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THE CALCULATION OF ELECTROSTATIC INTERACTIONS AND THEIR ROLE IN DETERMINING THE ENERGIES AND GEOMETRIES OF EXPLOSIVE MOLECULAR CRYSTALS

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Three different procedures were used to calculate electrostatic interactions in explosive molecular crystals. The use of Potential Derived Charges (PDC's) and atom-centered multipole expansions (ACME's) provides reasonable fits of the molecular electrostatic potential. The ability of these approaches to reproduce observed crystal structures was also evaluated.

INTRODUCTION

Properties of the crystalline phase are important in determining the behavior explosives. The CJ state of an explosive depends sensitively upon its density for example.[1] In addition, the shock sensitivity of PETN is found to depend upon the crystal orientation with respect to the shock direction.[2] Moreover, HE's with large amounts of hydrogen-bonding in the crystal (such as TATB and nitroguanidine) are frequently found to be less sensitive than those without. Finally, the heat of sublimation, which is the enthalpy difference between the gaseous and crystalline phases, is required to obtain the heat of formation of a condensed phase explosive from estimates of its gaseous heat of formation. The latter quantity is readily estimated using a number of approaches.

The atom-atom potential method can be used to calculate the energy and geometry of a molecular crystal.[3] In this approach, the intermolecular interaction between molecules A and B in the crystal lattice is taken as a sum over atom pairs. The interaction energy between atoms is then partitioned into distinct energetic components, as shown in Equation 1.

$$E_{AB} = \sum_{i \in A} \sum_{j \in B} \left(B_{ij} e^{-\alpha_{ij} R_{ij}} - \frac{A_{ij}}{R_{ij}^{6}} + E_{el,ij} \right) \quad (1)$$

These terms attempt to describe, respectively, the closed shell repulsion between the atoms resulting from the Pauli exclusion principle, van der Waals attractions, and the electrostatic interactions between the atomic charge distributions. The last term may be either attractive or repulsive. It is frequently represented as $q_i q_j / R_{ij}$, where the q's represent atomic charges.

A Raleigh-Schroedinger perturbation analysis of intermolecular interactions has shown that the electrostatic interaction is the leading order term.[4] Most HE's contain strongly polar functionalities (such as nitro groups), and many contain strong hydrogen-bonding moieties (such as amine groups). It is, therefore, important to represent the electrostatic interaction as accurately as possible if a realistic description of crystal properties is to be obtained. (It is well-recognized that electrostatic interactions are important in hydrogen bonds.[5])

In the past, a description of electrostatic interactions was difficult to obtain. The use of molecular electric moments for this purpose converges too slowly, if at all, for many common HE molecules. So, there was no reliable way of obtaining the atomic charges or multipoles that are required for the electrostatic calculation, except for the special case of small ions. More recently, however, it has become possible to obtain approximate charge distributions from ab initio molecular orbital theory for molecules the size of common explosives.[6] In addition, a number of procedures have been devised to obtain either atomic charges alone or multipoles for use in the electrostatic calculation.[7] In this paper, we examine three procedures for calculating electrostatic interactions. This has allowed us to characterize the role of these interactions in determining the crystalline geometry and energy of some explosives. In addition, diaminotetrazine, which is not an explosive, was examined. This molecule is of interest because of its high nitrogen content.

METHOD

Approximate molecular charge distributions were obtained from ab initio molecular orbital calculations for the molecules of interest using either the GAUSSIAN82[8] or GAUSSIAN92[9] computer program. The small split valence 3-21G basis was used throughout.[6] Molecular geometries were completely optimized within the common point group symmetry.

Atomic charges or multipoles were obtained from the approximate charge distributions using three different procedures. In the first of these, atomic charges are obtained from a mapping of the electron density onto the basis functions used in the molecular orbital calculation according to the prescription of Mulliken.[10] These Mulliken charges have been widely used in chemistry. A second procedure determines those atomic charges that best fit the electrostatic potential surrounding the molecule. Consequently, they are called potential derived charges (PDC's).[11] Finally, atom centered multipole expansions (ACME's) were determined from numerical integration of the charge distribution.[12] This procedure yields atomic multipole expansions truncated at an arbitrary level for use in calculating electrostatic interactions resulting from a charge distribution.

Calculations for molecular crystals require accurate treatment of interactions in an infinite periodic lattice. The use of atom-atom potentials commonly gives rise to terms in R^{-1} and R^{-6}. Consequently there exist well developed convergence schemes for these terms.[13] The exponential term used to describe overlap repulsion is a short ranged function and ment. However, the multipole-multipole interactions arising from the use of ACME's required additional consideration beyond that readily available in the literature. Theoretical treatment of these terms has appeared,^{14} but specific formula were unavailable. These are now presented in Table I without further discussion.^{15}

These formulas were implemented in the PCK83 code of Williams.^{16} This code performs lattice energy calculations using an input molecular geometry and Equation 1, as described in the program documentation and related publications. In addition to calculations of the energy, it was also desirable to energy optimize the cell parameters using the different treatments of the coulomb interactions. Consequently, derivatives of the multipole-multipole interactions were worked-out and implemented in the code.

RESULTS AND DISCUSSION

Fit of the Electrostatic Potential: It is important to determine how well the PDC's and ACME's reproduce a molecule's electrostatic potential. ACME's require considerably more computer time to evaluate and their use can only be justified in the current investigation if they yield a more accurate fit of the potential. PDC's were specifically designed to provide the best fit possible using a model limited to atomic charges. The ACME'S were truncated at quadrupoles for this comparison. MC's are not expected to be competitive with the other charge models and were consequently not considered in this comparison.

The evaluation was performed by comparing the differences in potential obtained from use of the above methods with that from analytical formulas on a grid of points surrounding the molecule. The grid points were 0.25 Å apart and formed a rectangular box. Grid points within a van der Waals distance of the molecule's atoms were ignored in this analysis. The fit of the potential was characterized by the root mean square (RMS) and relative root mean square (RRMS) error. These quantities were calculated for three ranges of potential values. In instances where the potential (V) ranges included positive and negative values these regions were: I V(r) < -1.15 kJ; and II [illegible] V(r) [illegible] 1.15; III V(r) > 1.15. For charged groups, the potential is uniformly positive or negative depending upon the molecular charge. Consequently the three ranges [illegible] over a wide range of potential values. The results of the comparison are shown in Table II. Drawings of the molecules examined are shown in Figure 1.

Inspection of Table II shows that in many instances the use of ACME's provides an improvement over PDC's of a factor of two or more in reproducing the electrostatic potential. In some cases, however, the use of PDC's provides a somewhat better fit. Nonetheless, the average RMS and RRMS for PDC's (ACME's) is 4.36 (1.85), 0.087 (0.038) for region I and 5.21 (5.23), 0.078 (0.053) for region III. Comparisons for region II are not particularly meaningful because of the small value of the potential for most molecules in this region. Thus, depending upon the molecule, the use of ACME's can provide a significantly better fit of the potential than PDC's.

Electrostatics at Fixed Crystal Geometries: To estimate the magnitude of the electrostatic energy in real crystals, the optimized molecular geometry was placed so that its center of mass and axes of the principle moments of inertia were in coinci dence with those of the molecular geometry found in the observed crystal structure. The electrostatic energy was then calculated at this molecular geometry, keeping all cell constants fixed at the observed values. In addition, the calculation was performed for two values of K, 0.0, and 0.2, to determine the effect of the procedure for accelerated convergence obtained with K=0.2 versus normal convergence obtained with K=0.0. The calculated electrostatic energies using MC's, PDC's and ACME's are shown in Table III. For the latter case, term energy increments for charges, (E_0), dipoles (E_1), quadrupoles (E_2), and octapoles (E_3) are shown.

The effect of the accelerated convergence procedure is seen by comparing the electrostatic energies obtained with K=0.0 and 0.2. The largest effect is found for the charge terms. A much smaller effect, on the order of a few tenths of a percent or less, is found in most cases for the dipole and quadrupole terms. This behavior is in accord with shorter range of the higher moments. For the monopole term, it is found that use of accelerated convergence results in changes as large as 10%, although many changes are much less. An exception to this generality is nitroguanidine (NQ), which has an ascentric cell and where an unusually large difference in the dipole term using normal and accelerated convergence is noted. Apparently, long range interactions which are slow to converge arise from the dipole moment of the unit cell. Nitromethane and NTODAG also show a significant effect when accelerated convergence is used to perform the lattice sums. Other molecules show a lesser, but noticeable effect. Thus, it is difficult to know in advance whether the use of the accelerated convergence procedure in calculating lattice sums will make a noticeable difference and, consequently, its use is required for accurate *a priori* calculations.

The results in Table III also provide information about the convergence of the multipole expansions. First, it is observed that the contribution attributable to each multipole is not monotonically decreasing with increasing order. Except for the organic salts NTODAG and NDAG, the dipole term makes the largest contribution. In these salts, the dipole term is significantly larger than in the neutrals, but the charge term predominates. The quadrupole term is less by a factor of two or more than the dipole term in all cases, except TATB. In this instance, its contribution is about 10% smaller than the dipole term. Finally, the octapole contribution to the total energy is normally relatively small, amounting in most cases to about 5% or less of the total electrostatic energy. The worst behavior is shown by diaminotetrazine, and may arise from the presence of a large number of unshared electron pairs on the nitrogens. Overall, however, truncation of the expansion at quadrupoles is a reasonable approximation.

It is interesting to compare the calculated electrostatic lattice energies obtained with different methods. Use of PDC's and ACME's gives results that are significantly different from those obtained using MC's. These large differences reflect the fact that MC's are not designed for calculating intermolecular interactions. The present results show that MC's should not be used for this purpose. On the other hand, PDC's and ACME's give results that are frequently in close agreement. Some significant differences are noticeable, however. An especially large difference is found for DAT. In this case, inspection of Table II shows that ACME's reproduce the electrostatic potential significantly better than do PDC's. This is also true for TATB, where a significant difference in the calculated lattice energies is found. Consequently, since the ACME's generally produce a better fit of the electrostatic potential, when differences in the lattice energy obtained from the two methods occurs, the ACME's seem likely to be a better approximation to the exact electrostatic lattice energy.

Finally, the size of the electrostatic lattice energy is noteworthy. For the uncharged explosives, it ranges from a low of about -36 kj/mol for nitromethane to a maximum of about -99 kj/mol for DAT. Heats of sublimation for compounds similar to these vary over a wide range, but a value of 100 kj/mol would certainly be reasonable. Thus, the electrostatic lattice energy is a significant fraction of a heat of sublimation of an explosive. It is also noteworthy that the computed lattice energies of the salts are much larger than those of the other HE's. This is in accord with expectations, since salts typically do have large electrostatic energies and heats of sublimations. A final point is that the electrostatic lattice energy is found to be stabilizing in all crystals that were examined. It is thus an important contribution to the energy of molecular crystals, in agreement with the arguments of Claverie.[4]

Calculation of Crystal Geometries: Rather than attempting to develop potential functions specifically designed for explosives, we decided to carry out a number of crystal structure optimizations to determine the effect of using an accurate treatment of electrostatics in conjunction with an existing set of potentials. This approach will allow us to assess the relative importance of electrostatic effects more accurately and determine, at least qualitatively, the sensitivity of structural parameters to the electrostatic calculation. Perhaps this will indicate fruitful strategies in the development of a more general and accurate semi-empirical model.

Initially, parameters for the Buckingham 6 function were those recommended by Williams, et al. and are shown in Table IV. This set of potential functions was supplemented by an electrostatic calculation using one of the three models: MC's, PDQ's, and ACME's truncated at the quadrupole level. After these optimization calculations were completed, which are summarized in Table V, we found that a number of crystals possessing extensive intermolecular hydrogen bonding were poorly calculated. We reasoned that a hydrogen on nitrogen or oxygen should be more positively charged and thus able to better penetrate an acceptor atom's electron cloud, thereby reducing its effective size. Accordingly, a set of crystal optimizations were performed in which the pre exponential parameter of the appropriate hydrogens was decreased by 30%. This model was used with both the PDC's and ACME's for elec the appropriate the P(N,O) or A(N,O) column of Table VI. Finally, Williams recommends a foreshortening of the X-H, X=C,N,O intramolecular bond lengths of ca. 0.07 Å from standard lengths to account in part for poorly determined hydrogen positions from x-ray structure determinations. This recommendation was followed in choosing the molecular geometries in a set of calculations labelled P(X-H) and A(X-H). This choice necessitated the use of two force centers for hydrogens. The nuclear center was used for the electrostatic calculation, while a center foreshortened by 0.07 Å, but in the same direction from the heavy atom, was used for the other terms. In this way we attempted to use the Williams parameter set in the manner originally intended, but with an improved treatment of electrostatics.

TABLE IV. POTENTIAL FUNCTION PARAMETERS USED IN THE BUCKINGHAM-6 EQUATION, $E_{ij} = B_{ij}\exp(-\alpha_{ij}R_{ij}) - A_{ij}/R^6$, with $A_{ij} = A_iA_j$, $B_{ij} = B_iB_j$, and $\alpha_{ij} = \alpha_i + \alpha_j$.

	B_i	α_i	A_i
H	11.68	1.87	109.41
C	49.39	1.80	608.07
N	37.13	1.89	504.51
O	33.60	1.98	479.66

Inspection of Table V shows that the use of different electrostatic models gives very different lattice energies, reflecting the trends found in Table IV. We were not able to find experimentally determined lattice energies or heats of sublimation for the compounds investigated here. Thus only a qualitative analysis of the calculated lattice energies can be given. In general, analogous models using either PDC's or ACME's yield very similar lattice energies. The MC's give crystal energies that differ from the other models significantly and are not expected to be very realistic. Lattice energies obtained using the other electrostatic models are of a reasonable magnitude and show larger values for the salts, as expected based upon the importance of coulomb interactions in them. Finally, a comparison of the electrostatic energies with the dispersion and repulsion energies can be made. The results in the table show that the electrostatic and repulsion energies are of opposite sign but frequently of similar magnitude. Thus these two components of the energy nearly cancel. The salts obviously do not follow this trend.

An error analysis of the computed cell constants is presented in Table VI. One quantity of particels give significantly different calculated densities. MC's yield the poorest results. The use of PDC's or ACME's with William's original parameters shows some improvement. The use of foreshortened X-H bonds provides an improvement over the use of the unaltered geometries. Additional improvement is found when the altered hydrogen parameters are used. This approach gives the best results, which are of comparable quality whether PDC's or ACME's are used. For these two models, the largest errors in the calculated densities are between 3-4%. For all the models a systematic underestimation of the density is apparent. Thus, for the purposes of density prediction alone, the model could be improved by applying a correction factor. Moreover, it is interesting to note that the difference in density of NQ at 25 C and -160 C is slightly over 2.5%.[17] Temperature is not included in our calculations at all, except insofar as the original derivation of the potential parameters was performed by fitting room temperature crystal of crystal density may need to account for temperature explicitly. Except for nitromethane, all the crystal structures shown in Table V appeared to have been determined at approximately room temperature. Nitromethane was studied at -45 C.

Also shown in Table VI is an error analysis of the cell lengths and angles. MC's yield the poorest results. Surprisingly, however, there is little difference in the accuracy among the remaining models. For both cell lengths and angles root-mean-square percent errors of between 5.42% and 8.72% are found. This error is larger than that found for the crystal density. Thus, the accuracy of the crystal density predictions depends upon a cancellation of errors in the cell structural parameters. However, the tendency to systematically overestimate the cell parameters is evident.

the asymmetric unit was allowed to undergo rigid rotation and translation to minimize the calculated energy. Any rotation or translation is measured relative to the observed orientation. The final rotations and translations are also shown in Table VI in degrees and Å, respectively. Here again there is little distinction between the various electrostatic models, although MC's are qualitatively poorer.

SUMMARY AND CONCLUSIONS

1. ACME's truncated at quadrupoles provide a fit of the electrostatic potential at least similar and many times superior to that given by PDC's. When unshared electron pairs are present in a molecule the improvement from the use of ACME's was most evident.
2. An efficient multipole treatment of electrostatic interactions on a periodic infinite lattice has been worked-out and implemented into a crystal modeling program.
3. The use of accelerated convergence techniques in the electrostatic lattice energy calculation results in reasonably small but noticeable differences when compared with explicit calculations within a given radius.
4. ACME's are reasonably well converged at the quadrupole level. Octapoles contribute less that 5% to the total electrostatic energies calculated.
5. PDC's and ACME's frequently give very similar electrostatic lattice energies. Some differences were noted, however, for diaminotetrazine where there is a large number of unshared electron pairs.
6. The electrostatic lattice energy is a significant fraction of the total lattice energy, and is an important stabilizing force operating in the crystal.
7. The use of Mulliken charges provides uniformly poor results compared with any of the other electrostatic models.
8. Calculation of a compound's crystal density proved sensitive to the electrostatic model employed. This is the result of a cancellation of errors. The use of a slightly altered set of hydrogen parameters gave highly accurate computed densities. Larger errors were, however, found in other crystal structure parameters.
9. The use of either PDC's or ACME's appears to offer promise for obtaining improved potential functions that include polarization, anisotropic

sity distribution.

10. Synthetic chemists can manipulate electron distributions in a molecule by substitution of polar groups, etc. With the ability of calculations to model these manipulations and to estimate their effect on the crystal lattice, as shown in this paper, a new approach to engineering dense explosives is now conceivable.

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TABLE I. ACCELERATED CONVERGENCE FORMULAS FOR LATTICE SUMS OF ELECTROSTATIC ENERGY USING ACME'S FOR TERMS UP TO QUADRUPOLES. THE ELECTROSTATIC TERM IN EQ. 1 IS EXPRESSED AS $E_{el} = \frac{1}{2}\sum_i \sum_j R(\mathbf{r}_{ij}) + \sum_{h} F(\mathbf{h}) \frac{\exp(-h^2)}{h^2} - K \sum_k^{cell} q_k^2 + \frac{2\pi}{3V}\mu^2_{cell}$ [1]

Real Space Term $R(\mathbf{r}_{ij})$	Reciprocal Space Term $F(\mathbf{h})$[1]
monopole-monopole	
[illegible]	[illegible]
monopole-dipole	
[illegible]	[illegible]
monopole-quadrupole	
[illegible]	[illegible]
dipole-dipole	
[illegible]	[illegible]
dipole-quadrupole	
[illegible]	[illegible]
quadrupole-quadrupole	
[illegible]	[illegible]

[1] where $\mathbf{r}$ is the vector from atom i to j; q, μ, Q are the monopole, dipole and quadrupole electric multipole moments

$f_0 = \mathrm{erfc}(a)$
$f_1 = \mathrm{erfc}(a) + 2A r_{ij} \exp(-a^2)$
$f_2 = \mathrm{erfc}(a) + A r_{ij} \exp(-a^2)(4a^2 + 6)/3$
$f_3 = \mathrm{erfc}(a) + A r_{ij} \exp(-a^2)(8a^4 + 20a^2 + 30)/15$
$f_4 = \mathrm{erfc}(a) + A r_{ij} \exp(-a^2)(16a^6 + 56a^4 + 140a^2 + 210)/105$

$S = \sum_k^{cell} q_k \exp(2\pi i\mathbf{h} \cdot \mathbf{r}_k)$
$\mathbf{L} = \sum_k^{cell} \mu_k \exp(2\pi i\mathbf{h} \cdot \mathbf{r}_k)$
$\mathbf{C} = \sum_k^{cell} Q_k \exp(2\pi i\mathbf{h} \cdot \mathbf{r}_k)$

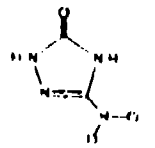
where [illegible]

TABLE II. FITS OF THE ELECTROSTATIC POTENTIAL OBTAINED FROM THE USE POTENTIAL DERIVED CHARGES (PDQ'S) AND FROM ACME'S TO QUADRUPOLE LEVEL (ME 2). ANALYSIS WAS PERFORMED IN THREE SEPARATE RANGES OF THE POTENTIALS, AS INDICATED. VALUES OF THE POTENTIAL ARE IN kJ/mol. ROOT MEAN SQUARE (RMS) AND RELATIVE ROOT MEAN SQUARE, (RRMS = $(N_{pts}^{-1} \sum_i ((x_{i,obs} - x_{i,calc})/x_{i,obs})^2)^{1/2}$) IN REGIONS SURROUNDING THE INDICATED MOLECULE ARE SHOWN.

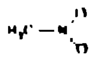
	Npts	RMS	RRMS	Npts	RMS	RRMS	Npts	RMS	RRMS
Nitroguanidine (NQ)									
RANGE	-2.179e+02 — -4.175e+00			-4.175e+00 — 4.175e+00			4.175e+00 — 3.439e+02		
PDQ	43997	2.162e+00	4.932e-02	2499	1.315e+00	6.284e+00	16598	2.498e+00	6.399e-02
ME 2	43997	1.104e+00	1.513e-02	2499	1.587e+00	4.161e+00	16598	2.226e+00	6.377e-02
3-nitrotriazol-5-one (NTO)									
RANGE	-1.859e+02 — -4.175e+00			-4.175e+00 — 4.175e+00			4.175e+00 — 2.397e+02		
PDQ	41490	2.459e+00	[illegible]	21009	4.809e-01	[illegible]	38416	4.116e+00	[illegible]
ME 2	41490	1.086e+00	4.814e-02	21009	4.634e-01	[illegible]	38416	2.516e+00	5.748e-02
Nitromethane									
RANGE	-1.385e+02 — -4.175e+00			-4.175e+00 — 4.175e+00			4.175e+00 — 1.667e+02		
PDQ	38839	1.843e+00	6.658e-02	6146	1.947e+00	5.382e+00	42102	1.782e+00	6.394e-02
ME 2	38839	6.583e-01	2.269e-02	6146	4.395e-01	1.433e+00	42102	2.148e+00	4.166e-02
Triaminotrinitrobenzene (TATB)									
RANGE	-1.599e+02 — -4.175e+00			-4.175e+00 — 4.175e+00			4.175e+00 — 2.164e+02		
PDQ	49338	2.163e+00	1.049e-01	28615	6.753e-01	[illegible]	49261	1.590e+00	4.508e-02
ME 2	49338	9.654e-01	4.479e-02	28615	1.544e-01	2.543e+01	49261	2.153e+00	4.954e-02
NTO anion									
RANGE	-6.406e+02 — -4.673e+02			-4.673e+02 — -2.943e+02			-2.241e+02 — -1.216e+02		
PDQ	1469	[illegible]	2.557e-02	3110	6.457e+00	1.747e-02	79101	1.525e+00	[illegible]
ME 2	1469	6.571e+00	1.233e-02	19110	3.096e+00	[illegible]	79101	6.532e-01	2.693e-03
Diaminoguanidinium cation (W configuration)									
RANGE	1.294e+02 — 3.387e+02			3.387e+02 — 5.461e+02			5.461e+02 — 7.535e+02		
PDQ	27081	1.564e+00	5.111e-03	31165	9.966e+00	2.345e-02	155	1.130e+01	2.112e-02
ME 2	97903	5.254e-01	1.730e-03	11165	5.595e+00	1.322e-02	152	2.049e+01	[illegible]
Diaminoguanidinium cation (S configuration)									
RANGE	1.739e+02 — 3.151e+02			3.151e+02 — 5.093e+02			5.093e+02 — 7.016e+02		
PDQ	102175	5.564e-01	3.147e-03	15647	7.423e+00	1.814e-02	257	1.747e+01	[illegible]
ME 2	102175	1.214e-01	1.147e-03	15647	4.513e+00	1.300e-02	257	1.610e+01	[illegible]
Nitrate anion									
RANGE	6.774e+02 — -5.015e+02			5.015e+02 — 3.256e+02			3.256e+02 — 1.496e+02		
PDQ	2564	7.485e+00	1.330e-02	13102	2.772e+00	5.299e-03	31465	[illegible]	[illegible]
ME 2	2564	3.479e+00	6.000e-03	13402	7.455e-01	1.761e-03	31465	[illegible]	[illegible]
1,4-dioxo-3,6-diaminotetrazine (TZX)									
RANGE	1.943e+02 — 4.175e+00			4.175e+00 — 4.175e+00			4.175e+00 — 2.861e+02		
PDQ	43912	1.745e+00	1.608e-01	15184	[illegible]	[illegible]	34956	2.536e+00	[illegible]
ME 2	43912	1.265e+00	8.841e-02	15184	7.001e-01	1.181e+01	34956	2.284e+00	[illegible]
Diaminotetrazine (DAT)									
RANGE	1.851e+02 — 4.175e+00			4.175e+00 — 4.175e+00			4.175e+00 — 1.804e+02		
PDQ	41130	7.400e+00	1.544e-01	27772	[illegible]	[illegible]	[illegible]	1.860e+00	[illegible]
ME 2	41130	2.330e+00	[illegible]	27772	[illegible]	[illegible]	11200	2.162e+00	[illegible]

FIGURE 1. MOLECULAR STRUCTURES MAKING UP THE CRYSTALS STUDIED IN THIS PAPER

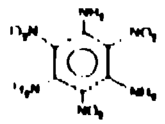
Nitroguanidine



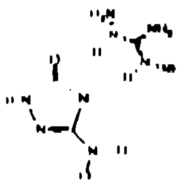
3-nitro-1,2,4-triazol-5-one (NTO)



Nitromethane



Triaminotrinitrobenzene (TATB)



NTO Diaminoguanidinium (NTODAG)

Diaminoguanidinium nitrate (NDAG)

3,6-diaminotetrazine (DAT)

3,6-diaminotetrazin-1,4-dioxide (TZX)

TABLE III. CALCULATED ELECTROSTATIC LATTICE ENERGIES FROM VARIOUS MODEL USING K=0.0 AND 0.2. WITH K=0.0 MOLECULES WITHIN A 10 Å SPHERE WERE INCLUDED. OPTIMIZED MOLECULAR GEOMETRIES WERE SUPERIMPOSED UPON OBSERVED CRYSTAL STRUCTURE COORDINATES AS DESCRIBED IN THE TEXT. ENERGIES IN kJ/mole. E_0, E_1, E_2, E_3 AND SUM REFER TO THE INDIVIDUAL TERMS INVOLVING MONOPOLES, DIPOLES, QUADRUPOLES, OCTAPOLES, AND THE SUM OF THESE TERMS.

	K	MC	PDC	E_0	E_1	E_2	E_3	SUM
NQ	0.0	[illegible]	[illegible]	[illegible]	[illegible]	6.7852	0.0176	[illegible]
	0.2	57.5404	-78.4917	[illegible]	47.3700	[illegible]	0.0119	-77.4916
NTO	0.0	-19.0554	69.0363	[illegible]	[illegible]	10.3494	-2.2446	80.4078
	0.2	52.9014	70.4728	[illegible]	50.6740	10.3536	-2.3439	61.7293
Nitro- methane	0.0	36.9821	33.3135	13.1324	18.4501	1.5044	-1.2855	-34.3724
	0.2	60.5602	35.2794	14.0745	-19.4050	[illegible]	-1.2845	36.2615
TATB	0.0	102.5832	[illegible]	11.1111	[illegible]	23.2284	-3.4906	-64.0014
	0.2	[illegible]	[illegible]	[illegible]	[illegible]	-23.3370	3.4911	63.8026
NTODAG	0.0	456.1045	-521.3867	-175.4469	142.5582	-26.6498	0.0919	547.7568
	0.2	477.3539	-536.3023	397.5094	145.3748	-24.6438	0.0908	567.6186
NDAG	0.0	515.6831	540.6456	485.6290	26.5280	-15.6098	2.3076	-575.1592
	0.2	537.2973	-566.7153	486.3985	77.3460	15.5230	-2.3099	576.9576
TZX	0.0	108.4899	-98.4557	38.4657	47.3883	-14.5291	1.1791	99.5617
	0.2	108.0632	98.1134	36.7184	47.2608	14.5351	1.1784	99.2227
DAT	0.0	45.6894	[illegible]	[illegible]	[illegible]	16.4739	5.3687	[illegible]
	0.2	47.4922	[illegible]	[illegible]	[illegible]	16.3241	5.5883	[illegible]

TABLE V. ENERGY OPTIMIZED CRYSTAL STRUCTURE OBTAINED USING THE INDICATED ELECTROSTATIC MODEL. MC'S USED MULLIKEN CHARGES ON EACH NUCLEUS, PDC USED POTENTIAL DERIVED CHARGES, AND ACME'S USED ATOM-CENTERED MULTIPOLE EXPANSIONS. P(N,O) AND A(N,O) INDICATE THAT THE A HYDROGEN PARAMETER WAS DECREAED BY 30% FROM THE VALUE SHOWN IN TABLE IV. THE USE OF P(X-H) AND A(X-H) INDICATE A FORSHORTENED X-H BONDS WITH THE INDICATED ELECTROSTATIC MODEL. CELL LENGHTS ARE IN Å, ANGLES IN DEGREES. ρ IS THE ANGLE BETWEEN THE AXIS OF THE ORIGINAL AND FINAL ORIENTATIONS OF THE ASYMMETRIC UNIT. T IS THE TRANSLATION OF THE ASYMMETRIC UNIT. D IS DENSITY IN g/cc. E(e) IS ELECTROSTATIC ENERGY, E(d) IS DISPERSION ENERGY, E(r) IS REPULSION ENERGY, E(t) IS SUM TOTAL. ALL ENERGIES IN kj/mol.

NQ Nitroguanidine located on Space Group Fdd2 (#43). The molecule is at a general position (Z=16).

	Obs	MC	PDC	P(N,O)	P(X-H)	ACME's	A(N,O)	A(X-H)
a	17.58	20.5200	17.1349	18.1700	18.8220	19.0668	18.3055	18.5872
b	24.92	24.7736	25.8965	25.4099	25.7079	25.9356	25.4469	25.7454
c	3.58	3.5095	3.4319	3.4077	3.4389	3.4587	3.4530	3.480
ρ		11.70	5.45	6.96	7.28	7.84	5.11	6.19
T		0.50	0.75	0.15	0.20	0.20	0.09	0.54
D	1.779	1.550	1.676	1.729	1.661	1.613	1.717	1.651
E(e)		-50.47	-63.33	-69.48	-65.65	-60.91	-67.78	-63.76
E(d)		-71.65	-61.58	-97.98	-96.77	-82.41	-96.49	-85.38
E(r)		49.73	49.10	59.29	51.59	47.65	56.23	50.41
E(t)		-55.73	-57.79	-108.17	-100.78	-95.87	-108.04	-98.73

NTO located in Space Group P2₁/a (#14). The molecule is on a general position (Z=4).

	Obs	MC	PDC	P(N,O)	P(X-H)	ACME's	A(N,O)	A(X-H)
a	9.3006	9.7995	9.5823	8.5626	8.5623	9.4787	10.2164	8.1553
b	5.5119	5.7815	6.0353	6.0760	6.0384	6.1742	5.0268	6.1601
c	9.1213	9.4289	9.5070	9.2405	9.1011	9.6877	9.8477	9.6937
β	100.48	95.64	98.52	96.78	98.71	98.64	117.27	94.69
ρ		29.48	15.74	15.78	15.55	15.36	16.82	15.54
T		1.89	0.15	0.09	0.40	0.59	0.55	0.44
D	1.881	1.713	[illegible]	1.815	1.787	1.680	1.646	1.770
E(e)		-56.19	-51.30	-67.44	-65.07	-61.89	-63.44	-64.69
E(d)		-71.74	-73.09	-107.09	-95.17	-86.69	-105.53	-69.87
E(r)		[illegible]	57.33	62.99	58.63	54.47	67.36	57.14
E(t)		-97.21	-79.28	-105.54	-101.56	-94.31	-101.56	-97.42

MENO2 Nitromethane located in Space Group P2₁2₁2₁ (#19). The molecule is on a general position (Z=4).

	Obs	MC	PDC	P(N,O)	P(X-H)	ACME's	A(N,O)	A(X-H)
a	5.244	5.2373	5.2751		5.2101	5.1838		5.2224
b	6.120	6.9146	6.1127		6.3024	6.1804		6.3069
c	8.730	8.9571	8.7753		8.6930	8.7011		8.8134
ρ		14.24	8.04		3.12	3.48		1.43
T		[illegible]	[illegible]		0.12	0.11		0.10
D	1.405	1.389	1.368		1.421	1.382		1.416
E(e)		-68.15	-15.56		-16.52	-14.25		-15.00
E(d)		-47.72	-58.39		-50.01	-17.82		-49.50
E(r)		11.5	21.20		10.18	28.47		29.46
E(t)		-92.1	-54.75		-56.37	-53.85		-55.14

TATB Triaminotrinitrobenzene located in Space Group P1 (#2). The molecule is on a general position (Z=2).

	Obs	MC	PDC	P(N,O)	P(X-H)	ACME's	A(N,O)	A(X-H)
a	9.010	9.4427	9.1777	9.3804	9.1438	9.1530	9.0300	9.1157
b	9.028	9.1427	9.1858	9.0485	9.1315	9.1873	9.0417	9.1118
c	6.812	5.8393	5.7854	6.717	6.7861	6.7361	6.1434	6.8015
α	108.59	80.80	110.76	110.28	110.77	110.37	110.22	111.19
β	91.82	90.30	88.13	88.62	88.86	90.23	89.69	90.18
γ	119.97	120.80	120.04	120.05	120.04	120.17	120.11	120.11
ρ		[illegible]	[illegible]	2.70	[illegible]	2.11	2.19	2.18
T		[illegible]	0.68	[illegible]	0.89	0.06	0.04	0.06
D	1.937	[illegible]	1.893	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
E(e)		-78.26	-81.18	-88.72	-61.35	-54.80	-62.18	-58.89
E(d)		[illegible]	-214.98	-214.54	[illegible]	-195.79	-217.04	-198.64
E(r)		138.18	[illegible]	114.75	[illegible]	21.08	112.02	79.18
E(t)		-160.19	-155.12	-168.51	-157.11	-153.11	-167.15	-155.85

NTODAQ 3-nitro-1,2,4-triazol-5-one-diaminoguanidine located in Space Group P1 (#2). The cell is on a general position (Z=2, Ion #1=DAG⁺, Ion #2=NTO⁻).

	Obs	MC	PDC	P(N,O)	P(X-H)	ACME's	A(N,O)	A(X-H)
a	8.235	8.5077	8.3410	8.1184	8.2203	8.1568	7.6496	7.2492
b	6.753	7.1796	6.5046	6.4717	6.5737	6.4913	6.4038	6.1174
c	9.844	10.5397	10.7210	9.9315	10.1109	10.0966	9.8461	[illegible]
α	98.79	103.63	96.98	98.66	98.43	96.51	96.96	[illegible]
β	77.17	63.47	67.81	69.56	66.94	69.9	71.70	[illegible]
γ	96.50	69.34	74.65	73.35	73.96	76.18	76.16	[illegible]
ρ1		25.40	21.74	15.66	14.18	25.68	26.46	[illegible]
ρ2		31.19	27.02	28.74	26.27	23.26	24.92	[illegible]
T1		4.79	2.56	2.13	2.47	2.17	[illegible]	[illegible]
T2		2.44	1.53	1.42	1.53	1.30	1.10	[illegible]
D	1.671	1.519	1.517	1.518	1.544	1.528	1.616	1.564
E(e)		-481.16	-509.99	-534.51	-520.15	-534.79	-577.16	-560.75
E(d)		-174.19	-171.64	-208.80	-179.99	-178.80	-216.66	-185.18
E(r)		122.53	125.53	150.56	129.46	137.70	172.28	136.13
E(t)		-533.12	-589.30	-592.56	-569.68	-575.89	-614.54	-586.70

NDAG Diaminoguanidine Nitrate located in Space Group P1 (#2). The cell is on a general position (Z=2, Ion #1=DAG⁺, Ion #2=NO3⁻).

	Obs	MC	PDC	P(N,O)	P(X-H)	ACME's	A(N,O)	A(X-H)
a	6.939	6.6995	6.6900	6.5702	6.6871	6.4434	6.7012	6.0101
b	6.272	7.3224	7.2786	6.9676	7.3009	7.0734	6.6101	[illegible]
c	7.764	7.4193	7.4200	7.3640	7.1760	7.0776	7.1020	7.0165
α	47.15	46.28	47.50	46.08	47.19	45.32	42.96	41.43
β	96.54	99.76	98.69	99.49	99.26	98.92	99.75	99.18
γ	107.74	106.71	105.98	107.15	106.75	107.79	108.73	108.15
ρ1		22.94	15.97	17.68	16.54	22.75	26.70	24.17
ρ2		16.10	[illegible]	10.20	11.09	8.07	8.19	[illegible]
T1		0.33	1.21	1.21	0.16	0.15	0.46	[illegible]
T2		0.84	1.87	0.65	0.65	0.41	0.46	[illegible]
D	1.611	1.448	1.488	1.610	1.526	1.488	1.604	[illegible]
E(e)		-520.58	-547.12	-565.68	-552.57	-549.26	-576.07	-562.17
E(d)		-124.10	-130.57	-163.24	-138.97	-131.76	-162.77	-114.58
E(r)		98.23	108.97	130.20	113.03	108.33	133.45	112.75
E(t)		-546.62	-568.72	-597.93	-577.76	-572.19	-604.79	[illegible]

TZX Space Group P2₁/c (#14), cell choice #3. Molecule is on an inversion center (Z=2).

	Obs	MC	PDC	P(N,O)	P(X-H)	ACME's	A(N,O)	A(X-H)
a	6.7709	7.0871	6.7210	6.8154	6.7031	6.4146	6.7155	6.7166
b	7.1189	7.1187	7.5401	7.4704	7.5718	7.5459	7.1541	7.5612
c	5.2514	5.0586	5.1751	5.2541	5.1727	5.1822	5.2044	5.1568
β	100.49	96.18	97.80	98.18	98.12	98.87	99.12	99.11
ρ		5.40	5.12	1.79	4.21	[illegible]	4.01	1.18
D	1.402	1.810	[illegible]	1.458	1.401	1.750	1.415	[illegible]
E(e)		-98.00	-99.78	-77.80	-92.19	-85.52	[illegible]	[illegible]
E(d)		-73.49	-115.41	-114.41	[illegible]	[illegible]	[illegible]	[illegible]
E(r)		40.31	[illegible]	[illegible]	78.42	72.28	[illegible]	[illegible]
E(t)		-142.28	-115.58	-145.12	-138.18	-128.44	[illegible]	[illegible]

UAT Space Group Amam (#63). Molecule is on two perpendicular [illegible] (Z=4).

	Obs	MC	PDC	P(N,O)	P(X-H)	ACME's	A(N,O)	A(X-H)
a	6.7570	5.7212	6.6097	[illegible]	6.1819	6.7174	6.7155	[illegible]
b	[illegible]	[illegible]	6.8641	[illegible]	[illegible]	6.1489	6.7188	[illegible]
c	9.1240	[illegible]	6.2414	[illegible]	6.7011	5.4814	7.1512	[illegible]
ρ		[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
D	1.610	1.585	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
E(e)		[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	
E(d)		[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
E(r)		[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
E(t)		[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]

[illegible] C. B., [illegible] J. S., [illegible] E. W. and [illegible] J. [illegible]

[illegible] H., private communication. The crystal [illegible] the [illegible]

[illegible] and [illegible] [illegible]

[illegible] and [illegible] [illegible]

[illegible] and [illegible] [illegible]

[illegible] and [illegible] [illegible]

[illegible] H. H. et al., private communication.

[illegible] and [illegible] [illegible]

TABLE VI. ERROR ANALYSIS OF CALCULATED CELL CONSTANTS. PERCENTAGE ERRORS $((x_{calc}/x_{obs})-1)*100$ ARE SHOWN FOR ALL PARAMETERS, EXCEPT ROTATION AND TRANSLATION OF THE ASYMMETRIC UNIT. IN THESE CASES, THEY ARE REPORTED IN DEGREE AND ANGSTROM. THEY WOULD BE ZERO FOR A PERFECT MATCH BETWEEN THE MODEL AND EXPERIMENT. ELECTROSTATIC MODELS ARE INDICATED AS IN TABLE V. <%Err> SIGNIFIES AVERAGE PERCENT ERROR. RMS %Err IS THE ROOT-MEAN-SQUARE PERCENT ERROR. n IS THE NUMBER OF OBSERVATIONS.

Densities n=8

Explosive	MC	PDC	P(N,O)	P(X-H)	ACME's	A(N,O)	A(X-H)
NQ	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
NTO	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
Nitromethane	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
TATB	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
NTODAG	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
NDAG	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
TZX	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
DAT	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
<%Err>	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
RMS %Err	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]

Cell Lengths n=24

Explosive		MC	PDC	P(N,O)	P(X-H)	ACME's	A(N,O)	A(X-H)
NQ	a	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
	b	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
	c	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
NTO	a	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
	b	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
	c	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
Nitromethane	a	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
	b	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
	c	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
TATB	a	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
	b	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
	c	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
NTODAG	a	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
	b	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
	c	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
NDAG	a	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
	b	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
	c	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
TZX	a	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
	b	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
	c	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
DAT	a	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
	b	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
	c	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
<%Err>		[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
RMS %Err		[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]

Cell Angles n=11

Explosive		MC	PDC	P(N,O)	P(X-H)	ACME's	A(N,O)	A(X-H)
NTO	β	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
TATB	α	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
	β	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
	γ	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
NTODAG	α	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
	β	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
	γ	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
NDAG	α	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
	β	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
	γ	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
TZX	β	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
<%Err>		[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
RMS %Err		[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]

Translations n=9

Explosive		MC	PDC	P(N,O)	P(X-H)	ACME's	A(N,O)	A(X-H)
NQ		[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
NTO		[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
Nitromethane		[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
TATB		[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
NTODAG	T1	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
	T2	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
NDAG	T1	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
	T2	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
DAT		[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
<%Err>		[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
RMS %Err		[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]

Rotations n=9

Explosive		MC	PDC	P(N,O)	P(X-H)	ACME's	A(N,O)	A(X-H)
NQ		[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
NTO		[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
Nitromethane		[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
TATB		[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
NTODAG	r1	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
	r2	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
NDAG	r1	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
	r2	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
TZX		[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
<%Err>		[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
RMS %Err		[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]