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CRDEC-TR-420

USE OF STATISTICS IN COMPUTATIONAL CHEMISTRY

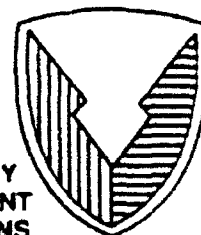
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PREFACE

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USE OF STATISTICS IN COMPUTATIONAL CHEMISTRY

1. INTRODUCTION

With increased concern for the environment and the tightening of regulatory requirements, it is becoming increasingly more difficult and more expensive to conduct exploratory experiments in the chemical laboratory. With the significant advancements that have been made in recent years in the area of computational chemistry, it is now possible to calculate many physical and chemical properties using one of the commonly available computational methods. However, at this time, it is not possible to estimate how close the calculated property of a new compound is to the true value.

In a previous report, Birenzvice and co-workers¹ use statistical methods to compare the ability of the three most commonly used computational methods (MNDO, PM3, and AM1) to predict the heat of formation, dipole moment, polarizability and ionization potential of 12 vanillic-type molecules. The result of that study shows that by using proper statistical tools, we can predict the precision and accuracy of the computational method. In addition, Birenzvice and co-workers show that not one method is suited to calculate all the physical properties.

Stewart² published an up-to-date summary of computed heat of formation (775 molecules), geometries (bond length and bond angle - 209 molecules, including 174 bond angles and 372 bond lengths), dipole moment (125 molecules), and ionization potential (256 molecules). In this report, we extend the methods used before to compare how well the three computational methods can predict the various physical/chemical properties.

2. PRINCIPLES OF STATISTICAL METHODS USED

As previously stated, the purpose of this study was to determine the ability of each of the three semi-empirical methods

¹Birenzvice, A., Sturdivan, L., Famini, G.R., Krishnan, P.N., and Morris, R.E., Predicting Polymer Properties by Computational Methods. 2: A Comparison of Semi-Empirical Methods, CRDEC-TR-361, U.S. Army Chemical Research, Development and Engineering Center, Aberdeen Proving Ground, MD, September 1992, UNCLASSIFIED Report (A256 856).

²Stewart, James J.P., "Optimization of Parameters for Semi-empirical Methods, II. Applications," J. Comput. Chem. Vol 10, p 221 (1989).

to calculate the physical/chemical property in question. To enable us to determine the accuracy of the calculation (i.e., the standard deviation of the error) in a statistically meaningful way, we need to show that the calculation errors are symmetrically distributed about the real (experimental) values. This is conventionally done by showing that the data follow the normal distribution function. One way of showing that a data set is normally distributed is to order it in an ascending order and plot the data on a normal distribution graph paper. For example, suppose we take the weight of nine people ($n=9$) selected at random. First, we sort them in ascending order; then we scale the linear Y axis so that all weights will fit. Finally, we plot the cumulative fraction on the probability axis versus the weight on the Y axis, letting the denominator of the fraction equal $n+1$ (for symmetry). Thus, the lightest weight would be plotted versus 0.1 ($1/n+1$), the next lightest versus 0.2, and so on until the heaviest would be plotted against 0.9 ($n/n+1$). If the weights were normally distributed, the resulting nine points would fall on a straight line. Alternatively, we can calculate the normal score that is the expected value of the normal order statistic of an ordered sample of size n . In the statistical package MINITAB^(tm), the normal score is abbreviated N-score. Plotting the N-score against normally distributed data will result in the points falling about a straight line.

Calculating the N-score requires numerical solution of integral equations. Calculation of N-score is available in some statistical packages on minicomputers but is not available in commonly used software packages for microcomputers. To enable us to perform the analysis on a desk-top microcomputer, we need to find a distribution function that will closely resemble the normal distribution but will be easier to compute. The logistic distribution is such a distribution. Its straight line transform, which we will call the L-score, is obtainable in closed form and is simple to calculate.

Figure 1 shows a comparison of L-score and N-score. It was produced as follows: First, we calculated the N-score of an ordered set of numbers from 1 to 1000 using minitab^(tm) on the VAX minicomputer. We then downloaded the data into a spread sheet on a desk-top PC and calculated the L-score according to the following equation:

$$L\text{-score}_{(i)} = \ln \frac{i}{n-i+1} \quad (1)$$

where i is the order of the item in the list, and n is the total number of items. The dashed line is the plot of L-score versus N-score. The solid line is a least-squares-fitted straight line

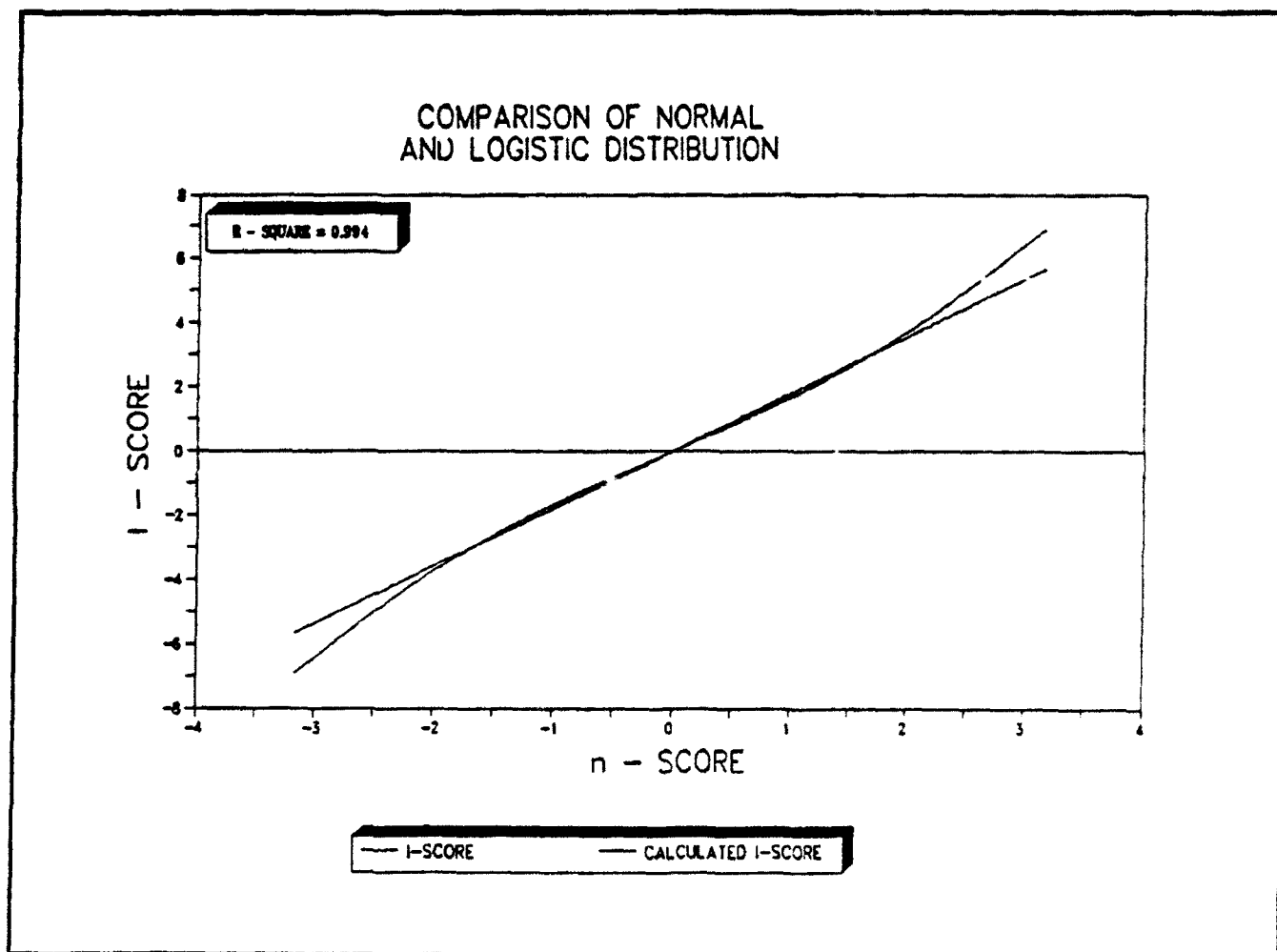


Figure 1. Comparison of Normal and Logistic Distribution

through the data. As can be seen, the two lines coincide except at the ends where the slightly heavier tails of the logistic distribution cause a bit of curvature away from the straight line. The correlation coefficient (R-squared) of the two measures is 0.994. When real data are plotted versus N-score and, separately, versus L-score, there is no visible difference in the "straightness," or lack of it, between the two plots.

For each molecule, the calculation errors (as reported by Stewart)² were plotted against L-score, and the correlation coefficient of the least squares regression line was determined. The plot was examined visually to determine any outliers and whether the fit will improve in a limited region. The average and standard deviation of the calculation errors were calculated in the region of symmetry as was the R-square for the least square regression line. To choose the best method for calculating the physical property in the region at a 95% confidence level, the following procedures should be followed:³

- For each of the three different methods, plot the difference between the calculated and experimental values of the property approximated versus its L-score. (Alternatively, plot the difference of the transformed data versus the L-score.)
- Determine a region (magnitude of calculated and experimental values) where the L-score plot forms a straight line, indicating a symmetrical "normal" distribution of errors. Transformed and untransformed data may have to be used for different regions (e.g., the data might be normally distributed in one region and lognormal in another).
- Calculate the R-square between the difference and the L-score for the appropriate region.
- Calculate the mean and standard deviation of the approximation error in the appropriate region.
- A method that has an R-square of 0.94 or larger is well approximated by the normal distribution. Among those that satisfy this criterion, choose the method that has the smallest standard deviation, unless that standard deviation is >2.28 times the size of the standard deviation of another method whose R-square is <0.94. In the latter case, choose the method with the smaller standard deviation regardless of the value of R-square.

³Mood, A.M., Graybill, F.A., and Boes, D.C., Introduction to the Theory of Statistics, 3rd ed., McGraw-Hill, New York, NY, 1974.

• Approximately 95% of the time, the experimental values will be in the range $\langle (\text{calculated value} - \text{bias}) \pm 2\sigma \rangle$.

3. RESULTS AND DISCUSSION

3.1 Heat of Formation.

Figures 2-4 are plots of the differences between the calculated experimental heat of formation for PM3, MNDO, and AM1, respectively. In each case, the straight line represents the least squares regression line of the calculation errors versus L-score. As clearly seen only in the case of PM3, the R-square is larger than 0.94. The PM3 calculation method has an average bias of 0.44 Kcal/mole (i.e., the calculation errors are normally distributed about an error of 0.44 Kcal/mole) and a standard deviation of 12.3 Kcal/mole. Thus, the true heat of formation for a compound with no experimental value will be as follows:

$$\text{True Value} = (\text{Calculated Value} - 0.44) \pm 12.3 \times 2 \quad (2) \\ \text{with 95\% confidence.}$$

Table 1 lists the seven compounds, which have the largest deviation (these compounds are marked in Figure 2). If these compounds are eliminated from the analysis, the precision (bias) and accuracy (standard deviation) of the method improve somewhat (0.37 Kcal/mole and 11.1 Kcal/mole, respectively).

3.2 Ionization Potential.

Figures 5-7 show that the calculated ionization potential for all three methods are normally distributed about the experimental values. MNDO provides slightly higher accuracy (standard deviations of 0.7 ev versus 0.73 ev for PM3 and AM1, respectively) and should be the preferred method even though it has higher bias (0.68 ev versus 0.12 ev and 0.40 ev for PM3 and AM1, respectively).

3.3 Dipole Moment.

The correlation coefficient of the calculation errors of the dipole moment versus L-score for PM3 (Figure 8) is only 0.92; thus, this method is not suitable for calculating the dipole moment. The correlation coefficient for both MNDO (Figure 9) and AM1 (Figure 10) is 0.96. The standard deviation for AM1 is smaller (0.49 deby) than the standard deviation for MNDO (0.63 deby). Thus, AM1 should be the preferred method for calculating dipole moment. The table under each figure (Tables 2-4) lists the compounds with the largest deviation from the regression line.

3.4 Bond Length.

As can be seen (Figures 11-13), none of the three methods evaluated in this study produces a data base of bond length, which is normally distributed about the true (experimental) values. In each case, there were few clear outliers, which are listed in Tables 5-7 (nine compounds for PM3, five compounds for MNDO, and seven compounds for AM1). When these outliers were removed from considerations, the correlation coefficient increased considerably (Figures 14-16). However, in the case of PM3 and MNDO, the correlation coefficient still remained below 0.94. In the case of AM1 when points 1-5 and point 8 were removed (these points show the largest deviation from the regression line), the correlation coefficient increased to 0.94.

3.5 Bond Angle.

Of the three methods evaluated (Figures 17-19), it appears that only AM1 shows a tendency for symmetry (Figure 19) even though there are few clear outliers. After removing the most extreme outliers from consideration in PM3 and MNDO (Tables 8-9), the correlation coefficient in PM3 increases to 0.92 (Figure 20) - not enough to show that the data are normally distributed. The correlation coefficient for MNDO remains very low (Figure 21). For AM1, once the six compounds listed in Table 10 are removed from consideration, the correlation coefficient between the computation errors and their corresponding L-score exceeds the required 0.94 (Figure 22).

4. CONCLUSIONS AND RECOMMENDATIONS

By using appropriate statistical tools, we show that semi-empirical computational methods can be used as screening methods to predict different physical or chemical compounds with a high degree of confidence. Furthermore, we show that not one of the commonly used computational methods is adequate for computing all of the properties.

For each of the properties studied, the computation error can be divided by a systematic error or bias (the precision of the calculation) and a random error (the accuracy of the calculation or standard deviation). Table 11 lists the different properties, the recommended computational method, and its bias and standard deviation. When calculating the property of an unknown compound, the true value can be evaluated as follows (with 95% confidence):

$$\text{True Value} = (\text{Computed Value} - \text{Bias}) \pm 2\sigma \quad (3)$$

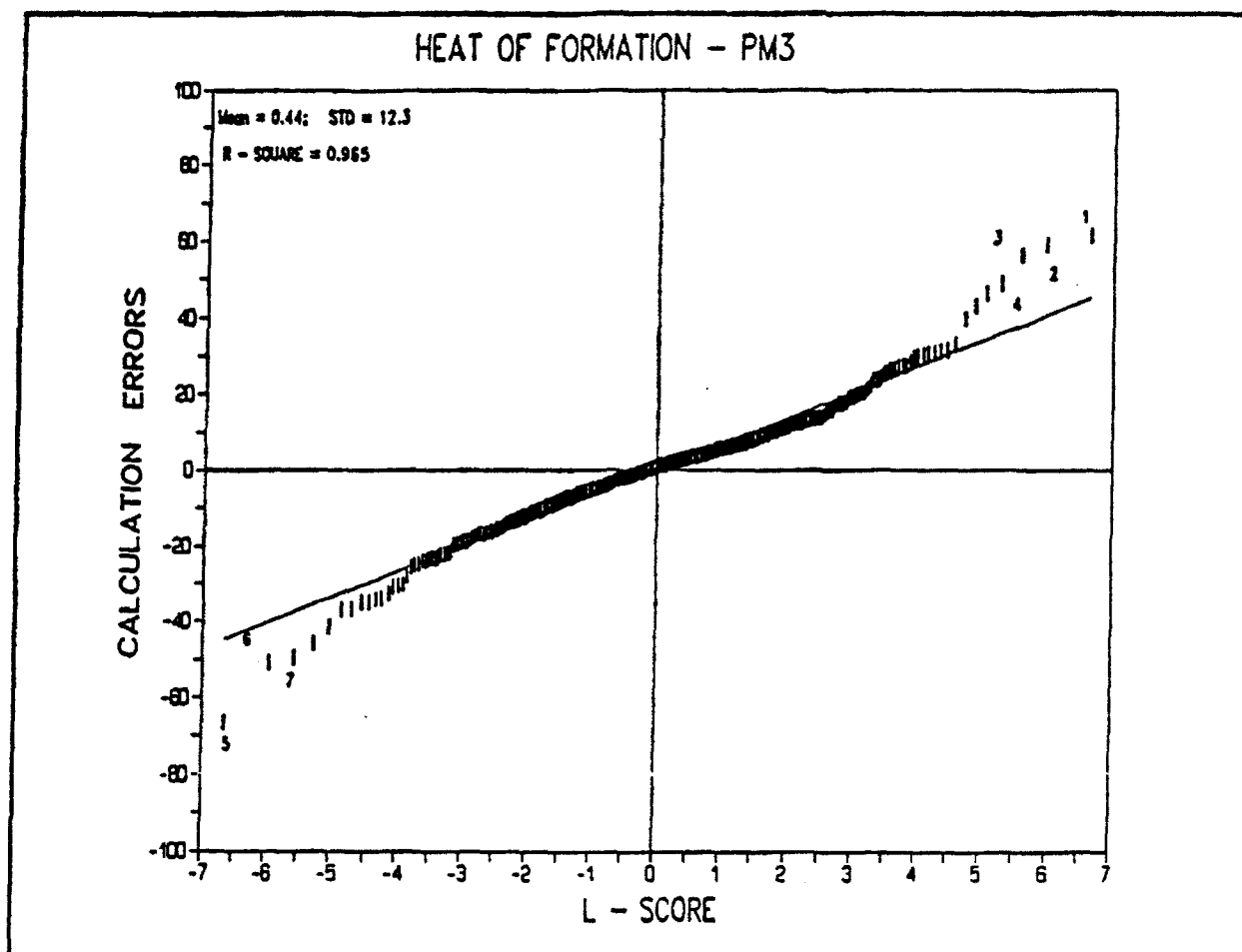


Figure 2. Test for Normal Distribution of Calculation Errors - Heat of Formation, PM3

Table 1. Compound with Largest Deviation of Calculated Error of Heat of Formation Using the PM3 Method

#	CHEMICAL	EXPERIMENTAL	CALC. ERRORS
1	Al ⁽⁺⁾	218.1	61.7
2	PSBr ₃	-67.2	59.4
3	AlOF ₂	-265	56.5
4	SiOI ₂	-99.4	49.2
5	COI	63.5	-66.4
6	AlOH ⁽⁻⁾	-55	-50.7
7	AlN	125	-49.5

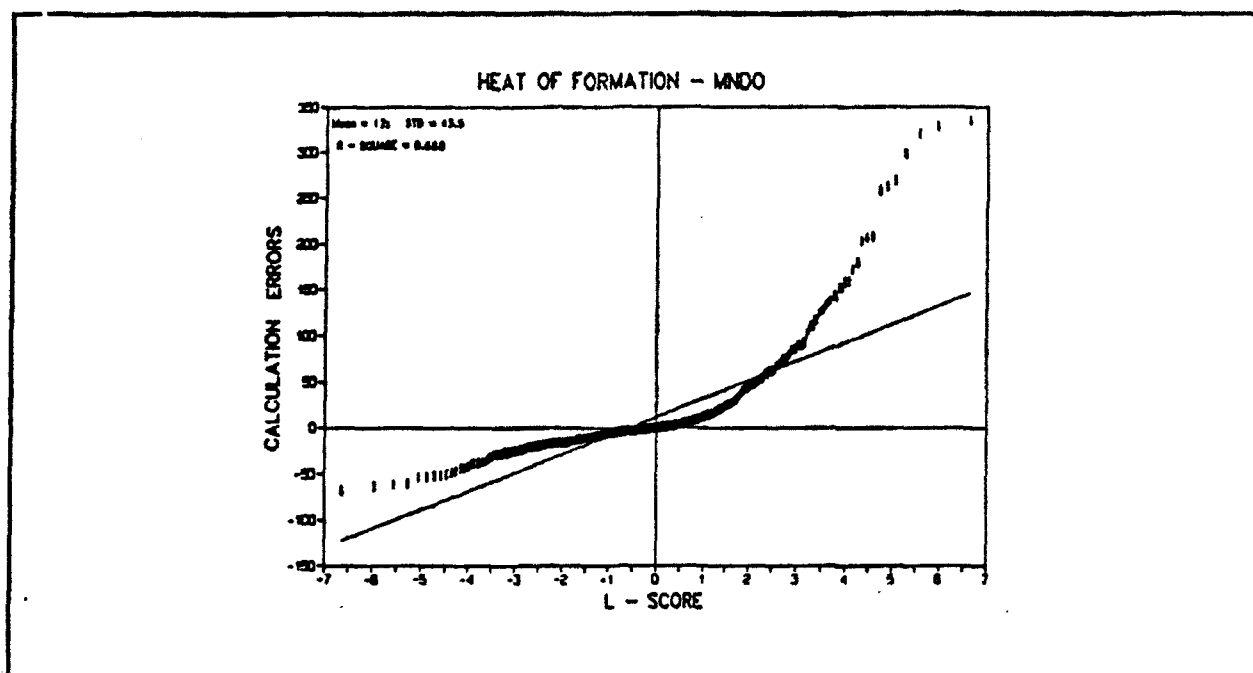


Figure 3. Test for Normal Distribution of Calculation Errors - Heat of Formation, MNDO

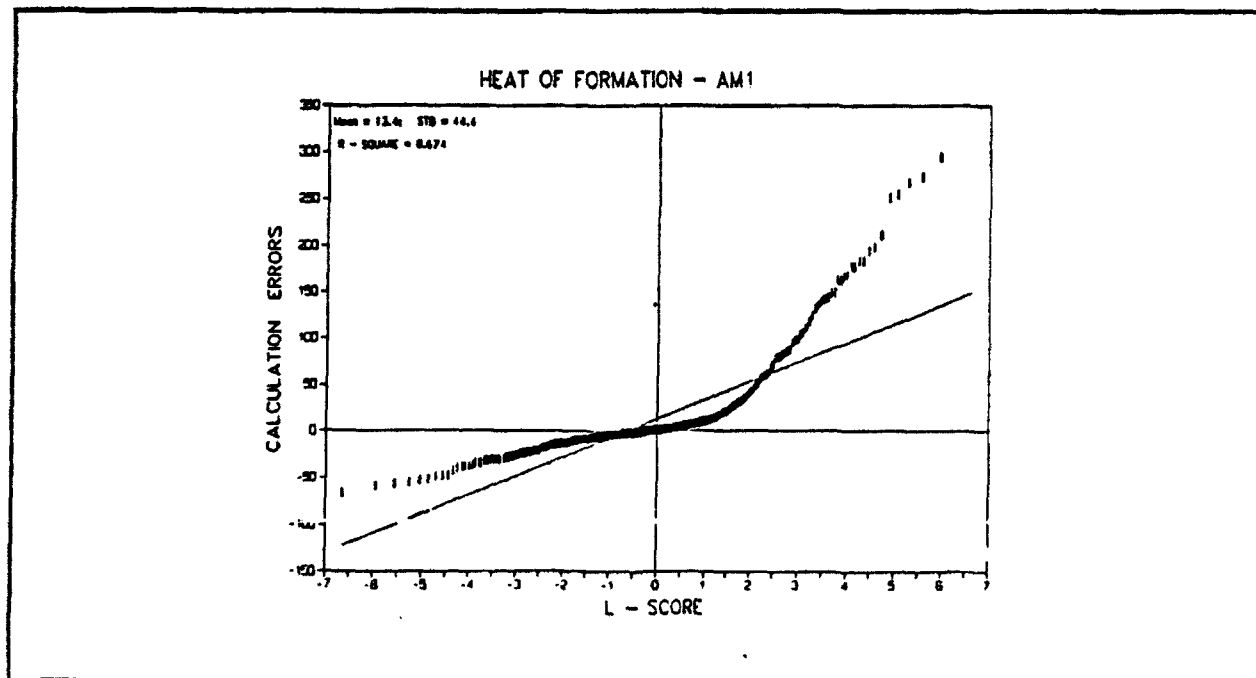


Figure 4. Test for Normal Distribution of Calculation Errors - Heat of Formation, AM1

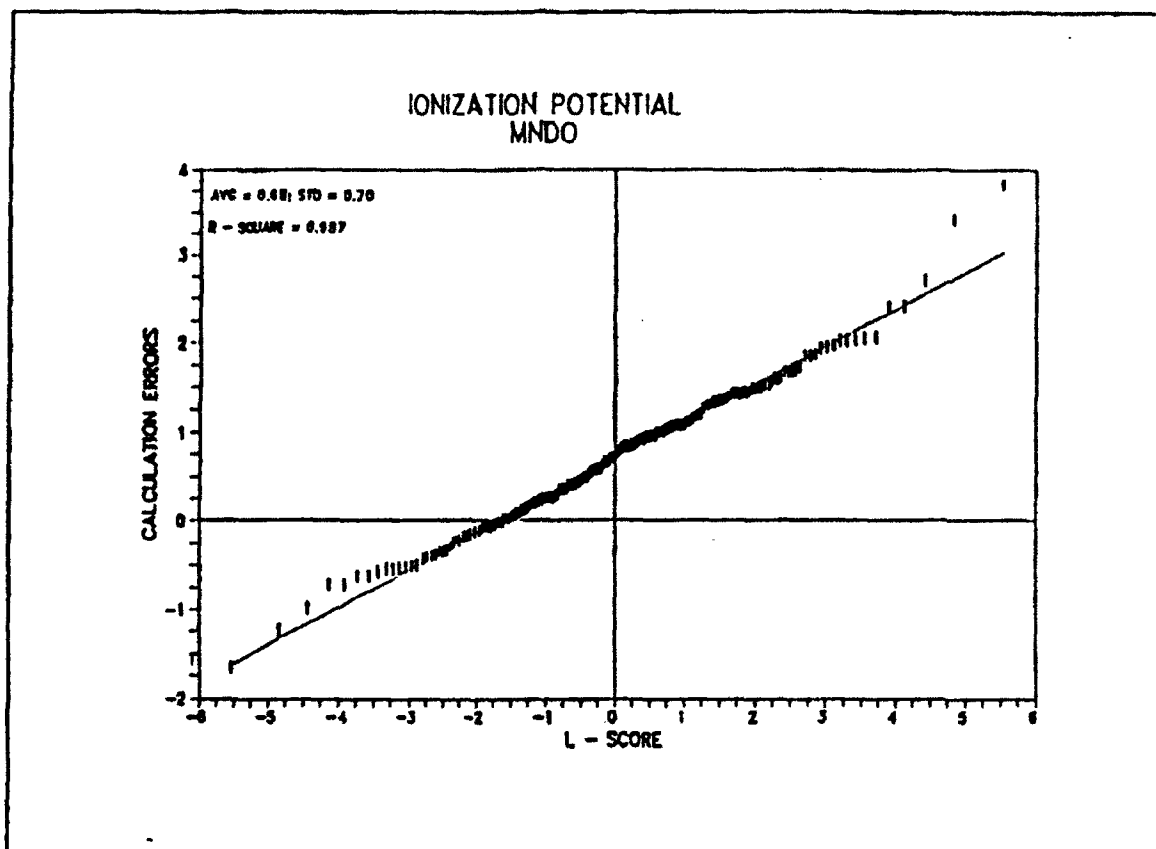


Figure 5. Test for Normal Distribution of Calculation Errors
- Ionization Potential, MNDO

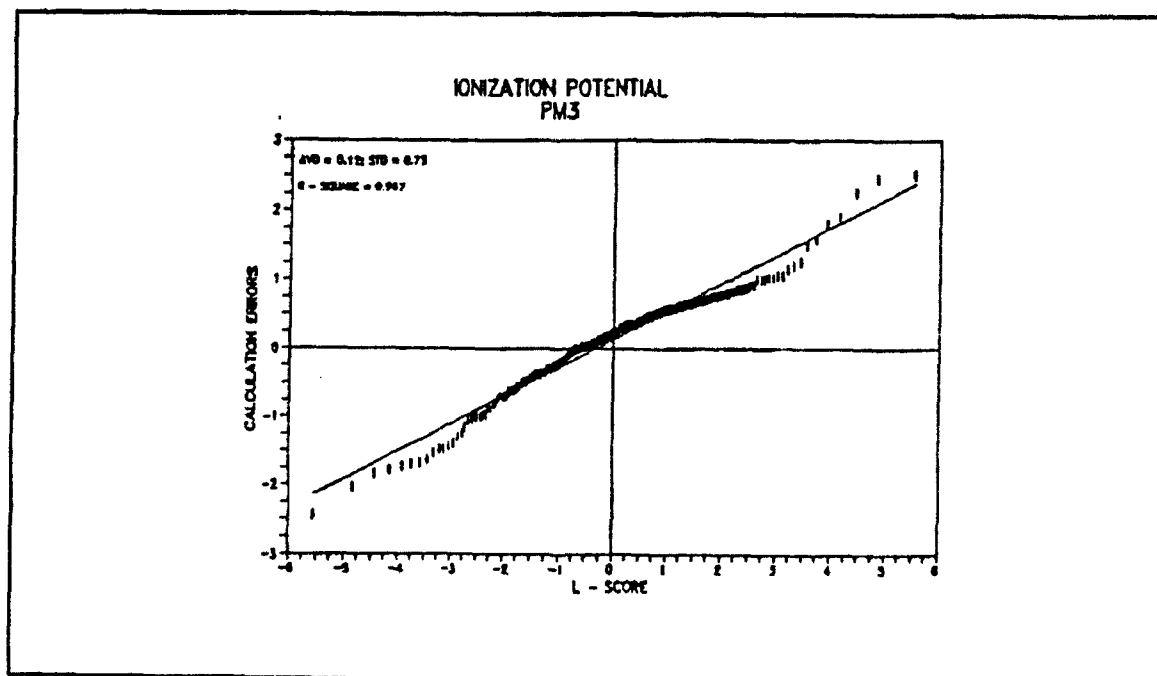


Figure 6. Test for Normal Distribution of Calculation Errors
- Ionization Potential, PM3

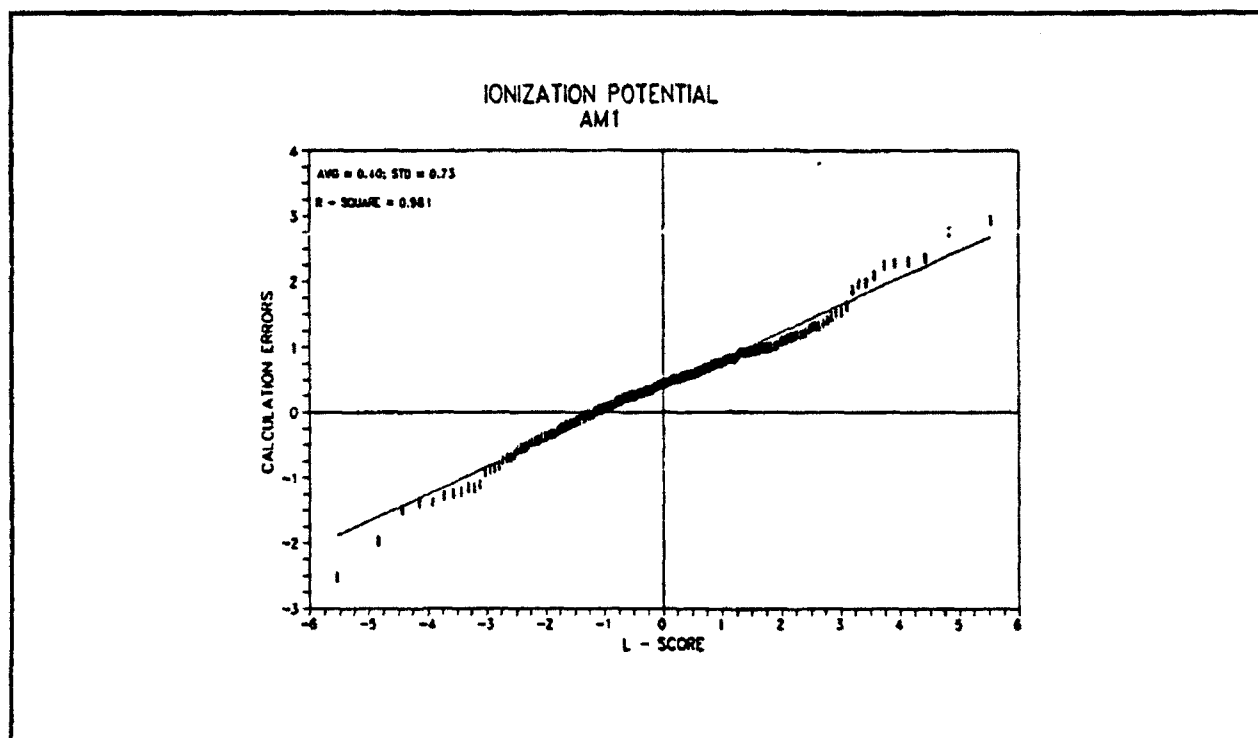


Figure 7. Test for Normal Distribution of Calculation Errors
- Ionization Potential, AM1

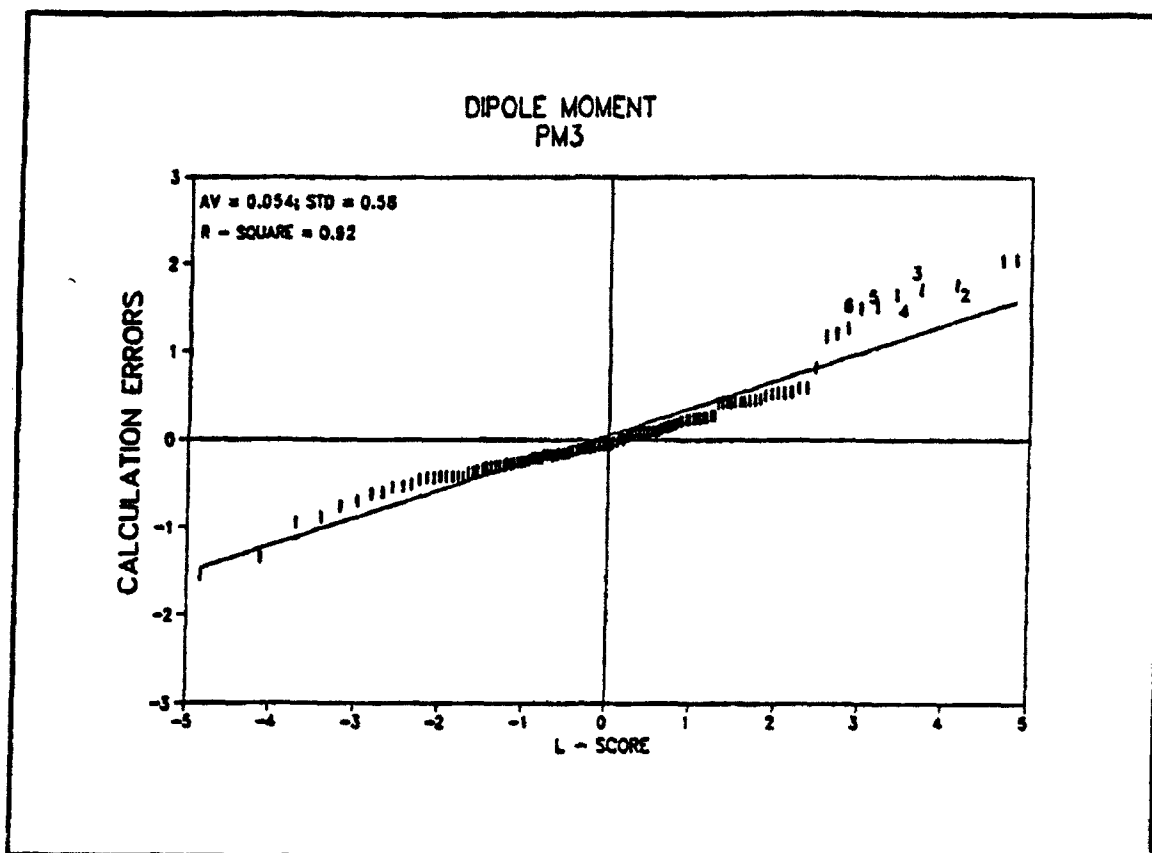


Figure 8. Test for Normal Distribution of Calculation Errors
- Dipole Moment, PM3

Table 2. Compound with Largest Deviation of Calculated Error
of Dipole Moment Using the PM3 Method

#	CHEMICAL	EXPERIMENTAL	CALC. ERRORS
1	SO ₂	1.57	2.06
2	AlF	1.53	1.76
3	BrO	1.61	1.71
4	H ₂ SiBr ₂	1.43	1.66
5	HSiCl ₃	0.86	1.52
6	H ₂ SiCl ₂	1.18	1.5

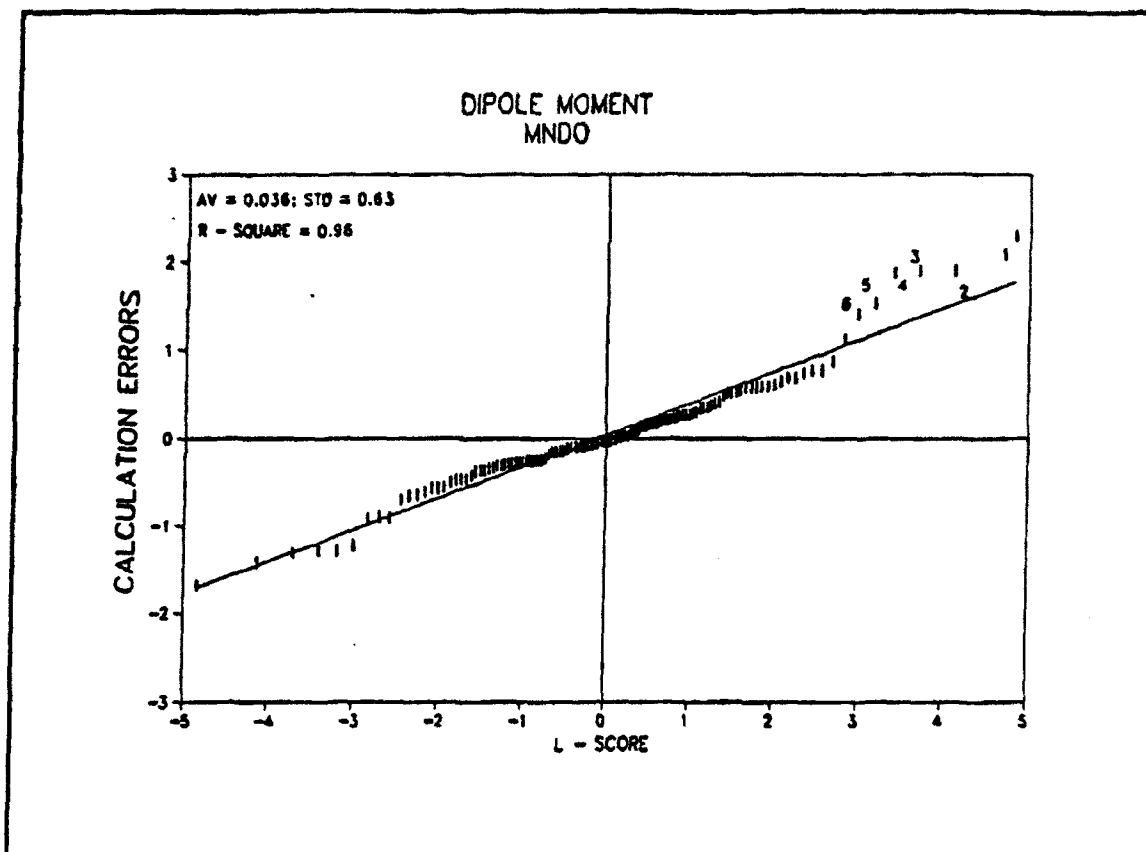


Figure 9. Test for Normal Distribution of Calculation Errors
- Dipole Moment, MNDO

Table 3. Compound with Largest Deviation of Calculated Error
of Dipole Moment Using the MNDO Method

#	CHEMICAL	EXPERIMENTAL	CALC. ERRORS
1	H ₂ SiCl ₂	1.18	2.29
2	H ₂ SiBr ₂	1.43	1.9
3	SO ₂	1.57	1.9
4	HSiCl ₃	0.86	1.87
5	HSiF ₃	1.27	1.53
6	PF ₃	1.03	1.22

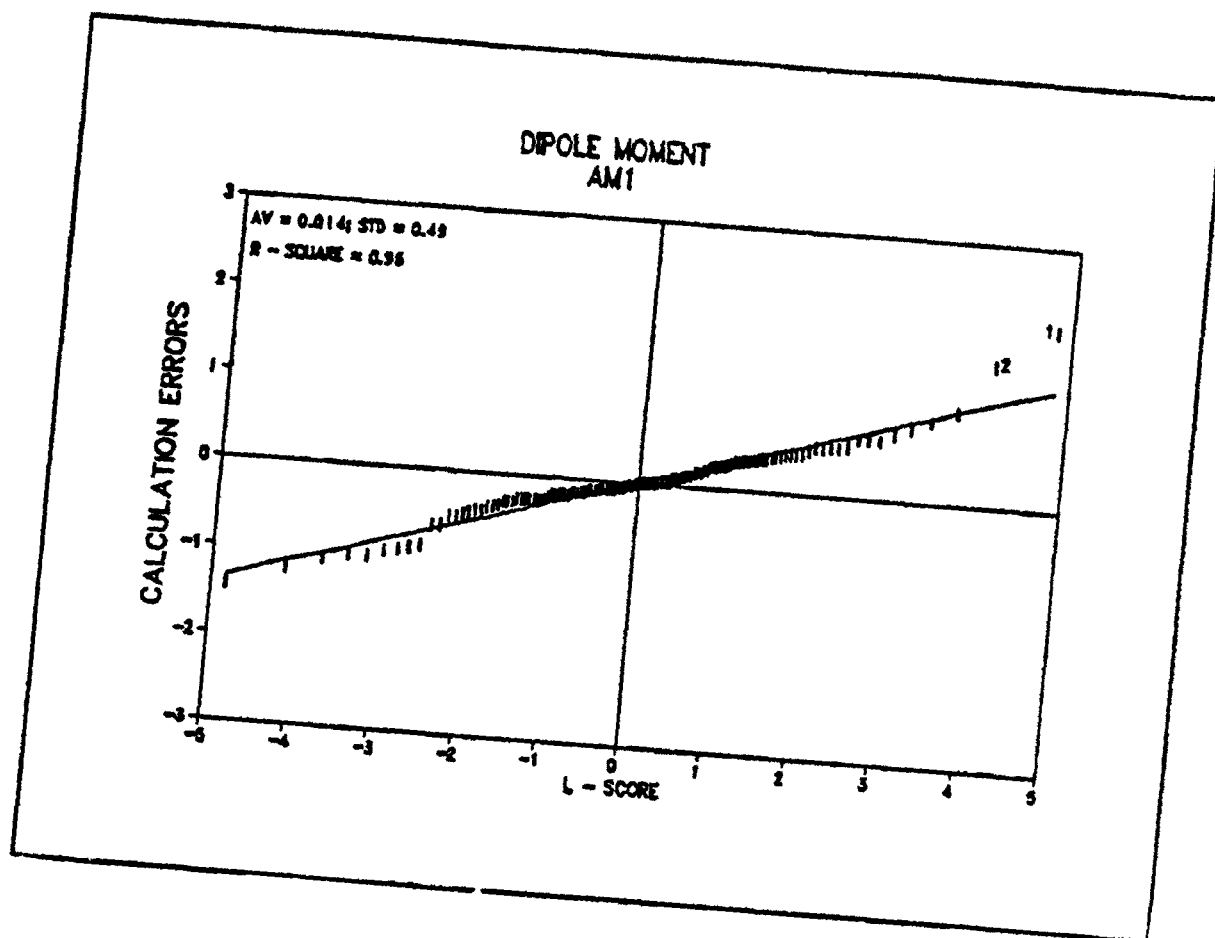


Figure 10. Test for Normal Distribution of Calculation Errors
- Dipole Moment, AM1

Table 4. Compound with Largest Deviation of Calculated Error
of Dipole Moment Using the AM1 Method

#	CHEMICAL	EXPERIMENTAL	CALC. ERRORS
1	SO ₂	1.57	2.06
2	H ₃ P	0.58	1.61

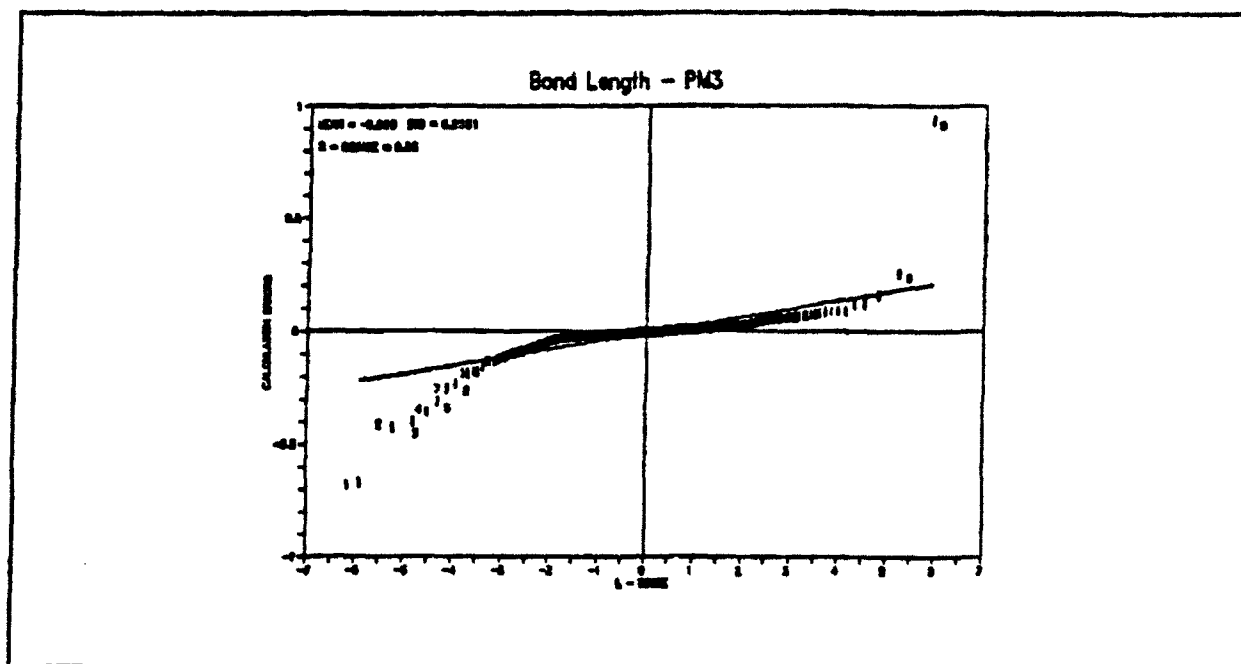


Figure 11. Test for Normal Distribution of Calculation Errors
- Bond Length, PM3

Table 5. Compound with Largest Deviation of Calculated Error
of Bond Length Using the PM3 Method

#	CHEMICAL	BOND	EXPERIMENTAL	CALC. ERRORS
1	N ₂ O ₃	N-N	2.08	-0.671
2	H ₃ SiI	Si-I	2.012	-0.425
3	AlBr ₃	Al-Br	2.27	-0.395
4	SiBr ₄	Si-Br	2.15	-0.354
5	F ₃ I	I-F(ax)	1.76	0.938
6	H ₃ SiBr	Si-Br	2.21	-0.309
7	NOBr	Br-N	2.14	-0.252
8	H ₂ O ₂ (H ₂ O Dimer)	O-O	3	-0.231
9	H ₂ SO ₄	S-O	1.42	0.248

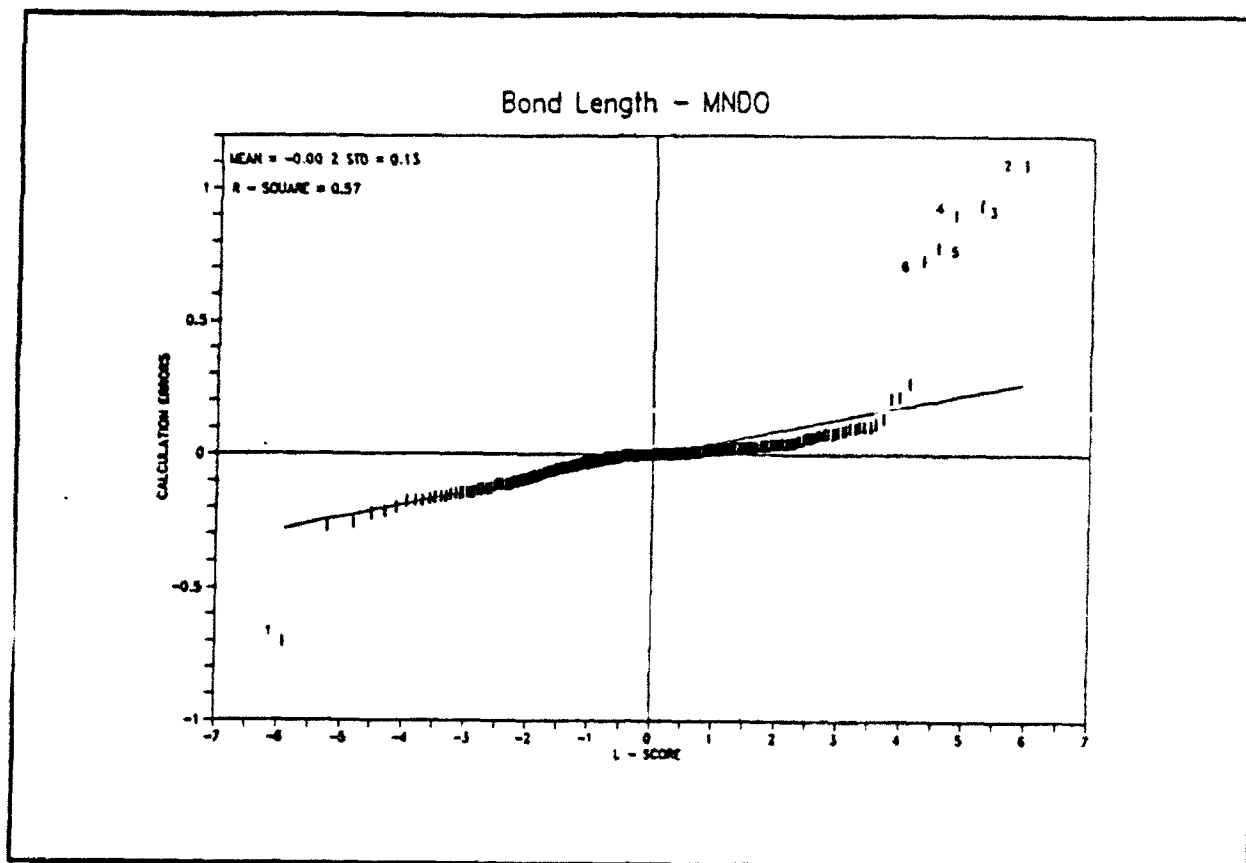


Figure 12. Test for Normal Distribution of Calculation Errors
- Bond Length, MNDO

Table 6. Compound with Largest Deviation of Calculated Error
of Bond Length Using the MNDO Method

#	CHEMICAL	BOND	EXPERIMENTAL	CALC. ERRORS
1	N ₂ O ₂	N-N	2.08	-0.706
2	H ₂ F ₂ (HF dimer)	H'-F	1.87	1.093
3	C ₇ H ₇ NO ₂ (salicylaldehyde)	N(14)-H(17)	1.834	0.94
4	H ₂ O ₂ (H ₂ O dimer)	O-O	3.0	0.905
5	C ₇ H ₇ NO ₂ (salicylaldehyde)	O(10)-N(14)	2.626	0.781
6	F ₂ I	I-F (ax)	1.76	0.731

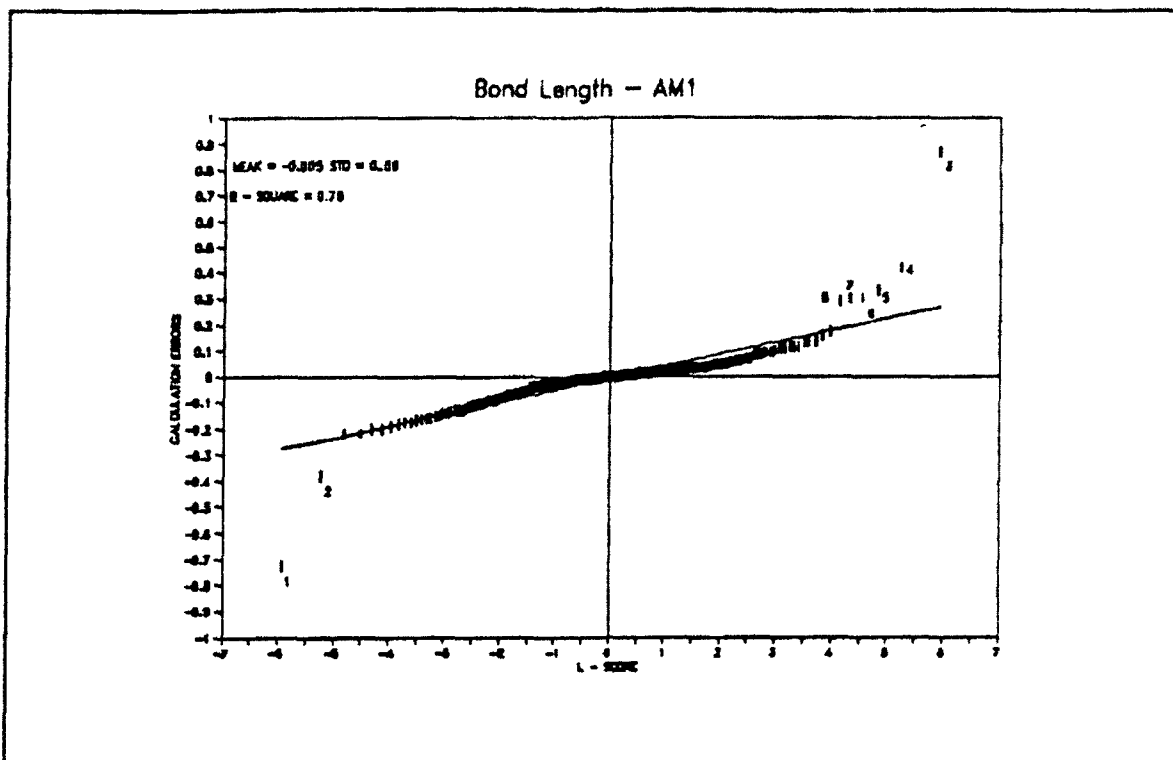


Figure 13. Test for Normal Distribution of Calculation Errors
- Bond Length, AM1

Table 7. Compound with Largest Deviation of Calculated Error
of Bond Length Using the AM1 Method

#	CHEMICAL	BOND	EXPERIMENTAL	CALC. ERRORS
1	N ₂ O ₃	N-N	2.08	-0.728
2	H ₂ O ₂ (H ₂ O dimer)	O-O	3.00	-0.383
3	F ₂ I	I-F (ax)	1.76	0.866
4	H ₂ F ₂ (HF dimer)	H'-F	1.87	0.417
5	O ₂ FC1	Cl-O	1.46	0.328
6	C ₇ H ₇ NO ₃ (Salicylaldehyde)	N(14)-H(17)	1.834	0.302
7	C ₇ H ₇ NO ₃ (Salicylaldehyde)	O(10)-N(14)	2.684	0.298
8	H ₂ SO ₄	S=O	1.42	0.287

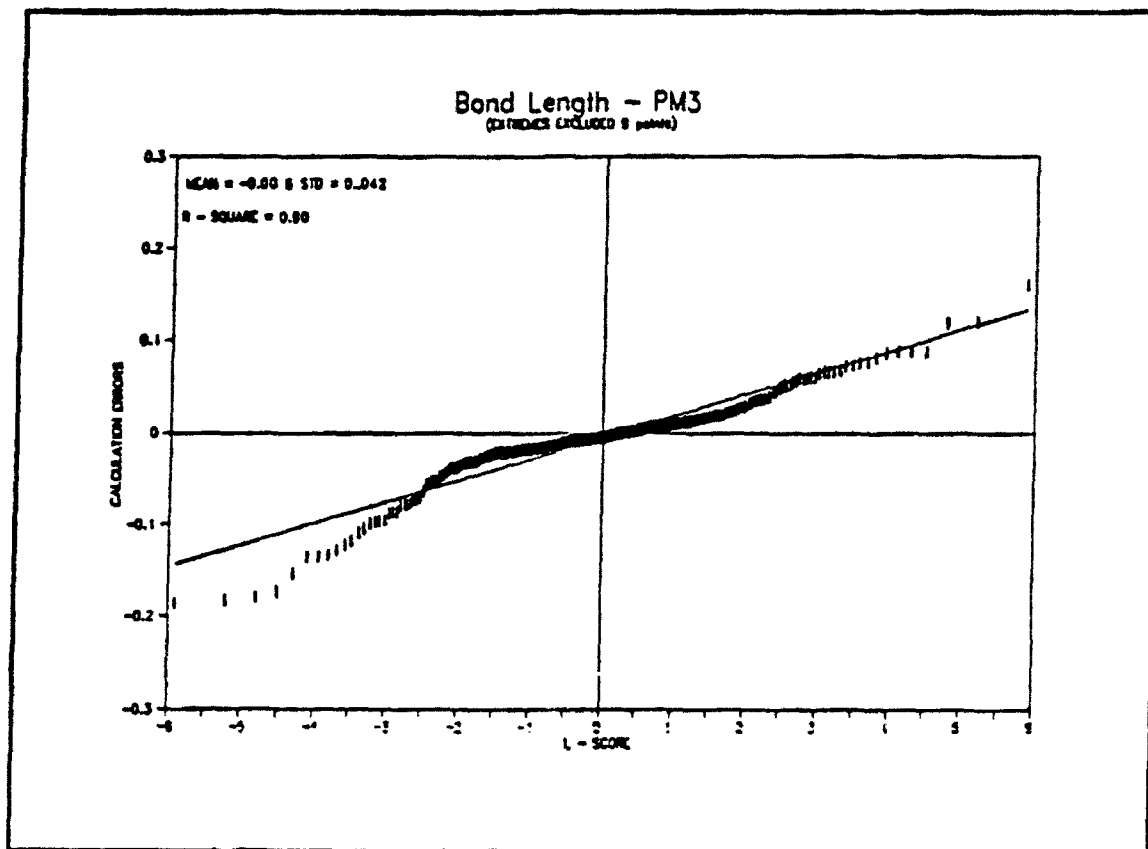


Figure 14. Test for Normal Distribution of Calculation Errors
- Bond Length, PM3 - Extremes Excluded

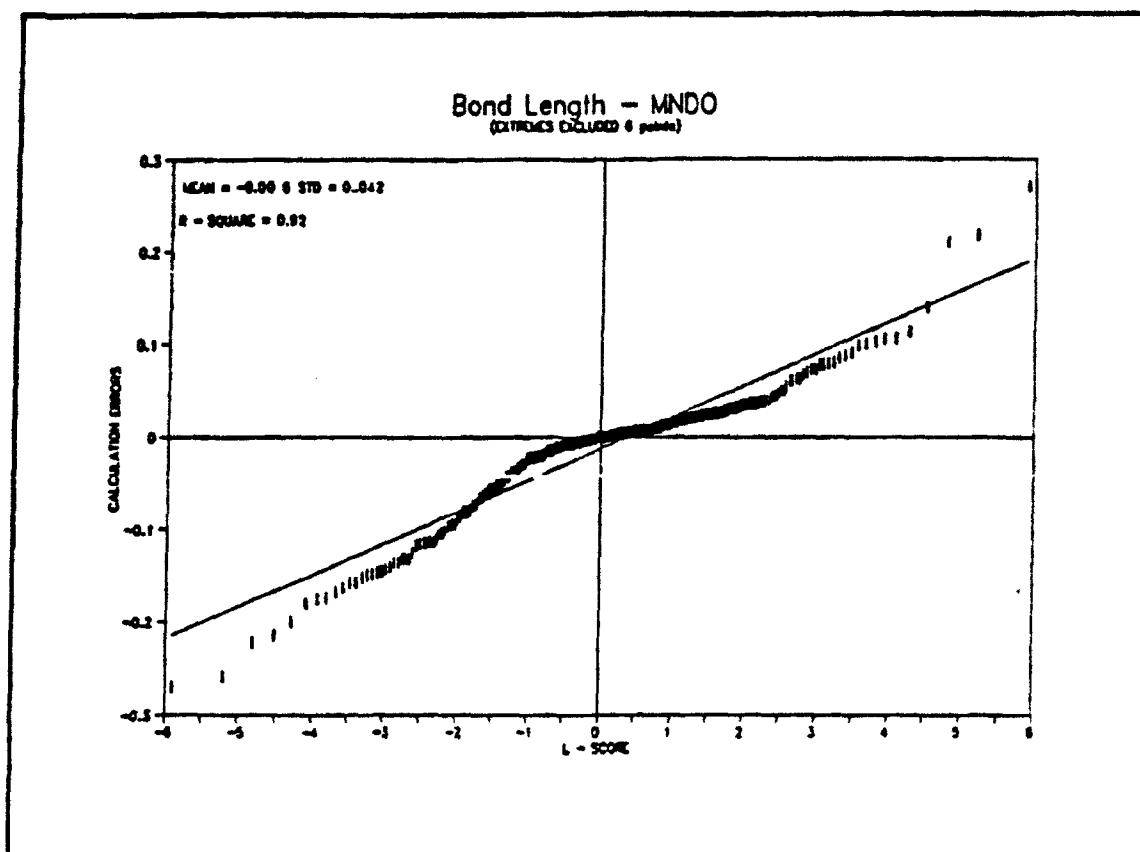


Figure 15. Test for Normal Distribution of Calculation Errors
- Bond Length, MNDO - Extremes Excluded

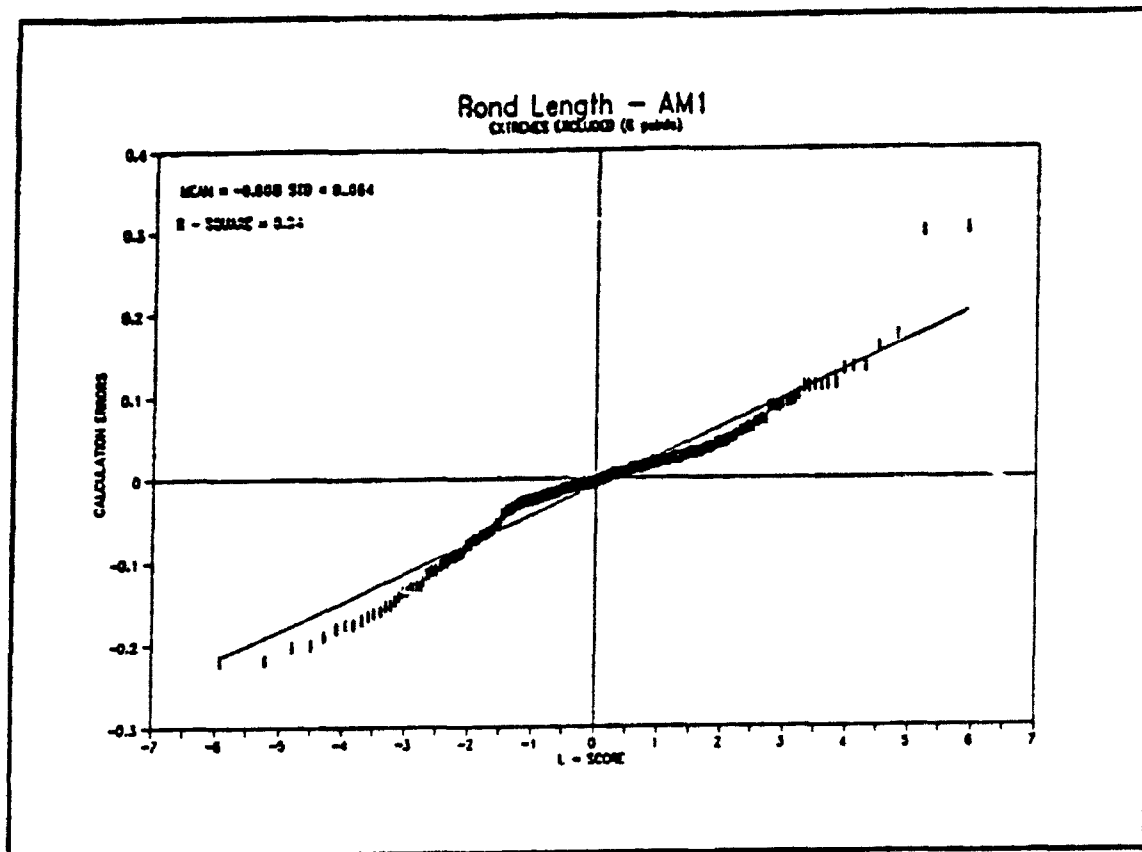


Figure 16. Test for Normal Distribution of Calculation Errors
- Bond Length, AM1 - Extremes Excluded

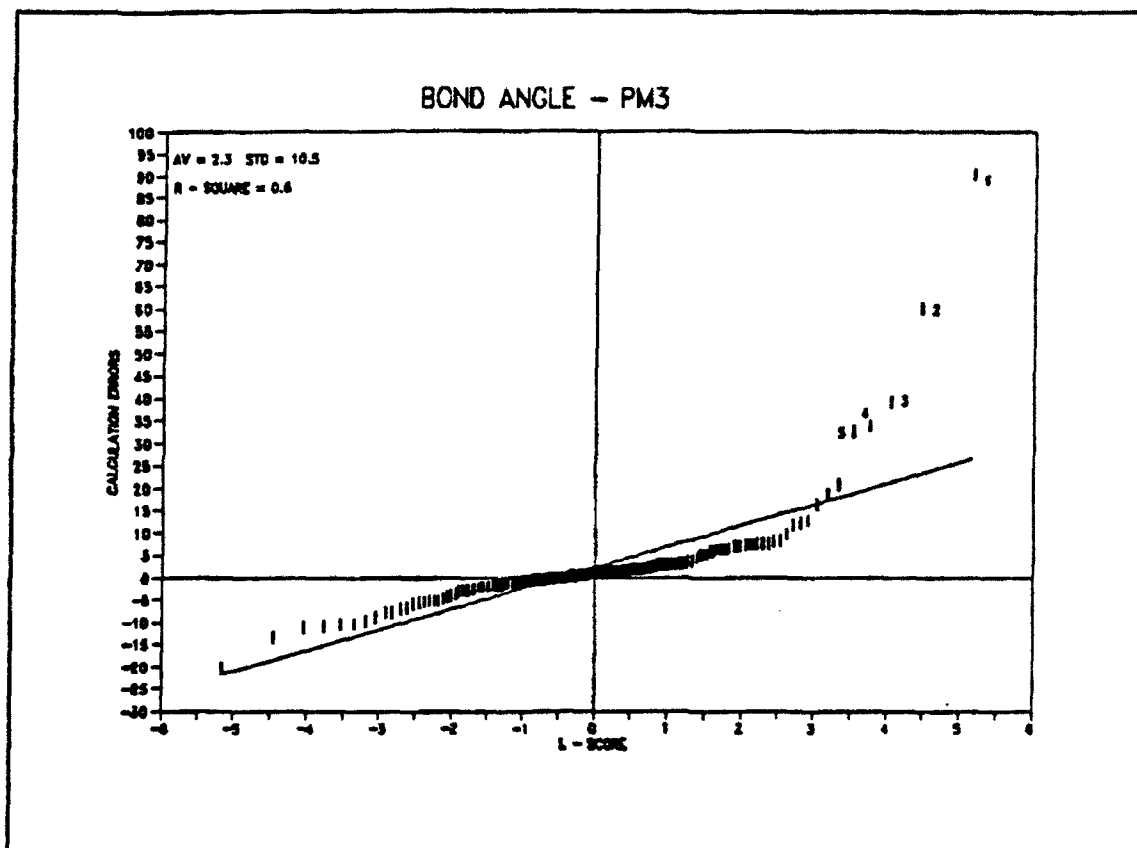


Figure 17. Test for Normal Distribution of Calculation Errors
- Bond Angle, PM3

Table 8. Compound with Largest Deviation of Calculated Error
of Bond Angle Using the PM3 Method

#	CHEMICAL	BOND	EXPERIMENTAL	CALC. ERRORS
1	H ₄ N ₂	HN-NH	90.0	90.3
2	H ₂ O ₂	HO-OH	119.8	60.2
3	H ₂ F ₂	H'FH	108.0	39.0
4	F ₃ Br ₂	F'BrF	86.2	33.8
5	F ₃ Cl	FClF'	87.5	32.5

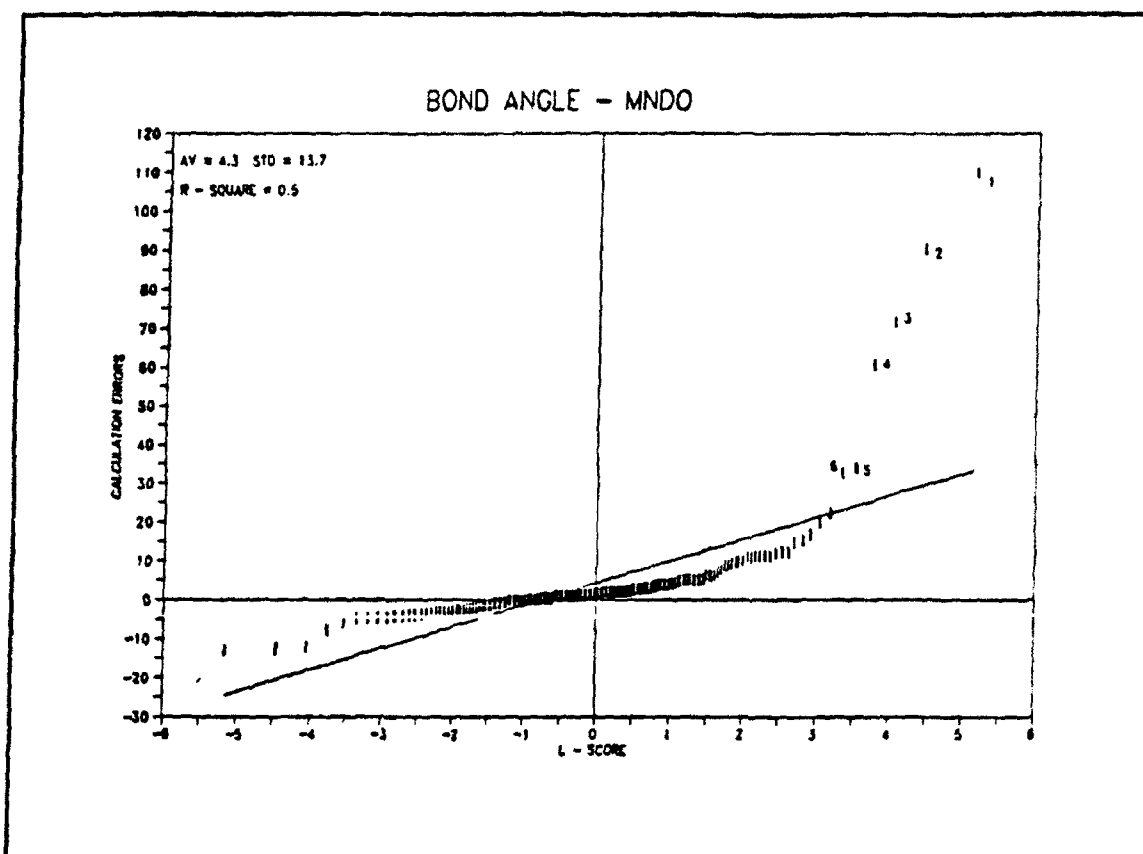


Figure 18. Test for Normal Distribution of Calculation Errors
- Bond Angle, MNDO

Table 9. Compound with Largest Deviation of Calculated Error
of Bond Angle Using the MNDO Method

#	CHEMICAL	BOND	EXPERIMENTAL	CALC. ERRORS
1	1,4 Pentadiene	C ₂ -C ₃ -C ₄ -C ₅	-4.3	110
2	H ₄ N ₂	HN-NH	90.0	90.2
3	H ₂ F ₂	H'FH	108.0	71.5
4	H ₂ O ₂	HO-OH	119.8	60.5
5	F ₃ Br ₂	F'BrF	86.2	33.8
6	F ₃ Cl	FClF'	87.5	32.5

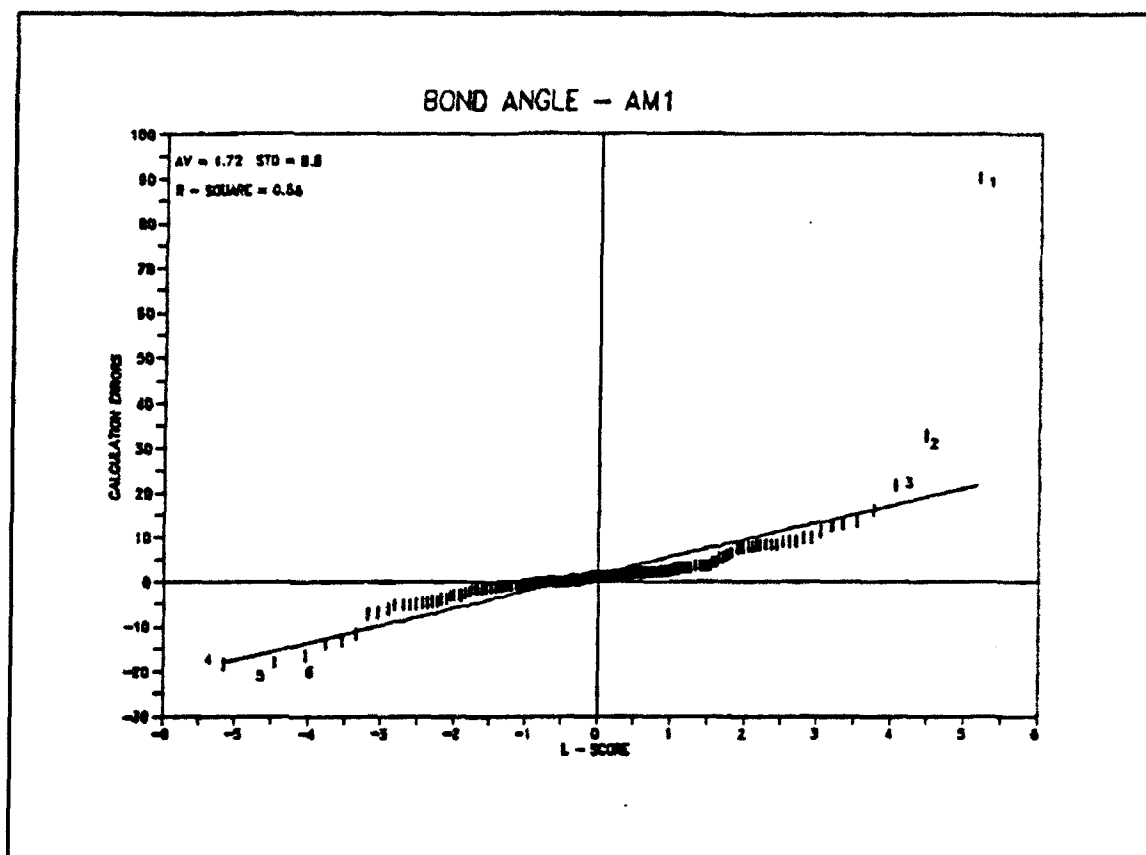


Figure 19. Test for Normal Distribution of Calculation Errors
- Bond Angle, AM1

Table 10. Compound with Largest Deviation of Calculated Error
of Bond Angle Using the AM1 Method

#	CHEMICAL	BOND	EXPERIMENTAL	CALC. ERRORS
1	H_4N_2	HN-NH	90.0	90.2
2	F_3Cl	FCIF'	87.5	32.5
3	H_2S_2	HS-SH	90.5	21.7
4	SF_4	FSF	101.6	-18.6
5	H_2F_2	H'FH	108	-18.1
6	SO_2	OSO	119.5	-16.6

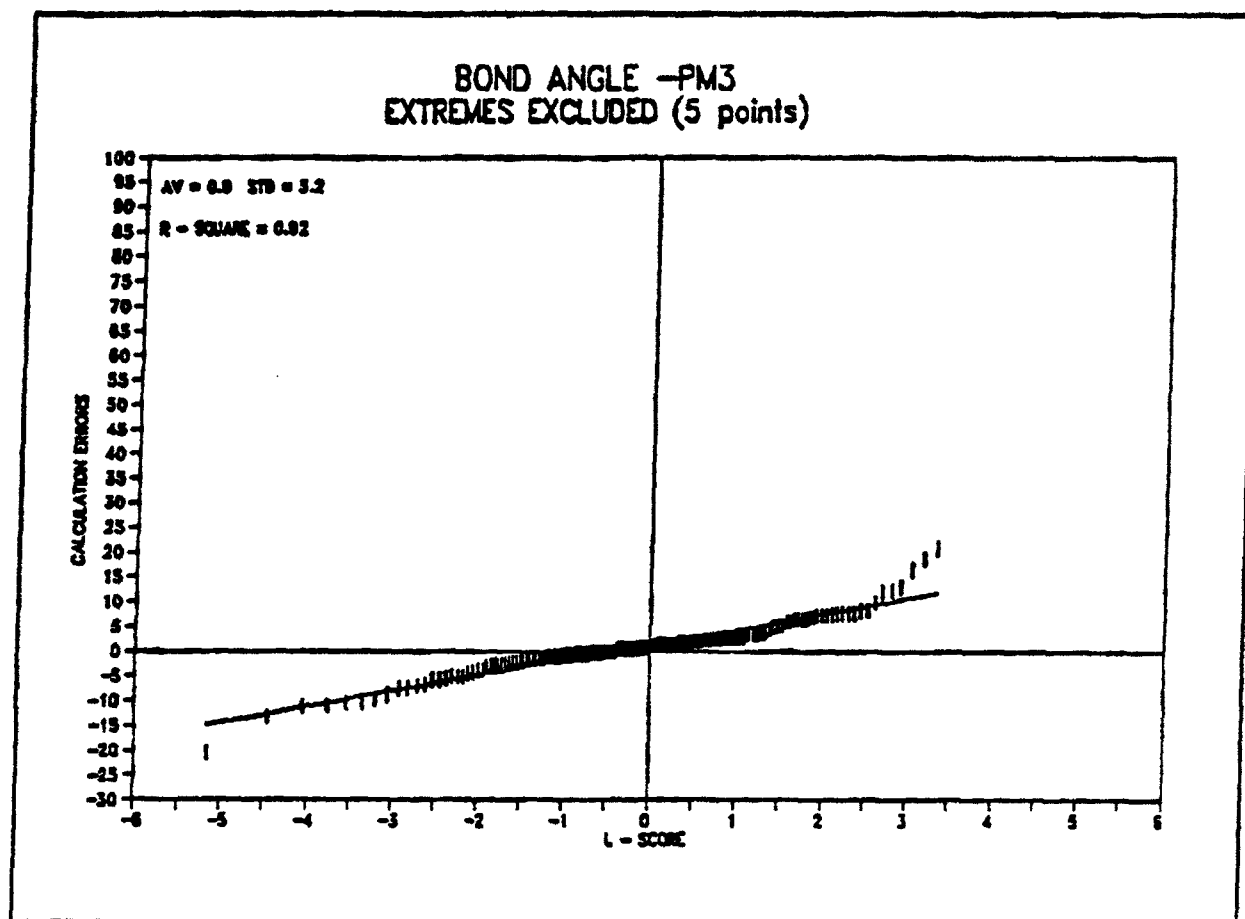


Figure 20. Test for Normal Distribution of Calculation Errors
- Bond Angle, PM3 - Extremes Excluded

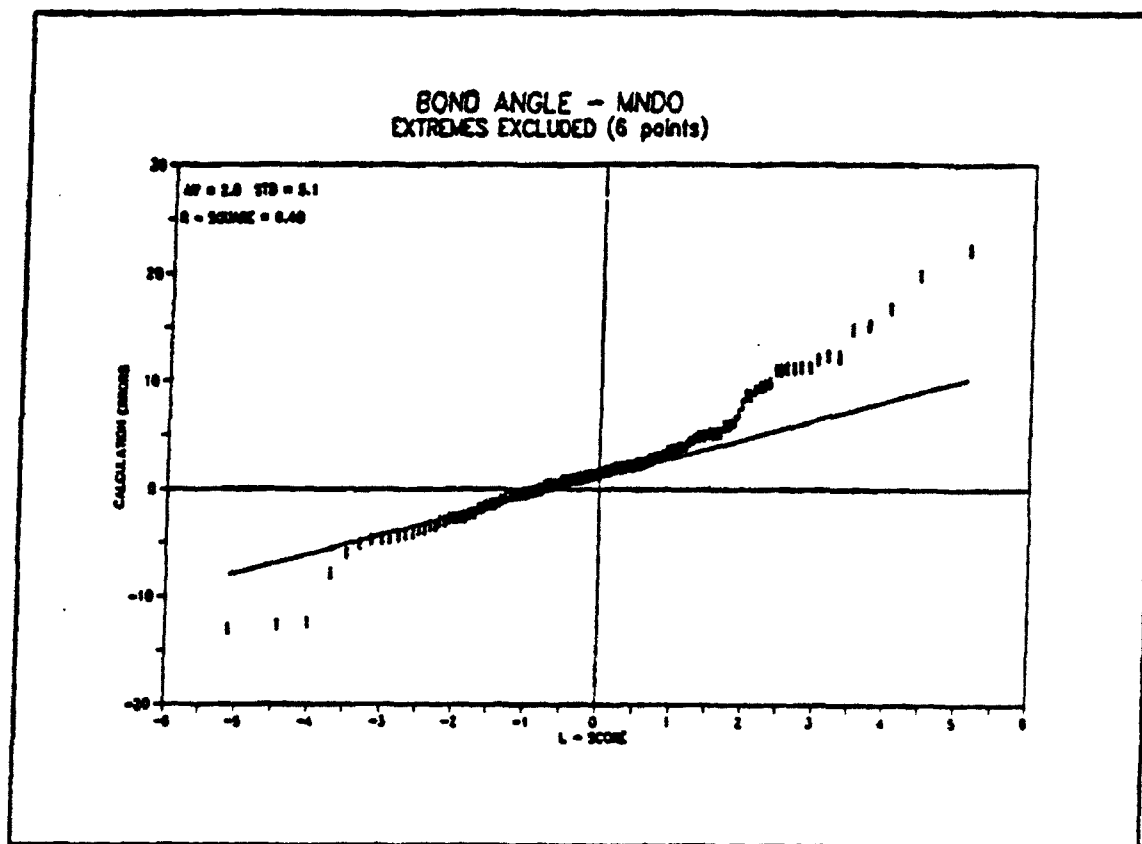


Figure 21. Test for Normal Distribution of Calculation Errors
- Bond Angle, MNDO - Extremes Excluded

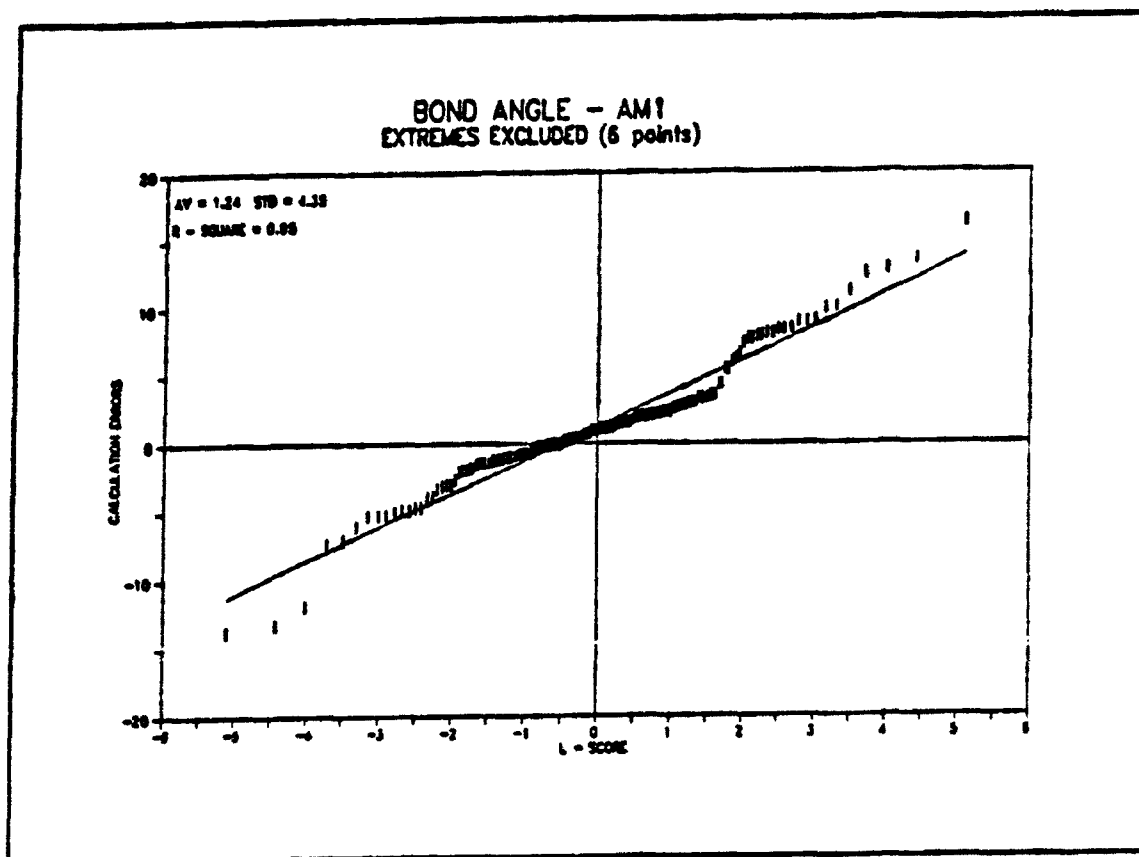


Figure 22. Test for Normal Distribution of Calculation Errors
- Bond Angle, AM1 - Extremes Excluded

Table 11. Recommended Computational Methods for the
Different Physical/Chemical Properties

COMPUTED PROPERTY	RECOMMENDED METHOD	BIAS	σ
HEAT OF FORMATION	PM3	0.44Kcal/mole	12.3Kcal/mole
IONIZATION POTENTIAL	MNDO	0.68 ev	0.70 ev
DIPOLE MOMENT	AM1	0.014 deby	0.49 deby
BOND LENGTH	AM1	0.08 Å	0.064 Å
BOND ANGLE	AM1	1.24°	4.35°