Supporting Information

Revisiting the Oxidation of Graphite: Reaction Mechanism, Chemical Stability, and Structure Self-regulation

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Discussion S1: the formation of oxonium ions

In the modified Hummers method, the oxidation of graphite occurs in the medium of concentrated sulfuric acid. In our experiment, the concentration of sulfuric acid is 18.4 mol/L. Sulfuric acid is a strong acid with pKₐ=-10 and will easily donate one of its two hydrogens. After the oxygen-containing functional groups are formed on graphene surface, part of them such as epoxide group will react with excess sulfuric acid.

For example:  \[ R-O-R + H_2SO_4 \rightleftharpoons R-OH-R^+ + HSO_4^- \]  (1)

For the forward reaction, \(H_2SO_4\) is functioning as an acid, and \(R-O-R\) is functioning as a base.

For the reverse reaction, \(R-OH-R^+\) is functioning as an acid, and \(HSO_4^-\) is functioning as a base.

For the forward reaction, \(pK_{eq} = pK_a L - pK_a R\) (2)

\[ = pK_a (H_2SO_4) - pK_a (R-OH-R^+) \]

\[ = -10 - (-3.6) \]

\[ = -6.4 \]

From \(pK_{eq} = - \log K_{eq} = -6.4\), we can get \(K_{eq} = 10^{6.4} \gg 1\). \(K_{eq} \gg 1\) indicates that the equilibrium lies to the right and favors the weaker acid.
Discussion S2: verification of the intercalating-oxidation and subsequent diffusive-oxidation processes of graphite

Experimental procedure: The whole procedure was conducted at room temperature. First, 100 mL of concentrated H$_2$SO$_4$ and 1 g of graphite were added into a 250 mL conical flask with vigorous stirring. Then, 0.5 g of KMnO$_4$ was added into the mixture to form electrically neutral oxidizing agent for the intercalating-oxidation of graphite. After 30 min stirring, 1 g of KNO$_3$ was added into the mixture to form electrophile for the diffusive-oxidation of H$_2$SO$_4$-GIC. 4 g of MnO$_2$ was subsequently added into the mixture to oxidize the reaction byproduct and form electrophile. The oxidation reaction took about one week. Finally, completely oxidized graphite oxide (without black graphite domain) could be obtained. To prepare unhydrolyzed sample, the oxidized graphite was washed as described in Section 4.2.

Sample characterization and analysis: the unhydrolyzed oxidized graphite sample was characterized with $^{13}$C SSNMR, TGA-DSC, and XPS (Figure S1). Figure S1a shows the $^{13}$C SSNMR spectrum of oxidized product. Besides the resonance signal of C=O bond (168.8 ppm), a strong resonance signal at 135.8 ppm also appears, which can be attributed to the formation of isolated sp$^2$ carbon pair. The resonance signals of monosulfate and disubstituted tert-butyl sulfate are also observed at 85.8 and 75.4 ppm, respectively, indicating the relatively high oxidation degree of graphite oxide. Figure S1b shows the TGA-DSC curves of oxidized graphite, and the sample has two major weight losses. The first major weight loss happens between 150 and 170 °C due to the decomposition of the labile oxygen-containing functional groups such as hydroxyl and epoxide groups. The second major weight loss happens between 620 and 760 °C, and the 31.6% weight loss can be attributed to the loss of sulfur.[32] Figures S1c and S1d show the XPS survey spectrum and high-resolution C 1s spectra of unhydrolyzed oxidized graphite, respectively. The atomic fractions of oxidized product are 39.18%, 46.49%, and 11.22% for C, O, and S atoms, respectively, indicating that the main oxygen-containing group is organosulfate. Meanwhile, the atomic fractions of C-C/C=C, C-O, and C=O are 61.9%, 29.1%, and 9.0%, respectively, indicating that the sample obtained with this method has a lower functional group content than that with the modified Hummers method.

For the modified Hummers method, 4 weight equivalent oxidizing agent KMnO$_4$ is needed for the oxidation of graphite. But in this procedure, only 0.5 weight equivalent KMnO$_4$ is used, which cannot realize the effective oxidation of graphite. Meanwhile, although nitric acid acting as a Bronsted-Lowry base in the medium of concentrated sulfuric acid and forming H$_2$NO$_3$, which in turn decomposes into nitronium ion, treating graphite with a mixture of concentrated nitric and sulfuric acids can only generate products similar to H$_2$SO$_4$-GIC due to the repulsive interaction between
electrophile $\text{NO}_2^+$ and positively charged $\text{H}_2\text{SO}_4\text{-GIC}$. The combination of the above two oxidizing agents can realize the complete oxidation of graphite, and the possible oxidation mechanism of this method is as follows: (i) the electrically neutral oxidizing agent forms in the medium of $\text{KMnO}_4$-$\text{H}_2\text{SO}_4$, and then intercalates into the interlayer spaces of graphite, damages the aromatic carbon skeleton, and transfers the charge of $\text{H}_2\text{SO}_4\text{-GIC}$ by forming oxygen-containing functional groups ($\text{C}=\text{O}$); (ii) electrophile $\text{NO}_2^+$ forms in the medium of $\text{KNO}_3$-$\text{H}_2\text{SO}_4$ and then diffuses into the interlayer spaces of $\text{H}_2\text{SO}_4\text{-GIC}$ through electron-rich domains, forming oxygen-containing groups by the oxidation of isolated $\text{C}=\text{C}$ bonds; (iii) the reaction by-product ($\text{NO}_2$) is oxidized by the decomposition product of $\text{MnO}_2$, forming electrophile $\text{NO}_2^+$. The feasibility of the above procedure indicates that the oxidation reaction of graphite indeed includes the intercalating-oxidation process of an electrically neutral oxidizing agent and the subsequent diffusive-oxidation process of an electrophile.

Figure S1. (a) Solid-sate $^{13}$C magic-angle spinning NMR spectrum, (b) TGA-DSC curves, (c) XPS survey scan, and (d) high-resolution C 1s scans of unhydrolyzed oxidized graphite.
Figure S2. XPS survey scans of unhydrolyzed oxidized graphite.
Figure S3. DSC curves of the unhydrolyzed oxidized graphite.
Figure S4. Deconvoluted C 1s X-ray photoelectron spectra of unhydrolyzed oxidized graphite.
Figure S5. Electron density distribution of (a) MnO$_3^+$, (b) HSO$_4^-$, (c) H$_2$SO$_4$-GIC, (d) epoxy-GO, (e) oxonium-GO, and (f) sulfate-GO.
Calculation data S1: the standard Gibbs free energy of formation ($\Delta_f G_m^\theta$) of each reactant and interim oxidized product and the calculation of Gibbs free energy ($\Delta_r G_m^\theta$) of each oxidation process (the formation of epoxy-GO, oxonium-GO, and sulfate-GO).

1. Epoxidation of graphite (the positive charge can be transferred to the aromatic domain, and the formed 19-rings oxidized microdomain doesn’t carry positive charge).

|                    | carbon skeleton | MnO$_3^+$  | epoxy-GO | MnO$_2$  |
|--------------------|----------------|------------|----------|----------|
| $\Delta_f G_m^\theta$ | -2068.384377   | -1376.089389 | -2143.579630 | -1301.293528 |
| $v_i$              | 1              | 1          | 1        | 1        |
| $\sum_i v_i \Delta_f G_m^\theta$ | -3444.473766 | -3444.873158 |

$$\Delta_r G_m^\theta = -3444.873158 - (-3444.473766) = -0.399392 \text{hartree} = -10.87 \text{eV} \quad (3)$$

2. Epoxidation of graphite (the positive charge cannot be transferred to the aromatic domain, and the formed 19-rings oxidized microdomain carries one positive charge).

|                    | carbon skeleton | MnO$_3^+$  | epoxy-GO | MnO$_2$  |
|--------------------|----------------|------------|----------|----------|
| $\Delta_f G_m^\theta$ | -2068.384377   | -1376.089389 | -2143.371596 | -1301.293528 |
| $v_i$              | 1              | 1          | 1        | 1        |
| $\sum_i v_i \Delta_f G_m^\theta$ | -3444.473766 | -3444.665124 |

$$\Delta_r G_m^\theta = -3444.665124 - (-3444.473766) = -0.191358 \text{hartree} = -5.21 \text{eV} \quad (4)$$

3. Transferring one positive charge from the oxidized microdomain with 19-rings to aromatic island.

| epoxy-GO with one positive charge | epoxy-GO without positive charge |
\[
\Delta_f G_m^\theta |_{v_i} \quad \Delta_f G_m^\theta |_{\sum v_i \Delta_f G_m^\theta}
\]

\[
\begin{array}{c|c|c}
\Delta_f G_m^\theta & -2068.255092 & -2068.384377 \\
v_i & 1 & 1 \\
\sum v_i \Delta_f G_m^\theta & -2068.255092 & -2068.384377 \\
\end{array}
\]

\[
\Delta_f G_m^\theta = -2068.384377 - (-2068.255092) = -0.129285 \text{hartree} = -3.52 \text{eV} \quad (5)
\]

4. Transferring two positive charges from the oxidized microdomain with 19-rings to aromatic island.

\[
\begin{array}{c|c|c}
\text{epoxy-GO with two positive charge} & \text{epoxy-GO without positive charge} \\
\Delta_f G_m^\theta & -2067.849522 & -2068.384377 \\
v_i & 1 & 1 \\
\sum v_i \Delta_f G_m^\theta & -2067.849522 & -2068.384377 \\
\end{array}
\]

\[
\Delta_f G_m^\theta = -2068.384377 - (-2067.849522) = -0.534855 \text{hartree} = -14.56 \text{eV} \quad (6)
\]

5. Protonation of epoxy-GO.

\[
\begin{array}{c|c|c|c|c}
\text{epoxy-GO} & \text{H}_3\text{SO}_4^+ & \text{oxonium-GO} & \text{H}_2\text{SO}_4 \\
\Delta_f G_m^\theta & -2143.579630 & -700.465639 & -2143.943972 & -700.154765 \\
v_i & 1 & 1 & 1 & 1 \\
\sum v_i \Delta_f G_m^\theta & -2844.045269 & -2844.098737 \\
\end{array}
\]

\[
\Delta_f G_m^\theta = -2844.098737 - (-2844.045269) = -0.053458 \text{hartree} = -1.45 \text{eV} \quad (7)
\]

6. Ring-opening of oxonium-GO.

\[
\begin{array}{c|c|c}
\text{oxonium-GO} & \text{HSO}_4^- & \text{sulfate-GO} \\
\end{array}
\]

810
\[
\begin{array}{|c|c|c|c|}
\hline
\Delta_f G_m^0 & -2143.943972 & -699.688188 & -2843.748627 \\
\hline
v_i & 1 & 1 & 1 \\
\hline
\sum v_i \Delta_f G_m^0 & -2843.63216 & -2843.748627 \\
\hline
\end{array}
\]

\[\Delta_f G_m^0 = -2843.748627 - (-2843.63216) = -0.116467 \text{hartree} = -3.17 \text{eV} \quad (8)\]
Figure S6. The intrinsic formation and conversion path of oxygen-containing functional groups on oxidized graphite with two possible routes. Route 1: the positive charge on the oxidized microdomain can be transferred to the adjacent aromatic domain; Route 2: the positive charge on the oxidized microdomain cannot be transferred to the adjacent aromatic domain.
Discussion S3: the reduction of MnO$_2$ by K$_2$S$_2$O$_8$-H$_2$SO$_4$

The standard electrode potential of K$_2$S$_2$O$_8$ (+1.96 V for S$_2$O$_8^{2-}$/SO$_4^{2-}$) is higher than that of MnO$_2$ (+1.69 V for MnO$_4^-$/MnO$_2$), so K$_2$S$_2$O$_8$ can chemically oxidize MnO$_2$ very slowly at room temperature as follows:

$$2\text{MnO}_2 + 3\text{K}_2\text{S}_2\text{O}_8 + 4\text{H}_2\text{O} \rightarrow 2\text{KMnO}_4 + 2\text{K}_2\text{SO}_4 + 4\text{H}_2\text{SO}_4$$ (9)

The reaction system exhibits the feature purple color of Mn(VII).

During the preparation of unhydrolyzed oxidized graphite, we dispersed oxidized graphite in K$_2$S$_2$O$_8$-H$_2$SO$_4$ mixture to chemically reduce the impurity of solid MnO$_2$. Because of the presence of concentrated sulfuric acid, the reaction is completely different from the above theoretical reaction between K$_2$S$_2$O$_8$ and MnO$_2$. In our reaction system, K$_2$S$_2$O$_8$ can only be decomposed to form H$_2$O$_2$ which then chemically reduce MnO$_2$. The reactions are given below:

$$\text{K}_2\text{S}_2\text{O}_8 + 2\text{H}_2\text{SO}_4 \rightarrow \text{H}_2\text{S}_2\text{O}_8 + 2\text{KHSO}_4$$ (10)

$$\text{H}_2\text{S}_2\text{O}_8 + 2\text{H}_2\text{O} \rightarrow 2\text{H}_2\text{SO}_4 + \text{H}_2\text{O}_2$$ (11)

$$\text{MnO}_2 + \text{H}_2\text{O}_2 + \text{H}_2\text{SO}_4 \rightarrow \text{MnSO}_4 + \text{O}_2 \uparrow + 2\text{H}_2\text{O}$$ (12)

This reaction process was experimentally observed. After adding oxidized graphite into the K$_2$S$_2$O$_8$-H$_2$SO$_4$ mixture, we observed that a lot of bubbles immediately generated, indicating the formation of O$_2$; meanwhile, the black color of mixture started to fade till the MnO$_2$ particles completely disappeared and turned to the natural white color. If reaction (9) occurred, the mixture should exhibit the feature dark green color of Mn(VII) in the medium of concentrated H$_2$SO$_4$, which is against the experimental phenomena.
Calculation data S2: the calculated atomic coordinates

\[ \text{MnO}_3^+ \]
Symbolic Z-matrix:
Charge = 1 Multiplicity = 1

| Element | X    | Y    | Z    |
|---------|------|------|------|
| Mn      | 0.41796 | 0.74303 | 0    |
| O       | -0.49704 | 2.32786  | 0    |
| O       | 2.24796  | 0.74303  | 0    |
| O       | -0.49704 | -0.84179 | 0    |

\[ \text{HSO}_4^- \]
Symbolic Z-matrix:
Charge = -1 Multiplicity = 1

| Element | X    | Y    | Z    |
|---------|------|------|------|
| S       | 0.31254 | -0.71732 | 1.10073 |
| O       | 0.80248  | -0.0297  | 2.30358 |
| O       | -1.15705 | -0.72297 | 1.10405 |
| O       | 0.86308  | 0.08001  | -0.25944 |
| O       | 0.87523  | -2.28964 | 1.09026 |
| H       | 0.55875  | -2.74799 | 1.87215 |

\[ \text{Carbon skeleton} \]
Symbolic Z-matrix:
Charge = 0 Multiplicity = 1

| Element | X    | Y    | Z    |
|---------|------|------|------|
| C       | 2.97251 | 2.21745  | -0.01839 |
|    |     C    |    X    |     Y    |     Z    |
|----|---------|---------|---------|---------|
|  C |  3.5778 |  0.9535 | -0.0133 |         |
|  C |  4.9750 |  0.8457 | -0.0120 |         |
|  C |   5.77 |   2.0018 | -0.0159 |         |
|  H |  6.8338 |  1.9195 | -0.0150 |         |
|  C |  5.1617 |  3.2658 | -0.0210 |         |
|  H |  5.7664 |  4.1486 | -0.0240 |         |
|  C |  3.7645 |  3.3736 | -0.0222 |         |
|  C |   5.58 |  -0.4182 | -0.0069 |         |
|  C |   2.78 |  -0.2026 | -0.0094 |         |
|  C |  3.3911 |  1.4665 | -0.0043 |         |
|  C |  4.7883 |  1.5743 | -0.0030 |         |
|  C |  5.3936 |  2.8383 |  0.0022 |         |
|  C |   2.59 |  -2.6227 | -0.0004 |         |
|  C |  3.2044 |  3.8867 |  0.0047 |         |
|  C |  4.6016 |  3.9445 |  0.0060 |         |
|  C |  3.1592 |  4.6375 | -0.0272 |         |
|  C |  1.7619 |  4.7453 | -0.0284 |         |
|  C |  1.5752 |  2.3252 | -0.0196 |         |
|  C |  0.9699 |  3.5891 | -0.0246 |         |
|  C |  0.7832 |  1.1691 | -0.0158 |         |
|  C |  1.3885 |  0.0948 | -0.0107 |         |
|  C |  0.5965 | -1.2509 | -0.0069 |         |
|  C |  1.2018 | -2.5149 | -0.0018 |         |
|  C |  0.4098 | -3.6711 |  0.0019 |         |
| C     | 1.01513 | -4.93501 | 0.00709 |
|-------|---------|----------|---------|
| C     | 2.41238 | -5.0428  | 0.00851 |
| C     | -0.42726| 3.69698  | -0.02583|
| C     | -0.61397| 1.2769   | -0.01709|
| C     | -0.80067| -1.14319 | -0.00832|
| C     | -0.98738| -3.56327 | 0.00051 |
| C     | -1.03253| 4.96093  | -0.03079|
| C     | -0.24054| 6.11707  | -0.03454|
| C     | 1.15671 | 6.00927  | -0.03338|
| C     | -1.77936| -4.71942 | 0.00421 |
| C     | -1.1741 | -5.98335 | 0.00938 |
| H     | -1.77879| -6.86609 | 0.01222 |
| C     | 0.22315 | -6.09115 | 0.01084 |
| C     | -1.21924| 2.54084  | -0.02209|
| C     | -1.40595| 0.12075  | -0.01337|
| C     | -1.59265| -2.29933 | -0.00461|
| C     | -2.61649| 2.64863  | -0.02335|
| C     | -2.42978| 5.06872  | -0.03199|
| C     | -3.22176| 3.91257  | -0.02829|
| C     | -3.40847| 1.49248  | -0.01968|
| C     | -2.8032 | 0.22855  | -0.0147 |
| C     | -3.59517| -0.9276  | -0.01105|
| C     | -2.9899 | -2.19154 | -0.00601|
| C     | -3.17661| -4.61162 | 0.00274 |
| Element | X         | Y         | Z         |
|---------|-----------|-----------|-----------|
| C       | -3.78187  | -3.34769  | -0.00237  |
| C       | -4.61901  | 4.02036   | -0.02954  |
| C       | -4.80572  | 1.60027   | -0.02099  |
| C       | -4.99242  | -0.81982  | -0.01244  |
| C       | -5.59769  | 0.44412   | -0.0174   |
| C       | -5.17912  | -3.2399   | -0.00383  |
| C       | -5.41099  | 2.86421   | -0.0259   |
| C       | -5.7844   | -1.97597  | -0.00886  |
| H       | 6.46042   | -2.92061  | 0.00323   |
| H       | 6.64713   | -0.50051  | 0.00595   |
| H       | 5.06375   | -4.9595   | 0.01007   |
| H       | 2.87451   | -6.00785  | 0.0125    |
| H       | 0.68528   | -7.0562   | 0.01481   |
| H       | -3.7813   | -5.49437  | 0.00552   |
| H       | -5.78381  | -4.12265  | 0.0011    |
| H       | -6.85122  | -1.89367  | 0.00996   |
| H       | -6.66452  | 0.52642   | -0.01844  |
| H       | -6.47782  | 2.94651   | -0.02687  |
| H       | -5.08115  | 4.98541   | -0.03327  |
| H       | -2.89191  | 6.03377   | -0.03573  |
| H       | -0.70267  | 7.08212   | -0.03831  |
| H       | 1.76141   | 6.89201   | -0.03627  |
| H       | 3.76391   | 5.52028   | -0.03021  |
Epoxy-GO
Symbolic Z-matrix:
Charge = 0 Multiplicity = 1

| Element | x   | y     | z     |
|---------|-----|-------|-------|
| C       | 0.0659 | -1.14385 | 3.49263 |
| C       | 0.01353 | -2.36213 | 2.79343 |
| C       | 0.16308 | -3.52233 | 3.461  |
| C       | 0.27576 | -3.54597 | 4.85857 |
| H       | 0.3716  | -4.47955 | 5.37253 |
| C       | 0.26413 | -2.34947 | 5.57861 |
| H       | 0.33168 | -2.3603  | 6.64642 |
| C       | 0.16773 | -1.13925 | 4.89021 |
| C       | 0.22314 | -4.66586 | 2.76987 |
| C       | -0.19514 | -2.36617 | 1.39972 |
| C       | -0.49695 | -3.55496 | 0.68234 |
| C       | 0.00432 | -4.677   | 1.38967 |
| C       | 0.28028 | -5.85853 | 0.69659 |
| C       | -0.49695 | -3.55496 | -0.68234 |
| C       | 0.00433 | -4.677   | -1.38967 |
| C       | 0.28028 | -5.85853 | -0.69659 |
| C       | 0.17283 | 0.07129  | 5.59398 |
| C       | 0.10402 | 1.28332  | 4.89761 |
| C       | 0.01621 | 0.06795  | 2.79654 |
| C       | 0.04229 | 1.28223  | 3.49796 |
| C       | -0.05119 | 0.06554  | 1.39922 |
| Element | X          | Y          | Z          |
|---------|------------|------------|------------|
| C       | -0.12992   | -1.14967   | 0.70062    |
| C       | -0.12992   | -1.14967   | -0.70062   |
| C       | -0.19514   | -2.36617   | -1.39972   |
| C       | 0.01354    | -2.36213   | -2.79343   |
| C       | 0.16307    | -3.52233   | -3.461     |
| C       | 0.22314    | -4.66586   | -2.76987   |
| C       | 0.00943    | 2.49532    | 2.79965    |
| C       | -0.03803   | 1.27981    | 0.69964    |
| C       | -0.05119   | 0.06554    | -1.39922   |
| C       | 0.0659     | -1.14385   | -3.49263   |
| C       | 0.01122    | 3.70891    | 3.5009     |
| C       | 0.04885    | 3.70905    | 4.90144    |
| C       | 0.09977    | 2.49582    | 5.59995    |
| C       | 0.16773    | -1.13925   | -4.89021   |
| C       | 0.26413    | -2.34947   | -5.57861   |
| H       | 0.33168    | -2.3603    | -6.64642   |
| C       | 0.27576    | -3.54597   | -4.85857   |
| C       | -0.02069   | 2.49448    | 1.39985    |
| C       | -0.03804   | 1.27981    | -0.69964   |
| C       | 0.01621    | 0.06795    | -2.79654   |
| C       | -0.03112   | 3.70837    | 0.70012    |
| C       | -0.02243   | 4.92227    | 2.8015     |
| C       | -0.0389    | 4.92215    | 1.40075    |
| C       | -0.03112   | 3.70837    | -0.70012   |
|   |   |   |   |
|---|---|---|---|
| C | -0.02069 | 2.49448 | -1.39985 |
| C | 0.00943 | 2.49532 | -2.79965 |
| C | 0.04229 | 1.28223 | -3.49796 |
| C | 0.17282 | 0.07129 | -5.59398 |
| C | 0.10402 | 1.28332 | -4.89761 |
| C | -0.06119 | 6.13572 | 0.70055 |
| C | -0.0389 | 4.92215 | -1.40075 |
| C | 0.01122 | 3.70891 | -3.5009 |
| C | -0.02243 | 4.92227 | -2.8015 |
| C | 0.09977 | 2.49582 | -5.59995 |
| C | -0.0612 | 6.13572 | -0.70055 |
| C | 0.04885 | 3.70905 | -4.90144 |
| H | 0.5064 | -6.75603 | 1.2335 |
| H | 0.44714 | -5.58047 | 3.27801 |
| H | 0.5064 | -6.75603 | -1.2335 |
| H | 0.44714 | -5.58047 | -3.27801 |
| H | 0.3716 | -4.47955 | -5.37253 |
| H | 0.23044 | 0.06973 | -6.66243 |
| H | 0.136 | 2.49507 | -6.66934 |
| H | 0.04048 | 4.63528 | -5.43711 |
| H | -0.03341 | 5.84861 | -3.3369 |
| H | -0.07707 | 7.06213 | -1.23571 |
| H | -0.07707 | 7.06213 | 1.23571 |
| H | -0.03341 | 5.84861 | 3.3369 |
Oxonium-GO
Symbolic Z-matrix:
Charge = 1 Multiplicity = 1

|   |  X     |  Y     |  Z    |
|---|--------|--------|-------|
| H | 0.04048| 4.63528| 5.43711|
| H | 0.136  | 2.49507| 6.66934|
| H | 0.23044| 0.06973| 6.66243|
| O | -1.83932| -3.67123| 0      |
| C | 2.26104| 2.96182| 0.03992|
| C | 3.19919| 1.92769| 0.11684|
| C | 4.54712| 2.21737| 0.00521|
| C | 4.99395| 3.54   |-0.09055|
| H | 6.04104| 3.75124|-0.15315|
| C | 4.0637 | 4.58375|-0.10569|
| H | 4.39601| 5.59927|-0.16247|
| C | 2.6949 | 4.29345|-0.05039|
| C | 5.43563| 1.16393|-0.02877|
| C | 2.77904| 0.60136| 0.30551|
| C | 3.66888| -0.45132| 0.6096 |
| C | 4.97307| -0.14079| 0.16771|
| C | 5.85797| -1.21093| -0.07251|
| C | 3.20317| -1.84405| 0.60988|
| C | 4.05819| -2.87678| 0.16826|
| C | 5.40878| -2.55426|-0.07223|

S21
| C   | 1.76146 | 5.33394  | -0.08526  |
|-----|---------|----------|-----------|
| C   | 0.39364 | 5.04484  | -0.05527  |
| C   | 0.89274 | 2.66811  | 0.05327   |
| C   | -0.04197| 3.7126   | -0.00075  |
| C   | 0.45887 | 1.33248  | 0.11331   |
| C   | 1.39809 | 0.28708  | 0.21529   |
| C   | 0.94492 | -1.0681  | 0.21555   |
| C   | 1.85906 | -2.14982 | 0.30604   |
| C   | 1.39686 | -3.46215 | 0.11786   |
| C   | 2.29938 | -4.50441 | 0.00652   |
| C   | 3.64285 | -4.19739 | -0.02768  |
| C   | -1.41157| 3.42735  | -0.00265  |
| C   | -0.9159 | 1.04716  | 0.07039   |
| C   | -0.43422| -1.33829 | 0.1138    |
| C   | 0.02535 | -3.72397 | 0.04114   |
| C   | -2.34429| 4.4743   | -0.03505  |
| C   | -1.90792| 5.80432  | -0.06826  |
| C   | -0.53834| 6.0896   | -0.08234  |
| C   | -0.42906| -5.04877 | -0.04869  |
| C   | 0.48978 | -6.10406 | -0.10372  |
| H   | 0.14439 | -7.11523 | -0.16014  |
| C   | 1.86075 | -5.82981 | -0.08876  |
| C   | -1.84954| 2.0966   | 0.02399   |
| C   | -1.36084| -0.28343 | 0.07064   |

822
C   -0.89104   -2.66627   0.05424
C   -3.22299    1.81662   0.00246
C   -3.71435    4.19266  -0.03616
C   -4.15418    2.86504  -0.02149
C   -3.66673    0.48963   0.00272
C   -2.73794   -0.56018   0.0245
C   -3.18856   -1.88672  -0.00164
C   -2.26604   -2.93844   0.00047
C   -1.80065   -5.31848  -0.08338
C   -2.71943   -4.26475  -0.0536
C   -5.52652    2.58688  -0.0324
C   -5.04126    0.21222  -0.02091
C   -4.56345   -2.16204  -0.03374
C   -5.48851   -1.11293  -0.03502
C   -4.0924    -4.53876  -0.08041
C   -5.97025    1.25992  -0.03211
C   -5.01489   -3.48702  -0.06648
H    6.88833   -1.00354  -0.27303
H    6.47447    1.34353  -0.21172
H    6.10714   -3.33979  -0.27253
H    4.36465   -4.96584  -0.21039
H    2.57014   -6.62843  -0.15112
H   -2.14669   -6.32972  -0.13375
H   -4.43572   -5.55168  -0.11207
| Element | X         | Y         | Z         |
|---------|-----------|-----------|-----------|
| H       | -6.06438  | -3.69496  | -0.08239  |
| H       | -6.5374   | -1.32393  | -0.0486   |
| H       | -7.0186   | 1.04592   | -0.04139  |
| H       | -6.23526  | 3.38845   | -0.04195  |
| H       | -4.42534  | 4.99215   | -0.05004  |
| H       | -2.62123  | 6.60171   | -0.08441  |
| H       | -0.20331  | 7.10527   | -0.11431  |
| O       | 3.5074    | -1.1713   | 1.89391   |
| H       | 4.51645   | -1.50852  | 2.8643    |

**sulfate-GO**

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

| Element | X         | Y         | Z         |
|---------|-----------|-----------|-----------|
| C       | 1.16962   | 3.25999   | -0.22838  |
| C       | 2.22265   | 2.32919   | -0.15391  |
| C       | 3.52825   | 2.75966   | -0.21438  |
| C       | 3.81217   | 4.13351   | -0.24036  |
| H       | 4.82897   | 4.46669   | -0.2397   |
| C       | 2.77405   | 5.06899   | -0.27422  |
| H       | 2.99439   | 6.11585   | -0.29156  |
| C       | 1.44862   | 4.63082   | -0.29049  |
| C       | 4.57798   | 1.88506   | -0.27879  |
| C       | 1.91498   | 0.96388   | -0.03178  |
| C       | 3.02582 | -0.05259 | 0.2278 |
|---------|---------|----------|-------|
| C       | 4.3748  | 0.5022   | -0.21625 |
| C       | 5.38909 | -0.40807 | -0.54346 |
| C       | 2.71771 | -1.28962 | -0.57813 |
| C       | 3.69748 | -2.28301 | -0.37746 |
| C       | 5.04415 | -1.90996 | -0.51751 |
| C       | 0.40486 | 5.5618   | -0.36934 |
| C       | -0.92469 | 5.12359 | -0.38705 |
| C       | -0.16533 | 2.82013 | -0.24166 |
| C       | -1.21104 | 3.75405 | -0.31579 |
| C       | -0.45872 | 1.44986 | -0.18054 |
| C       | 0.57933  | 0.50979  | -0.12186 |
| C       | 0.29092  | -0.83525 | -0.12004 |
| C       | 1.32272  | -1.78432 | -0.20345 |
| C       | 1.06595  | -3.13487 | 0.03624 |
| C       | 2.08921  | -4.02211 | 0.10692 |
| C       | 3.37407  | -3.61469 | -0.05689 |
| C       | -2.54411 | 3.31856 | -0.31697 |
| C       | -1.79144 | 1.02008 | -0.16255 |
| C       | -1.03451 | -1.27097 | -0.02056 |
| C       | -0.26281 | -3.56377 | 0.19 |
| C       | -3.58781 | 4.25033 | -0.401 |
| C       | -3.29933 | 5.61881 | -0.48592 |
| C       | -1.96789 | 6.05552 | -0.47585 |
|   |   |   |   |
|---|---|---|---|
| C | -0.54259 | -4.91847 | 0.39628 |
| C | 0.51139 | -5.8307 | 0.49314 |
| H | 0.31253 | -6.86665 | 0.67209 |
| C | 1.82957 | -5.38018 | 0.35202 |
| C | -2.83356 | 1.95168 | -0.23004 |
| C | -2.0791 | -0.34402 | -0.06399 |
| C | -1.31261 | -2.63563 | 0.12795 |
| C | -4.16525 | 1.5155 | -0.20465 |
| C | -4.92017 | 3.81333 | -0.39764 |
| C | -5.20892 | 2.44554 | -0.2925 |
| C | -4.45217 | 0.14874 | -0.08667 |
| C | -3.40748 | -0.78019 | -0.00577 |
| C | -3.68972 | -2.1448 | 0.13622 |
| C | -2.64132 | -3.07158 | 0.21982 |
| C | -1.87076 | -5.35579 | 0.50035 |
| C | -2.92143 | -4.43296 | 0.39588 |
| C | -6.54041 | 2.00736 | -0.27256 |
| C | -5.7824 | -0.28859 | -0.04699 |
| C | -5.01923 | -2.58181 | 0.19741 |
| C | -6.06659 | -1.65463 | 0.09538 |
| C | -4.25147 | -4.87 | 0.46748 |
| C | -6.8272 | 0.64042 | -0.14781 |
| C | -5.30039 | -3.94528 | 0.36178 |
| H | 6.37346 | -0.07154 | -0.79377 |
| Atom | X-coordinate | Y-coordinate | Z-coordinate |
|------|--------------|--------------|--------------|
| H    | 5.5714       | 2.26528      | -0.39439     |
| H    | 5.8128       | -2.65013     | -0.59743     |
| H    | 4.16365      | -4.32759     | 0.05769      |
| H    | 2.64127      | -6.0732      | 0.42829      |
| H    | -2.08237     | -6.39301     | 0.65684      |
| H    | -4.46641     | -5.90953     | 0.60186      |
| H    | -6.31555     | -4.28031     | 0.40773      |
| H    | -7.08244     | -1.9893      | 0.12762      |
| H    | -7.8436      | 0.30658      | -0.12873     |
| H    | -7.33801     | 2.71626      | -0.35101     |
| H    | -5.71646     | 4.52409      | -0.47297     |
| H    | -4.09542     | 6.33027      | -0.55717     |
| H    | -1.74746     | 7.10089      | -0.53575     |
| H    | 0.62378      | 6.60813      | -0.41672     |
| O    | 2.72054      | -0.91347     | -1.95778     |
| H    | 3.58817      | -0.5786      | -2.19624     |
| O    | 3.07855      | -0.34447     | 1.62658      |
| O    | 4.33562      | -1.76758     | 3.35278      |
| O    | 5.75143      | -0.84377     | 1.42241      |
| O    | 3.99475      | -2.69677     | 1.16664      |
| H    | 5.93885      | -0.0394      | 1.91175      |
| S    | 4.28207      | -1.4655      | 1.91557      |