Supporting Information

Solid-State and Gas-Phase Structures and Energetic Properties of the Dangerous Methyl and Fluoromethyl Nitrates

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Table of contents

1.1. General procedures ........................................................................................................ 3
1.2. Synthesis .......................................................................................................................... 3
  1.2.1. Fluoromethyl nitrate (FMN) ......................................................................................... 3
  1.2.2. Methyl nitrate (MN) .................................................................................................... 4
  1.2.3. Methylene dinitrate (MDN) .......................................................................................... 4
1.3. NMR spectra (CD$_2$CN, 26 °C) ...................................................................................... 5
  1.3.1. NMR spectra (FMN) ..................................................................................................... 5
  1.3.2. NMR spectra (MN) ..................................................................................................... 9
  1.3.3. NMR spectra (MDN) .................................................................................................. 11
  1.3.4. NMR spectra of MDN decomposition products ........................................................... 12
1.4. Raman spectra .................................................................................................................. 15
  1.4.1. IR spectrum (FMN) ....................................................................................................... 14
  1.4.2. IR spectrum (MN) ....................................................................................................... 14
  1.4.3. IR spectrum (MDN) ..................................................................................................... 15
1.5. Raman spectra .................................................................................................................. 15
  1.5.1. Raman spectrum (FMN) ............................................................................................... 15
  1.5.2. Raman spectrum (MN) ............................................................................................... 16
  1.5.3. Raman spectrum (MDN) ............................................................................................. 16
2. Calculations ......................................................................................................................... 17
  2.1. Theory ............................................................................................................................. 17
    2.1.1. Enthalpy of formation ................................................................................................. 17
    2.1.2. Enthalpy of sublimation / vaporization ..................................................................... 17
    2.1.3. Heat of formation (Enthalpy of formation) ............................................................... 17
  2.2. Heat of formation calculation results ............................................................................ 18
  2.3. EXPLO05 calculation results ......................................................................................... 19
    2.3.1. Results for FMN ........................................................................................................ 19
    2.3.2. Results for MN .......................................................................................................... 21
    2.3.3. Results for NG ........................................................................................................... 23
  2.4. Calculations for structure determination ....................................................................... 25
    2.4.1. Calculated Cartesian Coordinates of MN ................................................................. 27
    2.4.2. Calculated Cartesian Coordinates of FMN ................................................................. 28
  3. Structure Determination .................................................................................................... 31
  3.1. X-ray Crystallography .................................................................................................. 31
  3.2. Gas-phase electron diffraction ....................................................................................... 34
    3.2.1. Experiment ................................................................................................................. 34
3.2.2 Experimental (black dots) and model (red line) radial distribution curve as well as difference curve (below) for the refinement of FMN. Vertical bars (blue) indicate individual diatomic contributions to the total intensity. .................................................. 35

3.2.3 First sets of experimental reduced electron diffraction intensities and background lines of MN (top) and FMN (bottom) for middle and long camera settings. ........................................... 36

3.2.5 Structural Analysis of MN .................................................................................................................. 37

3.2.5 Structural Analysis of FMN ............................................................................................................... 41

3.2.6 Electron diffraction intensities of MN .............................................................................................. 43

3.2.7 Electron diffraction intensities of FMN ............................................................................................ 53

Bibliography .................................................................................................................................................. 62
1.1. General procedures

All compounds were handled using Schlenk techniques under dry Ar. Silver nitrate, purchased from VWR, was dried in vacuo at room temperature for 30 min and fluoroiodomethane (donation from F-Select GmbH) was distilled under inert conditions before use. Melting points were determined on the X-ray diffractometer with an Oxford Cryosystem/ Cryostream controller of the 700 series. Boiling points were determined using the Siwoloboff method in a Büchi B-540 apparatus using a heating rate of 1 °C min⁻¹.¹ The sensitivities towards impact and friction were determined with a BAM ball-drop and a BAM friction tester, respectively (method 1 out of 6).² The samples for infrared spectroscopy were placed under ambivalent conditions without further preparation onto an Smith DuraSampLIR II ATR device using a Perkin Elmer BX II FR-IR System spectrometer. Samples for Raman spectroscopy were sealed in glass tubes. The measurement was carried out on a Bruker MultiRam FT Raman device using a neodymium-doped yttrium aluminum garnet (Nd:YAG) laser (λ = 1064 nm) with 1074 mW. The samples for NMR spectroscopy were prepared under inert atmosphere using Ar as protective gas. The solvent CD₃CN was dried using 3 Å mol sieve and stored under Ar atmosphere. Spectra were recorded on a Bruker Avance III spectrometer operating at 400.1 MHz (¹H), 376.4 MHz (¹⁹F), 100.6 MHz (¹³C), 54.2 MHz (¹⁷O), 40.6 MHz (¹⁵N) and 28.9 MHz (¹⁴N). Chemical shifts are referred to TMS (¹H/¹³C), CFCl₃ (¹⁹F), H₂O (¹⁷O), MeNO₂ (¹⁴N/¹⁵N). All spectra were recorded at 299.15 K (26 °C). Elemental analyses were performed with an Elemental Vario EL Analyzer.

Caution! MN and FMN are highly energetic materials with high sensitivities towards impact and friction. Even if no accident has occurred during the synthesis and manipulation of these compounds, additional proper protective precautions like ear plugs, Kevlar gloves, face shield, shatterproof jacket and helmet, Kevlar arm guards and heavy armored blast shields should be used when undertaking work with these compounds.

1.2. Synthesis

1.2.1. Fluoromethyl nitrate (FMN)

The reaction was performed under Argon as inert gas. Finely mortared AgNO₃ (9.42 g, 55.5 mmol, 15 eq) was placed into a small Schlenk tube. Fluoroiodomethane (0.25 mL, 3.7 mmol, 1 eq) was slowly injected through a septum on top of the silver nitrate under cooling at 0 °C. The mixture was reacted without stirring for 45 min at room temperature. Then the septum was replaced by another Schlenk tube, into which the product was condensed. The product was obtained in quantitative yield (0.35 g, 99.7%) as a colorless liquid with high vapor pressure.

\[ T_{\text{melting}} = -91 \degree \text{C}; \quad T_{\text{boiling}} = 58 \degree \text{C}; \]

¹H NMR: \( \delta = 5.99 \) (d, \( 2J(F,H) = 52.0 \) Hz, 2H, CH₂F);
¹³C NMR: \( \delta = 99.1 \) (dt, \( 1J(F,C) = 228.8 \) Hz, \( 1J(C,H) = 182 \) Hz, CH₂F);
¹³C\{¹H\} NMR: \( \delta = 99.1 \) (d, \( 1J(F,C) = 228.8 \) Hz, CH₂F);
¹⁹F\{¹H\} NMR: \( \delta = -155.9 \) (s, CH₂F);
¹⁹F NMR: \( \delta = -155.9 \) (t, \( 2J(F,H) = 52.0 \) Hz, CH₂F);
¹⁷O NMR: \( \delta = 446 \) (2O, NO₂), 363 (1O, FCH₂O);
¹⁵N\{¹H\} NMR: \( \delta = -52.3 \) (d, \( 3J(N,H) = 1.7 \) Hz, NO₂);
¹⁵N NMR: \( \delta = -52.3 \) (td, \( 3J(N,H) = 7.0 \) Hz, \( 3J(F,N) = 1.7 \) Hz, NO₂).
IR: $\tilde{\nu} = 1670$ (s, $\nu_{as}$NO$_2$), 1461 (w), 1291 (s, $\nu_{s}$NO$_2$), 1047 (m, $\nu$CF), 997 (s), 811 (s, $\nu$NO), 760 (m, $\gamma$wNO$_2$), 654 (m, $\delta$NO$_2$), 575 (m), 456 (w) cm$^{-1}$.

Raman: $\tilde{\nu} = 3054$ (w), 2997 (s), 2906 (w), 2799 (w), 1689 (w, $\nu_{as}$NO$_2$), 1462 (w), 1412 (w), 1296 (m, $\nu_{s}$NO$_2$), 1049 (w, $\nu$CF), 1005 (w), 822 (m, $\nu$NO), 660 (w, $\delta$NO$_2$), 579 (m), 458 (m), 364 (m) cm$^{-1}$.

EA calcd (%) for CH$_2$FNO$_3$: C 12.64, H 2.12, N 14.74; found: C 12.83, H 2.17, N 15.03.

1.2.2. Methyl nitrate (MN)
The reaction was performed analogous to the above for FMN, by using AgNO$_3$ (10.6 g, 62.6 mmol, 15 eq) and iodomethane (0.26 mL, 4.1 mmol, 1 eq) instead of fluoriodomethane. The product was obtained in nearly quantitative yield (0.32 g, 99.5%) as a colorless liquid. $T_{melt} \sim$83°C; $T_{boil}$ 65°C;

$^1$H NMR: $\delta = 4.10$ (s, CH$_3$);

$^{13}$C($^1$H) NMR: $\delta = 61.1$ (s, CH$_3$);

$^{17}$O NMR: $\delta = 446$ (2O, NO$_2$), 310 (1O, H$_3$CO);

$^{15}$N($^1$H) NMR: $\delta = -39.9$ (s, ONO$_2$);

$^{15}$N NMR: $\delta = -39.9$ (q, $^3$$J$(N,H) = 3.9 Hz, ONO$_2$);

IR: $\tilde{\nu} = 1622$ (s, $\nu_{as}$NO$_2$), 1428 (w), 1281 (s, $\nu_{s}$NO$_2$), 989 (s), 854 (s, $\nu$NO), 760 (m, $\gamma$wNO$_2$), 652 (m, $\delta$NO$_2$), 578 (w) cm$^{-1}$.

Raman: $\tilde{\nu} = 3041$ (w), 2963 (s), 2902 (w), 2833 (w), 1636 (w, $\nu_{as}$NO$_2$), 1525 (w), 1438 (w), 1285 (m, $\nu_{s}$NO$_2$), 1176 (w), 991 (w), 860 (m, $\nu$NO), 664 (w, $\delta$NO$_2$), 579 (m), 354 (w) cm$^{-1}$.

EA calcd (%) for CH$_3$NO$_3$: C 15.59, H 3.93, N 18.18; found: C 15.77, H 3.89, N 18.55.

1.2.3. Methylene dinitrate (MDN)
The reaction was performed under Argon as inert gas. Finely mortared AgNO$_3$ (0.807 g, 4.75 mmol, 2.5 eq) was placed into a Schlenk flask containing 5 mL dry acetonitrile. Subsequently, diiodomethane (0.15 mL, 1.9 mmol, 1 eq) was slowly added under cooling. The solution was reacted at 50°C for 48 h. Acetonitrile was removed under reduced pressure and MDN was obtained as a slightly yellowish liquid.

$^1$H NMR: $\delta = 6.29$ (s, CH$_3$);

$^{13}$C($^1$H) NMR: $\delta = 89.7$ (s, CH$_3$);

$^{14}$N NMR: $\delta = -18$ (ONO$_2$);

IR: $\tilde{\nu} = 3056$ (w), 2947 (w), 1759 (w), 1657 (s, $\nu_{as}$NO$_2$), 1422 (m), 1276 (s, $\nu_{s}$NO$_2$), 1227 (w), 1118 (w), 1071 (w), 1015 (m), 958 (s, $\nu$CON), 838 (w, $\nu$NO), 782 (s, $\nu$NO), 745 (s, $\gamma$wNO$_2$) cm$^{-1}$.

Raman: $\tilde{\nu} = 3056$ (w), 2998 (s), 2946 (w), 1685 (w, $\nu_{as}$NO$_2$), 1426 (w), 1298 (m, $\nu_{s}$NO$_2$), 1023 (w), 840 (s, $\nu$NO), 605 (s, $\delta$NO$_2$), 569 (m), 419 (w), 250 (m) cm$^{-1}$.
1.3. NMR spectra (CD$_2$CN, 26 °C)

1.3.1. NMR spectra (FMN)

$^1$H NMR

$^{19}$F($^1$H) NMR
$^{19}$F NMR

$^{13}$C(¹H) NMR
$^{17}$O NMR
1.3.2. NMR spectra (MN)

$^1$H NMR

$^{13}$C($^1$H) NMR

$^{15}$N NMR
$^{17}O$ NMR
1.3.3. NMR spectra (MDN)

$^1$H NMR

$^{13}$C NMR

$^{14}$N NMR
1.3.4. NMR spectra of MDN decomposition products

$^1$H NMR

$^{19}$F$^1$H) NMR

$^{19}$F NMR
$^{13}$C NMR

$^{14}$N NMR
1.4. IR spectra

1.4.1. IR spectrum (FMN)

1.4.2. IR spectrum (MN)
1.4.3. IR spectrum (MDN)

1.5. Raman spectra

1.5.1. Raman spectrum (FMN)
1.5.2. Raman spectrum (MN)

![Raman spectrum (MN)](image)

1.5.3. Raman spectrum (MDN)

![Raman spectrum (MDN)](image)
2. Calculations

2.1. Theory

2.1.1. Enthalpy of formation
Using the atomization energy method, based on the atomization energies in Table 1, the enthalpy of formation of the molecule in the gas phase can first be calculated.\[3\]

\[
\Delta H^\circ_{f,\text{gas,298K,Molecule}} = H_{\text{Molecule,298K}} - \sum n \cdot H^\circ_{\text{Atom,298K}} + \sum n \cdot \Delta H^\circ_{f,\text{Atom,298K}}
\]

\[
\Delta H^\circ_{f,\text{gas,298K,Molecule}} = \text{Enthalpy of formation of the gas phase species molecule}
\]

\[H_{\text{Molecule,298K}} = \text{Total energy of the gas phase (formation from atomic nuclei and electrons)}\]

\[H^\circ_{\text{Atom,298K}} = \text{CBS - 4M electronic enthalpies}\]

\[\Delta H^\circ_{f,\text{Atom,298K}} = \text{Standard enthalpy of formation of gaseous atoms}\]

\[n = \text{atomic number}\]

| \(H^\circ_{\text{Atom,298K}} [\text{a.u.}]\) | \(\Delta H^\circ_{f,\text{Atom,298K}} [\text{kJ mol}^{-1}]\) |
|---|---|
| H | -0.500991 | 217.998 |
| C | -37.786156 | 716.68 |
| N | -54.522462 | 472.68 |
| O | -74.991202 | 249.18 |
| F | -99.649394 | 79.38 |

2.1.2. Enthalpy of sublimation / vaporization
In order to obtain the energy of formation at the condensed (liquid/ solid) phase, the corresponding enthalpy of sublimation must first be calculated (Trouton’s Rule).\[4\]

\[\Delta H^\circ_v = 90 \cdot T_{\text{boil}}\]

\[\Delta H^\circ_v = \text{Enthalpy of vaporisation}\]

\[T_{\text{boil}} = \text{Boiling point of the compound}\]

2.1.3. Heat of formation (Enthalpy of formation)
The heat of formation of the compound results from the subtraction of the heat of formation vaporization from the heat of formation of the gas phase species.\[4\]

\[\Delta H^\circ_f (\text{liquid}) = \Delta H^\circ_{f,\text{gas,298K,Molecule}} - \Delta H^\circ_v\]

\[\Delta H^\circ_f (\text{liquid}) = \text{Heat of formation of the liquid product}\]
2.2. Heat of formation calculation results
The results of the calculation for the heat of formation are shown in Table 2. The theoretical value of MN is in good agreement compared to the experimentally determined value of $\Delta H^\circ_f (\text{liquid})$ of MN ($-156.3 \text{ kJ mol}^{-1}$). [5]

Table 2. Heat of formation calculation results

| M    | $H_{(\text{molecule},298K)}$ [a.u.] | $\Delta H^\circ_f (\text{gas,298K,molecule})$ [kJ mol$^{-1}$] | $\Delta H^\circ_v$ [kJ mol$^{-1}$] | $\Delta H^\circ_f (\text{liquid})$ [kJ mol$^{-1}$] | $\Delta n$ | $\Delta U^\circ$ [kJ mol$^{-1}$] |
|------|-------------------------------------|-------------------------------------------------|-----------------------------------|----------------------------------|---------|-------------------------------|
| FMN  | -418.994048                         | -331.9                                          | 29.8                              | -361.7                           | -3.5    | -353.1                        |
| MN   | -319.822235                         | -131.8                                          | 30.4                              | -162.3                           | -3.5    | -153.6                        |
### 2.3. EXPLO05 calculation results

#### 2.3.1. Results for FMN

Reactant information: FMN, 100 %, C₁ H₂ N₁ O₃ F

|                          |                |
|--------------------------|----------------|
| Molecular weight         | 95.03          |
| Density of explosive     | 1.28 g/cm³     |
| Oxygen balance           | 8.41778 %      |
| Enthalpy of formation    | -3806.13 kJ/kg |
| Internal energy of formation | -3714.83 kJ/kg |

Detonation parameters (at the C-J point):

|                          |                |
|--------------------------|----------------|
| Heat of detonation        | -4449.915 kJ/kg |
| Detonation temperature   | 3827.314 K     |
| Detonation pressure      | 12.29527 GPa   |
| Detonation velocity      | 6132.644 m/s   |
| Particle velocity        | 1566.32 m/s    |
| Sound velocity           | 4566.323 m/s   |
| Density of products      | 1.71906 g/cm³  |
| Volume of products       | 0.5817133 cm³/g |
| Exponent ‘Gamma’         | 2.915319       |
| Moles of gaseous products| 3.251744 mol/mol explosive |
| Moles of condensed products | 0 mol/mol explosive |
| Volume of gas at STP     | 836.8284 dm³/kg |
| Mean molecular mass of gas. prod. | 29.2243 g/mol |
| Mean molecular mass of cond.prod. | 12.011 g/mol |
| Mean molecular mass of all prod. | 29.2243 g/mol |
| Entropy of products      | 7.15572 kJ/kg K |
| Internal energy of products | 5676.604 kJ/kg, i.e. 7.266053 kJ/cm³ |
| Compression energy       | 1226.689 kJ/kg, i.e. 1.570162 kJ/cm³ |
| Total heat energy        | -4449.9151 kJ/kg, i.e. -5.69589 kJ/cm³ |
### Composition of detonation products:

| Products | mol/mol | mol/kg | Mol % |
|----------|---------|--------|-------|
| HF       | 0.9892425 | 10.40968 | 30.42191 |
| CO₂      | 0.9786295 | 10.298 | 30.09553 |
| H₂O      | 0.5026178 | 5.288989 | 15.45687 |
| N₂       | 0.4798901 | 5.049828 | 14.75793 |
| O₂       | 0.2335356 | 2.457467 | 7.181857 |
| CO       | 0.02864648 | 0.3014435 | 0.8809574 |
| NO       | 0.01903141 | 0.2002653 | 0.5852679 |
| O        | 0.00586574 | 0.06172444 | 0.1803874 |
| NFO      | 0.00557624 | 0.0587814 | 0.1714874 |
| NO₂      | 0.00311801 | 0.03281048 | 0.0958874 |
| OH       | 0.00214027 | 0.02252176 | 0.06581901 |
| CH₂O₂    | 0.00119556 | 0.01258075 | 0.03676677 |
| FO       | 0.00103945 | 0.01093796 | 0.03196578 |
| H₂       | 0.00043724 | 0.00460101 | 0.01344627 |
| CF₄      | 0.000014397 | 0.000435614 | 0.01273064 |
| CFO      | 0.00010483 | 0.00110308 | 0.00322372 |
| H        | 0.000010304 | 0.000108424 | 0.000316864 |
| HFO      | 6.05E−05 | 0.00063662 | 0.0018605 |
| F₂       | 4.30E−05 | 0.00045231 | 0.00132187 |
| N₂O      | 4.17E−05 | 0.00043851 | 0.00128153 |
| NH₃      | 5.25E−06 | 5.52E−05 | 0.00016144 |
| N        | 2.23E−06 | 2.35E−05 | 6.87E−05 |
| NF       | 2.09E−06 | 2.19E−05 | 6.41E−05 |
| CNO      | 4.86E−07 | 5.11E−06 | 1.49E−05 |
| HCN      | 2.81E−07 | 2.96E−06 | 8.66E−06 |
| CHNO     | 1.03E−07 | 1.08E−06 | 3.16E−06 |
| CH₂F₂    | 9.35E−08 | 9.83E−07 | 2.87E−06 |
| CF₂O     | 3.85E−08 | 4.05E−07 | 1.18E−06 |
| C₂F₂     | 8.85E−09 | 9.31E−08 | 2.72E−07 |
| CFN      | 2.82E−09 | 2.97E−08 | 8.67E−08 |
| CF       | 1.63E−10 | 1.71E−09 | 5.01E−09 |
| CH₂OH    | 1.03E−10 | 1.08E−09 | 3.17E−09 |

### Running parameters:
- Equation of state: BKW EOS
- 'BKWN' set of constants
- Covolumes set 1 (Alpha=0.5, Beta=0.38, Kappa=9.32, Theta=4120)
- Activity: Model 1: Condensed products form pure phase (Default)
### 2.3.2. Results for MN

Reactant information: MN, 100 %, C\textsubscript{1} H\textsubscript{3} N\textsubscript{1} O\textsubscript{3}

| Property                                    | Value                        |
|---------------------------------------------|------------------------------|
| Molecular weight                            | 77.04                        |
| Density of explosive                        | 1.21 g/cm\textsuperscript{3}  |
| Oxygen balance                              | −10.3837 %                   |
| Enthalpy of formation                       | −2106.73 kJ/kg               |
| Internal energy of formation                | −1994.11 kJ/kg               |
| Detonation parameters (at the C-J point):   |                              |
| Heat of detonation                          | −6020.894 kJ/kg              |
| Detonation temperature                      | 4151.1 K                     |
| Detonation pressure                         | 14.16645 GPa                 |
| Detonation velocity                         | 6652.552 m/s                 |
| Particle velocity                           | 1759.897 m/s                 |
| Sound velocity                              | 4892.655 m/s                 |
| Density of products                         | 1.645239 g/cm\textsuperscript{3}|
| Volume of products                          | 0.6078143 cm\textsuperscript{3}/g |
| Exponent 'Gamma'                            | 2.780081                     |
| Moles of gaseous products                   | 2.909729 mol/mol explosive   |
| Moles of condensed products                 | 5.163047E−12 mol/mol explosive|
| Volume of gas at STP                        | 923.6923 dm\textsuperscript{3}/kg |
| Mean molecular mass of gas. prod.           | 26.47651 g/mol               |
| Mean molecular mass of cond.prod.           | 12.011 g/mol                 |
| Mean molecular mass of all prod.            | 26.47651 g/mol               |
| Entropy of products                         | 8.351068 kJ/kg K             |
| Internal energy of products                 | 7569.523 kJ/kg, i.e. 9.159123 kJ/cm\textsuperscript{3} |
| Compression energy                          | 1548.629 kJ/kg, i.e. 1.873842 kJ/cm\textsuperscript{3} |
| Total heat energy                           | −6020.894 kJ/kg, i.e. −7.285282 kJ/cm\textsuperscript{3} |
Composition of detonation products:

| Products | mol/mol | mol/kg | Mol %  |
|----------|---------|--------|--------|
| H₂O      | 1.370607| 17.79107| 47.10427 |
| CO₂      | 0.5459073| 7.086115| 18.76145 |
| N₂       | 0.4969358| 6.450445| 17.07842 |
| CO       | 0.3687748| 4.786858| 12.67385 |
| H₂O₂     | 0.08433607| 1.094719| 2.898417 |
| H₂       | 0.03632341| 0.4714938| 1.248343 |
| NH₃      | 0.00513521| 0.06665727| 0.1764841 |
| H        | 0.00081916| 0.01063305| 0.02815243 |
| HCN      | 0.00060218| 0.00781662| 0.002069554 |
| NH₂      | 9.71E−05| 0.00126092| 0.00333844 |
| NO₂      | 6.62E−05| 0.00085876| 0.0027369 |
| CNO      | 3.38E−05| 0.00043863| 0.00116132 |
| CH₄      | 2.13E−05| 0.00027611| 0.00073104 |
| CH₂O     | 2.01E−05| 0.00026104| 0.00069114 |
| CHNO     | 1.93E−05| 0.0002504| 0.00066296 |
| CH₂OH    | 1.68E−05| 0.00021798| 0.00057712 |
| N        | 6.38E−06| 8.28E−05| 0.00021916 |
| N₂O      | 3.94E−06| 5.11E−05| 0.00013543 |
| N₂H₄     | 2.63E−06| 3.41E−05| 9.04E−05 |
| C₂H₄     | 9.51E−07| 1.23E−05| 3.27E−05 |
| C₂H₅     | 8.40E−08| 1.09E−06| 2.89E−06 |
| C(gr)    | 2.83E−12| 3.67E−11| 9.72E−11 |
| C(d)     | 2.34E−12| 3.03E−11| 8.03E−11 |

Running parameters:
- Equation of state: BKW EOS
- 'BKWN' set of constants
- Covolumes set 1 (Alpha=0.5, Beta=0.38, Kappa=9.32, Theta=4120)
- Activity: Model 1: Condensed products form pure phase (Default)
### Results for NG

Reactant information: Nitroglycerine (NG), 100 %, $C_3H_5N_3O_9$

| Property                                      | Value                        |
|-----------------------------------------------|------------------------------|
| Molecular weight                              | 227.09                       |
| Density of explosive                          | 1.6 g/cm$^3$                 |
| Oxygen balance                                | 3.52269 %                    |
| Enthalpy of formation                         | $-1632.76$ kJ/kg             |
| Internal energy of formation                  | $-1539.98$ kJ/kg             |

Detonation parameters (at the C–J point):

| Property                                      | Value                        |
|-----------------------------------------------|------------------------------|
| Heat of detonation                            | $-6099.163$ kJ/kg            |
| Detonation temperature                        | 4316.724 K                   |
| Detonation pressure                           | 23.73653 GPa                 |
| Detonation velocity                           | 7850.276 m/s                 |
| Particle velocity                             | 1889.785 m/s                 |
| Sound velocity                                | 5960.492 m/s                 |
| Density of products                           | 2.107283 g/cm$^3$            |
| Volume of products                            | 0.4745447 cm$^3$/g           |
| Exponent ‘Gamma’                              | 3.154059                     |
| Moles of gaseous products                     | 7.26082 mol/mol explosive    |
| Moles of condensed products                   | 0 mol/mol explosive          |
| Volume of gas at STP                          | 781.9567 dm$^3$/kg           |
| Mean molecular mass of gas. prod.             | 31.27573 g/mol               |
| Mean molecular mass of cond.prod.             | 0 g/mol                      |
| Mean molecular mass of all prod.              | 31.27573 g/mol               |
| Entropy of products                            | 7.165994 KJ/kg K             |
| Internal energy of products                   | 7884.813 KJ/kg. i.e. 12.6157 kJ/cm$^3$ |
| Compression energy                            | 1785.651 KJ/kg. i.e. 2.857041 kJ/cm$^3$ |
| Total energy of detonation                    | $-6099.163$ KJ/kg. i.e. $-9.75866$ KJ/cm$^3$ |
Composition of detonation products:

| Products | mol/mol     | mol/kg     | Mol %  |
|----------|-------------|------------|--------|
| CO₂      | 2.854252 E00 | 1.256909 E01 | 39.3103 |
| H₂O      | 2.436451 E00 | 1.072925 E01 | 33.5561 |
| N₂       | 1.468932 E00 | 6.468644 E00 | 20.2309 |
| O₂       | 2.809613 E-01| 1.237252 E00 | 3.8696  |
| CO       | 8.584561 E-02| 3.780330 E-01| 1.1823  |
| CH₃O₂    | 5.988686 E-02| 2.637200 E-01| 0.8248  |
| NO       | 4.629133 E-02| 2.038502 E-01| 0.6375  |
| NO₂      | 1.536168 E-02| 6.764727 E-02| 0.2116  |
| O        | 7.806584 E-03| 3.437737 E-02| 0.1075  |
| OH       | 2.554218 E-03| 1.124785 E-02| 0.0352  |
| H₂       | 1.997825 E-03| 8.797699 E-03| 0.0275  |
| NH₃      | 2.185473 E-04| 9.624031 E-04| 0.0030  |
| N₂O      | 1.164172 E-04| 5.126593 E-04| 0.0016  |
| H        | 1.121857 E-04| 4.940254 E-04| 0.0015  |
| N        | 1.650913 E-05| 7.270021 E-05| 0.0002  |
| CNO      | 1.019812 E-05| 4.490884 E-05| 0.0001  |
| HCN      | 5.271434 E-06| 2.321348 E-05| 0.0001  |
| N₂H₄     | 7.717688 E-08| 3.398590 E-07| 0.0000  |
| CH₃OH    | 2.566241 E-08| 1.130080 E-07| 0.0000  |

Running parameters:
- Equation of state: BKW EOS
- 'BKWN' standard set of constants
- Covolumes set 1 (Alpha=0.5, Beta=0.38, Kappa=9.4, Theta=4120)
- Activity: Model 1: Condensed products form pure phase (Default)
2.4. Calculations for structure determination
The conformational landscape of MN and FMN were elucidated using molecular structures of MN and FMN were optimized with the Gaussian 09 program suite\(^6\) using different DFT functionals (B3LYP, B3PW91, M06-2X, PBE0, TPSSh) in combination with Ahlrichs’ def2-TZVP basis set, and using second order perturbation theory (MP2) in combination with Dunning’s cc-pVTZ for frozen core calculations (fc) and cc-pwCVTZ for calculations with all electrons correlated. The stationary points were located with the Berny algorithm using redundant internal coordinates. Analytical Hessians were computed to determine the nature of stationary points (zero imaginary frequencies for minima). Cubic force fields were calculated at all of the DFT levels mentioned above.

According to these calculations, for MN only the anti-conformer of \(C_\text{s}\) symmetry is a minimum on the potential hypersurface, whereas for FMN the calculations suggest the existence of two minima, one anti conformer of \(C_\text{s}\) symmetry and one asymmetric gauche conformer. The two dimensional scan of the FCON and CONO dihedral angles is shown in the Figure below, calculated relative energies of these are listed in Table 11.
Table 3. Relative electronic ($\Delta E$) and Gibbs free energies ($\Delta G$) in kJ mol$^{-1}$ of the two possible conformers of FMN. Negative values indicate energetic preference for the gauche-conformer.

| Method                  | $\Delta E$ | $\Delta G$ (298 K) |
|-------------------------|------------|---------------------|
| B3LYP-D3/def2-TZVP      | -18.5      | -17.1               |
| B3PW91-D3/def2-TZVP     | -17.8      | -16.6               |
| M06-2X/def2-TZVP        | -15.6      | -14.5               |
| MP2(fc)/cc-pVTZ         | -19.1      | -18.4               |
| MP2(full)/cc-pwCVTZ     | -19.2      | -18.5               |
| PBE0-D3/def2-TZVP       | -17.1      | -16.0               |
| TPSSh/def2-TZVP         | -18.4      | -17.3               |
### 2.4.1. Calculated Cartesian Coordinates of MN

| Method          | Vibration | E (cm⁻¹) |
|-----------------|-----------|----------|
| B3LYP-D3/def2-TZVP | νₙ₉₅ = 140 | E = -320,340669 |
|                 | C         | -0.142295 | -1.7568700 0.000000 |
|                 | O         | 0.708840  | -0.601033 0.000000 |
|                 | N         | 0.000000  | 0.623880 0.000000 |
|                 | O         | 0.722249  | 1.576915 0.000000 |
|                 | O         | -1.203223 | 0.565029 0.000000 |
|                 | H         | 0.561107  | -2.586144 0.000000 |
|                 | H         | -0.765129 | -1.783540 -0.892521 |
|                 | H         | -0.765129 | -1.783540 0.892521 |
| B3PW91-D3/def2-TZVP | νₙ₉₅ = 145 | E = -320,2168415 |
|                 | C         | 0.706633  | -0.593143 0.000000 |
|                 | O         | -0.137915 | -1.743591 0.000000 |
|                 | N         | 0.000000  | 0.617667 0.000000 |
|                 | O         | 0.715752  | 1.571254 0.000000 |
|                 | O         | -1.199013 | 0.554235 0.000000 |
|                 | H         | 0.564938  | -2.574555 0.000000 |
|                 | H         | -0.762211 | -1.773169 -0.892848 |
|                 | H         | -0.762211 | -1.773169 0.892848 |
| M06-2X/def2-TZVP | νₙ₉₅ = 141 | E = -320,1957239 |
|                 | C         | -1.743609 | -0.004963 0.000000 |
|                 | O         | -0.522513 | -0.746131 0.000000 |
|                 | N         | 0.607488  | 0.045685 0.000000 |
|                 | O         | 1.618805  | -0.579515 0.000000 |
|                 | O         | 0.448350  | 1.233221 0.000000 |
|                 | H         | -2.508036 | -0.776600 -0.000011 |
|                 | H         | -1.819925 | 0.612994 -0.891909 |
|                 | H         | -1.819934 | 0.612978 0.891919 |
| MP2(fc)/cc-pVTZ  | νₙ₉₅ = 146 | E = -319.6982628 |
|                 | C         | -1.741774 | -0.006503 0.0000002 |
|                 | O         | -0.531845 | -0.768976 -0.000003 |
|                 | N         | 0.612747  | 0.053058 -0.000003 |
|                 | O         | 1.636808  | -0.580751 0.0000003 |
|                 | O         | 0.433638  | 1.250255 0.000000 |
|                 | H         | -2.517085 | -0.765080 0.0000008 |
|                 | H         | -1.815155 | 0.612633 -0.899352 |
|                 | H         | -1.815145 | 0.612636 0.899354 |
| MP2(full)/cc-pwCVTZ | νₙ₉₅ = 146 | E = -319.9679348 |
|                 | C         | -1.738465 | -0.006354 0.0000002 |
|                 | O         | -0.531407 | -0.766135 -0.000003 |
|                 | N         | 0.612080  | 0.052920 -0.000002 |
|                 | O         | 1.632944  | -0.580195 0.0000003 |
|                 | O         | 0.433972  | 1.247194 0.000000 |
|                 | H         | -2.512918 | -0.763089 0.0000008 |
|                 | H         | -1.812472 | 0.611928 -0.887636 |
|                 | H         | -1.812462 | 0.611932 0.887638 |
| PBE0-D3/def2-TZVP | νₙ₉₅ = 147 | E = -319.9950741 |
|                 | C         | -1.741623 | -0.004342 0.0000001 |
|                 | O         | -0.527709 | -0.748377 -0.000002 |
|                 | N         | 0.610694  | 0.048158 0.000001 |
|                 | O         | 1.619151  | -0.583279 0.000001 |
|                 | O         | 0.450055  | 1.235407 -0.000001 |
|                 | H         | -2.511996 | -0.773240 -0.000012 |
|                 | H         | -1.822547 | 0.616097 -0.892579 |
|                 | H         | -1.822555 | 0.616075 0.892596 |
| TPSSh/def2-TZVP  | νₙ₉₅ = 145 | E = -320.3413971 |
|                 | C         | -0.147932 | -1.753798 0.000000 |
|                 | O         | 0.718035  | -0.605506 0.000000 |
|                 | N         | 0.000000  | 0.625612 0.000000 |
|                 | O         | 0.722523  | 1.582169 0.000000 |
|                 | O         | -1.205855 | 0.557537 0.000000 |
|                 | H         | 0.550386  | -2.589334 0.000000 |
|                 | H         | -0.770208 | -1.770482 -0.894648 |
|                 | H         | -0.770208 | -1.770482 0.894648 |
2.4.2. Calculated Cartesian Coordinates of FMN

B3LYP-D3/def2-TZVP \_ gauche $\nu_{\text{min}} = 83 \text{ cm}^{-1}$ $E = -419.6235876$

|        |        |        |        |
|--------|--------|--------|--------|
| C      | 1.331435 | -0.209463 | 0.498826 |
| O      | 0.118982 | -0.846498 | 0.218478 |
| N      | -1.004735 | 0.070415  | 0.009661 |
| O      | -1.977411 | -0.509019 | -0.349704 |
| O      | -0.810187 | 1.229775  | 0.229345 |
| F      | 1.915972  | 0.235727  | -0.660040 |
| H      | 1.953134  | -0.992899 | 0.931125 |
| H      | 1.196582  | 0.641162  | 1.163691 |

B3LYP-D3/def2-TZVP \_ anti $\nu_{\text{min}} = 61 \text{ cm}^{-1}$ $E = -419.6165405$

|        |        |        |        |
|--------|--------|--------|--------|
| C      | -1.238394 | 0.419756  | 0.000004 |
| O      | -0.196550 | -0.572570 | 0.000009 |
| N      | 1.100783  | -0.011633 | 0.000010 |
| O      | 1.964968  | -0.832493 | -0.000008 |
| O      | 1.170601  | 1.193478  | -0.000005 |
| F      | -2.379873 | -0.310064 | -0.000008 |
| H      | -1.184201 | 1.023077  | -0.905467 |
| H      | -1.184215 | 1.023070  | 0.905480 |

B3PW91-D3/def2-TZVP \_ gauche $\nu_{\text{min}} = 85 \text{ cm}^{-1}$ $E = -419.4623719$

|        |        |        |        |
|--------|--------|--------|--------|
| C      | 1.321003 | -0.211700 | 0.495656 |
| O      | 0.110147  | -0.840728 | 0.210485 |
| N      | -0.996120 | 0.069740  | 0.009345 |
| O      | -1.972295 | -0.501863 | -0.343618 |
| O      | -0.796416 | 1.225551  | 0.225280 |
| F      | 1.910375  | 0.231258  | -0.652671 |
| H      | 1.936486  | -0.999901 | 0.931778 |
| H      | 1.185471  | 0.636917  | 1.165737 |

B3PW91-D3/def2-TZVP \_ anti $\nu_{\text{min}} = 67 \text{ cm}^{-1}$ $E = -419.4555812$

|        |        |        |        |
|--------|--------|--------|--------|
| C      | -1.229001 | 0.415132 | 0.000004 |
| O      | -0.191092 | -0.571641 | 0.000009 |
| N      | 1.091060  | -0.011756 | 0.000011 |
| O      | 1.957322  | -0.825817 | -0.000008 |
| O      | 1.156076  | 1.189774  | -0.000006 |
| F      | -2.366151 | -0.309982 | -0.000008 |
| H      | -1.173243 | 1.021407  | -0.905586 |
| H      | -1.173257 | 1.021400  | 0.905600 |

M06-2X/def2-TZVP \_ gauche $\nu_{\text{min}} = 88 \text{ cm}^{-1}$ $E = -419.450253$

|        |        |        |        |
|--------|--------|--------|--------|
| C      | 1.318338 | -0.262226 | 0.480570 |
| O      | 0.086598  | -0.857174 | 0.172140 |
| N      | -0.972438 | 0.066863  | 0.015315 |
| O      | -1.971062 | -0.457528 | -0.341596 |
| O      | -0.744194 | 1.210996  | 0.258846 |
| F      | 1.865019  | 0.274112  | -0.639245 |
| H      | 1.931398  | -1.094954 | 0.819285 |
| H      | 1.209733  | 0.519457  | 1.228166 |
M06-2X/def2-TZVP \textit{anti} $\nu_{\text{min}} = 85 \text{ cm}^{-1}$ $E = -419.4443139$

|   |     |       |       |
|---|-----|-------|-------|
| C | -1.224008 | 0.417674 | -0.000001 |
| O | -0.183203 | -0.566052 | -0.000004 |
| N | 1.078736  | -0.014904 | -0.000013 |
| O | 1.948934  | -0.819599 | 0.000008  |
| O | 1.145355  | 1.184441  | 0.000005  |
| F | -2.351058 | -0.314760 | 0.000005  |
| H | -1.168139 | 1.020399  | -0.904799 |
| H | -1.168132 | 1.020402  | 0.904793  |

MP2(fc)/cc-pVTZ \textit{gauche} $\nu_{\text{min}} = 88 \text{ cm}^{-1}$ $E = -418.8311737$

|   |     |       |       |
|---|-----|-------|-------|
| C | 1.316669 | -0.255769 | 0.482448 |
| O | 0.102541 | -0.874769 | 0.178932 |
| N | -0.986851 | 0.077514  | 0.014379 |
| O | -1.990625 | -0.468957 | -0.342766 |
| O | -0.744664 | 1.230412  | 0.254759  |
| F | 1.882632  | 0.268910  | -0.642471 |
| H | 1.940255  | -1.063535 | 0.853317  |
| H | 1.185984  | 0.541866  | 1.206178  |

MP2(fc)/cc-pVTZ \textit{anti} $\nu_{\text{min}} = 80 \text{ cm}^{-1}$ $E = -418.8239176$

|   |     |       |       |
|---|-----|-------|-------|
| C | -1.221605 | 0.408816 | 0.000002 |
| O | -0.193192 | -0.588938 | 0.000005 |
| N | 1.088751  | -0.008079 | 0.000005 |
| O | -1.971704 | -0.822660 | -0.000004 |
| O | 1.136317  | 1.203917  | -0.000003 |
| F | -2.365747 | -0.306489 | -0.000004 |
| H | -1.159261 | 1.011749  | -0.901221 |
| H | -1.159269 | 1.011746  | 0.901227  |

MP2(full)/cc-pwCVTZ \textit{gauche} $\nu_{\text{min}} = 88 \text{ cm}^{-1}$ $E = -419.1618758$

|   |     |       |       |
|---|-----|-------|-------|
| C | 1.314524 | -0.250856 | 0.482286 |
| O | 0.104027 | -0.870708 | 0.183369 |
| N | -0.985951 | 0.077044  | 0.014130 |
| O | -1.984667 | -0.471504 | -0.343392 |
| O | -0.747434 | 1.227888  | 0.252491  |
| F | 1.879770  | 0.264860  | -0.643531 |
| H | 1.937563  | -1.053605 | 0.859919  |
| H | 1.183613  | 0.550282  | 1.199493  |

MP2(full)/cc-pwCVTZ \textit{anti} $\nu_{\text{min}} = 78 \text{ cm}^{-1}$ $E = -419.1545618$

|   |     |       |       |
|---|-----|-------|-------|
| C | -1.219565 | 0.407861 | 0.000002 |
| O | -0.193161 | -0.586590 | 0.000005 |
| N | 1.087118  | -0.008158 | 0.000005 |
| O | 1.966993  | -0.821499 | -0.000004 |
| O | 1.135289  | 1.200811  | -0.000003 |
| F | -2.361179 | -0.305889 | -0.000004 |
| H | -1.157391 | 1.010584  | -0.899289 |
| H | -1.157399 | 1.010580  | 0.899295  |
### PBE0-D3/def2-TZVP \_gauche \( \nu_{\text{min}} = 87 \text{ cm}^{-1} \) \( E = -419.1887742 \)

| Atom | \( x \)  | \( y \)  | \( z \)  |
|------|---------|---------|---------|
| C    | 1.315284| -0.223131| 0.491512|
| O    | 0.100702| -0.839277| 0.198418|
| N    | -0.986637| 0.068695| 0.010454|
| O    | -1.969037| -0.489514| -0.340158|
| O    | -0.779211| 1.220463| 0.229917|
| F    | 1.898165| 0.237521| -0.646361|
| H    | 1.926518| -1.024552| 0.909301|
| H    | 1.185117| 0.611410| 1.180282|

### PBE0-D3/def2-TZVP \_anti \( \nu_{\text{min}} = 73 \text{ cm}^{-1} \) \( E = -419.1822466 \)

| Atom | \( x \)  | \( y \)  | \( z \)  |
|------|---------|---------|---------|
| C    | 1.291700| -0.011693| 0.000000|
| O    | 0.000000| 0.598542| 0.000000|
| N    | -1.033240| -0.325850| 0.000000|
| O    | -2.109846| 0.172461| 0.000000|
| O    | -0.720146| -1.485105| 0.000000|
| F    | 2.140750| 1.030663| 0.000000|
| H    | 1.427827| -0.606020| -0.90534|
| H    | 1.427827| -0.606020| 0.90534|

### TPSSh/def2-TZVP \_gauche \( \nu_{\text{min}} = 84 \text{ cm}^{-1} \) \( E = -419.6209576 \)

| Atom | \( x \)  | \( y \)  | \( z \)  |
|------|---------|---------|---------|
| C    | 1.330206| -0.199701| 0.502865|
| O    | 0.124830| -0.852851| 0.221628|
| N    | -1.010561| 0.072622| 0.008092|
| O    | -1.984011| -0.513550| -0.347162|
| O    | -0.811660| 1.234890| 0.222785|
| F    | 1.925023| 0.227372| -0.661416|
| H    | 1.955434| -0.970550| 0.954763|
| H    | 1.178787| 0.666135| 1.146142|

### TPSSh/def2-TZVP \_anti \( \nu_{\text{min}} = 64 \text{ cm}^{-1} \) \( E = -419.6139557 \)

| Atom | \( x \)  | \( y \)  | \( z \)  |
|------|---------|---------|---------|
| C    | -1.234234| 0.418662| 0.000001|
| O    | -0.199296| -0.585051| 0.000001|
| N    | 1.102886| -0.010096| -0.000004|
| O    | 1.974785| -0.827097| 0.000001|
| O    | 1.157895| 1.198999| 0.000001|
| F    | -2.380873| -0.308200| -0.000001|
| H    | -1.177004| 1.018846| -0.908397|
| H    | -1.177004| 1.018844| 0.908402|
3. Structure Determination

3.1 X-ray Crystallography

3.1.1 Crystal growth

3.1.1.1 MN
Crystals of CH$_3$NO$_3$ [MN] were grown in-situ inside of a sealed capillary. At 245 K, a small crystal could be manually grown. It turned out to be oxonium nitrate, see below. Slowly chilling with 10 K/h to 100 K methyl nitrate crystallizes as oligocrystalline material.

3.1.1.2 FMN
A twinned crystal was grown in-situ inside of a sealed capillary at 182.5 K by manually growing a crystal seed, chilling to 162 K with 1 K/h and to 100 K with 20 K/h.

3.1.1.3 Oxonium nitrate dihydrate
A crystal of H$_3$O$^+$NO$_3^-$ x 2 H$_2$O was grown in-situ inside of a sealed capillary at 245 K. Chilling fast to 180 K the methyl nitrate acted as undercooled solvent.

3.1.2 Structure determination and refinement

All measurements were examined on a Rigaku Supernova diffractometer using MoKα (λ = 0.71073 Å) radiation. Using Olex2 [1], the structures were solved with the ShelXT [2] structure solution program using Intrinsic Phasing and refined with the ShelXL [3] refinement package using Least Squares minimization. All hydrogen atoms were refined isotropically.

3.1.2.1 For MN seven domains were indexed and taken into account for data reduction, only none or minor overlapping reflections of the main domain (quota ca. 27%) were used for structure solution and refinement.

3.1.2.2 The crystal of FMN was twinned by a rotation of 180 ° around 100 with ratio 58:42. Both domains were taken into account during data reduction and refinement.
## Crystal data and structure refinement

|                              | MN          | FMN         | H$_3$O$^+$ NO$_3^-$ · 2 H$_2$O |
|------------------------------|-------------|-------------|-------------------------------|
| **Empirical formula**        | CH$_3$NO$_3$ | CH$_3$FNO$_3$ | H$_3$NO$_6$                   |
| **Formula weight**           | 77.04       | 95.04       | 117.07                        |
| **Temperature/K**            | 100.0(1)    | 100.0(1)    | 180.0(1)                      |
| **Cryst. system**            | orthorhombic| monoclinic  | orthorhombic                  |
| **Space group**              | $Pbca$      | $Cc$        | $P2_12_12_1$                  |
| **$a$/Å**                    | 4.6169(2)   | 5.0962(16)  | 3.48643(15)                   |
| **$b$/Å**                    | 11.2184(6)  | 14.28632(3) | 9.5040(4)                     |
| **$c$/Å**                    | 12.5130(7)  | 4.8520(10)  | 14.7100(5)                    |
| **$\beta$/°**               | 90          | 103.57(3)   | 90                            |
| **Volume/Å$^3$**             | 648.10(6)   | 343.40(16)  | 487.42(3)                     |
| **Z**                        | 8           | 4           | 4                             |
| **$\rho$ calc/g/cm$^3$**     | 1.579       | 1.838       | 1.595                         |
| **$\mu$/mm$^{-1}$**          | 0.161       | 0.211       | 0.180                         |
| **F(000)**                   | 320         | 192         | 248                           |
| **Crystal size/mm**          | 0.51 x 0.32 x 0.27 | 0.63 x 0.33 x 0.27 | 0.24 x 0.15 x 0.10 |
| **2$\Theta$ range /°**      | 6.5 to 61.7 | 5.7 to 73.6 | 5.1 to 64.5                   |
| **Index ranges**             | $-6 \leq h \leq 6$ | $-8 \leq h \leq 8$ | $-5 \leq h \leq 5$ |
|                             | $-15 \leq k \leq 16$ | $-23 \leq k \leq 23$ | $-14 \leq k \leq 13$ |
|                             | $-17 \leq l \leq 17$ | $-8 \leq l \leq 8$ | $-21 \leq l \leq 21$ |
| **Refl. collected**          | 8968        | 13818       | 9655                          |
| **Unique refl.**             | 1002        | 3370        | 1638                          |
| **$R_{int}$**                | 0.0576      | 0.0214      | 0.0339                        |
| **Refl. with I > 2$\sigma$(I)** | 764        | 3225        | 1390                          |
| **Data/restraints/parameters** | 1002/0/59  | 3370/2/64   | 1638/0/93                     |
| **Goof on $F^2$**            | 0.929       | 1.061       | 1.079                         |
| **Final $R$ indices**        | $R_1 = 0.0283$, $R_1 = 0.0329$, $R_1 = 0.0307$, | $R_1 = 0.0407$, $R_1 = 0.0349$, $R_1 = 0.0411$, | $R_1 = 0.0407$, $R_1 = 0.0349$, $R_1 = 0.0411$, |
| [for $I > 2\sigma(I)$]      | $wR_2 = 0.0645$, $wR_2 = 0.1007$, $wR_2 = 0.0603$, | $wR_2 = 0.0670$, $wR_2 = 0.1074$, $wR_2 = 0.0649$, | $wR_2 = 0.0670$, $wR_2 = 0.1074$, $wR_2 = 0.0649$, |
| **Final $R$ indices**        | $R_1 = 0.0047$, $R_1 = 0.0049$, $R_1 = 0.00411$, | $R_1 = 0.0047$, $R_1 = 0.0049$, $R_1 = 0.00411$, | $R_1 = 0.0047$, $R_1 = 0.0049$, $R_1 = 0.00411$, |
| [for all data]               | $wR_2 = 0.0645$, $wR_2 = 0.1007$, $wR_2 = 0.0603$, | $wR_2 = 0.0670$, $wR_2 = 0.1074$, $wR_2 = 0.0649$, | $wR_2 = 0.0670$, $wR_2 = 0.1074$, $wR_2 = 0.0649$, |
| **Resid. electron density/ e Å$^{-3}$** | 0.13/ -0.20, 0.36/ -0.30, 0.16/ -0.21 | 0.13/ -0.20, 0.36/ -0.30, 0.16/ -0.21 |
| **Flack parameter**          | -0.1(5)     | 0.3(10)     |                               |
| **CCDC number**              | 1936407     | 1936406     | 1936408                       |

1. O. V. Dolomanov, L. J. Bourhis, R. J. Gildea, J. A. K. Howard, H. Puschmann, *J. Appl. Crystallogr.* 2009, 42, 339–341.

2. G. M. Sheldrick, *Acta Crystallogr.* 2015, A71, 3–8.

3. G. M. Sheldrick, *Acta Crystallogr.* 2015, C71, 3–8.
Fig. S1 Asymmetric unit of H$_3$O$^+$ NO$_3^-$ x 2 H$_2$O

Fig. S2 Hydrogen bond network of H$_3$O$^+$ NO$_3^-$ : 2 H$_2$O
3.2. Gas-phase electron diffraction

3.2.1 Experiment

The electron diffraction patterns were recorded on the heavily improved Balzers Eldigraph KD-G2 gas-phase electron diffractometer at Bielefeld University. Experimental details are listed in Table 4, instrumental details are reported elsewhere.\cite{10}

| Table 4. Details of the gas-phase electron diffraction experiment for methyl nitrate and fluoromethyl nitrate. |
|---|---|---|---|---|
| Parameters | Methyl nitrate | Fluoromethyl nitrate |
| nozzle-to-plate distance, mm | short detector distance | long detector distance | short detector distance | long detector distance |
| nozzle temperature, K | 297 | 298 | 297 | 298 |
| accelerating voltage, kV | 60 | 60 | 60 | 60 |
| fast electron current, μA | 1.54 | 1.53 | 1.54 | 1.53 |
| electron wavelength, Å | 0.048672 | 0.048629 | 0.048672 | 0.048629 |
| Sample pressure, mbar | 2.8×10^{-6} | 4.2×10^{-6} | 5.0×10^{-6} | 4.7×10^{-6} |
| residual gas pressure, mbar | 7.0×10^{-7} | 1.2×10^{-6} | 7.0×10^{-7} | 1.2×10^{-6} |
| exposure time, s | 10 | 10 | 10 | 10 |
| used s range, Å^{-1} | 7.4–32.2 | 2.0–16.4 | 9.2–30.0 | 3.0–16.0 |
| number of inflection points | 7 | 4 | 7 | 5 |
| R factor | 6.3 | 3.2 | 6.9 | 1.9 |

\(a\) Determined from CCl₄ diffraction patterns measured in the same experiment. \(b\) During the measurement. \(c\) Between measurements. \(d\) Number of inflection points on the reduced background lines.

The electron diffraction patterns, four for each, long and short nozzle-to-plate distance (with the exception of only three for the medium distance for FMN) were measured on the Fuji BAS-IP MP 2025 imaging plates, which were scanned by using calibrated Fuji BAS 1800II scanner. The intensity curves (see below) were obtained by applying the method described earlier.\cite{11} Electron wavelengths were refined\cite{12} using carbon tetrachloride diffraction patterns, recorded in the same experiment as the substance under investigation.
3.2.2 Experimental (black dots) and model (red line) radial distribution curve as well as difference curve (below) for the refinement of FMN. Vertical bars (blue) indicate individual diatomic contributions to the total intensity.
3.2.3 First sets of experimental reduced electron diffraction intensities and background lines of MN (top) and FMN (bottom) for middle and long camera settings.
3.2.4 Experimental and model molecular electron diffraction intensities of MN (top) and FMN (bottom) in the main refinement; in case of MN combined with rotational constants.

3.2.5 Structural Analysis of MN

Two types of experimental data were available for structural analysis: (a) electron diffraction intensities measured in this work and (b) published earlier rotational constants.\textsuperscript{[13]}

Molecular structure of methyl nitrate has been refined from published rotational constants for eight isotopologues. The parameters were refined unconstrained within $C_\text{s}$ symmetry point group. The experimental $B_0$ rotational constants have been corrected to equilibrium geometry using theoretically computed differences ($B_\text{e}$-$B_0$) at the DFT level and VPT2 theory as implemented in
Gaussian program package. The obtained results are listed in Table 5. Interestingly, the differences between results obtained with PBE0 and TPSSh corrections were negligible, although the corrections themselves deviated by 5-10%. To assess the influence of uncertainties in corrections ($B_e-B_0$) onto the errors of refined molecular structure parameters Monte-Carlo simulations have been done as described earlier. Assumed standard deviations for rotational constants were 5% of their respective corrections. The obtained in this way total errors are provided in Table 5.

Table 5. Structural parameters of methyl nitrate (Å and degrees) refined from experimental $B_0$ rotational constants using theoretical corrections ($B_e-B_0$) from VPT2 calculations with PBE0 and TPSSh DFT functionals. Uncertainties are standard deviations from least squares method (LSQ) or total errors from Monte-Carlo simulations.

| Parameter | PBE0/def2-TZVP, LSQ errors | TPSSh/def2-TZVP, LSQ errors | TPSSh/def2-TZVP, total errors |
|-----------|----------------------------|----------------------------|-------------------------------|
| C1-O1     | 1.433(5)                   | 1.433(5)                   | 1.433(22)                     |
| O1-N1     | 1.399(8)                   | 1.397(8)                   | 1.397(38)                     |
| N1-O2     | 1.206(5)                   | 1.205(5)                   | 1.207(22)                     |
| N1-O3     | 1.203(6)                   | 1.203(6)                   | 1.203(29)                     |
| Average C–H | 1.078(4)               | 1.078(4)                   | 1.079(21)                     |
| C1–O1–N1  | 112.6(2)                   | 112.5(2)                   | 112.5(11)                     |
| O1N1O2    | 117.7(7)                   | 117.8(7)                   | 117.8(33)                     |
| O1N1O3    | 112.8(4)                   | 112.7(4)                   | 112.7(21)                     |
| O2N1O3    | 129.5(9)                   | 129.5(9)                   | 129.5(45)                     |
| wRMSD, MHz | 0.42                      | 0.41                      | 0.41                          |

Next, molecular structure of MN has been refined from electron diffraction intensities. The procedure was as follows. Background procedure has been applied for each of the measured total intensity functions, extracting molecular intensity. The individual intensities, four from each nozzle-to-detector distance, were averaged. The averaged molecular intensity functions $s_M(s)$, one from middle and one from the long camera setting, were used in structural analysis. The geometry of the molecule has been defined using a Z-matrix, which also contains grouping of the parameters:

- C
- O 1 Reco
- O 2 Rno1 1 Acon
- O 3 Rno2 2 Aono1 1 D180
- O 3 Rno3 2 Aono2 4 D180
- H 1 Rch1 2 Aoch1 3 D180
- H 1 Rch2 2 Aoch2 6 Ahch -1
- H 1 Rch2 2 Aoch2 6 Ahch 1

Variable: Value: Group:
Rco 1.429925 1
Rno1 1.408961 2
Rno2 1.204332 3
Rno3 1.210520 3
Rch1 1.084687 5
Rch2 1.086124 5
Acon 112.122997 7
Aono1 112.973586 8
Aono2 117.163526 9
Aoch1 103.420346
Aoch2 111.159491
Ahch 110.510013
D180 180.0

The initial values of parameters have been taken from MP2(fc)/cc-pVTZ calculations. The differences between parameters in groups were fixed on the values also taken from this level of theory. In preliminary calculations of anharmonic vibrational frequencies using VPT2 theory it was found that TPSSh/def2-TZVP level of theory reproduces experimental values most closely. Therefore, force fields from this level were used to calculate interatomic vibrational mean square amplitudes and corrections, required in structural analysis. The corrections were calculated for equilibrium structure.
taking into account cubic force fields. This type of calculations was done in VibModule program. In the refinement amplitudes have been divided into four groups (see Table below). The ratios of amplitudes in each group were fixed at the theoretical values. Thus scale factors for theoretical amplitudes have been refined to the values 1.06(1), 1.13(7), 0.99(5), 1.19(7). The values of refined geometrical parameters are listed in Table 8. The largest correlation 0.81 was between the first scale factor for the amplitudes and the scale factor for the molecular intensity from middle camera measurements.

Finally, a combined refinement of molecular model has been done utilizing both GED data and rotational constants. The model and grouping of parameters was the same as in the refinement based on only GED data. The relative weighting of the rotational constants has been adjusted manually so that their average contributions to the refined parameters were possibly similar to those from GED data. In the least squares method the maximal correlation -0.83 was between parameters in groups 7 and 8 (see Z-matrix above). As expected, the quality of fit for GED data and rotational constants was worse than in case of using only one type of data in the least squares refinement. However, it is expected that the overall accuracy of the refined parameters in this model was higher. The refined geometrical parameters of MN are listed in Tables 2 and 3 of the paper. Table 8 lists Cartesian coordinates of atoms in MN corresponding to the final structure. Note, the final values were corrected by the Monte-Carlo procedure, which was used to assess the influence of uncertainties in different parameters of the model and in data and also for calculation of total errors. For this reason, a series of quantum-chemical calculations has been performed for computing the possible ranges of geometrical constraints. The approximations were MP2(fc)/cc-pVTZ, MP2(full)/cc-pwCVTZ, B3LYP-D3/def2-TZVP, B3PW91-D3/def2-TZVP, M06-2X/def2-TZVP, TPSSh/def2-TZVP, PBE0-D3/def2-TZVP. The obtained from these calculations ranges for constraints were additionally extended by 30%. The same procedure was used for obtaining ranges of possible values for vibrational amplitudes and corrections, where the tested quantum-chemical approximations were PBE0-D3/def2-TZVP, B3LYP-D3/def2-TZVP, M06-2X/def2-TZVP, B3PW91-D3/def2-TZVP and TPSSh/def2-TZVP.

Table 6. Equilibrium structural parameters of methyl nitrate (Å and degrees) refined from GED data. Uncertainties are total standard deviations from Monte-Carlo simulations.

| Parameter (GED numbering) | Parameter (XRD numbering) | GED, total errors |
|--------------------------|---------------------------|-------------------|
| C1–O2                    | C1–O1                     | 1.425(3)          |
| O2–N3                    | O1–N1                     | 1.404(2)          |
| N3–O4                    | N1–O2                     | 1.205(1)          |
| N3–O5                    | N1–O3                     | 1.199(1)          |
| Average C–H              |                           | 1.081(4)          |
| C1–O2–N3                 | C1–O1–N1                  | 113.7(3)          |
| O2–N3–O4                 | O1–N1–O2                  | 116.4(3)          |
| O2–N3–O5                 | O1–N1–O3                  | 110.8(4)          |
| O4–N3–O5                 | O2–N1–O3                  | 132.8(5)          |
| R-factor, %              |                           | 4.6               |
Table 7. Thermally averaged distances between atoms, refined amplitudes, vibrational corrections (all in Å) and group numbers for amplitudes in the refinement of MN.

| At1 | At2 | r_a | l | corr | Gln |
|-----|-----|-----|---|------|-----|
| C1  | H6  | 1.096753 | 0.080934 | -0.016500 | 20  |
| C1  | H8  | 1.098090 | 0.081253 | -0.016400 | 20  |
| C1  | H7  | 1.098090 | 0.081253 | -0.016400 | 20  |
| N3  | O4  | 1.203219 | 0.040361 | -0.004400 | 20  |
| N3  | O5  | 1.208707 | 0.041104 | -0.003700 | 20  |
| O2  | N3  | 1.420663 | 0.059160 | -0.016500 | 20  |
| C1  | O2  | 1.432633 | 0.053000 | -0.007700 | 20  |
| H7  | H8  | 1.791448 | 0.138053 | -0.020000 | 21  |
| H6  | H8  | 1.794662 | 0.138960 | -0.018200 | 21  |
| H6  | H7  | 1.794662 | 0.138960 | -0.018200 | 21  |
| O2  | H6  | 1.994952 | 0.118445 | -0.017100 | 21  |
| O2  | H8  | 2.092830 | 0.115044 | -0.016000 | 21  |
| O2  | O4  | 2.158492 | 0.064606 | -0.012100 | 21  |
| O2  | O5  | 2.239864 | 0.064039 | -0.020000 | 21  |
| C1  | N3  | 2.397757 | 0.063626 | -0.028600 | 22  |
| O5  | H7  | 2.566145 | 0.243423 | -0.045400 | 22  |
| O5  | H8  | 2.566145 | 0.243423 | -0.045400 | 22  |
| C1  | O5  | 2.697317 | 0.166339 | -0.033500 | 22  |
| N3  | H7  | 2.697317 | 0.166339 | -0.033500 | 22  |
| N3  | H6  | 3.261634 | 0.122652 | -0.024500 | 23  |
| C1  | O4  | 3.431927 | 0.073687 | -0.017200 | 23  |
| O5  | H6  | 3.613451 | 0.135670 | -0.037200 | 23  |
| O4  | H8  | 3.784779 | 0.192637 | -0.024900 | 23  |
| O4  | H7  | 3.784779 | 0.192637 | -0.024900 | 23  |
| O4  | H6  | 4.133893 | 0.133640 | -0.010800 | 23  |

Table 8. Cartesian coordinates (Å) of atoms in MN. The values correspond to equilibrium structure refined from combined GED+RotC data and corrected in Monte-Carlo procedure. Internal numeration is used.

| At | X | Y | Z |
|----|---|---|---|
| C  | -1.824975055240 | -0.001855788015 | 0.000000000000 |
| O  | -0.608446978339 | -0.743987070143 | 0.000000000000 |
| N  | 0.5407524291990 | 0.060453265649 | 0.000000000000 |
| O  | 1.548866909894 | -0.587398959595 | 0.000000000000 |
| O  | 0.358301273211 | 1.251076311740 | 0.000000000000 |
| H  | -2.582484077838 | -0.764532680668 | 0.000000000000 |
| H  | -1.906646055559 | 0.610621432175 | -0.881373123432 |
| H  | -1.906646055559 | 0.610621432175 | 0.881373123432 |
3.2.5 Structural Analysis of FMN

Even the lowest predicted energy difference of 14.5 kJ mol$^{-1}$ (see chapter 2.5) between the two possible conformers would result in a Boltzmann distribution based ratio of 99.99:0.01 favoring the \textit{gauche} conformer. Therefore, and due to an insufficient agreement of the experimental data with the \textit{anti}-conformer, we decided to refine the structure of FMN taking into account only the \textit{gauche} conformer.

The refinement procedure based on the electron diffraction intensities was in close analogy to the one described for MN with the following differences: For the medium distance only three individual intensities were used for averaging, the initial values of parameters have been taken from MP2(full)/cc-pwCVTZ calculations and the Z-matrix was modified as follows:

```
1 C
2 O 1 rOC1
3 N 2 rNO1 1 aNOC1
4 O 3 rON1 2 aONO1 1 dONOC1
5 O 3 rON2 2 aONO2 1 dONOC2
6 F 1 rFC 2 aFCO 3 dFCON
7 H 1 rHC1 2 aHCO1 6 aHCF1 -1
8 H 1 rHC2 2 aHCO2 6 aHCF2 1
```

Variables:
- \( rOC1 = 1.39243385 \) 1
- \( rNO1 = 1.45427839 \) 7
- \( rON1 = 1.19421928 \) 2
- \( rON2 = 1.19922852 \) 2
- \( rFC = 1.36122395 \) 3
- \( rHC1 = 1.08406195 \)
- \( rHC2 = 1.08321029 \)
- \( aNOC1 = 112.73326344 \) 4
- \( aONO1 = 111.24084116 \) 5
- \( aONO2 = 116.94953757 \) 6
- \( aFCO = 110.61566405 \) 8
- \( aHCO1 = 104.16845212 \)
- \( aHCO2 = 108.51703562 \)
- \( dONOC1 = 174.54393828 \)
- \( dONOC2 = -5.82750348 \)
- \( dFCON = -78.77859396 \) 9

In the refinement amplitudes have been divided into five groups (see Table below). The ratios of amplitudes in each group were fixed at the theoretical values. Thus, scale factors for theoretical amplitudes have been refined to the values 0.95(2), 1.12(4), 0.92(2), 1.40(5), 1.21(6). The values of refined geometrical parameters are listed in Table 11. The largest correlation 0.88 was between the first scale factor for the amplitudes and the scale factor for the molecular intensity from middle camera measurements.
Table 9. Equilibrium structural parameters of methyl nitrate (Å and degrees) refined from GED data. Uncertainties are total standard deviations from Monte-Carlo simulations. In this table, the numbering is chosen to fit the solid state structural data.

| Parameter | GED, total errors |
|-----------|-------------------|
| C1–O1     | 1.385(3)          |
| O1–N1     | 1.454(2)          |
| N1–O2     | 1.190(2)          |
| N1–O3     | 1.185(1)          |
| C1–F      | 1.336(2)          |
| Average C–H | 1.083            |
| C1–O1–N1  | 115.3(2)          |
| O1–N1–O2  | 115.1(3)          |
| O1–N1–O3  | 111.9(11)         |
| O2–N1–O3  | 133.0(13)         |
| F–C1–O2–N1| −74.7(8)          |
| R-factor, % | 3.5              |

Table 10. Thermally averaged distances between atoms, refined amplitudes, vibrational corrections (all in Å) and group numbers for amplitudes in the refinement of FMN.

| At1 | At2 | r_e_l corr Gl | lcorr |
|-----|-----|---------------|-------|
| C1  | H8  | 1.100410 0.071353 −0.017200 200 |
| C1  | H7  | 1.101162 0.071446 −0.017100 200 |
| N3  | O4  | 1.189511 0.035162 −0.004100 200 |
| N3  | O5  | 1.194420 0.035817 −0.004000 200 |
| C1  | F6  | 1.346761 0.044139 −0.008600 200 |
| C1  | O2  | 1.398348 0.046758 −0.005200 200 |
| O2  | N3  | 1.461679 0.058541 −0.019600 200 |
| H7  | H8  | 1.790545 0.137091 −0.020500 201 |
| O2  | H7  | 1.980416 0.116471 −0.016900 201 |
| F6  | H8  | 1.986867 0.112392 −0.019900 201 |
| F6  | H7  | 1.994431 0.112845 −0.013700 201 |
| O2  | H8  | 2.069210 0.113072 −0.015000 201 |
| O4  | O5  | 2.227805 0.052231 −0.007100 201 |
| O2  | O4  | 2.138358 0.066886 −0.017000 201 |
| O5  | H8  | 2.414875 0.201898 −0.024600 201 |
| O2  | F6  | 2.296927 0.069792 −0.009200 201 |
| O2  | O5  | 2.236097 0.068772 −0.019600 201 |
| C1  | N3  | 2.423914 0.074551 −0.024100 201 |
| N3  | H8  | 2.649422 0.164056 −0.016600 201 |
| C1  | O5  | 2.586385 0.104461 −0.041900 201 |
| N3  | F6  | 2.991327 0.127744 −0.040600 202 |
| O5  | F6  | 2.933700 0.203986 −0.079600 202 |
| N3  | H7  | 3.295109 0.147248 −0.024900 203 |
| C1  | O4  | 3.391905 0.089697 −0.013000 203 |
| O5  | H7  | 3.613197 0.140179 −0.029000 204 |
| O4  | H8  | 3.739134 0.172658 −0.011400 204 |
| O4  | F6  | 3.948417 0.197048 −0.008200 204 |
| O4  | H7  | 4.099151 0.136919 −0.015300 204 |

Table 11. Cartesian coordinates (Å) of atoms in FMN. The values correspond to equilibrium structure refined from GED data and corrected in Monte-Carlo procedure. Internal numbering is used.

| At | X | Y | Z |
|----|---|---|---|
| C  | −1.3258997970795 | −0.322922259206 | −0.512318804835 |
| O  | −0.094195203689 | −0.870917632317 | −0.193829995850 |
| N  | 0.985534186486 | 0.086477713116 | −0.016220235555 |
| O  | 1.983034410001 | −0.435533501590 | 0.354718935236 |
| O  | 0.706870079031 | 1.215213166122 | −0.271761929045 |
| F  | −1.9065168333931 | 0.257496320177 | 0.541940554242 |
| H  | −1.921390517964 | −1.172815527223 | −0.825787382163 |
| H  | −1.240947552253 | 0.410220741584 | −1.305180068695 |
### 3.2.6 Electron diffraction intensities of MN

**Middle camera 1:**

| Total Int. | Background |
|------------|------------|
| 21.80000000 | 15.54767982e-01 |
| 21.60000000 | 15.54767982e-01 |
| 20.80000000 | 15.54767982e-01 |
| 20.00000000 | 15.54767982e-01 |
| 19.40000000 | 15.54767982e-01 |
| 19.20000000 | 15.54767982e-01 |
| 18.80000000 | 15.54767982e-01 |
| 18.40000000 | 15.54767982e-01 |
| 17.80000000 | 15.54767982e-01 |
| 17.60000000 | 15.54767982e-01 |
| 17.40000000 | 15.54767982e-01 |
| 17.20000000 | 15.54767982e-01 |
| 16.60000000 | 15.54767982e-01 |
| 16.00000000 | 15.54767982e-01 |
| 15.80000000 | 15.54767982e-01 |
| 15.60000000 | 15.54767982e-01 |
| 15.40000000 | 15.54767982e-01 |
| 14.00000000 | 15.54767982e-01 |
| 13.80000000 | 15.54767982e-01 |
| 13.40000000 | 15.54767982e-01 |
| 13.20000000 | 15.54767982e-01 |
| 12.00000000 | 15.54767982e-01 |
| 11.40000000 | 15.54767982e-01 |
| 11.20000000 | 15.54767982e-01 |
| 10.80000000 | 15.54767982e-01 |
| 9.80000000  | 15.54767982e-01 |
| 9.40000000  | 15.54767982e-01 |
| 9.00000000  | 15.54767982e-01 |
| 8.20000000  | 15.54767982e-01 |
| 8.00000000  | 15.54767982e-01 |
| 7.60000000  | 15.54767982e-01 |
| 7.40000000  | 15.54767982e-01 |
| 7.20000000  | 15.54767982e-01 |
| 7.00000000  | 15.54767982e-01 |
| 6.80000000  | 15.54767982e-01 |
| 6.60000000  | 15.54767982e-01 |
| 6.40000000  | 15.54767982e-01 |
| 6.20000000  | 15.54767982e-01 |
| 6.00000000  | 15.54767982e-01 |
| 5.80000000  | 15.54767982e-01 |
| 5.60000000  | 15.54767982e-01 |
| 5.40000000  | 15.54767982e-01 |
| 5.20000000  | 15.54767982e-01 |
| 5.00000000  | 15.54767982e-01 |
| 4.80000000  | 15.54767982e-01 |
| 4.60000000  | 15.54767982e-01 |
| 4.40000000  | 15.54767982e-01 |
| 4.20000000  | 15.54767982e-01 |
| 4.00000000  | 15.54767982e-01 |
| 3.80000000  | 15.54767982e-01 |
| 3.60000000  | 15.54767982e-01 |
| 3.40000000  | 15.54767982e-01 |
| 3.20000000  | 15.54767982e-01 |
| 3.00000000  | 15.54767982e-01 |
| 2.80000000  | 15.54767982e-01 |
| 2.60000000  | 15.54767982e-01 |
| 2.40000000  | 15.54767982e-01 |
| 2.20000000  | 15.54767982e-01 |
| 2.00000000  | 15.54767982e-01 |
| 1.80000000  | 15.54767982e-01 |
| 1.60000000  | 15.54767982e-01 |
| 1.40000000  | 15.54767982e-01 |
| 1.20000000  | 15.54767982e-01 |
| 1.00000000  | 15.54767982e-01 |
| 0.80000000  | 15.54767982e-01 |
| 0.60000000  | 15.54767982e-01 |
| 0.40000000  | 15.54767982e-01 |
| 0.20000000  | 15.54767982e-01 |
| 0.00000000  | 15.54767982e-01 |
Middle camera 2:

| 11.20000000 | 11.00000000 | 10.80000000 | 10.60000000 | 10.20000000 | 9.80000000 | 9.60000000 | 9.20000000 | 9.00000000 | 8.60000000 | 8.40000000 |
|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|
| 29.20000000 | 28.80000000 | 28.60000000 | 28.40000000 | 28.20000000 | 28.00000000 | 27.80000000 | 27.20000000 | 27.00000000 | 25.00000000 | 23.80000000 |
| 0.00000000  | 0.00000000  | 0.00000000  | 0.00000000  | 0.00000000  | 0.00000000  | 0.00000000  | 0.00000000  | 0.00000000  | 0.00000000  | 0.00000000  |

| Total Int. | 7.18303890e+00 | 7.46013837e+00 | 8.05269650e+00 | 8.91579058e+00 | 6.13839323e+00 | 1.43970994e+00 | 1.48562982e+00 | 1.51730927e+00 | 1.54883883e+00 | 1.57004283e+00 |

| | 1.43712957e+00 | 9.74879528e-01 | - | - | - | - | - | - | - | - |

| | 6.20793252e-01 | 5.84425899e-01 | 5.15113232e-01 | 2.59601801e-01 | 2.76351763e-01 | 2.59601801e-01 | 3.49403235e-01 |
### Middle camera 3:

| S | Total Int. | Background | Exp. m(s) |
|---|-------------|------------|-----------|
| 7.0000000 | 1.11055314e+01 | 1.14407610e+00 | -2.16829885e-01 |
| 7.6000000 | 1.03833212e+01 | 1.09249386e+01 | -3.76779400e-01 |
| 7.8000000 | 9.73288005e+00 | 1.04545342e+01 | -5.30762819e-01 |
| 8.0000000 | 9.22935350e+00 | 9.93828272e+00 | -6.31957831e-01 |
| 8.2000000 | 8.53276501e+00 | 9.57335350e+00 | -6.34346377e-01 |
| 8.6000000 | 5.38290999e+00 | 1.02115819e+00 | -2.36783272e+01 |
| 8.8000000 | 5.61848236e+00 | 8.81029399e+00 | -4.82357810e+01 |
| 9.0000000 | 8.14252235e+00 | 8.46951285e+00 | -3.39749393e-01 |
| 9.2000000 | 8.0090316e+00 | 8.14770580e+00 | -1.62158899e-01 |
| 9.4000000 | 7.83904522e+00 | 7.84547025e+00 | -1.11297587e-03 |
| 9.6000000 | 7.64713496e+00 | 7.56100508e+00 | 1.07081619e-01 |
| 9.8000000 | 7.40659191e+00 | 7.29255996e+00 | 1.50112823e-01 |
| 10.0000000 | 7.12136538e+00 | 7.03842833e+00 | 1.15477920e-01 |
| 10.2000000 | 6.84291541e+00 | 6.79695097e+00 | 6.76250962e-02 |
| 10.4000000 | 6.54849482e+00 | 5.66671600e+00 | -2.82971352e-02 |
| 10.6000000 | 5.30322699e+00 | 6.34722105e+00 | -7.20848052e-02 |
| 10.8000000 | 5.08661922e+00 | 6.13819830e+00 | -8.90716427e-02 |
| 11.0000000 | 5.09089498e+00 | 5.93940344e+00 | -5.36587463e-02 |
| 11.2000000 | 5.76935464e+00 | 5.70585300e+00 | 2.93625383e-02 |
| 11.4000000 | 5.64746247e+00 | 5.57108122e+00 | 1.53215165e-01 |
| 11.6000000 | 5.42356261e+00 | 5.40137799e+00 | 2.52333496e-02 |
| 11.8000000 | 5.39669275e+00 | 5.23991536e+00 | 3.47070059e-01 |
| 12.0000000 | 5.24457549e+00 | 5.08638488e+00 | 3.66989376e-01 |
| 12.2000000 | 5.09115161e+00 | 4.94010205e+00 | 3.66914243e-01 |
| 12.4000000 | 4.92627586e+00 | 4.80039623e+00 | 3.19917481e-01 |
| 12.6000000 | 4.75878278e+00 | 4.66687283e+00 | 2.41696998e-01 |
| 12.8000000 | 4.59080825e+00 | 4.53910718e+00 | 1.43337139e-01 |
| 13.0000000 | 4.43509995e+00 | 4.41688926e+00 | 5.27739715e-02 |
| 13.2000000 | 4.28555339e+00 | 4.29906078e+00 | -5.45852899e-02 |
| 13.4000000 | 4.13062093e+00 | 4.18694785e+00 | -1.77579318e-01 |
| 13.6000000 | 4.00717330e+00 | 4.07871673e+00 | -2.52980849e-01 |
| 13.8000000 | 3.88038675e+00 | 3.97476665e+00 | -3.22928778e-01 |
| 14.0000000 | 3.78053478e+00 | 3.87496356e+00 | -3.36291475e-01 |
| 14.2000000 | 3.69507229e+00 | 3.77916727e+00 | -1.15315151e-01 |
| 14.4000000 | 3.62585979e+00 | 3.68723540e+00 | -2.37404911e-01 |
| 14.6000000 | 3.57110003e+00 | 3.59095379e+00 | -1.11844413e-01 |
| 14.8000000 | 3.52007230e+00 | 3.51448476e+00 | 2.32119899e-02 |
| 15.0000000 | 3.47547498e+00 | 3.43336262e+00 | 9.21928646e-02 |
| 15.2000000 | 3.38781074e+00 | 3.35550778e+00 | 1.44402667e-01 |
| 15.4000000 | 3.20723528e+00 | 3.20703689e+00 | 1.22723533e-01 |
| 15.6000000 | 3.22098711e+00 | 3.17458294e+00 | 2.56719366e-02 |
| 15.8000000 | 3.12682287e+00 | 3.12488238e+00 | 3.05060231e-02 |
| 16.0000000 | 3.08379995e+00 | 3.07621811e+00 | -1.73913192e-01 |
| 16.2000000 | 3.04616214e+00 | 3.00989516e+00 | -2.56613475e-01 |
| 16.4000000 | 2.90412824e+00 | 2.94860936e+00 | -2.64772436e-01 |
Long camera 1:

| S  | Total Int. | Background | Exp. aM(s) |
|----|------------|------------|------------|
| 2.0000000 | 1.4351081e+01 | 1.49394530e+01 | -7.81886486e-02 |
| 2.2000000 | 1.32607575e+01 | 1.40447378e+01 | -1.22880447e-01 |
| 2.4000000 | 1.23595797e+01 | 1.34606857e+01 | -1.96327995e-01 |
| 2.6000000 | 1.16567894e+01 | 1.29745826e+01 | -2.64074960e-01 |
| 2.8000000 | 1.11862984e+01 | 1.25693267e+01 | -3.08089622e+00 |
| 3.0000000 | 1.09786841e+01 | 1.22140305e+01 | -3.03427499e+00 |
| 3.2000000 | 1.08244585e+01 | 1.18679026e+01 | -2.85414757e+00 |
| 3.4000000 | 1.05981751e+01 | 1.15775852e+01 | -2.87516927e+00 |
| 3.6000000 | 1.02932951e+01 | 1.12778010e+01 | -3.14265271e+00 |
| 3.8000000 | 0.98542829e+00 | 1.09833169e+01 | -3.96223797e+00 |
| 4.0000000 | 0.932610553e+00 | 1.06922973e+01 | -5.11087954e+00 |
| 4.2000000 | 0.87950243e+00 | 1.00403363e+01 | -6.9495128e+00 |
| 4.4000000 | 0.84016384e+00 | 0.91165025e+01 | -7.45850845e+00 |
| 4.6000000 | 0.82210414e+00 | 0.87268575e+00 | -7.50214660e+00 |
| 4.8000000 | 0.82560487e+00 | 0.93563833e+00 | -6.44439993e+00 |
| 5.0000000 | 0.84497561e+00 | 0.92423932e+00 | -4.28805131e+00 |
| 5.2000000 | 0.87604672e+00 | 0.94642673e+00 | -1.08086659e+00 |
| S | Total Int. | Background | Exp. | sM(s) |
|---|---|---|---|---|
| 2.0000000000 | 1.63951108e+01 | 1.70205876e+01 | -7.34965013e-02 |
| 2.2000000000 | 1.51987051e+01 | 1.61345431e+01 | -1.27604704e-01 |
| 2.4000000000 | 1.41219002e+01 | 1.55528620e+01 | -2.20815206e-01 |
| 2.6000000000 | 1.33877641e+01 | 1.50388623e+01 | -2.85450803e-01 |
| 2.8000000000 | 1.29189120e+01 | 1.45993314e+01 | -3.20588674e-01 |
| 3.0000000000 | 1.27333455e+01 | 1.41056770e+01 | -3.07135611e-01 |
| 3.2000000000 | 1.26324229e+01 | 1.38106328e+01 | -2.75083094e-01 |
| 3.4000000000 | 1.23769290e+01 | 1.34548868e+01 | -2.72395933e-01 |
| 3.6000000000 | 1.20135667e+01 | 1.31104816e+01 | -3.01201257e-01 |
| 3.8000000000 | 1.15062734e+01 | 1.27723634e+01 | -3.76683764e-01 |
| 4.0000000000 | 1.08600051e+01 | 1.24368787e+01 | -5.07163112e-01 |
| 4.2000000000 | 1.01944081e+01 | 1.21037062e+01 | -6.60722996e-01 |
| 4.4000000000 | 9.72593920e+00 | 1.17116462e+01 | -7.64643330e-01 |
| 4.6000000000 | 9.51374564e+00 | 1.14365612e+01 | -7.73392576e-01 |
| 4.8000000000 | 9.50362090e+00 | 1.10935968e+01 | -6.67292926e-01 |
| 5.0000000000 | 9.77448871e+00 | 1.07417899e+01 | -4.50065227e-01 |
Long camera 4:

| S | Total Int. | Background | Exp. sM(s) |
|---|------------|------------|------------|
| 2.00000000 | 1.61642449e+01 | 1.67727627e+01 | -7.25602303e-02 |
| 2.20000000 | 1.48708761e+01 | 1.57742641e+01 | -1.25993427e+00 |
| 2.40000000 | 1.38236609e+01 | 1.31198373e+01 | -2.05751225e+00 |
| 2.60000000 | 1.30627671e+01 | 1.49761563e+01 | -2.69966848e-01 |
| 2.80000000 | 1.24543347e+01 | 1.33303670e+01 | 8.58261708e-02 |
| 3.00000000 | 1.25983050e+01 | 1.08950511e+01 | 1.47070304e-07 |
| 3.20000000 | 2.09892358e+01 | 2.08594998e+01 | 9.45733119e-02 |
| 3.40000000 | 2.06981400e+01 | 2.06390201e+01 | 4.36774145e-02 |
| 3.60000000 | 2.03732111e+01 | 2.04251635e+01 | -5.18155660e-02 |
| 3.80000000 | 1.99995967e+01 | 2.02121623e+01 | -1.68971574e-01 |
| 4.00000000 | 1.97196578e+01 | 1.99843212e+00 | -2.23036903e-01 |
| 4.20000000 | 1.94504756e+01 | 1.97835955e+00 | -2.72776387e-01 |
| 4.40000000 | 1.90779722e+01 | 1.95697375e+00 | -2.10500810e-01 |

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Long camera 4:
### 3.2.7 Electron diffraction intensities of FMN

| S   | Total Int. | Background | Exp. a.m(s) |
|-----|------------|------------|-------------|
| 9.20000000 | 1.38840579e+01 | 1.3891784e+01 | -5.07329461e-03 |
| 9.40000000 | 1.35029888e+01 | 1.3405670e+01 | 7.18451148e-02 |
| 9.60000000 | 1.30510493e+01 | 1.2936152e+01 | 8.53010271e-02 |
| 9.80000000 | 1.2693868e+01 | 1.24957289e+01 | 8.91382346e-02 |
| 10.00000000 | 1.21306437e+01 | 1.20766487e+01 | 4.4698724e-02 |
| 10.20000000 | 1.1677013e+01 | 1.16572848e+01 | 4.21904672e-04 |
| 10.40000000 | 1.12870968e+01 | 1.12947785e+01 | -6.79710341e-03 |
| 10.60000000 | 1.09643817e+01 | 1.09301830e+01 | 3.31656653e-02 |
| 10.80000000 | 1.06867862e+01 | 1.05835128e+01 | 1.05385988e-01 |
|               | Total Int. | Background Exp. aM(s) |
|---------------|------------|-----------------------|
| 9.6860141e+00 | 9.6868555e+00 | -2.50793452e-03 |
| 9.4123371e+00 | 9.3354061e+00 | 7.7463308e-02 |
| 9.1154509e+00 | 9.0015303e+00 | 1.2159063e-01 |
| 8.7571019e+00 | 8.6851279e+00 | 8.1221106e-02 |
| 8.4214117e+00 | 8.3843563e+00 | 4.4195198e-03 |
| 8.0840025e+00 | 8.0976700e+00 | -1.1676427e-02 |
| 7.8027239e+00 | 7.8246112e+00 | -2.9092421e-02 |
| 7.5834250e+00 | 7.5650510e+00 | 4.6119494e-03 |
| 7.3189236e+00 | 7.0839857e+00 | 1.7425175e-01 |
| 7.0861814e+00 | 7.0861814e+00 | 1.7425175e-01 |
| 7.0332923e+00 | 6.8666397e+00 | 2.7178231e-02 |
| 6.8610747e+00 | 6.6959664e+00 | 3.4424117e-01 |
| 6.6786208e+00 | 6.4654590e+00 | 3.8244411e-01 |
| 6.4707630e+00 | 6.2822926e+00 | 3.5399219e-01 |
| 6.2508968e+00 | 6.1094589e+00 | 2.7780796e-02 |
| 6.0366572e+00 | 5.9458240e+00 | 1.8637696e-04 |
| 5.8225869e+00 | 5.7904969e+00 | 6.8718679e-06 |
| 5.6232983e+00 | 5.6422585e+00 | -2.2687930e-02 |
| 5.4523490e+00 | 5.5010122e+00 | -1.1323152e-01 |
| 5.2912574e+00 | 5.3648799e+00 | -1.7839946e-03 |
| 5.1439914e+00 | 5.2333125e+00 | -2.2529171e-02 |
| 5.0114116e+00 | 5.1057839e+00 | -2.4767766e-01 |
| 4.8954985e+00 | 4.9381987e+00 | -2.3610378e-02 |
| 4.7888223e+00 | 4.8618337e+00 | -2.3548201e-04 |
| 4.6518739e+00 | 4.7451688e+00 | -1.7699405e-05 |
| 4.5981566e+00 | 4.6321996e+00 | -1.0439001e-01 |
| 4.5201094e+00 | 4.5229484e+00 | -9.1535055e-03 |
| 4.4346760e+00 | 4.4175949e+00 | 5.6452530e-02 |
| 4.3454410e+00 | 4.3160368e+00 | 1.0082989e-01 |
| 4.2502027e+00 | 4.2182239e+00 | 1.1306922e-01 |
| 4.1495049e+00 | 4.1239910e+00 | 9.4037646e-02 |
| 4.0372238e+00 | 4.0381835e+00 | 1.5402145e-02 |
| 3.9425006e+00 | 3.9456253e+00 | -8.3628395e-02 |
| 3.8191484e+00 | 3.8612285e+00 | -1.7219001e-03 |
| 3.7278438e+00 | 3.7797438e+00 | -2.1967393e-01 |
| 3.6528930e+00 | 3.7010468e+00 | -2.1077577e-01 |
| 3.5864571e+00 | 3.6250678e+00 | -1.7467673e-00 |
| 3.5355417e+00 | 3.5517997e+00 | -7.5984748e-02 |
| 3.4879361e+00 | 3.4812647e+00 | 3.2196521e-02 |
| 3.4384726e+00 | 3.4134981e+00 | 1.2624537e-01 |
| 3.3963555e+00 | 3.3485240e+00 | 2.5740224e-02 |
| 3.3388812e+00 | 3.2864341e+00 | 2.7816450e-04 |
| 3.2883258e+00 | 3.2269199e+00 | 3.3491466e-05 |
| 3.2252431e+00 | 3.1701293e+00 | 3.0945886e-05 |
| 3.1607786e+00 | 3.1150603e+00 | 2.5893723e-04 |
| 3.1395642e+00 | 3.0067331e+00 | 1.9524091e-02 |
| 3.0530458e+00 | 3.0170843e+00 | 1.3027389e-01 |
| 2.9700214e+00 | 2.9655277e+00 | 2.8222299e-01 |
| 2.9143141e+00 | 2.9189614e+00 | -2.9931600e-07 |
| 2.8596143e+00 | 2.8738109e+00 | -9.3809767e-02 |
| 2.8081367e+00 | 2.8298651e+00 | -1.4742257e-01 |
| 2.7636181e+00 | 2.7869546e+00 | -1.6244542e-01 |
| 2.7204167e+00 | 2.7492733e+00 | -1.7501650e-01 |
| 2.6764837e+00 | 2.7036620e+00 | -1.9903786e-01 |
### Long camera 2:

| S | Total Int. | Background | Exp. sM(s) |
|---|------------|------------|------------|
| 3.00000000 | 1.43583753e+01 | 1.62521534e+01 | -3.49574247e-01 |
| 3.20000000 | 1.42181684e+01 | 1.59899933e+01 | -3.54582742e-01 |
| 3.60000000 | 1.39145888e+01 | 1.57275574e+01 | -3.9132906e-01 |
| 3.80000000 | 1.35734038e+01 | 1.54502029e+01 | -4.35688623e-01 |
| 4.00000000 | 1.30598578e+01 | 1.51480391e+01 | -5.23863038e-01 |
| 4.20000000 | 1.24460357e+01 | 1.48152447e+01 | -6.39667872e-01 |
| 4.40000000 | 1.19473605e+01 | 1.44512678e+01 | -7.27715246e-01 |
| 4.60000000 | 1.16131581e+01 | 1.40572259e+01 | -7.65509386e-01 |
| 4.80000000 | 1.15552066e+01 | 1.36374143e+01 | -7.02343904e-01 |
| 5.00000000 | 1.16811523e+01 | 1.31983524e+01 | -5.51777992e-01 |
| 5.20000000 | 1.19172685e+01 | 1.27477657e+01 | -3.25742228e-01 |
| 5.40000000 | 1.21267737e+01 | 1.22931401e+01 | -3.19226755e-02 |
| 5.60000000 | 1.24624444e+01 | 1.18043976e+01 | 2.83649258e-01 |
| 5.80000000 | 1.26142099e+01 | 1.13940509e+01 | 5.98802644e-01 |
| 6.00000000 | 1.26409070e+01 | 1.09574281e+01 | 8.90669161e-01 |
| 6.20000000 | 1.24583287e+01 | 1.05330309e+01 | 1.09672008e+00 |
| 6.40000000 | 1.20911549e+01 | 1.01230596e+01 | 1.20538565e+00 |
| 6.60000000 | 1.15306762e+01 | 9.72918133e+00 | 1.18509919e+01 |
| 6.80000000 | 1.07923707e+01 | 9.35197760e+00 | 1.01653622e+01 |
| 7.00000000 | 9.94375132e+00 | 8.99169805e+00 | 7.19993290e-01 |
| 7.20000000 | 9.05674053e+00 | 8.64782269e+00 | 3.30999492e-01 |
| 7.40000000 | 8.25566073e+00 | 8.31961091e+00 | -5.54306295e-02 |
| 7.60000000 | 7.50722721e+00 | 8.00650340e+00 | -4.03239333e-02 |
| 7.80000000 | 7.04031552e+00 | 7.70828677e+00 | -6.58587532e-03 |
| 8.00000000 | 6.66572867e+00 | 7.42443740e+00 | -7.97087750e-04 |
| 8.20000000 | 6.42907503e+00 | 7.13447138e+00 | -8.11125019e-04 |
| 8.40000000 | 6.27913148e+00 | 6.89756459e+00 | -7.35208991e-04 |
| 8.60000000 | 6.18180527e+00 | 6.65311345e+00 | -5.95085082e-04 |
| 8.80000000 | 6.09928700e+00 | 6.42046318e+00 | -4.30204960e-04 |
| 9.00000000 | 6.02037050e+00 | 6.19888225e+00 | -2.53410746e-04 |
| 9.20000000 | 5.92750560e+00 | 5.89752493e+00 | -8.99397919e-05 |
| 9.40000000 | 5.80107979e+00 | 5.78558167e+00 | 3.99548467e-04 |
| 9.60000000 | 5.65307322e+00 | 5.59265521e+00 | 9.70140243e-04 |
| 9.80000000 | 5.47341160e+00 | 5.40867726e+00 | 1.14858643e-04 |
| 10.00000000 | 5.27583549e+00 | 5.23364018e+00 | 7.90107742e-05 |

### Long camera 3:

| S | Total Int. | Background | Exp. sM(s) |
|---|------------|------------|------------|

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| Background | Exp. sM(s) |
|------------|-----------|
| 242e+00    | 1.06462718e+01 |
| 200e+00    | 1.12224793e+01 |
| 190e+00    | 1.13775376e+01 |
| 180e+00    | 1.13982674e+01 |
| 170e+00    | 1.15093255e+01 |
| 160e+00    | 1.16133044e+01 |
| 150e+00    | 1.16133044e+01 |
| 140e+00    | 1.16133044e+01 |
| 130e+00    | 1.16133044e+01 |
| 120e+00    | 1.16133044e+01 |
| 110e+00    | 1.16133044e+01 |
| 100e+00    | 1.16133044e+01 |
| 90e+00     | 1.16133044e+01 |
| 80e+00     | 1.16133044e+01 |
| 70e+00     | 1.16133044e+01 |
| 60e+00     | 1.16133044e+01 |
| 50e+00     | 1.16133044e+01 |
| 40e+00     | 1.16133044e+01 |
| 30e+00     | 1.16133044e+01 |
| 20e+00     | 1.16133044e+01 |
| 10e+00     | 1.16133044e+01 |

| Total Int. | 1.02070765e+01 |
|------------|----------------|
| 9.81177253e+00 | -3.40366484e-01 |
| 9.65525268e+00 | -3.57553098e-01 |
| 9.30015318e+00 | -3.95286791e-01 |
| 9.37994788e+00 | -4.46847531e-01 |
| 9.1133044e+01 | -5.26712970e-01 |
| 8.96437209e+00 | -6.3979281e-01 |
| 8.47509336e+00 | -7.28431551e-01 |
| 8.50302383e+00 | -7.69474894e-01 |
| 8.24313935e+00 | -7.05278261e-01 |
| 7.96876012e+00 | -5.45462165e-01 |
| 7.86563645e+00 | -3.28780624e-01 |
| 7.40285862e+00 | -2.92720700e-02 |
| 7.12236751e+00 | 2.79404403e+00 |
| 6.84584581e+00 | 4.01286832e+00 |
| 6.58359125e+00 | 8.84117659e-01 |
| 6.3290101e+00 | 1.10196080e+00 |
| 6.08595253e+00 | 1.20507459e+00 |
| 5.85529976e+00 | 1.17530651e+00 |
| 5.6722232e+00 | 1.10619797e+00 |
| 5.4310172e+00 | 7.17393124e-01 |
| 5.23558991e+00 | 3.27056693e-01 |
| 5.04962133e+00 | -5.58625647e-02 |
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| 4.53672459e+00 | -7.83480435e-01 |
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| 3.91777250e+00 | -3.21333505e+00 |
| 3.80927997e+00 | -2.54928276e+00 |
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| 2.54114910e+00 | 4.13000357e-01 |
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| 1.80859115e-01 | 2.03895115e-02 |
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| 1.75387540e-01 | -1.77591775e-01 |
| 1.72857547e+00 | -2.23532522e-01 |

Long camera 4:
S | Total Int. | Background | Exp. sM(s)
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