# Supplementary Information

## Kinetics of tautomerisation of thiouracils and cognate species at low temperatures: theory *versus* experiment

Judith Wurmel[‡] and John M. Simmie

Table 1: High-level rate constants, $k$ / $s^{-1}$, at various temperatures

| *T*/K | SU3 | SU2 | MeSU3 | NSU3 | NNSH | 5SH |
|---|---|---|---|---|---|---|
| **3.5** | 2.10E-06 | | 1.44E-04 | 6.97E-08 | | |
| **15** | 2.10E-06 | 6.90E-11 | 1.45E-04 | 7.01E-08 | 6.45E-11 | 1.85E-17 |
| **50** | 2.50E-06 | 9.55E-11 | 2.16E-04 | 8.64E-08 | 7.01E-11 | 2.18E-17 |
| **100** | 7.37E-06 | 1.18E-09 | 6.89E-04 | 2.74E-07 | 2.37E-10 | 2.65E-16 |
| **150** | 4.40E-05 | 4.13E-08 | 3.00E-03 | 2.05E-06 | 4.63E-09 | 2.63E-14 |
| **200** | 4.06E-04 | 1.37E-06 | 1.91E-02 | 2.85E-05 | 2.03E-07 | 3.21E-12 |
| **250** | 5.77E-03 | 4.39E-05 | 1.96E-01 | 5.68E-04 | 1.05E-05 | 4.58E-10 |
| **300** | 1.22E-01 | 1.58E-03 | 3.08E+00 | 1.48E-02 | 5.62E-04 | 5.80E-08 |

Table 2: Formation enthalpies kJ/mol

| Species | $\Delta H_f$(0 K) |
|---|---|
| **SU1** | -42.92 |
| **SU2** | -10.37 |
| **SU3** | +23.80 |
| **MeSU1** | -43.75 |
| **MeSU3** | +25.00 |
| **NSU1** | +85.10 |
| **NSU3** | 139.40 |
| **NNSH** | 302.29 |
| **NNHS** | 285.00 |
| **5SH** | 164.52 |
| **5HS** | 140.56 |

[‡] Judith.wurmel@atu.ie

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!LIST OF PROCESSED FILES
!++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
5HS-m062x.log
5SH-5HS-H2O-TS-d3bj.log
5SH-m062x.log
MeSU1-apf.log
MeSU1-apfd.log
MeSU1-b2plyp.log
MeSU1-b2plypd3.log
MeSU1-wb97xd.log
MeSU3-apf.log
MeSU3-apfd.log
MeSU3-b2plyp.log
MeSU3-b2plypd3.log
MeSU3-MeSU1-H2O-TS-d3bj.log
MeSU3-MeSU1-m062x-product.log
MeSU3-MeSU1-m062x-reactant.log
MeSU3-wb97xd.log
NNHS-m062x.log
NNSH-m062x.log
NNSH-NNHS-H2O-TS-d3bj.log
NSU3-dimer-reactant-qb3.log
NSU3-dimer-reactant-v2.log
NSU3-NSU1-H2O-TS-d3bj.log
NSU3-NSU1-m062x-product.log
NSU3-NSU1-m062x-reactant.log
NSU3-qb3.log
SU1-m062x.log
SU2-m062x.log
SU3-SU1-H2O-TS.log
TS-5SH-5HS-m062x.log
TS-MeSU3-MeSU1-apf.log
TS-MeSU3-MeSU1-apfd.log
TS-MeSU3-MeSU1-b2plyp.log
TS-MeSU3-MeSU1-wb97xd.log
TS-NNSH-NNHS-m062x.log
TS-NSU3-dimer-qb3.log
TS-NSU3-NSU1-m062x.log
TS-SU2-SU1-m062x.log
TS-SU2-SU1.log
TS-SU3-SU1-m062x.log

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 GAUSSIAN OUTPUT FILENAME: 5HS-m062x.log
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 1)LEVEL OF THEORY: OPT=VTIGHT
 Charge = 0 Multiplicity = 1  Stoichiometry    C3H4N2S

 ---------------------------------------------------------------------
 ---------------------- OPTIMIZED GEOMETRY ---------------------------
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          7           0        1.068879   -0.493993   -0.000000
      2          6           0        0.000000    0.350639    0.000000
      3          6           0        0.672736   -1.819199   -0.000000
      4          6           0       -0.672708   -1.819207    0.000000
      5          7           0       -1.068868   -0.494010    0.000000
      6          1           0       -2.010404   -0.141361    0.000000
      7          1           0       -1.372252   -2.634443    0.000000
      8          1           0        1.372296   -2.634421   -0.000000
      9         16           0       -0.000018    2.012137    0.000000
     10          1           0        2.010412   -0.141337   -0.000000
 ---------------------------------------------------------------------
 Rotational constants (GHZ):           9.2221519           2.1885885           1.7688156

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-------------------- FREQUENCIES AND ROTATIONAL CONSTANTS ----------------------
--------------------------------------------------------------------------------
INDEX NO. DOF TYPE  CM-1(UNSCALED)  CM-1(SCALED BY ) SYMMETRY IR-INTENSITY
   1        vib         216.35           0.00               A"        2.1310
   2        vib         321.95           0.00               A'        1.6936
   3        vib         543.53           0.00               A'       18.6598
   4        vib         556.37           0.00               A"        0.0000
   5        vib         600.83           0.00               A"       95.4249
   6        vib         633.85           0.00               A"        0.0000
   7        vib         692.87           0.00               A"       44.7509
   8        vib         730.94           0.00               A"       91.8471
   9        vib         859.21           0.00               A"        0.0000
  10        vib         925.95           0.00               A'        4.3633
  11        vib         974.91           0.00               A'        0.1216
  12        vib        1074.80           0.00               A'       49.3972
  13        vib        1136.50           0.00               A'       10.3893
  14        vib        1152.84           0.00               A'        0.0079
  15        vib        1220.78           0.00               A'      126.1465
  16        vib        1267.54           0.00               A'        0.2663
  17        vib        1396.00           0.00               A'       19.4001
  18        vib        1439.72           0.00               A'        2.1198
  19        vib        1538.62           0.00               A'      455.9253
  20        vib        1646.63           0.00               A'       48.3747
  21        vib        3310.58           0.00               A'        5.7594
  22        vib        3330.78           0.00               A'        1.0902
  23        vib        3682.90           0.00               A'      214.5619
  24        vib        3683.72           0.00               A'        0.0466
  25        rot      0.3076179           -
  26        rot      0.0730035           -
  27        rot      0.0590013           -
--------------------------------------------------------------------------------

--------------------------------------------------------------------------------
------------------------ ZPE & THERMAL CONTRIBUTIONS ---------------------------
--------------------------------------------------------------------------------
Eelectronic                    [kJ/mol]   = -1639402.189
Ezpe                           [kJ/mol]   = +197.015
Eelectronic+Ezpe               [kJ/mol]   = -1639205.174

Eelectronic                    [hartrees] = -624.415231
Ezpe                           [hartrees] = +0.075039
Eelectronic+Ezpe               [hartrees] = -624.340192

Thermal Correction to Energy   [kJ/mol]   = +209.959
Thermal Correction to Enthalpy [kJ/mol]   = +212.437
Thermal Correction to Gibbs    [kJ/mol]   = +121.605
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 END OF GAUSSIAN OUTPUT FILENAME: 5HS-m062x.log
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 GAUSSIAN OUTPUT FILENAME: 5SH-5HS-H2O-TS-d3bj.log
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 1)LEVEL OF THEORY: B3LYP/DEF2TZVP
 Charge = 0 Multiplicity = 1  Stoichiometry    C3H6N2OS

 ---------------------------------------------------------------------
 ---------------------- OPTIMIZED GEOMETRY ---------------------------
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          6           0       -1.677340    1.171311   -0.008924
      2          7           0       -0.321913    0.922397   -0.010452
      3          6           0       -0.151044   -0.404270    0.003855
      4         16           0        1.369365   -1.228927   -0.003561
      5          7           0       -1.373977   -0.992920    0.016379
      6          6           0       -2.349944   -0.009148    0.008097
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     7          1          0        0.958348    1.528990   -0.039322
     8          8          0        2.073290    1.505700   -0.084829
     9          1          0        2.430180    1.817571    0.756825
    10          1          0        2.048193    0.270409   -0.056718
    11          1          0       -3.399570   -0.239058    0.014540
    12          1          0       -1.521418   -1.986940    0.022205
    13          1          0       -2.070702    2.172568   -0.021582
 ---------------------------------------------------------------------
 Rotational constants (GHZ):           3.5190272           1.7596905           1.1768135

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 -------------------- FREQUENCIES AND ROTATIONAL CONSTANTS ----------------------
 --------------------------------------------------------------------------------
 INDEX NO. DOF TYPE  CM-1(UNSCALED)  CM-1(SCALED BY ) SYMMETRY IR-INTENSITY
    1        vib       -1230.73           0.00                A      874.3200
    2        vib          98.67           0.00                A        9.9311
    3        vib         227.99           0.00                A        1.9373
    4        vib         311.85           0.00                A       52.9106
    5        vib         408.75           0.00                A       45.4442
    6        vib         457.91           0.00                A       19.7805
    7        vib         474.89           0.00                A      100.3448
    8        vib         531.24           0.00                A       72.3690
    9        vib         547.47           0.00                A       56.1143
   10        vib         577.48           0.00                A       62.0233
   11        vib         634.71           0.00                A       10.4369
   12        vib         693.92           0.00                A       54.4364
   13        vib         729.36           0.00                A       17.9222
   14        vib         843.46           0.00                A        7.7634
   15        vib         956.99           0.00                A       12.8641
   16        vib         983.85           0.00                A       38.9824
   17        vib        1089.50           0.00                A       56.3693
   18        vib        1140.17           0.00                A      154.2108
   19        vib        1167.79           0.00                A       34.6858
   20        vib        1182.56           0.00                A      834.9261
   21        vib        1240.85           0.00                A      216.8823
   22        vib        1261.00           0.00                A      517.7970
   23        vib        1342.32           0.00                A      340.5363
   24        vib        1413.50           0.00                A      516.8781
   25        vib        1483.15           0.00                A      130.8353
   26        vib        1512.30           0.00                A      981.9063
   27        vib        1534.59           0.00                A      112.7959
   28        vib        1570.15           0.00                A       33.5601
   29        vib        1877.85           0.00                A      661.6805
   30        vib        3262.53           0.00                A        2.1049
   31        vib        3288.52           0.00                A        0.3561
   32        vib        3656.58           0.00                A       73.0310
   33        vib        3794.49           0.00                A       60.6379
   34        rot      0.1173821           -
   35        rot      0.0586970           -
   36        rot      0.0392543           -
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 ----------------------- ZPE & THERMAL CONTRIBUTIONS ----------------------------
 --------------------------------------------------------------------------------
 Eelectronic                    [kJ/mol]   = -1840509.878
 Ezpe                           [kJ/mol]   = +241.026
 Eelectronic+Ezpe               [kJ/mol]   = -1840268.852

 Eelectronic                    [hartrees] = -701.013094
 Ezpe                           [hartrees] = +0.091802
 Eelectronic+Ezpe               [hartrees] = -700.921292

 Thermal Correction to Energy   [kJ/mol]   = +258.134
 Thermal Correction to Enthalpy [kJ/mol]   = +260.612
 Thermal Correction to Gibbs    [kJ/mol]   = +159.693
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GAUSSIAN OUTPUT FILENAME: 5SH-m062x.log
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1)LEVEL OF THEORY: OPT
Charge = 0 Multiplicity = 1  Stoichiometry    C3H4N2S

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---------- OPTIMIZED GEOMETRY ----------

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| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 7 | 0 | -0.483343 | -1.150861 | -0.003329 |
| 2 | 6 | 0 | 0.219815 | -0.052471 | -0.000601 |
| 3 | 6 | 0 | -1.796245 | -0.740473 | -0.001303 |
| 4 | 6 | 0 | -1.874923 | 0.617296 | 0.001505 |
| 5 | 7 | 0 | -0.567574 | 1.053318 | 0.002300 |
| 6 | 1 | 0 | -0.254402 | 2.008543 | 0.012373 |
| 7 | 1 | 0 | -2.705754 | 1.299376 | 0.002452 |
| 8 | 1 | 0 | -2.604287 | -1.452097 | -0.002495 |
| 9 | 16 | 0 | 1.968975 | 0.070969 | -0.004263 |
| 10 | 1 | 0 | 2.125385 | -1.254631 | 0.065476 |

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Rotational constants (GHZ):  9.2117979  2.1784750  1.7618888

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---------- FREQUENCIES AND ROTATIONAL CONSTANTS ----------

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| INDEX NO. | DOF TYPE | CM-1(UNSCALED) | CM-1(SCALED BY ) | SYMMETRY | IR-INTENSITY |
|---|---|---|---|---|---|
| 1 | vib | 184.80 | 0.00 | A | 30.1884 |
| 2 | vib | 232.41 | 0.00 | A | 4.7557 |
| 3 | vib | 286.33 | 0.00 | A | 8.5954 |
| 4 | vib | 495.01 | 0.00 | A | 0.1881 |
| 5 | vib | 535.45 | 0.00 | A | 67.7014 |
| 6 | vib | 645.13 | 0.00 | A | 7.3621 |
| 7 | vib | 714.13 | 0.00 | A | 10.4158 |
| 8 | vib | 753.24 | 0.00 | A | 49.7285 |
| 9 | vib | 894.97 | 0.00 | A | 6.9250 |
| 10 | vib | 909.66 | 0.00 | A | 15.6949 |
| 11 | vib | 929.85 | 0.00 | A | 4.5201 |
| 12 | vib | 983.75 | 0.00 | A | 11.1288 |
| 13 | vib | 1107.31 | 0.00 | A | 33.6142 |
| 14 | vib | 1137.04 | 0.00 | A | 0.2235 |
| 15 | vib | 1193.20 | 0.00 | A | 3.3864 |
| 16 | vib | 1254.35 | 0.00 | A | 4.0494 |
| 17 | vib | 1389.69 | 0.00 | A | 25.7968 |
| 18 | vib | 1476.80 | 0.00 | A | 51.7065 |
| 19 | vib | 1511.34 | 0.00 | A | 51.2242 |
| 20 | vib | 1590.67 | 0.00 | A | 44.1020 |
| 21 | vib | 2746.61 | 0.00 | A | 9.4259 |
| 22 | vib | 3283.88 | 0.00 | A | 3.6458 |
| 23 | vib | 3312.83 | 0.00 | A | 0.2282 |
| 24 | vib | 3684.03 | 0.00 | A | 82.6106 |
| 25 | rot | 0.3072725 | - | | |
| 26 | rot | 0.0726661 | - | | |
| 27 | rot | 0.0587703 | - | | |

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---------- ZPE & THERMAL CONTRIBUTIONS ----------

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Eelectronic  [kJ/mol]  = -1639363.683
Ezpe  [kJ/mol]  = +186.930
Eelectronic+Ezpe  [kJ/mol]  = -1639176.753

Eelectronic  [hartrees] = -624.400565
Ezpe  [hartrees] = +0.071198
Eelectronic+Ezpe  [hartrees] = -624.329367

Thermal Correction to Energy  [kJ/mol]  = +201.168

Thermal Correction to Enthalpy [kJ/mol] = +203.647
Thermal Correction to Gibbs [kJ/mol] = +110.253

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END OF GAUSSIAN OUTPUT FILENAME: 5SH-m062x.log
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GAUSSIAN OUTPUT FILENAME: MeSU1-apf.log
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1)LEVEL OF THEORY: OPT=VTIGHT
Charge = 0 Multiplicity = 1 Stoichiometry C5H6N2OS

OPTIMIZED GEOMETRY

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 7 | 0 | -1.176538 | 0.041741 | 0.000000 |
| 2 | 7 | 0 | 1.123545 | -0.060672 | 0.000000 |
| 3 | 6 | 0 | -0.000000 | 0.730223 | 0.000000 |
| 4 | 6 | 0 | -1.382648 | -1.342262 | 0.000000 |
| 5 | 6 | 0 | -0.143654 | -2.087611 | 0.000000 |
| 6 | 6 | 0 | 1.025385 | -1.426189 | 0.000000 |
| 7 | 1 | 0 | -0.184127 | -3.166097 | 0.000000 |
| 8 | 1 | 0 | 1.973742 | -1.948377 | 0.000000 |
| 9 | 16 | 0 | 0.048828 | 2.380786 | 0.000000 |
| 10 | 1 | 0 | -2.009986 | 0.613546 | 0.000000 |
| 11 | 8 | 0 | -2.504914 | -1.796049 | 0.000000 |
| 12 | 6 | 0 | 2.430088 | 0.575722 | 0.000000 |
| 13 | 1 | 0 | 2.541982 | 1.206626 | 0.881854 |
| 14 | 1 | 0 | 3.190394 | -0.203302 | 0.000000 |
| 15 | 1 | 0 | 2.541982 | 1.206626 | -0.881854 |

Rotational constants (GHZ): 2.4084459 1.1830627 0.7972791

FREQUENCIES AND ROTATIONAL CONSTANTS

| INDEX NO. | DOF TYPE | CM-1(UNSCALED) | CM-1(SCALED BY ) | SYMMETRY | IR-INTENSITY |
|---|---|---|---|---|---|
| 1 | vib | 107.51 | 0.00 | A" | 0.1574 |
| 2 | vib | 123.97 | 0.00 | A" | 0.7473 |
| 3 | vib | 154.30 | 0.00 | A" | 1.4347 |
| 4 | vib | 256.88 | 0.00 | A" | 3.1725 |
| 5 | vib | 274.23 | 0.00 | A' | 8.7074 |
| 6 | vib | 352.77 | 0.00 | A' | 1.0052 |
| 7 | vib | 409.00 | 0.00 | A" | 7.3130 |
| 8 | vib | 457.89 | 0.00 | A' | 22.0280 |
| 9 | vib | 503.41 | 0.00 | A' | 10.7189 |
| 10 | vib | 551.62 | 0.00 | A' | 0.3696 |
| 11 | vib | 661.68 | 0.00 | A" | 4.6372 |
| 12 | vib | 717.10 | 0.00 | A" | 27.1014 |
| 13 | vib | 729.18 | 0.00 | A' | 2.5451 |
| 14 | vib | 758.90 | 0.00 | A" | 10.0672 |
| 15 | vib | 792.91 | 0.00 | A' | 0.8886 |
| 16 | vib | 830.28 | 0.00 | A" | 66.3108 |
| 17 | vib | 936.56 | 0.00 | A' | 8.3622 |
| 18 | vib | 978.53 | 0.00 | A" | 0.4354 |
| 19 | vib | 1049.47 | 0.00 | A' | 6.3399 |
| 20 | vib | 1146.44 | 0.00 | A" | 0.0000 |
| 21 | vib | 1151.82 | 0.00 | A' | 103.8540 |
| 22 | vib | 1187.45 | 0.00 | A' | 40.4257 |
| 23 | vib | 1236.02 | 0.00 | A' | 34.2270 |
| 24 | vib | 1252.57 | 0.00 | A' | 56.9958 |
| 25 | vib | 1333.01 | 0.00 | A' | 63.8119 |
| 26 | vib | 1406.75 | 0.00 | A' | 59.0447 |
| 27 | vib | 1450.85 | 0.00 | A' | 24.0847 |
| 28 | vib | 1458.00 | 0.00 | A" | 14.7388 |

| | | | | | |
|---|---|---|---|---|---|
| 29 | vib | 1471.07 | 0.00 | A' | 69.6989 |
| 30 | vib | 1489.08 | 0.00 | A' | 71.4153 |
| 31 | vib | 1533.43 | 0.00 | A' | 483.8751 |
| 32 | vib | 1686.58 | 0.00 | A' | 127.0296 |
| 33 | vib | 1802.89 | 0.00 | A' | 700.2803 |
| 34 | vib | 3069.66 | 0.00 | A' | 20.0208 |
| 35 | vib | 3143.88 | 0.00 | A" | 4.0211 |
| 36 | vib | 3166.40 | 0.00 | A' | 6.9434 |
| 37 | vib | 3216.78 | 0.00 | A' | 3.6540 |
| 38 | vib | 3260.07 | 0.00 | A' | 2.2477 |
| 39 | vib | 3604.25 | 0.00 | A' | 63.1930 |
| 40 | rot | 0.0803371 | - | | |
| 41 | rot | 0.0394627 | - | | |
| 42 | rot | 0.0265944 | - | | |

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---------- ZPE & THERMAL CONTRIBUTIONS ----------
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Eelectronic [kJ/mol] = -2039575.49
Ezpe [kJ/mol] = +297.351
Eelectronic+Ezpe [kJ/mol] = -2039278.139

Eelectronic [hartrees] = -776.833171
Ezpe [hartrees] = +0.113255
Eelectronic+Ezpe [hartrees] = -776.719916

Thermal Correction to Energy [kJ/mol] = +318.263
Thermal Correction to Enthalpy [kJ/mol] = +320.742
Thermal Correction to Gibbs [kJ/mol] = +210.276

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END OF GAUSSIAN OUTPUT FILENAME: MeSU1-apf.log
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GAUSSIAN OUTPUT FILENAME: MeSU1-apfd.log
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1)LEVEL OF THEORY: OPT=VTIGHT
Charge = 0 Multiplicity = 1 Stoichiometry C5H6N2OS

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---------- OPTIMIZED GEOMETRY ----------
---

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 7 | 0 | -1.176955 | 0.042297 | 0.000000 |
| 2 | 7 | 0 | 1.123371 | -0.060660 | 0.000000 |
| 3 | 6 | 0 | 0.000000 | 0.733638 | 0.000000 |
| 4 | 6 | 0 | -1.381837 | -1.344494 | 0.000000 |
| 5 | 6 | 0 | -0.141892 | -2.088928 | 0.000000 |
| 6 | 6 | 0 | 1.026501 | -1.425931 | 0.000000 |
| 7 | 1 | 0 | -0.182875 | -3.167873 | 0.000000 |
| 8 | 1 | 0 | 1.976810 | -1.944697 | 0.000000 |
| 9 | 16 | 0 | 0.045376 | 2.387479 | 0.000000 |
| 10 | 1 | 0 | -2.012174 | 0.612322 | 0.000000 |
| 11 | 8 | 0 | -2.502152 | -1.804583 | 0.000000 |
| 12 | 6 | 0 | 2.431573 | 0.571175 | 0.000000 |
| 13 | 1 | 0 | 2.544549 | 1.201407 | 0.881969 |
| 14 | 1 | 0 | 3.189361 | -0.209771 | 0.000000 |
| 15 | 1 | 0 | 2.544549 | 1.201407 | -0.881969 |

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Rotational constants (GHZ): 2.4015427 1.1805580 0.7953860

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---------- FREQUENCIES AND ROTATIONAL CONSTANTS ----------
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INDEX NO. DOF TYPE CM-1(UNSCALED) CM-1(SCALED BY ) SYMMETRY IR-INTENSITY

```
    1        vib         105.96           0.00              A"        0.1486
    2        vib         124.20           0.00              A"        0.9877
    3        vib         158.72           0.00              A"        1.3128
    4        vib         256.48           0.00              A"        3.0694
    5        vib         281.77           0.00              A'        9.4217
    6        vib         353.74           0.00              A'        0.8758
    7        vib         408.47           0.00              A"        7.3766
    8        vib         457.20           0.00              A'       22.0679
    9        vib         502.59           0.00              A'       10.3551
   10        vib         544.39           0.00              A'        0.5805
   11        vib         662.33           0.00              A"        4.7429
   12        vib         715.85           0.00              A"       27.3248
   13        vib         724.04           0.00              A'        2.9175
   14        vib         758.52           0.00              A"        9.9789
   15        vib         790.00           0.00              A'        0.8178
   16        vib         831.09           0.00              A"       66.0136
   17        vib         931.00           0.00              A'        8.1543
   18        vib         978.36           0.00              A"        0.4093
   19        vib        1051.92           0.00              A'        5.5000
   20        vib        1147.08           0.00              A"        0.0003
   21        vib        1152.65           0.00              A'      120.2985
   22        vib        1187.71           0.00              A'       25.6220
   23        vib        1237.58           0.00              A'       48.5263
   24        vib        1251.66           0.00              A'       57.2897
   25        vib        1338.80           0.00              A'       77.7794
   26        vib        1404.81           0.00              A'       57.3016
   27        vib        1447.56           0.00              A'       21.8222
   28        vib        1460.16           0.00              A"       14.6990
   29        vib        1470.86           0.00              A'       64.2562
   30        vib        1488.45           0.00              A'       74.7086
   31        vib        1533.17           0.00              A'      459.2049
   32        vib        1682.41           0.00              A'      116.4187
   33        vib        1798.51           0.00              A'      714.1304
   34        vib        3071.46           0.00              A'       19.8473
   35        vib        3145.57           0.00              A"        4.0701
   36        vib        3169.37           0.00              A'        6.6593
   37        vib        3216.09           0.00              A'        3.8454
   38        vib        3257.06           0.00              A'        2.1928
   39        vib        3602.43           0.00              A'       63.0196
   40        rot      0.0801068           -
   41        rot      0.0393792           -
   42        rot      0.0265312           -
 --------------------------------------------------------------------------------

 --------------------------------------------------------------------------------
 ------------------------ ZPE & THERMAL CONTRIBUTIONS ---------------------------
 --------------------------------------------------------------------------------
 Eelectronic                    [kJ/mol]   = -2039598.371
 Ezpe                           [kJ/mol]   = +297.272
 Eelectronic+Ezpe               [kJ/mol]   = -2039301.099

 Eelectronic                    [hartrees] = -776.841886
 Ezpe                           [hartrees] = +0.113225
 Eelectronic+Ezpe               [hartrees] = -776.728661

 Thermal Correction to Energy   [kJ/mol]   = +318.169
 Thermal Correction to Enthalpy [kJ/mol]   = +320.647
 Thermal Correction to Gibbs    [kJ/mol]   = +210.229
 --------------------------------------------------------------------------------

!++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
 END OF GAUSSIAN OUTPUT FILENAME: MeSU1-apfd.log
!++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++


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 GAUSSIAN OUTPUT FILENAME: MeSU1-b2plyp.log
!++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++

 1)LEVEL OF THEORY: OPT=VTIGHT
 Charge = 0 Multiplicity = 1  Stoichiometry    C5H6N2OS
```

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---------- OPTIMIZED GEOMETRY ----------

---

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 7 | 0 | -1.180519 | 0.040259 | 0.000000 |
| 2 | 7 | 0 | 1.127095 | -0.059003 | 0.000000 |
| 3 | 6 | 0 | -0.000000 | 0.735321 | 0.000000 |
| 4 | 6 | 0 | -1.384189 | -1.349277 | 0.000000 |
| 5 | 6 | 0 | -0.142483 | -2.093351 | 0.000000 |
| 6 | 6 | 0 | 1.029802 | -1.430271 | 0.000000 |
| 7 | 1 | 0 | -0.180672 | -3.170284 | 0.000000 |
| 8 | 1 | 0 | 1.976246 | -1.951215 | 0.000000 |
| 9 | 16 | 0 | 0.043825 | 2.390886 | 0.000000 |
| 10 | 1 | 0 | -2.016720 | 0.609525 | 0.000000 |
| 11 | 8 | 0 | -2.510617 | -1.808210 | 0.000000 |
| 12 | 6 | 0 | 2.442431 | 0.578568 | 0.000000 |
| 13 | 1 | 0 | 2.554246 | 1.205935 | 0.881408 |
| 14 | 1 | 0 | 3.196992 | -0.203131 | 0.000000 |
| 15 | 1 | 0 | 2.554246 | 1.205935 | -0.881408 |

---

Rotational constants (GHZ): 2.3891898 1.1744831 0.7912686

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---------- FREQUENCIES AND ROTATIONAL CONSTANTS ----------

---

| INDEX NO. | DOF TYPE | CM-1(UNSCALED) | CM-1(SCALED BY ) | SYMMETRY | IR-INTENSITY |
|---|---|---|---|---|---|
| 1 | vib | 106.42 | 0.00 | A" | 0.1498 |
| 2 | vib | 122.14 | 0.00 | A" | 0.7126 |
| 3 | vib | 155.73 | 0.00 | A" | 1.1903 |
| 4 | vib | 251.60 | 0.00 | A" | 3.2355 |
| 5 | vib | 274.24 | 0.00 | A' | 8.2755 |
| 6 | vib | 351.45 | 0.00 | A' | 0.9016 |
| 7 | vib | 407.46 | 0.00 | A" | 6.8782 |
| 8 | vib | 455.93 | 0.00 | A' | 22.5195 |
| 9 | vib | 499.44 | 0.00 | A' | 10.2603 |
| 10 | vib | 548.25 | 0.00 | A' | 0.4031 |
| 11 | vib | 653.84 | 0.00 | A" | 4.5739 |
| 12 | vib | 711.89 | 0.00 | A" | 26.6202 |
| 13 | vib | 722.93 | 0.00 | A' | 2.0035 |
| 14 | vib | 750.48 | 0.00 | A" | 14.6599 |
| 15 | vib | 783.03 | 0.00 | A' | 1.0516 |
| 16 | vib | 824.11 | 0.00 | A" | 62.1984 |
| 17 | vib | 927.81 | 0.00 | A' | 10.3295 |
| 18 | vib | 970.86 | 0.00 | A" | 0.5375 |
| 19 | vib | 1049.57 | 0.00 | A' | 5.1123 |
| 20 | vib | 1153.12 | 0.00 | A' | 134.6702 |
| 21 | vib | 1158.39 | 0.00 | A" | 0.0708 |
| 22 | vib | 1183.96 | 0.00 | A' | 21.2071 |
| 23 | vib | 1217.39 | 0.00 | A' | 50.4007 |
| 24 | vib | 1246.81 | 0.00 | A' | 60.0675 |
| 25 | vib | 1334.77 | 0.00 | A' | 73.5010 |
| 26 | vib | 1396.67 | 0.00 | A' | 91.1892 |
| 27 | vib | 1448.58 | 0.00 | A' | 10.9744 |
| 28 | vib | 1479.54 | 0.00 | A' | 147.1673 |
| 29 | vib | 1482.24 | 0.00 | A" | 13.0840 |
| 30 | vib | 1497.86 | 0.00 | A' | 159.9825 |
| 31 | vib | 1536.71 | 0.00 | A' | 286.9233 |
| 32 | vib | 1665.79 | 0.00 | A' | 82.2810 |
| 33 | vib | 1765.27 | 0.00 | A' | 667.1936 |
| 34 | vib | 3079.75 | 0.00 | A' | 20.2413 |
| 35 | vib | 3155.38 | 0.00 | A" | 4.4244 |
| 36 | vib | 3174.59 | 0.00 | A' | 6.7122 |
| 37 | vib | 3225.84 | 0.00 | A' | 4.0973 |
| 38 | vib | 3262.79 | 0.00 | A' | 1.7084 |
| 39 | vib | 3577.82 | 0.00 | A' | 64.0984 |
| 40 | rot | 0.0796948 | - | | |
| 41 | rot | 0.0391765 | - | | |
| 42 | rot | 0.0263939 | - | | |

---

```
-------------------------------------------------------------------------------
----------------------- ZPE & THERMAL CONTRIBUTIONS ---------------------------
-------------------------------------------------------------------------------
Eelectronic                    [kJ/mol]   = -2039520.261
Ezpe                           [kJ/mol]   = +296.737
Eelectronic+Ezpe               [kJ/mol]   = -2039223.524

Eelectronic                    [hartrees] = -776.812135
Ezpe                           [hartrees] = +0.113021
Eelectronic+Ezpe               [hartrees] = -776.699114

Thermal Correction to Energy   [kJ/mol]   = +317.749
Thermal Correction to Enthalpy [kJ/mol]   = +320.227
Thermal Correction to Gibbs    [kJ/mol]   = +209.541
-------------------------------------------------------------------------------

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 END OF GAUSSIAN OUTPUT FILENAME: MeSU1-b2plyp.log
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!+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
 GAUSSIAN OUTPUT FILENAME: MeSU1-b2plypd3.log
!+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++

 1)LEVEL OF THEORY: OPT=VTIGHT
 Charge = 0 Multiplicity = 1  Stoichiometry    C5H6N2OS

 ---------------------------------------------------------------------
 ---------------------- OPTIMIZED GEOMETRY ---------------------------
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          7           0       -1.180494    0.040804    0.000000
      2          7           0        1.126290   -0.059510    0.000000
      3          6           0        0.000000    0.734685    0.000000
      4          6           0       -1.384143   -1.348115    0.000000
      5          6           0       -0.142977   -2.092529    0.000000
      6          6           0        1.029377   -1.430186    0.000000
      7          1           0       -0.181901   -3.169271    0.000000
      8          1           0        1.975787   -1.950813    0.000000
      9         16           0        0.045842    2.389370    0.000000
     10          1           0       -2.016238    0.610456    0.000000
     11          8           0       -2.510567   -1.806901    0.000000
     12          6           0        2.440386    0.578758    0.000000
     13          1           0        2.550848    1.206282    0.881311
     14          1           0        3.195290   -0.202394    0.000000
     15          1           0        2.550848    1.206282   -0.881311
 ---------------------------------------------------------------------
 Rotational constants (GHZ):           2.3929277           1.1752338           0.7920184

 -------------------------------------------------------------------------------
 -------------------- FREQUENCIES AND ROTATIONAL CONSTANTS ----------------------
 -------------------------------------------------------------------------------
 INDEX NO. DOF TYPE  CM-1(UNSCALED)  CM-1(SCALED BY ) SYMMETRY IR-INTENSITY
    1        vib         106.30           0.00              A"        0.1561
    2        vib         122.18           0.00              A"        0.7724
    3        vib         157.58           0.00              A"        1.1385
    4        vib         250.92           0.00              A"        3.2200
    5        vib         275.28           0.00              A'        8.3179
    6        vib         352.52           0.00              A'        0.8781
    7        vib         406.90           0.00              A"        6.8703
    8        vib         456.60           0.00              A'       22.4240
    9        vib         499.99           0.00              A'       10.2489
   10        vib         548.94           0.00              A'        0.3984
   11        vib         653.52           0.00              A"        4.5848
   12        vib         711.65           0.00              A"       26.8162
   13        vib         724.39           0.00              A'        2.0272
   14        vib         750.20           0.00              A"       14.4545
   15        vib         784.59           0.00              A'        1.0173
   16        vib         823.88           0.00              A"       62.2171
```

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  17        vib         929.40           0.00              A'       10.2114
  18        vib         970.63           0.00              A"        0.5328
  19        vib        1050.87           0.00              A'        5.1402
  20        vib        1154.71           0.00              A'      132.4965
  21        vib        1158.99           0.00              A"        0.0706
  22        vib        1185.32           0.00              A'       22.0004
  23        vib        1219.87           0.00              A'       49.4045
  24        vib        1248.43           0.00              A'       60.4732
  25        vib        1336.01           0.00              A'       72.5734
  26        vib        1398.62           0.00              A'       88.5781
  27        vib        1449.58           0.00              A'       11.4932
  28        vib        1480.38           0.00              A'      140.0925
  29        vib        1482.33           0.00              A"       13.1252
  30        vib        1498.64           0.00              A'      159.2899
  31        vib        1537.63           0.00              A'      298.2898
  32        vib        1667.33           0.00              A'       82.5189
  33        vib        1766.14           0.00              A'      668.0595
  34        vib        3080.57           0.00              A'       20.2988
  35        vib        3156.26           0.00              A"        4.4170
  36        vib        3175.74           0.00              A'        6.7489
  37        vib        3226.72           0.00              A'        4.0942
  38        vib        3263.80           0.00              A'        1.7116
  39        vib        3579.64           0.00              A'       64.1631
  40        rot      0.0798195           -
  41        rot      0.0392016           -
  42        rot      0.0264189           -
 ---------------------------------------------------------------------------

 ---------------------------------------------------------------------------
 ----------------------- ZPE & THERMAL CONTRIBUTIONS -----------------------
 ---------------------------------------------------------------------------
 Eelectronic                    [kJ/mol]   = -2039556.222
 Ezpe                           [kJ/mol]   = +296.931
 Eelectronic+Ezpe               [kJ/mol]   = -2039259.291

 Eelectronic                    [hartrees] = -776.825832
 Ezpe                           [hartrees] = +0.113095
 Eelectronic+Ezpe               [hartrees] = -776.712737

 Thermal Correction to Energy   [kJ/mol]   = +317.924
 Thermal Correction to Enthalpy [kJ/mol]   = +320.403
 Thermal Correction to Gibbs    [kJ/mol]   = +209.764
 ---------------------------------------------------------------------------

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 END OF GAUSSIAN OUTPUT FILENAME: MeSU1-b2plypd3.log
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!+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
 GAUSSIAN OUTPUT FILENAME: MeSU1-wb97xd.log
!+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++

 1)LEVEL OF THEORY: OPT=VTIGHT
 Charge = 0 Multiplicity = 1  Stoichiometry    C5H6N2OS

 ---------------------------------------------------------------------
 ---------------------- OPTIMIZED GEOMETRY ---------------------------
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          7           0       -1.177271    0.041485    0.000000
      2          7           0        1.123491   -0.057849    0.000000
      3          6           0        0.000000    0.729846    0.000000
      4          6           0       -1.379877   -1.342668    0.000000
      5          6           0       -0.137315   -2.088505    0.000000
      6          6           0        1.026565   -1.427192    0.000000
      7          1           0       -0.177090   -3.165754    0.000000
      8          1           0        1.973713   -1.948554    0.000000
      9         16           0        0.038796    2.382131    0.000000
     10          1           0       -2.010695    0.610810    0.000000
```

```
    11          8           0       -2.497809   -1.799064    0.000000
    12          6           0        2.434446    0.576736    0.000000
    13          1           0        2.548226    1.204785    0.882167
    14          1           0        3.192904   -0.202422    0.000000
    15          1           0        2.548226    1.204785   -0.882167
---------------------------------------------------------------------
Rotational constants (GHZ):           2.3991524           1.1849434           0.7971123

--------------------------------------------------------------------------------
-------------------- FREQUENCIES AND ROTATIONAL CONSTANTS ----------------------
--------------------------------------------------------------------------------
INDEX NO. DOF TYPE  CM-1(UNSCALED)  CM-1(SCALED BY ) SYMMETRY IR-INTENSITY
   1        vib         106.16           0.00               A"        0.1880
   2        vib         123.16           0.00               A"        0.6318
   3        vib         154.84           0.00               A"        1.7059
   4        vib         256.76           0.00               A"        3.3790
   5        vib         279.58           0.00               A'        8.8383
   6        vib         357.87           0.00               A'        1.1064
   7        vib         412.30           0.00               A"        7.4928
   8        vib         461.79           0.00               A'       25.2527
   9        vib         508.90           0.00               A'       11.3292
  10        vib         557.40           0.00               A'        0.5018
  11        vib         669.87           0.00               A"        5.2029
  12        vib         720.81           0.00               A"       28.8817
  13        vib         732.36           0.00               A'        3.4428
  14        vib         766.25           0.00               A"       10.0861
  15        vib         796.84           0.00               A'        0.9969
  16        vib         839.46           0.00               A"       69.5557
  17        vib         939.83           0.00               A'        9.8837
  18        vib         997.47           0.00               A"        0.2751
  19        vib        1058.29           0.00               A'        7.7222
  20        vib        1157.96           0.00               A"        0.0257
  21        vib        1161.51           0.00               A'      136.3273
  22        vib        1197.79           0.00               A'       43.2701
  23        vib        1241.44           0.00               A'       37.9530
  24        vib        1262.43           0.00               A'       47.6793
  25        vib        1343.70           0.00               A'       89.9407
  26        vib        1421.76           0.00               A'       73.5448
  27        vib        1463.97           0.00               A'       30.5337
  28        vib        1474.17           0.00               A"       14.6123
  29        vib        1486.30           0.00               A'       74.7391
  30        vib        1502.26           0.00               A'       64.7487
  31        vib        1545.43           0.00               A'      549.2092
  32        vib        1706.78           0.00               A'      132.3863
  33        vib        1823.54           0.00               A'      749.9340
  34        vib        3075.86           0.00               A'       19.7974
  35        vib        3152.68           0.00               A"        4.5047
  36        vib        3173.32           0.00               A'        7.0485
  37        vib        3227.46           0.00               A'        3.6885
  38        vib        3267.28           0.00               A'        1.8570
  39        vib        3628.04           0.00               A'       63.1837
  40        rot      0.0800271           -
  41        rot      0.0395255           -
  42        rot      0.0265888           -
--------------------------------------------------------------------------------

--------------------------------------------------------------------------------
------------------------ ZPE & THERMAL CONTRIBUTIONS ---------------------------
--------------------------------------------------------------------------------
Eelectronic                    [kJ/mol]   = -2040306.39
Ezpe                           [kJ/mol]   = +299.388
Eelectronic+Ezpe               [kJ/mol]   = -2040007.002

Eelectronic                    [hartrees] = -777.111556
Ezpe                           [hartrees] = +0.114031
Eelectronic+Ezpe               [hartrees] = -776.997525

Thermal Correction to Energy   [kJ/mol]   = +320.180
Thermal Correction to Enthalpy [kJ/mol]   = +322.658
Thermal Correction to Gibbs    [kJ/mol]   = +212.356
--------------------------------------------------------------------------------
```

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 END OF GAUSSIAN OUTPUT FILENAME: MeSU1-wb97xd.log
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 GAUSSIAN OUTPUT FILENAME: MeSU3-apf.log
!+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++

 1)LEVEL OF THEORY: OPT=VTIGHT
 Charge = 0 Multiplicity = 1  Stoichiometry    C5H6N2OS

 ---------------------------------------------------------------------
 ---------------------- OPTIMIZED GEOMETRY ---------------------------
 ---------------------------------------------------------------------

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 7 | 0 | -1.223339 | 0.217216 | 0.000000 |
| 2 | 7 | 0 | 1.089190 | -0.231026 | 0.000000 |
| 3 | 6 | 0 | -0.000000 | 0.598503 | 0.000000 |
| 4 | 6 | 0 | -1.549995 | -1.146396 | 0.000000 |
| 5 | 6 | 0 | -0.413293 | -2.061732 | 0.000000 |
| 6 | 6 | 0 | 0.838266 | -1.581833 | 0.000000 |
| 7 | 1 | 0 | -0.600050 | -3.126568 | 0.000000 |
| 8 | 1 | 0 | 1.716786 | -2.215141 | 0.000000 |
| 9 | 16 | 0 | 0.376770 | 2.326940 | 0.000000 |
| 10 | 1 | 0 | -0.925594 | 2.649559 | 0.000000 |
| 11 | 8 | 0 | -2.704245 | -1.517145 | 0.000000 |
| 12 | 6 | 0 | 2.448377 | 0.275589 | 0.000000 |
| 13 | 1 | 0 | 2.639520 | 0.879657 | 0.889568 |
| 14 | 1 | 0 | 3.134375 | -0.569155 | 0.000000 |
| 15 | 1 | 0 | 2.639520 | 0.879657 | -0.889568 |

 ---------------------------------------------------------------------
 Rotational constants (GHZ):           2.4218298           1.1764851           0.7958057

 ---------------------------------------------------------------------------------
 -------------------- FREQUENCIES AND ROTATIONAL CONSTANTS ----------------------
 ---------------------------------------------------------------------------------

| INDEX NO. | DOF TYPE | CM-1(UNSCALED) | CM-1(SCALED BY ) | SYMMETRY | IR-INTENSITY |
|---|---|---|---|---|---|
| 1 | vib | 76.54 | 0.00 | A" | 0.6993 |
| 2 | vib | 90.82 | 0.00 | A" | 0.2227 |
| 3 | vib | 169.32 | 0.00 | A" | 0.3525 |
| 4 | vib | 221.83 | 0.00 | A" | 4.2892 |
| 5 | vib | 247.45 | 0.00 | A' | 4.1592 |
| 6 | vib | 338.50 | 0.00 | A" | 19.7798 |
| 7 | vib | 339.63 | 0.00 | A' | 1.2931 |
| 8 | vib | 425.43 | 0.00 | A" | 0.1949 |
| 9 | vib | 438.04 | 0.00 | A' | 12.9961 |
| 10 | vib | 482.06 | 0.00 | A' | 2.1244 |
| 11 | vib | 551.78 | 0.00 | A' | 0.0235 |
| 12 | vib | 656.75 | 0.00 | A" | 2.8581 |
| 13 | vib | 711.43 | 0.00 | A' | 5.9221 |
| 14 | vib | 757.74 | 0.00 | A" | 0.5274 |
| 15 | vib | 775.67 | 0.00 | A' | 0.9859 |
| 16 | vib | 848.37 | 0.00 | A" | 48.4433 |
| 17 | vib | 881.68 | 0.00 | A' | 10.0548 |
| 18 | vib | 952.75 | 0.00 | A' | 33.7461 |
| 19 | vib | 972.94 | 0.00 | A" | 0.0042 |
| 20 | vib | 1037.05 | 0.00 | A' | 1.1564 |
| 21 | vib | 1128.59 | 0.00 | A' | 83.6891 |
| 22 | vib | 1141.19 | 0.00 | A" | 0.0001 |
| 23 | vib | 1177.85 | 0.00 | A' | 11.0630 |
| 24 | vib | 1220.66 | 0.00 | A' | 50.9001 |
| 25 | vib | 1298.87 | 0.00 | A' | 36.4503 |
| 26 | vib | 1391.16 | 0.00 | A' | 98.2518 |
| 27 | vib | 1456.78 | 0.00 | A' | 149.7645 |
| 28 | vib | 1467.68 | 0.00 | A' | 1.9191 |
| 29 | vib | 1476.97 | 0.00 | A" | 13.8166 |
| 30 | vib | 1512.94 | 0.00 | A' | 94.3634 |
| 31 | vib | 1574.46 | 0.00 | A' | 271.9155 |
| 32 | vib | 1705.13 | 0.00 | A' | 246.3344 |

```
  33        vib        1774.01           0.00              A'      530.2058
  34        vib        2720.97           0.00              A'       11.8818
  35        vib        3053.18           0.00              A'       20.5842
  36        vib        3120.25           0.00              A"        6.1577
  37        vib        3162.39           0.00              A'        4.9940
  38        vib        3208.78           0.00              A'        3.1876
  39        vib        3238.64           0.00              A'        0.8918
  40        rot      0.0807835           -
  41        rot      0.0392433           -
  42        rot      0.0265452           -
 -------------------------------------------------------------------------------

 -------------------------------------------------------------------------------
 ----------------------- ZPE & THERMAL CONTRIBUTIONS ---------------------------
 -------------------------------------------------------------------------------
 Eelectronic                    [kJ/mol]   = -2039491.724
 Ezpe                           [kJ/mol]   = +285.946
 Eelectronic+Ezpe               [kJ/mol]   = -2039205.778

 Eelectronic                    [hartrees] = -776.801266
 Ezpe                           [hartrees] = +0.108911
 Eelectronic+Ezpe               [hartrees] = -776.692355

 Thermal Correction to Energy   [kJ/mol]   = +308.284
 Thermal Correction to Enthalpy [kJ/mol]   = +310.762
 Thermal Correction to Gibbs    [kJ/mol]   = +196.873
 -------------------------------------------------------------------------------

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 END OF GAUSSIAN OUTPUT FILENAME: MeSU3-apf.log
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 GAUSSIAN OUTPUT FILENAME: MeSU3-apfd.log
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 1)LEVEL OF THEORY: OPT=VTIGHT
 Charge = 0 Multiplicity = 1  Stoichiometry    C5H6N2OS

 ---------------------------------------------------------------------
 ---------------------- OPTIMIZED GEOMETRY ---------------------------
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          7           0       -1.222399    0.214236    0.000000
      2          7           0        1.091165   -0.229635    0.000000
      3          6           0        0.000000    0.599710    0.000000
      4          6           0       -1.546681   -1.151439    0.000000
      5          6           0       -0.407399   -2.063299    0.000000
      6          6           0        0.843074   -1.580316    0.000000
      7          1           0       -0.592569   -3.128923    0.000000
      8          1           0        1.724439   -2.209778    0.000000
      9         16           0        0.365898    2.336709    0.000000
     10          1           0       -0.938562    2.650925    0.000000
     11          8           0       -2.698962   -1.529892    0.000000
     12          6           0        2.451288    0.273237    0.000000
     13          1           0        2.643097    0.876543    0.889663
     14          1           0        3.134771   -0.573078    0.000000
     15          1           0        2.643097    0.876543   -0.889663
 ---------------------------------------------------------------------
 Rotational constants (GHZ):           2.4091089           1.1748879           0.7936995

 -------------------------------------------------------------------------------
 -------------------- FREQUENCIES AND ROTATIONAL CONSTANTS ----------------------
 -------------------------------------------------------------------------------
 INDEX NO. DOF TYPE  CM-1(UNSCALED)  CM-1(SCALED BY ) SYMMETRY IR-INTENSITY
   1        vib          74.68           0.00              A"        0.7721
   2        vib         101.65           0.00              A"        0.1740
   3        vib         168.11           0.00              A"        0.2873
   4        vib         221.66           0.00              A"        4.5749
```

```
    5        vib         253.69           0.00              A'        4.1835
    6        vib         331.73           0.00              A"       19.4333
    7        vib         336.97           0.00              A'        1.4148
    8        vib         424.91           0.00              A"        0.2052
    9        vib         434.15           0.00              A'       13.2937
   10        vib         485.65           0.00              A'        2.1240
   11        vib         554.00           0.00              A'        0.1689
   12        vib         657.09           0.00              A"        2.8666
   13        vib         711.33           0.00              A'        6.1963
   14        vib         757.50           0.00              A"        0.4790
   15        vib         776.38           0.00              A'        1.0272
   16        vib         849.03           0.00              A"       48.4108
   17        vib         888.54           0.00              A'        9.8983
   18        vib         962.56           0.00              A'       35.7733
   19        vib         973.13           0.00              A"        0.0006
   20        vib        1031.35           0.00              A'        0.6069
   21        vib        1125.57           0.00              A'       82.3036
   22        vib        1141.57           0.00              A"        0.0000
   23        vib        1175.90           0.00              A'       18.5364
   24        vib        1221.37           0.00              A'       42.0882
   25        vib        1296.19           0.00              A'       30.7349
   26        vib        1386.45           0.00              A'      120.6173
   27        vib        1455.41           0.00              A'      100.4836
   28        vib        1458.76           0.00              A'       39.5389
   29        vib        1479.06           0.00              A"       13.6953
   30        vib        1511.00           0.00              A'       89.2137
   31        vib        1574.42           0.00              A'      279.0000
   32        vib        1704.86           0.00              A'      263.8231
   33        vib        1773.38           0.00              A'      510.2013
   34        vib        2721.29           0.00              A'       12.0886
   35        vib        3055.01           0.00              A'       20.9370
   36        vib        3122.38           0.00              A"        6.2558
   37        vib        3165.11           0.00              A'        4.8147
   38        vib        3207.84           0.00              A'        3.0700
   39        vib        3235.52           0.00              A'        1.0596
   40        rot      0.0803592           -
   41        rot      0.0391900           -
   42        rot      0.0264750           -
 --------------------------------------------------------------------------------

 --------------------------------------------------------------------------------
 ------------------------ ZPE & THERMAL CONTRIBUTIONS ---------------------------
 --------------------------------------------------------------------------------
 Eelectronic                    [kJ/mol]   = -2039513.479
 Ezpe                           [kJ/mol]   = +285.938
 Eelectronic+Ezpe               [kJ/mol]   = -2039227.541

 Eelectronic                    [hartrees] = -776.809552
 Ezpe                           [hartrees] = +0.108908
 Eelectronic+Ezpe               [hartrees] = -776.700644

 Thermal Correction to Energy   [kJ/mol]   = +308.236
 Thermal Correction to Enthalpy [kJ/mol]   = +310.717
 Thermal Correction to Gibbs    [kJ/mol]   = +197.015
 --------------------------------------------------------------------------------

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 GAUSSIAN OUTPUT FILENAME: MeSU3-b2plyp.log
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 1)LEVEL OF THEORY: OPT=VTIGHT
 Charge = 0 Multiplicity = 1  Stoichiometry    C5H6N2OS

 ---------------------------------------------------------------------
 ---------------------- OPTIMIZED GEOMETRY ---------------------------
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
```

| Number | Number | Type | X | Y | Z |
|---|---|---|---|---|---|
| 1 | 7 | 0 | -1.229031 | 0.218350 | 0.000000 |
| 2 | 7 | 0 | 1.093002 | -0.231043 | 0.000000 |
| 3 | 6 | 0 | -0.000000 | 0.601058 | 0.000000 |
| 4 | 6 | 0 | -1.553027 | -1.153244 | 0.000000 |
| 5 | 6 | 0 | -0.414189 | -2.067550 | 0.000000 |
| 6 | 6 | 0 | 0.841803 | -1.586874 | 0.000000 |
| 7 | 1 | 0 | -0.599359 | -3.130924 | 0.000000 |
| 8 | 1 | 0 | 1.718081 | -2.219375 | 0.000000 |
| 9 | 16 | 0 | 0.374933 | 2.337497 | 0.000000 |
| 10 | 1 | 0 | -0.924621 | 2.660641 | 0.000000 |
| 11 | 8 | 0 | -2.712499 | -1.526710 | 0.000000 |
| 12 | 6 | 0 | 2.461516 | 0.275111 | 0.000000 |
| 13 | 1 | 0 | 2.650925 | 0.876892 | 0.888363 |
| 14 | 1 | 0 | 3.140692 | -0.572540 | 0.000000 |
| 15 | 1 | 0 | 2.650925 | 0.876892 | -0.888363 |

Rotational constants (GHZ): 2.4015963 1.1678067 0.7896395

---------- FREQUENCIES AND ROTATIONAL CONSTANTS ----------

| INDEX NO. | DOF TYPE | CM-1(UNSCALED) | CM-1(SCALED BY ) | SYMMETRY | IR-INTENSITY |
|---|---|---|---|---|---|
| 1 | vib | 75.42 | 0.00 | A" | 0.5352 |
| 2 | vib | 89.85 | 0.00 | A" | 0.4386 |
| 3 | vib | 168.63 | 0.00 | A" | 0.3338 |
| 4 | vib | 218.27 | 0.00 | A" | 4.1682 |
| 5 | vib | 250.16 | 0.00 | A' | 4.1636 |
| 6 | vib | 333.43 | 0.00 | A" | 20.0040 |
| 7 | vib | 338.88 | 0.00 | A' | 1.1330 |
| 8 | vib | 424.39 | 0.00 | A" | 0.2262 |
| 9 | vib | 434.04 | 0.00 | A' | 12.8524 |
| 10 | vib | 480.08 | 0.00 | A' | 1.9947 |
| 11 | vib | 548.48 | 0.00 | A' | 0.0366 |
| 12 | vib | 648.54 | 0.00 | A" | 2.4133 |
| 13 | vib | 706.13 | 0.00 | A' | 5.6067 |
| 14 | vib | 750.41 | 0.00 | A" | 0.2232 |
| 15 | vib | 767.90 | 0.00 | A' | 0.7537 |
| 16 | vib | 842.48 | 0.00 | A" | 47.7781 |
| 17 | vib | 876.46 | 0.00 | A' | 8.6565 |
| 18 | vib | 949.07 | 0.00 | A' | 36.6744 |
| 19 | vib | 965.71 | 0.00 | A" | 0.0089 |
| 20 | vib | 1034.31 | 0.00 | A' | 1.5487 |
| 21 | vib | 1129.60 | 0.00 | A' | 81.6160 |
| 22 | vib | 1153.12 | 0.00 | A" | 0.0558 |
| 23 | vib | 1175.26 | 0.00 | A' | 31.7330 |
| 24 | vib | 1219.69 | 0.00 | A' | 39.9305 |
| 25 | vib | 1283.02 | 0.00 | A' | 44.3642 |
| 26 | vib | 1393.16 | 0.00 | A' | 121.6475 |
| 27 | vib | 1452.14 | 0.00 | A' | 128.7965 |
| 28 | vib | 1482.07 | 0.00 | A' | 24.3626 |
| 29 | vib | 1499.40 | 0.00 | A" | 12.4015 |
| 30 | vib | 1527.98 | 0.00 | A' | 81.3474 |
| 31 | vib | 1546.03 | 0.00 | A' | 257.6275 |
| 32 | vib | 1679.03 | 0.00 | A' | 154.9870 |
| 33 | vib | 1731.19 | 0.00 | A' | 518.1962 |
| 34 | vib | 2726.70 | 0.00 | A' | 11.6962 |
| 35 | vib | 3065.09 | 0.00 | A' | 21.1470 |
| 36 | vib | 3133.48 | 0.00 | A" | 6.4038 |
| 37 | vib | 3170.37 | 0.00 | A' | 5.3013 |
| 38 | vib | 3217.98 | 0.00 | A' | 2.9035 |
| 39 | vib | 3242.61 | 0.00 | A' | 1.2658 |
| 40 | rot | 0.0801086 | - | | |
| 41 | rot | 0.0389538 | - | | |
| 42 | rot | 0.0263395 | - | | |

---------- ZPE & THERMAL CONTRIBUTIONS ----------

Eelectronic [kJ/mol] = -2039439.138

```
 Ezpe                             [kJ/mol]   = +285.492
 Eelectronic+Ezpe                 [kJ/mol]   = -2039153.646

 Eelectronic                      [hartrees] = -776.781237
 Ezpe                             [hartrees] = +0.108738
 Eelectronic+Ezpe                 [hartrees] = -776.672499

 Thermal Correction to Energy   [kJ/mol]   = +307.927
 Thermal Correction to Enthalpy [kJ/mol]   = +310.408
 Thermal Correction to Gibbs    [kJ/mol]   = +196.277
 ---------------------------------------------------------------------------

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 GAUSSIAN OUTPUT FILENAME: MeSU3-b2plypd3.log
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 1)LEVEL OF THEORY: OPT=VTIGHT
 Charge = 0 Multiplicity = 1  Stoichiometry    C5H6N2OS

 ---------------------------------------------------------------------
 ---------------------- OPTIMIZED GEOMETRY ---------------------------
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          7           0       -1.229287    0.219534    0.000000
      2          7           0        1.091882   -0.231546    0.000000
      3          6           0        0.000000    0.600925    0.000000
      4          6           0       -1.553314   -1.151628    0.000000
      5          6           0       -0.415116   -2.066506    0.000000
      6          6           0        0.840979   -1.586902    0.000000
      7          1           0       -0.601307   -3.129530    0.000000
      8          1           0        1.717186   -2.219186    0.000000
      9         16           0        0.377798    2.335168    0.000000
     10          1           0       -0.921309    2.659719    0.000000
     11          8           0       -2.712756   -1.524980    0.000000
     12          6           0        2.459257    0.275331    0.000000
     13          1           0        2.647433    0.877344    0.888319
     14          1           0        3.138837   -0.571781    0.000000
     15          1           0        2.647433    0.877344   -0.888319
 ---------------------------------------------------------------------
 Rotational constants (GHZ):           2.4061911           1.1684796           0.7904432

 ---------------------------------------------------------------------------
 -------------------- FREQUENCIES AND ROTATIONAL CONSTANTS ----------------
 ---------------------------------------------------------------------------
 INDEX NO. DOF TYPE  CM-1(UNSCALED)  CM-1(SCALED BY ) SYMMETRY IR-INTENSITY
    1        vib          75.50           0.00              A"        0.5864
    2        vib          92.49           0.00              A"        0.4227
    3        vib         168.21           0.00              A"        0.3335
    4        vib         217.70           0.00              A"        4.0664
    5        vib         251.47           0.00              A'        4.1868
    6        vib         334.67           0.00              A"       20.0668
    7        vib         340.03           0.00              A'        1.1313
    8        vib         423.90           0.00              A"        0.2209
    9        vib         435.17           0.00              A'       12.7507
   10        vib         480.92           0.00              A'        1.9935
   11        vib         548.93           0.00              A'        0.0362
   12        vib         648.24           0.00              A"        2.4247
   13        vib         707.67           0.00              A'        5.7021
   14        vib         750.22           0.00              A"        0.2390
   15        vib         769.38           0.00              A'        0.7413
   16        vib         842.23           0.00              A"       47.7558
   17        vib         878.10           0.00              A'        8.8997
   18        vib         950.31           0.00              A'       36.1846
   19        vib         965.45           0.00              A"        0.0081
   20        vib        1035.71           0.00              A'        1.5063
```

| | | | | | |
|---|---|---|---|---|---|
| 21 | vib | 1131.75 | 0.00 | A' | 82.1268 |
| 22 | vib | 1153.67 | 0.00 | A" | 0.0554 |
| 23 | vib | 1176.49 | 0.00 | A' | 29.6581 |
| 24 | vib | 1220.84 | 0.00 | A' | 40.9385 |
| 25 | vib | 1285.00 | 0.00 | A' | 43.9173 |
| 26 | vib | 1394.44 | 0.00 | A' | 118.6809 |
| 27 | vib | 1453.44 | 0.00 | A' | 132.2774 |
| 28 | vib | 1482.46 | 0.00 | A' | 23.4395 |
| 29 | vib | 1499.63 | 0.00 | A" | 12.4453 |
| 30 | vib | 1528.66 | 0.00 | A' | 78.5694 |
| 31 | vib | 1547.37 | 0.00 | A' | 260.9020 |
| 32 | vib | 1680.51 | 0.00 | A' | 156.1802 |
| 33 | vib | 1732.15 | 0.00 | A' | 517.0345 |
| 34 | vib | 2727.23 | 0.00 | A' | 11.6619 |
| 35 | vib | 3065.87 | 0.00 | A' | 21.1050 |
| 36 | vib | 3134.30 | 0.00 | A" | 6.3852 |
| 37 | vib | 3171.62 | 0.00 | A' | 5.3010 |
| 38 | vib | 3218.87 | 0.00 | A' | 2.9121 |
| 39 | vib | 3243.66 | 0.00 | A' | 1.2528 |
| 40 | rot | 0.0802619 | - | | |
| 41 | rot | 0.0389763 | - | | |
| 42 | rot | 0.0263663 | - | | |

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---------- ZPE & THERMAL CONTRIBUTIONS ----------

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Eelectronic [kJ/mol] = -2039475.047
Ezpe [kJ/mol] = +285.694
Eelectronic+Ezpe [kJ/mol] = -2039189.353

Eelectronic [hartrees] = -776.794914
Ezpe [hartrees] = +0.108815
Eelectronic+Ezpe [hartrees] = -776.686099

Thermal Correction to Energy [kJ/mol] = +308.097
Thermal Correction to Enthalpy [kJ/mol] = +310.576
Thermal Correction to Gibbs [kJ/mol] = +196.553

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END OF GAUSSIAN OUTPUT FILENAME: MeSU3-b2plypd3.log
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GAUSSIAN OUTPUT FILENAME: MeSU3-MeSU1-H2O-TS-d3bj.log
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1)LEVEL OF THEORY: B3LYP/DEF2TZVP
Charge = 0 Multiplicity = 1 Stoichiometry C5H8N2O2S

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---------- OPTIMIZED GEOMETRY ----------

---

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 2.327061 | 0.332924 | -0.008063 |
| 2 | 6 | 0 | 1.646848 | -0.955381 | -0.001663 |
| 3 | 7 | 0 | 0.250818 | -0.883158 | -0.015061 |
| 4 | 6 | 0 | -0.421007 | 0.249302 | -0.003778 |
| 5 | 16 | 0 | -2.160176 | 0.252393 | 0.000240 |
| 6 | 7 | 0 | 0.229339 | 1.457253 | 0.004336 |
| 7 | 6 | 0 | 1.607190 | 1.465103 | -0.003065 |
| 8 | 1 | 0 | 3.405815 | 0.354054 | -0.011984 |
| 9 | 1 | 0 | -0.675439 | -2.060047 | -0.057184 |
| 10 | 8 | 0 | -1.651659 | -2.516933 | -0.092065 |
| 11 | 1 | 0 | -1.790764 | -3.002371 | 0.731556 |
| 12 | 1 | 0 | -2.143795 | -1.365017 | -0.024725 |
| 13 | 8 | 0 | 2.216394 | -2.032081 | 0.016953 |
| 14 | 1 | 0 | 2.059917 | 2.446331 | -0.003444 |

| | | | | | |
|---|---|---|---|---|---|
| 15 | 6 | 0 | -0.509638 | 2.716780 | 0.014401 |
| 16 | 1 | 0 | -1.137814 | 2.783057 | 0.901501 |
| 17 | 1 | 0 | 0.207394 | 3.533547 | 0.016729 |
| 18 | 1 | 0 | -1.144200 | 2.793230 | -0.867301 |

Rotational constants (GHZ): 1.3057321 1.1535701 0.6158332

---------- FREQUENCIES AND ROTATIONAL CONSTANTS ----------

| INDEX NO. | DOF TYPE | CM-1(UNSCALED) | CM-1(SCALED BY ) | SYMMETRY | IR-INTENSITY |
|---|---|---|---|---|---|
| 1 | vib | -1052.04 | 0.00 | A | 1032.9611 |
| 2 | vib | 77.49 | 0.00 | A | 10.3680 |
| 3 | vib | 91.83 | 0.00 | A | 0.3662 |
| 4 | vib | 124.77 | 0.00 | A | 0.2388 |
| 5 | vib | 164.09 | 0.00 | A | 1.5044 |
| 6 | vib | 223.65 | 0.00 | A | 24.9806 |
| 7 | vib | 245.34 | 0.00 | A | 1.6918 |
| 8 | vib | 332.39 | 0.00 | A | 26.5348 |
| 9 | vib | 384.01 | 0.00 | A | 41.1809 |
| 10 | vib | 423.05 | 0.00 | A | 3.4531 |
| 11 | vib | 457.24 | 0.00 | A | 20.3946 |
| 12 | vib | 464.76 | 0.00 | A | 2.1442 |
| 13 | vib | 480.46 | 0.00 | A | 106.9469 |
| 14 | vib | 535.78 | 0.00 | A | 30.1407 |
| 15 | vib | 563.21 | 0.00 | A | 83.4018 |
| 16 | vib | 579.55 | 0.00 | A | 32.2777 |
| 17 | vib | 666.10 | 0.00 | A | 2.3008 |
| 18 | vib | 734.60 | 0.00 | A | 13.3721 |
| 19 | vib | 756.07 | 0.00 | A | 1.9390 |
| 20 | vib | 802.52 | 0.00 | A | 3.8239 |
| 21 | vib | 840.71 | 0.00 | A | 47.1554 |
| 22 | vib | 936.41 | 0.00 | A | 82.6632 |
| 23 | vib | 972.26 | 0.00 | A | 0.0812 |
| 24 | vib | 1049.56 | 0.00 | A | 3.6202 |
| 25 | vib | 1090.99 | 0.00 | A | 382.1779 |
| 26 | vib | 1145.13 | 0.00 | A | 86.6283 |
| 27 | vib | 1149.19 | 0.00 | A | 0.0895 |
| 28 | vib | 1181.78 | 0.00 | A | 11.6117 |
| 29 | vib | 1215.50 | 0.00 | A | 549.4835 |
| 30 | vib | 1231.84 | 0.00 | A | 34.7457 |
| 31 | vib | 1281.44 | 0.00 | A | 21.0456 |
| 32 | vib | 1387.96 | 0.00 | A | 240.6102 |
| 33 | vib | 1433.49 | 0.00 | A | 374.6794 |
| 34 | vib | 1466.80 | 0.00 | A | 332.7715 |
| 35 | vib | 1479.22 | 0.00 | A | 13.4427 |
| 36 | vib | 1480.52 | 0.00 | A | 27.5392 |
| 37 | vib | 1520.82 | 0.00 | A | 73.5605 |
| 38 | vib | 1543.65 | 0.00 | A | 175.8749 |
| 39 | vib | 1610.58 | 0.00 | A | 351.3221 |
| 40 | vib | 1681.02 | 0.00 | A | 114.5058 |
| 41 | vib | 1746.90 | 0.00 | A | 770.0922 |
| 42 | vib | 2153.47 | 0.00 | A | 1816.8796 |
| 43 | vib | 3058.51 | 0.00 | A | 20.5346 |
| 44 | vib | 3122.00 | 0.00 | A | 6.4087 |
| 45 | vib | 3147.87 | 0.00 | A | 8.9067 |
| 46 | vib | 3203.88 | 0.00 | A | 4.1456 |
| 47 | vib | 3232.21 | 0.00 | A | 0.7331 |
| 48 | vib | 3794.49 | 0.00 | A | 75.9861 |
| 49 | rot | 0.0435545 | - | | |
| 50 | rot | 0.0384790 | - | | |
| 51 | rot | 0.0205420 | - | | |

---------- ZPE & THERMAL CONTRIBUTIONS ----------

Eelectronic [kJ/mol] = -2241482.676
Ezpe [kJ/mol] = +342.523
Eelectronic+Ezpe [kJ/mol] = -2241140.153

Eelectronic [hartrees] = -853.735546

```
 Ezpe                             [hartrees] = +0.130460
 Eelectronic+Ezpe                 [hartrees] = -853.605086

 Thermal Correction to Energy   [kJ/mol]   = +368.087
 Thermal Correction to Enthalpy [kJ/mol]   = +370.566
 Thermal Correction to Gibbs    [kJ/mol]   = +249.457
 ---------------------------------------------------------------------------

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 END OF GAUSSIAN OUTPUT FILENAME: MeSU3-MeSU1-H2O-TS-d3bj.log
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 GAUSSIAN OUTPUT FILENAME: MeSU3-MeSU1-m062x-product.log
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 1)LEVEL OF THEORY: M062X/DEF2TZVP
 Charge = 0 Multiplicity = 1  Stoichiometry    C5H6N2OS

 ---------------------------------------------------------------------
 ---------------------- OPTIMIZED GEOMETRY ---------------------------
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          7           0       -1.178469    0.042220    0.000000
      2          7           0        1.121879   -0.059618    0.000000
      3          6           0        0.000000    0.731413    0.000000
      4          6           0       -1.382238   -1.342654    0.000000
      5          6           0       -0.139548   -2.092603    0.000000
      6          6           0        1.024852   -1.430133    0.000000
      7          1           0       -0.183374   -3.169365    0.000000
      8          1           0        1.973368   -1.949013    0.000000
      9         16           0        0.045512    2.382732    0.000000
     10          1           0       -2.014630    0.611840    0.000000
     11          8           0       -2.499900   -1.797747    0.000000
     12          6           0        2.433581    0.579040    0.000000
     13          1           0        2.540310    1.207869    0.881891
     14          1           0        3.191260   -0.199534    0.000000
     15          1           0        2.540310    1.207869   -0.881891
 ---------------------------------------------------------------------
 Rotational constants (GHZ):           2.4038318           1.1823694           0.7964586

 ---------------------------------------------------------------------------
 -------------------- FREQUENCIES AND ROTATIONAL CONSTANTS ----------------
 ---------------------------------------------------------------------------
 INDEX NO. DOF TYPE  CM-1(UNSCALED)  CM-1(SCALED BY ) SYMMETRY IR-INTENSITY
    1        vib         106.76           0.00              A"        0.2433
    2        vib         129.21           0.00              A"        0.9264
    3        vib         174.74           0.00              A"        1.2427
    4        vib         257.18           0.00              A"        3.2747
    5        vib         281.62           0.00              A'        8.2800
    6        vib         360.99           0.00              A'        0.9980
    7        vib         408.39           0.00              A"        7.2693
    8        vib         460.08           0.00              A'       25.5470
    9        vib         505.12           0.00              A'       11.6713
   10        vib         556.54           0.00              A'        0.4134
   11        vib         666.32           0.00              A"        4.7197
   12        vib         721.04           0.00              A"       27.0334
   13        vib         732.19           0.00              A'        3.7533
   14        vib         765.77           0.00              A"       12.4855
   15        vib         794.79           0.00              A'        0.8961
   16        vib         838.25           0.00              A"       69.6427
   17        vib         942.09           0.00              A'       10.1432
   18        vib         997.29           0.00              A"        0.2838
   19        vib        1056.64           0.00              A'        5.9466
   20        vib        1154.08           0.00              A"        0.0731
   21        vib        1157.27           0.00              A'      142.4880
   22        vib        1193.88           0.00              A'       56.2918
   23        vib        1238.48           0.00              A'       41.6551
   24        vib        1253.65           0.00              A'       49.4896
```

| | | | | | |
|---|---|---|---|---|---|
| 25 | vib | 1341.61 | 0.00 | A' | 86.1179 |
| 26 | vib | 1415.22 | 0.00 | A' | 76.9723 |
| 27 | vib | 1459.00 | 0.00 | A' | 31.1651 |
| 28 | vib | 1474.25 | 0.00 | A" | 13.6636 |
| 29 | vib | 1485.37 | 0.00 | A' | 75.9794 |
| 30 | vib | 1498.75 | 0.00 | A' | 122.5547 |
| 31 | vib | 1542.05 | 0.00 | A' | 539.4995 |
| 32 | vib | 1707.20 | 0.00 | A' | 144.9884 |
| 33 | vib | 1831.13 | 0.00 | A' | 766.5887 |
| 34 | vib | 3089.17 | 0.00 | A' | 15.3747 |
| 35 | vib | 3161.27 | 0.00 | A" | 2.6869 |
| 36 | vib | 3187.73 | 0.00 | A' | 5.1991 |
| 37 | vib | 3235.71 | 0.00 | A' | 3.0148 |
| 38 | vib | 3278.57 | 0.00 | A' | 3.8822 |
| 39 | vib | 3601.03 | 0.00 | A' | 73.4497 |
| 40 | rot | 0.0801832 | - | | |
| 41 | rot | 0.0394396 | - | | |
| 42 | rot | 0.0265670 | - | | |

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---------- ZPE & THERMAL CONTRIBUTIONS ----------

---

Eelectronic [kJ/mol] = -2040205.075
Ezpe [kJ/mol] = +299.428
Eelectronic+Ezpe [kJ/mol] = -2039905.647

Eelectronic [hartrees] = -777.072967
Ezpe [hartrees] = +0.114046
Eelectronic+Ezpe [hartrees] = -776.958921

Thermal Correction to Energy [kJ/mol] = +320.117
Thermal Correction to Enthalpy [kJ/mol] = +322.595
Thermal Correction to Gibbs [kJ/mol] = +212.689

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END OF GAUSSIAN OUTPUT FILENAME: MeSU3-MeSU1-m062x-product.log
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!++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
GAUSSIAN OUTPUT FILENAME: MeSU3-MeSU1-m062x-reactant.log
!++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++

1)LEVEL OF THEORY: M062X/DEF2TZVP
Charge = 0 Multiplicity = 1 Stoichiometry C5H6N2OS

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---------- OPTIMIZED GEOMETRY ----------

---

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 7 | 0 | -1.224433 | 0.225832 | 0.000000 |
| 2 | 7 | 0 | 1.085078 | -0.236547 | 0.000000 |
| 3 | 6 | 0 | -0.000000 | 0.598294 | 0.000000 |
| 4 | 6 | 0 | -1.555607 | -1.140670 | 0.000000 |
| 5 | 6 | 0 | -0.420342 | -2.065707 | 0.000000 |
| 6 | 6 | 0 | 0.829930 | -1.590108 | 0.000000 |
| 7 | 1 | 0 | -0.615943 | -3.127094 | 0.000000 |
| 8 | 1 | 0 | 1.706023 | -2.224253 | 0.000000 |
| 9 | 16 | 0 | 0.388670 | 2.326587 | 0.000000 |
| 10 | 1 | 0 | -0.906154 | 2.659057 | 0.000000 |
| 11 | 8 | 0 | -2.706917 | -1.506846 | 0.000000 |
| 12 | 6 | 0 | 2.450023 | 0.269564 | 0.000000 |
| 13 | 1 | 0 | 2.636599 | 0.872635 | 0.888888 |
| 14 | 1 | 0 | 3.130953 | -0.576844 | 0.000000 |
| 15 | 1 | 0 | 2.636599 | 0.872635 | -0.888888 |

---

Rotational constants (GHZ): 2.4229148 1.1749578 0.7952174

```
-------------------------------------------------------------------------------
-------------------- FREQUENCIES AND ROTATIONAL CONSTANTS ----------------------
-------------------------------------------------------------------------------
 INDEX NO. DOF TYPE  CM-1(UNSCALED)  CM-1(SCALED BY ) SYMMETRY IR-INTENSITY
    1        vib          78.42           0.00              A"        0.7307
    2        vib         118.85           0.00              A"        0.7448
    3        vib         172.60           0.00              A"        0.2970
    4        vib         228.89           0.00              A"        2.5888
    5        vib         261.45           0.00              A'        4.5464
    6        vib         350.06           0.00              A'        1.2324
    7        vib         403.27           0.00              A"       22.1485
    8        vib         428.32           0.00              A"        0.1205
    9        vib         441.25           0.00              A'       12.6871
   10        vib         485.38           0.00              A'        2.1608
   11        vib         557.70           0.00              A'        0.1486
   12        vib         659.94           0.00              A"        2.6960
   13        vib         714.88           0.00              A'        7.0876
   14        vib         764.78           0.00              A"        0.2250
   15        vib         778.24           0.00              A'        1.0927
   16        vib         855.66           0.00              A"       51.8163
   17        vib         894.14           0.00              A'        8.8544
   18        vib         960.81           0.00              A'       37.6023
   19        vib         994.13           0.00              A"        0.0628
   20        vib        1043.17           0.00              A'        1.0994
   21        vib        1135.89           0.00              A'       80.1588
   22        vib        1149.93           0.00              A"        0.0560
   23        vib        1184.69           0.00              A'       16.3060
   24        vib        1225.27           0.00              A'       61.0645
   25        vib        1308.25           0.00              A'       35.2205
   26        vib        1402.38           0.00              A'      103.7718
   27        vib        1466.86           0.00              A'      185.6890
   28        vib        1479.50           0.00              A'        7.6228
   29        vib        1491.19           0.00              A"       13.1783
   30        vib        1525.12           0.00              A'       92.6502
   31        vib        1590.30           0.00              A'      323.7062
   32        vib        1723.23           0.00              A'      305.5921
   33        vib        1808.08           0.00              A'      575.7831
   34        vib        2745.23           0.00              A'       14.9103
   35        vib        3074.28           0.00              A'       17.0958
   36        vib        3141.36           0.00              A"        4.2421
   37        vib        3180.94           0.00              A'        3.6254
   38        vib        3226.35           0.00              A'        2.3161
   39        vib        3259.35           0.00              A'        0.3077
   40        rot      0.0808197           -
   41        rot      0.0391924           -
   42        rot      0.0265256           -
-------------------------------------------------------------------------------

-------------------------------------------------------------------------------
------------------------ ZPE & THERMAL CONTRIBUTIONS --------------------------
-------------------------------------------------------------------------------
 Eelectronic                    [kJ/mol]   = -2040121.849
 Ezpe                           [kJ/mol]   = +288.960
 Eelectronic+Ezpe               [kJ/mol]   = -2039832.889

 Eelectronic                    [hartrees] = -777.041268
 Ezpe                           [hartrees] = +0.110059
 Eelectronic+Ezpe               [hartrees] = -776.931209

 Thermal Correction to Energy   [kJ/mol]   = +310.762
 Thermal Correction to Enthalpy [kJ/mol]   = +313.241
 Thermal Correction to Gibbs    [kJ/mol]   = +200.811
 -------------------------------------------------------------------------------

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 END OF GAUSSIAN OUTPUT FILENAME: MeSU3-MeSU1-m062x-reactant.log
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 GAUSSIAN OUTPUT FILENAME: MeSU3-wb97xd.log
!+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
```

1)LEVEL OF THEORY: OPT=VTIGHT
Charge = 0 Multiplicity = 1  Stoichiometry  C5H6N2OS

---

---------- OPTIMIZED GEOMETRY ----------

---

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 7 | 0 | -1.222003 | 0.216973 | 0.000000 |
| 2 | 7 | 0 | 1.088885 | -0.230487 | 0.000000 |
| 3 | 6 | 0 | -0.000000 | 0.598363 | 0.000000 |
| 4 | 6 | 0 | -1.547389 | -1.148149 | 0.000000 |
| 5 | 6 | 0 | -0.407716 | -2.064953 | 0.000000 |
| 6 | 6 | 0 | 0.839469 | -1.583804 | 0.000000 |
| 7 | 1 | 0 | -0.594127 | -3.128355 | 0.000000 |
| 8 | 1 | 0 | 1.716528 | -2.216675 | 0.000000 |
| 9 | 16 | 0 | 0.367767 | 2.331043 | 0.000000 |
| 10 | 1 | 0 | -0.930438 | 2.655465 | 0.000000 |
| 11 | 8 | 0 | -2.698038 | -1.519414 | 0.000000 |
| 12 | 6 | 0 | 2.451930 | 0.275075 | 0.000000 |
| 13 | 1 | 0 | 2.643261 | 0.876796 | 0.889461 |
| 14 | 1 | 0 | 3.135611 | -0.570003 | 0.000000 |
| 15 | 1 | 0 | 2.643261 | 0.876796 | -0.889461 |

---

Rotational constants (GHZ):  2.4115864  1.1779382  0.7953583

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---------- FREQUENCIES AND ROTATIONAL CONSTANTS ----------

---

| INDEX NO. | DOF TYPE | CM-1(UNSCALED) | CM-1(SCALED BY ) | SYMMETRY | IR-INTENSITY |
|---|---|---|---|---|---|
| 1 | vib | 75.67 | 0.00 | A" | 0.7453 |
| 2 | vib | 86.85 | 0.00 | A" | 0.2368 |
| 3 | vib | 171.36 | 0.00 | A" | 0.3504 |
| 4 | vib | 222.95 | 0.00 | A" | 4.0829 |
| 5 | vib | 253.58 | 0.00 | A' | 4.5425 |
| 6 | vib | 343.95 | 0.00 | A" | 21.3831 |
| 7 | vib | 344.69 | 0.00 | A' | 1.2730 |
| 8 | vib | 429.98 | 0.00 | A" | 0.1970 |
| 9 | vib | 441.72 | 0.00 | A' | 12.7691 |
| 10 | vib | 488.15 | 0.00 | A' | 2.1251 |
| 11 | vib | 558.74 | 0.00 | A' | 0.0434 |
| 12 | vib | 663.03 | 0.00 | A" | 3.0651 |
| 13 | vib | 715.11 | 0.00 | A' | 6.1129 |
| 14 | vib | 766.36 | 0.00 | A" | 0.3196 |
| 15 | vib | 780.67 | 0.00 | A' | 0.8222 |
| 16 | vib | 855.75 | 0.00 | A" | 51.9434 |
| 17 | vib | 891.00 | 0.00 | A' | 8.0886 |
| 18 | vib | 963.74 | 0.00 | A' | 38.7176 |
| 19 | vib | 990.52 | 0.00 | A" | 0.0045 |
| 20 | vib | 1045.85 | 0.00 | A' | 0.6791 |
| 21 | vib | 1140.47 | 0.00 | A' | 79.7535 |
| 22 | vib | 1153.23 | 0.00 | A" | 0.0279 |
| 23 | vib | 1187.85 | 0.00 | A' | 16.9804 |
| 24 | vib | 1232.76 | 0.00 | A' | 48.5616 |
| 25 | vib | 1308.13 | 0.00 | A' | 34.7248 |
| 26 | vib | 1406.09 | 0.00 | A' | 105.6050 |
| 27 | vib | 1470.36 | 0.00 | A' | 156.7859 |
| 28 | vib | 1483.30 | 0.00 | A' | 5.6583 |
| 29 | vib | 1490.73 | 0.00 | A" | 13.9213 |
| 30 | vib | 1524.54 | 0.00 | A' | 98.4547 |
| 31 | vib | 1588.14 | 0.00 | A' | 301.7228 |
| 32 | vib | 1721.52 | 0.00 | A' | 269.7321 |
| 33 | vib | 1797.54 | 0.00 | A' | 575.0221 |
| 34 | vib | 2746.90 | 0.00 | A' | 10.9843 |
| 35 | vib | 3060.89 | 0.00 | A' | 21.1594 |
| 36 | vib | 3130.98 | 0.00 | A" | 6.5635 |
| 37 | vib | 3169.84 | 0.00 | A' | 5.6603 |
| 38 | vib | 3219.63 | 0.00 | A' | 2.9407 |
| 39 | vib | 3248.77 | 0.00 | A' | 0.7738 |
| 40 | rot | 0.0804419 | - | | |

```
  41        rot      0.0392918           -
  42        rot      0.0265303           -
 -------------------------------------------------------------------------------

 -------------------------------------------------------------------------------
 ------------------------ ZPE & THERMAL CONTRIBUTIONS --------------------------
 -------------------------------------------------------------------------------
 Eelectronic                    [kJ/mol]   = -2040222.488
 Ezpe                           [kJ/mol]   = +288.128
 Eelectronic+Ezpe               [kJ/mol]   = -2039934.360

 Eelectronic                    [hartrees] = -777.079599
 Ezpe                           [hartrees] = +0.109742
 Eelectronic+Ezpe               [hartrees] = -776.969857

 Thermal Correction to Energy   [kJ/mol]   = +310.318
 Thermal Correction to Enthalpy [kJ/mol]   = +312.797
 Thermal Correction to Gibbs    [kJ/mol]   = +199.073
 -------------------------------------------------------------------------------

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 END OF GAUSSIAN OUTPUT FILENAME: MeSU3-wb97xd.log
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 GAUSSIAN OUTPUT FILENAME: NNHS-m062x.log
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 1)LEVEL OF THEORY: OPT=VTIGHT
 Charge = 0 Multiplicity = 1  Stoichiometry    C4H4N2S

 ---------------------------------------------------------------------
 ---------------------- OPTIMIZED GEOMETRY ---------------------------
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          6           0        1.264011   -0.087362    0.000000
      2          7           0       -1.072135   -0.249731    0.000000
      3          6           0        0.000000    0.600922    0.000000
      4          6           0        1.301941   -1.436830    0.000000
      5          6           0        0.075907   -2.166210    0.000000
      6          7           0       -1.076847   -1.578182    0.000000
      7          1           0        0.053209   -3.247040    0.000000
      8         16           0       -0.204390    2.240665    0.000000
      9          1           0       -1.988876    0.178702    0.000000
     10          1           0        2.241847   -1.972625    0.000000
     11          1           0        2.155779    0.522600    0.000000
 ---------------------------------------------------------------------
 Rotational constants (GHZ):           5.9018673           1.6972436           1.3181682

 -------------------------------------------------------------------------------
 -------------------- FREQUENCIES AND ROTATIONAL CONSTANTS ----------------------
 -------------------------------------------------------------------------------
 INDEX NO. DOF TYPE  CM-1(UNSCALED)  CM-1(SCALED BY ) SYMMETRY IR-INTENSITY
    1        vib         147.83           0.00              A"        1.0380
    2        vib         311.40           0.00              A'        4.0735
    3        vib         369.24           0.00              A"        1.6533
    4        vib         468.12           0.00              A'       10.8309
    5        vib         506.45           0.00              A"        6.9272
    6        vib         632.38           0.00              A'        5.9123
    7        vib         736.26           0.00              A"        6.3073
    8        vib         770.67           0.00              A'        5.8864
    9        vib         789.80           0.00              A"       82.6958
   10        vib         844.19           0.00              A"        3.4376
   11        vib         950.53           0.00              A"        0.2674
   12        vib        1029.92           0.00              A'       49.3626
   13        vib        1044.20           0.00              A"        0.0008
   14        vib        1044.73           0.00              A'        9.1304
   15        vib        1117.32           0.00              A'       84.5969
   16        vib        1193.74           0.00              A'       11.8632
```

| | | | | | |
|---|---|---|---|---|---|
| 17 | vib | 1228.60 | 0.00 | A' | 150.7407 |
| 18 | vib | 1309.42 | 0.00 | A' | 77.7520 |
| 19 | vib | 1402.73 | 0.00 | A' | 4.5970 |
| 20 | vib | 1419.65 | 0.00 | A' | 1.6399 |
| 21 | vib | 1516.21 | 0.00 | A' | 79.9953 |
| 22 | vib | 1620.97 | 0.00 | A' | 161.2372 |
| 23 | vib | 1690.81 | 0.00 | A' | 38.1856 |
| 24 | vib | 3223.58 | 0.00 | A' | 1.7443 |
| 25 | vib | 3239.53 | 0.00 | A' | 0.6267 |
| 26 | vib | 3251.85 | 0.00 | A' | 0.9260 |
| 27 | vib | 3585.89 | 0.00 | A' | 77.2030 |
| 28 | rot | 0.1968651 | - | | |
| 29 | rot | 0.0566140 | - | | |
| 30 | rot | 0.0439694 | - | | |

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---------- ZPE & THERMAL CONTRIBUTIONS ----------
---

Eelectronic [kJ/mol] = -1739334.285
Ezpe [kJ/mol] = +212.014
Eelectronic+Ezpe [kJ/mol] = -1739122.271

Eelectronic [hartrees] = -662.477351
Ezpe [hartrees] = +0.080752
Eelectronic+Ezpe [hartrees] = -662.396599

Thermal Correction to Energy [kJ/mol] = +226.195
Thermal Correction to Enthalpy [kJ/mol] = +228.673
Thermal Correction to Gibbs [kJ/mol] = +133.832

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GAUSSIAN OUTPUT FILENAME: NNSH-m062x.log
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1)LEVEL OF THEORY: OPT=VTIGHT
Charge = 0 Multiplicity = 1 Stoichiometry C4H4N2S

---
---------- OPTIMIZED GEOMETRY ----------
---

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 1.235528 | -0.197855 | 0.000000 |
| 2 | 7 | 0 | -1.160456 | -0.181731 | -0.000000 |
| 3 | 6 | 0 | 0.000000 | 0.460026 | -0.000000 |
| 4 | 6 | 0 | 1.203631 | -1.566637 | 0.000000 |
| 5 | 6 | 0 | -0.049217 | -2.180185 | 0.000000 |
| 6 | 7 | 0 | -1.182623 | -1.501559 | -0.000000 |
| 7 | 1 | 0 | -0.153864 | -3.257514 | 0.000000 |
| 8 | 16 | 0 | -0.042327 | 2.216929 | -0.000000 |
| 9 | 1 | 0 | -1.379411 | 2.273676 | -0.000000 |
| 10 | 1 | 0 | 2.110211 | -2.156669 | 0.000000 |
| 11 | 1 | 0 | 2.162198 | 0.360586 | 0.000000 |

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Rotational constants (GHZ): 5.9353891 1.6874750 1.3139183

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---------- FREQUENCIES AND ROTATIONAL CONSTANTS ----------
---

| INDEX NO. | DOF TYPE | CM-1(UNSCALED) | CM-1(SCALED BY ) | SYMMETRY | IR-INTENSITY |
|---|---|---|---|---|---|
| 1 | vib | 176.81 | 0.00 | A" | 1.4020 |
| 2 | vib | 280.23 | 0.00 | A' | 8.5472 |
| 3 | vib | 298.90 | 0.00 | A" | 22.2969 |
| 4 | vib | 384.66 | 0.00 | A" | 0.1840 |

```
    5        vib         439.44           0.00              A'        0.4695
    6        vib         499.18           0.00              A"        0.5151
    7        vib         641.89           0.00              A'        0.1171
    8        vib         761.79           0.00              A'       11.1047
    9        vib         777.25           0.00              A"        9.1083
   10        vib         829.13           0.00              A"       26.0279
   11        vib         911.79           0.00              A'        9.8251
   12        vib         967.49           0.00              A"        0.0097
   13        vib        1028.66           0.00              A"        0.0457
   14        vib        1042.60           0.00              A'        4.5978
   15        vib        1072.69           0.00              A'        2.3147
   16        vib        1123.75           0.00              A'       24.5229
   17        vib        1180.81           0.00              A'       48.9611
   18        vib        1184.67           0.00              A'        1.8022
   19        vib        1239.11           0.00              A'       25.6091
   20        vib        1439.52           0.00              A'       28.5083
   21        vib        1464.25           0.00              A'       58.1258
   22        vib        1621.40           0.00              A'        0.5135
   23        vib        1650.39           0.00              A'       39.6660
   24        vib        2739.18           0.00              A'        8.3515
   25        vib        3215.32           0.00              A'        0.3208
   26        vib        3223.85           0.00              A'        3.1603
   27        vib        3237.45           0.00              A'        3.2594
   28        rot      0.1979833           -
   29        rot      0.0562881           -
   30        rot      0.0438276           -
 ---------------------------------------------------------------------------

 ---------------------------------------------------------------------------
 ----------------------- ZPE & THERMAL CONTRIBUTIONS -----------------------
 ---------------------------------------------------------------------------
 Eelectronic                    [kJ/mol]   = -1739301.081
 Ezpe                           [kJ/mol]   = +199.969
 Eelectronic+Ezpe               [kJ/mol]   = -1739101.112

 Eelectronic                    [hartrees] = -662.464704
 Ezpe                           [hartrees] = +0.076164
 Eelectronic+Ezpe               [hartrees] = -662.388540

 Thermal Correction to Energy   [kJ/mol]   = +215.144
 Thermal Correction to Enthalpy [kJ/mol]   = +217.622
 Thermal Correction to Gibbs    [kJ/mol]   = +121.314
 ---------------------------------------------------------------------------

!+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
 END OF GAUSSIAN OUTPUT FILENAME: NNSH-m062x.log
!+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++


!+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
 GAUSSIAN OUTPUT FILENAME: NNSH-NNHS-H2O-TS-d3bj.log
!+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++

 1)LEVEL OF THEORY: B3LYP/DEF2TZVP
 Charge = 0 Multiplicity = 1  Stoichiometry    C4H6N2OS

 ---------------------------------------------------------------------
 ---------------------- OPTIMIZED GEOMETRY ---------------------------
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          6           0       -2.337900    0.743744    0.001084
      2          7           0       -1.236018    1.464219   -0.014384
      3          7           0       -0.067021    0.841168   -0.017910
      4          6           0        0.060434   -0.503120   -0.000940
      5         16           0        1.641580   -1.211825   -0.005267
      6          6           0       -1.111336   -1.294012    0.015407
      7          6           0       -2.321371   -0.660511    0.015421
      8          1           0       -3.263599    1.303938    0.002188
      9          1           0        1.191171    1.482357   -0.033519
     10          8           0        2.311346    1.521667   -0.076732
```

```
    11          1           0        2.659148    1.874987    0.752353
    12          1           0        2.311039    0.288591   -0.035850
    13          1           0       -3.249152   -1.217380    0.026462
    14          1           0       -1.022338   -2.370936    0.026723
 -------------------------------------------------------------------
 Rotational constants (GHZ):           2.9069462           1.3453621           0.9219276

 --------------------------------------------------------------------------------
 -------------------- FREQUENCIES AND ROTATIONAL CONSTANTS ----------------------
 --------------------------------------------------------------------------------
 INDEX NO. DOF TYPE  CM-1(UNSCALED)  CM-1(SCALED BY ) SYMMETRY IR-INTENSITY
    1        vib       -1297.78           0.00                A      544.2205
    2        vib          94.07           0.00                A        8.1191
    3        vib         167.85           0.00                A        1.0414
    4        vib         281.27           0.00                A       44.8230
    5        vib         387.63           0.00                A        1.8727
    6        vib         393.25           0.00                A       55.3269
    7        vib         438.79           0.00                A        8.1720
    8        vib         468.75           0.00                A       50.9676
    9        vib         492.58           0.00                A      102.2588
   10        vib         509.76           0.00                A        9.4765
   11        vib         596.43           0.00                A       65.1954
   12        vib         675.64           0.00                A       10.0207
   13        vib         765.01           0.00                A       11.4023
   14        vib         766.10           0.00                A       18.9896
   15        vib         821.02           0.00                A       29.2511
   16        vib         941.60           0.00                A        0.0305
   17        vib        1016.93           0.00                A        0.1251
   18        vib        1051.18           0.00                A      217.9944
   19        vib        1055.16           0.00                A       28.8746
   20        vib        1112.81           0.00                A      126.6240
   21        vib        1163.25           0.00                A       78.4705
   22        vib        1181.76           0.00                A       32.4548
   23        vib        1212.27           0.00                A      680.6125
   24        vib        1246.10           0.00                A      458.2369
   25        vib        1258.93           0.00                A     1252.0023
   26        vib        1389.38           0.00                A      240.8980
   27        vib        1449.73           0.00                A      286.6804
   28        vib        1460.63           0.00                A      755.1771
   29        vib        1541.53           0.00                A      125.2013
   30        vib        1566.36           0.00                A       17.7242
   31        vib        1628.69           0.00                A       66.9933
   32        vib        1914.09           0.00                A      730.7416
   33        vib        3182.96           0.00                A        1.6956
   34        vib        3196.63           0.00                A        7.9473
   35        vib        3210.57           0.00                A        2.1760
   36        vib        3792.16           0.00                A       61.6777
   37        rot      0.0969653           -
   38        rot      0.0448764           -
   39        rot      0.0307522           -
 --------------------------------------------------------------------------------

 --------------------------------------------------------------------------------
 ------------------------ ZPE & THERMAL CONTRIBUTIONS ---------------------------
 --------------------------------------------------------------------------------
 Eelectronic                    [kJ/mol]   = -1940502.327
 Ezpe                           [kJ/mol]   = +253.794
 Eelectronic+Ezpe               [kJ/mol]   = -1940248.533

 Eelectronic                    [hartrees] = -739.098201
 Ezpe                           [hartrees] = +0.096665
 Eelectronic+Ezpe               [hartrees] = -739.001536

 Thermal Correction to Energy   [kJ/mol]   = +272.309
 Thermal Correction to Enthalpy [kJ/mol]   = +274.790
 Thermal Correction to Gibbs    [kJ/mol]   = +170.046
 --------------------------------------------------------------------------------

!+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
 END OF GAUSSIAN OUTPUT FILENAME: NNSH-NNHS-H2O-TS-d3bj.log
!+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
```

!+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
GAUSSIAN OUTPUT FILENAME: NSU3-dimer-reactant-qb3.log
!+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++

1)LEVEL OF THEORY: CBS-QB3
Charge = 0 Multiplicity = 1  Stoichiometry  C6H6N6O2S2

---

---------- OPTIMIZED GEOMETRY ----------

---

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 7 | 0 | 0.466742 | 1.772637 | 0.000045 |
| 2 | 7 | 0 | 2.680555 | 2.499203 | -0.000054 |
| 3 | 6 | 0 | 1.742230 | 1.507871 | 0.000013 |
| 4 | 6 | 0 | 0.045497 | 3.104122 | 0.000009 |
| 5 | 6 | 0 | 1.127439 | 4.111979 | -0.000063 |
| 6 | 7 | 0 | 2.382499 | 3.819735 | -0.000090 |
| 7 | 1 | 0 | 0.864271 | 5.163389 | -0.000092 |
| 8 | 16 | 0 | 2.382499 | -0.128940 | 0.000055 |
| 9 | 1 | 0 | 1.149901 | -0.736682 | 0.000110 |
| 10 | 8 | 0 | -1.132596 | 3.408121 | 0.000014 |
| 11 | 1 | 0 | 3.667713 | 2.289341 | -0.000075 |
| 12 | 7 | 0 | -0.466742 | -1.772637 | 0.000045 |
| 13 | 7 | 0 | -2.680555 | -2.499203 | -0.000054 |
| 14 | 6 | 0 | -1.742230 | -1.507871 | 0.000013 |
| 15 | 6 | 0 | -0.045497 | -3.104122 | 0.000009 |
| 16 | 6 | 0 | -1.127439 | -4.111979 | -0.000063 |
| 17 | 7 | 0 | -2.382499 | -3.819735 | -0.000090 |
| 18 | 1 | 0 | -0.864271 | -5.163389 | -0.000092 |
| 19 | 16 | 0 | -2.382499 | 0.128940 | 0.000055 |
| 20 | 1 | 0 | -1.149901 | 0.736682 | 0.000110 |
| 21 | 8 | 0 | 1.132596 | -3.408121 | 0.000014 |
| 22 | 1 | 0 | -3.667713 | -2.289341 | -0.000075 |

---

Rotational constants (GHZ): 0.7619320 0.2473812 0.1867484

---

---------- FREQUENCIES AND ROTATIONAL CONSTANTS ----------

---

| INDEX NO. | DOF TYPE | CM-1(UNSCALED) | CM-1(SCALED BY 0.99) | SYMMETRY | IR-INTENSITY |
|---|---|---|---|---|---|
| 1 | vib | 25.25 | 24.99 | A | 0.7224 |
| 2 | vib | 36.54 | 36.17 | A | 7.5956 |
| 3 | vib | 60.43 | 59.83 | B | 0.0000 |
| 4 | vib | 76.46 | 75.70 | B | 23.3149 |
| 5 | vib | 76.59 | 75.82 | A | 0.0000 |
| 6 | vib | 96.95 | 95.98 | A | 0.0000 |
| 7 | vib | 112.62 | 111.49 | B | 0.0000 |
| 8 | vib | 117.45 | 116.27 | A | 0.3764 |
| 9 | vib | 161.24 | 159.63 | A | 0.2877 |
| 10 | vib | 169.75 | 168.05 | B | 0.0000 |
| 11 | vib | 265.96 | 263.30 | A | 0.0000 |
| 12 | vib | 280.89 | 278.08 | B | 5.9411 |
| 13 | vib | 413.99 | 409.85 | A | 0.0000 |
| 14 | vib | 418.06 | 413.88 | B | 8.1942 |
| 15 | vib | 430.42 | 426.12 | B | 0.0000 |
| 16 | vib | 430.60 | 426.29 | A | 0.0055 |
| 17 | vib | 495.73 | 490.77 | A | 0.0000 |
| 18 | vib | 498.32 | 493.34 | B | 9.4197 |
| 19 | vib | 535.33 | 529.97 | B | 0.0000 |
| 20 | vib | 569.07 | 563.38 | A | 206.5087 |
| 21 | vib | 579.03 | 573.24 | A | 0.0000 |
| 22 | vib | 583.93 | 578.09 | B | 36.2658 |
| 23 | vib | 623.24 | 617.00 | A | 1.9574 |
| 24 | vib | 623.73 | 617.50 | B | 0.0000 |
| 25 | vib | 663.88 | 657.24 | A | 28.2393 |
| 26 | vib | 664.20 | 657.56 | B | 0.0000 |
| 27 | vib | 699.33 | 692.34 | B | 7.6291 |
| 28 | vib | 700.97 | 693.96 | A | 0.0000 |
| 29 | vib | 774.18 | 766.44 | B | 0.0000 |

```
  30        vib         776.31         768.54                A        0.9056
  31        vib         908.64         899.56                A        0.0000
  32        vib         917.54         908.36                B        7.9970
  33        vib         925.02         915.77                B        0.0000
  34        vib         925.03         915.78                A       30.2121
  35        vib        1008.31         998.22                A        0.0000
  36        vib        1008.34         998.25                B      107.1077
  37        vib        1038.04        1027.66                B       95.1879
  38        vib        1038.28        1027.90                A        0.0000
  39        vib        1102.98        1091.95                B       19.2218
  40        vib        1118.92        1107.73                A        0.0000
  41        vib        1175.97        1164.21                B       72.2511
  42        vib        1176.60        1164.84                A        0.0000
  43        vib        1292.24        1279.32                B      306.4616
  44        vib        1293.45        1280.51                A        0.0000
  45        vib        1354.39        1340.85                A        0.0000
  46        vib        1354.43        1340.89                B      197.5534
  47        vib        1467.55        1452.87                B      397.3180
  48        vib        1468.01        1453.33                A        0.0000
  49        vib        1541.69        1526.28                A        0.0000
  50        vib        1585.91        1570.05                B      632.7527
  51        vib        1649.00        1632.51                A        0.0000
  52        vib        1649.13        1632.64                B       22.6574
  53        vib        1750.38        1732.88                A        0.0000
  54        vib        1750.64        1733.14                B      560.7695
  55        vib        2252.87        2230.34                A        0.0000
  56        vib        2306.19        2283.13                B     2537.5404
  57        vib        3191.86        3159.94                B        4.0361
  58        vib        3191.88        3159.96                A        0.0000
  59        vib        3621.84        3585.63                B      209.3348
  60        vib        3622.06        3585.84                A        0.0000
  61        rot      0.0254153              -
  62        rot      0.0082517              -
  63        rot      0.0062293              -
 --------------------------------------------------------------------------------

 --------------------------------------------------------------------------------
 ------------------------ ZPE & THERMAL CONTRIBUTIONS ---------------------------
 --------------------------------------------------------------------------------
 Eelectronic                    [kJ/mol]   = -3958666.426
 Ezpe                           [kJ/mol]   = +362.752
 Eelectronic+Ezpe               [kJ/mol]   = -3958303.674

 Eelectronic                    [hartrees] = -1507.776205
 Ezpe                           [hartrees] = +0.138165
 Eelectronic+Ezpe               [hartrees] = -1507.638040

 Thermal Correction to Energy   [kJ/mol]   = +402.166
 Thermal Correction to Enthalpy [kJ/mol]   = +404.645
 Thermal Correction to Gibbs    [kJ/mol]   = +245.731
 --------------------------------------------------------------------------------

 --------------------------------------------------------------------------------
 ------------------------------ ENERGETICS --------------------------------------
 --------------------------------------------------------------------------------
 Temperature=              298.150000
 E(ZPE)=                     0.136784 E(Thermal)=                     0.151901
 E(SCF)=                 -1502.372794 DE(MP2)=                       -2.912395
 DE(CBS)=                   -0.287627 DE(MP34)=                      -0.063511
 DE(CCSD)=                  -0.103441 DE(Int)=                        0.094654
 DE(Empirical)=             -0.127469
 CBS-QB3 (0 K)=          -1505.635799 CBS-QB3 Energy=             -1505.620682
 CBS-QB3 Enthalpy=       -1505.619738 CBS-QB3 Free Energy=        -1505.680494
 --------------------------------------------------------------------------------
!++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
 END OF GAUSSIAN OUTPUT FILENAME: NSU3-dimer-reactant-qb3.log
!++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++


!++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
 GAUSSIAN OUTPUT FILENAME: NSU3-dimer-reactant-v2.log
!++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
```

1)LEVEL OF THEORY: B3LYP/DEF2TZVP
Charge = 0 Multiplicity = 1  Stoichiometry  C6H6N6O2S2

---
---------- OPTIMIZED GEOMETRY ----------
---

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 7 | 0 | 0.362057 | -1.770087 | 0.000000 |
| 2 | 7 | 0 | -1.313978 | -3.377237 | 0.000000 |
| 3 | 6 | 0 | -0.902430 | -2.081136 | 0.000000 |
| 4 | 6 | 0 | 1.313978 | -2.781673 | 0.000000 |
| 5 | 6 | 0 | 0.781104 | -4.156024 | 0.000000 |
| 6 | 7 | 0 | -0.474064 | -4.431928 | 0.000000 |
| 7 | 1 | 0 | 1.472455 | -4.988655 | 0.000000 |
| 8 | 16 | 0 | -2.177625 | -0.891646 | 0.000000 |
| 9 | 1 | 0 | -1.326473 | 0.193049 | 0.000000 |
| 10 | 8 | 0 | 2.507274 | -2.543304 | 0.000000 |
| 11 | 1 | 0 | -2.293353 | -3.613360 | 0.000000 |
| 12 | 7 | 0 | -0.362057 | 1.770087 | 0.000000 |
| 13 | 7 | 0 | 1.313978 | 3.377237 | 0.000000 |
| 14 | 6 | 0 | 0.902430 | 2.081136 | 0.000000 |
| 15 | 6 | 0 | -1.313978 | 2.781673 | 0.000000 |
| 16 | 6 | 0 | -0.781104 | 4.156024 | 0.000000 |
| 17 | 7 | 0 | 0.474064 | 4.431928 | 0.000000 |
| 18 | 1 | 0 | -1.472455 | 4.988655 | 0.000000 |
| 19 | 16 | 0 | 2.177625 | 0.891646 | 0.000000 |
| 20 | 1 | 0 | 1.326473 | -0.193049 | 0.000000 |
| 21 | 8 | 0 | -2.507274 | 2.543304 | 0.000000 |
| 22 | 1 | 0 | 2.293353 | 3.613360 | 0.000000 |

---
Rotational constants (GHZ):  0.7704707  0.2531149  0.1905240

---
---------- FREQUENCIES AND ROTATIONAL CONSTANTS ----------
---

| INDEX NO. | DOF TYPE | CM-1(UNSCALED) | CM-1(SCALED BY ) | SYMMETRY | IR-INTENSITY |
|---|---|---|---|---|---|
| 1 | vib | 23.31 | 0.00 | AU | 0.4876 |
| 2 | vib | 32.42 | 0.00 | AU | 8.0019 |
| 3 | vib | 57.79 | 0.00 | BG | 0.0000 |
| 4 | vib | 79.38 | 0.00 | AG | 0.0000 |
| 5 | vib | 81.93 | 0.00 | BU | 26.5209 |
| 6 | vib | 101.27 | 0.00 | AG | 0.0000 |
| 7 | vib | 114.43 | 0.00 | BG | 0.0000 |
| 8 | vib | 117.99 | 0.00 | AU | 0.5569 |
| 9 | vib | 160.74 | 0.00 | AU | 0.2945 |
| 10 | vib | 169.99 | 0.00 | BG | 0.0000 |
| 11 | vib | 269.21 | 0.00 | AG | 0.0000 |
| 12 | vib | 289.12 | 0.00 | BU | 8.4382 |
| 13 | vib | 422.39 | 0.00 | AG | 0.0000 |
| 14 | vib | 427.01 | 0.00 | BU | 7.2054 |
| 15 | vib | 429.17 | 0.00 | AU | 0.2161 |
| 16 | vib | 430.03 | 0.00 | BG | 0.0000 |
| 17 | vib | 500.68 | 0.00 | AG | 0.0000 |
| 18 | vib | 503.77 | 0.00 | BU | 9.6297 |
| 19 | vib | 548.86 | 0.00 | BG | 0.0000 |
| 20 | vib | 575.87 | 0.00 | AU | 186.3447 |
| 21 | vib | 582.77 | 0.00 | AG | 0.0000 |
| 22 | vib | 587.63 | 0.00 | BU | 37.1373 |
| 23 | vib | 639.30 | 0.00 | BG | 0.0000 |
| 24 | vib | 641.89 | 0.00 | AU | 1.3019 |
| 25 | vib | 672.20 | 0.00 | AU | 14.8583 |
| 26 | vib | 672.54 | 0.00 | BG | 0.0000 |
| 27 | vib | 702.88 | 0.00 | BU | 7.4803 |
| 28 | vib | 705.12 | 0.00 | AG | 0.0000 |
| 29 | vib | 781.76 | 0.00 | BG | 0.0000 |
| 30 | vib | 783.43 | 0.00 | AU | 0.0552 |
| 31 | vib | 921.04 | 0.00 | AG | 0.0000 |
| 32 | vib | 930.48 | 0.00 | BU | 9.5765 |
| 33 | vib | 932.56 | 0.00 | AU | 28.6715 |

```
  34        vib         932.61           0.00              BG        0.0000
  35        vib        1024.12           0.00              AG        0.0000
  36        vib        1026.28           0.00              BU       79.6837
  37        vib        1045.99           0.00              BU      122.7786
  38        vib        1046.12           0.00              AG        0.0000
  39        vib        1110.23           0.00              BU       30.3189
  40        vib        1128.38           0.00              AG        0.0000
  41        vib        1189.99           0.00              BU       73.0037
  42        vib        1191.20           0.00              AG        0.0000
  43        vib        1300.82           0.00              BU      291.2843
  44        vib        1302.24           0.00              AG        0.0000
  45        vib        1362.08           0.00              AG        0.0000
  46        vib        1362.36           0.00              BU      187.7720
  47        vib        1463.88           0.00              AG        0.0000
  48        vib        1464.61           0.00              BU      423.1387
  49        vib        1535.21           0.00              AG        0.0000
  50        vib        1583.34           0.00              BU      640.2495
  51        vib        1649.68           0.00              AG        0.0000
  52        vib        1649.76           0.00              BU       19.7135
  53        vib        1735.61           0.00              BU      556.3851
  54        vib        1735.78           0.00              AG        0.0000
  55        vib        2175.34           0.00              AG        0.0000
  56        vib        2243.93           0.00              BU     3093.8182
  57        vib        3197.82           0.00              BU        2.6832
  58        vib        3197.84           0.00              AG        0.0000
  59        vib        3611.86           0.00              BU      207.9579
  60        vib        3612.09           0.00              AG        0.0000
  61        rot      0.0257001           -
  62        rot      0.0084430           -
  63        rot      0.0063552           -
 ---------------------------------------------------------------------------

 ---------------------------------------------------------------------------
 ------------------------ ZPE & THERMAL CONTRIBUTIONS ----------------------
 ---------------------------------------------------------------------------
 Eelectronic                    [kJ/mol]   = -3959072.208
 Ezpe                           [kJ/mol]   = +363.474
 Eelectronic+Ezpe               [kJ/mol]   = -3958708.734

 Eelectronic                    [hartrees] = -1507.930759
 Ezpe                           [hartrees] = +0.138440
 Eelectronic+Ezpe               [hartrees] = -1507.792319

 Thermal Correction to Energy   [kJ/mol]   = +402.586
 Thermal Correction to Enthalpy [kJ/mol]   = +405.065
 Thermal Correction to Gibbs    [kJ/mol]   = +246.458
 ---------------------------------------------------------------------------

!+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
 END OF GAUSSIAN OUTPUT FILENAME: NSU3-dimer-reactant-v2.log
!+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++


!+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
 GAUSSIAN OUTPUT FILENAME: NSU3-NSU1-H2O-TS-d3bj.log
!+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++

 1)LEVEL OF THEORY: B3LYP/DEF2TZVP
 Charge = 0 Multiplicity = 1  Stoichiometry    C3H5N3O2S

 ---------------------------------------------------------------------
 ---------------------- OPTIMIZED GEOMETRY ---------------------------
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          6           0       -2.292754   -0.345620   -0.005600
      2          6           0       -1.462188    0.874415   -0.003064
      3          7           0       -0.093101    0.647626   -0.012823
      4          6           0        0.385914   -0.584033    0.000729
      5         16           0        2.080341   -0.927764    0.002124
      6          7           0       -0.467773   -1.639840    0.013205
```

```
     7          7          0       -1.812870   -1.536809    0.004177
     8          1          0       -3.369852   -0.242445   -0.012782
     9          1          0        1.058078    1.653084   -0.055023
    10          8          0        2.097132    1.887387   -0.092520
    11          1          0        2.343850    2.338015    0.726382
    12          1          0        2.369046    0.685535   -0.031514
    13          8          0       -1.940855    1.990678    0.009461
    14          1          0       -0.106421   -2.579897    0.019126
---------------------------------------------------------------------
Rotational constants (GHZ):           1.9834694           1.1654198           0.7355062

--------------------------------------------------------------------------------
-------------------- FREQUENCIES AND ROTATIONAL CONSTANTS ----------------------
--------------------------------------------------------------------------------
INDEX NO. DOF TYPE  CM-1(UNSCALED)  CM-1(SCALED BY ) SYMMETRY IR-INTENSITY
   1        vib        -969.84           0.00                A     1217.0229
   2        vib          76.39           0.00                A        8.1570
   3        vib         134.78           0.00                A        0.3643
   4        vib         158.11           0.00                A        1.5101
   5        vib         226.65           0.00                A       36.0192
   6        vib         375.86           0.00                A       87.2371
   7        vib         432.73           0.00                A        7.3904
   8        vib         434.64           0.00                A        7.9701
   9        vib         457.49           0.00                A        1.1608
  10        vib         475.34           0.00                A      114.1813
  11        vib         549.11           0.00                A       64.5589
  12        vib         557.91           0.00                A       53.4563
  13        vib         590.68           0.00                A       21.8020
  14        vib         621.03           0.00                A       82.6462
  15        vib         675.18           0.00                A       10.6300
  16        vib         711.83           0.00                A       11.3857
  17        vib         779.82           0.00                A        1.1054
  18        vib         929.60           0.00                A       15.5803
  19        vib         946.95           0.00                A       94.3287
  20        vib        1053.05           0.00                A       18.1015
  21        vib        1076.56           0.00                A      247.0170
  22        vib        1093.55           0.00                A       97.2059
  23        vib        1195.76           0.00                A       63.0287
  24        vib        1224.18           0.00                A      390.6136
  25        vib        1310.37           0.00                A      170.1880
  26        vib        1363.30           0.00                A      135.3599
  27        vib        1430.02           0.00                A      389.8095
  28        vib        1524.23           0.00                A      160.2949
  29        vib        1567.76           0.00                A      348.9461
  30        vib        1628.69           0.00                A      349.0989
  31        vib        1649.90           0.00                A        0.4906
  32        vib        1758.57           0.00                A      505.7405
  33        vib        2269.49           0.00                A     1777.1775
  34        vib        3200.28           0.00                A        0.7798
  35        vib        3618.87           0.00                A      100.2714
  36        vib        3788.05           0.00                A       86.5329
  37        rot      0.0661614           -
  38        rot      0.0388742           -
  39        rot      0.0245338           -
--------------------------------------------------------------------------------

--------------------------------------------------------------------------------
------------------------ ZPE & THERMAL CONTRIBUTIONS ---------------------------
--------------------------------------------------------------------------------
Eelectronic                    [kJ/mol]   = -2180282.988
Ezpe                           [kJ/mol]   = +238.577
Eelectronic+Ezpe               [kJ/mol]   = -2180044.411

Eelectronic                    [hartrees] = -830.425819
Ezpe                           [hartrees] = +0.090869
Eelectronic+Ezpe               [hartrees] = -830.334950

Thermal Correction to Energy   [kJ/mol]   = +259.783
Thermal Correction to Enthalpy [kJ/mol]   = +262.261
Thermal Correction to Gibbs    [kJ/mol]   = +150.601
--------------------------------------------------------------------------------
```

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END OF GAUSSIAN OUTPUT FILENAME: NSU3-NSU1-H2O-TS-d3bj.log
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GAUSSIAN OUTPUT FILENAME: NSU3-NSU1-m062x-product.log
!+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++

1)LEVEL OF THEORY: M062X/DEF2TZVP
Charge = 0 Multiplicity = 1  Stoichiometry    C3H3N3OS

---

---------- OPTIMIZED GEOMETRY ----------

---

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 7 | 0 | -0.896150 | -0.173280 | 0.000000 |
| 2 | 7 | 0 | 1.298217 | 0.438817 | -0.000000 |
| 3 | 6 | 0 | 0.000000 | 0.860295 | 0.000000 |
| 4 | 6 | 0 | -0.580639 | -1.525823 | 0.000000 |
| 5 | 6 | 0 | 0.872963 | -1.766757 | -0.000000 |
| 6 | 7 | 0 | 1.738023 | -0.826367 | -0.000000 |
| 7 | 1 | 0 | 1.225580 | -2.788410 | -0.000000 |
| 8 | 16 | 0 | -0.419805 | 2.447262 | 0.000000 |
| 9 | 1 | 0 | -1.877194 | 0.076817 | 0.000000 |
| 10 | 8 | 0 | -1.422213 | -2.384549 | 0.000000 |
| 11 | 1 | 0 | 2.011615 | 1.151312 | -0.000000 |

---

Rotational constants (GHZ):  3.6773322  1.3349671  0.9794143

---

---------- FREQUENCIES AND ROTATIONAL CONSTANTS ----------

---

| INDEX NO. | DOF TYPE | CM-1(UNSCALED) | CM-1(SCALED BY ) | SYMMETRY | IR-INTENSITY |
|---|---|---|---|---|---|
| 1 | vib | 133.58 | 0.00 | A" | 2.0403 |
| 2 | vib | 157.32 | 0.00 | A" | 2.1971 |
| 3 | vib | 274.61 | 0.00 | A' | 10.0471 |
| 4 | vib | 427.77 | 0.00 | A" | 0.0900 |
| 5 | vib | 463.97 | 0.00 | A' | 8.3378 |
| 6 | vib | 488.19 | 0.00 | A' | 19.1347 |
| 7 | vib | 553.67 | 0.00 | A' | 22.8511 |
| 8 | vib | 653.66 | 0.00 | A" | 6.5300 |
| 9 | vib | 671.01 | 0.00 | A" | 27.9991 |
| 10 | vib | 705.32 | 0.00 | A' | 11.6462 |
| 11 | vib | 735.64 | 0.00 | A" | 102.0172 |
| 12 | vib | 782.31 | 0.00 | A" | 22.4422 |
| 13 | vib | 920.43 | 0.00 | A" | 17.3069 |
| 14 | vib | 950.98 | 0.00 | A' | 7.6515 |
| 15 | vib | 1042.99 | 0.00 | A' | 22.5244 |
| 16 | vib | 1114.48 | 0.00 | A' | 26.7624 |
| 17 | vib | 1201.25 | 0.00 | A' | 267.6497 |
| 18 | vib | 1274.75 | 0.00 | A' | 44.3711 |
| 19 | vib | 1361.71 | 0.00 | A' | 45.9187 |
| 20 | vib | 1417.42 | 0.00 | A' | 51.5196 |
| 21 | vib | 1439.76 | 0.00 | A' | 120.6659 |
| 22 | vib | 1566.61 | 0.00 | A' | 663.9610 |
| 23 | vib | 1693.92 | 0.00 | A' | 10.8840 |
| 24 | vib | 1850.05 | 0.00 | A' | 583.5974 |
| 25 | vib | 3246.89 | 0.00 | A' | 2.2202 |
| 26 | vib | 3594.33 | 0.00 | A' | 80.4090 |
| 27 | vib | 3644.98 | 0.00 | A' | 116.9276 |
| 28 | rot | 0.1226626 | - | | |
| 29 | rot | 0.0445297 | - | | |
| 30 | rot | 0.0326697 | - | | |

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---------- ZPE & THERMAL CONTRIBUTIONS ----------

---

Eelectronic  [kJ/mol]  = -1979058.296

```
 Ezpe                             [kJ/mol]   = +193.602
 Eelectronic+Ezpe                 [kJ/mol]   = -1978864.694

 Eelectronic                      [hartrees] = -753.783392
 Ezpe                             [hartrees] = +0.073739
 Eelectronic+Ezpe                 [hartrees] = -753.709653

 Thermal Correction to Energy   [kJ/mol]   = +210.148
 Thermal Correction to Enthalpy [kJ/mol]   = +212.626
 Thermal Correction to Gibbs    [kJ/mol]   = +111.613
 --------------------------------------------------------------------------------

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 END OF GAUSSIAN OUTPUT FILENAME: NSU3-NSU1-m062x-product.log
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 GAUSSIAN OUTPUT FILENAME: NSU3-NSU1-m062x-reactant.log
!++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++

 1)LEVEL OF THEORY: M062X/DEF2TZVP
 Charge = 0 Multiplicity = 1  Stoichiometry    C3H3N3OS

 ---------------------------------------------------------------------
 ---------------------- OPTIMIZED GEOMETRY ---------------------------
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          7           0       -0.976664   -0.131198    0.000000
      2          7           0        1.306661    0.345939   -0.000000
      3          6           0       -0.000000    0.703387    0.000000
      4          6           0       -0.666425   -1.491953   -0.000000
      5          6           0        0.779973   -1.816914   -0.000000
      6          7           0        1.710063   -0.939219   -0.000000
      7          1           0        1.078394   -2.857387   -0.000000
      8         16           0       -0.277664    2.443696    0.000000
      9          1           0       -1.605661    2.287443    0.000000
     10          8           0       -1.505139   -2.356403   -0.000000
     11          1           0        2.049295    1.026262   -0.000000
 ---------------------------------------------------------------------
 Rotational constants (GHZ):           3.6877298           1.3253394           0.9749504

 --------------------------------------------------------------------------------
 -------------------- FREQUENCIES AND ROTATIONAL CONSTANTS ----------------------
 --------------------------------------------------------------------------------
 INDEX NO. DOF TYPE  CM-1(UNSCALED)  CM-1(SCALED BY ) SYMMETRY IR-INTENSITY
    1        vib         101.54           0.00               A"        0.0508
    2        vib         169.14           0.00               A"        0.0229
    3        vib         254.27           0.00               A'        5.4036
    4        vib         316.92           0.00               A"       39.5449
    5        vib         419.14           0.00               A'        3.5584
    6        vib         434.97           0.00               A"        1.2322
    7        vib         495.21           0.00               A'        3.5475
    8        vib         565.78           0.00               A"       78.0079
    9        vib         578.89           0.00               A'       12.5227
   10        vib         675.80           0.00               A"        8.4172
   11        vib         704.24           0.00               A'        9.4272
   12        vib         792.43           0.00               A"        0.1764
   13        vib         900.91           0.00               A'       20.4278
   14        vib         938.54           0.00               A'       13.1255
   15        vib         952.02           0.00               A"       14.7315
   16        vib        1044.47           0.00               A'       40.0870
   17        vib        1119.26           0.00               A'        2.2066
   18        vib        1197.25           0.00               A'       32.3306
   19        vib        1310.12           0.00               A'      127.4014
   20        vib        1377.07           0.00               A'       90.0961
   21        vib        1512.69           0.00               A'      192.4098
   22        vib        1620.56           0.00               A'      517.2372
   23        vib        1703.40           0.00               A'       20.3751
   24        vib        1827.00           0.00               A'      443.8853
```

| | | | | | |
|---|---|---|---|---|---|
| 25 | vib | 2751.67 | 0.00 | A' | 17.9463 |
| 26 | vib | 3230.66 | 0.00 | A' | 0.2377 |
| 27 | vib | 3644.90 | 0.00 | A' | 123.9765 |
| 28 | rot | 0.1230094 | - | | |
| 29 | rot | 0.0442086 | - | | |
| 30 | rot | 0.0325208 | - | | |

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---------- ZPE & THERMAL CONTRIBUTIONS ----------
---

Eelectronic [kJ/mol] = -1978988.912
Ezpe [kJ/mol] = +183.260
Eelectronic+Ezpe [kJ/mol] = -1978805.652

Eelectronic [hartrees] = -753.756965
Ezpe [hartrees] = +0.069800
Eelectronic+Ezpe [hartrees] = -753.687165

Thermal Correction to Energy [kJ/mol] = +201.016
Thermal Correction to Enthalpy [kJ/mol] = +203.495
Thermal Correction to Gibbs [kJ/mol] = +100.137

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END OF GAUSSIAN OUTPUT FILENAME: NSU3-NSU1-m062x-reactant.log
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GAUSSIAN OUTPUT FILENAME: NSU3-qb3.log
!++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++

1)LEVEL OF THEORY: CBS-QB3
Charge = 0 Multiplicity = 1 Stoichiometry C3H3N3OS

---
---------- OPTIMIZED GEOMETRY ----------
---

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 7 | 0 | 0.157265 | -0.972148 | -0.000003 |
| 2 | 7 | 0 | -0.375807 | 1.308953 | 0.000064 |
| 3 | 6 | 0 | -0.704295 | -0.014915 | -0.000004 |
| 4 | 6 | 0 | 1.521488 | -0.632765 | 0.000139 |
| 5 | 6 | 0 | 1.808710 | 0.823169 | 0.000068 |
| 6 | 7 | 0 | 0.908959 | 1.745150 | 0.000083 |
| 7 | 1 | 0 | 2.843192 | 1.147689 | 0.000033 |
| 8 | 16 | 0 | -2.458516 | -0.341301 | -0.000085 |
| 9 | 1 | 0 | -2.269209 | -1.670343 | -0.000143 |
| 10 | 8 | 0 | 2.405388 | -1.460589 | -0.000104 |
| 11 | 1 | 0 | -1.069181 | 2.041562 | 0.000073 |

---

Rotational constants (GHZ): 3.6387674 1.3050257 0.9605347

---
---------- FREQUENCIES AND ROTATIONAL CONSTANTS ----------
---

| INDEX NO. | DOF | TYPE | CM-1(UNSCALED) | CM-1(SCALED BY 0.99) | SYMMETRY | IR-INTENSITY |
|---|---|---|---|---|---|---|
| 1 | vib | | 91.91 | 90.99 | A | 0.0344 |
| 2 | vib | | 160.55 | 158.95 | A | 0.5822 |
| 3 | vib | | 226.78 | 224.51 | A | 38.4711 |
| 4 | vib | | 245.49 | 243.03 | A | 4.7100 |
| 5 | vib | | 398.24 | 394.26 | A | 7.0361 |
| 6 | vib | | 424.67 | 420.42 | A | 0.0926 |
| 7 | vib | | 487.47 | 482.60 | A | 3.4820 |
| 8 | vib | | 550.60 | 545.09 | A | 83.3638 |
| 9 | vib | | 572.08 | 566.36 | A | 11.1931 |
| 10 | vib | | 658.05 | 651.47 | A | 13.2997 |
| 11 | vib | | 693.04 | 686.11 | A | 8.9299 |
| 12 | vib | | 774.63 | 766.88 | A | 0.4074 |

```
  13        vib         876.58         867.81               A       17.9007
  14        vib         911.80         902.69               A       13.4349
  15        vib         931.28         921.96               A       14.9581
  16        vib        1020.11        1009.91               A       37.9160
  17        vib        1090.67        1079.77               A        0.9815
  18        vib        1155.07        1143.52               A       43.1491
  19        vib        1278.82        1266.03               A      190.8604
  20        vib        1346.04        1332.58               A       65.5143
  21        vib        1479.87        1465.08               A      131.1524
  22        vib        1591.10        1575.19               A      454.2214
  23        vib        1650.89        1634.38               A       17.3195
  24        vib        1776.16        1758.40               A      352.3679
  25        vib        2690.10        2663.20               A       11.9233
  26        vib        3188.14        3156.25               A        2.5954
  27        vib        3626.02        3589.76               A       97.7758
  28        rot      0.1213762           -
  29        rot      0.0435310           -
  30        rot      0.0320400           -
 -------------------------------------------------------------------------------

 -------------------------------------------------------------------------------
 ------------------------ ZPE & THERMAL CONTRIBUTIONS --------------------------
 -------------------------------------------------------------------------------
 Eelectronic                    [kJ/mol]   = -1979299.143
 Ezpe                           [kJ/mol]   = +178.820
 Eelectronic+Ezpe               [kJ/mol]   = -1979120.323

 Eelectronic                    [hartrees] = -753.875126
 Ezpe                           [hartrees] = +0.068109
 Eelectronic+Ezpe               [hartrees] = -753.807017

 Thermal Correction to Energy   [kJ/mol]   = +197.254
 Thermal Correction to Enthalpy [kJ/mol]   = +199.735
 Thermal Correction to Gibbs    [kJ/mol]   = +94.788
 -------------------------------------------------------------------------------

 -------------------------------------------------------------------------------
 ------------------------------ ENERGETICS -------------------------------------
 -------------------------------------------------------------------------------
 Temperature=              298.150000
 E(ZPE)=                     0.067427 E(Thermal)=                     0.074499
 E(SCF)=                  -751.181027 DE(MP2)=                       -1.447117
 DE(CBS)=                   -0.143522 DE(MP34)=                      -0.033744
 DE(CCSD)=                  -0.050698 DE(Int)=                        0.047314
 DE(Empirical)=             -0.063827
 CBS-QB3 (0 K)=           -752.805192 CBS-QB3 Energy=              -752.798121
 CBS-QB3 Enthalpy=        -752.797177 CBS-QB3 Free Energy=         -752.837240
 -------------------------------------------------------------------------------
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 END OF GAUSSIAN OUTPUT FILENAME: NSU3-qb3.log
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 GAUSSIAN OUTPUT FILENAME: SU1-m062x.log
!+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++

 1)LEVEL OF THEORY: OPT=VTIGHT
 Charge = 0 Multiplicity = 1  Stoichiometry    C4H4N2OS

 ---------------------------------------------------------------------
 ---------------------- OPTIMIZED GEOMETRY ---------------------------
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          7           0       -0.873491   -0.173500    0.000000
      2          7           0        1.312103    0.483012   -0.000000
      3          6           0       -0.000000    0.870968   -0.000000
      4          6           0       -0.580181   -1.547994    0.000000
      5          6           0        0.846311   -1.838717   -0.000000
      6          6           0        1.720451   -0.824126   -0.000000
```

```
      7          1           0        1.159168   -2.869739   -0.000000
      8          1           0        2.791538   -0.971892   -0.000000
      9         16           0       -0.454745    2.454061    0.000000
     10          1           0       -1.856064    0.067902    0.000000
     11          8           0       -1.473739   -2.356892    0.000000
     12          1           0        1.981423    1.236518   -0.000000
 ---------------------------------------------------------------------
 Rotational constants (GHZ):           3.5897210           1.3214615           0.9658933

 --------------------------------------------------------------------------------
 -------------------- FREQUENCIES AND ROTATIONAL CONSTANTS ----------------------
 --------------------------------------------------------------------------------
 INDEX NO. DOF TYPE  CM-1(UNSCALED)  CM-1(SCALED BY ) SYMMETRY IR-INTENSITY
    1        vib         135.77           0.00               A"        0.8116
    2        vib         164.67           0.00               A"        1.0561
    3        vib         277.91           0.00               A'        9.6477
    4        vib         406.22           0.00               A"       13.3794
    5        vib         460.52           0.00               A'       15.0484
    6        vib         503.82           0.00               A'       11.0803
    7        vib         541.77           0.00               A'        8.9546
    8        vib         635.56           0.00               A"       29.7378
    9        vib         668.87           0.00               A"       17.4448
   10        vib         727.30           0.00               A"       57.4183
   11        vib         728.93           0.00               A'        5.9704
   12        vib         763.98           0.00               A"       11.0353
   13        vib         838.25           0.00               A"       70.1044
   14        vib         931.38           0.00               A'        5.8729
   15        vib         998.95           0.00               A"        0.0641
   16        vib        1013.15           0.00               A'       11.0356
   17        vib        1094.65           0.00               A'        4.4143
   18        vib        1182.77           0.00               A'      222.3090
   19        vib        1225.31           0.00               A'      123.5327
   20        vib        1247.88           0.00               A'       56.2580
   21        vib        1400.64           0.00               A'       13.2906
   22        vib        1420.99           0.00               A'       58.3087
   23        vib        1474.30           0.00               A'       50.7452
   24        vib        1587.37           0.00               A'      819.3915
   25        vib        1706.30           0.00               A'       87.8235
   26        vib        1833.20           0.00               A'      678.0644
   27        vib        3240.33           0.00               A'        2.2186
   28        vib        3281.99           0.00               A'        5.4770
   29        vib        3599.44           0.00               A'       77.4520
   30        vib        3642.44           0.00               A'      109.6420
   31        rot      0.1197402           -
   32        rot      0.0440792           -
   33        rot      0.0322187           -
 --------------------------------------------------------------------------------

 --------------------------------------------------------------------------------
 ------------------------ ZPE & THERMAL CONTRIBUTIONS ---------------------------
 --------------------------------------------------------------------------------
 Eelectronic                    [kJ/mol]   = -1937017.84
 Ezpe                           [kJ/mol]   = +225.704
 Eelectronic+Ezpe               [kJ/mol]   = -1936792.136

 Eelectronic                    [hartrees] = -737.771030
 Ezpe                           [hartrees] = +0.085966
 Eelectronic+Ezpe               [hartrees] = -737.685064

 Thermal Correction to Energy   [kJ/mol]   = +242.478
 Thermal Correction to Enthalpy [kJ/mol]   = +244.959
 Thermal Correction to Gibbs    [kJ/mol]   = +143.707
 --------------------------------------------------------------------------------

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 END OF GAUSSIAN OUTPUT FILENAME: SU1-m062x.log
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 GAUSSIAN OUTPUT FILENAME: SU2-m062x.log
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```

1)LEVEL OF THEORY: OPT=VTIGHT
Charge = 0 Multiplicity = 1  Stoichiometry  C4H4N2OS

---

---------- OPTIMIZED GEOMETRY ----------

---

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 7 | 0 | -0.801184 | -0.322729 | 0.000000 |
| 2 | 7 | 0 | 1.289183 | 0.711934 | -0.000000 |
| 3 | 6 | 0 | 0.000000 | 0.769852 | -0.000000 |
| 4 | 6 | 0 | -0.321900 | -1.648805 | 0.000000 |
| 5 | 6 | 0 | 1.122371 | -1.697839 | 0.000000 |
| 6 | 6 | 0 | 1.831809 | -0.547797 | 0.000000 |
| 7 | 1 | 0 | 1.593869 | -2.668548 | 0.000000 |
| 8 | 1 | 0 | 2.914988 | -0.570848 | -0.000000 |
| 9 | 16 | 0 | -0.836955 | 2.315771 | -0.000000 |
| 10 | 1 | 0 | 0.305873 | 3.009314 | -0.000000 |
| 11 | 8 | 0 | -1.103042 | -2.571204 | 0.000000 |
| 12 | 1 | 0 | -1.808777 | -0.229530 | 0.000000 |

---

Rotational constants (GHZ):  3.5951095  1.3127084  0.9615945

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---------- FREQUENCIES AND ROTATIONAL CONSTANTS ----------

---

| INDEX NO. | DOF TYPE | CM-1(UNSCALED) | CM-1(SCALED BY ) | SYMMETRY | IR-INTENSITY |
|---|---|---|---|---|---|
| 1 | vib | 152.40 | 0.00 | A" | 2.2036 |
| 2 | vib | 183.14 | 0.00 | A" | 3.0427 |
| 3 | vib | 248.46 | 0.00 | A' | 0.4585 |
| 4 | vib | 264.29 | 0.00 | A" | 35.7624 |
| 5 | vib | 413.88 | 0.00 | A" | 7.8800 |
| 6 | vib | 435.23 | 0.00 | A' | 2.2745 |
| 7 | vib | 493.68 | 0.00 | A' | 10.0637 |
| 8 | vib | 543.39 | 0.00 | A' | 1.4239 |
| 9 | vib | 635.91 | 0.00 | A" | 31.4756 |
| 10 | vib | 723.79 | 0.00 | A' | 12.0891 |
| 11 | vib | 724.31 | 0.00 | A" | 18.9109 |
| 12 | vib | 779.64 | 0.00 | A" | 6.4891 |
| 13 | vib | 859.86 | 0.00 | A" | 46.7033 |
| 14 | vib | 886.93 | 0.00 | A' | 0.5211 |
| 15 | vib | 954.78 | 0.00 | A' | 31.2181 |
| 16 | vib | 1011.89 | 0.00 | A' | 40.3048 |
| 17 | vib | 1033.05 | 0.00 | A" | 0.2023 |
| 18 | vib | 1090.22 | 0.00 | A' | 17.3350 |
| 19 | vib | 1192.77 | 0.00 | A' | 30.2958 |
| 20 | vib | 1229.27 | 0.00 | A' | 5.6108 |
| 21 | vib | 1303.71 | 0.00 | A' | 96.3874 |
| 22 | vib | 1443.49 | 0.00 | A' | 16.3789 |
| 23 | vib | 1486.89 | 0.00 | A' | 21.5421 |
| 24 | vib | 1589.07 | 0.00 | A' | 583.6128 |
| 25 | vib | 1668.46 | 0.00 | A' | 66.2645 |
| 26 | vib | 1824.64 | 0.00 | A' | 736.2746 |
| 27 | vib | 2753.31 | 0.00 | A' | 13.5700 |
| 28 | vib | 3210.46 | 0.00 | A' | 12.6100 |
| 29 | vib | 3261.94 | 0.00 | A' | 0.2556 |
| 30 | vib | 3591.21 | 0.00 | A' | 66.5160 |
| 31 | rot | 0.1199199 | - | | |
| 32 | rot | 0.0437872 | - | | |
| 33 | rot | 0.0320753 | - | | |

---

---

---------- ZPE & THERMAL CONTRIBUTIONS ----------

---

Eelectronic  [kJ/mol]  = -1936971.089
Ezpe  [kJ/mol]  = +215.267
Eelectronic+Ezpe  [kJ/mol]  = -1936755.822

Eelectronic  [hartrees] = -737.753224

```
 Ezpe                             [hartrees] = +0.081991
 Eelectronic+Ezpe                 [hartrees] = -737.671233

 Thermal Correction to Energy   [kJ/mol]   = +233.021
 Thermal Correction to Enthalpy [kJ/mol]   = +235.499
 Thermal Correction to Gibbs    [kJ/mol]   = +132.724
 ---------------------------------------------------------------------------

!+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
 END OF GAUSSIAN OUTPUT FILENAME: SU2-m062x.log
!+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++


!+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
 GAUSSIAN OUTPUT FILENAME: SU3-SU1-H2O-TS.log
!+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++

 1)LEVEL OF THEORY: B3LYP/DEF2TZVP
 Charge = 0 Multiplicity = 1  Stoichiometry    C4H6N2O2S

 ---------------------------------------------------------------------
 ---------------------- OPTIMIZED GEOMETRY ---------------------------
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          6           0       -2.346951   -0.257107   -0.006416
      2          6           0       -1.461807    0.907734   -0.001955
      3          7           0       -0.085293    0.625091   -0.011859
      4          6           0        0.388818   -0.600115    0.000913
      5         16           0        2.092766   -0.939670    0.004836
      6          7           0       -0.460041   -1.669986    0.010621
      7          6           0       -1.823005   -1.492695    0.001818
      8          1           0       -3.413723   -0.094731   -0.011867
      9          1           0        1.055127    1.619953   -0.056246
     10          8           0        2.096042    1.876362   -0.096958
     11          1           0        2.332632    2.340059    0.717234
     12          1           0        2.378784    0.652150   -0.026075
     13          8           0       -1.857025    2.058237    0.012306
     14          1           0       -2.414133   -2.398088    0.002944
     15          1           0       -0.060069   -2.594056    0.016350
 ---------------------------------------------------------------------
 Rotational constants (GHZ):           1.9501150           1.1649455           0.7306856

 ---------------------------------------------------------------------------
 -------------------- FREQUENCIES AND ROTATIONAL CONSTANTS ----------------------
 ---------------------------------------------------------------------------
 INDEX NO. DOF TYPE  CM-1(UNSCALED)  CM-1(SCALED BY ) SYMMETRY IR-INTENSITY
    1        vib       -1039.86           0.00                A     1067.3894
    2        vib          78.15           0.00                A       12.7925
    3        vib         145.00           0.00                A        0.2860
    4        vib         160.62           0.00                A        1.9964
    5        vib         222.17           0.00                A       38.3429
    6        vib         373.85           0.00                A       76.3448
    7        vib         417.69           0.00                A        6.9558
    8        vib         429.05           0.00                A       13.7123
    9        vib         458.90           0.00                A        7.6735
   10        vib         480.12           0.00                A      105.6686
   11        vib         557.13           0.00                A       65.4892
   12        vib         563.91           0.00                A       43.7725
   13        vib         573.04           0.00                A       44.2580
   14        vib         585.69           0.00                A       71.4774
   15        vib         664.94           0.00                A        1.1179
   16        vib         721.07           0.00                A       20.1050
   17        vib         757.04           0.00                A        6.6552
   18        vib         841.90           0.00                A       46.5323
   19        vib         917.47           0.00                A      109.9549
   20        vib         971.68           0.00                A        0.0407
   21        vib        1021.74           0.00                A       25.5675
   22        vib        1077.83           0.00                A      344.5189
   23        vib        1081.35           0.00                A        3.7945
   24        vib        1164.06           0.00                A       25.7957
```

```
  25        vib        1201.00           0.00               A      467.0743
  26        vib        1221.86           0.00               A        8.9748
  27        vib        1288.42           0.00               A      280.6196
  28        vib        1418.95           0.00               A       44.2856
  29        vib        1444.99           0.00               A      468.7887
  30        vib        1531.98           0.00               A       32.7780
  31        vib        1575.01           0.00               A      480.5669
  32        vib        1615.09           0.00               A      334.6671
  33        vib        1678.64           0.00               A       56.6249
  34        vib        1748.43           0.00               A      642.4480
  35        vib        2182.20           0.00               A     1746.1772
  36        vib        3204.03           0.00               A        3.4057
  37        vib        3233.39           0.00               A        0.4909
  38        vib        3620.22           0.00               A       87.0722
  39        vib        3791.44           0.00               A       78.1746
  40        rot      0.0650488           -
  41        rot      0.0388584           -
  42        rot      0.0243730           -
 -------------------------------------------------------------------------------

 -------------------------------------------------------------------------------
 ------------------------ ZPE & THERMAL CONTRIBUTIONS --------------------------
 -------------------------------------------------------------------------------
 Eelectronic                    [kJ/mol]   = -2138156.27
 Ezpe                           [kJ/mol]   = +269.279
 Eelectronic+Ezpe               [kJ/mol]   = -2137886.991

 Eelectronic                    [hartrees] = -814.380602
 Ezpe                           [hartrees] = +0.102563
 Eelectronic+Ezpe               [hartrees] = -814.278039

 Thermal Correction to Energy   [kJ/mol]   = +290.785
 Thermal Correction to Enthalpy [kJ/mol]   = +293.266
 Thermal Correction to Gibbs    [kJ/mol]   = +181.354
 -------------------------------------------------------------------------------

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 END OF GAUSSIAN OUTPUT FILENAME: SU3-SU1-H2O-TS.log
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 GAUSSIAN OUTPUT FILENAME: TS-5SH-5HS-m062x.log
!+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++

 1)LEVEL OF THEORY: OPT=(TS,CALCFC,NOEIGENTEST,VTIGHT)
 Charge = 0 Multiplicity = 1  Stoichiometry    C3H4N2S

 ---------------------------------------------------------------------
 ---------------------- OPTIMIZED GEOMETRY ---------------------------
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          7           0        0.670822   -0.823412   -0.000000
      2          6           0       -0.000000    0.321632    0.000000
      3          6           0       -0.241266   -1.855847   -0.000000
      4          6           0       -1.486480   -1.314035   -0.000000
      5          7           0       -1.317566    0.066215   -0.000000
      6          1           0       -2.045844    0.758480   -0.000000
      7          1           0       -2.460539   -1.768987   -0.000000
      8          1           0        0.046597   -2.891790   -0.000000
      9         16           0        1.102811    1.640260    0.000000
     10          1           0        1.708496    0.048012    0.000000
 ---------------------------------------------------------------------
 Rotational constants (GHZ):           9.2824906           2.2327991           1.7998624

 -------------------------------------------------------------------------------
 -------------------- FREQUENCIES AND ROTATIONAL CONSTANTS ---------------------
 -------------------------------------------------------------------------------
 INDEX NO. DOF TYPE  CM-1(UNSCALED)  CM-1(SCALED BY ) SYMMETRY IR-INTENSITY
    1        vib       -1670.60           0.00               A'     1762.8056
```

```
    2        vib         191.09           0.00              A"        3.8428
    3        vib         375.08           0.00              A'        5.4372
    4        vib         567.10           0.00              A'        5.6869
    5        vib         576.75           0.00              A"       60.0674
    6        vib         624.74           0.00              A"       15.8143
    7        vib         675.37           0.00              A"        1.4843
    8        vib         731.42           0.00              A"       74.2266
    9        vib         851.76           0.00              A"       19.2515
   10        vib         881.10           0.00              A"        4.9406
   11        vib         939.05           0.00              A'        0.7044
   12        vib         984.51           0.00              A'       15.2904
   13        vib        1083.95           0.00              A'       32.8411
   14        vib        1143.72           0.00              A'        5.2557
   15        vib        1184.65           0.00              A'        0.5993
   16        vib        1267.53           0.00              A'       18.1253
   17        vib        1366.09           0.00              A'       39.8121
   18        vib        1484.97           0.00              A'       36.2610
   19        vib        1514.69           0.00              A'      187.6054
   20        vib        1590.62           0.00              A'       59.8127
   21        vib        1786.09           0.00              A'       27.3867
   22        vib        3300.03           0.00              A'        3.3905
   23        vib        3319.57           0.00              A'        0.0052
   24        vib        3689.84           0.00              A'      112.3264
   25        rot      0.3096306           -
   26        rot      0.0744782           -
   27        rot      0.0600369           -
 ---------------------------------------------------------------------------

 ---------------------------------------------------------------------------
 ----------------------- ZPE & THERMAL CONTRIBUTIONS -----------------------
 ---------------------------------------------------------------------------
 Eelectronic                    [kJ/mol]   = -1639230.55
 Ezpe                           [kJ/mol]   = +180.217
 Eelectronic+Ezpe               [kJ/mol]   = -1639050.333

 Eelectronic                    [hartrees] = -624.349857
 Ezpe                           [hartrees] = +0.068641
 Eelectronic+Ezpe               [hartrees] = -624.281216

 Thermal Correction to Energy   [kJ/mol]   = +192.751
 Thermal Correction to Enthalpy [kJ/mol]   = +195.230
 Thermal Correction to Gibbs    [kJ/mol]   = +104.965
 ---------------------------------------------------------------------------

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 END OF GAUSSIAN OUTPUT FILENAME: TS-5SH-5HS-m062x.log
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!+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
 GAUSSIAN OUTPUT FILENAME: TS-MeSU3-MeSU1-apf.log
!+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++

 1)LEVEL OF THEORY: OPT=(TS,CALCFC,NOEIGENTEST,VTIGHT)
 Charge = 0 Multiplicity = 1  Stoichiometry    C5H6N2OS

 ---------------------------------------------------------------------
 ---------------------- OPTIMIZED GEOMETRY ---------------------------
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          7           0       -1.156985   -0.010556    0.000000
      2          7           0        1.195599    0.017231    0.000000
      3          6           0        0.000000    0.634041    0.000000
      4          6           0       -1.252405   -1.402245    0.000000
      5          6           0        0.054223   -2.068429    0.000000
      6          6           0        1.193913   -1.363426    0.000000
      7          1           0        0.072955   -3.149293    0.000000
      8          1           0        2.173674   -1.824315    0.000000
      9         16           0       -0.323781    2.314867    0.000000
     10          1           0       -1.609891    1.337955    0.000000
```

```
    11          8           0       -2.312755   -1.986063    0.000000
    12          6           0        2.428325    0.784948    0.000000
    13          1           0        2.480292    1.417348    0.887384
    14          1           0        3.270589    0.095526    0.000000
    15          1           0        2.480292    1.417348   -0.887384
---------------------------------------------------------------------
Rotational constants (GHZ):           2.2328918           1.2498790           0.8053826

--------------------------------------------------------------------------------
-------------------- FREQUENCIES AND ROTATIONAL CONSTANTS ----------------------
--------------------------------------------------------------------------------
INDEX NO. DOF TYPE  CM-1(UNSCALED)  CM-1(SCALED BY ) SYMMETRY IR-INTENSITY
   1        vib       -1549.30           0.00               A'     1253.1392
   2        vib          28.32           0.00               A"        0.0231
   3        vib         100.11           0.00               A"        0.8129
   4        vib         154.77           0.00               A"        0.1168
   5        vib         235.24           0.00               A"        3.4104
   6        vib         258.79           0.00               A'        3.0429
   7        vib         347.55           0.00               A'        2.3892
   8        vib         419.54           0.00               A"        1.3864
   9        vib         458.34           0.00               A'       19.9908
  10        vib         529.73           0.00               A'        3.6837
  11        vib         568.01           0.00               A'        1.4701
  12        vib         645.27           0.00               A"        0.3283
  13        vib         717.11           0.00               A'       12.5565
  14        vib         739.83           0.00               A"        2.3412
  15        vib         802.93           0.00               A'        3.2163
  16        vib         839.57           0.00               A"       48.5418
  17        vib         885.28           0.00               A"       13.2264
  18        vib         952.29           0.00               A'       12.4898
  19        vib         971.10           0.00               A"        0.0906
  20        vib        1042.75           0.00               A'        1.4482
  21        vib        1146.08           0.00               A"        0.0064
  22        vib        1149.96           0.00               A'       79.6843
  23        vib        1204.25           0.00               A'        4.6468
  24        vib        1234.51           0.00               A'       52.1860
  25        vib        1291.11           0.00               A'       31.1335
  26        vib        1405.11           0.00               A'       68.6061
  27        vib        1460.43           0.00               A'       72.7227
  28        vib        1465.71           0.00               A'      254.6611
  29        vib        1472.64           0.00               A"       14.1014
  30        vib        1510.51           0.00               A'      136.5747
  31        vib        1519.29           0.00               A'      231.0434
  32        vib        1692.38           0.00               A'       95.9056
  33        vib        1782.20           0.00               A'      585.9646
  34        vib        1827.18           0.00               A'       73.4848
  35        vib        3063.70           0.00               A'       19.1559
  36        vib        3136.54           0.00               A"        4.7449
  37        vib        3165.90           0.00               A'        4.6049
  38        vib        3214.14           0.00               A'        2.7146
  39        vib        3241.37           0.00               A'        0.3077
  40        rot      0.0744813           -
  41        rot      0.0416915           -
  42        rot      0.0268647           -
--------------------------------------------------------------------------------

--------------------------------------------------------------------------------
------------------------ ZPE & THERMAL CONTRIBUTIONS ---------------------------
--------------------------------------------------------------------------------
Eelectronic                    [kJ/mol]   = -2039410.748
Ezpe                           [kJ/mol]   = +279.206
Eelectronic+Ezpe               [kJ/mol]   = -2039131.542

Eelectronic                    [hartrees] = -776.770424
Ezpe                           [hartrees] = +0.106344
Eelectronic+Ezpe               [hartrees] = -776.664080

Thermal Correction to Energy   [kJ/mol]   = +300.578
Thermal Correction to Enthalpy [kJ/mol]   = +303.056
Thermal Correction to Gibbs    [kJ/mol]   = +188.763
--------------------------------------------------------------------------------
```

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 END OF GAUSSIAN OUTPUT FILENAME: TS-MeSU3-MeSU1-apf.log
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 GAUSSIAN OUTPUT FILENAME: TS-MeSU3-MeSU1-apfd.log
!+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++

 1)LEVEL OF THEORY: OPT=(TS,CALCFC,NOEIGENTEST,VTIGHT)
 Charge = 0 Multiplicity = 1  Stoichiometry    C5H6N2OS

 ---------------------------------------------------------------------
 ---------------------- OPTIMIZED GEOMETRY ---------------------------
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          7           0       -1.156194   -0.011178    0.000000
      2          7           0        1.196781    0.018209    0.000000
      3          6           0        0.000000    0.634154    0.000000
      4          6           0       -1.248985   -1.404053    0.000000
      5          6           0        0.059065   -2.067871    0.000000
      6          6           0        1.198343   -1.361779    0.000000
      7          1           0        0.077885   -3.149238    0.000000
      8          1           0        2.179301   -1.820267    0.000000
      9         16           0       -0.331522    2.315339    0.000000
     10          1           0       -1.611789    1.335836    0.000000
     11          8           0       -2.306360   -1.994170    0.000000
     12          6           0        2.426030    0.789834    0.000000
     13          1           0        2.473383    1.422453    0.887212
     14          1           0        3.272238    0.105780    0.000000
     15          1           0        2.473383    1.422453   -0.887212
 ---------------------------------------------------------------------
 Rotational constants (GHZ):           2.2305139           1.2498696           0.8050676

 --------------------------------------------------------------------------------
 -------------------- FREQUENCIES AND ROTATIONAL CONSTANTS ----------------------
 --------------------------------------------------------------------------------
 INDEX NO. DOF TYPE  CM-1(UNSCALED)  CM-1(SCALED BY ) SYMMETRY IR-INTENSITY
    1        vib       -1543.70           0.00              A'     1253.4805
    2        vib          31.94           0.00              A"        0.0382
    3        vib          98.76           0.00              A"        0.8233
    4        vib         153.33           0.00              A"        0.1052
    5        vib         233.85           0.00              A"        3.3697
    6        vib         269.44           0.00              A'        3.2274
    7        vib         357.08           0.00              A'        2.2653
    8        vib         418.57           0.00              A"        1.3909
    9        vib         458.29           0.00              A'       19.9036
   10        vib         533.23           0.00              A'        4.1140
   11        vib         581.17           0.00              A'        0.7861
   12        vib         645.43           0.00              A"        0.3366
   13        vib         716.53           0.00              A'       12.9645
   14        vib         739.48           0.00              A"        2.3542
   15        vib         804.22           0.00              A'        3.1881
   16        vib         840.15           0.00              A"       48.4198
   17        vib         884.73           0.00              A"       13.2409
   18        vib         961.35           0.00              A'       14.9262
   19        vib         970.79           0.00              A"        0.0610
   20        vib        1049.78           0.00              A'        2.1722
   21        vib        1146.86           0.00              A"        0.0035
   22        vib        1153.13           0.00              A'       85.5108
   23        vib        1208.78           0.00              A'        3.0934
   24        vib        1238.56           0.00              A'       48.8460
   25        vib        1300.70           0.00              A'       38.2075
   26        vib        1409.41           0.00              A'       62.1680
   27        vib        1464.40           0.00              A'      299.9770
   28        vib        1473.53           0.00              A"       14.2238
   29        vib        1474.35           0.00              A'       32.0809
   30        vib        1513.11           0.00              A'      153.0427
   31        vib        1524.47           0.00              A'      210.1520
   32        vib        1693.43           0.00              A'      100.9809

```
  33        vib        1781.74           0.00              A'      579.3780
  34        vib        1829.72           0.00              A'       67.9858
  35        vib        3065.60           0.00              A'       19.1796
  36        vib        3138.39           0.00              A"        4.7615
  37        vib        3168.75           0.00              A'        4.5122
  38        vib        3213.25           0.00              A'        2.6858
  39        vib        3238.15           0.00              A'        0.3831
  40        rot      0.0744019           -
  41        rot      0.0416912           -
  42        rot      0.0268542           -
 -------------------------------------------------------------------------------

 -------------------------------------------------------------------------------
 ----------------------- ZPE & THERMAL CONTRIBUTIONS ---------------------------
 -------------------------------------------------------------------------------
 Eelectronic                    [kJ/mol]   = -2039433.848
 Ezpe                           [kJ/mol]   = +279.834
 Eelectronic+Ezpe               [kJ/mol]   = -2039154.014

 Eelectronic                    [hartrees] = -776.779222
 Ezpe                           [hartrees] = +0.106583
 Eelectronic+Ezpe               [hartrees] = -776.672639

 Thermal Correction to Energy   [kJ/mol]   = +301.100
 Thermal Correction to Enthalpy [kJ/mol]   = +303.579
 Thermal Correction to Gibbs    [kJ/mol]   = +189.706
 -------------------------------------------------------------------------------

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 END OF GAUSSIAN OUTPUT FILENAME: TS-MeSU3-MeSU1-apfd.log
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 GAUSSIAN OUTPUT FILENAME: TS-MeSU3-MeSU1-b2plyp.log
!+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++

 1)LEVEL OF THEORY: OPT=(TS,CALCFC,NOEIGENTEST,VTIGHT)
 Charge = 0 Multiplicity = 1  Stoichiometry    C5H6N2OS

 ---------------------------------------------------------------------
 ---------------------- OPTIMIZED GEOMETRY ---------------------------
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          7           0       -1.161567   -0.012405    0.000000
      2          7           0        1.199259    0.019530    0.000000
      3          6           0       -0.000000    0.638210    0.000000
      4          6           0       -1.252981   -1.411905    0.000000
      5          6           0        0.056579   -2.074362    0.000000
      6          6           0        1.199638   -1.365779    0.000000
      7          1           0        0.078859   -3.153492    0.000000
      8          1           0        2.177638   -1.825112    0.000000
      9         16           0       -0.328928    2.323877    0.000000
     10          1           0       -1.623100    1.333892    0.000000
     11          8           0       -2.317415   -1.999928    0.000000
     12          6           0        2.438826    0.791818    0.000000
     13          1           0        2.487629    1.421739    0.886417
     14          1           0        3.277296    0.100861    0.000000
     15          1           0        2.487629    1.421739   -0.886417
 ---------------------------------------------------------------------
 Rotational constants (GHZ):           2.2175259           1.2398137           0.7991956

 -------------------------------------------------------------------------------
 ------------------- FREQUENCIES AND ROTATIONAL CONSTANTS ----------------------
 -------------------------------------------------------------------------------
 INDEX NO. DOF TYPE  CM-1(UNSCALED)  CM-1(SCALED BY ) SYMMETRY IR-INTENSITY
    1        vib       -1587.40           0.00              A'     1262.4607
    2        vib          36.50           0.00              A"        0.0398
    3        vib          99.52           0.00              A"        0.7719
    4        vib         152.90           0.00              A"        0.1471
```

```
    5        vib         230.47           0.00              A"        3.5058
    6        vib         259.82           0.00              A'        3.2896
    7        vib         344.40           0.00              A'        2.2245
    8        vib         418.71           0.00              A"        1.3384
    9        vib         455.19           0.00              A'       20.2871
   10        vib         523.18           0.00              A'        3.9223
   11        vib         563.51           0.00              A'        1.3212
   12        vib         638.30           0.00              A"        0.1826
   13        vib         712.04           0.00              A'       12.3799
   14        vib         732.35           0.00              A"        1.4654
   15        vib         792.96           0.00              A'        2.1819
   16        vib         833.72           0.00              A"       50.4869
   17        vib         880.50           0.00              A"       11.3325
   18        vib         938.60           0.00              A'       11.3912
   19        vib         962.99           0.00              A"        0.1272
   20        vib        1039.93           0.00              A'        2.4512
   21        vib        1156.37           0.00              A'       95.5676
   22        vib        1158.11           0.00              A"        0.1048
   23        vib        1192.84           0.00              A'        4.8331
   24        vib        1229.33           0.00              A'       41.2422
   25        vib        1277.51           0.00              A'       48.4382
   26        vib        1405.39           0.00              A'      117.2761
   27        vib        1457.02           0.00              A'      357.4193
   28        vib        1463.87           0.00              A'      113.8987
   29        vib        1494.24           0.00              A"       12.7520
   30        vib        1495.58           0.00              A'       43.7272
   31        vib        1531.15           0.00              A'      114.4232
   32        vib        1665.38           0.00              A'       51.9602
   33        vib        1741.59           0.00              A'      581.6996
   34        vib        1807.63           0.00              A'       41.2425
   35        vib        3073.73           0.00              A'       19.4558
   36        vib        3147.85           0.00              A"        4.9682
   37        vib        3173.34           0.00              A'        4.8028
   38        vib        3222.81           0.00              A'        2.5151
   39        vib        3244.84           0.00              A'        0.4361
   40        rot      0.0739687           -
   41        rot      0.0413557           -
   42        rot      0.0266583           -
 -------------------------------------------------------------------------------

 -------------------------------------------------------------------------------
 ------------------------ ZPE & THERMAL CONTRIBUTIONS --------------------------
 -------------------------------------------------------------------------------
 Eelectronic                    [kJ/mol]   = -2039350.658
 Ezpe                           [kJ/mol]   = +278.455
 Eelectronic+Ezpe               [kJ/mol]   = -2039072.203

 Eelectronic                    [hartrees] = -776.747537
 Ezpe                           [hartrees] = +0.106058
 Eelectronic+Ezpe               [hartrees] = -776.641479

 Thermal Correction to Energy   [kJ/mol]   = +299.890
 Thermal Correction to Enthalpy [kJ/mol]   = +302.371
 Thermal Correction to Gibbs    [kJ/mol]   = +188.469
 -------------------------------------------------------------------------------

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 END OF GAUSSIAN OUTPUT FILENAME: TS-MeSU3-MeSU1-b2plyp.log
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 GAUSSIAN OUTPUT FILENAME: TS-MeSU3-MeSU1-wb97xd.log
!+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++

 1)LEVEL OF THEORY: OPT=(TS,CALCFC,NOEIGENTEST,VTIGHT)
 Charge = 0 Multiplicity = 1  Stoichiometry    C5H6N2OS

 ---------------------------------------------------------------------
 ---------------------- OPTIMIZED GEOMETRY ---------------------------
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
```

| Number | Number | Type | X | Y | Z |
|---|---|---|---|---|---|
| 1 | 7 | 0 | -1.154848 | -0.012245 | 0.000000 |
| 2 | 7 | 0 | 1.195280 | 0.019903 | 0.000000 |
| 3 | 6 | 0 | -0.000000 | 0.632779 | 0.000000 |
| 4 | 6 | 0 | -1.247029 | -1.404700 | 0.000000 |
| 5 | 6 | 0 | 0.063573 | -2.070290 | 0.000000 |
| 6 | 6 | 0 | 1.197898 | -1.363488 | 0.000000 |
| 7 | 1 | 0 | 0.084306 | -3.149686 | 0.000000 |
| 8 | 1 | 0 | 2.177090 | -1.822188 | 0.000000 |
| 9 | 16 | 0 | -0.336724 | 2.314336 | 0.000000 |
| 10 | 1 | 0 | -1.614830 | 1.328979 | 0.000000 |
| 11 | 8 | 0 | -2.303534 | -1.988837 | 0.000000 |
| 12 | 6 | 0 | 2.428627 | 0.792211 | 0.000000 |
| 13 | 1 | 0 | 2.477913 | 1.422814 | 0.887340 |
| 14 | 1 | 0 | 3.272031 | 0.105907 | 0.000000 |
| 15 | 1 | 0 | 2.477913 | 1.422814 | -0.887340 |

Rotational constants (GHZ): 2.2260835 1.2522917 0.8054936

---------- FREQUENCIES AND ROTATIONAL CONSTANTS ----------

| INDEX NO. | DOF TYPE | CM-1(UNSCALED) | CM-1(SCALED BY ) | SYMMETRY | IR-INTENSITY |
|---|---|---|---|---|---|
| 1 | vib | -1616.94 | 0.00 | A' | 1420.1512 |
| 2 | vib | 49.04 | 0.00 | A" | 0.0391 |
| 3 | vib | 100.19 | 0.00 | A" | 0.8698 |
| 4 | vib | 157.98 | 0.00 | A" | 0.1127 |
| 5 | vib | 237.13 | 0.00 | A" | 3.5609 |
| 6 | vib | 266.52 | 0.00 | A' | 3.1979 |
| 7 | vib | 352.89 | 0.00 | A' | 2.4164 |
| 8 | vib | 424.11 | 0.00 | A" | 1.4083 |
| 9 | vib | 461.67 | 0.00 | A' | 22.1758 |
| 10 | vib | 534.05 | 0.00 | A' | 3.7816 |
| 11 | vib | 575.38 | 0.00 | A' | 1.8211 |
| 12 | vib | 650.71 | 0.00 | A" | 0.2990 |
| 13 | vib | 719.92 | 0.00 | A' | 13.4713 |
| 14 | vib | 748.05 | 0.00 | A" | 2.0590 |
| 15 | vib | 806.35 | 0.00 | A' | 3.3578 |
| 16 | vib | 847.80 | 0.00 | A" | 50.7190 |
| 17 | vib | 895.69 | 0.00 | A" | 16.1826 |
| 18 | vib | 955.38 | 0.00 | A' | 14.6710 |
| 19 | vib | 989.70 | 0.00 | A" | 0.0615 |
| 20 | vib | 1052.63 | 0.00 | A' | 1.1489 |
| 21 | vib | 1158.14 | 0.00 | A" | 0.0464 |
| 22 | vib | 1162.76 | 0.00 | A' | 84.9355 |
| 23 | vib | 1213.34 | 0.00 | A' | 4.7633 |
| 24 | vib | 1246.80 | 0.00 | A' | 52.8251 |
| 25 | vib | 1299.33 | 0.00 | A' | 27.7185 |
| 26 | vib | 1418.66 | 0.00 | A' | 72.3704 |
| 27 | vib | 1476.43 | 0.00 | A' | 102.0000 |
| 28 | vib | 1480.66 | 0.00 | A' | 258.6088 |
| 29 | vib | 1487.46 | 0.00 | A" | 14.2506 |
| 30 | vib | 1521.65 | 0.00 | A' | 158.8778 |
| 31 | vib | 1532.37 | 0.00 | A' | 256.6957 |
| 32 | vib | 1710.90 | 0.00 | A' | 112.3298 |
| 33 | vib | 1804.98 | 0.00 | A' | 619.6981 |
| 34 | vib | 1854.57 | 0.00 | A' | 80.6662 |
| 35 | vib | 3069.64 | 0.00 | A' | 19.0216 |
| 36 | vib | 3145.29 | 0.00 | A" | 5.0564 |
| 37 | vib | 3172.47 | 0.00 | A' | 5.0041 |
| 38 | vib | 3224.79 | 0.00 | A' | 2.4463 |
| 39 | vib | 3250.94 | 0.00 | A' | 0.2837 |
| 40 | rot | 0.0742542 | - | | |
| 41 | rot | 0.0417720 | - | | |
| 42 | rot | 0.0268684 | - | | |

---------- ZPE & THERMAL CONTRIBUTIONS ----------

Eelectronic [kJ/mol] = -2040133.052

```
 Ezpe                             [kJ/mol]   = +281.459
 Eelectronic+Ezpe                 [kJ/mol]   = -2039851.593

 Eelectronic                      [hartrees] = -777.045535
 Ezpe                             [hartrees] = +0.107202
 Eelectronic+Ezpe                 [hartrees] = -776.938333

 Thermal Correction to Energy   [kJ/mol]   = +302.552
 Thermal Correction to Enthalpy [kJ/mol]   = +305.033
 Thermal Correction to Gibbs    [kJ/mol]   = +192.394
 ---------------------------------------------------------------------------

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 END OF GAUSSIAN OUTPUT FILENAME: TS-MeSU3-MeSU1-wb97xd.log
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 GAUSSIAN OUTPUT FILENAME: TS-NNSH-NNHS-m062x.log
!+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++

 1)LEVEL OF THEORY: OPT=(TS,CALCFC,NOEIGENTEST,VTIGHT)
 Charge = 0 Multiplicity = 1  Stoichiometry    C4H4N2S

 ---------------------------------------------------------------------
 ---------------------- OPTIMIZED GEOMETRY ---------------------------
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          6           0        1.359127    0.218220    0.000000
      2          7           0       -0.924015   -0.427079   -0.000000
      3          6           0        0.000000    0.560400   -0.000000
      4          6           0        1.648988   -1.122296    0.000000
      5          6           0        0.604644   -2.057464    0.000000
      6          7           0       -0.668890   -1.701875    0.000000
      7          1           0        0.793044   -3.121879    0.000000
      8         16           0       -0.894651    2.019229   -0.000000
      9          1           0       -1.804105    0.612571   -0.000000
     10          1           0        2.674205   -1.468541    0.000000
     11          1           0        2.125067    0.979695    0.000000
 ---------------------------------------------------------------------
 Rotational constants (GHZ):           5.9089909           1.7426513           1.3457648

 ---------------------------------------------------------------------------
 -------------------- FREQUENCIES AND ROTATIONAL CONSTANTS ----------------
 ---------------------------------------------------------------------------
 INDEX NO. DOF TYPE  CM-1(UNSCALED)  CM-1(SCALED BY ) SYMMETRY IR-INTENSITY
    1        vib       -1600.64           0.00               A'     1126.8491
    2        vib         160.62           0.00               A"        0.3364
    3        vib         364.36           0.00               A'        7.2994
    4        vib         395.74           0.00               A"        0.4459
    5        vib         476.07           0.00               A"        1.3189
    6        vib         507.82           0.00               A'        3.4546
    7        vib         667.94           0.00               A'        4.6894
    8        vib         759.42           0.00               A"        9.0772
    9        vib         761.82           0.00               A'       20.9537
   10        vib         825.89           0.00               A"       35.4521
   11        vib         946.54           0.00               A"        2.9143
   12        vib         954.61           0.00               A"        3.9359
   13        vib        1033.83           0.00               A"        0.0330
   14        vib        1053.80           0.00               A'       13.0931
   15        vib        1081.95           0.00               A'        1.2064
   16        vib        1123.21           0.00               A'       68.4949
   17        vib        1177.67           0.00               A'       51.1919
   18        vib        1221.73           0.00               A'       25.4176
   19        vib        1264.67           0.00               A'       66.3729
   20        vib        1409.10           0.00               A'       28.0003
   21        vib        1473.78           0.00               A'      117.3081
   22        vib        1600.92           0.00               A'        1.2500
   23        vib        1639.00           0.00               A'      115.8556
   24        vib        1824.93           0.00               A'       35.6306
```

```
  25        vib        3222.51           0.00              A'        1.1107
  26        vib        3240.32           0.00              A'        1.4825
  27        vib        3250.86           0.00              A'        0.1836
  28        rot      0.1971027           -
  29        rot      0.0581286           -
  30        rot      0.0448899           -
 ---------------------------------------------------------------------------

 ---------------------------------------------------------------------------
 ----------------------- ZPE & THERMAL CONTRIBUTIONS -----------------------
 ---------------------------------------------------------------------------
 Eelectronic                    [kJ/mol]   = -1739192.062
 Ezpe                           [kJ/mol]   = +194.030
 Eelectronic+Ezpe               [kJ/mol]   = -1738998.032

 Eelectronic                    [hartrees] = -662.423181
 Ezpe                           [hartrees] = +0.073902
 Eelectronic+Ezpe               [hartrees] = -662.349279

 Thermal Correction to Energy   [kJ/mol]   = +207.743
 Thermal Correction to Enthalpy [kJ/mol]   = +210.221
 Thermal Correction to Gibbs    [kJ/mol]   = +116.325
 ---------------------------------------------------------------------------

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 END OF GAUSSIAN OUTPUT FILENAME: TS-NNSH-NNHS-m062x.log
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 GAUSSIAN OUTPUT FILENAME: TS-NSU3-dimer-qb3.log
!+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++

 1)LEVEL OF THEORY: CBS-QB3
 Charge = 0 Multiplicity = 1  Stoichiometry    C6H6N6O2S2

 ---------------------------------------------------------------------
 ---------------------- OPTIMIZED GEOMETRY ---------------------------
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          7           0        1.778677   -0.343756   -0.000027
      2          7           0        3.200405    1.487368    0.000039
      3          6           0        1.939990    0.963275    0.000007
      4          6           0        2.884322   -1.198247   -0.000024
      5          6           0        4.196162   -0.519611   -0.000005
      6          7           0        4.341011    0.759934    0.000026
      7          1           0        5.095777   -1.123651   -0.000016
      8         16           0        0.641325    2.112912    0.000010
      9          1           0       -0.494279    1.139062   -0.000014
     10          8           0        2.763001   -2.407444   -0.000038
     11          1           0        3.334165    2.487941    0.000059
     12          7           0       -1.778677    0.343756   -0.000024
     13          7           0       -3.200404   -1.487368    0.000031
     14          6           0       -1.939990   -0.963274    0.000005
     15          6           0       -2.884323    1.198247   -0.000024
     16          6           0       -4.196162    0.519611    0.000001
     17          7           0       -4.341011   -0.759935    0.000027
     18          1           0       -5.095777    1.123650   -0.000003
     19         16           0       -0.641324   -2.112912    0.000011
     20          1           0        0.494278   -1.139061   -0.000016
     21          8           0       -2.763002    2.407444   -0.000043
     22          1           0       -3.334164   -2.487941    0.000051
 ---------------------------------------------------------------------
 Rotational constants (GHZ):           0.7981956           0.2576413           0.1947727

 ---------------------------------------------------------------------------
 -------------------- FREQUENCIES AND ROTATIONAL CONSTANTS -----------------
 ---------------------------------------------------------------------------
 INDEX NO. DOF TYPE  CM-1(UNSCALED)  CM-1(SCALED BY 0.99) SYMMETRY IR-INTENSITY
    1        vib        -643.14        -636.71               A        0.0000
```

| | | | | | |
|---|---|---|---|---|---|
| 2 | vib | 22.40 | 22.18 | A | 0.0578 |
| 3 | vib | 38.54 | 38.15 | A | 7.2432 |
| 4 | vib | 65.55 | 64.89 | A | 0.0000 |
| 5 | vib | 96.25 | 95.29 | A | 0.0000 |
| 6 | vib | 99.14 | 98.15 | A | 97.7965 |
| 7 | vib | 123.56 | 122.32 | A | 0.0000 |
| 8 | vib | 128.34 | 127.06 | A | 0.6745 |
| 9 | vib | 158.21 | 156.63 | A | 0.7506 |
| 10 | vib | 169.64 | 167.95 | A | 0.0000 |
| 11 | vib | 279.15 | 276.36 | A | 0.0000 |
| 12 | vib | 291.40 | 288.48 | A | 407.4345 |
| 13 | vib | 409.55 | 405.45 | A | 0.0000 |
| 14 | vib | 427.64 | 423.36 | A | 0.0000 |
| 15 | vib | 432.11 | 427.79 | A | 0.0000 |
| 16 | vib | 432.85 | 428.52 | A | 1.7142 |
| 17 | vib | 435.91 | 431.55 | A | 42.4978 |
| 18 | vib | 507.85 | 502.77 | A | 7.5708 |
| 19 | vib | 520.04 | 514.84 | A | 0.0000 |
| 20 | vib | 585.44 | 579.59 | A | 109.5770 |
| 21 | vib | 593.88 | 587.95 | A | 0.0000 |
| 22 | vib | 602.77 | 596.74 | A | 0.0000 |
| 23 | vib | 609.53 | 603.43 | A | 164.0016 |
| 24 | vib | 660.00 | 653.40 | A | 0.0000 |
| 25 | vib | 662.43 | 655.81 | A | 42.4271 |
| 26 | vib | 702.38 | 695.36 | A | 47.9607 |
| 27 | vib | 713.28 | 706.15 | A | 0.0000 |
| 28 | vib | 765.41 | 757.76 | A | 0.1812 |
| 29 | vib | 767.42 | 759.74 | A | 0.0000 |
| 30 | vib | 900.32 | 891.31 | A | 0.0000 |
| 31 | vib | 920.27 | 911.07 | A | 45.7619 |
| 32 | vib | 920.80 | 911.59 | A | 374.8905 |
| 33 | vib | 922.03 | 912.81 | A | 0.0000 |
| 34 | vib | 922.35 | 913.12 | A | 0.0000 |
| 35 | vib | 928.78 | 919.50 | A | 8.3527 |
| 36 | vib | 1030.22 | 1019.92 | A | 6778.8842 |
| 37 | vib | 1052.87 | 1042.34 | A | 140.0984 |
| 38 | vib | 1057.42 | 1046.85 | A | 0.0000 |
| 39 | vib | 1074.23 | 1063.49 | A | 0.0000 |
| 40 | vib | 1089.26 | 1078.37 | A | 723.6271 |
| 41 | vib | 1183.72 | 1171.89 | A | 289.2187 |
| 42 | vib | 1188.91 | 1177.02 | A | 0.0000 |
| 43 | vib | 1266.62 | 1253.95 | A | 388.6594 |
| 44 | vib | 1273.16 | 1260.43 | A | 0.0000 |
| 45 | vib | 1305.45 | 1292.40 | A | 116.6194 |
| 46 | vib | 1345.05 | 1331.60 | A | 0.0000 |
| 47 | vib | 1360.76 | 1347.15 | A | 185.9834 |
| 48 | vib | 1362.37 | 1348.75 | A | 0.0000 |
| 49 | vib | 1465.04 | 1450.39 | A | 0.0000 |
| 50 | vib | 1465.29 | 1450.64 | A | 101.9813 |
| 51 | vib | 1561.37 | 1545.76 | A | 0.0000 |
| 52 | vib | 1577.71 | 1561.94 | A | 547.5411 |
| 53 | vib | 1650.66 | 1634.15 | A | 0.0000 |
| 54 | vib | 1650.88 | 1634.37 | A | 16.6194 |
| 55 | vib | 1762.54 | 1744.92 | A | 0.0000 |
| 56 | vib | 1771.82 | 1754.10 | A | 1014.6139 |
| 57 | vib | 3195.42 | 3163.46 | A | 2.0131 |
| 58 | vib | 3195.44 | 3163.48 | A | 0.0000 |
| 59 | vib | 3620.61 | 3584.41 | A | 209.3380 |
| 60 | vib | 3620.93 | 3584.72 | A | 0.0000 |
| 61 | rot | 0.0266249 | - | | |
| 62 | rot | 0.0085940 | - | | |
| 63 | rot | 0.0064969 | - | | |

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---------- ZPE & THERMAL CONTRIBUTIONS ----------

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Eelectronic [kJ/mol] = -3958657.948
Ezpe [kJ/mol] = +352.557
Eelectronic+Ezpe [kJ/mol] = -3958305.391

Eelectronic [hartrees] = -1507.772976

```
 Ezpe                             [hartrees] = +0.134282
 Eelectronic+Ezpe                 [hartrees] = -1507.638694

 Thermal Correction to Energy   [kJ/mol]   = +389.509
 Thermal Correction to Enthalpy [kJ/mol]   = +391.987
 Thermal Correction to Gibbs    [kJ/mol]   = +237.836
 ---------------------------------------------------------------------------

 ---------------------------------------------------------------------------
 ------------------------------ ENERGETICS ---------------------------------
 ---------------------------------------------------------------------------
 Temperature=              298.150000
 E(ZPE)=                     0.132939 E(Thermal)=                    0.147118
 E(SCF)=                 -1502.352182 DE(MP2)=                      -2.930215
 DE(CBS)=                   -0.288818 DE(MP34)=                     -0.058655
 DE(CCSD)=                  -0.105138 DE(Int)=                       0.094921
 DE(Empirical)=             -0.127199
 CBS-QB3 (0 K)=          -1505.634346 CBS-QB3 Energy=            -1505.620168
 CBS-QB3 Enthalpy=       -1505.619223 CBS-QB3 Free Energy=       -1505.678155
 ---------------------------------------------------------------------------
!+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
 END OF GAUSSIAN OUTPUT FILENAME: TS-NSU3-dimer-qb3.log
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 GAUSSIAN OUTPUT FILENAME: TS-NSU3-NSU1-m062x.log
!+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++

 1)LEVEL OF THEORY: M062X/DEF2TZVP
 Charge = 0 Multiplicity = 1  Stoichiometry    C3H3N3OS

 ---------------------------------------------------------------------
 ---------------------- OPTIMIZED GEOMETRY ---------------------------
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          7           0       -0.841605   -0.227949   -0.000000
      2          7           0        1.323597    0.625141    0.000000
      3          6           0        0.000000    0.799723    0.000000
      4          6           0       -0.369710   -1.530435   -0.000000
      5          6           0        1.120030   -1.606360   -0.000000
      6          7           0        1.906721   -0.601272    0.000000
      7          1           0        1.572712   -2.589767   -0.000000
      8         16           0       -0.906419    2.243706    0.000000
      9          1           0       -1.750181    0.840944    0.000000
     10          8           0       -1.062745   -2.513155   -0.000000
     11          1           0        1.959222    1.405756    0.000000
 ---------------------------------------------------------------------
 Rotational constants (GHZ):           3.4328916           1.4114974           1.0002330

 ---------------------------------------------------------------------------
 -------------------- FREQUENCIES AND ROTATIONAL CONSTANTS -----------------
 ---------------------------------------------------------------------------
 INDEX NO. DOF TYPE  CM-1(UNSCALED)  CM-1(SCALED BY ) SYMMETRY IR-INTENSITY
    1        vib       -1615.61           0.00               A'     1532.2104
    2        vib         140.89           0.00               A"        0.9230
    3        vib         156.50           0.00               A"        0.0222
    4        vib         304.95           0.00               A'        6.7675
    5        vib         440.22           0.00               A"        2.1482
    6        vib         448.09           0.00               A'        6.6233
    7        vib         538.50           0.00               A'        9.1700
    8        vib         585.84           0.00               A'       32.7082
    9        vib         608.79           0.00               A"       56.5121
   10        vib         655.17           0.00               A"       48.7119
   11        vib         698.80           0.00               A'       12.1536
   12        vib         769.17           0.00               A"        0.6676
   13        vib         881.62           0.00               A"       21.2600
   14        vib         951.46           0.00               A"        9.9742
   15        vib         960.47           0.00               A'        1.7126
   16        vib        1060.34           0.00               A'       42.7513
```

| | | | | | |
|---|---|---|---|---|---|
| 17 | vib | 1088.16 | 0.00 | A' | 2.3310 |
| 18 | vib | 1233.00 | 0.00 | A' | 33.8319 |
| 19 | vib | 1321.99 | 0.00 | A' | 150.9829 |
| 20 | vib | 1360.68 | 0.00 | A' | 169.1611 |
| 21 | vib | 1518.08 | 0.00 | A' | 209.3523 |
| 22 | vib | 1546.35 | 0.00 | A' | 522.0013 |
| 23 | vib | 1705.31 | 0.00 | A' | 8.8472 |
| 24 | vib | 1802.96 | 0.00 | A' | 23.9008 |
| 25 | vib | 1842.46 | 0.00 | A' | 526.4285 |
| 26 | vib | 3224.16 | 0.00 | A' | 0.2037 |
| 27 | vib | 3658.28 | 0.00 | A' | 146.2294 |
| 28 | rot | 0.1145089 | - | | |
| 29 | rot | 0.0470825 | - | | |
| 30 | rot | 0.0333642 | - | | |

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---------- ZPE & THERMAL CONTRIBUTIONS ----------
---

Eelectronic [kJ/mol] = -1978886.559
Ezpe [kJ/mol] = +176.462
Eelectronic+Ezpe [kJ/mol] = -1978710.097

Eelectronic [hartrees] = -753.717981
Ezpe [hartrees] = +0.067211
Eelectronic+Ezpe [hartrees] = -753.650770

Thermal Correction to Energy [kJ/mol] = +192.678
Thermal Correction to Enthalpy [kJ/mol] = +195.156
Thermal Correction to Gibbs [kJ/mol] = +94.773

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GAUSSIAN OUTPUT FILENAME: TS-SU2-SU1-m062x.log
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1)LEVEL OF THEORY: OPT=(TS,CALCFC,NOEIGENTEST,VTIGHT)
Charge = 0 Multiplicity = 1 Stoichiometry C4H4N2OS

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---------- OPTIMIZED GEOMETRY ----------
---

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 7 | 0 | -0.971847 | -0.139562 | -0.000000 |
| 2 | 7 | 0 | 1.282300 | 0.423312 | -0.000000 |
| 3 | 6 | 0 | 0.000000 | 0.777406 | -0.000000 |
| 4 | 6 | 0 | -0.733758 | -1.541525 | 0.000000 |
| 5 | 6 | 0 | 0.675576 | -1.875774 | 0.000000 |
| 6 | 6 | 0 | 1.611151 | -0.899279 | 0.000000 |
| 7 | 1 | 0 | 0.938070 | -2.921769 | 0.000000 |
| 8 | 1 | 0 | 2.670160 | -1.121626 | 0.000000 |
| 9 | 16 | 0 | -0.074963 | 2.483346 | -0.000000 |
| 10 | 1 | 0 | 1.422698 | 1.798160 | -0.000000 |
| 11 | 8 | 0 | -1.672503 | -2.298007 | 0.000000 |
| 12 | 1 | 0 | -1.942491 | 0.144534 | -0.000000 |

---

Rotational constants (GHZ): 3.8585658 1.2880472 0.9656865

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---------- FREQUENCIES AND ROTATIONAL CONSTANTS ----------
---

| INDEX NO. | DOF TYPE | CM-1(UNSCALED) | CM-1(SCALED BY ) | SYMMETRY | IR-INTENSITY |
|---|---|---|---|---|---|
| 1 | vib | -1622.57 | 0.00 | A' | 1458.1710 |
| 2 | vib | 138.80 | 0.00 | A" | 0.9629 |
| 3 | vib | 179.48 | 0.00 | A" | 5.2643 |

```
    4        vib         303.56           0.00              A'        2.4270
    5        vib         412.83           0.00              A"       13.7792
    6        vib         478.37           0.00              A'       20.7286
    7        vib         533.32           0.00              A'        2.4834
    8        vib         553.29           0.00              A'        5.2717
    9        vib         633.81           0.00              A"        4.6729
   10        vib         722.63           0.00              A"       51.9697
   11        vib         738.79           0.00              A'       15.2217
   12        vib         769.22           0.00              A"        6.0141
   13        vib         844.10           0.00              A"       57.1592
   14        vib         867.86           0.00              A"       15.8955
   15        vib         900.59           0.00              A'       11.3065
   16        vib        1017.07           0.00              A"        0.2552
   17        vib        1028.81           0.00              A'       26.6730
   18        vib        1108.24           0.00              A'       21.5281
   19        vib        1175.21           0.00              A'       47.8526
   20        vib        1222.07           0.00              A'       25.8980
   21        vib        1298.98           0.00              A'      137.8138
   22        vib        1436.00           0.00              A'        0.5680
   23        vib        1509.77           0.00              A'       36.1318
   24        vib        1538.51           0.00              A'      802.5079
   25        vib        1659.26           0.00              A'      147.8476
   26        vib        1822.98           0.00              A'      325.2428
   27        vib        1834.62           0.00              A'      396.7832
   28        vib        3229.74           0.00              A'        6.1758
   29        vib        3269.18           0.00              A'        1.9717
   30        vib        3603.80           0.00              A'       84.2119
   31        rot      0.1287079           -
   32        rot      0.0429646           -
   33        rot      0.0322118           -
 ---------------------------------------------------------------------------

 ---------------------------------------------------------------------------
 ------------------------ ZPE & THERMAL CONTRIBUTIONS --------------------------
 ---------------------------------------------------------------------------
 Eelectronic                    [kJ/mol]   = -1936863.153
 Ezpe                           [kJ/mol]   = +208.336
 Eelectronic+Ezpe               [kJ/mol]   = -1936654.817

 Eelectronic                    [hartrees] = -737.712113
 Ezpe                           [hartrees] = +0.079351
 Eelectronic+Ezpe               [hartrees] = -737.632762

 Thermal Correction to Energy   [kJ/mol]   = +224.617
 Thermal Correction to Enthalpy [kJ/mol]   = +227.095
 Thermal Correction to Gibbs    [kJ/mol]   = +126.820
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 GAUSSIAN OUTPUT FILENAME: TS-SU2-SU1.log
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 1)LEVEL OF THEORY: OPT=(TS,CALCFC,NOEIGENTEST,VTIGHT)
 Charge = 0 Multiplicity = 1  Stoichiometry    C4H4N2OS

 ---------------------------------------------------------------------
 ---------------------- OPTIMIZED GEOMETRY ---------------------------
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          7           0       -0.978382   -0.131991    0.000000
      2          7           0        1.286005    0.412031   -0.000000
      3          6           0       -0.000000    0.781602    0.000000
      4          6           0       -0.747220   -1.544357   -0.000000
      5          6           0        0.657837   -1.884254   -0.000000
      6          6           0        1.605963   -0.911004   -0.000000
```

```
      7          1           0        0.917258   -2.931526   -0.000000
      8          1           0        2.663439   -1.141923   -0.000000
      9         16           0       -0.047929    2.493257    0.000000
     10          1           0        1.459538    1.788822    0.000000
     11          8           0       -1.697292   -2.296785   -0.000000
     12          1           0       -1.947875    0.154587    0.000000
 ---------------------------------------------------------------------
 Rotational constants (GHZ):           3.8498870           1.2773895           0.9591457

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 -------------------- FREQUENCIES AND ROTATIONAL CONSTANTS ----------------------
 --------------------------------------------------------------------------------
 INDEX NO. DOF TYPE  CM-1(UNSCALED)  CM-1(SCALED BY ) SYMMETRY IR-INTENSITY
    1        vib       -1622.43           0.00               A'     1329.5291
    2        vib         133.67           0.00               A"        0.9435
    3        vib         178.84           0.00               A"        4.8891
    4        vib         298.09           0.00               A'        2.1722
    5        vib         414.12           0.00               A"       13.4740
    6        vib         473.54           0.00               A'       20.0482
    7        vib         525.26           0.00               A'        1.9580
    8        vib         553.33           0.00               A'        5.8639
    9        vib         625.67           0.00               A"        6.0406
   10        vib         710.37           0.00               A"       50.4785
   11        vib         733.34           0.00               A'       11.1688
   12        vib         755.98           0.00               A"        3.8709
   13        vib         831.85           0.00               A"       52.7049
   14        vib         862.80           0.00               A"       14.2887
   15        vib         874.29           0.00               A'        8.8477
   16        vib         994.95           0.00               A"        0.2883
   17        vib        1015.67           0.00               A'       18.5064
   18        vib        1097.44           0.00               A'       25.8876
   19        vib        1149.92           0.00               A'       33.3687
   20        vib        1211.78           0.00               A'       42.3409
   21        vib        1291.78           0.00               A'      154.4907
   22        vib        1423.91           0.00               A'        1.9991
   23        vib        1483.62           0.00               A'       35.8905
   24        vib        1505.36           0.00               A'      597.9554
   25        vib        1613.76           0.00               A'      121.2851
   26        vib        1775.23           0.00               A'      635.6522
   27        vib        1810.26           0.00               A'        8.5806
   28        vib        3194.07           0.00               A'        7.7159
   29        vib        3233.58           0.00               A'        0.2115
   30        vib        3577.80           0.00               A'       67.1892
   31        rot      0.1284184           -
   32        rot      0.0426091           -
   33        rot      0.0319937           -
 --------------------------------------------------------------------------------

 --------------------------------------------------------------------------------
 ------------------------ ZPE & THERMAL CONTRIBUTIONS ---------------------------
 --------------------------------------------------------------------------------
 Eelectronic                    [kJ/mol]   = -1937313.533
 Ezpe                           [kJ/mol]   = +205.461
 Eelectronic+Ezpe               [kJ/mol]   = -1937108.072

 Eelectronic                    [hartrees] = -737.883654
 Ezpe                           [hartrees] = +0.078256
 Eelectronic+Ezpe               [hartrees] = -737.805398

 Thermal Correction to Energy   [kJ/mol]   = +221.902
 Thermal Correction to Enthalpy [kJ/mol]   = +224.380
 Thermal Correction to Gibbs    [kJ/mol]   = +123.790
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 GAUSSIAN OUTPUT FILENAME: TS-SU3-SU1-m062x.log
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1)LEVEL OF THEORY: M062X/DEF2TZVP
Charge = 0 Multiplicity = 1  Stoichiometry  C4H4N2OS

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---------- OPTIMIZED GEOMETRY ----------

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 7 | 0 | -0.823697 | -0.222908 | 0.000000 |
| 2 | 7 | 0 | 1.336791 | 0.666041 | -0.000000 |
| 3 | 6 | 0 | 0.000000 | 0.808042 | 0.000000 |
| 4 | 6 | 0 | -0.376064 | -1.550951 | 0.000000 |
| 5 | 6 | 0 | 1.092410 | -1.683434 | -0.000000 |
| 6 | 6 | 0 | 1.881872 | -0.605635 | -0.000000 |
| 7 | 1 | 0 | 1.505538 | -2.680320 | -0.000000 |
| 8 | 1 | 0 | 2.961525 | -0.650572 | -0.000000 |
| 9 | 16 | 0 | -0.922621 | 2.249592 | 0.000000 |
| 10 | 1 | 0 | -1.748477 | 0.854715 | 0.000000 |
| 11 | 8 | 0 | -1.132445 | -2.488983 | 0.000000 |
| 12 | 1 | 0 | 1.921947 | 1.484500 | -0.000000 |

Rotational constants (GHZ):  3.3513045  1.3989569  0.9869627

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---------- FREQUENCIES AND ROTATIONAL CONSTANTS ----------

| INDEX NO. | DOF TYPE | CM-1(UNSCALED) | CM-1(SCALED BY ) | SYMMETRY | IR-INTENSITY |
|---|---|---|---|---|---|
| 1 | vib | -1590.74 | 0.00 | A' | 1472.0234 |
| 2 | vib | 144.58 | 0.00 | A" | 0.7232 |
| 3 | vib | 158.01 | 0.00 | A" | 0.4367 |
| 4 | vib | 304.88 | 0.00 | A' | 6.4448 |
| 5 | vib | 416.85 | 0.00 | A" | 5.4612 |
| 6 | vib | 445.32 | 0.00 | A' | 10.5303 |
| 7 | vib | 547.73 | 0.00 | A' | 4.1993 |
| 8 | vib | 571.21 | 0.00 | A' | 11.8250 |
| 9 | vib | 575.88 | 0.00 | A" | 78.3845 |
| 10 | vib | 641.35 | 0.00 | A" | 0.6327 |
| 11 | vib | 712.43 | 0.00 | A' | 15.0271 |
| 12 | vib | 745.73 | 0.00 | A" | 7.9075 |
| 13 | vib | 848.51 | 0.00 | A" | 52.2550 |
| 14 | vib | 881.29 | 0.00 | A" | 13.3862 |
| 15 | vib | 937.10 | 0.00 | A' | 8.4011 |
| 16 | vib | 992.43 | 0.00 | A" | 0.0089 |
| 17 | vib | 1030.93 | 0.00 | A' | 45.5564 |
| 18 | vib | 1076.34 | 0.00 | A' | 9.8010 |
| 19 | vib | 1206.32 | 0.00 | A' | 8.5995 |
| 20 | vib | 1217.37 | 0.00 | A' | 6.7842 |
| 21 | vib | 1304.01 | 0.00 | A' | 290.5481 |
| 22 | vib | 1423.02 | 0.00 | A' | 2.1820 |
| 23 | vib | 1523.12 | 0.00 | A' | 189.1160 |
| 24 | vib | 1569.12 | 0.00 | A' | 607.4026 |
| 25 | vib | 1714.05 | 0.00 | A' | 71.4062 |
| 26 | vib | 1807.17 | 0.00 | A' | 157.1438 |
| 27 | vib | 1830.53 | 0.00 | A' | 472.2374 |
| 28 | vib | 3240.07 | 0.00 | A' | 2.0672 |
| 29 | vib | 3262.22 | 0.00 | A' | 0.9616 |
| 30 | vib | 3665.06 | 0.00 | A' | 128.8569 |
| 31 | rot | 0.1117875 | - | | |
| 32 | rot | 0.0466642 | - | | |
| 33 | rot | 0.0329215 | - | | |

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---------- ZPE & THERMAL CONTRIBUTIONS ----------

Eelectronic  [kJ/mol]  = -1936837.806
Ezpe  [kJ/mol]  = +208.105
Eelectronic+Ezpe  [kJ/mol]  = -1936629.701

Eelectronic  [hartrees] = -737.702459

```
 Ezpe                             [hartrees] = +0.079263
 Eelectronic+Ezpe                 [hartrees] = -737.623196

 Thermal Correction to Energy   [kJ/mol]   = +224.659
 Thermal Correction to Enthalpy [kJ/mol]   = +227.137
 Thermal Correction to Gibbs    [kJ/mol]   = +126.315
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