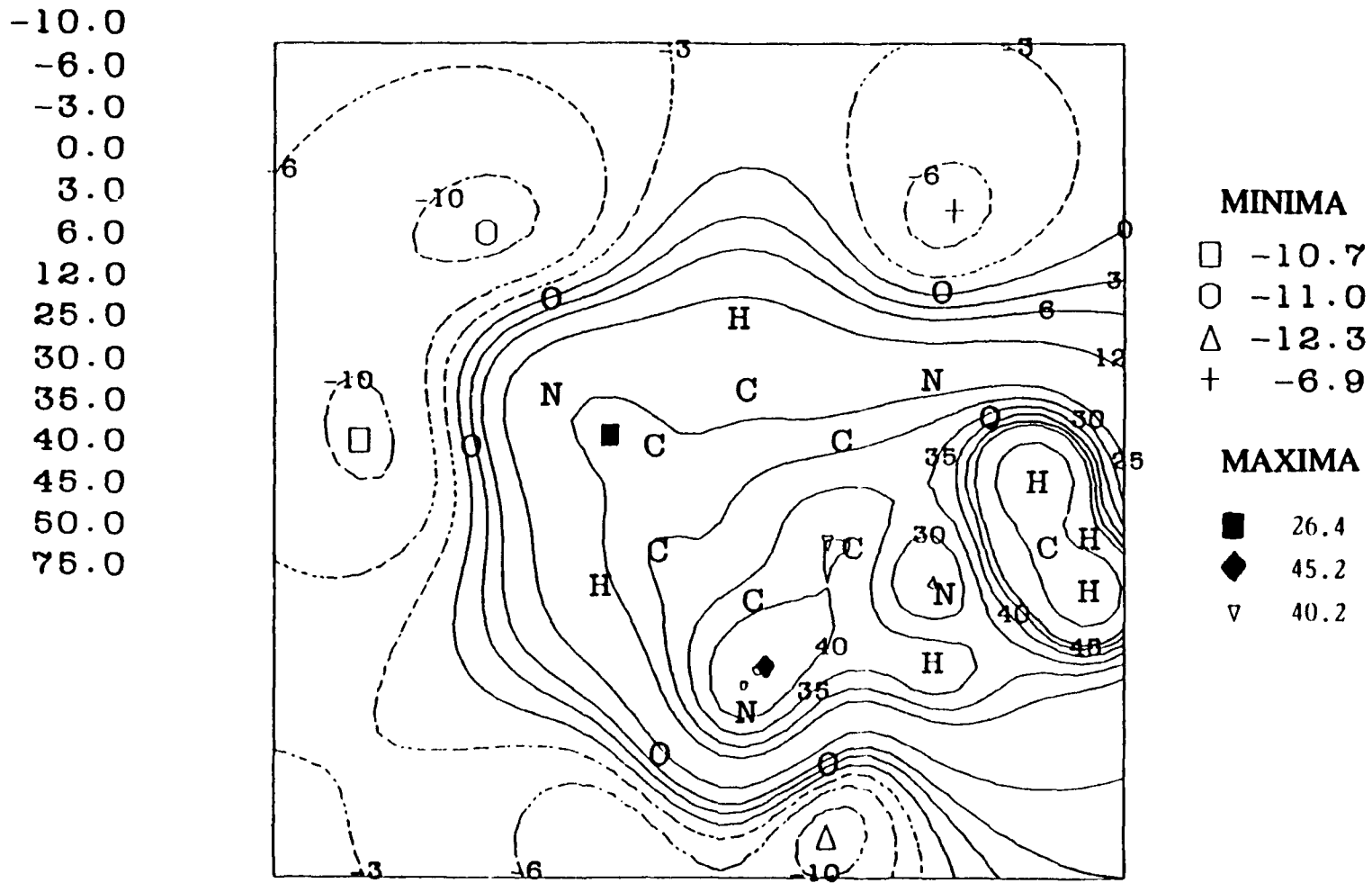


Figure FF-1. Calculated electrostatic potential, in kcal/mole, of N-methylpicramide, in the plane 1.75Å above the N9 nitro group located in the upper left corner. Projected positions of nuclei are shown. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

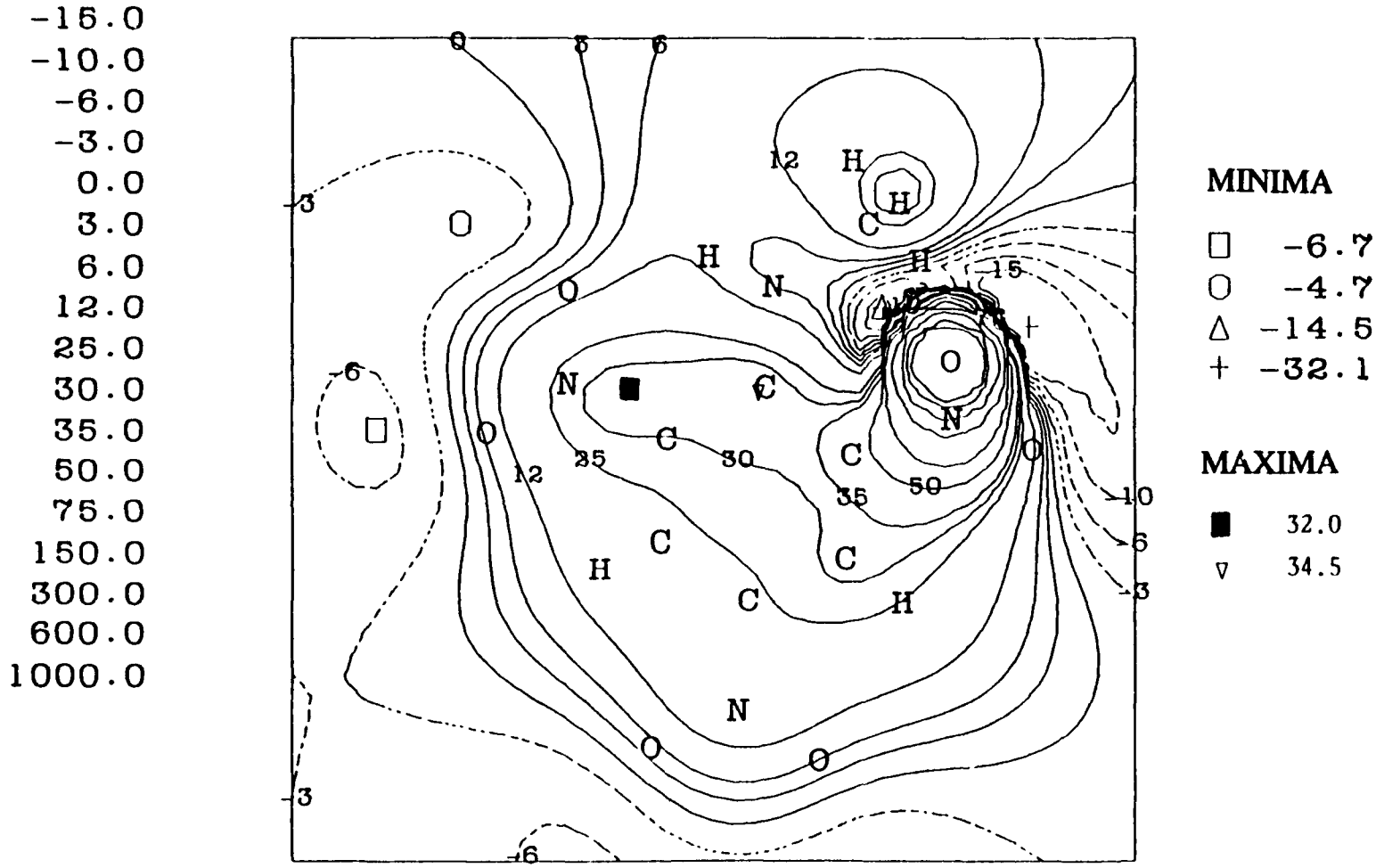
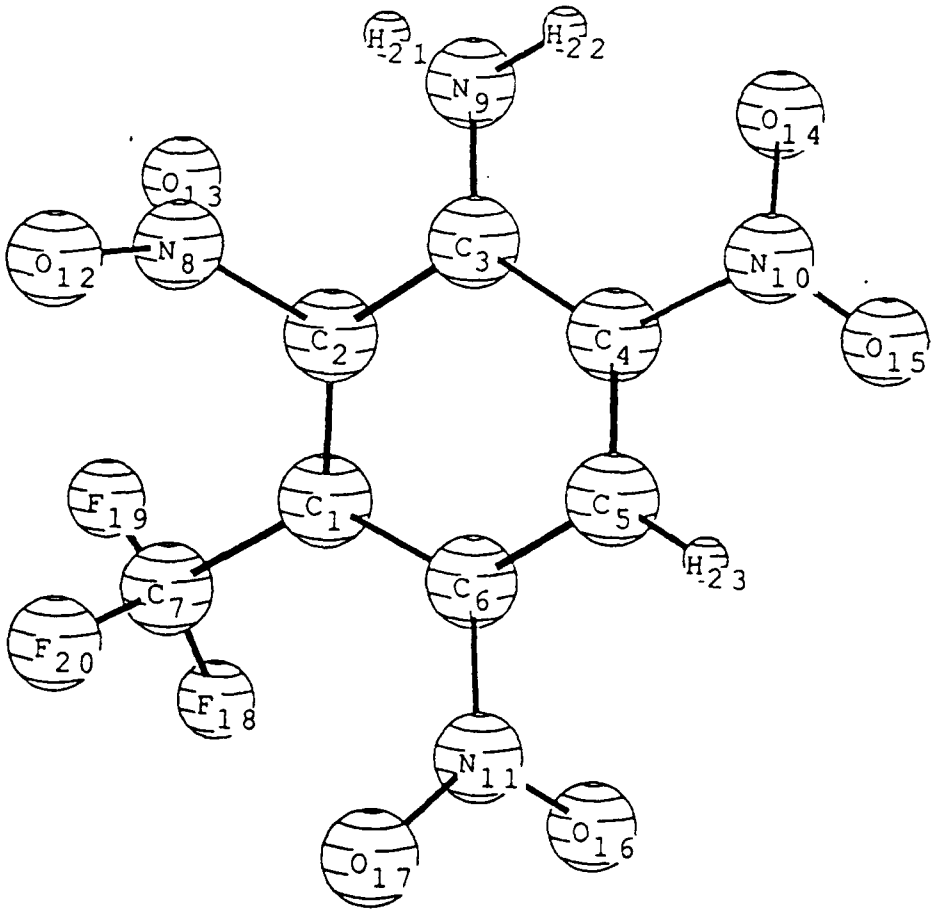


Figure FF-2. Calculated electrostatic potential, in kcal/mole, of N-methylpicramide, in the plane 1.75Å above the N8 nitro group located in the upper left corner. Projected positions of nuclei are shown. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

APPENDIX GG
3-TRIFLUOROMETHYL-2,4,6-TRINITROANILINE

The short distances between non-bonded hydrogens and oxygens are H21-O13 (2.21 Å), H22-O14 (1.94 Å), H23-O15 (2.36 Å) and H23-O16 (2.45 Å).

The N10 nitro group is rotated by only about 6°, while the N8 and N11 nitro groups are rotated by approximately 55° and 37°, respectively.



Z-MATRIX (ANGSTROMS AND DEGREES)

CD	CENT	ATOM	N1	LENGTH	N2	ALPHA	N3	BETA	J
1	1	C							
2	2	C	1	1.377000 (1)					
3	3	C	2	1.423341 (2)	1	124.869 (23)			
4	4	C	3	1.414991 (3)	2	113.914 (24)	1	-3.607 (44)	0
5	5	C	4	1.368284 (4)	3	122.473 (25)	2	2.014 (45)	0
6	6	C	5	1.370912 (5)	4	120.672 (26)	3	-0.585 (46)	0
7	7	C	1	1.526463 (6)	2	120.289 (27)	3	-167.190 (47)	0
8	8	N	2	1.475356 (7)	3	116.159 (28)	4	172.719 (48)	0
9	9	N	3	1.328759 (8)	4	124.273 (29)	5	-178.928 (49)	0
10	10	N	4	1.459222 (9)	5	116.478 (30)	6	178.033 (50)	0
11	11	N	6	1.464138 (10)	5	117.502 (31)	4	-176.072 (51)	0
12	12	O	8	1.219998 (11)	2	116.274 (32)	3	-123.853 (52)	0
13	13	O	8	1.224792 (12)	2	118.839 (33)	3	55.066 (53)	0
14	14	O	10	1.217181 (13)	4	119.193 (34)	5	173.113 (54)	0
15	15	O	10	1.210136 (14)	4	118.346 (35)	5	-6.139 (55)	0
16	16	O	11	1.226621 (15)	6	117.128 (36)	5	-35.466 (56)	0
17	17	O	11	1.220246 (16)	6	118.049 (37)	5	140.211 (57)	0
18	18	F	7	1.336189 (17)	1	111.715 (38)	2	142.156 (58)	0
19	19	F	7	1.335440 (18)	1	111.454 (39)	2	24.746 (59)	0
20	20	F	7	1.327102 (19)	1	112.764 (40)	2	-96.090 (60)	0
21	21	H	9	0.828794 (20)	3	121.524 (41)	4	173.273 (61)	0
22	22	H	9	0.916242 (21)	3	118.686 (42)	4	0.225 (62)	0
23	23	H	5	0.930860 (22)	4	121.966 (43)	3	179.783 (63)	0

STOICHIOMETRY C7H3F3N4O6

SCF DONE: E(RHF) = -1226.15046963

EIGENVALUES — -0.32830 -0.32454 -0.32219 -0.31111 0.10521

Estimated ionization potential: 8.47 ev

TOTAL ATOMIC CHARGES.

		1	Net Charge
1	C	5.984284	0.016
2	C	5.929704	0.070
3	C	5.784771	0.215
4	C	5.931482	0.069
5	C	6.056998	-0.057
6	C	5.915220	0.085
7	C	5.508179	0.492
8	N	6.832628	0.167
9	N	7.547599	-0.548
10	N	6.820424	0.180
11	N	6.831440	0.169
12	O	8.177611	-0.178
13	O	8.199445	-0.199
14	O	8.220131	-0.220
15	O	8.182812	-0.183
16	O	8.190944	-0.191
17	O	8.187893	-0.188
18	F	9.152070	-0.152
19	F	9.156847	-0.157
20	F	9.140736	-0.141
21	H	0.700174	0.300
22	H	0.700424	0.300
23	H	0.848186	0.152

DIPOLE MOMENT (DEBYE): X= 0.6634 Y= 0.4913 Z= 2.8708 TOTAL= 2.9871

Bond Order:		V-mid:	
C2-N8:	1.23	C2-N8:	0.170
C4-N10:	1.27	C4-N10:	0.181
C6-N11:	1.25	C6-N11:	0.184
N8-O12:	1.94		
N8-O13:	1.91		
N10-O14:	1.95		
N10-O15:	1.99		
N11-O16:	1.91		
N11-O17:	1.94		

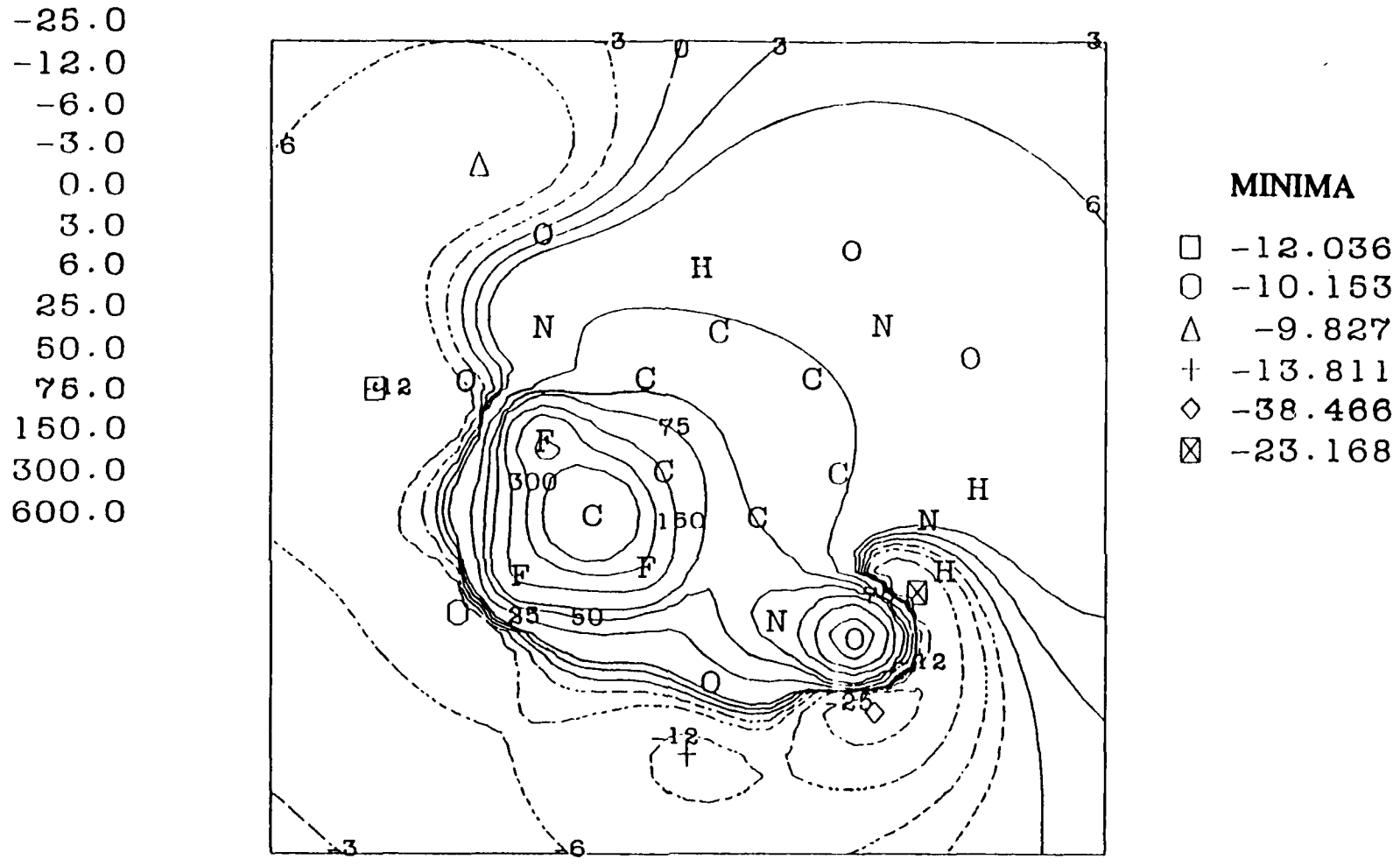


Figure GG-1. Calculated electrostatic potential, in kcal/mole, of 3-trifluoromethyl-2,4,5-trinitroaniline, in the plane 1.75Å above the N11 nitro group located in the upper left corner. Projected positions of nuclei are shown. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

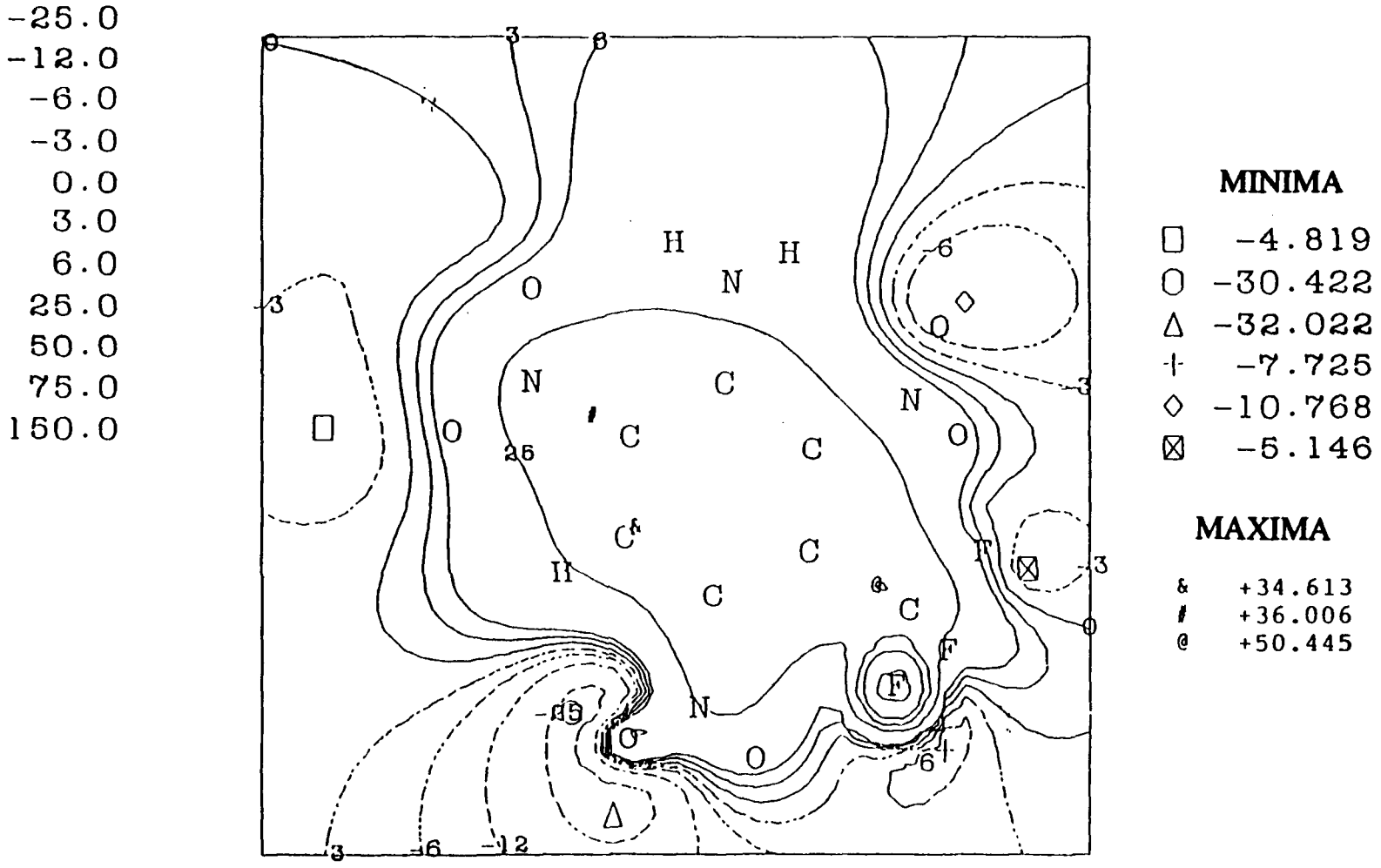
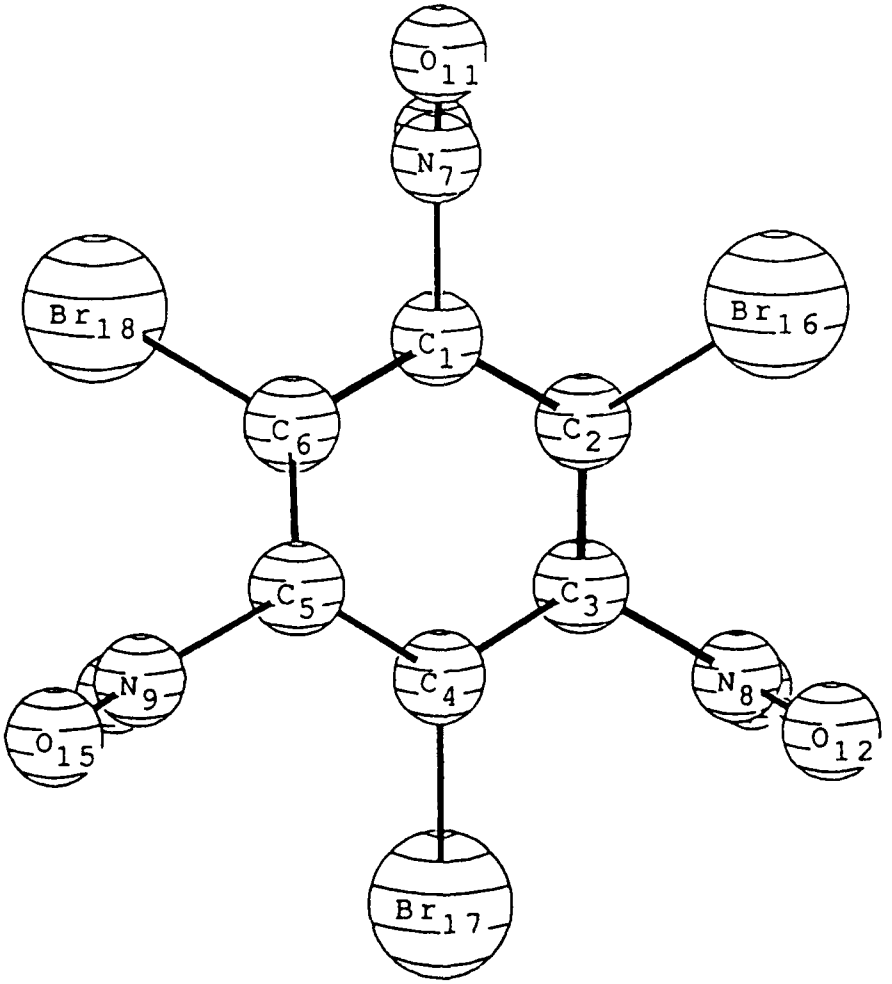


Figure GG-2. Calculated electrostatic potential, in kcal/mole, of 3-trifluoromethyl-2,4,5-trinitroaniline, in the plane 1.75Å above the N10 nitro group located in the upper left corner. Projected positions of nuclei are shown. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

APPENDIX HH
1,3,5-TRIBROMO-2,4,6-TRINITROBENZENE

All three nitro groups are essentially perpendicular to the mean plane of the benzene ring.



Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.393000(1)					
3	3	C	2	1.348241(2)	1	118.314(18)			
4	4	C	3	1.391096(3)	2	123.257(19)	1	-1.997(34)	0
5	5	C	4	1.391208(4)	3	116.077(20)	2	1.075(35)	0
6	6	C	5	1.348499(5)	4	123.244(21)	3	0.999(36)	0
7	7	N	1	1.478230(6)	2	119.616(22)	3	-179.033(37)	0
8	8	N	3	1.493504(7)	2	118.852(23)	1	177.130(38)	0
9	9	N	5	1.493336(8)	4	117.850(24)	3	-178.112(39)	0
10	10	O	7	1.217902(9)	1	115.518(25)	2	90.887(40)	0
11	11	O	7	1.218270(10)	1	115.515(26)	2	-89.181(41)	0
12	12	O	8	1.214312(11)	3	114.720(27)	2	90.325(42)	0
13	13	O	8	1.187091(12)	3	118.131(28)	2	-91.002(43)	0
14	14	O	9	1.214241(13)	5	114.710(29)	6	90.276(44)	0
15	15	O	9	1.187406(14)	5	118.122(30)	6	-90.997(45)	0
16	16	Br	2	1.872735(15)	3	121.701(31)	4	175.775(46)	0
17	17	Br	4	1.856453(16)	3	121.948(32)	2	-178.987(47)	0
18	18	Br	6	1.872691(17)	5	121.677(33)	4	175.825(48)	0

STOICHIOMETRY C6Br3N3O6

SCF DONE: E(RHF) = -8512.21818058

Alpha eigenvalues — -0.34212 -0.33284 -0.33243 -0.33020 0.12972

Estimated ionization potential: 8.99 ev

Total atomic charges:

		1
1	C	0.102297
2	C	-0.031984
3	C	0.092852
4	C	-0.027379
5	C	0.092918
6	C	-0.031978
7	N	0.175023
8	N	0.190006
9	N	0.189896
10	O	-0.173694
11	O	-0.173812
12	O	-0.186747
13	O	-0.176726
14	O	-0.186619
15	O	-0.176734
16	Br	0.103060
17	Br	0.116546
18	Br	0.103074

Dipole moment (Debye):

X= -0.0006 Y= 0.0299 Z= 0.0019 Tot= 0.0299

Bond Order:		V-mid:	
C1–N7:	1.22	C1–N7:	0.198
C3–N8:	1.18	C3–N8:	0.201
C5–N9:	1.18	C5–N9:	0.201
N7–O10:	1.95		
N7–O11:	1.95		
N8–O12:	1.97		
N8–O13:	2.10		
N9–O14:	1.97		
N9–O15:	2.10		

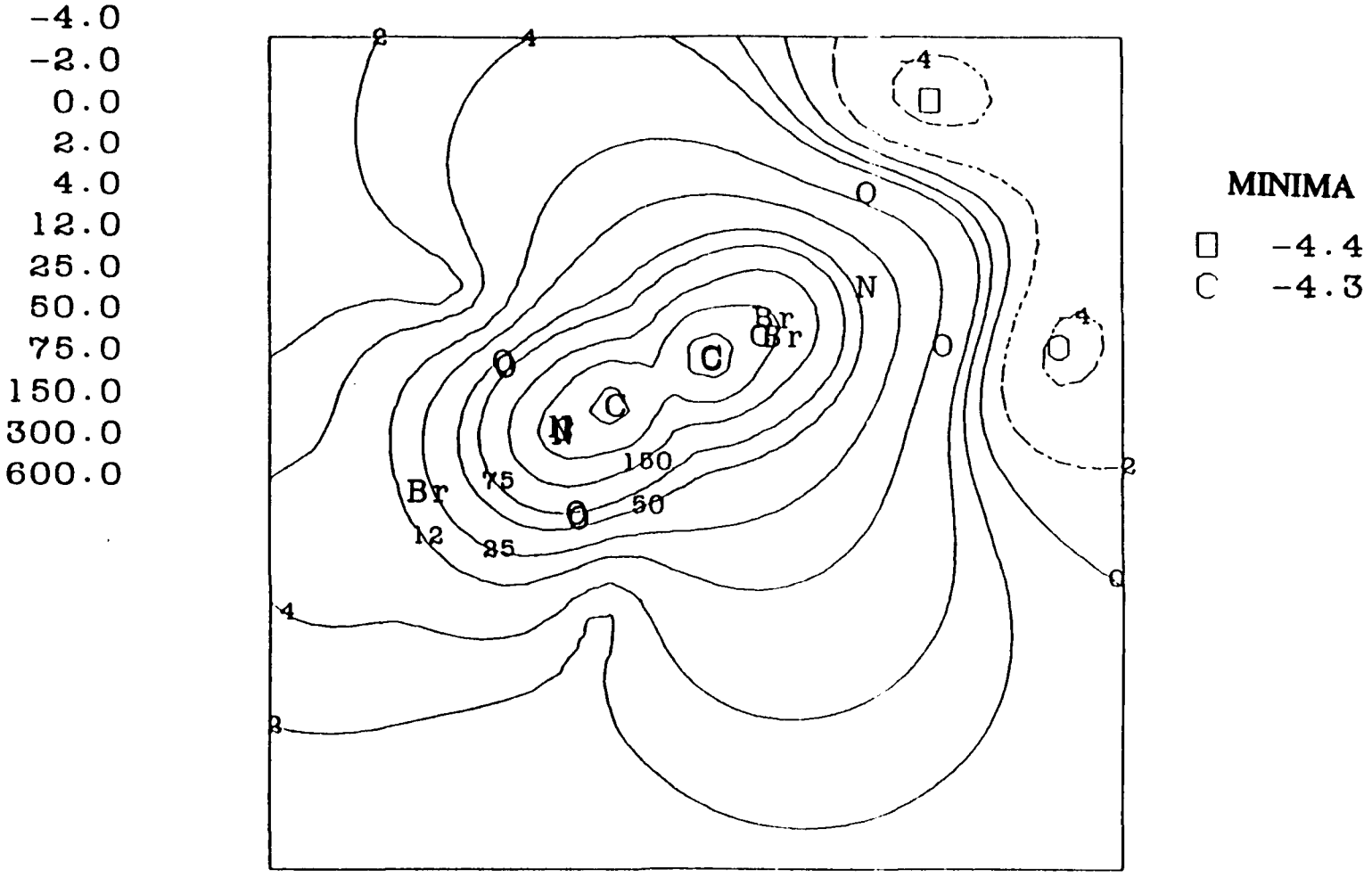


Figure HH-1. Calculated electrostatic potential, in kcal/mole, of 1,3,5-tribromo-2,4,6-trinitrobenzene, in the plane 1.75Å above the N7 nitro group located in the upper right corner. Projected positions of nuclei are shown. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

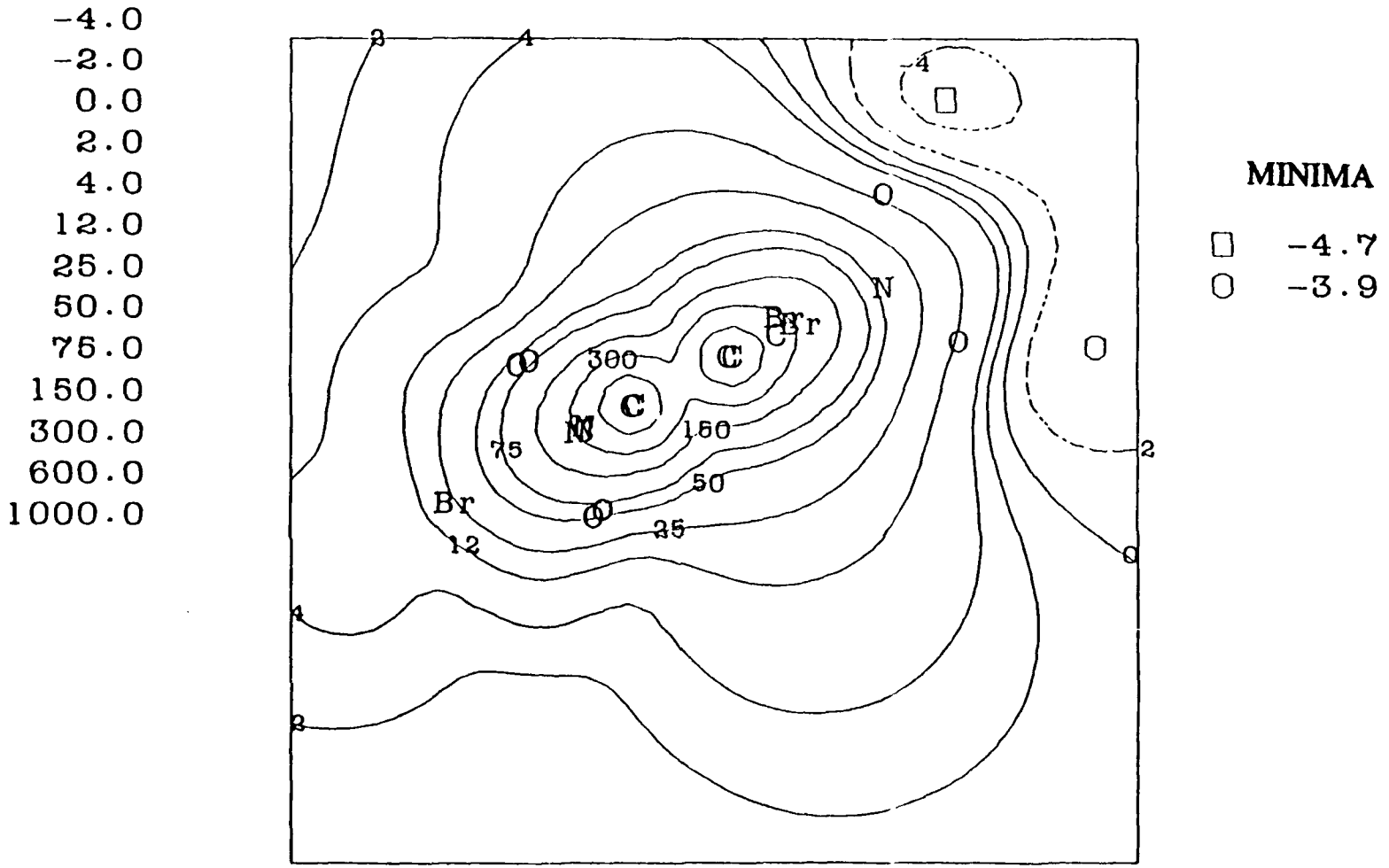
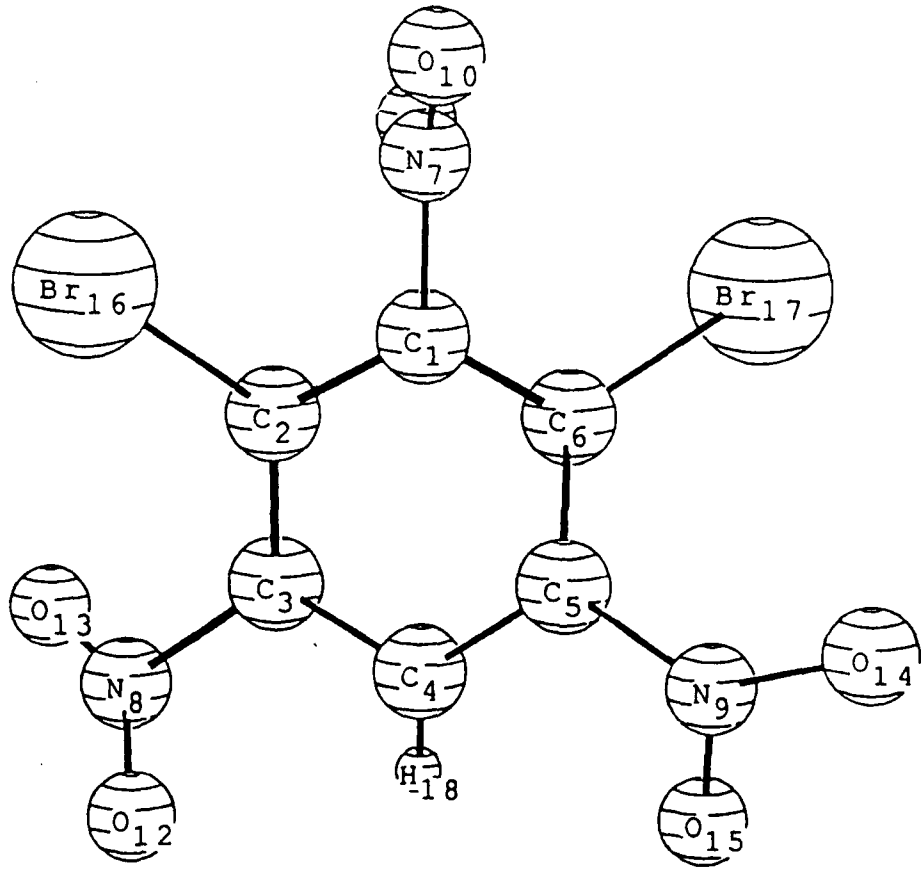


Figure HH-2. Calculated electrostatic potential, in kcal/mole, of 1,3,5-tribromo-2,4,6-trinitrobenzene, in the plane 1.75Å above the N8 nitro group located in the upper right corner. Projected positions of nuclei are shown. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

APPENDIX II
2,4-DIBROMO-1,3,5-TRINITROBENZENE

The short distances between non-bonded hydrogens and oxygens are H18-O12 (2.44 Å) and H18-O15 (2.44 Å).

The N8 and N9 nitro groups are rotated out of the mean plane of the benzene ring by 30°, while the N7 nitro group is approximately perpendicular to the ring (~95°).



Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.380000(1)					
3	3	C	2	1.390498(2)	1	116.357(18)			
4	4	C	3	1.382818(3)	2	122.441(19)	1	1.111(34)	0
5	5	C	4	1.382818(4)	3	118.020(20)	2	-0.584(35)	0
6	6	C	5	1.390498(5)	4	122.441(21)	3	-0.584(36)	0
7	7	N	1	1.480000(6)	2	117.814(22)	3	179.466(37)	0
8	8	N	3	1.479386(7)	4	115.151(23)	5	178.818(38)	0
9	9	N	5	1.479386(8)	4	115.151(24)	3	178.818(39)	0
10	10	O	7	1.210060(9)	1	117.034(25)	2	94.656(40)	0
11	11	O	7	1.210740(10)	1	117.018(26)	2	-85.379(41)	0
12	12	O	8	1.208234(11)	3	116.904(27)	4	29.845(42)	0
13	13	O	8	1.211220(12)	3	118.132(28)	4	-149.941(43)	0
14	14	O	9	1.211322(13)	5	118.154(29)	4	-149.989(44)	0
15	15	O	9	1.207948(14)	5	116.948(30)	4	29.831(45)	0
16	16	Br	2	1.891338(15)	3	125.206(31)	4	-175.584(46)	0
17	17	Br	6	1.891866(16)	5	125.196(32)	4	-175.555(47)	0
18	18	H	4	0.807000(17)	5	120.990(33)	6	179.416(48)	0

STOICHIOMETRY C6HBr2N3O6

SCF DONE: E(RHF) = -5953.87892238

Alpha eigenvalues -- -0.32804 -0.32390 -0.32381 0.10685 0.12158

Estimated ionization potential: 8.82 ev

```
Total atomic charges:
                1
 1  C    0.100374
 2  C   -0.025497
 3  C    0.115873
 4  C   -0.105965
 5  C    0.115836
 6  C   -0.025324
 7  N    0.178433
 8  N    0.181801
 9  N    0.181819
10  O   -0.179373
11  O   -0.179622
12  O   -0.187011
13  O   -0.185362
14  O   -0.185495
15  O   -0.187001
16  Br   0.115126
17  Br   0.115026
18  H    0.156362
Dipole moment (Debye):
   X=    -0.0043    Y=    -0.2721    Z=    -0.0025  Tot=     0.2721

    Bond Order: C1-N7: 1.21       V-mid: C1-N7: 0.199
                C3-N8: 1.22              C3-N8: 0.213
                C5-N9: 1.22              C5-N9: 0.213
               N7-O10: 1.99
               N7-O11: 1.98
               N8-O12: 2.00
               N8-O13: 1.99
               N9-O14: 1.99
               N9-O15: 2.00
```

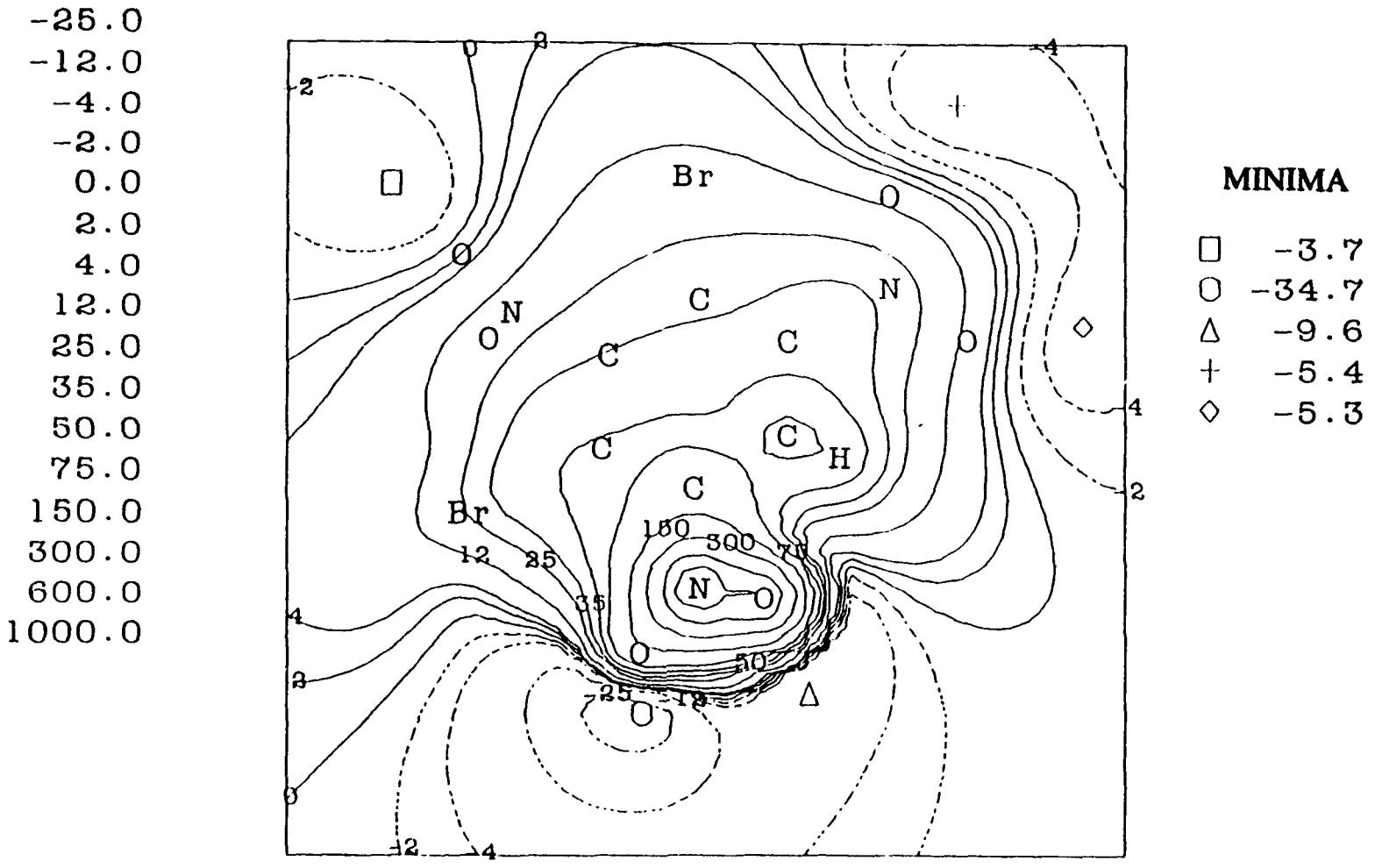


Figure II-1. Calculated electrostatic potential, in kcal/mole, of 2,4-dibromo-1,3,5-trinitrobenzene, in the plane 1.75Å above the N9 nitro group located in the upper right corner. Projected positions of nuclei are shown. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

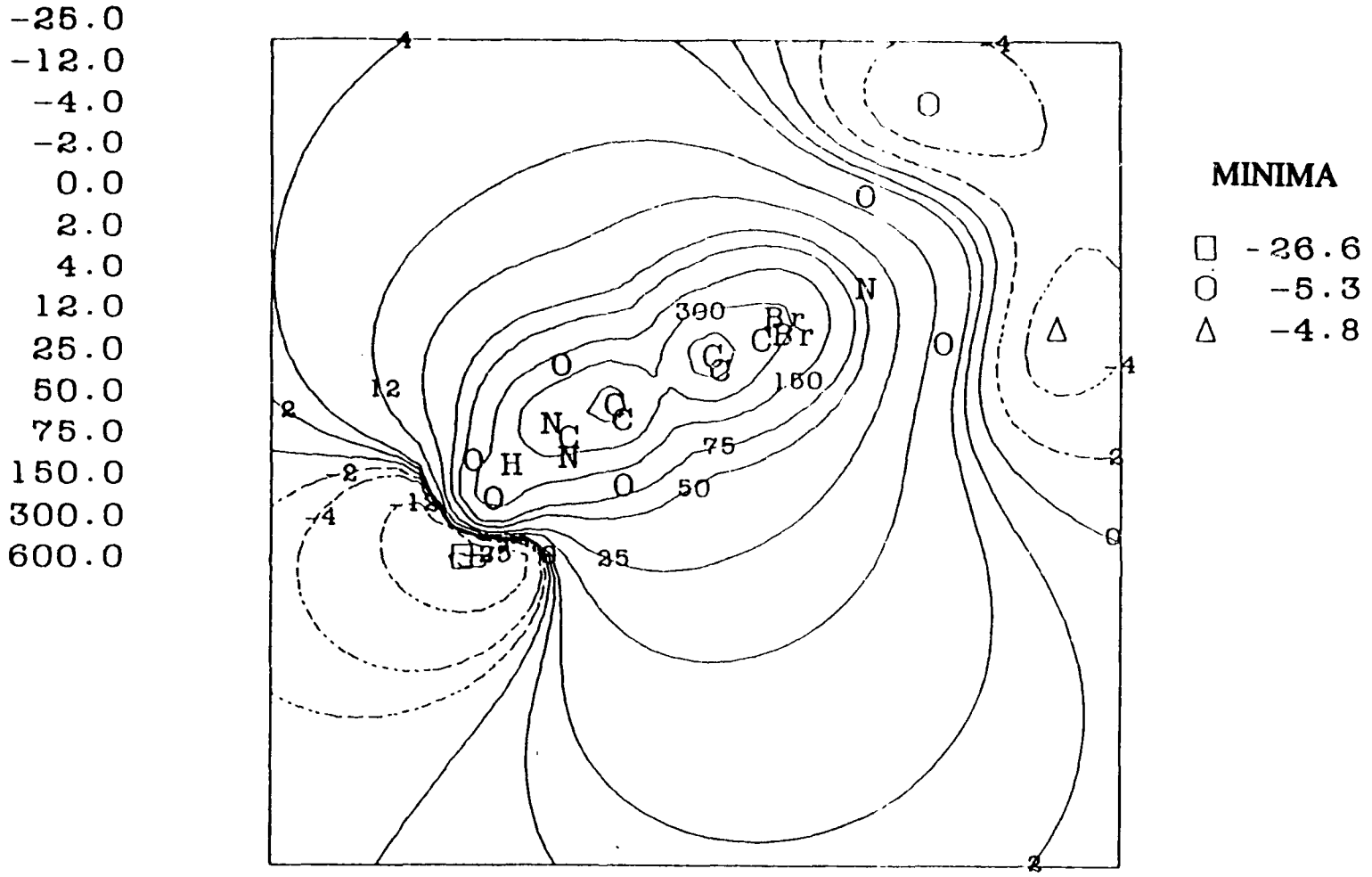
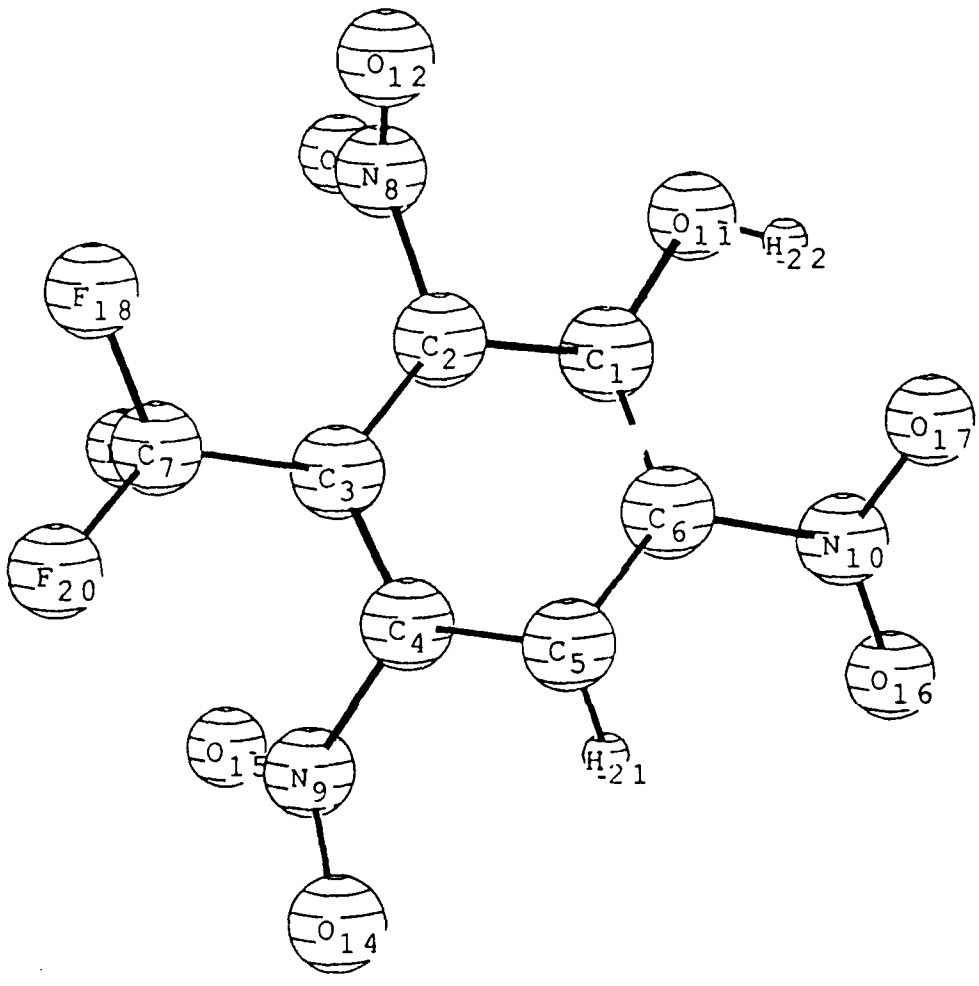


Figure II-2. Calculated electrostatic potential, in kcal/mole, of 2,4-dibromo-1,3,5-trinitrobenzene, in the plane 1.75Å above the N7 nitro group located in the upper right corner. Projected positions of nuclei are shown. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

APPENDIX JJ
3-TRIFLUOROMETHYL-2,4,6-TRINITROPHENOL

The short distances between non-bonded hydrogens and oxygens are H21-O16 (2.46 Å), H21-O14 (2.51 Å) and H22-O17 (1.90 Å).

The N10 nitro group is essentially planar, while the N8 and N9 nitro groups are rotated out of the plane by about 75° and 47°, respectively.



Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.404000(1)					
3	3	C	2	1.377935(2)	1	123.606(22)			
4	4	C	3	1.389770(3)	2	116.643(23)	1	0.328(42)	0
5	5	C	4	1.371750(4)	3	122.259(24)	2	1.301(43)	0
6	6	C	5	1.372874(5)	4	119.185(25)	3	-1.787(44)	0
7	7	C	3	1.528478(6)	4	122.350(26)	5	-174.260(45)	0
8	8	N	2	1.470356(7)	3	121.911(27)	4	179.191(46)	0
9	9	N	4	1.474082(8)	5	115.956(28)	6	176.116(47)	0
10	10	N	6	1.473645(9)	5	117.657(29)	4	-177.434(48)	0
11	11	O	1	1.326126(10)	2	117.062(30)	3	178.427(49)	0
12	12	O	8	1.215598(11)	2	117.138(31)	3	105.300(50)	0
13	13	O	8	1.209973(12)	2	117.510(32)	3	-75.519(51)	0
14	14	O	9	1.214281(13)	4	117.277(33)	5	46.276(52)	0
15	15	O	9	1.217971(14)	4	117.477(34)	5	-131.208(53)	0
16	16	O	10	1.199587(15)	6	118.296(35)	5	1.764(54)	0
17	17	O	10	1.221103(16)	6	117.472(36)	5	-177.931(55)	0
18	18	F	7	1.331131(17)	3	110.958(37)	4	150.137(56)	0
19	19	F	7	1.316372(18)	3	111.025(38)	4	-90.833(57)	0
20	20	F	7	1.310814(19)	3	111.626(39)	4	31.997(58)	0
21	21	H	5	0.972101(20)	4	115.616(40)	3	-177.819(59)	0
22	22	H	11	0.819230(21)	1	107.493(41)	6	-11.126(60)	0

SCF DONE: E(RHF) = -1245.86368404

Alpha eigenvalues — -0.35002 -0.34604 -0.32175 -0.31498 0.10080

Estimated ionization potential: 8.58 ev

Total atomic charges:

		1
1	C	0.203108
2	C	0.086656
3	C	0.006774
4	C	0.093541
5	C	-0.047036
6	C	0.061299
7	C	0.506982
8	N	0.184475
9	N	0.174856
10	N	0.185986
11	O	-0.362201
12	O	-0.179356
13	O	-0.183966
14	O	-0.186585
15	O	-0.187443
16	O	-0.166619
17	O	-0.225928
18	F	-0.156473
19	F	-0.145043
20	F	-0.154374
21	H	0.146811
22	H	0.344536

Dipole moment (Debye):

X= 2.1028 Y= 0.6998 Z= -0.3858 Tot= 2.2495

Bond Order:		V-mid:	
	C2-N8: 1.24		C2-N8: 0.195
	C4-N9: 1.23		C4-N9: 0.193
	C6-N10: 1.23		C6-N10: 0.177
	N8-O12: 1.96		
	N8-O13: 1.99		
	N9-O14: 1.97		
	N9-O15: 1.95		
	N10-O16: 2.04		
	N10-O17: 1.93		

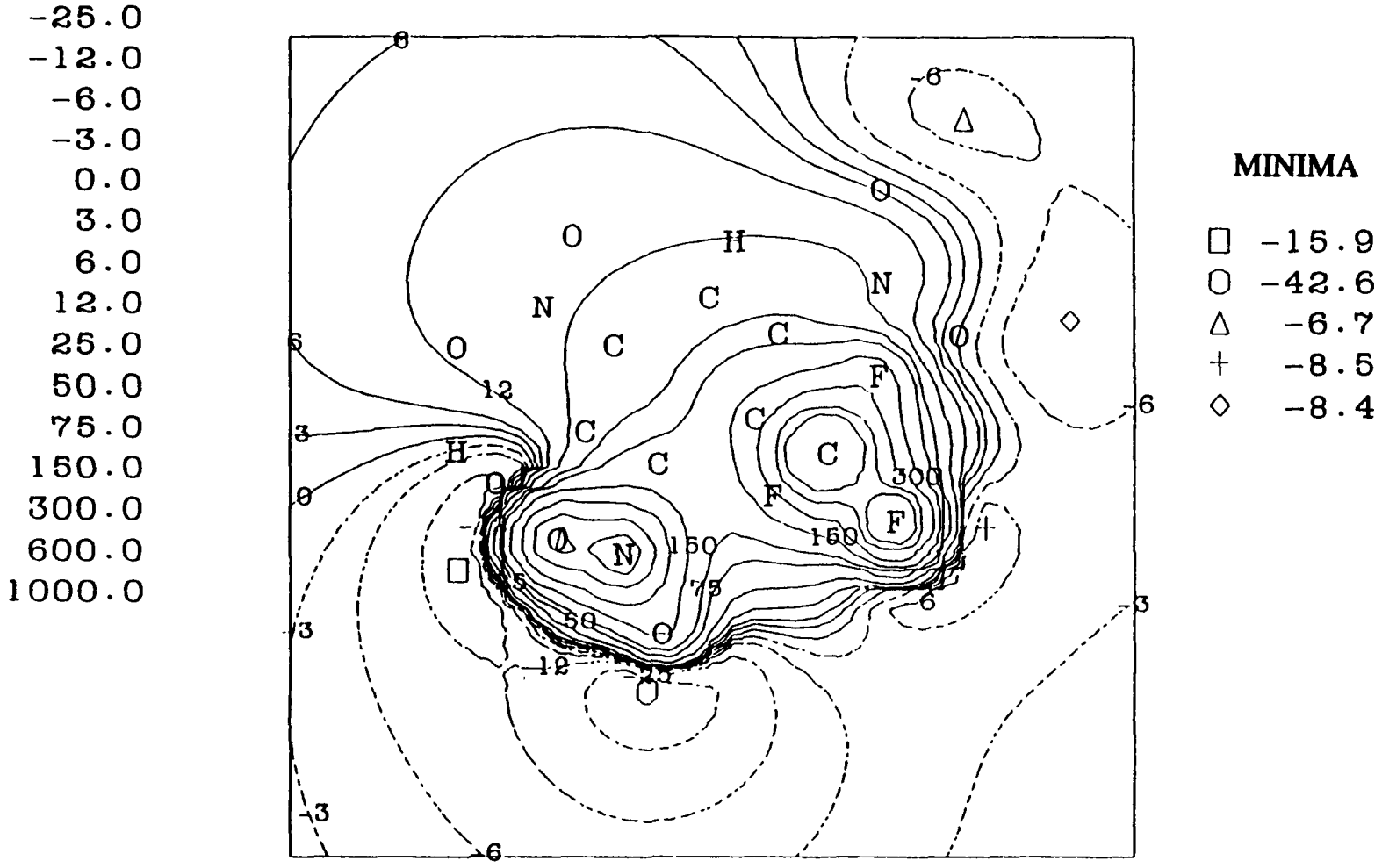


Figure JJ-1. Calculated electrostatic potential, in kcal/mole, of 3-trifluoromethyl-2,4,6-trinitrophenol, in the plane 1.75Å above the N9 nitro group located in the upper right corner. Projected positions of nuclei are shown. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

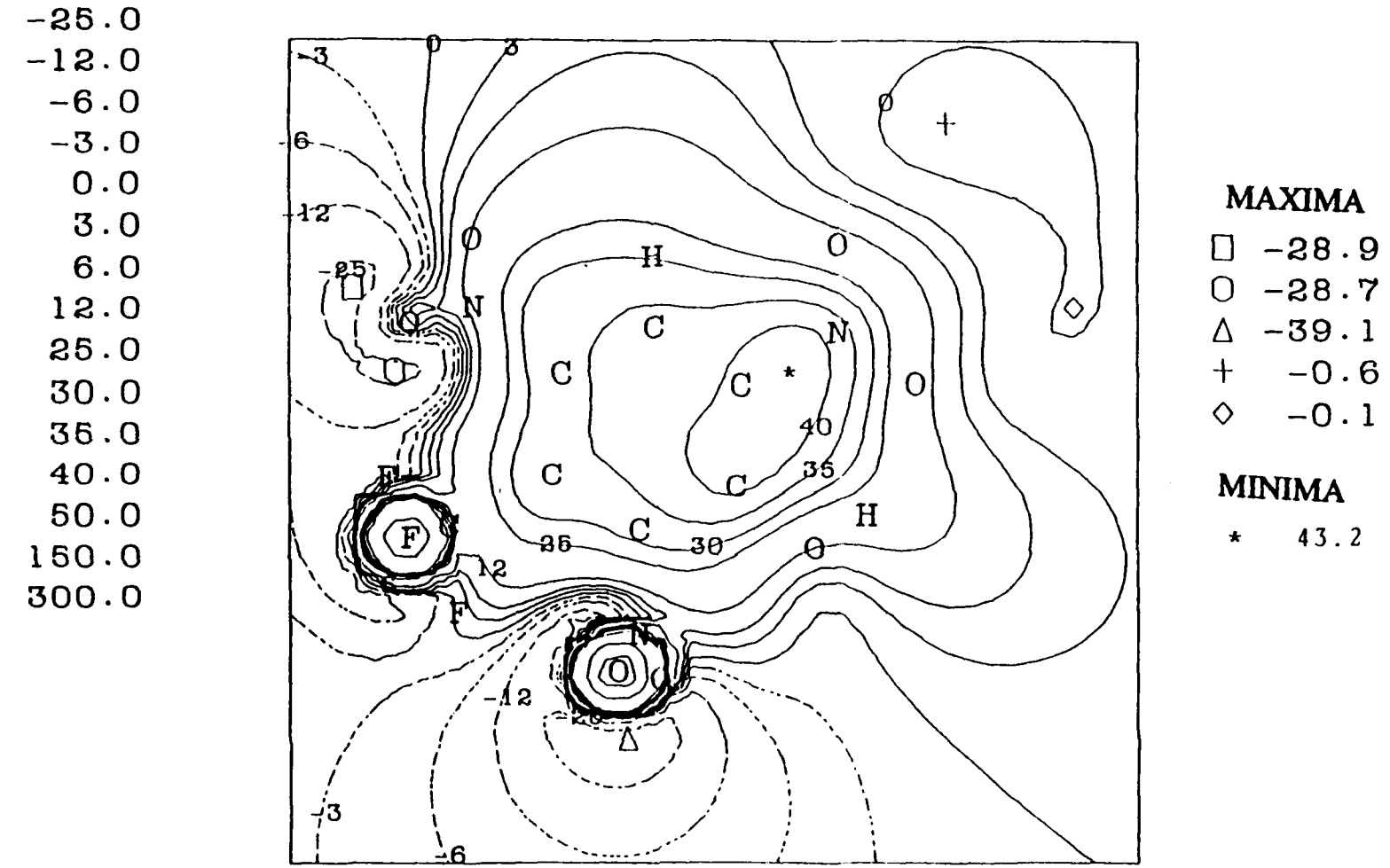
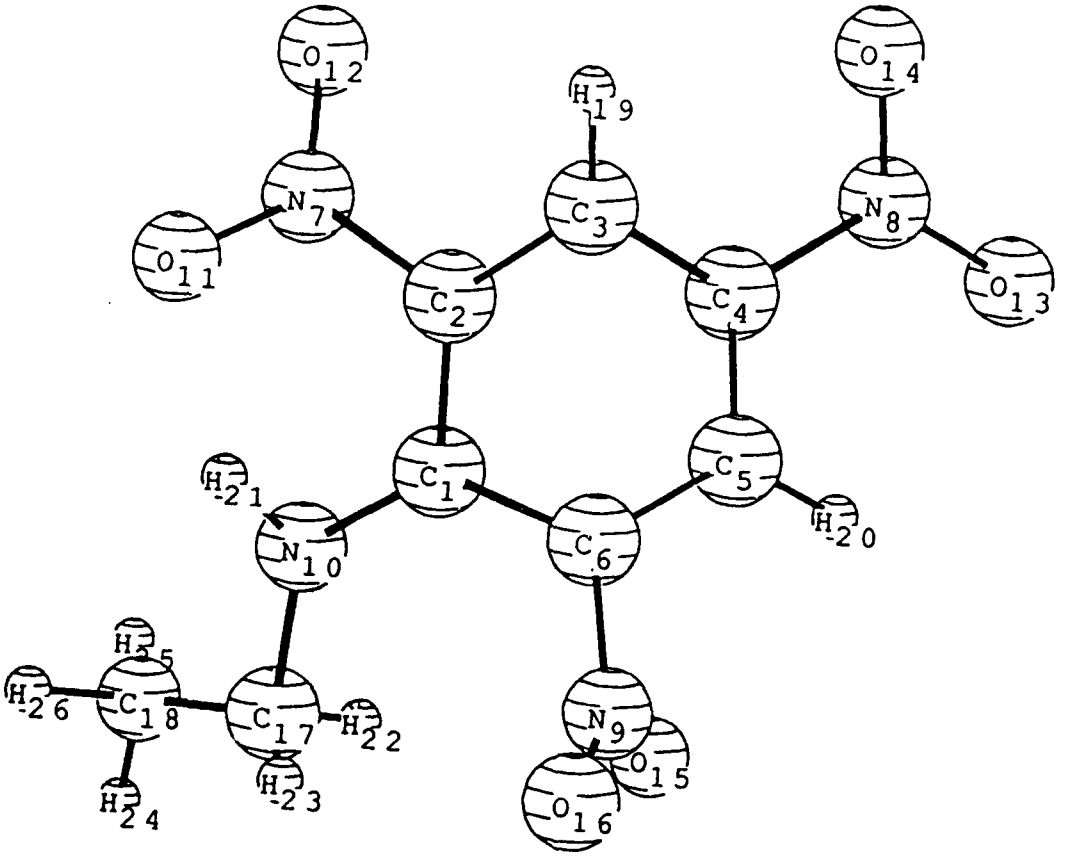


Figure JJ-2. Calculated electrostatic potential, in kcal/mole, of 3-trifluoromethyl-2,4,6-trinitrophenol, in the plane 1.75Å above the N10 nitro group located in the upper right corner. Projected positions of nuclei are shown. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

APPENDIX KK
N-ETHYLPICRAMIDE

The short distances between non-bonded hydrogens and oxygens are H21-O11 (1.86 Å), H19-O12 (2.30 Å), H20-O13 (2.43 Å) and H19-O14 (2.42 Å).

The N7 and N9 nitro groups are rotated by approximately 16° and 63°, while the N8 nitro group is almost planar.



Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.452000(1)					
3	3	C	2	1.383366(2)	1	125.488(26)			
4	4	C	3	1.375288(3)	2	117.056(27)	1	0.466(50)	0
5	5	C	4	1.385204(4)	3	122.328(28)	2	-1.217(51)	0
6	6	C	5	1.357979(5)	4	118.178(29)	3	-0.371(52)	0
7	7	N	2	1.444456(6)	3	113.303(30)	4	-175.605(53)	0
8	8	N	4	1.472789(7)	5	119.316(31)	6	-178.995(54)	0
9	9	N	6	1.474800(8)	5	114.736(32)	4	-173.377(55)	0
10	10	N	1	1.311624(9)	2	122.669(33)	3	-177.952(56)	0
11	11	O	7	1.219191(10)	2	119.271(34)	1	16.622(57)	0
12	12	O	7	1.218956(11)	2	119.482(35)	1	-164.796(58)	0
13	13	O	8	1.223478(12)	4	117.155(36)	3	-175.437(59)	0
14	14	O	8	1.227899(13)	4	118.349(37)	3	2.636(60)	0
15	15	O	9	1.217938(14)	6	117.621(38)	1	118.997(61)	0
16	16	O	9	1.206604(15)	6	117.433(39)	1	-63.474(62)	0
17	17	C	10	1.457236(16)	1	127.715(40)	2	162.809(63)	0
18	18	C	17	1.519795(17)	10	107.228(41)	1	-150.949(64)	0
19	19	H	3	0.959378(18)	4	121.418(42)	5	178.855(65)	0
20	20	H	5	0.960549(19)	4	121.006(43)	3	179.444(66)	0
21	21	H	10	0.891037(20)	1	107.469(44)	2	-13.213(67)	0
22	22	H	17	0.960053(21)	10	109.853(45)	1	-31.507(68)	0
23	23	H	17	0.959400(22)	10	110.263(46)	1	89.275(69)	0
24	24	H	18	0.959927(23)	17	109.454(47)	10	179.758(70)	0
25	25	H	18	0.960684(24)	17	109.538(48)	10	59.752(71)	0
26	26	H	18	0.959818(25)	17	109.486(49)	10	-60.235(72)	0

STOICHIOMETRY C8H8N4O6

SCF DONE: E(RHF) = -970.057729827 A.U. AFTER 22 CYCLES

Alpha eigenvalues — -0.29392 0.12726 0.14741 0.19115 0.23185

Estimated ionization potential: 8.01 ev

Total atomic charges:

		1
1	C	0.199520
2	C	0.057593
3	C	-0.047819
4	C	0 077816
5	C	-0.049395
6	C	0.065943
7	N	0.168615
8	N	0.167424
9	N	0.171636
10	N	-0.404492
11	O	-0.229021
12	O	-0.188108
13	O	-0.200677
14	O	-0.201120
15	O	-0.199962
16	O	-0.198314
17	C	-0.046327
18	C	-0.293763
19	H	0.151310
20	H	0.141052
21	H	0.291566
22	H	0.112157
23	H	0.120304
24	H	0.113478
25	H	0.110211
26	H	0.110374

Dipole moment (Debye):

X= -3.7803 Y= 0.2872 Z= -0.1971 Tot= 3.7963

V-mid: C2-N7: 0.167
C4-N8: 0.176
C6-N9: 0.172

Bond Order: C2-N7: 1.32
C4-N8: 1.24
C6-N9: 1.24
N7-O11: 1.94
N7-O12: 1.94
N8-O13: 1.92
N8-O14: 1.90
N9-O15: 1.95
N9-O16: 2.00

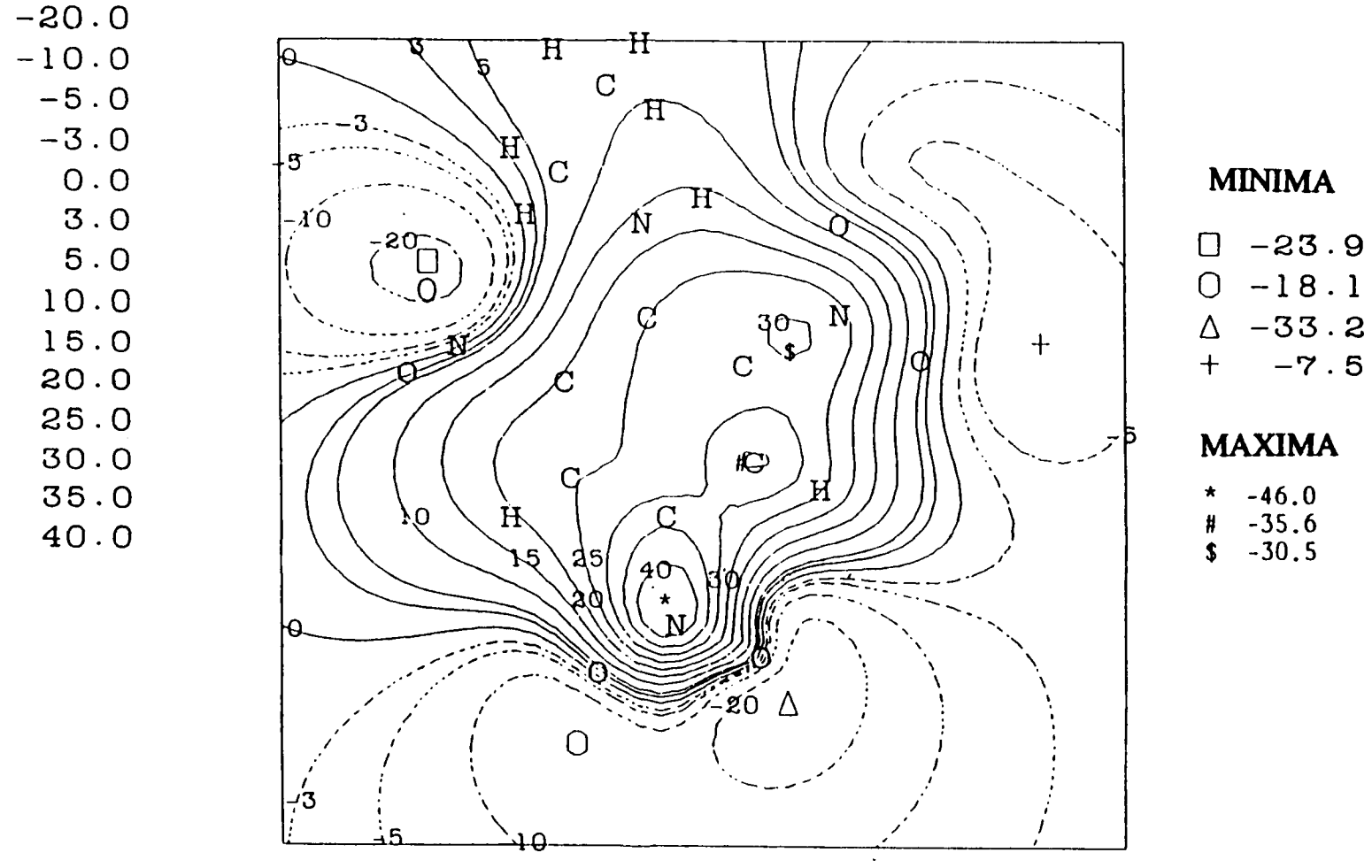


Figure KK-1. Calculated electrostatic potential, in kcal/mole, of N-ethylpicramide, in the plane 1.75Å above the N7 nitro group located in the upper right corner. Projected positions of nuclei are shown. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

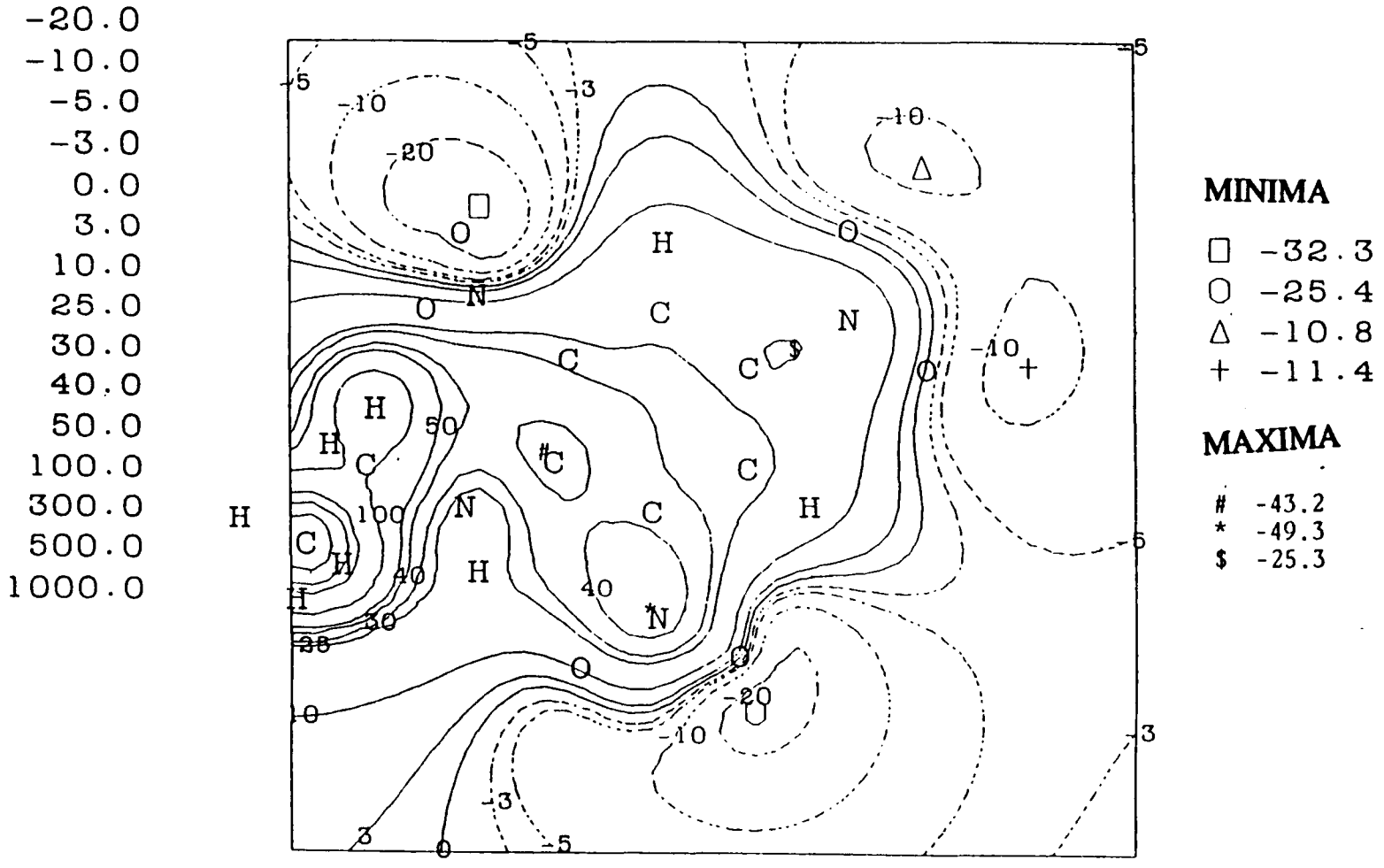
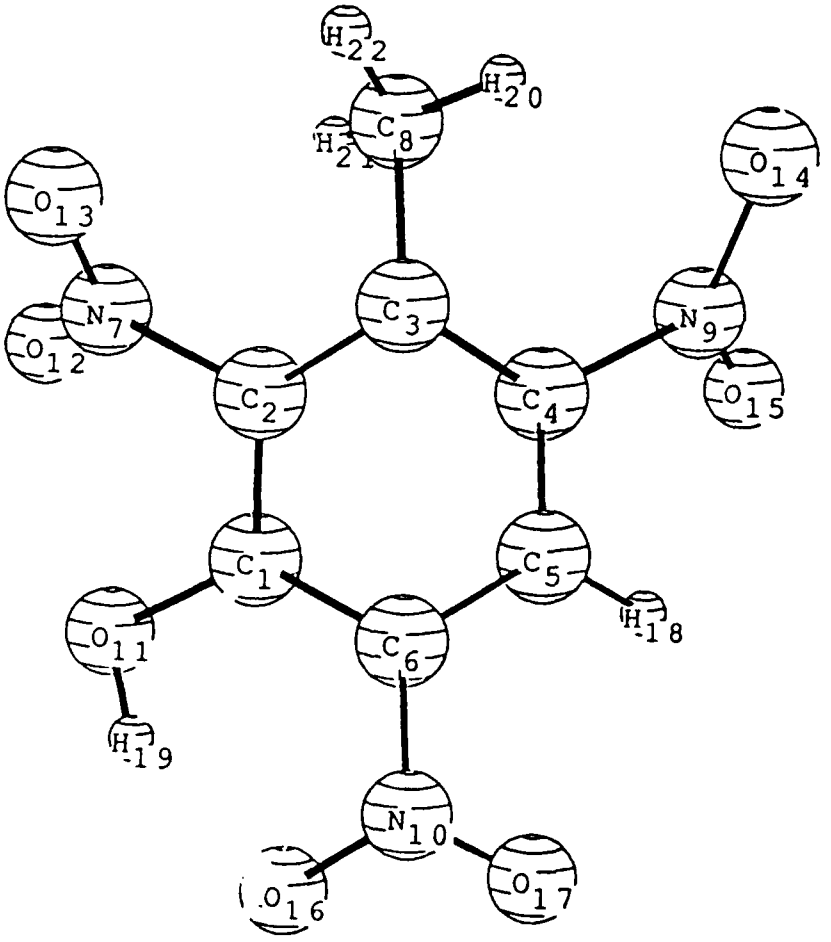


Figure KK-2. Calculated electrostatic potential, in kcal/mole, of N-ethylpicramide, in the plane 1.75Å above the N8 nitro group located in the upper right corner. Projected positions of nuclei are shown. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

APPENDIX LL
3-HYDROXY-2,4,6-TRINITROTOLUENE

The short distances between non-bonded hydrogens and oxygens are H21-O14 (2.18 Å), H20-O17 (2.42 Å) and H19-O16 (1.81 Å).

The N7, N9 and N10 nitro groups are rotated by approximately 67°, 42°and 17°, respectively.



Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.389000(1)					
3	3	C	2	1.390802(2)	1	123.323(22)			
4	4	C	3	1.380522(3)	2	116.382(23)	1	0.514(42)	0
5	5	C	4	1.363861(4)	3	122.528(24)	2	-1.787(43)	0
6	6	C	5	1.374531(5)	4	120.144(25)	3	-0.410(44)	0
7	7	N	2	1.462911(6)	3	120.070(26)	4	-178.974(45)	0
8	8	C	3	1.519220(7)	4	124.283(27)	5	-177.010(46)	0
9	9	N	4	1.472782(8)	5	116.667(28)	6	-178.754(47)	0
10	10	N	6	1.446781(9)	5	118.634(29)	4	-179.909(48)	0
11	11	O	1	1.342890(10)	2	118.042(30)	3	-179.786(49)	0
12	12	O	7	1.233874(11)	2	118.357(31)	3	111.651(50)	0
13	13	O	7	1.226798(12)	2	117.357(32)	3	-66.311(51)	0
14	14	O	9	1.222853(13)	4	117.759(33)	5	-136.877(52)	0
15	15	O	9	1.230465(14)	4	117.131(34)	5	42.557(53)	0
16	16	O	10	1.236648(15)	6	118.257(35)	5	-164.844(54)	0
17	17	O	10	1.215929(16)	6	117.749(36)	5	19.357(55)	0
18	18	H	5	0.960418(17)	4	119.896(37)	3	179.771(56)	0
19	19	H	11	0.908336(18)	1	104.888(38)	6	1.857(57)	0
20	20	H	8	0.960301(19)	3	109.532(39)	4	-4.787(58)	0
21	21	H	8	0.959471(20)	3	109.528(40)	4	115.323(59)	0
22	22	H	8	0.960519(21)	3	109.413(41)	4	-124.715(60)	0

STOICHIOMETRY C7H5N3O7

SCF DONE: E(RHF) = -950.909243802 A.U. AFTER 22 CYCLES

Alpha eigenvalues -- -0.31314 -0.30340 0.11238 0.14601 0.17979

Estimated ionization potential: 8.26 ev

Total atomic charges:

		1
1	C	0.192800
2	C	0.064872
3	C	0.087716
4	C	0.075010
5	C	-0.046299
6	C	0.052624
7	N	0.165141
8	C	-0.318260
9	N	0.166690
10	N	0.169700
11	O	-0.315936
12	O	-0.179456
13	O	-0.189917
14	O	-0.191096
15	O	-0.190489
16	O	-0.224933
17	O	-0.161141
18	H	0.142403
19	H	0.302241
20	H	0.135493
21	H	0.125994
22	H	0.136842

Dipole moment (Debye):

X= 0.1044 Y= -0.6909 Z= -0.1543 Tot= 0.7156

V-mid: C2-N7: 0.167
C4-N9: 0.174
C6-N10: 0.163

Bond Order: C2-N7: 1.27
C4-N9: 1.24
C6-N10: 1.29
N7-O12: 1.87
N7-O13: 1.91
N9-O14: 1.92
N9-O15: 1.89
N10-O16: 1.86
N10-O17: 1.96

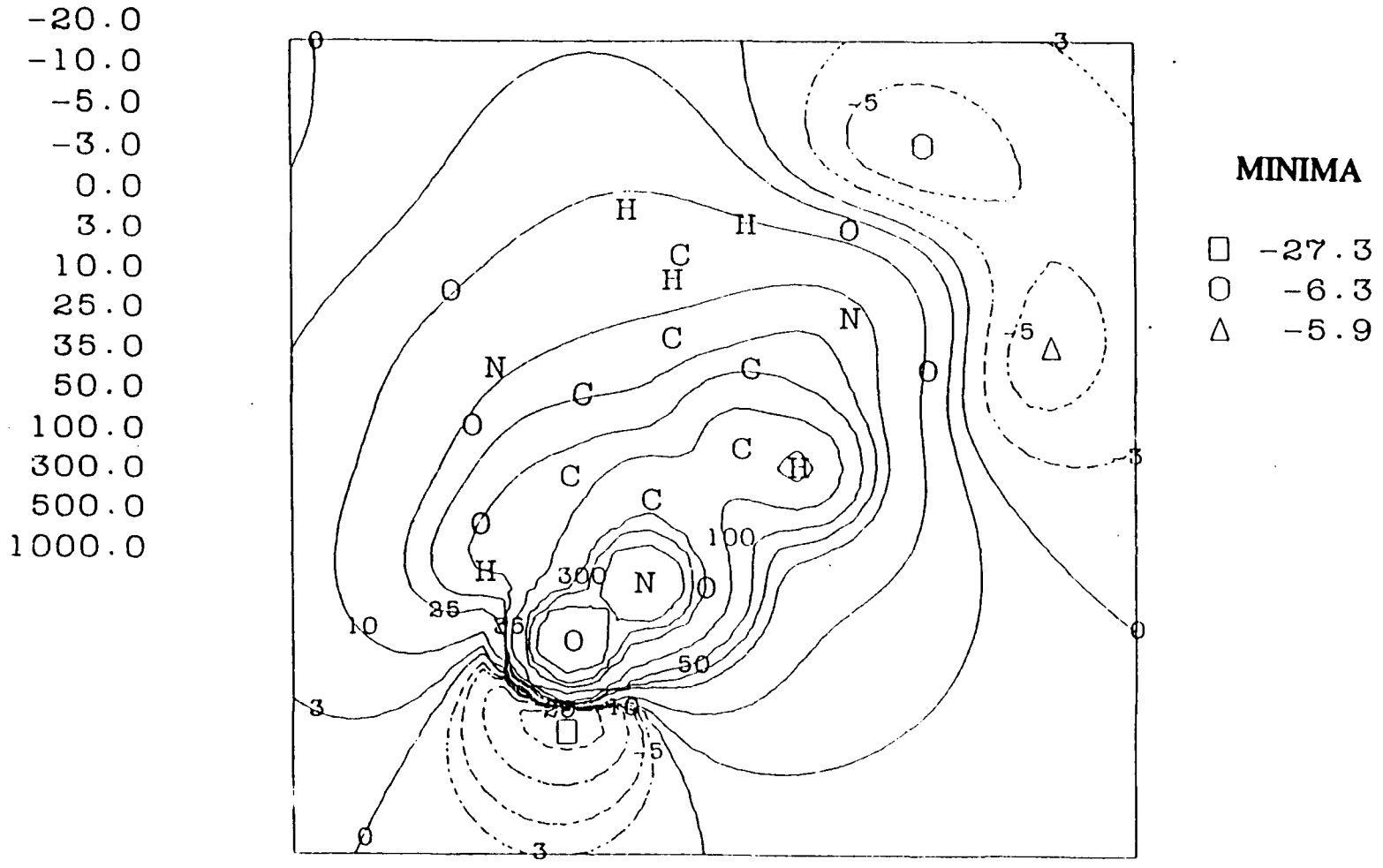


Figure LL-1. Calculated electrostatic potential, in kcal/mole, of 3-hydroxy-2,4,6-trinitrotoluene, in the plane 1.75Å above the N9 nitro group located in the upper right corner. Projected positions of nuclei are shown. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

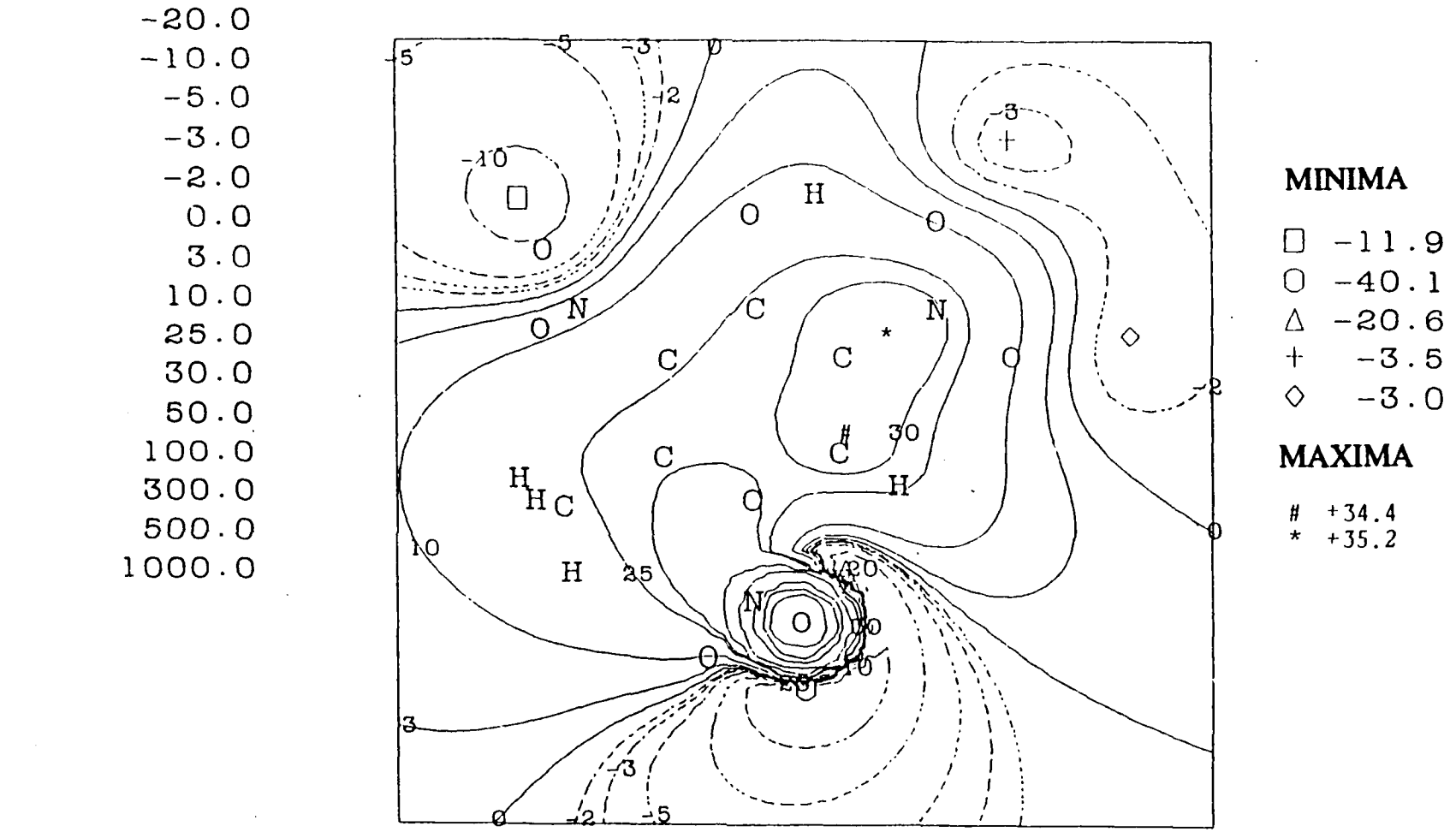
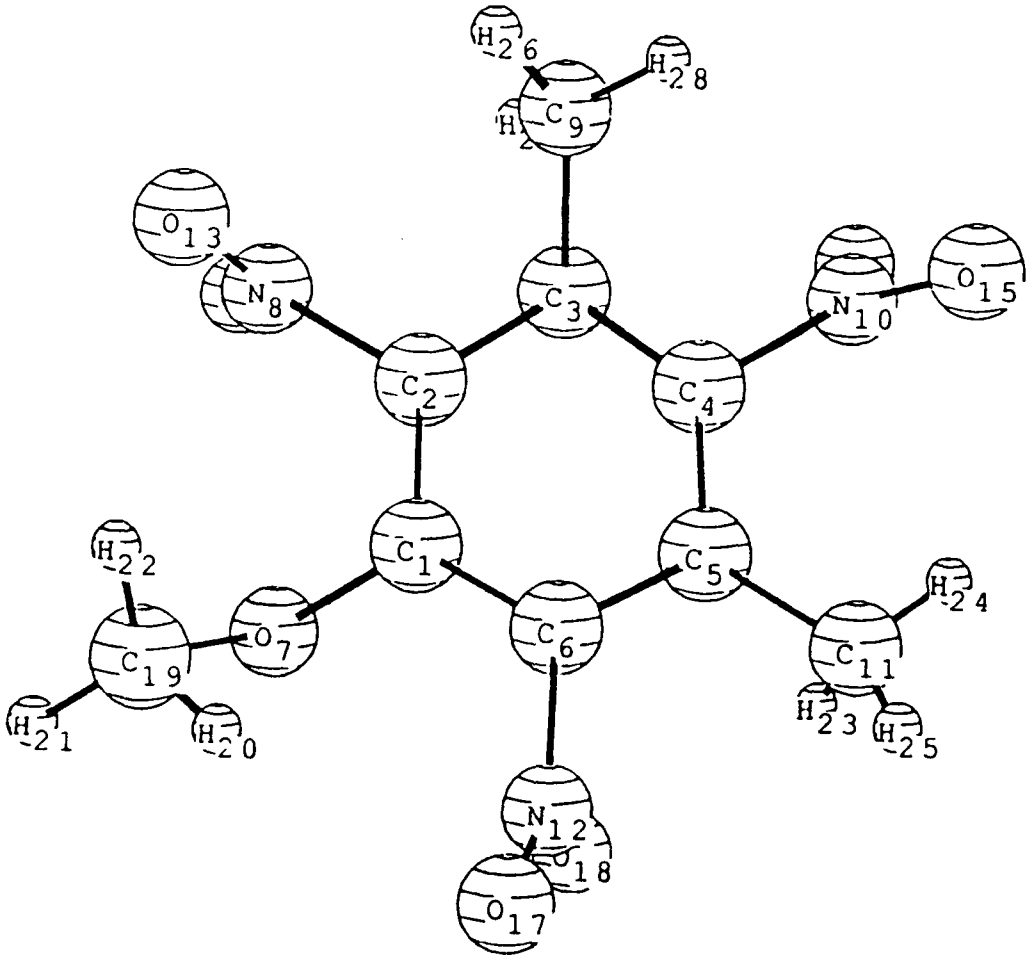


Figure LL-2. Calculated electrostatic potential, in kcal/mole, of 3-hydroxy-2,4,6-trinitrotoluene, in the plane 1.75Å above the N10 nitro group located in the upper right corner. Projected positions of nuclei are shown. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

APPENDIX MM
3,5-DIMETHYL-2,4,6-TRINITROANISOLE

All distances between non-bonded hydrogen and oxygen atoms are greater than 2.50 Å.

The N8 nitro group is almost perpendicular to the plane of the benzene ring, while the N10 and N12 nitro groups are both rotated by about 71° and 75°, respectively.



Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.358000(1)					
3	3	C	2	1.399318(2)	1	123.009(28)			
4	4	C	3	1.381244(3)	2	113.706(29)	1	-0.330(54)	0
5	5	C	4	1.374427(4)	3	127.264(30)	2	-0.536(55)	0
6	6	C	5	1.380457(5)	4	113.220(31)	3	0.276(56)	0
7	7	O	1	1.381053(6)	2	122.235(32)	3	-173.505(57)	0
8	8	N	2	1.494392(7)	3	118.242(33)	4	-178.931(58)	0
9	9	C	3	1.514005(8)	2	121.506(34)	1	-178.302(59)	0
10	10	N	4	1.474365(9)	5	117.024(35)	6	-178.217(60)	0
11	11	C	5	1.488442(10)	4	123.677(36)	3	-178.810(61)	0
12	12	N	6	1.488545(11)	5	118.590(37)	4	-179.717(62)	0
13	13	O	8	1.195761(12)	2	117.026(38)	3	-86.755(63)	0
14	14	O	8	1.176405(13)	2	117.908(39)	3	94.062(64)	0
15	15	O	10	1.221266(14)	4	119.364(40)	3	109.150(65)	0
16	16	O	10	1.227326(15)	4	118.185(41)	3	-71.237(66)	0
17	17	O	12	1.217146(16)	6	115.962(42)	5	105.055(67)	0
18	18	O	12	1.202357(17)	6	119.010(43)	5	-75.058(68)	0
19	19	C	7	1.410976(18)	1	117.800(44)	2	-78.553(69)	0
20	20	H	19	0.960738(19)	7	98.207(45)	1	-65.863(70)	0
21	21	H	13	0.959901(20)	7	114.169(46)	1	178.350(71)	0
22	22	H	19	0.960835(21)	7	115.396(47)	1	50.294(72)	0
23	23	H	11	0.959732(22)	5	103.633(48)	4	-125.713(73)	0
24	24	H	11	0.960368(23)	5	113.210(49)	4	-7.302(74)	0
25	25	H	11	0.959800(24)	5	111.280(50)	4	116.792(75)	0
26	26	H	9	0.960337(25)	3	106.135(51)	4	-124.700(76)	0
27	27	H	9	0.960321(26)	3	107.094(52)	4	118.482(77)	0
28	28	H	9	0.959719(27)	3	115.051(53)	4	-3.471(78)	0

STOICHIOMETRY C9H9N3O7

SCF DONE: E(RHF) = -1028.63317892 A.U. AFTER 22 CYCLES

Alpha eigenvalues -- -0.34989 -0.32387 -0.31355 -0.30780 0.15926

Estimated ionization energy: 8.34 ev

Total atomic charges:

		1
1	C	0.158660
2	C	0.067981
3	C	0.073648
4	C	0.080800
5	C	0.070937
6	C	0.073606
7	O	-0.241150
8	N	0.199707
9	C	-0.315982
10	N	0.159940
11	C	-0.320361
12	N	0.184359
13	O	-0.212092
14	O	-0.186413
15	O	-0.193336
16	O	-0.194589
17	O	-0.201273
18	O	-0.186486
19	C	-0.179946
20	H	0.123724
21	H	0.131548
22	H	0.117949
23	H	0.134896
24	H	0.129555
25	H	0.132281
26	H	0.130789
27	H	0.132034
28	H	0.129215

Dipole moment (Debye):
X= 0.1680 Y= -0.3563 Z= -1.2833 Tot= 1.3424

Bond Order: C2-N8: 1.18
C4-N10: 1.23
C6-N12: 1.19
N8-O13: 2.06
N8-O14: 2.16
N10-O15: 1.93
N10-O16: 1.91
N11-O17: 1.95
N11-O18: 2.03

V-mid: C2-N8: 0.190
C4-N10: 0.173
C6-N12: 0.184

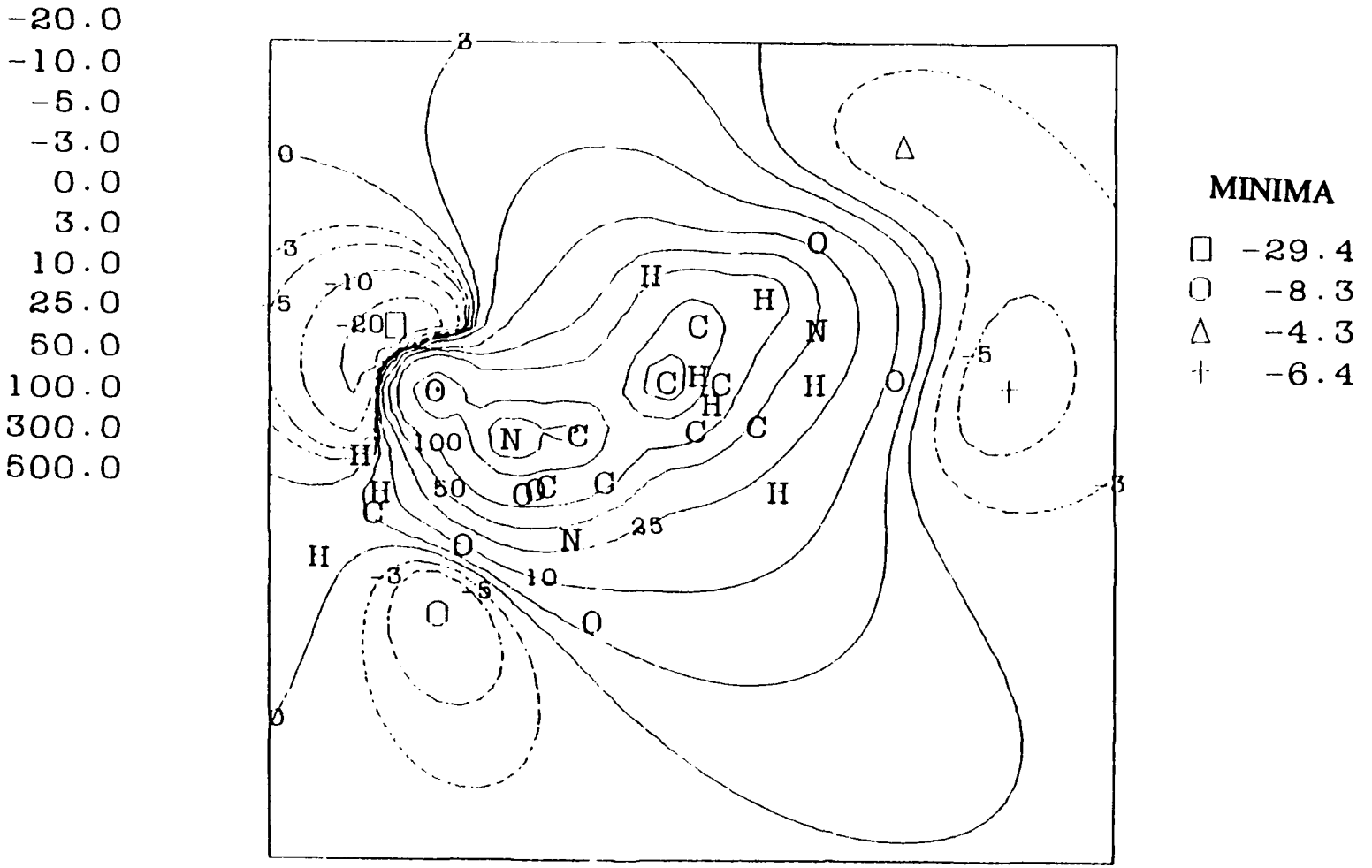


Figure MM-1. Calculated electrostatic potential, in kcal/mole, of 3,5-dimethyl-2,4,6-trinitroanisole, in the plane 1.75Å above the N10 nitro group located in the upper right corner. Projected positions of nuclei are shown. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

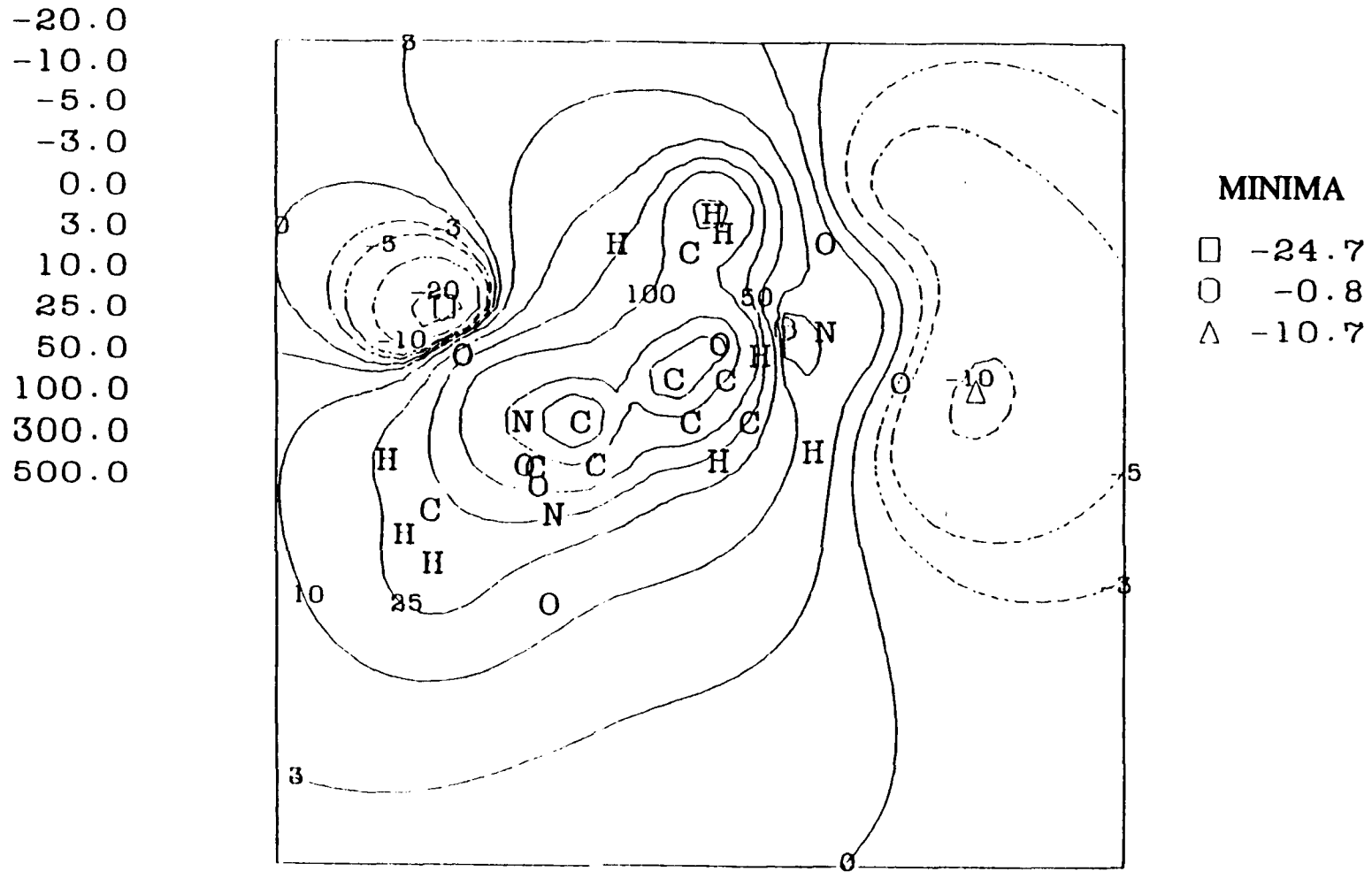
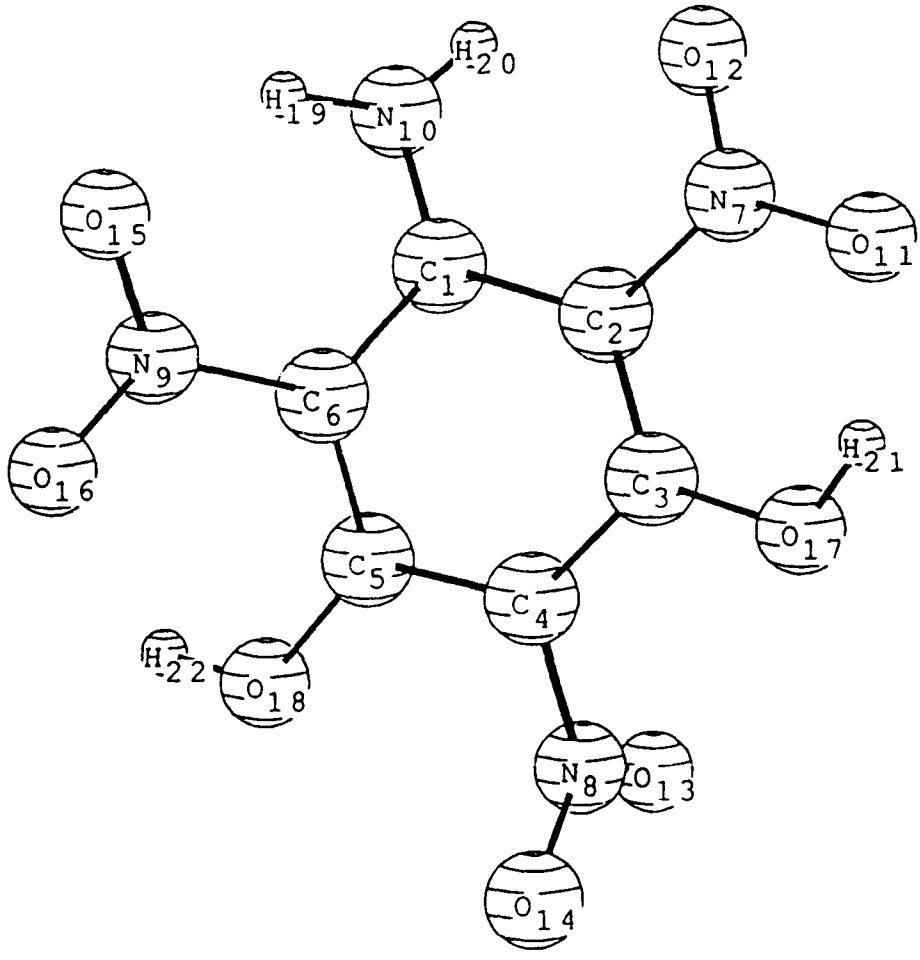


Figure MM-2. Calculated electrostatic potential, in kcal/mole, of 3,5-dimethyl-2,4,6-trinitroanisole, in the plane 1.75Å above the N12 nitro group located in the upper right corner. Projected positions of nuclei are shown. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

APPENDIX NN
2,4,6-TRINITRO-3,5-DIHYDROXYANILINE

The short distances between non-bonded hydrogens and oxygens are H22-O11 (1.68 Å), H20-O12 (1.89 Å), H19-O15 (1.77 Å) and H22-O16 (1.76 Å).

The N7 and N8 nitro groups are rotated out of the mean plane of the benzene ring by about 10° and 57°, respectively, while the N9 nitro group is approximately planar.



Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.433000(1)					
3	3	C	2	1.401292(2)	1	122.054(22)			
4	4	C	3	1.392566(3)	2	119.184(23)	1	3.757(42)	0
5	5	C	4	1.389651(4)	3	121.683(24)	2	-3.991(43)	0
6	6	C	5	1.406808(5)	4	119.432(25)	3	0.574(44)	0
7	7	N	2	1.419691(6)	3	117.928(26)	4	-178.310(45)	0
8	8	N	4	1.451284(7)	3	118.574(27)	2	176.053(46)	0
9	9	N	6	1.429487(8)	5	118.653(28)	4	-176.904(47)	0
10	10	N	1	1.312041(9)	2	122.472(29)	3	178.899(48)	0
11	11	O	7	1.246641(10)	2	119.706(30)	3	-9.464(49)	0
12	12	O	7	1.226492(11)	2	121.595(31)	3	170.181(50)	0
13	13	O	8	1.231708(12)	4	117.251(32)	3	-57.207(51)	0
14	14	O	8	1.200124(13)	4	118.786(33)	3	123.278(52)	0
15	15	O	9	1.231430(14)	6	121.497(34)	5	-179.019(53)	0
16	16	O	9	1.250106(15)	6	118.600(35)	5	1.307(54)	0
17	17	O	3	1.320112(16)	2	124.265(36)	1	-176.920(55)	0
18	18	O	5	1.325487(17)	4	116.486(37)	3	-179.929(56)	0
19	19	H	10	0.959025(18)	1	114.320(38)	2	-171.925(57)	0
20	20	H	10	0.845067(19)	1	114.298(39)	2	3.019(58)	0
21	21	H	17	0.895016(20)	3	106.611(40)	4	-171.735(59)	0
22	22	H	18	0.868143(21)	3	134.968(41)	4	179.432(60)	0

STOICHIOMETRY C6H4N4O8

SCF DONE: E(RHF) = -1041.29860035

Alpha eigenvalues — -0.28233 0.11816 0.13663 0.19340 0.24411

Estimated ionization potential: 7.69 ev

Total atomic charges:

		1
1	C	0.237769
2	C	−0.015954
3	C	0.228912
4	C	0.013388
5	C	0.233026
6	C	−0.014067
7	N	0.161212
8	N	0.181797
9	N	0.162517
10	N	−0.530495
11	O	−0.231007
12	O	−0.193961
13	O	−0.202589
14	O	−0.189842
15	O	−0.203892
16	O	−0.223215
17	O	−0.328231
18	O	−0.344611
19	H	0.301574
20	H	0.309182
21	H	0.318936
22	H	0.329549

Dipole moment (Debye):

X= −1.5662 Y= −4.1003 Z= −0.3683 Tot= 4.4046

Bond Order:	C2–N7:	1.37	V-mid: C2–N7:	0.108
	C4–N8:	1.29	C4–N8:	0.142
	C6–N9:	1.35	C6–N9:	0.110
	N7–O11:	1.82		
	N7–O12:	1.91		
	N8–O13:	1.88		
	N8–O14:	2.04		
	N9–O15:	1.89		
	N9–O16:	1.80		

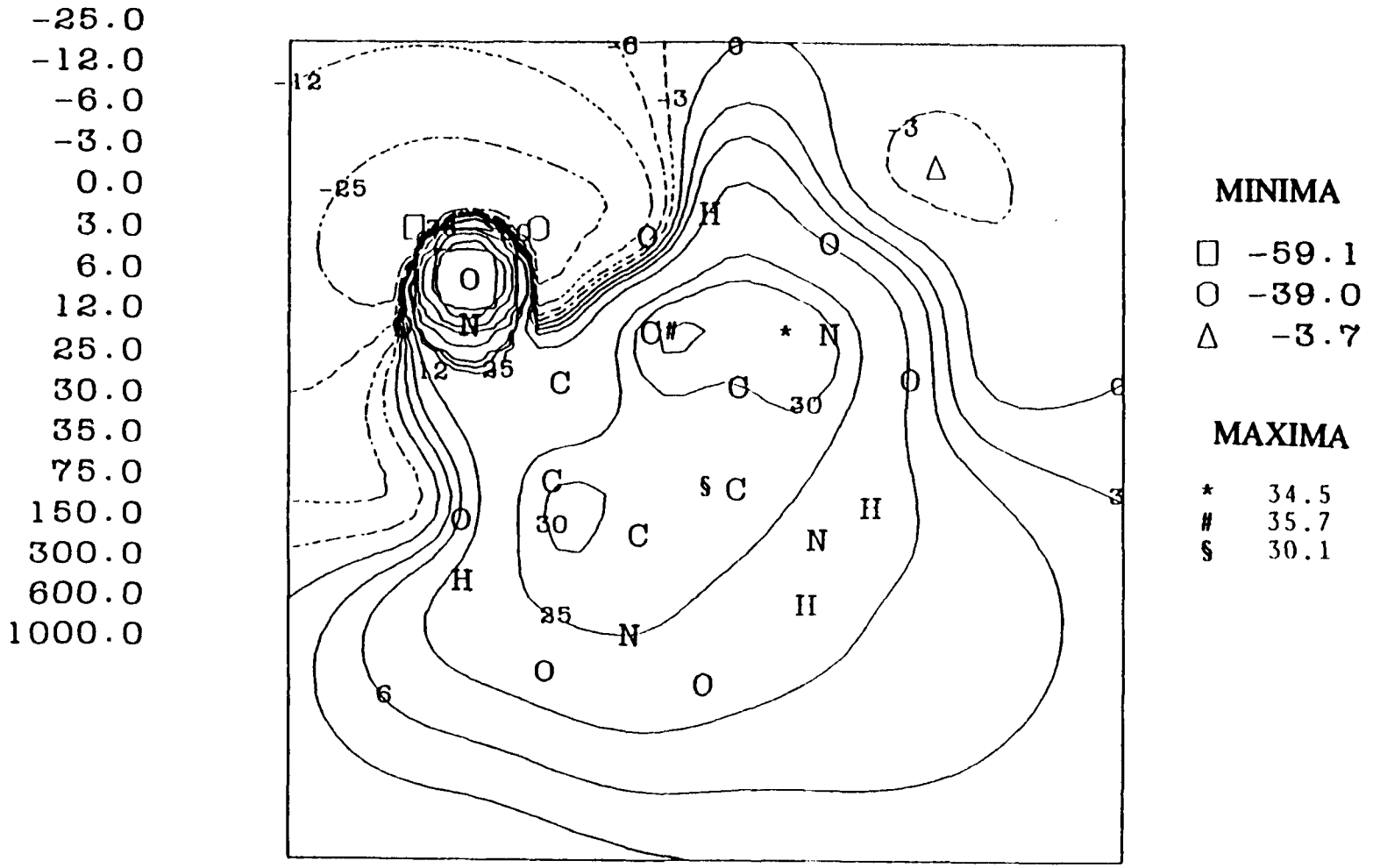


Figure NN-1. Calculated electrostatic potential, in kcal/mole, of 2,4,6-trinitro-3,5-dihydroxyaniline, in the plane 1.75Å above the N7 nitro group located in the upper left corner. Projected positions of nuclei are shown. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

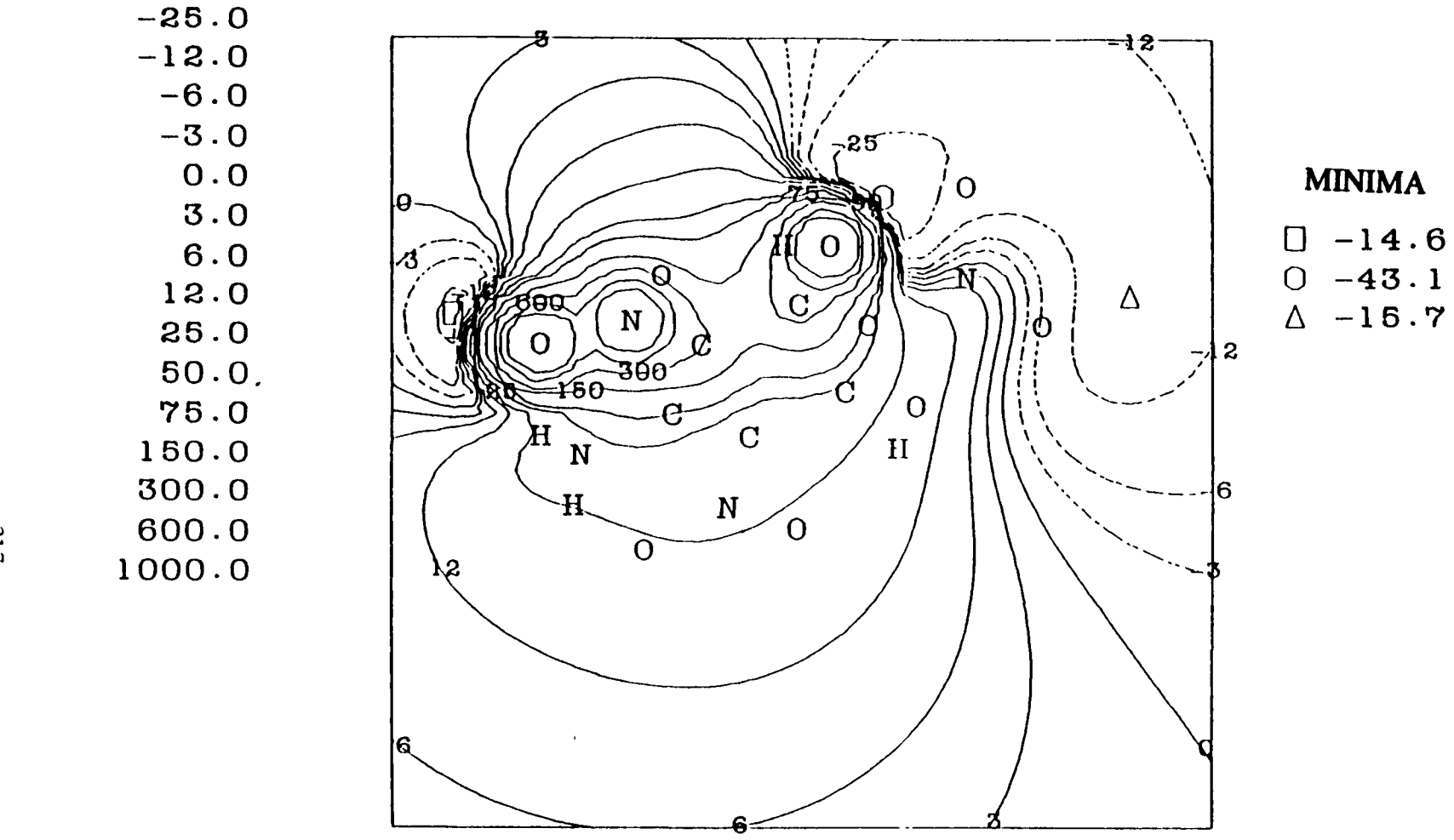
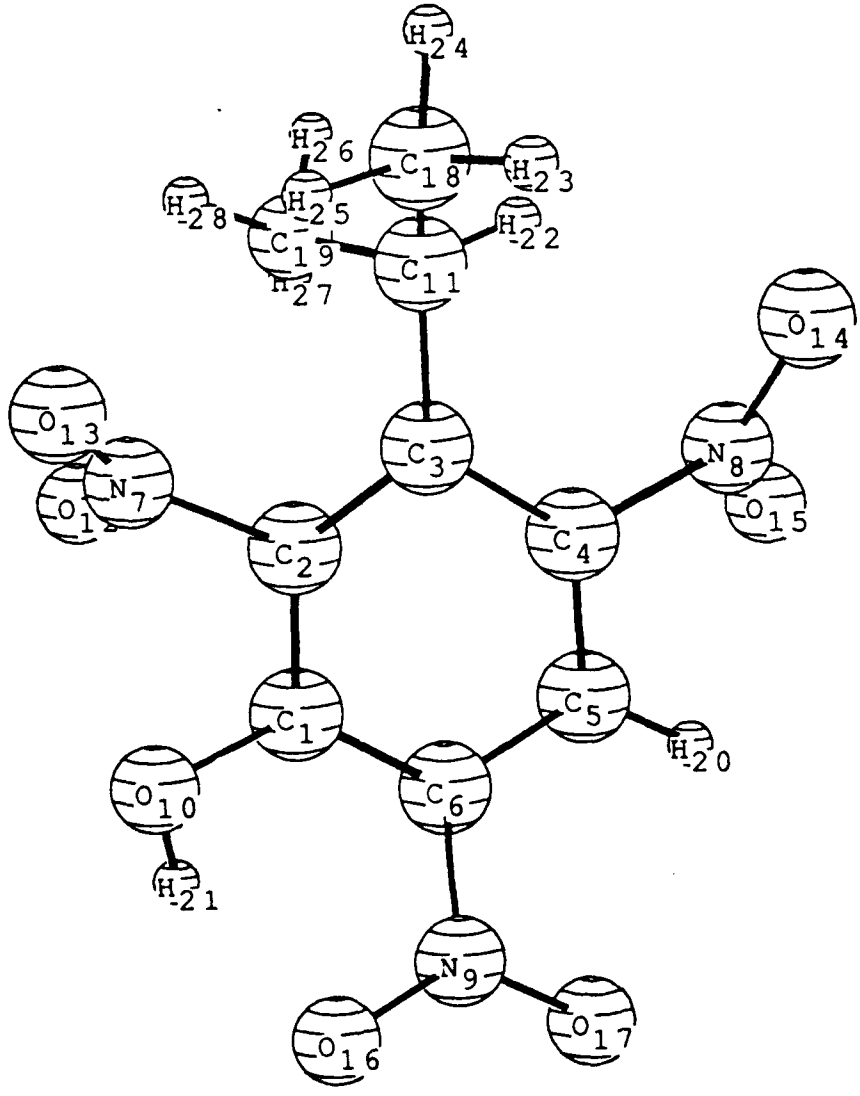


Figure NN-2. Calculated electrostatic potential, in kcal/mole, of 2,4,6-trinitro-3,5-dihydroxyaniline, in the plane 1.75Å above the N8 nitro group located in the upper right corner. Projected positions of nuclei are shown. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

APPENDIX OO
1-HYDROXY-3-ISOPROPYL-2,4,6-TRINITROBENZENE

The short distances between non-bonded hydrogens and oxygens are H21-O16 (1.89 Å), H20-O17 (2.46 Å) and H22-O14 (2.51 Å).

The N7 nitro group is rotated out of the plane by about 80° and the N8 nitro group is rotated by about 55°, while the N9 nitro group is essentially planar.



Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.388000(1)					
3	3	C	2	1.387669(2)	1	125.921(28)			
4	4	C	3	1.405766(3)	2	112.354(29)	1	4.635(54)	0
5	5	C	4	1.358591(4)	3	125.030(30)	2	-1.979(55)	0
6	6	C	5	1.383269(5)	4	119.124(31)	3	-1.896(56)	0
7	7	N	2	1.485838(6)	3	121.698(32)	4	-178.485(57)	0
8	8	N	4	1.480845(7)	5	114.723(33)	6	177.753(58)	0
9	9	N	6	1.457886(8)	5	116.408(34)	4	-176.960(59)	0
10	10	O	1	1.338471(9)	2	116.876(35)	3	175.275(60)	0
11	11	C	3	1.516254(10)	2	124.647(36)	1	-175.831(61)	0
12	12	O	7	1.213447(11)	2	117.125(37)	3	102.887(62)	0
13	13	O	7	1.207865(12)	2	117.419(38)	3	-79.577(63)	0
14	14	O	8	1.210975(13)	4	118.600(39)	3	55.976(64)	0
15	15	O	8	1.215999(14)	4	117.321(40)	3	-126.918(65)	0
16	16	O	9	1.235425(15)	6	117.244(41)	5	176.488(66)	0
17	17	O	9	1.202063(16)	6	119.247(42)	5	-3.129(67)	0
18	18	C	11	1.544227(17)	3	110.25 (43)	2	84.399(68)	0
19	19	C	11	1.531956(18)	3	115.001(44)	2	-42.333(69)	0
20	20	H	5	0.978625(19)	4	118.069(45)	3	175.972(70)	0
21	21	H	10	0.793650(20)	1	104.145(46)	2	179.251(71)	0
22	22	H	11	0.960347(21)	3	108.571(47)	4	21.738(72)	0
23	23	H	18	0.959416(22)	11	111.938(48)	3	53.237(73)	0
24	24	H	18	0.960172(23)	11	108.037(49)	3	173.942(74)	0
25	25	H	18	0.960073(24)	11	108.334(50)	3	-67.580(75)	0
26	26	H	19	0.960102(25)	11	107.446(51)	3	-166.508(76)	0
27	27	H	19	0.960241(26)	11	110.618(52)	3	-47.132(77)	0
28	28	H	19	0.960081(27)	11	110.504(53)	3	74.208(78)	0

STOICHIOMETRY C9H9N3O7

CF DONE: E(RHF) = -1028.63602740 A.U. AFTER 22 CYCLES

Alpha eigenvalues -- -0.33832 -0.33330 -0.31251 -0.30798 0.11642

Estimated ionization potential: 8.39 ev

Total atomic charges:

		1
1	C	0.192208
2	C	0.068542
3	C	0.064438
4	C	0.079993
5	C	-0.049027
6	C	0.052344
7	N	0.186430
8	N	0.172991
9	N	0.176261
10	O	-0.379352
11	C	-0.034239
12	O	-0.190142
13	O	-0.194737
14	O	-0.196555
15	O	-0.197313
16	O	-0.230134
17	O	-0.167135
18	C	-0.299204
19	C	-0.303012
20	H	0.140570
21	H	0.350573
22	H	0.100882
23	H	0.111085
24	H	0.109257
25	H	0.111096
26	H	0.110161
27	H	0.105843
28	H	0.108075

Dipole moment (Debye):
X= -0.6133 Y= 0.5527 Z= -0.0293 Tot= 0.8261

V-mid: C2-N7: 0.182
C4-N8: 0.181
C6-N9: 0.165

Bond Order: C2-N7: 1.20
C4-N8: 1.21
C6-N9: 1.27
N7-O12: 1.97
N7-O13: 2.00
N8-O14: 1.98
N8-O15: 1.96
N9-O16: 1.87
N9-O17: 2.03

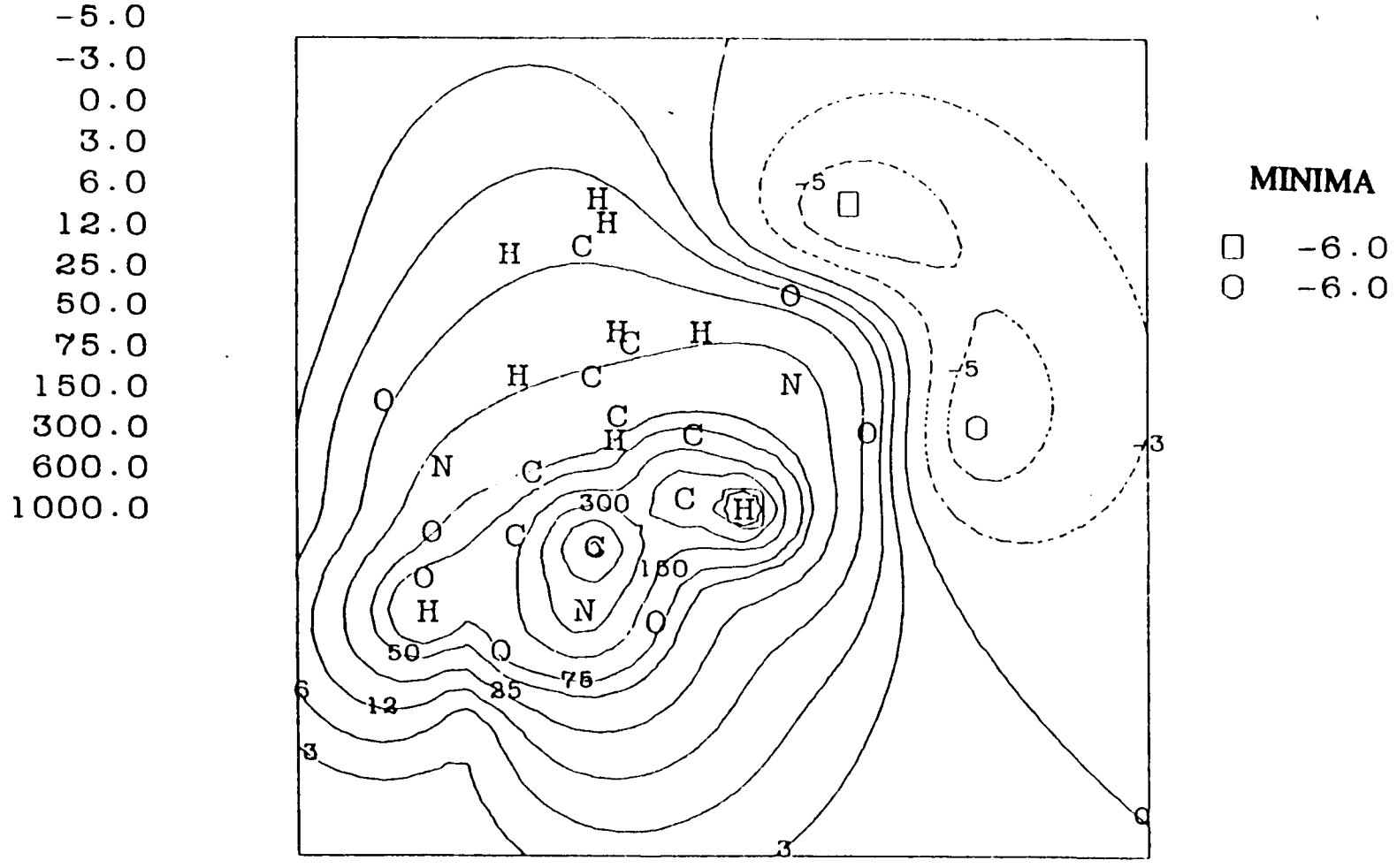


Figure OO-1. Calculated electrostatic potential, in kcal/mole, of 1-hydroxy-3-isopropyl-2,4,6-trinitrobenzene, in the plane 1.75Å above the N8 nitro group located in the upper right corner. Projected positions of nuclei are shown. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

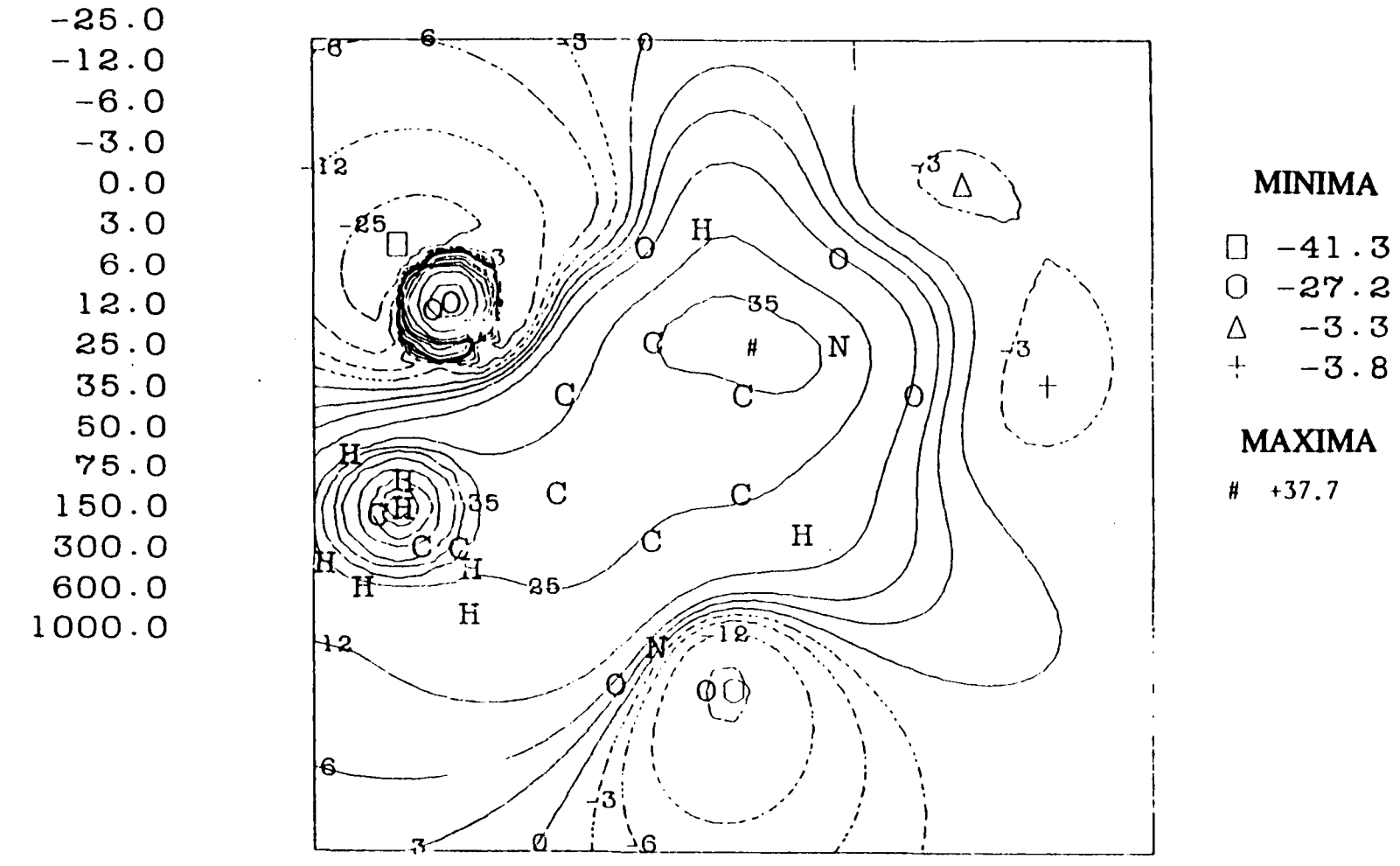
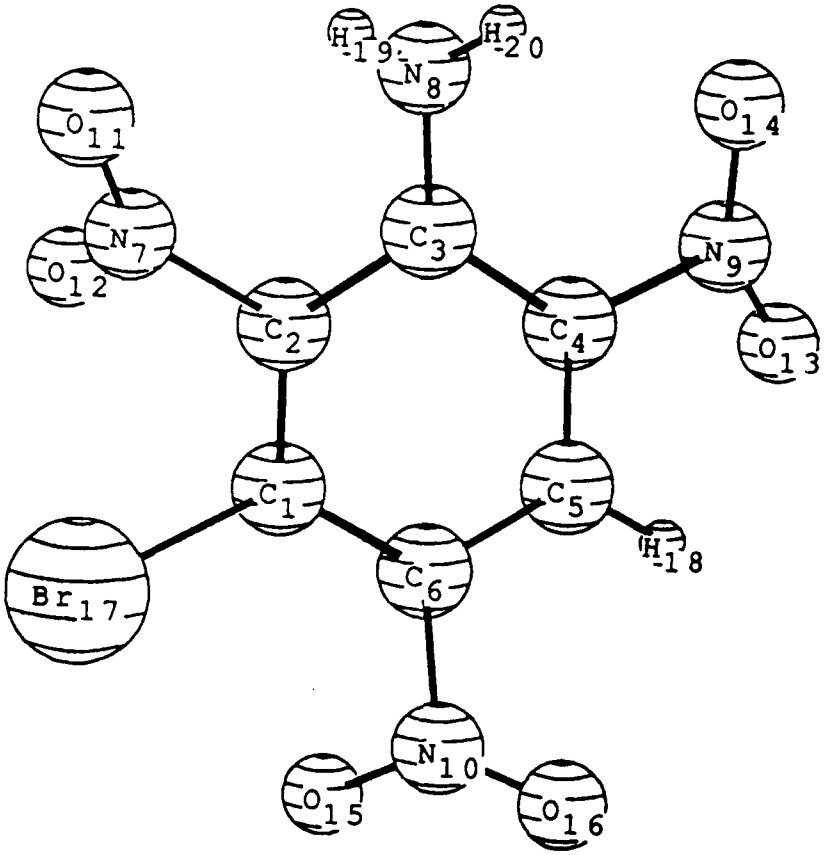


Figure OO-2. Calculated electrostatic potential, in kcal/mole, of 1-hydroxy-3-isopropyl-2,4,6-trinitrobenzene, in the plane 1.75Å above the N9 nitro group located in the upper right corner. Projected positions of nuclei are shown. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

APPENDIX PP
3-BROMO-2,4,6-TRINITROANILINE

The short distances between non-bonded hydrogens and oxygens are H18-O13 (2.36 Å), H20-O14 (2.08 Å) and H19-O11 (2.43 Å).

The N7, N9 and N10 nitro groups are rotated by approximately 65°, 18°, and 28°, respectively.



Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.372000(1)					
3	3	C	2	1.424368(2)	1	124.674(20)			
4	4	C	3	1.405510(3)	2	113.461(21)	1	7.533(38)	0
5	5	C	4	1.366465(4)	3	122.424(22)	2	-7.636(39)	0
6	6	C	5	1.369559(5)	4	120.969(23)	3	3.834(40)	0
7	7	N	2	1.477968(6)	3	116.350(24)	4	-173.750(41)	0
8	8	N	3	1.346803(7)	2	121.284(25)	1	-174.924(42)	0
9	9	N	4	1.454183(8)	5	116.924(26)	6	-176.688(43)	0
10	10	N	6	1.473321(9)	5	116.102(27)	4	-178.449(44)	0
11	11	O	7	1.204854(10)	2	117.583(28)	1	115.162(45)	0
12	12	O	7	1.209212(11)	2	117.654(29)	1	-66.867(46)	0
13	13	O	9	1.212505(12)	4	117.722(30)	5	18.395(47)	0
14	14	O	9	1.216814(13)	4	119.350(31)	5	-162.578(48)	0
15	15	O	10	1.224901(14)	6	118.331(32)	5	-149.334(49)	0
16	16	O	10	1.218068(15)	6	117.218(33)	5	27.587(50)	0
17	17	Br	1	1.878236(16)	2	118.492(34)	3	172.183(51)	0
18	18	H	5	0.922872(17)	4	119.131(35)	3	-177.317(52)	0
19	19	H	8	0.677042(18)	3	118.041(36)	2	0.621(53)	0
20	20	H	8	0.732741(19)	3	115.600(37)	2	174.196(54)	0

STOICHIOMETRY C6H3BrN4O6

SCF DONE: E(RHF) = -3450.13321750 A.U. AFTER 27 CYCLES

Alpha eigenvalues — -0.33612 -0.32384 -0.32244 -0.31168 0.11827

Estimated ionization potential: 8.49 ev

Total atomic charges:

		1
1	C	-0.017044
2	C	0.069692
3	C	0.241481
4	C	0.072043
5	C	-0.058216
6	C	0.081735
7	N	0.176424
8	N	-0.761201
9	N	0.176836
10	N	0.171671
11	O	-0.195344
12	O	-0.183900
13	O	-0.186679
14	O	-0.211035
15	O	-0.186568
16	O	-0.191160
17	Br	0.112995
18	H	0.152885
19	H	0.367661
20	H	0.367844

Dipole moment (Debye):

X= 0.8162 Y= -1.3947 Z= -0.5005 Tot= 1.6917

V-mid: C2-N7: 0.176
C4-N8: 0.181
C6-N9: 0.183

Bond Order: C2-N7: 1.22
C4-N8: 1.28
C6-N9: 1.23
N7-O11: 2.01
N7-O12: 1.99
N8-O13: 1.97
N9-O14: 1.95
N10-O15: 1.91
N10-O16: 1.95

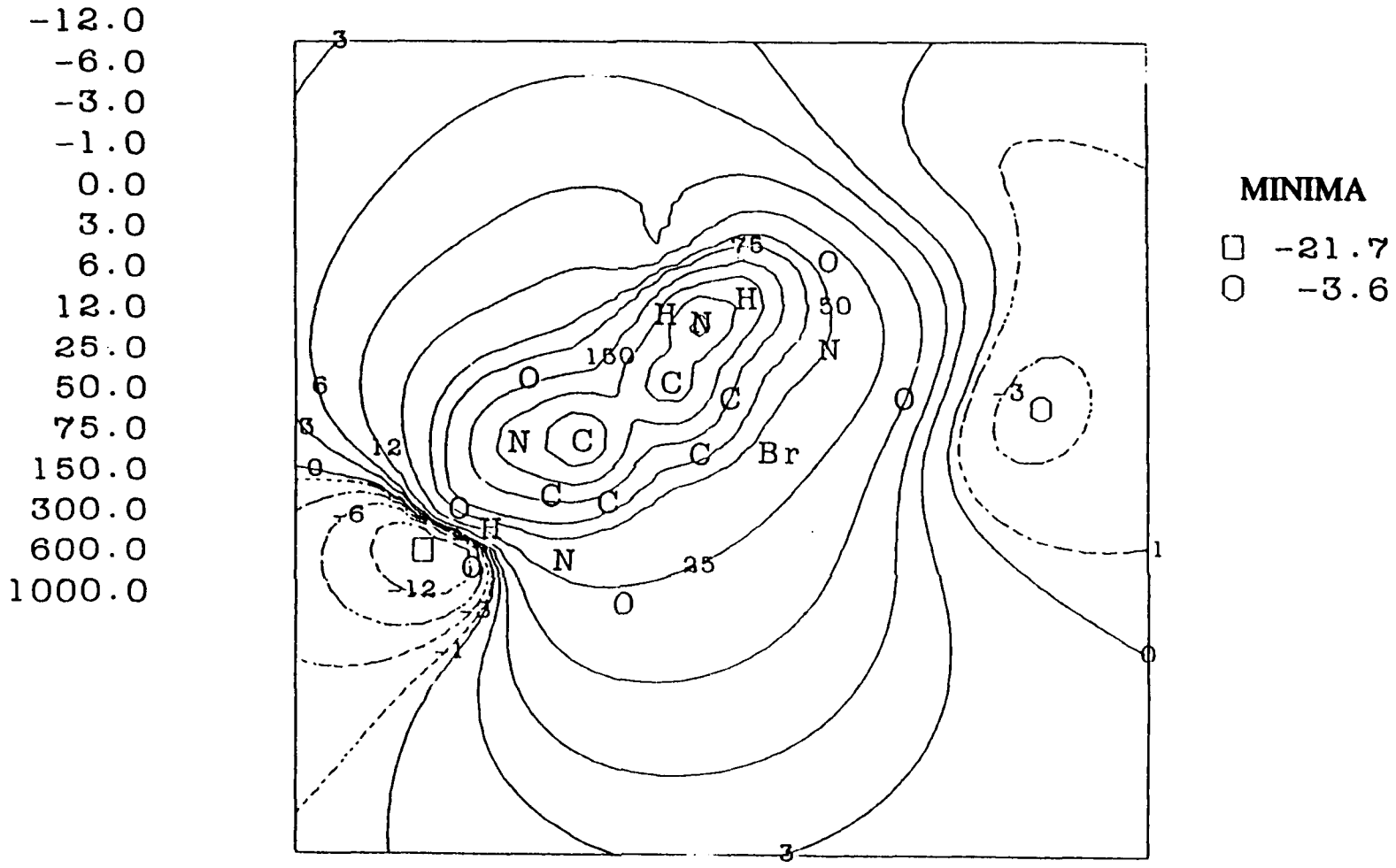


Figure PP-1. Calculated electrostatic potential, in kcal/mole, of 3-bromo-2,4,6-trinitroaniline, in the plane 1.75Å above the N7 nitro group located in the upper right corner. Projected positions of nuclei are shown. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

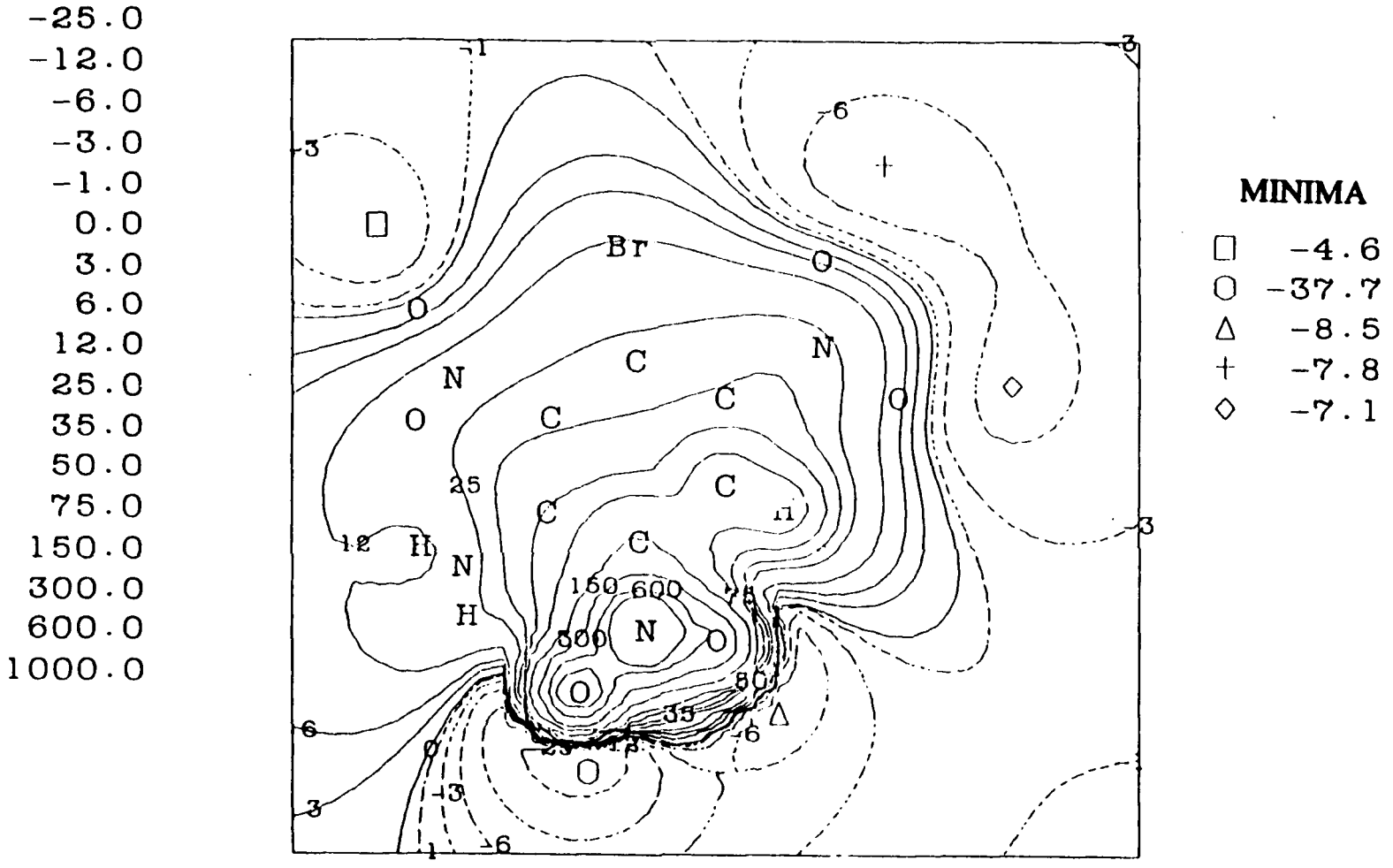
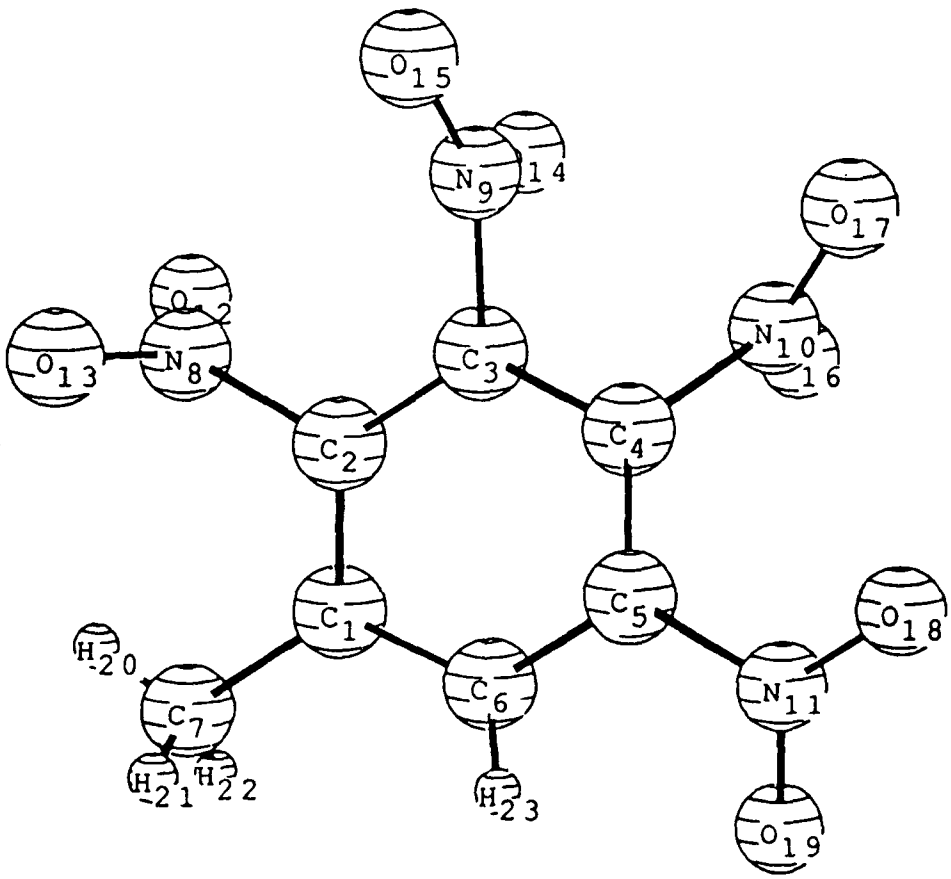


Figure PP-2. Calculated electrostatic potential, in kcal/mole, of 3-bromo-2,4,6-trinitroaniline, in the plane 1.75Å above the N10 nitro group located in the upper right corner. Projected positions of nuclei are shown. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

APPENDIX QQ
2,3,4,5-TETRANITROTOLUENE

The short distances between a non-bonded hydrogen and oxygen are H20-O13 (2.41 Å) and H23-O19 (2.37 Å).

The N8, N9, N10 and N11 nitro groups are rotated out of the mean plane of the benzene ring by about 52°, 57°, 70° and 17°, respectively.



Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.386000(1)					
3	3	C	2	1.389914(2)	1	122.670(23)			
4	4	C	3	1.386169(3)	2	120.086(24)	1	-0.531(44)	0
5	5	C	4	1.388959(4)	3	117.977(25)	2	-1.559(45)	0
6	6	C	5	1.372667(5)	4	121.030(26)	3	1.832(46)	0
7	7	C	1	1.499494(6)	2	123.471(27)	3	-175.907(47)	0
8	8	N	2	1.476841(7)	3	117.175(28)	4	-175.195(48)	0
9	9	N	3	1.469061(8)	4	119.387(29)	5	177.288(49)	0
10	10	N	4	1.472367(9)	5	123.988(30)	6	-177.134(50)	0
11	11	N	5	1.476757(10)	4	121.230(31)	3	-176.260(51)	0
12	12	O	8	1.220058(11)	2	116.667(32)	3	52.701(52)	0
13	13	O	8	1.220096(12)	2	117.668(33)	3	-127.694(53)	0
14	14	O	9	1.215757(13)	3	117.034(34)	4	56.748(54)	0
15	15	O	9	1.213007(14)	3	116.934(35)	4	-121.648(55)	0
16	16	O	10	1.203945(15)	4	117.557(36)	5	70.280(56)	0
7	17	O	10	1.215721(16)	4	116.552(37)	5	-111.938(57)	0
18	18	O	11	1.218650(17)	5	116.738(38)	6	-161.648(58)	0
19	19	O	11	1.207000(18)	5	118.200(39)	6	16.600(59)	0
20	20	H	7	0.960042(19)	1	111.415(40)	2	10.127(60)	0
21	21	H	7	0.959226(20)	1	108.817(41)	2	-110.677(61)	0
22	22	H	7	0.960381(21)	1	108.144(42)	2	130.423(62)	0
23	23	H	6	0.899000(22)	5	117.121(43)	4	178.993(63)	0

STOICHIOMETRY C7H4N4O8

SCF DONE: E(RHF) = -1078.84669927 A.U. AFTER 23 CYCLES

Alpha eigenvalues -- -0.33526 -0.33225 -0.32882 -0.32413 0.09313

Estimated ionization potential: 8.83 ev

Total atomic charges:

		1
1	C	0.086743
2	C	0.104312
3	C	0.117021
4	C	0.111062
5	C	0.120064
6	C	-0.090093
7	C	-0.314426
8	N	0.173332
9	N	0.182791
10	N	0.194078
11	N	0.183363
12	O	-0.180278
13	O	-0.174823
14	O	-0.168316
15	O	-0.170357
16	O	-0.163796
17	O	-0.177225
18	O	-0.180773
19	O	-0.180193
20	H	0.129860
21	H	0.132950
22	H	0.127817
23	H	0.136886

Dipole moment (Debye):

X= -1.1539 Y= 6.0775 Z= 0.1396 Tot= 6.1877

V-mid: C2-N8: 0.198
C3-N9: 0.216
C4-N10: 0.220
C5-N11: 0.217

Bond Order: C2-N8: 1.22
C3-N9: 1.24
C4-N10: 1.23
C5-N11: 1.22
N8-O12: 1.94
N8-O13: 1.94
N9-O14: 1.96
N9-O15: 1.97
N10-O16: 2.02
N10-O17: 1.96
N11-O18: 1.94
N11-O19: 2.00

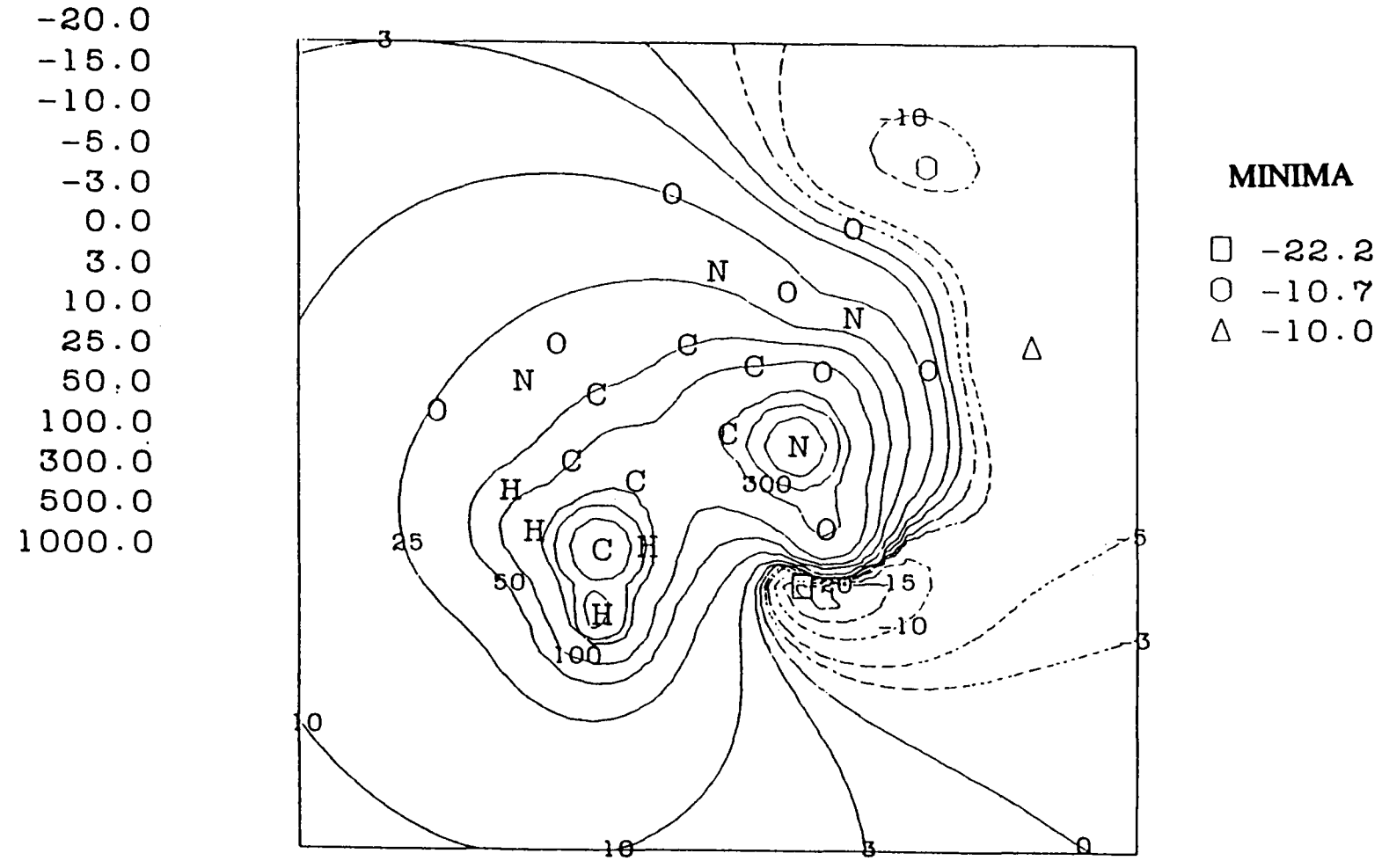


Figure QQ-1. Calculated electrostatic potential, in kcal/mole, of 2,3,4,5-tetranitrotoluene, in the plane 1.75Å above the N9 nitro group located in the upper right corner. Projected positions of nuclei are shown. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

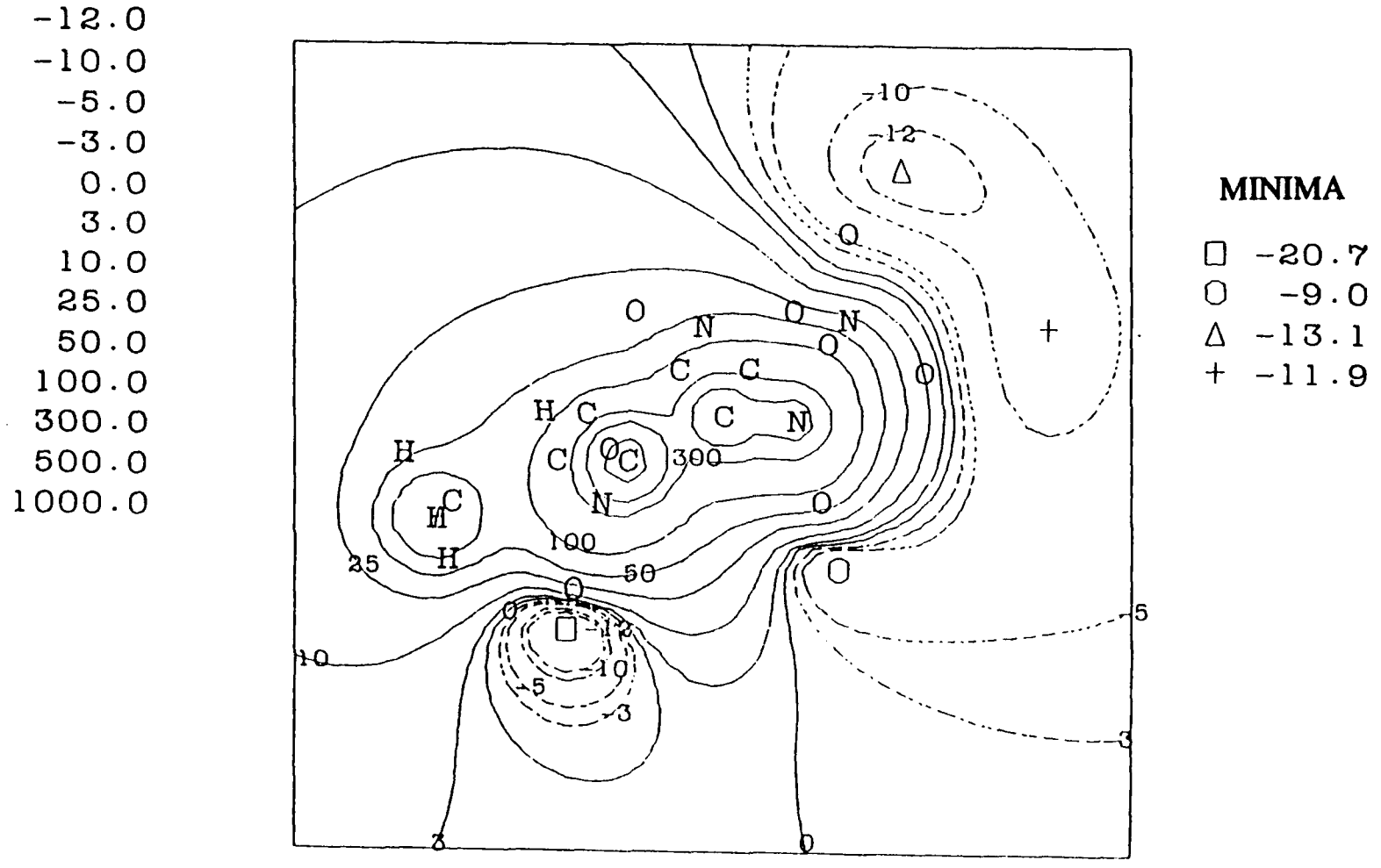
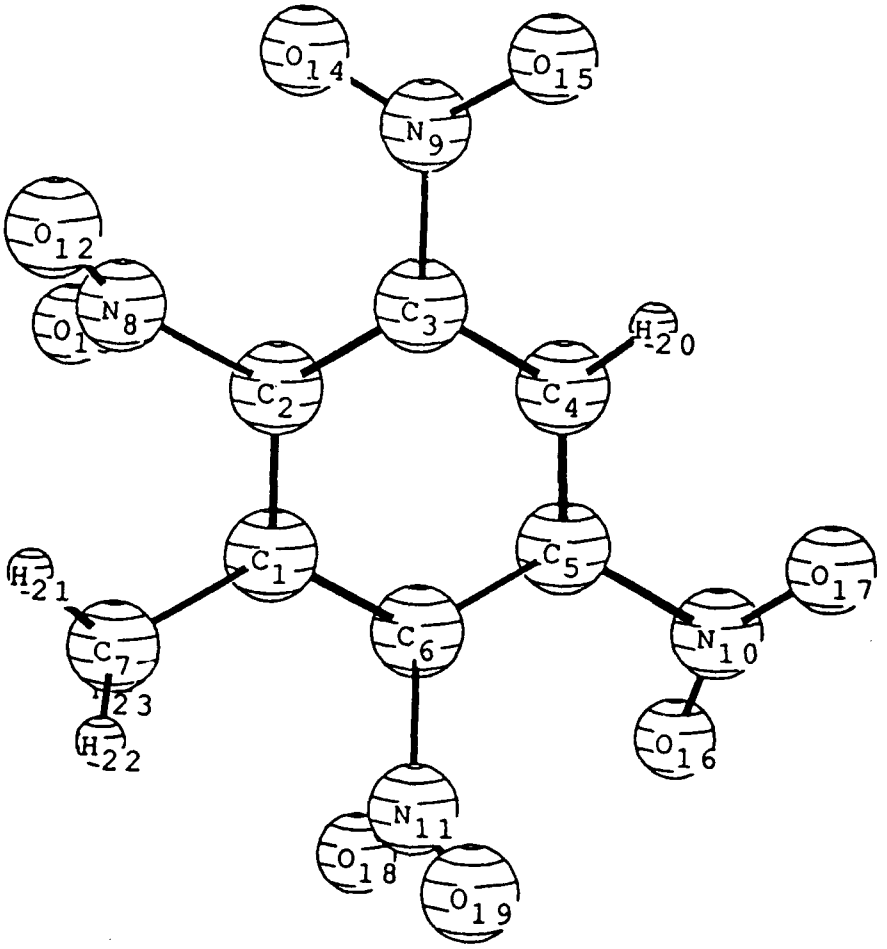


Figure QQ-2. Calculated electrostatic potential, in kcal/mole, of 2,3,4,5-tetranitrotoluene, in the plane 1.75Å above the N10 nitro group located in the upper right corner. Projected positions of nuclei are shown. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

APPENDIX RR
2,3,5,6-TETRANITROTOLUENE

The short non-bonded oxygen hydrogen distance is H20-O15 (2.36 Å).

The N8, N9, N10, and N11 nitro groups are both rotated by approximately 80°, 15°, 32° and 70°, respectively.



Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.400000(1)					
3	3	C	2	1.381443(2)	1	121.398(23)			
4	4	C	3	1.373904(3)	2	120.468(24)	1	2.503(44)	0
5	5	C	4	1.345872(4)	3	119.936(25)	2	-1.597(45)	0
6	6	C	5	1.393176(5)	4	119.747(26)	3	-0.917(46)	0
7	7	C	1	1.515595(6)	2	122.117(27)	3	176.670(47)	0
8	8	N	2	1.466849(7)	3	122.671(28)	4	-178.772(48)	0
9	9	N	3	1.461898(8)	4	118.559(29)	5	178.408(49)	0
10	10	N	5	1.470476(9)	4	119.310(30)	3	-179.517(50)	0
11	11	N	6	1.483591(10)	5	120.979(31)	4	-173.462(51)	0
12	12	O	8	1.206716(11)	2	117.742(32)	3	-80.970(52)	0
13	13	O	8	1.229347(12)	2	116.005(33)	3	102.264(53)	0
14	14	O	9	1.212008(13)	3	118.626(34)	2	-14.555(54)	0
15	15	O	9	1.218880(14)	3	118.289(35)	2	164.893(55)	0
16	16	O	10	1.206272(15)	5	117.139(36)	4	-146.656(56)	0
17	17	O	10	1.190841(16)	5	117.324(37)	4	30.116(57)	0
18	18	O	11	1.213804(17)	6	117.883(38)	5	-111.442(58)	0
19	19	O	11	1.216086(18)	6	115.667(39)	5	72.188(59)	0
20	20	H	4	0.921252(19)	3	115.638(40)	2	-178.564(60)	0
21	21	H	7	0.959480(20)	1	107.768(41)	2	-7.718(61)	0
22	22	H	7	0.960219(21)	1	110.985(42)	2	-127.608(62)	0
23	23	H	7	0.960329(22)	1	109.673(43)	2	111.411(63)	0

STOICHIOMETRY C7H4N4O8

SCF DONE: E(RHF) = -1078.85136659 A.U. AFTER 23 CYCLES

Alpha eigenvalues — -0.33701 -0.33399 -0.33046 -0.32624 0.08686

ESTIMATED IONIZATION POTENTIAL: 8.88 ev

```
 Total atomic charges:
                1
  1  C    0.070719
  2  C    0.112801
  3  C    0.118821
  4  C   -0.079733
  5  C    0.116625
  6  C    0.110954
  7  C   -0.314021
  8  N    0.181539
  9  N    0.177002
 10  N    0.195248
 11  N    0.183539
 12  O   -0.170716
 13  O   -0.179174
 14  O   -0.178712
 15  O   -0.180401
 16  O   -0.188083
 17  O   -0.177373
 18  O   -0.172127
 19  O   -0.181751
 20  H    0.155393
 21  H    0.127928
 22  H    0.131383
 23  H    0.140140
 Dipole moment (Debye):
    X=     0.0105    Y=    -0.9166    Z=    -0.1413  Tot=     0.9275


 V-mid: C2-N8: 0.212
        C3-N9: 0.214
       C5-N10: 0.225
       C6-N11: 0.211


 Bond order: C2-N8: 1.24
             C3-N9: 1.27
            C5-N10: 1.24
            C6-N11: 1.21
            N8-O12: 2.00
            N8-O13: 1.90
            N9-O14: 1.98
            N9-O15: 1.94
           N10-O16: 2.01
           N10-O17: 2.04
           N11-O18: 1.97
           N11-O19: 1.96
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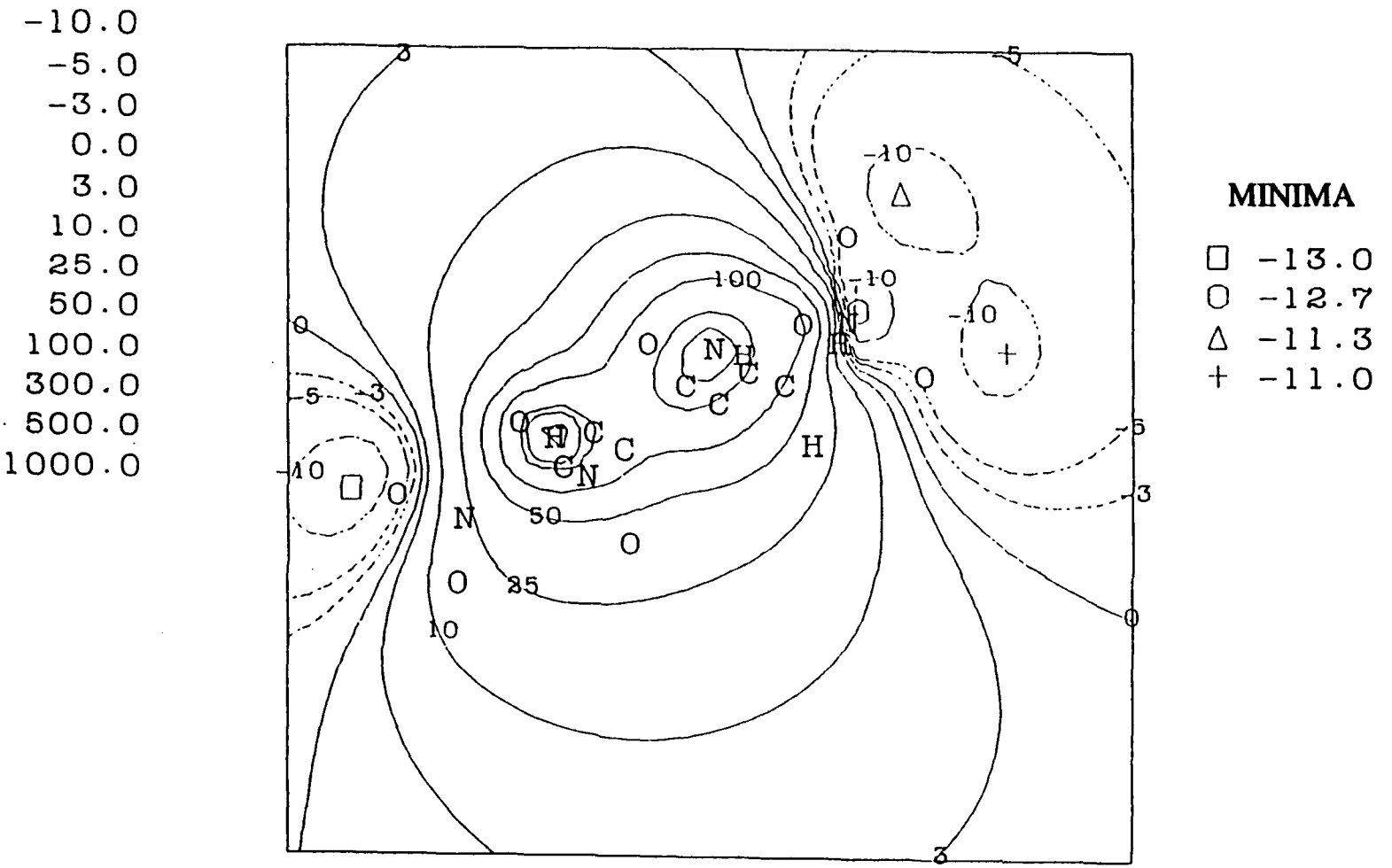


Figure RR-1. Calculated electrostatic potential, in kcal/mole, of 2,3,5,6-tetranitrotoluene, in the plane 1.75Å above the N8 nitro group located in the upper right corner. Projected positions of nuclei are shown. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

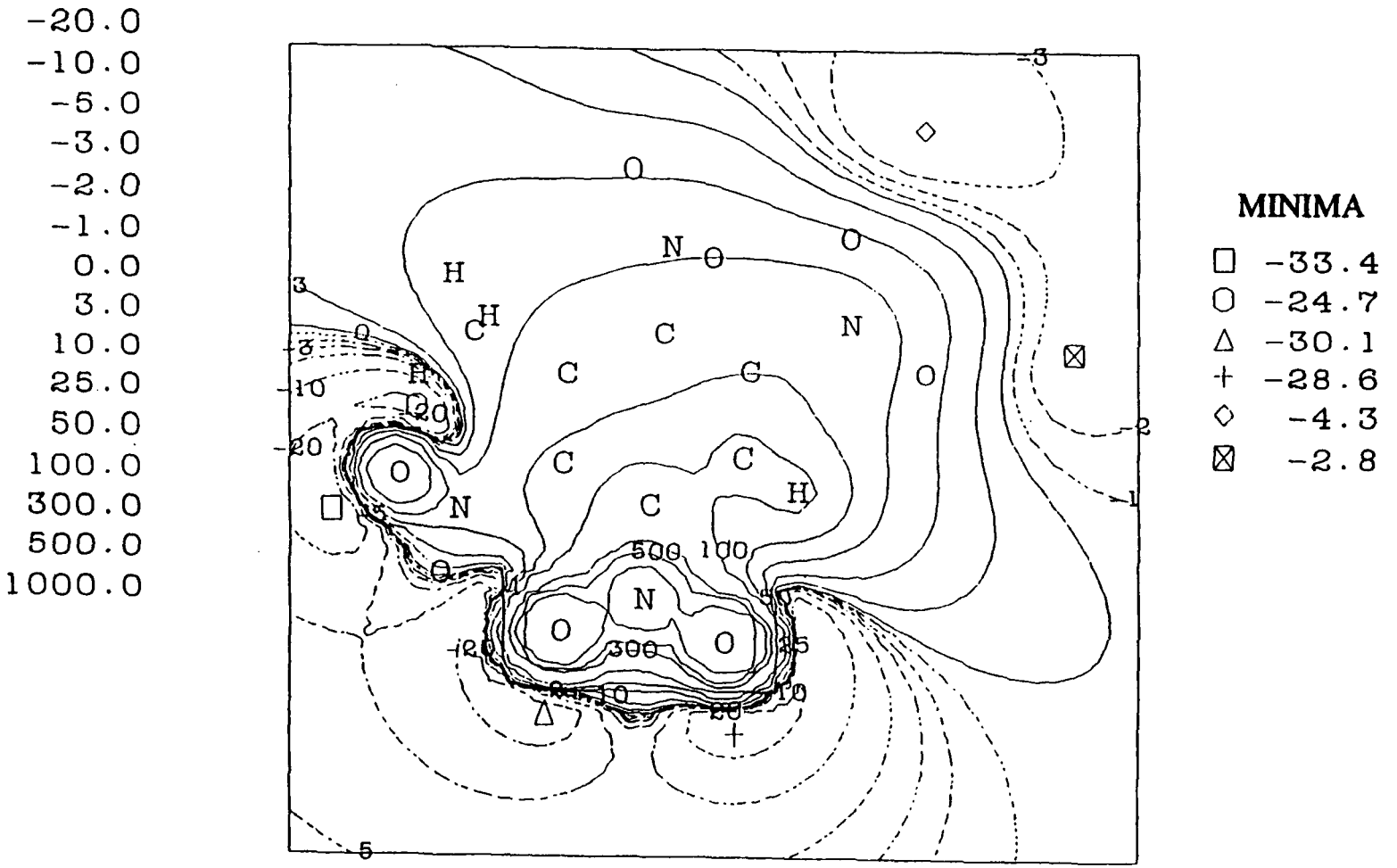
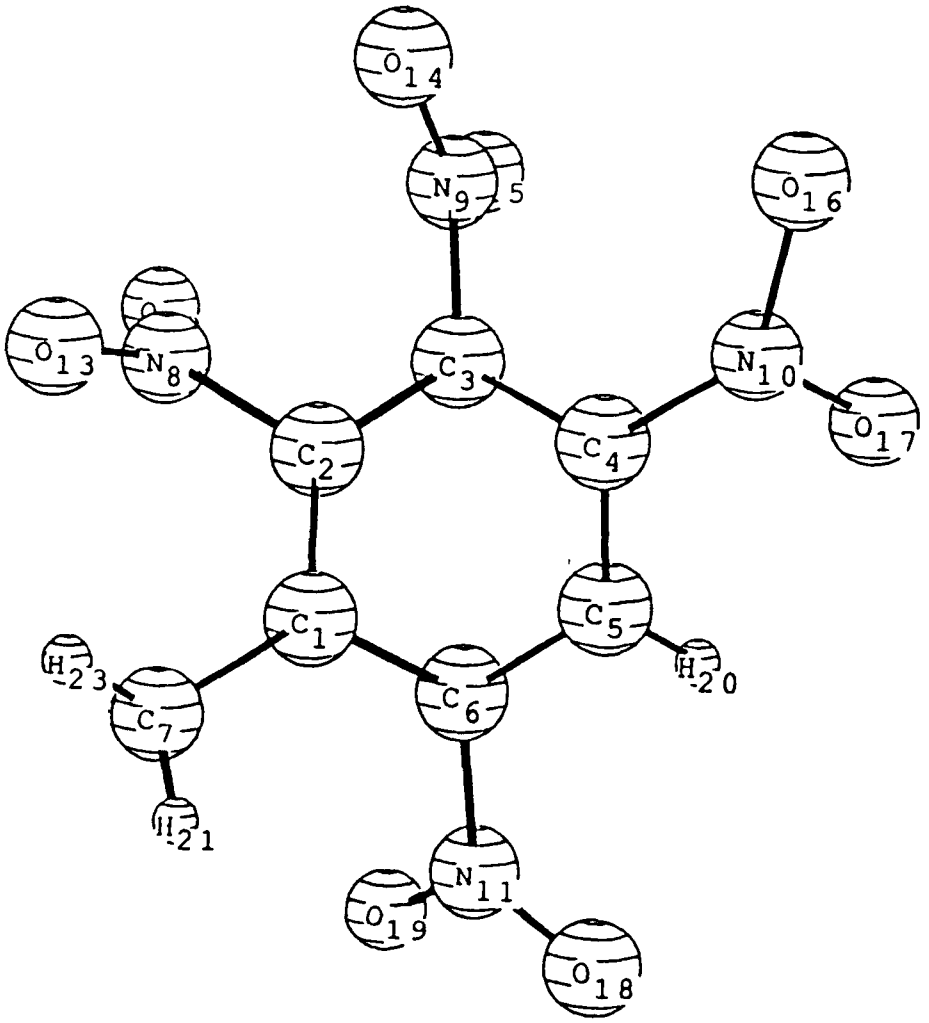


Figure RR-2. Calculated electrostatic potential, in kcal/mole, of 2,3,5,6-tetranitrotoluene, in the plane 1.75Å above the N9 nitro group located in the upper right corner. Projected positions of nuclei are shown. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

APPENDIX SS
2,3,4,6-TETRANITROTOLUENE

The short distances between non-bonded hydrogens and oxygens are H20-O17 (2.47 Å), H21-O19 (2.44 Å) and H23-O13 (2.36 Å)

The N8, N9, N10 and N11 nitro groups are rotated out of the mean plane of the benzene ring by approximately 62°, 68°, 27° and 47°, respectively.



Z-MATRIX (ANGSTROMS AND DEGREES)

CO	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.389000(1)					
3	3	C	2	1.375172(2)	1	123.720(23)			
4	4	C	3	1.383634(3)	2	119.370(24)	1	-1.863(44)	0
5	5	C	4	1.371733(4)	3	119.918(25)	2	2.169(45)	0
6	6	C	5	1.373445(5)	4	118.712(26)	3	0.223(46)	0
7	7	C	1	1.492121(6)	2	123.285(27)	3	178.926(47)	0
8	8	N	2	1.476720(7)	3	117.177(28)	4	179.615(48)	0
9	9	N	3	1.480007(8)	2	119.428(29)	1	175.896(49)	0
10	10	N	4	1.467231(9)	5	117.991(30)	6	179.848(50)	0
11	11	N	6	1.476320(10)	5	115.613(31)	4	177.197(51)	0
12	12	O	8	1.214278(11)	2	116.939(32)	3	61.362(52)	0
13	13	O	8	1.216425(12)	2	117.471(33)	3	-117.043(53)	0
14	14	O	9	1.207692(13)	3	117.447(34)	2	66.722(54)	0
15	15	O	9	1.213542(14)	3	116.207(35)	2	-111.979(55)	0
16	16	O	10	1.229370(15)	4	116.467(36)	5	-151.248(56)	0
17	17	O	10	1.197508(16)	4	118.170(37)	5	26.392(57)	0
18	18	O	11	1.204533(17)	6	117.327(38)	1	-134.095(58)	0
19	19	O	11	1.214875(18)	6	117.637(39)	1	48.037(59)	0
20	20	H	5	0.896227(19)	4	120.717(40)	3	169.875(60)	0
21	21	H	7	0.952914(20)	1	109.751(41)	2	-157.606(61)	0
22	22	H	7	0.960115(21)	1	112.638(42)	2	80.017(62)	0
23	23	H	7	0.959605(22)	1	105.684(43)	2	-39.439(63)	0

STOICHIOMETRY C7H4N4O8

SCF DONE: E(RHF) = -1078.84031213 A.U. AFTER 23 CYCLES

Alpha eigenvalues -- -0.33499 -0.33329 -0.33118 -0.32700 0.09702

Estimated ionization potential: 8.91 ev

Total atomic charges:

		1
1	C	0.081413
2	C	0.101510
3	C	0.118168
4	C	0.116989
5	C	-0.079623
6	C	0.114700
7	C	-0.322111
8	N	0.176597
9	N	0.193826
10	N	0.183033
11	N	0.178602
12	O	-0.176888
13	O	-0.177513
14	O	-0.169090
15	O	-0.168483
16	O	-0.185679
17	O	-0.173604
18	O	-0.183706
19	O	-0.190938
20	H	0.150989
21	H	0.133745
22	H	0.138560
23	H	0.139503

Dipole moment (Debye): X = -3.4811 Y = -0.6377 Z = -0.1966 Tot = 3.5445

V-mid: C2-N8: 0.200
C3-N9: 0.223
C4-N10: 0.217
C6-N11: 0.211

Bond Order: C2-N8: 1.22
C3-N9: 1.21
C4-N10: 1.25
C6-N11: 1.22
N8-O12: 1.97
N8-O13: 1.96
N9-O14: 2.00
N9-O15: 1.97
N10-O16: 1.90
N10-O17: 2.05
N11-O18: 2.02
N11-O19: 1.96

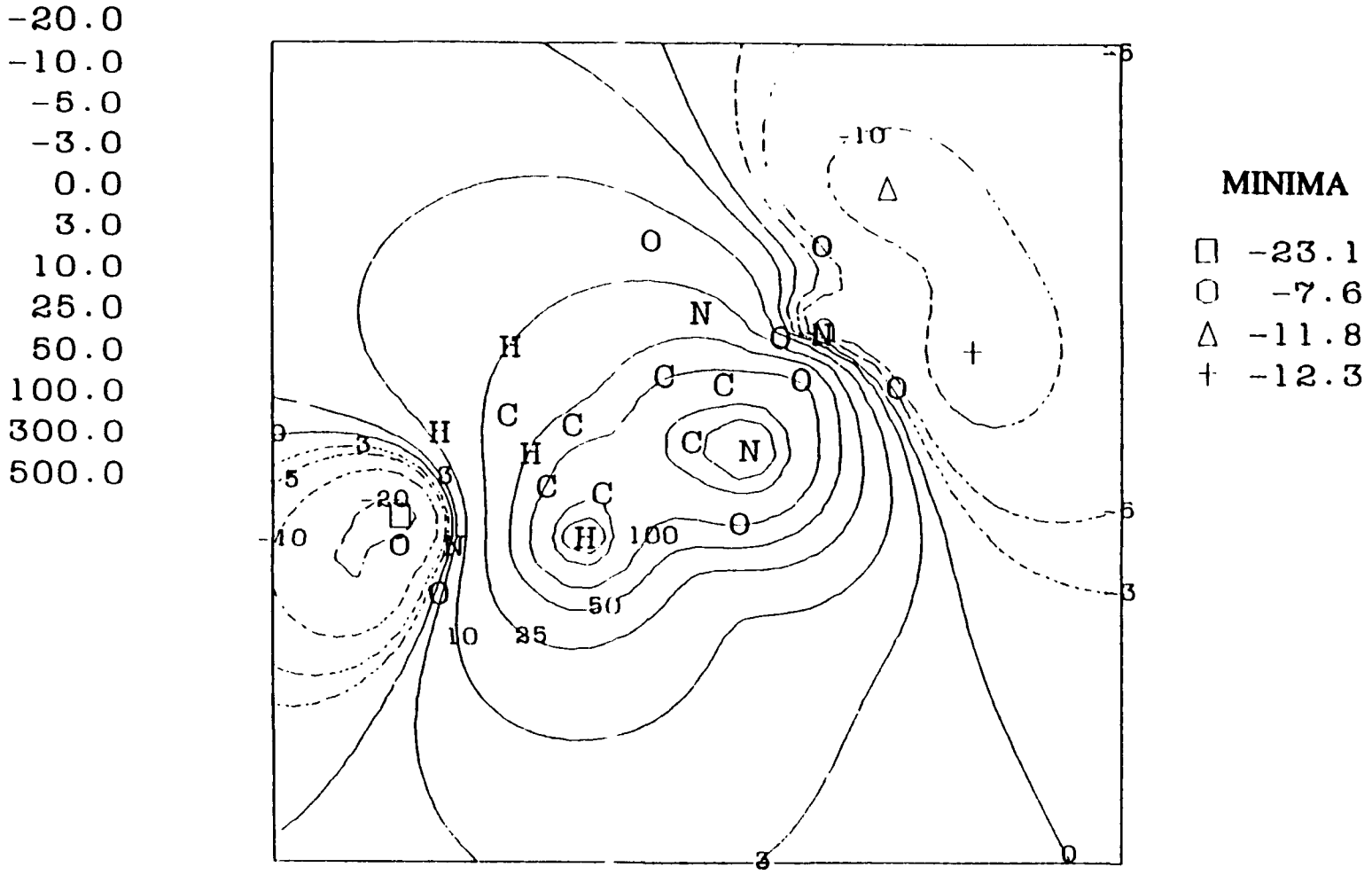


Figure SS-1. Calculated electrostatic potential, in kcal/mole, of 2,3,4,6-tetranitrotoluene, in the plane 1.75Å above the N9 nitro group located in the upper right corner. Projected positions of nuclei are shown. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

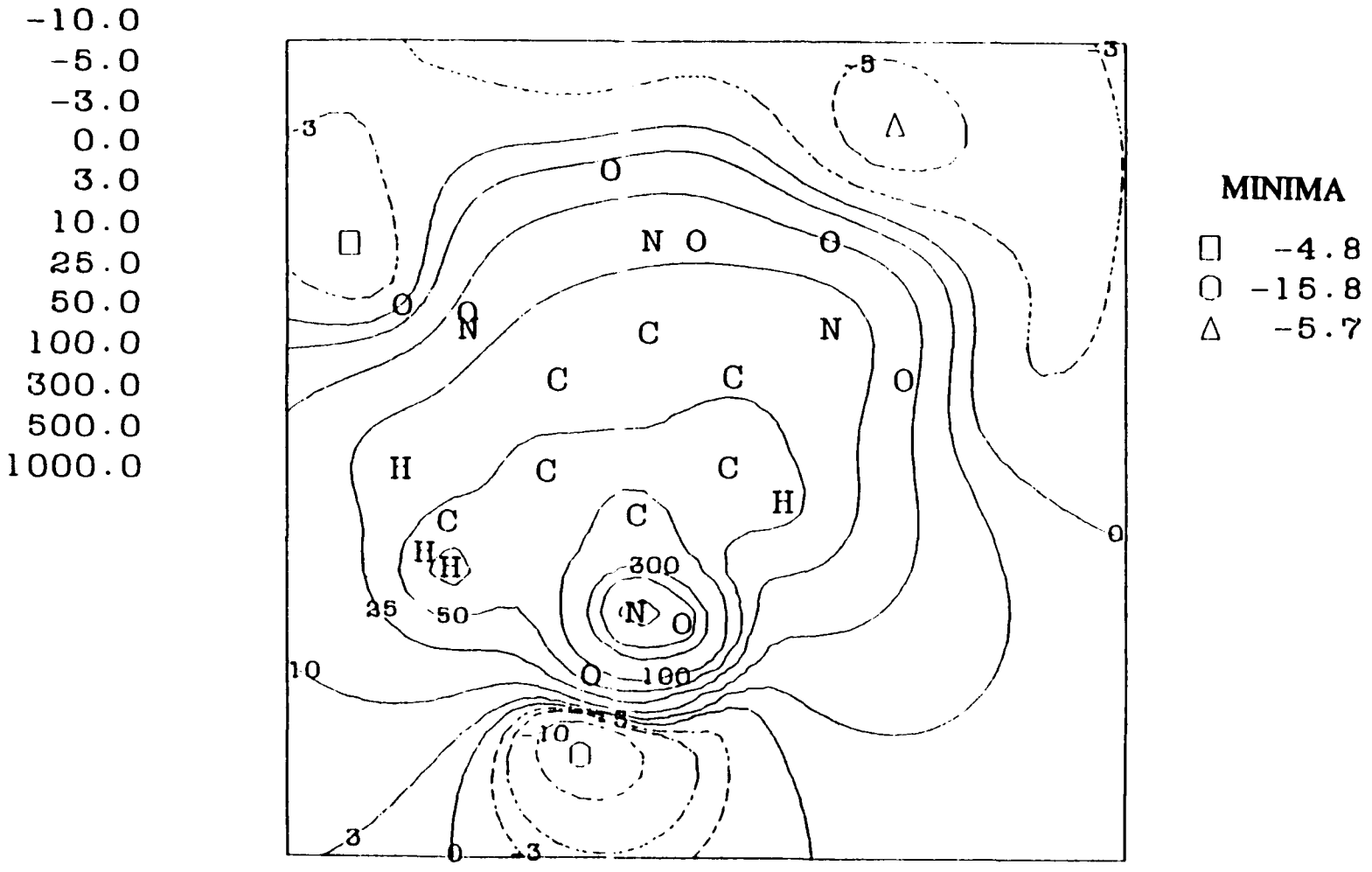
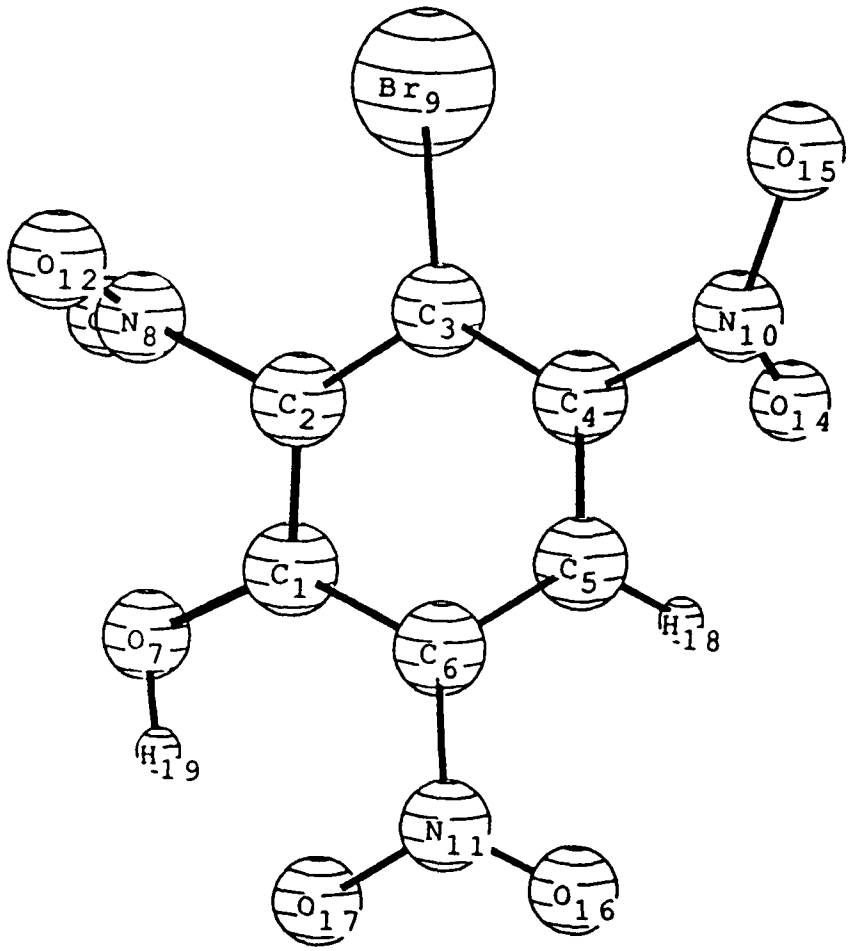


Figure SS-2. Calculated electrostatic potential, in kcal/mole, of 2,3,4,6-tetranitrotoluene, in the plane 1.75Å above the N10 nitro group located in the upper right corner. Projected positions of nuclei are shown. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

APPENDIX TT
3-BROMOPICRIC ACID

The short distances between non-bonded hydrogens and oxygens are H19-O17 (1.81 Å), H18-O16 (2.39 Å) and H18-O14 (2.46 Å)

The N10 nitro group is rotated out of the plane of the benzene ring by about 35°. The N8 nitro group is approximately perpendicular to to the ring and the N11 nitro group is approximately coplanar with the ring.



Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.393000(1)					
3	3	C	2	1.379119(2)	1	124.840(19)			
4	4	C	3	1.398896(3)	2	116.142(20)	1	-0.767(36)	0
5	5	C	4	1.370097(4)	3	121.720(21)	2	0.418(37)	0
6	6	C	5	1.378388(5)	4	119.955(22)	3	-0.908(38)	0
7	7	O	1	1.317921(6)	2	116.370(23)	3	-177.983(39)	0
8	8	N	2	1.479396(7)	3	119.965(24)	4	-178.983(40)	0
9	9	Br	3	1.871273(8)	4	125.348(25)	5	-177.755(41)	0
10	10	N	4	1.477524(9)	3	121.840(26)	2	-179.934(42)	0
11	11	N	6	1.452290(10)	5	118.380(27)	4	-178.339(43)	0
12	12	O	8	1.208843(11)	2	117.272(28)	3	-91.929(44)	0
13	13	O	8	1.209434(12)	2	116.731(29)	3	88.373(45)	0
14	14	O	10	1.212246(13)	4	117.269(30)	3	-146.439(46)	0
15	15	O	10	1.217925(14)	4	117.484(31)	3	35.977(47)	0
16	16	O	11	1.211311(15)	6	118.604(32)	5	3.421(48)	0
17	17	O	11	1.236546(16)	6	117.855(33)	5	-176.069(49)	0
18	18	H	5	0.960447(17)	4	120.034(34)	3	179.026(50)	0
19	19	H	7	0.950660(18)	1	107.542(35)	2	-178.636(51)	0

STOICHIOMETRY C6H2BrN3O7

SCF DONE: E(RHF) = -3470.25461235 A.U. AFTER 26 CYCLES

Alpha eigenvalues — -0.34290 -0.33656 -0.31560 -0.31353 0.10586

Estimated ionization potential 8.54 ev

Total atomic charges:

		1
1	C	0.201612
2	C	0.071464
3	C	-0.016561
4	C	0.080536
5	C	-0.046379
6	C	0.053573
7	O	-0.304134
8	N	0.186047
9	Br	0.118185
10	N	0.176623
11	N	0.173891
12	O	-0.185136
13	O	-0.186380
14	O	-0.193281
15	O	-0.189150
16	O	-0.160008
17	O	-0.230146
18	H	0.148479
19	H	0.300765

Dipole moment (Debye):

X= -1.6305 Y= 0.3220 Z= -0.0124 Tot= 1.6620

V-mid: C2-N8: 0.184
C4-N10: 0.185
C5-N11: 0.166

Bond Order: C2-N8: 1.22
C4-N10: 1.22
C5-N11: 1.29
N8-O12: 1.99
N8-O13: 1.99
N10-O14: 1.98
N10-O15: 1.95
N11-O16: 1.98
N11-O17: 1.86

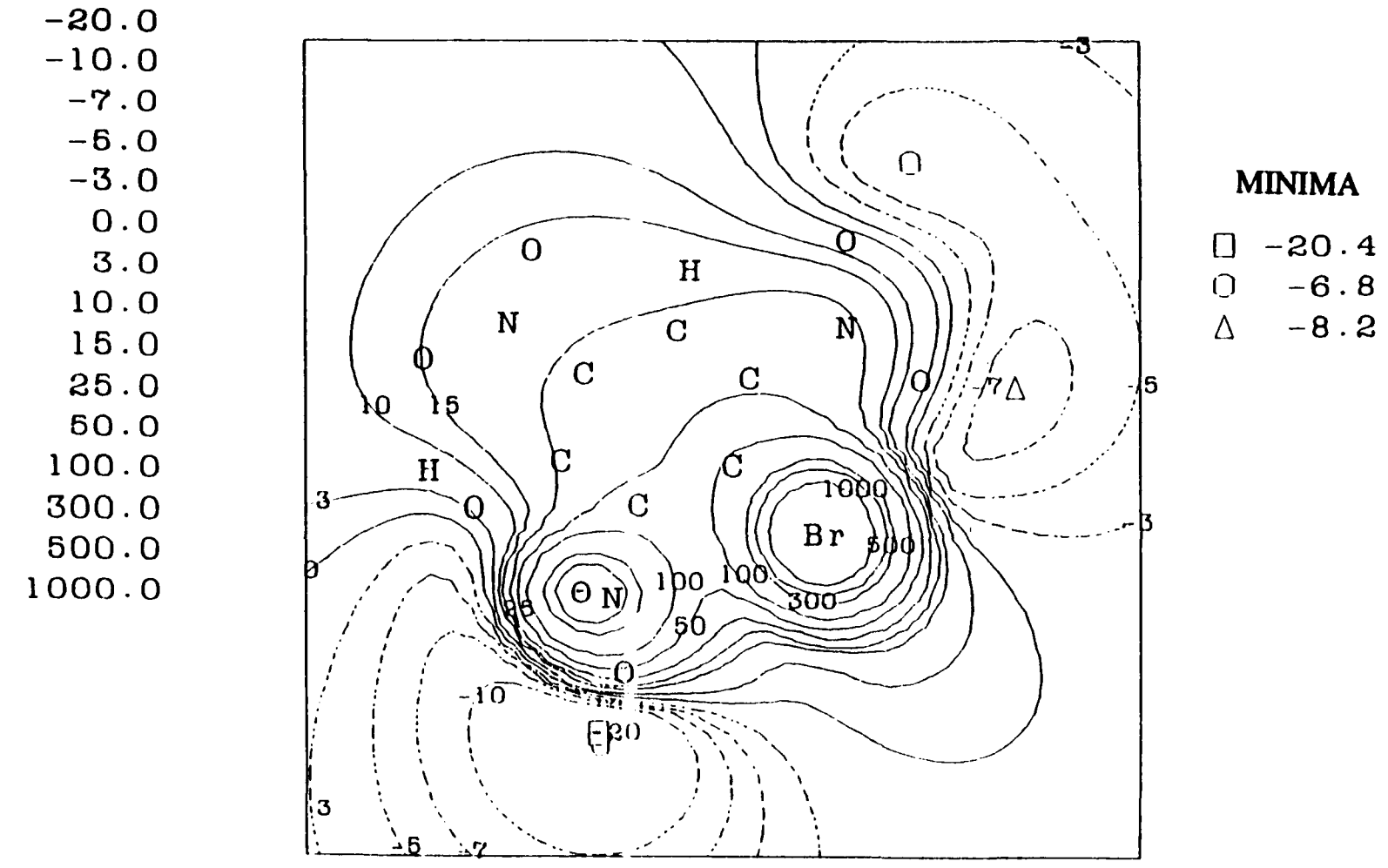


Figure TT-1. Calculated electrostatic potential, in kcal/mole, of 3-bromopicric acid, in the plane 1.75Å above the N10 nitro group located in the upper right corner. Projected positions of nuclei are shown. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

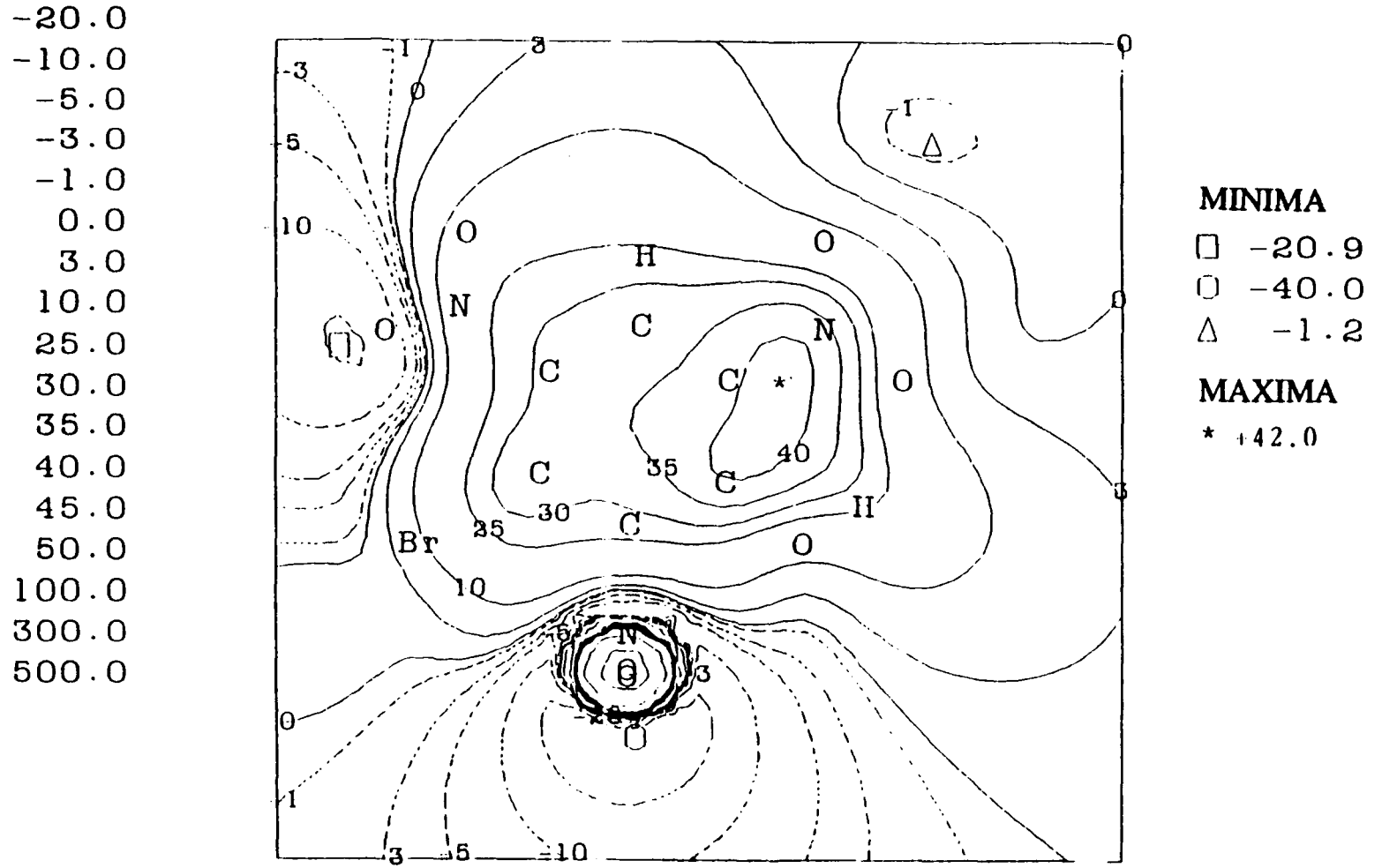
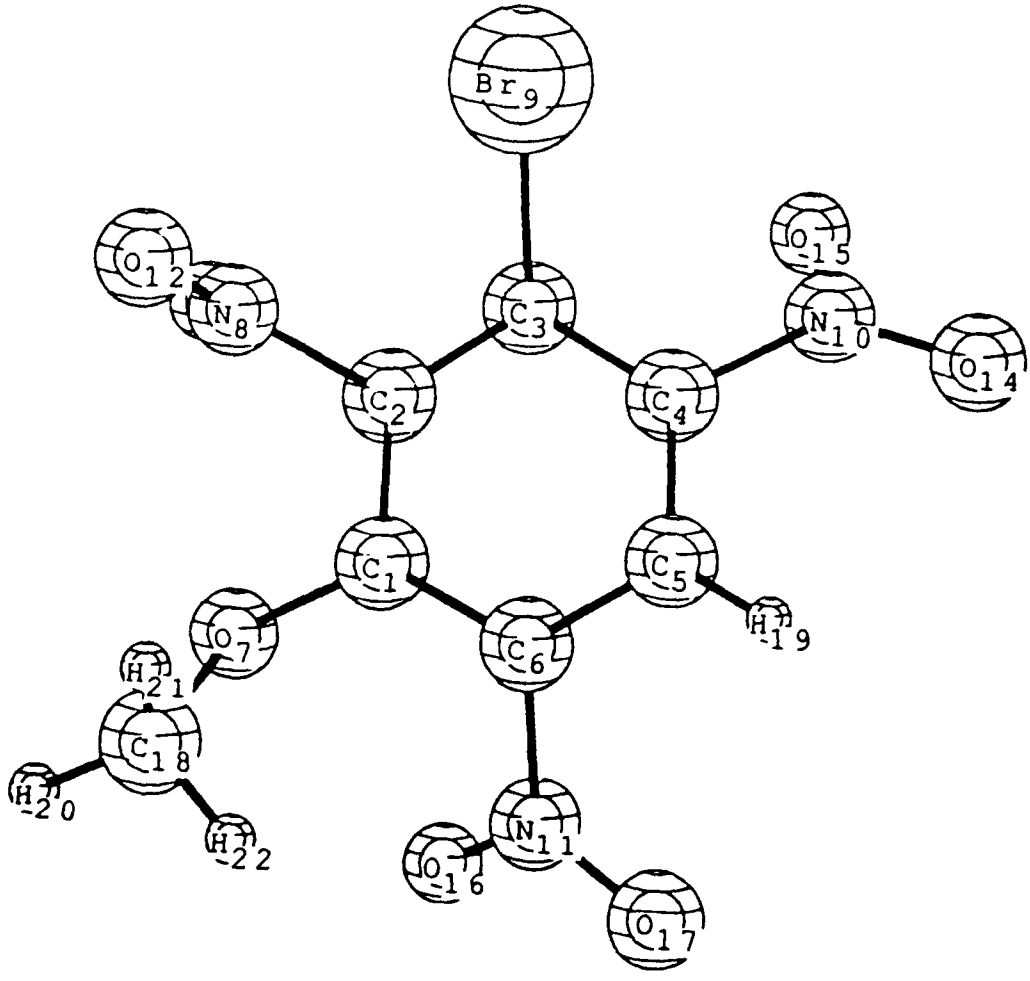


Figure TT-2. Calculated electrostatic potential, in kcal/mole, of 3-bromopicric acid, in the plane 1.75Å above the N11 nitro group located in the upper right corner. Projected positions of nuclei are shown. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

APPENDIX UU
3-BROMO-2,4,6-TRINITROANISOLE

The short distances between non-bonded hydrogens and oxygens are H19-O14 (2.45 Å), H19-O17 (2.49 Å) and H22-O16 (2.47 Å)

The N8 nitro group is essentially perpendicular to the mean plane of the benzene ring, while the N10 and N11 nitro groups are both rotated by about 36°.



Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.379000(1)					
3	3	C	2	1.379116(2)	1	124.442(22)			
4	4	C	3	1.395400(3)	2	116.406(23)	1	-1.379(42)	0
5	5	C	4	1.368293(4)	3	121.775(24)	2	-1.346(43)	0
6	6	C	5	1.382808(5)	4	119.307(25)	3	3.569(44)	0
7	7	O	1	1.351355(6)	2	117.977(26)	3	-176.200(45)	0
8	8	N	2	1.476378(7)	3	119.163(27)	4	176.735(46)	0
9	9	Br	3	1.872958(8)	4	124.246(28)	5	175.728(47)	0
10	10	N	4	1.476587(9)	5	116.492(29)	6	-175.714(48)	0
11	11	N	6	1.477025(10)	5	116.722(30)	4	175.269(49)	0
12	12	O	8	1.201329(11)	2	117.202(31)	3	-92.123(50)	0
13	13	O	8	-1.200812(12)	2	116.353(32)	3	88.446(51)	0
14	14	O	10	1.212974(13)	4	115.902(33)	5	-35.462(52)	0
15	15	O	10	1.209142(14)	4	118.232(34)	5	143.432(53)	0
16	16	O	11	1.209457(15)	6	117.747(35)	5	-143.725(54)	0
17	17	O	11	1.209442(16)	6	116.999(36)	5	35.373(55)	0
18	18	C	7	1.398537(17)	1	117.875(37)	2	-115.577(56)	0
19	19	H	5	0.959648(18)	4	120.314(38)	3	-176.408(57)	0
20	20	H	18	0.959867(19)	7	109.535(39)	1	179.959(58)	0
21	21	H	18	0.960615(20)	7	109.472(40)	1	59.984(59)	0
22	22	H	18	0.960007(21)	7	109.495(41)	1	-59.944(60)	0

STOICHIOMETRY C7H4BrN3O7

SCF DONE: E(RHF) = -3509.10229704 A.U. AFTER 25 CYCLES

Alpha eigenvalues — -0.34044 -0.32306 -0.32168 -0.31901 0.11836

Estimated ionization potential: 8.69 ev

Total atomic charges:

		1
1	C	0.185275
2	C	0.080447
3	C	-0.024495
4	C	0.092655
5	C	-0.055062
6	C	0.078798
7	O	-0.237359
8	N	0.192271
9	Br	0.111449
10	N	0.180334
11	N	0.179910
12	O	-0.195012
13	O	-0.180095
14	O	-0.192763
15	O	-0.185360
16	O	-0.188450
17	O	-0.193487
18	C	-0.166343
19	H	0.145739
20	H	0.137222
21	H	0.117720
22	H	0.116606

Dipole moment (Debye):

X= 1.1326 Y= -0.3745 Z= 1.3379 Tot= 1.7925

V-mid: C2-N8: 0.195
C4-N10: 0.196
C6-N11: 0.186

Bond Order: C2-N8: 1.22
C4-N10: 1.22
C6-N11: 1.22
N8-O12: 2.03
N8-O13 2.03
N10-O14: 1.97
N10-O15: 1.99
N11-O16: 1.99
N11-O17: 1.99

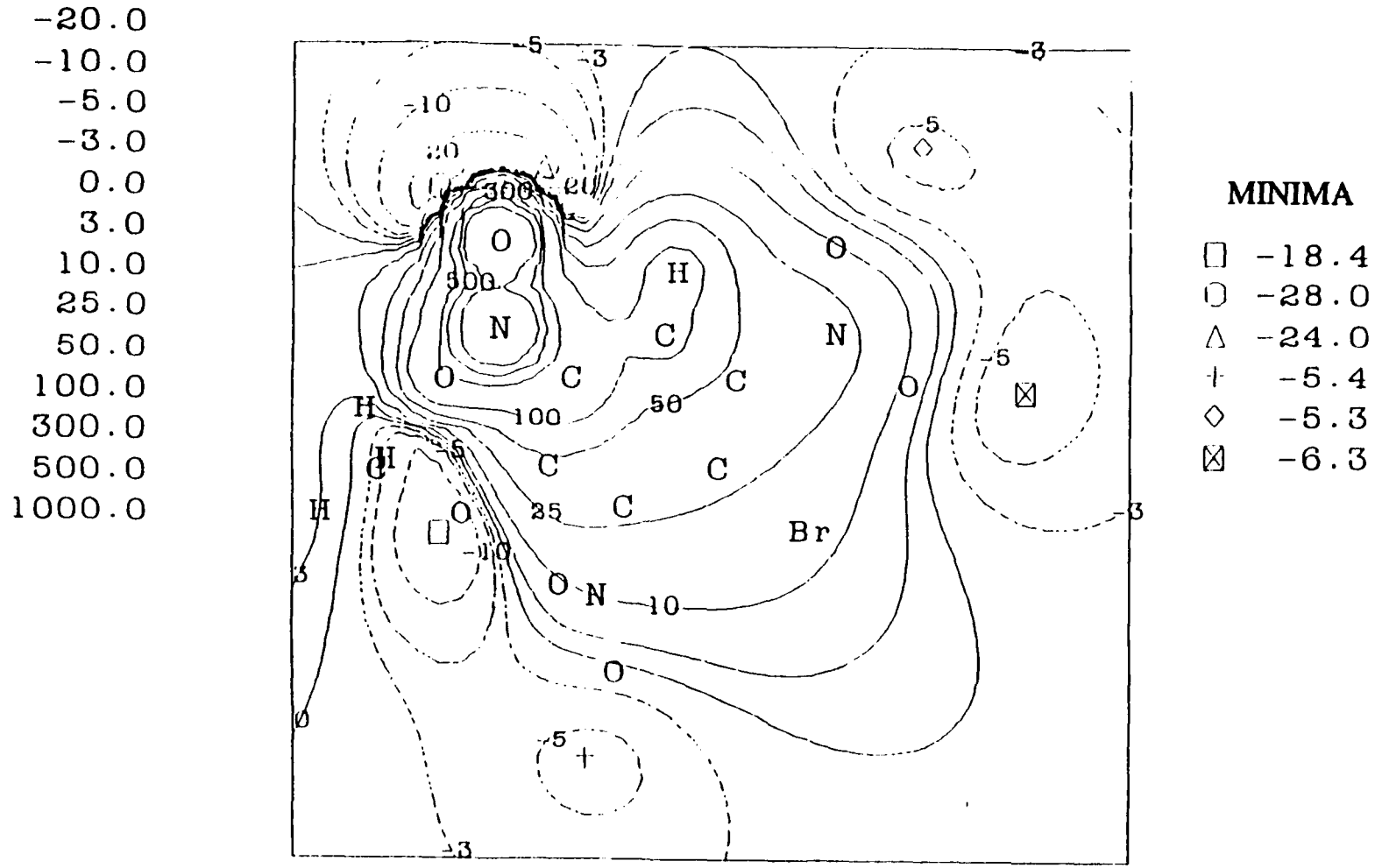


Figure UU-1. Calculated electrostatic potential, in kcal/mole, of 3-bromo-2,4,6-trinitroanisole, in the plane 1.75Å above the N10 nitro group located in the upper right corner. Projected positions of nuclei are shown. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

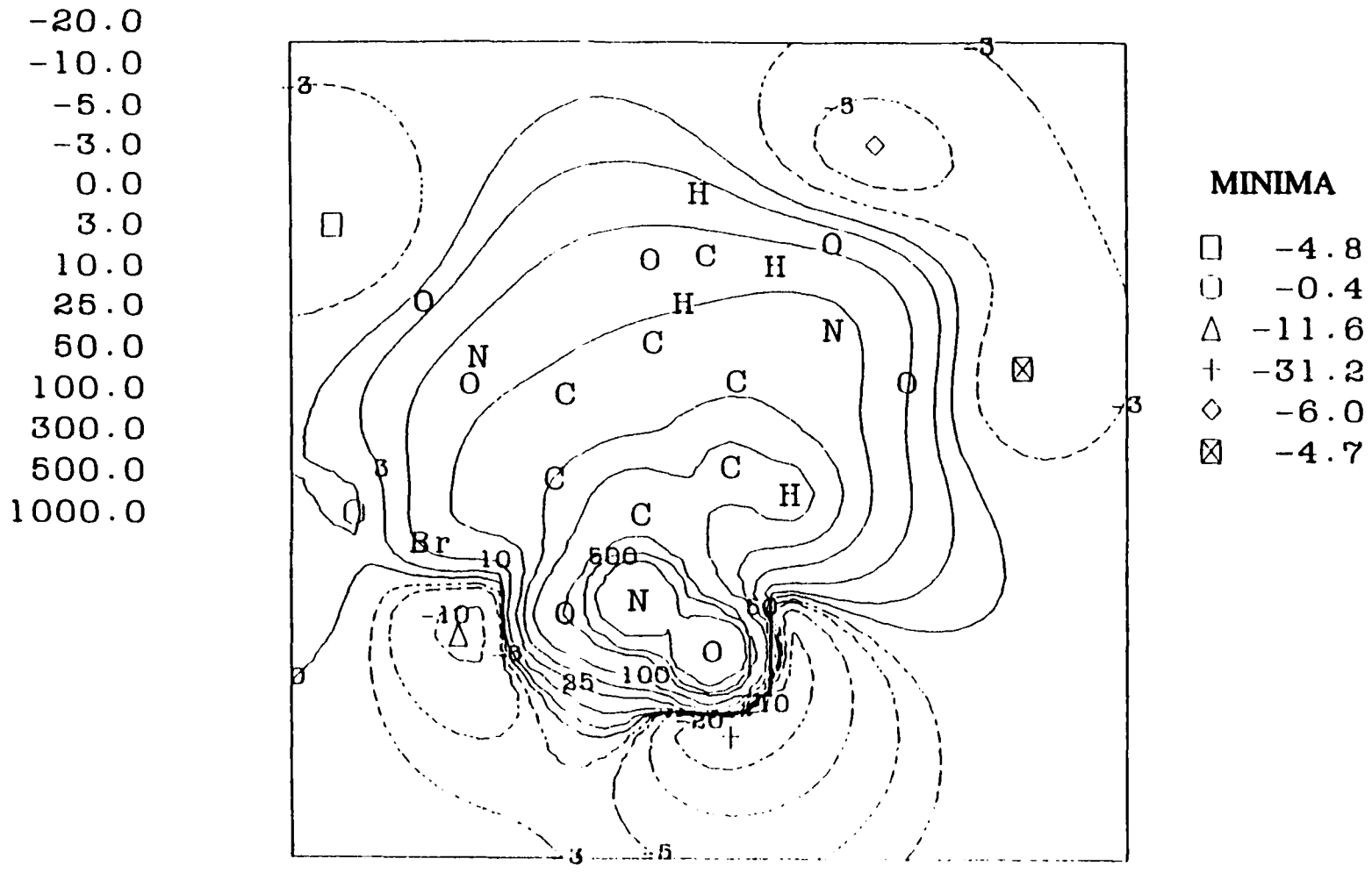
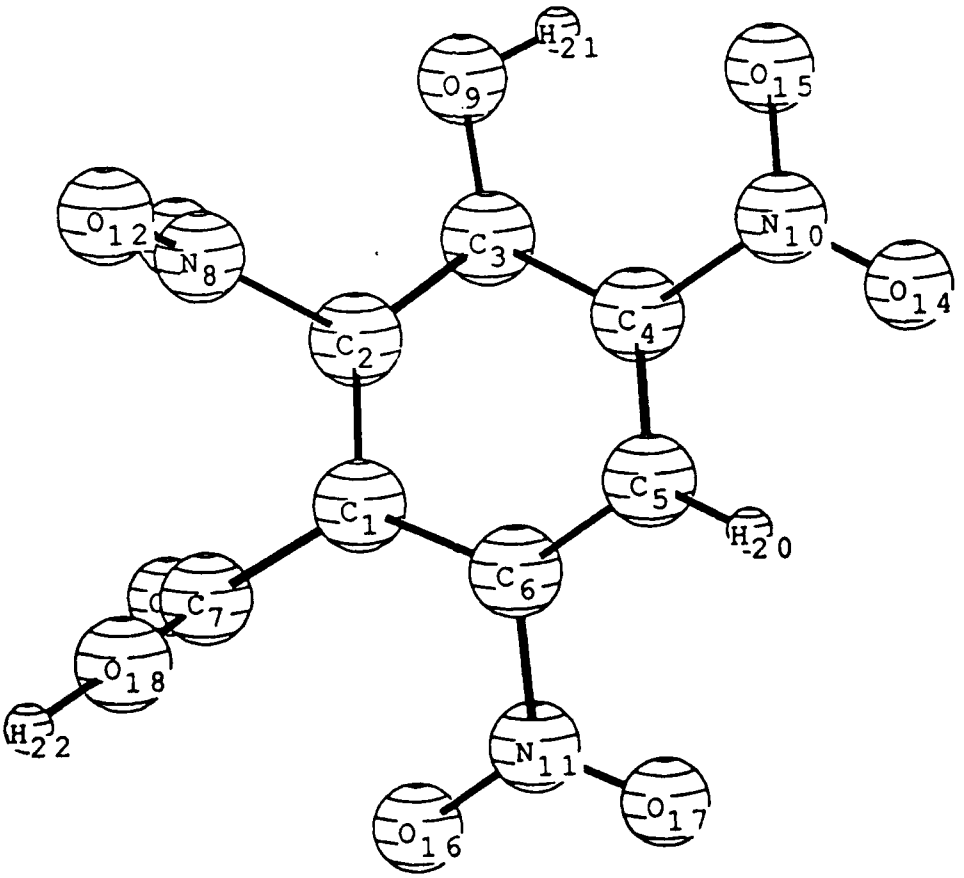


Figure UU-2. Calculated electrostatic potential, in kcal/mole, of 3-bromo-2,4,6-trinitroanisole, in the plane 1.75Å above the N11 nitro group located in the upper right corner. Projected positions of nuclei are shown. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

APPENDIX VV
2,4,6-TRINITRO-3-HYDROXYBENZOIC ACID

The short distances between non-bonded hydrogens and oxygens are H21-O15 (1.82 Å), H20-O14 (2.42 Å) and H20-O17 (2.38 Å)

The N8 and N11 nitro groups are rotated out of the mean plane of the benzene ring by about 85° and 15°, respectively, while the N10 nitro group is coplanar.



Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.380000(1)					
3	3	C	2	1.375419(2)	1	125.708(22)			
4	4	C	3	1.410745(3)	2	116.196(23)	1	-2.263(42)	0
5	5	C	4	1.379572(4)	3	120.865(24)	2	1.200(43)	0
6	6	C	5	1.358087(5)	4	119.608(25)	3	0.587(44)	0
7	7	C	1	1.504014(6)	2	119.832(26)	3	-176.905(45)	0
8	8	N	2	1.477542(7)	3	115.445(27)	4	175.716(46)	0
9	9	O	3	1.326100(8)	4	126.004(28)	5	179.890(47)	0
10	10	N	4	1.443422(9)	5	119.204(29)	6	-179.408(48)	0
11	11	N	6	1.478447(10)	5	117.605(30)	4	177.563(49)	0
12	12	O	8	1.206366(11)	2	116.582(31)	3	-95.761(50)	0
13	13	O	8	1.207174(12)	2	118.128(32)	3	83.498(51)	0
14	14	O	10	1.209020(13)	4	118.876(33)	5	-1.472(52)	0
15	15	O	10	1.232903(14)	4	118.891(34)	5	-179.861(53)	0
16	16	O	11	1.218424(15)	6	117.372(35)	5	-165.606(54)	0
17	17	O	11	1.224370(16)	6	117.658(36)	5	15.063(55)	0
18	18	O	7	1.276162(17)	1	114.312(37)	2	-98.637(56)	0
19	19	O	7	1.232137(18)	1	119.602(38)	2	74.313(57)	0
20	20	H	5	0.938906(19)	4	120.737(39)	3	179.296(58)	0
21	21	H	9	0.898851(20)	3	107.772(40)	4	5.968(59)	0
22	22	H	18	0.875728(21)	7	120.356(41)	1	-177.756(60)	0

STOICHIOMETRY C7H3N3O9

SCF DONE: E(RHF) = -1098.71997240

Alpha eigenvalues — -0.34245 -0.33877 -0.31967 -0.31152 0.10020

Estimated ionization potential: 8.48 ev

Total atomic charges:

		1
1	C	0.042209
2	C	0.078744
3	C	0.200410
4	C	0.062703
5	C	-0.058925
6	C	0.089312
7	C	0.380530
8	N	0.185185
9	O	-0.324553
10	N	0.172504
11	N	0.174672
12	O	-0.192965
13	O	-0.180343
14	O	-0 161448
15	O	-0 229640
16	O	-0.197011
17	O	-0.189305
18	O	-0.374100
19	O	-0.257961
20	H	0.153092
21	H	0.314924
22	H	0.311966

Dipole moment (Debye):

X= -0.4087 Y= 0.7248 Z= 0.9239 Tot= 1.2434

Bond Order:		V-mid:	
C2–N8:	1.22	C2–N8:	0.189
C4–N10:	1.31	C4–N10:	0.173
C6–N11:	1.22	C6–N11:	0.189
N8–O12:	2.01		
N8–O13:	2.00		
N10–O14:	1.99		
N10–O15:	1.88		
N11–O16:	1.95		
N11–O17:	1.92		

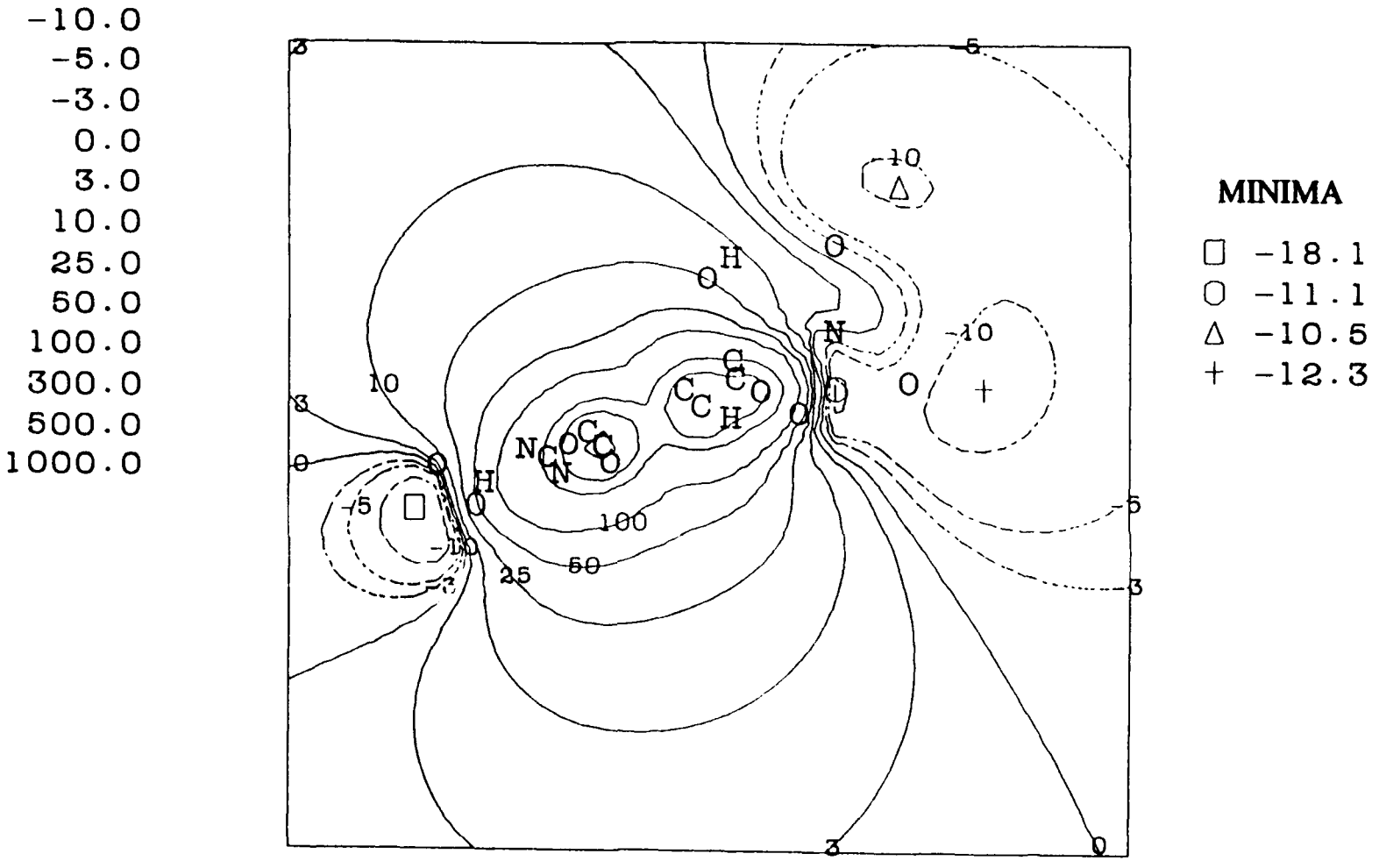


Figure VV-1. Calculated electrostatic potential, in kcal/mole, of 2,4,6-trinitro-3-hydroxybenzoic acid, in the plane 1.75Å above the N8 nitro group located in the upper right corner. The zero contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

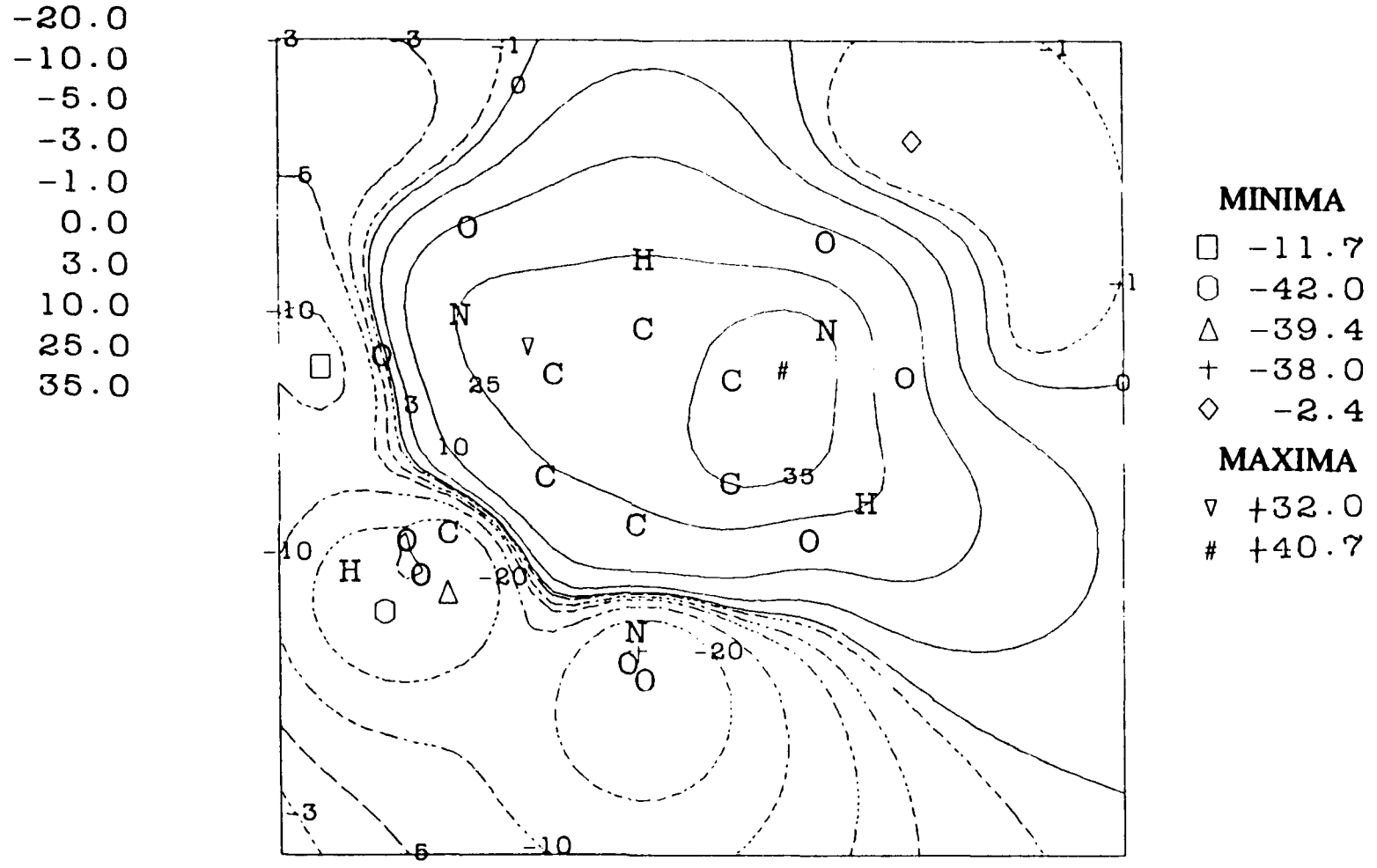


Figure VV-2. Calculated electrostatic potential, in kcal/mole, of 2,4,6-trinitro-3-hydroxybenzoic acid, in the plane 1.75Å above the N10 nitro group located in the upper right corner. The zero contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

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