Title Page

Title (1 pts)

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Two Hypotheses (4 pts)

Due to the lack of proper hypotheses prepared before the lab setting, newer hypotheses were thought up before any of the data was calculated.

It is not believed that the readings for the physical dimensions of the graphite sample will be very accurate. At such a small system, the smallest of values can lead to a significant change in the overall calculations. Also, it is assumed that the unit cell has a perfect arrangement of geometry, but in reality, atoms are constantly in motion, and constantly changing their locations, which leads to constantly shifting bond lengths.

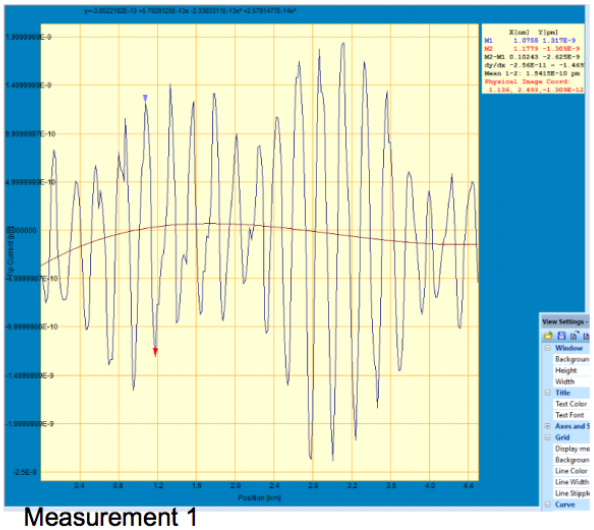
Another prediction for the lab is that the reading from the scanning-tunneling microscope will be quite noisy, which could also cause some errors. This is hypothesized because of interactions from the air. It is possible that particles in the air could interfere with the sample, and possibly interfere with the readings.

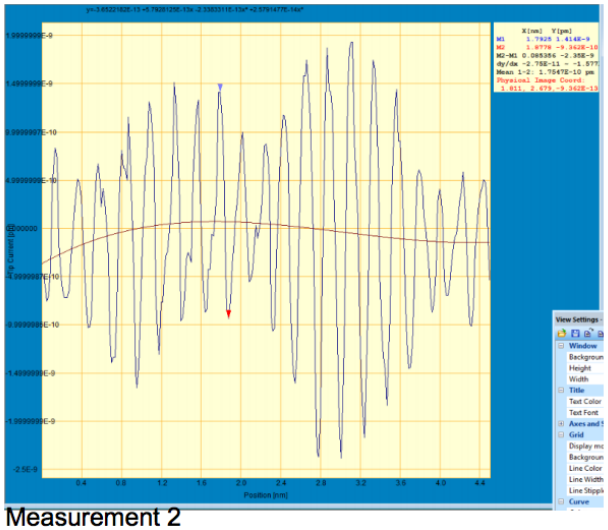
Abstract (5 pts)

Scanning-tunneling microscopy is a fairly new invention introduced into the field of chemistry, originating as recent as the late 80's. Scanning-tunneling microscopy as a whole has a number of benefits that come from its use over other types of microscopy. For one, the STM instrument is much smaller compared to an electron microscope, yet STM still manages to have accuracy near that of an electron microscope. For another, it is much easier to alter the operating parameters of the STM compared to the other instruments. Most of the properties of the STM come from the wire tip used in the instrument, which can easily be replaced with a wire tip of another material. Lastly, STM is able to alter the position of the scans in real-time. This is unlike an electron microscope, which takes much longer to run. In this experiment, the utility of the scanning-tunneling microscope is used to examine the structure of a sample of graphite, which is in turn used to determine physical properties of the sample, including bond length and density. The readings received gave an ideas to how the STM works, and how accurate the microscope is compared to other instruments. The data received from the experiment gave semi-inaccurate results, but still show the convenience that STM holds.

Results (35 pts)

After the scan of the graphite sample is complete, the reading can be analyzed to determine possible values needed to determine the a-parameters of the graphite unit cell.


Measurement 1


Measurement 2

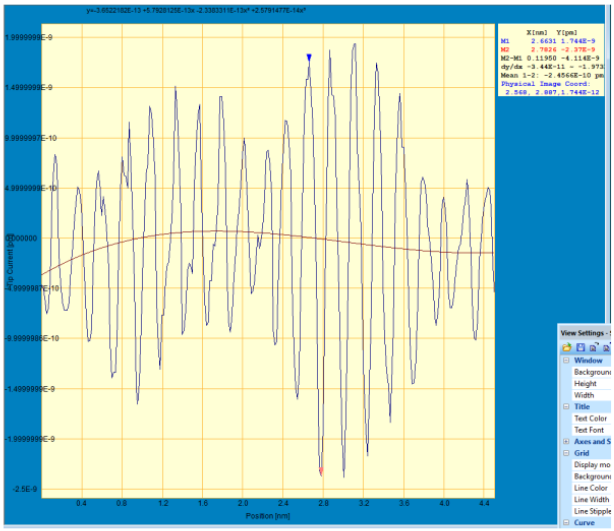

Measurement 3

Figure 1 – Analysis of the scans of graphite in the STM. In each measurement, there are two data points, which correlate to the M1 and M2 values. These values are used to determine the partial a-parameters of the graphite. In the case of this experiment, three measurements are taken.

Table 1 – M1 and M2 values gathered from the measurements in **Figure 1**, and calculated partial a-parameters.

Measurement #	M1x (nm)	M1y (pm)	M2x (nm)	M2y (pm)	a (nm) [1] {1}	a (m) [1] {1}
1	$1.0755 \pm 5\times10^{-5}$	$1.317\times10^{-9} \pm 5\times10^{-13}$	$1.1779 \pm 5\times10^{-5}$	$-1.309\times10^{-9} \pm 5\times10^{-13}$	$0.1024 \pm 7\times10^{-5}$	$1.024\times10^{-10} \pm 7\times10^{-14}$
2	$1.7925 \pm 5\times10^{-5}$	$1.414\times10^{-9} \pm 5\times10^{-13}$	$1.8778 \pm 5\times10^{-5}$	$-9.362\times10^{-10} \pm 5\times10^{-13}$	$0.0853 \pm 7\times10^{-5}$	$0.853\times10^{-10} \pm 7\times10^{-14}$
3	$2.6631 \pm 5\times10^{-5}$	$1.744\times10^{-9} \pm 5\times10^{-13}$	$2.7826 \pm 5\times10^{-5}$	$-2.37\times10^{-9} \pm 5\times10^{-13}$	$0.1195 \pm 7\times10^{-5}$	$1.195\times10^{-10} \pm 7\times10^{-14}$

After the partial a-parameters are found, the total a-parameter of the graphite cell can be determined. This is simply done by take the sum of the individual parts.

Table 2 – Partial a-parameters, and the total a-parameter calculated.				
#	1 [1] {1}	2 [1] {1}	3 [1] {1}	Total [2] {2}
a (m)	$1.024\times10^{-10} \pm 7\times10^{-14}$	$0.853\times10^{-10} \pm 7\times10^{-14}$	$1.195\times10^{-10} \pm 7\times10^{-14}$	$3.072\times10^{-10} \pm 1\times10^{-13}$

With the a-parameter now determined, the volume of the unit cell can be found. For this experiment, the c-parameter is given, as it is not possible for the c-parameter to be determined from scanning-tunneling microscopy.

Table 3 – Determination of the volume of the graphite unit cell.			
a (m) [2] {2}	c (m)	V (m^3) [3] {3}	V (cm^3) [3] {3}
$3.072\times10^{-10} \pm 1\times10^{-13}$	$6.7079\times10^{-10} \pm 5\times10^{-15}$	$5.482\times10^{-29} \pm 4\times10^{-32}$	$5.482\times10^{-23} \pm 4\times10^{-26}$

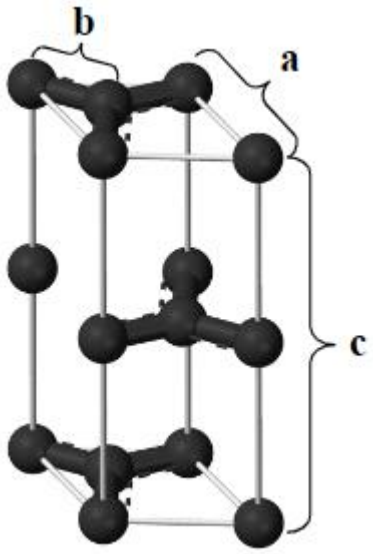


Figure 2 – Unit cell diagram of graphite assumed in the experiment.

Now with the volume known, as well as the mass and number of carbons in the unit cell, the density of the unit cell can be determined.

Table 4 – Determination of density using V, m, and Z.			
Z	m (g) [4] {4}	V (cm^3) [3] {3}	ρ (g/cm^3) [5] {5}
4	$7.978\times10^{-23} \pm 3\times10^{-28}$	$5.482\times10^{-23} \pm 4\times10^{-26}$	1.455 ± 0.001

It is assumed that Z is equal to 4 in the unit cell, rather than 15. This is because the carbons that lie on the corners, the edges, and the faces of the unit cell are also interacting with other unit cells present around the one shown above. The carbons on the corners are also a part of eight other unit cells, the carbons on the edges are a part of four other unit cells, and the carbons on the faces are a part of two other unit cells. Because of this, it can be believed that ⅛, ¼, and ½ of each carbon on the corners, edges, and faces of the unit cell are actually present in the unit cell shown above. This gives a total count of carbons present in the unit cell of four.

Lastly, going back to the determined a-parameter, the value received can be used to determine the bond length of the carbon-carbon bonds in the unit cell. This can be achieved through simple geometric calculations. It is believed

that the structure of the graphite is a 100% uniform hexagonal pattern. The process for determining the value of b is shown below.

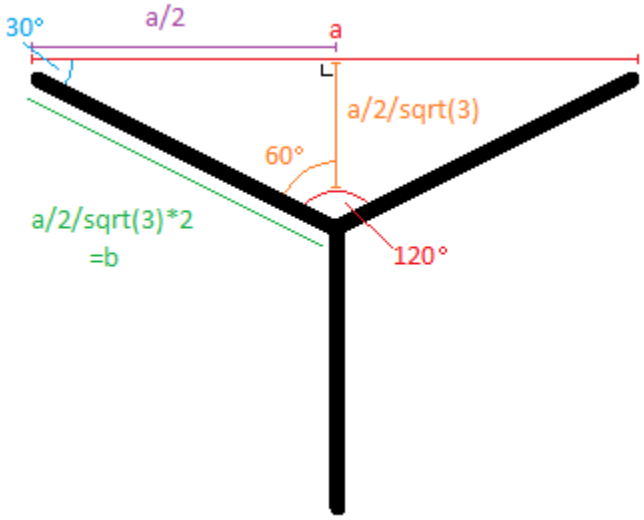


Figure 3 – Cross section of a layer of the unit cell of graphite.

Table 5 – a-parameter and bond length b determined.	
a (m) [2] {2}	b (m) [6] {6}
$3.072\times10^{-10} \pm 1\times10^{-13}$	$1.774\times10^{-10} \pm 7\times10^{-14}$

Sample Calculations (15 pts)

[1]

$$a_n = M2_n - M1_n$$

$$a_1 = 1.1779 \cdot 10^{-9}\ \text{m} - 1.0755 \cdot 10^{-9}\ \text{m} = 1.024 \cdot 10^{-10}\ \text{m}$$

[2]

$$a = \sum a_n$$

$$a = 1.024 \cdot 10^{-10}\ \text{m} + 8.53 \cdot 10^{-11}\ \text{m} + 1.195 \cdot 10^{-10}\ \text{m} = 3.072 \cdot 10^{-10}\ \text{m}$$

[3]

$$V = a^2 c \sin\left(\frac{120°\pi}{180}\right)$$

$$V = (3.072 \cdot 10^{-10}\ \text{m})^2 (6.7079 \cdot 10^{-10}\ \text{m}) \sin\left(\frac{120°\pi}{180}\right) = 5.482 \cdot 10^{-29}\ \text{m}^3 = 5.482 \cdot 10^{-23}\ \text{cm}^3$$

[4]

$$m = Z \cdot \frac{MM}{NA}$$

$$m = 4 \cdot \frac{12.0107\ \frac{\text{g}}{\text{mol}}}{6.022 \cdot 10^{23}\ \text{mol}^{-1}} = 7.978 \cdot 10^{-23}\ \text{g}$$

[5]

$$\rho = \frac{m}{V}$$

$$\rho = \frac{7.978 \cdot 10^{-23}\ \text{g}}{5.482 \cdot 10^{-23}\ \text{cm}^3} = 1.455\ \frac{\text{g}}{\text{cm}^3}$$

[6]

$$b = \frac{\frac{a}{2}}{\sqrt{3}} \cdot 2 = \frac{a}{\sqrt{3}}$$

$$b = \frac{3.072 \cdot 10^{-10}\ \mathrm{m}}{\sqrt{3}} = 1.774 \cdot 10^{-10}\ \mathrm{m}$$

{1}

$$\delta a_n = \sqrt{(\delta M2_n)^2 + (\delta M1_n)^2}$$

$$\delta a_1 = \sqrt{(5 \cdot 10^{-14}\ \mathrm{m})^2 + (5 \cdot 10^{-14}\ \mathrm{m})^2} = 7 \cdot 10^{-14}\ \mathrm{m}$$

{2}

$$\delta a = \sqrt{{\delta a_1}^2 + {\delta a_2}^2 + {\delta a_3}^2}$$

$$\delta a = \sqrt{(7 \cdot 10^{-14}\ \mathrm{m})^2 + (7 \cdot 10^{-14}\ \mathrm{m})^2 + (7 \cdot 10^{-14}\ \mathrm{m})^2} = 1 \cdot 10^{-13}\ \mathrm{m}$$

{3}

$$\delta V = a^2 c \sin\left(\frac{120° \pi}{180}\right) \sqrt{\left[\frac{2\left(\frac{\delta a}{a}\right)}{a^2}\right]^2 + \left[\frac{\delta c}{c}\right]^2}$$

$$\delta V = (3.072 \cdot 10^{-10}\ \mathrm{m})^2 \cdot 6.7079 \cdot 10^{-10}\ \mathrm{m} \cdot \sin\left(\frac{120° \pi}{180}\right) \sqrt{\left[\frac{2\left(\frac{1 \cdot 10^{-13}\ \mathrm{m}}{3.072 \cdot 10^{-10}\ \mathrm{m}}\right)}{(3.072 \cdot 10^{-10}\ \mathrm{m})^2}\right]^2 + \left[\frac{5 \cdot 10^{-15}\ \mathrm{m}}{6.7079 \cdot 10^{-10}\ \mathrm{m}}\right]^2} = 4 \cdot 10^{-32}\ \mathrm{m}^3$$

$$= 4 \cdot 10^{-26}\ \mathrm{cm}^3$$

{4}

$$\delta m = Z \cdot \frac{\delta MM}{NA}$$

$$\delta m = 4 \cdot \frac{0.00005\ \frac{\mathrm{g}}{\mathrm{mol}}}{6.022 \cdot 10^{23}\ \mathrm{mol}^{-1}} = 3 \cdot 10^{-28}\ \mathrm{g}$$

{5}

$$\delta \rho = \rho \sqrt{\left(\frac{\delta m}{m}\right)^2 + \left(\frac{\delta V}{V}\right)^2}$$

$$\delta \rho = 1.455\ \frac{\mathrm{g}}{\mathrm{cm}^3} \sqrt{\left(\frac{3 \cdot 10^{-28}\ \mathrm{g}}{7.978 \cdot 10^{-23}\ \mathrm{g}}\right)^2 + \left(\frac{4 \cdot 10^{-26}\ \mathrm{cm}^3}{5.482 \cdot 10^{-23}\ \mathrm{cm}^3}\right)^2} = 0.001\ \frac{\mathrm{g}}{\mathrm{cm}^3}$$

{6}

$$\delta b = \frac{\frac{a}{2}}{\sqrt{3}} \cdot 2 = \frac{\delta a}{\sqrt{3}}$$

$$\delta b = \frac{1 \cdot 10^{-13}\ \mathrm{m}}{\sqrt{3}} = 7 \cdot 10^{-14}\ \mathrm{m}$$

Discussion, 1 (min) – 2 (max) pages, single spaced (35 pts)

The first hypothesis supposed stated that the values would not be accurate because of the small-scale system that the lab is focusing on. At microscopic levels, the values that would normally cause indistinguishable error at normal levels become values that could drastically affect the readings received from the lab. Looking at the results and comparing them to literature values found online, the error gathered from the experiment can be discovered.

Table 6 – Error calculations for determined values.

Value	Experimental	Theoretical	Error (%)
ρ	1.455 ± 0.001 g/cm^3	2.26 g/cm^3	35.6
b	$1.774\times10^{-10} \pm 7\times10^{-14}$ m	1.42×10^{-10} m	24.9

The error shown above has proven to be less than ideal for determining these values. This goes to show that the hypothesis was correct. That being said, however, the amount of error was actually less than what was expected. It was believed that the values would show little correlation to the literature values. In the experimental run, the values received seemed to lie right in the middle between accurate and inaccurate. Also, the uncertainties of the values obtained are not very large, so the percent error cannot really be blamed on the lack of precision.

The second hypothesis states that the scans of the samples through the scanning-tunneling microscope would come out noisy and overall not very sharp. As with the first hypothesis, it was proven to be true, but not necessarily outright. The scans received still have a sense of distinction between the two, as it is possible to tell which scan is graphite and which is gold. That being said, the readings are not clear enough for the bond length of the carbon-carbon bonds in graphite to be found. As shown in the figure below, the graphite and gold samples have significantly different structures. The graphite shows the carbon molecules neatly arranged in somewhat of a hexagonal pattern, as to be expected, and the gold lacks any uniformity in its structure.

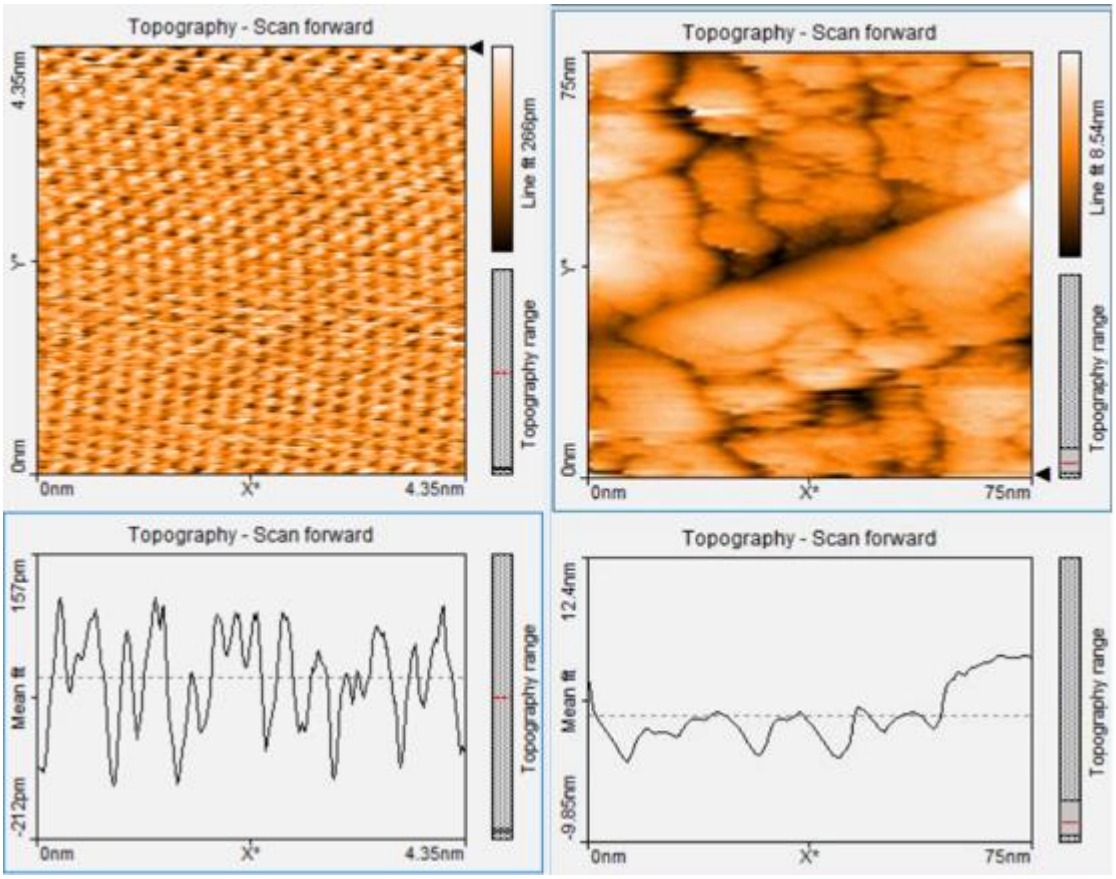


Figure 4 – Scans of the samples used in the lab. The scan on the left is graphite, and the scan on the right is gold.

The reason why graphite has an organized structure and gold does not is due to the crystallinity of the two samples. Crystals have an overall much more uniform in structure, and the gold used is most likely not in its crystalline form. The uniformity of graphite makes it a much better sample to scan, as the data is much more significant than gold, and the repeating crystalline structure allows for bulk properties to be obtained.

The way that scanning-tunneling spectroscopy works is through the transfer of electrons from the wire tip to the samples being scanned. The readings from the electrons traveling from the samples show a variation in the distance from the tip to the individual molecules through the electrical interaction. Areas where molecules are will show a brighter color and areas without a molecule will show a darker color. This idea comparing a difference of color to a difference of energy can be seen more clearly in **Figure 5**. Because of the transfer of electrons, only samples that are conductors or semiconductors can be analyzed, as insulators will not receive electrons transferred through the electrical current. The precision of the STM relies on the wire tip used to conduct the electricity. This is why the edge is sharpened before the STM is run. If the tip has more surface area, the electric current is spread over a large amount of the sample, and therefore less concentrated. The less surface area confines the flow to a much narrower area, which results in a more concentrated flow.

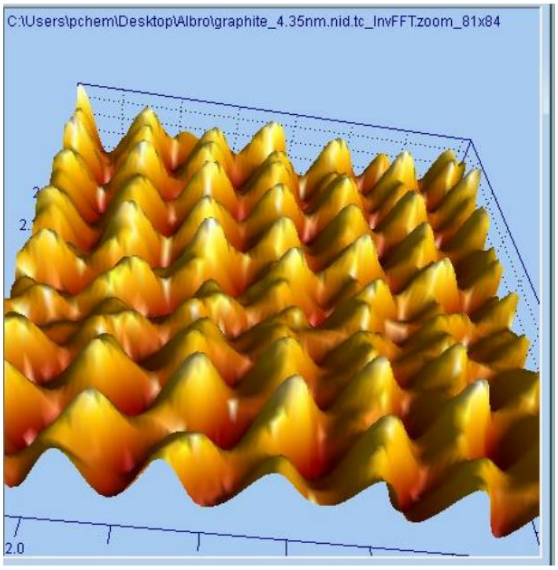


Figure 5 – 3D scan of a portion of the reading of graphite received from the STM. The peaks show a difference in energy, which in turn imply the positions of the carbon atoms in graphite. This also explains why the c lattice parameter needs to be given; the energy only comes into contact with the first layers of the graphite, and the subsequent layers are shielded.

The STM's feature of using electricity is also significant for another number of reasons. In the experiment, the amount of electricity run through the sample was altered for the different samples used (0.5 V for graphite and 50 mV for gold). This compensates for the difference in conductivity between the two samples. Gold is a much better conductor of electricity compared to graphite, so less over voltage is needed to obtain the reading of the gold sample.

The use of conductive materials can also be used to scan materials that do not conduct. If a non-conductive sample is covered in a layer of conductive material, the structure of the non-conductive material can be seen in the readings. However, this can only be achieved to determine a more macroscopic scale of structure, as looking for the atomic structure of a non-conductive sample would only show the atomic structure of the conductive sample coating it. Larger materials such as DNA have been observed through STM by this procedure.

Lab Notebook (5 pts)

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O
1		x (nm)	y (pm)		a (nm)	d	a^2	da^2	V (m^3)	dV (m^3)	V (cm^3)	dV (cm^3)	D (g/cm^3)	dD (g/cm^3)	
2	M11	1.0755	1.317E-09		1.02E-10	7E-14			6.091E-30						
3	M12	1.1779	-1.309E-09		8.53E-11	7E-14			4.227E-30						
4	M21	1.7925	1.414E-09		1.2E-10	7E-14			8.296E-30						
5	M22	1.8778	-9.362E-10		-7.5E-11										
6	M31	2.6631	1.744E-09		3.07E-10	1E-13	9.437E-20	8E-23	5.482E-29	4E-32	5.482E-23	4E-26	1.455	0.00116	-35.6%
7	M32	2.7826	-2.37E-09												24.9%
8	dM1	0.1024	-2.63E-09		c (nm)										
9	dM2	0.0853	-2.35E-09		6.71E-10	5.00E-15									
10	dM3	0.1195	-4.11E-09		m				m (g)	dm (g)					
11					12.0107	5.00E-05			7.978E-23	3.321E-28					
12		5.00E-14			Z										
13		7.071E-14			4										
14															
15							1.774E-10	7E-14							
16															
17							1.7743E-10	1.7729E-10							