Electronic Supplementary Material (ESI) for Chemical Science.


# Tribochemical Nanolithography: Photolithography without Optics Supplementary information

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**CONTENTS**

# S1. METHODS

## S1.1. Surface Preparation

(Methoxyheptaethyleneglycol)nitrophenylethoxycarbonyl-protected aminopropyl(triethoxy silane) (OEG-NPEOC-APTES) was synthesized by AF ChemPharm Ltd (Sheffield, UK). {*N*-[2-(2-Nitrophenyl)propan-1-oxycarbonyl]-3-aminopropyl}-triethoxysilane (NPPOC-APTES) was synthesized according to our previously reported methodology.[1] Glass slides (Menzel-Glaser, Braunschweig, Germany) and silicon wafers (PI-KEM Ltd, Tamworth, UK) were used as substrates. A thermal oxide was grown on the silicon wafers by heating them in a furnace for 6 h at 950 °C and allowing them to slowly cool to room temperature. Prior to use, all substrates were cleaned in piranha solution, a 1:3 mixture of hydrogen peroxide and sulfuric acid (***Caution! Piranha solution is an extremely strong oxidizing agent and can detonate upon contact with organic materials***) and rinsed thoroughly in deionized water (Veolia Water Technologies, High Wycombe, UK). The substrates were placed in an RCAII bath (hydrogen peroxide, ammonia, and water in the ratio 1:2:5) for 20 min, allowed to cool and rinsed thoroughly with deionized water. The substrates were dried at 120 °C for 2 h. Films of adsorbed silanes were formed by immersing clean, dry substrates in a solution of the silane in toluene (30 μL in 30 mL) for 48 h. The substrates were removed from the silane solution and washed in toluene, then a 50:50 (vol/vol) mix of toluene and ethanol, and finally with pure ethanol. The substrates were annealed at 120 °C for 20 minutes under vacuum. Samples were stored sealed in the dark until needed and used within one month of preparation.

## S1.2. Tribochemical Nanolithography

Tribochemical removal of nitrophenyl protecting groups was performed using a Nanoscope IIIa with nanolithography module. Tapping mode AFM probes (OTESPA-R3, Bruker, Karlsruhe, Germany) with nominal spring constants of 26 N $m^{-1}$ and a tip radius of 7-10 nm were used. The spring constant $k$ was measured for each cantilever using the thermal tune method, and the deflection sensitivity $\sigma$ was determined by bringing the probe into contact with a mica surface. Nanolithography was performed in contact mode. The applied load normal to the surface $F_N$ was calculated using the following equation:

$$F_N = k\sigma \times \text{setpoint} \quad (1)$$

After nanolithography, the substrates were washed with ethanol or deionized water and dried under a stream of nitrogen.

### S1.3 Surface Functionalization

To enable attachment of green fluorescent protein (GFP) to amine patterns formed by nanolithography, samples were first placed in a 25% (v/v) glutaraldehyde solution (pH 5) for 1 h in order to form an aldehyde-functionalized surface. Subsequently, the samples were immersed in a 10 mM aqueous solution of N-(5-amino-1-carboxypentyl)iminodiacetic acid (ABNTA) at pH 5 for 18 h to produce NTA functional surfaces. $Ni^{2+}$-chelated surfaces were prepared by immersing the samples in 100 mM $NiCl_2$ for 4 h, and complexed to His-GFP by immersion in a solution of the protein in buffer for 18 h. To remove the His-tagged GFP from the surface, samples were immersed in imadazole (100 mM, pH 7.4) solution for 4 h, and then rinsed with ammonium acetate and dried gently with a stream of nitrogen.

### S1.4. Density Functional Theory

The ground-state geometry of a simpler NPPOC molecule (without oligoethylene glycol sidechain, and with a methyl replacing the APTES group) in the gas-phase and in water was calculated for a number of different functionals and basis sets using Gaussian 09. From excited-state energy calculations, theoretical UV-Vis spectra were obtained and compared to the experimental value obtained in acetonitrile. The functional and basis set that resulted in spectra that most closely resembled empirical data were selected for use in further calculations.

The ground-state geometries for a variety of different conformations along the proposed NPEOC deprotection pathway were optimized. Additionally, geometries as various bonds in NPEOC were stretched by scanning across a range of separation values were also obtained. The resulting ground-state energy vs. bond length plots were fitted with a Morse oscillator potential to obtain a relative measure of the bond-dissociation energy.

Calculations in the excited-state geometry optimizations were performed using the "Optimization" job type and "TD-SCF" method, with 6 excited-state levels being investigated to arrive at a final geometry for the n = 2 energy level (N = 6, with state of interest root N = 1). UV-Vis spectra (and associated energy level transitions) were calculated using the "Energy" job type and "TD-SCF" method for 100 excited-state energy levels (N = 100), with resulting data exported into CSV files.

Results given above are for simulations run *in vacuo*. However, simulations run in a water environment were also performed using the integral equation formulism polarizable continuum model (IEFPCM), developed by Tomasi *et al.*[2] and Pascual-Ahuir *et al.*[3] These give similar results.

## S2. LITHOGRAPHIC PROCESS

To test whether pattern formation occurred via mechanical wear of the surface, behaviour was compared for APTES films at loads of 500 nN and 15 N (Figure S1). For these silanes that do not have a photoremovable protecting group, patterning was not observed at a load of 500 nN (the load typically selected in the lithographic experiments described in the main manuscript). However, modification of APTES films was observed on increasing the load above 12.5 μN, suggesting that there was a very high load threshold for mechanical wear. Thus, the patterning process observed for OEG-NPEOC-APTES films at lower loads is not attributable to mechanical wear. In contrast, feature formation is observed at loads of 500 nN for OEG-NPEOC-APTES films. Moreover, modification of APTES films at high loads leads to the accumulation of debris along the edge of the patterned structures (bright features in Figure S1(b)), indicative of tip-induced wear. In contrast, such accumulations of debris are not observed for OEG-NPEOC-APTES films even at a load of 15 μN, suggesting a different mechanism of surface modification.

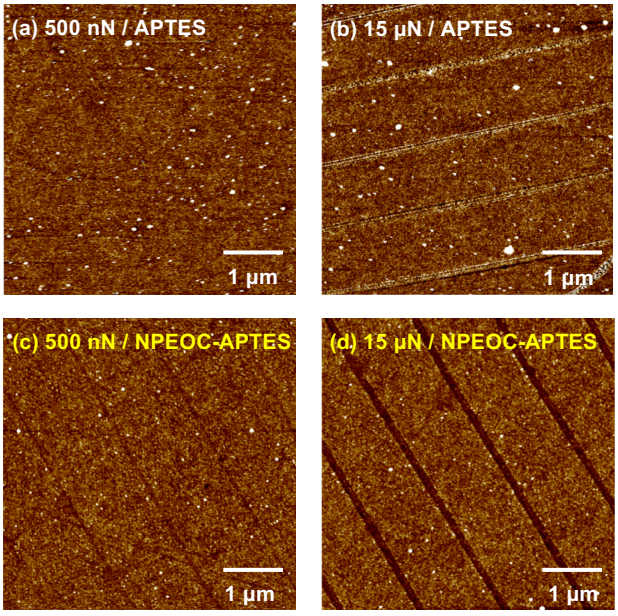



***Figure S1**: Tapping mode images showing the effect of the load on tip-induced modification of siloxane films. Top: APTES. Bottom: OEG-NPEOC-APTES.*

## S3. DENSITY FUNCTIONAL THEORY

A number of density functionals and basis sets were compared, by testing their ability to reproduce the absorption spectrum on the NPPOC functional group. The ω-B97XD functional[4] was selected. Figure S2 shows the experimental spectrum for NPEOC-APTES (black) together with calculated spectra produced using the ω-B97XD functional in conjunction with three different basis sets. The 6-311++G(d,p) was judged to be the best. This basis set includes a diffuse function in order to better represent orbitals further from the nucleus, including those of lighter atoms.

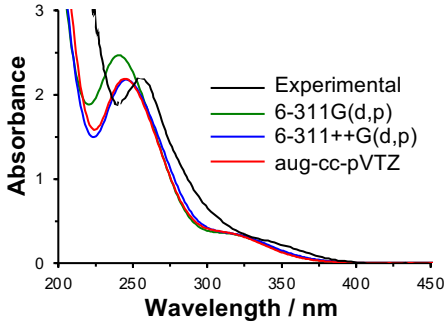



***Figure S2**: Absorption spectra for NPPOC calculated using the ω-B97XD functional in conjunction with three different basis sets.*

Two optimised ground-state configurations were determined from the DFT calculations (Supporting Information), described as “straight” and “folded”. The folded

conformation had slightly lower energy than the "straight" conformation and was thus used as the starting conformation for subsequent calculations.

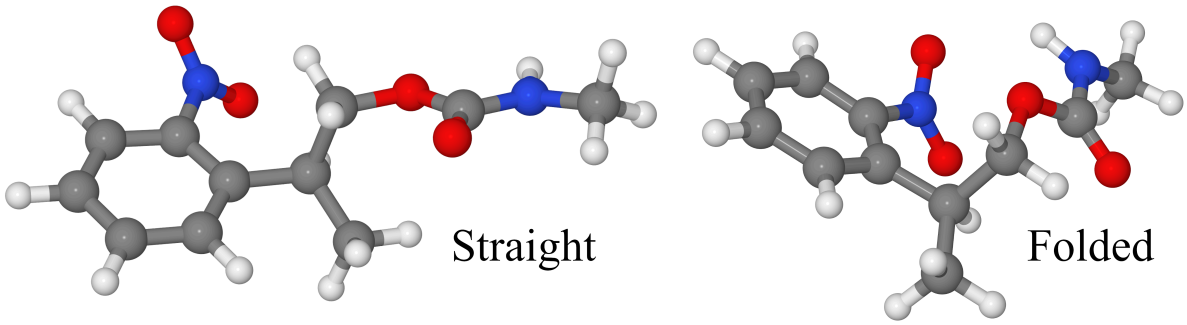



***Figure S3**: Straight and folded conformations for NPPOC determined from DFT calculations.*

After initial excitation by absorption of a photon, there is a change in the conformation of the $NO_2$ group; in the ground state it is planar, but it is no longer planar in the excited state, moving towards a pyramidal conformation (the ONO bond angle changes from 124.3º to 105.4º), and there is a small lengthening of the N–O bonds, suggesting a change in local electronic configuration (Figure S4).

The absorption spectrum was calculated after formation of the aci-nitro intermediate (Figure S5). The literature reports a substantial red-shift in the position of the $\pi \rightarrow \pi^*$ peak for the intermediate, something that is clearly replicated in the calculated spectrum. In the calculated spectrum, the $\pi \rightarrow \pi^*$ transition is seen at 390 nm with an oscillator strength of 0.178, compared to 320 nm (0.015) for the ground state. This $S_0 \rightarrow S_1$ transition has a strength an order of magnitude greater than in the initial ground-state conformation, albeit at a lower energy, but is unlikely to be a factor in subsequent steps in the decomposition of the molecule.

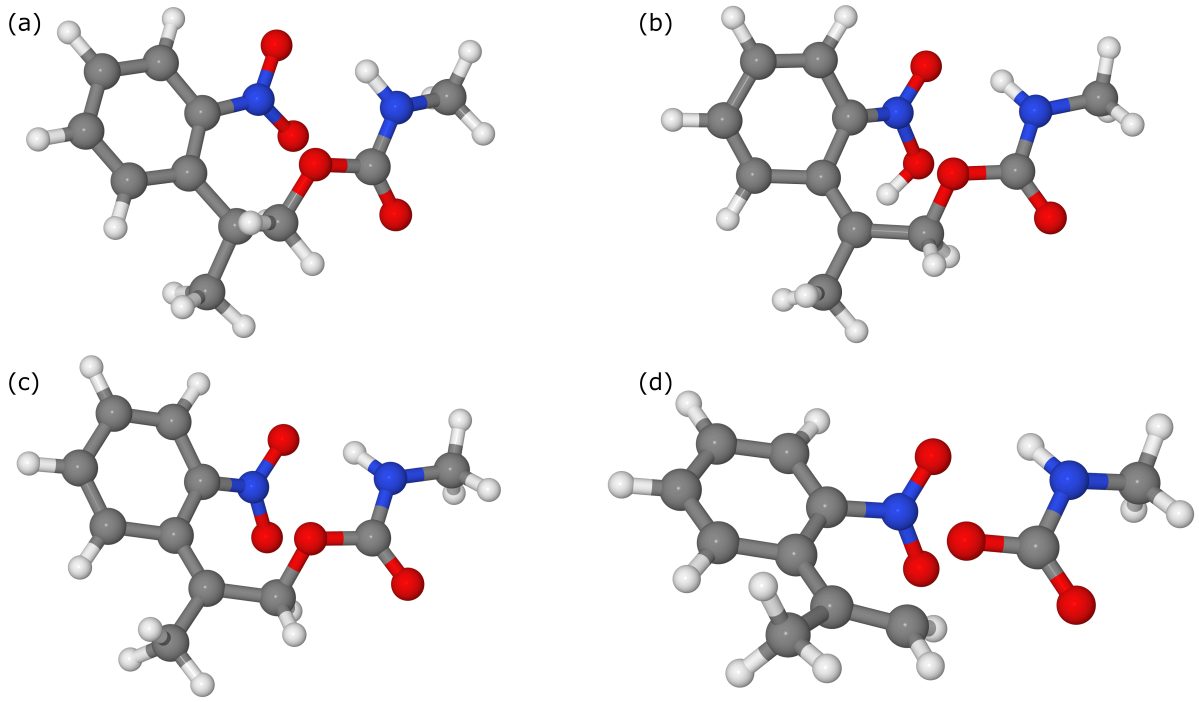



*Figure S4: Optimized geometries at different steps along the proposed photo-deprotection pathway. (a) After irradiation with UV light. (b) After proton transfer and relaxation (intermediate formation). (c) After proton loss (ionic form). (d) After decomposition of intermediate.*

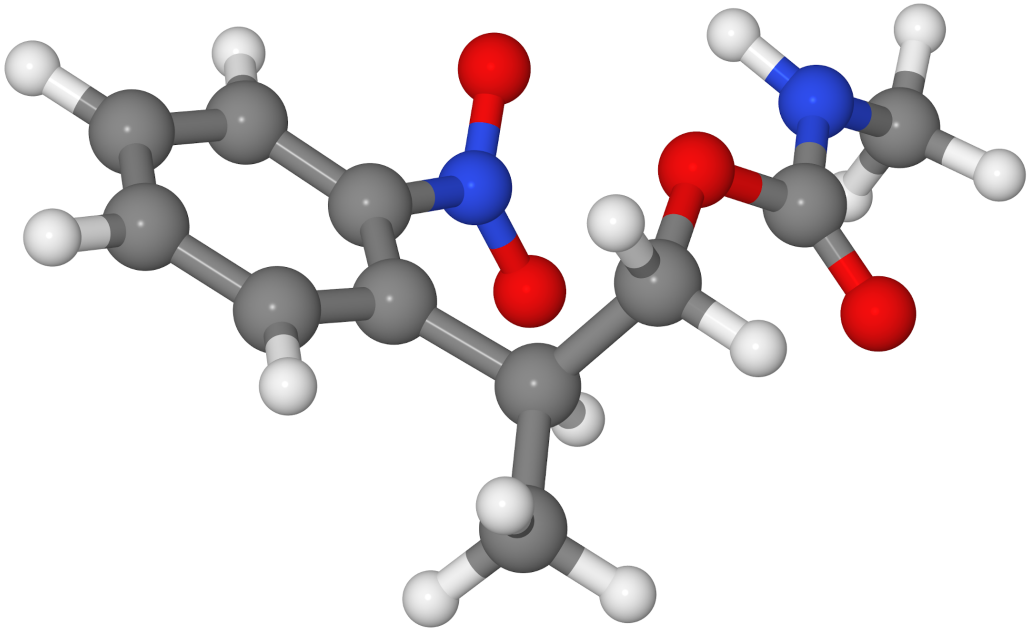

1 Alang-Ahmad, S. A. *et al.* Micrometer- and Nanometer-Scale Photopatterning Using 2-Nitrophenylpropyloxycarbonyl-Protected Aminosiloxane Monolayers. *J. Am Chem. Soc.* **131**, 1513–1522 (2009).

2 Miertuš, S., Scrocco, E. & Tomasi, J. Electrostatic interaction of a solute with a continuum. A direct utilizaion of AB initio molecular potentials for the prevision of solvent effects. *Chemical Physics* **55**, 117-129, doi:https://doi.org/10.1016/0301-0104(81)85090-2 (1981).

3 Pascual-ahuir, J. L., Silla, E. & Tuñon, I. GEPOL: An improved description of molecular surfaces. III. A new algorithm for the computation of a solvent-excluding surface. *Journal of Computational Chemistry* **15**, 1127-1138, doi:https://doi.org/10.1002/jcc.540151009 (1994).

4 Mardirossian, N. & Head-Gordon, M. ωB97X-V: A 10-parameter, range-separated hybrid, generalized gradient approximation density functional with nonlocal correlation, designed by a survival-of-the-fittest strategy. *Physical Chemistry Chemical Physics* **16**, 9904-9924, doi:10.1039/C3CP54374A (2014).

## S4. CALCULATIONS ON NPPOC (FOLDED FORM; $S_0$)



| | | |
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| SMILES | : CC(COC(=O)NC)c1ccccc1N(=O)=O | |
| Formula | : $C_{11}H_{14}N_2O_4$ | |
| Charge | : 0 | |
| Multiplicity | : 1 | |
| Dipole | : 11.4787 | Debye |
| Energy | : -837.89556198 | a.u. |
| Gibbs Energy | : -837.68941400 | a.u. |
| Number of imaginary frequencies | : 0 | |

### S4.1. Cartesian Co-ordinates (XYZ format)

31

| | | | |
|---|---|---|---|
| C | 3.83181906 | -0.11519900 | 0.50298500 |
| C | 2.86214900 | 0.82782698 | 0.19079000 |
| C | 1.56898999 | 0.47289801 | -0.20184501 |
| C | 1.31238794 | -0.90280700 | -0.24029800 |
| C | 2.25747204 | -1.86417699 | 0.09128400 |
| C | 3.53369808 | -1.46973300 | 0.45401001 |
| H | 4.82389688 | 0.21398801 | 0.79010600 |
| H | 3.12104988 | 1.87700295 | 0.25349799 |
| H | 1.98114705 | -2.90989399 | 0.05584300 |
| H | 4.28265715 | -2.21307397 | 0.69794202 |
| N | 0.00264400 | -1.44217300 | -0.64833099 |
| O | -0.43630999 | -2.37853289 | -0.00402400 |
| O | -0.55119902 | -0.95740098 | -1.61332595 |
| C | 0.51871902 | 1.54634500 | -0.44354999 |
| H | -0.14104100 | 1.21987998 | -1.24654305 |

| | | | |
|---|---|---|---|
| C | 1.09878194 | 2.90407491 | -0.84441602 |
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| H | 0.28789699 | 3.55715895 | -1.17307103 |
| H | 1.60404396 | 3.40451598 | -0.01243000 |
| C | -0.34633601 | 1.72408998 | 0.81304598 |
| H | -0.99615401 | 2.59180188 | 0.69191200 |
| H | 0.27970201 | 1.85467696 | 1.69842899 |
| O | -1.13978004 | 0.56979501 | 1.06660295 |
| C | -2.36596704 | 0.55329603 | 0.46953499 |
| O | -2.84265208 | 1.49803901 | -0.11510200 |
| N | -2.95404005 | -0.64915800 | 0.65510899 |
| H | -2.34631705 | -1.39757502 | 0.95099998 |
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| H | -3.93546295 | -1.24915302 | -1.12033999 |
| H | -4.63600206 | -1.84178305 | 0.40711600 |
| H | -4.83806181 | -0.14406800 | -0.06510400 |

### S4.2. Frequencies

| Mode | IR frequency | IR intensity | Raman intensity |
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| 3 | 71.68430000 | 1.74060000 | 0.00000000 |
| 4 | 79.18040000 | 0.56160000 | 0.00000000 |
| 5 | 88.10130000 | 7.10640000 | 0.00000000 |
| 6 | 98.84240000 | 3.30950000 | 0.00000000 |
| 7 | 108.33450000 | 0.97500000 | 0.00000000 |
| 8 | 148.46310000 | 0.85210000 | 0.00000000 |
| 9 | 177.04150000 | 2.27230000 | 0.00000000 |
| 10 | 184.72260000 | 2.37980000 | 0.00000000 |
| 11 | 226.75680000 | 6.06850000 | 0.00000000 |
| 12 | 260.02090000 | 1.55880000 | 0.00000000 |
| 13 | 265.11070000 | 2.79330000 | 0.00000000 |
| 14 | 275.88310000 | 1.56270000 | 0.00000000 |
| 15 | 310.31140000 | 1.45510000 | 0.00000000 |
| 16 | 370.03070000 | 32.09800000 | 0.00000000 |
| 17 | 383.66750000 | 0.94550000 | 0.00000000 |
| 18 | 396.13320000 | 3.44380000 | 0.00000000 |
| 19 | 407.88650000 | 2.09700000 | 0.00000000 |
| 20 | 446.68800000 | 0.08990000 | 0.00000000 |
| 21 | 555.82240000 | 3.12770000 | 0.00000000 |
| 22 | 574.63000000 | 73.46850000 | 0.00000000 |
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| 24 | 591.72020000 | 45.59370000 | 0.00000000 |
| 25 | 609.48530000 | 0.37260000 | 0.00000000 |
| 26 | 685.82020000 | 6.70730000 | 0.00000000 |
| 27 | 713.88210000 | 27.10290000 | 0.00000000 |
| 28 | 741.63500000 | 23.42450000 | 0.00000000 |
| 29 | 773.22490000 | 21.92860000 | 0.00000000 |
| 30 | 783.80940000 | 15.50480000 | 0.00000000 |
| 31 | 795.80940000 | 19.07210000 | 0.00000000 |
| 32 | 821.09170000 | 11.50780000 | 0.00000000 |
| 33 | 891.31790000 | 20.46240000 | 0.00000000 |
| 34 | 899.08910000 | 9.59700000 | 0.00000000 |
| 35 | 915.13120000 | 14.73380000 | 0.00000000 |
| 36 | 930.70270000 | 8.39670000 | 0.00000000 |
| 37 | 983.12320000 | 12.81110000 | 0.00000000 |
| 38 | 989.17240000 | 0.87080000 | 0.00000000 |
| 39 | 1023.09930000 | 0.21240000 | 0.00000000 |
| 40 | 1058.27150000 | 34.56950000 | 0.00000000 |
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| 42 | 1083.15620000 | 7.64750000 | 0.00000000 |
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| 44 | 1132.16300000 | 0.76120000 | 0.00000000 |
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| 46 | 1154.39080000 | 13.55950000 | 0.00000000 |
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| 48 | 1188.60240000 | 2.15160000 | 0.00000000 |
| 49 | 1200.25120000 | 2.86540000 | 0.00000000 |
| 50 | 1202.68720000 | 13.46800000 | 0.00000000 |
| 51 | 1233.38580000 | 8.45990000 | 0.00000000 |
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| 53 | 1293.66620000 | 33.12950000 | 0.00000000 |
| 54 | 1321.12470000 | 10.99350000 | 0.00000000 |
| 55 | 1340.59980000 | 14.84970000 | 0.00000000 |
| 56 | 1355.47040000 | 7.35850000 | 0.00000000 |
| 57 | 1389.55040000 | 1.30040000 | 0.00000000 |
| 58 | 1417.71700000 | 8.38960000 | 0.00000000 |
| 59 | 1423.82750000 | 5.79300000 | 0.00000000 |
| 60 | 1458.28990000 | 225.30500000 | 0.00000000 |

| | | | |
|---|---|---|---|
| 61 | 1461.18690000 | 10.61920000 | 0.00000000 |
| 62 | 1480.70650000 | 10.62910000 | 0.00000000 |
| 63 | 1490.08260000 | 1.64250000 | 0.00000000 |
| 64 | 1494.46620000 | 27.85810000 | 0.00000000 |
| 65 | 1506.55320000 | 9.52740000 | 0.00000000 |
| 66 | 1509.26360000 | 9.00900000 | 0.00000000 |
| 67 | 1513.82720000 | 17.79830000 | 0.00000000 |
| 68 | 1534.52290000 | 9.51580000 | 0.00000000 |
| 69 | 1584.56300000 | 306.49960000 | 0.00000000 |
| 70 | 1643.64820000 | 106.41690000 | 0.00000000 |
| 71 | 1657.16860000 | 92.96190000 | 0.00000000 |
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| 73 | 1830.67010000 | 366.01790000 | 0.00000000 |
| 74 | 3045.04900000 | 34.66670000 | 0.00000000 |
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| 76 | 3080.34090000 | 31.88380000 | 0.00000000 |
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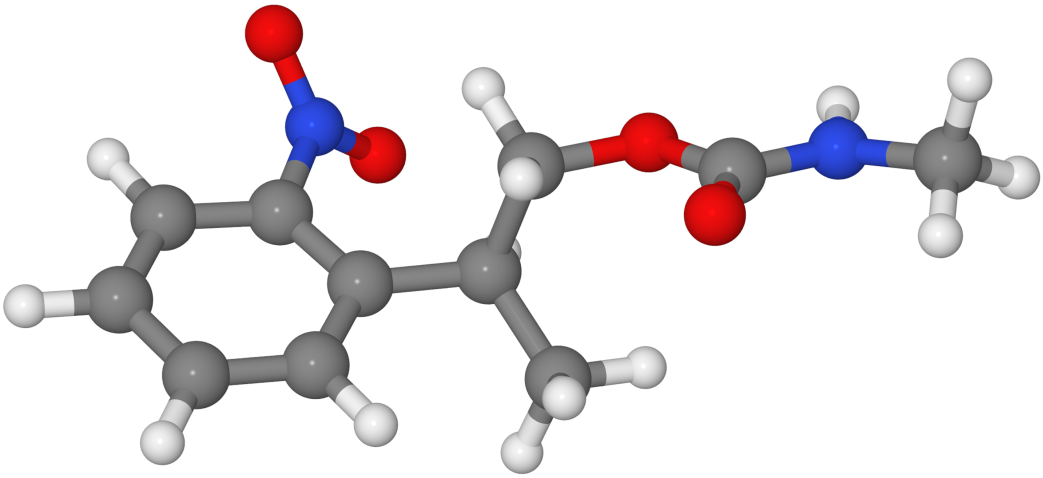
| 81 | 3149.92700000 | 9.91630000 | 0.00000000 |
| 82 | 3163.02960000 | 7.91250000 | 0.00000000 |
| 83 | 3197.88510000 | 2.38720000 | 0.00000000 |
| 84 | 3215.27980000 | 6.97830000 | 0.00000000 |
| 85 | 3225.93940000 | 5.07750000 | 0.00000000 |
| 86 | 3233.74030000 | 3.00660000 | 0.00000000 |
| 87 | 3654.82090000 | 50.94170000 | 0.00000000 |

## S5. CALCULATIONS ON NPPOC (STRAIGHT FORM; $S_0$)



| | | |
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| Formula | : $C_{11}H_{14}N_2O_4$ | |
| Charge | : 0 | |
| Multiplicity | : 1 | |
| Dipole | : 5.9868 | Debye |
| Energy | : -837.89045085 | a.u. |
| Gibbs Energy | : -837.68782300 | a.u. |
| Number of imaginary frequencies | : 0 | |

### S5.1. Cartesian Co-ordinates (XYZ format)

31

| | | | |
|---|---|---|---|
| C | -2.61938095 | -1.74748397 | 0.07618600 |
| C | -2.31463695 | -0.39372799 | 0.13432001 |
| C | -1.07577205 | 0.07062900 | 0.58009601 |
| C | -0.15383001 | -0.91917700 | 0.93807101 |
| C | -0.42469299 | -2.27741790 | 0.86495101 |
| C | -1.67565596 | -2.69671702 | 0.44329801 |
| H | -3.59964395 | -2.05931497 | -0.26543799 |
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| H | -1.90545702 | -3.75415111 | 0.39695400 |
| N | 1.19797599 | -0.57461500 | 1.42426002 |
| O | 2.12914705 | -1.19592297 | 0.95130098 |
| O | 1.30101001 | 0.28093201 | 2.28110504 |
| C | -0.74066401 | 1.55359399 | 0.56174499 |
| H | -0.13085701 | 1.77529097 | 1.43737698 |
| C | -1.96510196 | 2.46817803 | 0.59816098 |
| H | -2.61973310 | 2.20991707 | 1.43391001 |
| H | -1.64273095 | 3.50198102 | 0.73601401 |
| H | -2.53862810 | 2.43202710 | -0.33103400 |
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| H | -0.44903600 | 1.61653495 | -1.59259605 |

| | | | |
|---|---|---|---|
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| N | 0.48873100 | 5.26752806 | -1.39170003 |
| H | 1.28928900 | 5.35468388 | -0.78905100 |
| C | 0.11919900 | 6.35918379 | -2.26666689 |
| H | 0.71900499 | 6.37603092 | -3.18245602 |
| H | -0.92883199 | 6.25047302 | -2.54367304 |
| H | 0.24852200 | 7.30421209 | -1.73761594 |

### S5.2. Frequencies

| Mode | IR frequency | IR intensity | Raman intensity |
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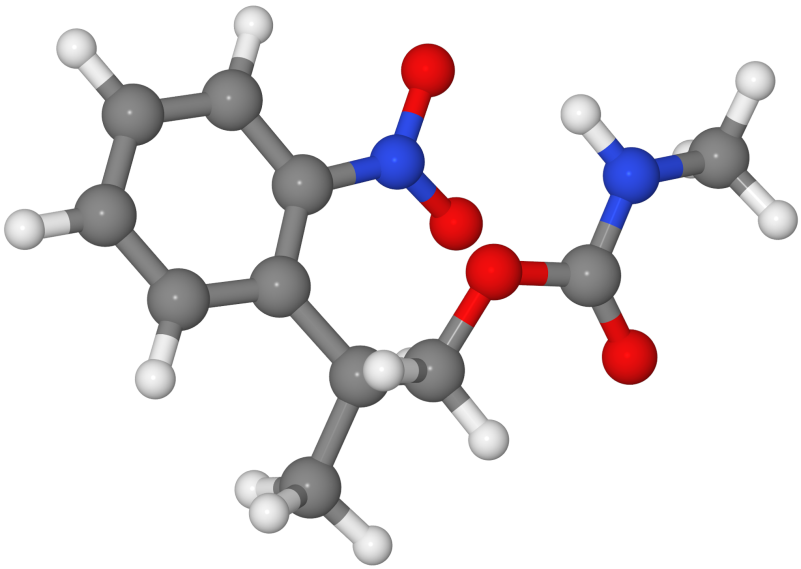
| 22 | 525.69580000 | 10.44340000 | 0.00000000 |
| 23 | 559.12390000 | 3.89380000 | 0.00000000 |
| 24 | 598.60370000 | 1.35920000 | 0.00000000 |
| 25 | 636.84920000 | 0.23310000 | 0.00000000 |
| 26 | 695.70240000 | 7.10290000 | 0.00000000 |
| 27 | 707.16250000 | 6.99540000 | 0.00000000 |
| 28 | 743.51630000 | 17.79170000 | 0.00000000 |
| 29 | 768.18730000 | 35.96230000 | 0.00000000 |
| 30 | 791.99330000 | 10.27730000 | 0.00000000 |
| 31 | 805.70100000 | 19.07400000 | 0.00000000 |
| 32 | 819.83840000 | 6.30230000 | 0.00000000 |
| 33 | 886.23360000 | 22.42240000 | 0.00000000 |
| 34 | 898.42900000 | 8.55250000 | 0.00000000 |
| 35 | 905.74920000 | 1.10240000 | 0.00000000 |
| 36 | 926.71910000 | 9.20050000 | 0.00000000 |
| 37 | 966.30550000 | 13.23180000 | 0.00000000 |
| 38 | 988.01360000 | 1.74650000 | 0.00000000 |
| 39 | 1023.69860000 | 0.40260000 | 0.00000000 |
| 40 | 1048.23370000 | 85.92470000 | 0.00000000 |
| 41 | 1059.22000000 | 9.28280000 | 0.00000000 |
| 42 | 1087.85760000 | 2.41590000 | 0.00000000 |
| 43 | 1101.78500000 | 4.03980000 | 0.00000000 |
| 44 | 1143.32400000 | 1.42930000 | 0.00000000 |
| 45 | 1155.67220000 | 23.73500000 | 0.00000000 |
| 46 | 1164.04340000 | 23.67300000 | 0.00000000 |
| 47 | 1188.28930000 | 10.83320000 | 0.00000000 |
| 48 | 1193.87830000 | 28.87340000 | 0.00000000 |
| 49 | 1202.67870000 | 3.98110000 | 0.00000000 |
| 50 | 1207.54650000 | 111.66150000 | 0.00000000 |
| 51 | 1234.92740000 | 3.61990000 | 0.00000000 |
| 52 | 1273.91080000 | 455.46820000 | 0.00000000 |
| 53 | 1302.92460000 | 8.80990000 | 0.00000000 |
| 54 | 1324.07430000 | 9.01850000 | 0.00000000 |
| 55 | 1340.88200000 | 19.11960000 | 0.00000000 |
| 56 | 1354.59420000 | 8.39830000 | 0.00000000 |
| 57 | 1402.14020000 | 9.74580000 | 0.00000000 |
| 58 | 1417.39200000 | 4.17070000 | 0.00000000 |
| 59 | 1435.47710000 | 2.86330000 | 0.00000000 |
| 60 | 1458.10430000 | 173.49480000 | 0.00000000 |

| | | | |
|---|---|---|---|
| 61 | 1461.32380000 | 18.45100000 | 0.00000000 |
| 62 | 1489.14930000 | 3.05500000 | 0.00000000 |
| 63 | 1492.85290000 | 2.25720000 | 0.00000000 |
| 64 | 1497.05260000 | 34.80310000 | 0.00000000 |
| 65 | 1501.55680000 | 15.69550000 | 0.00000000 |
| 66 | 1514.87210000 | 42.34220000 | 0.00000000 |
| 67 | 1517.40630000 | 7.12280000 | 0.00000000 |
| 68 | 1535.73460000 | 9.01710000 | 0.00000000 |
| 69 | 1581.62390000 | 433.23940000 | 0.00000000 |
| 70 | 1647.12220000 | 92.74980000 | 0.00000000 |
| 71 | 1658.87700000 | 169.26890000 | 0.00000000 |
| 72 | 1690.91970000 | 73.91400000 | 0.00000000 |
| 73 | 1826.31300000 | 335.74120000 | 0.00000000 |
| 74 | 3042.54960000 | 65.14380000 | 0.00000000 |
| 75 | 3052.91680000 | 15.13400000 | 0.00000000 |
| 76 | 3080.15300000 | 27.14950000 | 0.00000000 |
| 77 | 3120.64770000 | 22.40780000 | 0.00000000 |
| 78 | 3121.24650000 | 5.27250000 | 0.00000000 |
| 79 | 3133.94130000 | 18.52720000 | 0.00000000 |
| 80 | 3135.93550000 | 15.09800000 | 0.00000000 |
| 81 | 3146.15880000 | 6.67270000 | 0.00000000 |
| 82 | 3163.00300000 | 6.46980000 | 0.00000000 |
| 83 | 3198.68900000 | 2.15010000 | 0.00000000 |
| 84 | 3214.87760000 | 6.80050000 | 0.00000000 |
| 85 | 3227.73730000 | 1.99720000 | 0.00000000 |
| 86 | 3231.72640000 | 4.08060000 | 0.00000000 |
| 87 | 3692.58730000 | 46.57330000 | 0.00000000 |

## S6. CALCULATIONS ON NPPOC (FOLDED FORM; $S_1$)



| | | |
|---|---|---|
| Route | : # opt=maxstep=3 td=(nstates=6,root=1) wb97xd/6-311++g(d,p) nosymm geom | |
| | : =connectivity int=ultrafine iop(1/19=15) | |
| SMILES | : CC(COC(=O)NC)c1ccccc1N(=O)=O | |
| Formula | : $C_{11}H_{14}N_2O_4$ | |
| Charge | : 0 | |
| Multiplicity | : 1 | |
| Energy | : -837.77915912 | a.u. |

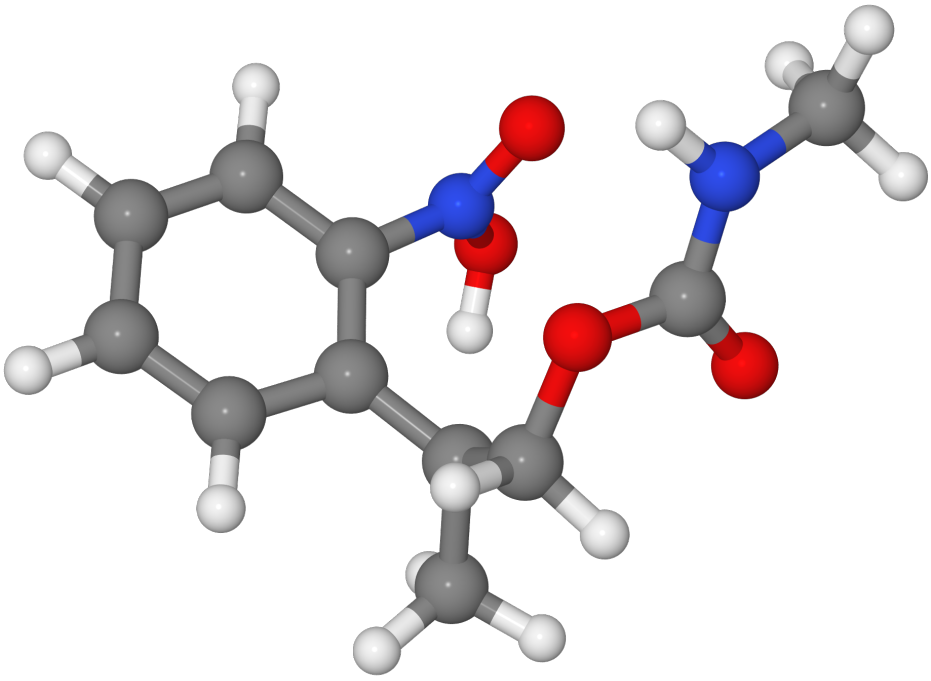
### S6.1. Cartesian Co-ordinates (XYZ format)

31

| | | | |
|---|---|---|---|
| C | -3.70653391 | -0.17038199 | -0.67987102 |
| C | -2.79748011 | 0.80764902 | -0.29493099 |
| C | -1.53932297 | 0.50033301 | 0.21765700 |
| C | -1.24501002 | -0.87108397 | 0.34884700 |
| C | -2.14392805 | -1.86970103 | -0.04307500 |
| C | -3.37474298 | -1.51427996 | -0.56195301 |
| H | -4.67281818 | 0.12050100 | -1.07469797 |
| H | -3.07489896 | 1.84820604 | -0.41001001 |
| H | -1.86791503 | -2.90851212 | 0.08531500 |
| H | -4.07638216 | -2.28468704 | -0.85792601 |
| N | -0.02196700 | -1.31957901 | 0.84134400 |
| O | 0.38219699 | -2.54053497 | 0.79329401 |
| O | 0.76874298 | -0.73165298 | 1.66492796 |
| C | -0.52657002 | 1.59934402 | 0.49058300 |
| H | 0.14937100 | 1.28088295 | 1.28725195 |
| C | -1.15001905 | 2.92762399 | 0.92395401 |
| H | -1.85785699 | 2.78282499 | 1.74258006 |
| H | -0.36450300 | 3.60369992 | 1.26782596 |
| H | -1.67373204 | 3.42717290 | 0.10325500 |
| C | 0.33583799 | 1.82919002 | -0.75981897 |
| H | 1.01836395 | 2.66357207 | -0.59044701 |
| H | -0.29746300 | 2.04002905 | -1.62447500 |

| | | | |
|---|---|---|---|
| O | 1.08054602 | 0.66616601 | -1.10131502 |
| C | 2.30862403 | 0.55734199 | -0.52247399 |
| O | 2.84129906 | 1.44351006 | 0.10244200 |
| N | 2.83560395 | -0.66145098 | -0.78326601 |
| H | 2.18926692 | -1.35738397 | -1.11811602 |
| C | 4.01550007 | -1.10988700 | -0.07107800 |
| H | 3.78075099 | -1.40403795 | 0.95663500 |
| H | 4.44751120 | -1.95934606 | -0.60082000 |
| H | 4.74531794 | -0.30157101 | -0.04566800 |

## S7. CALCULATIONS ON NPPOC (H-TRANSFER; RELAXED; $S_1$)



Route : # opt=maxstep=3 td=(nstates=6,root=1) wb97xd/6-311++g(d,p) nosymm geom =connectivity density=current int=ultrafine iop(1/19=15)
SMILES : C[C](COC(=O)NC)c1ccccc1N(O)[O]
Formula : $C_{11}H_{14}N_2O_4$
Charge : 0
Multiplicity : 1
Energy : -837.716697352 a.u.

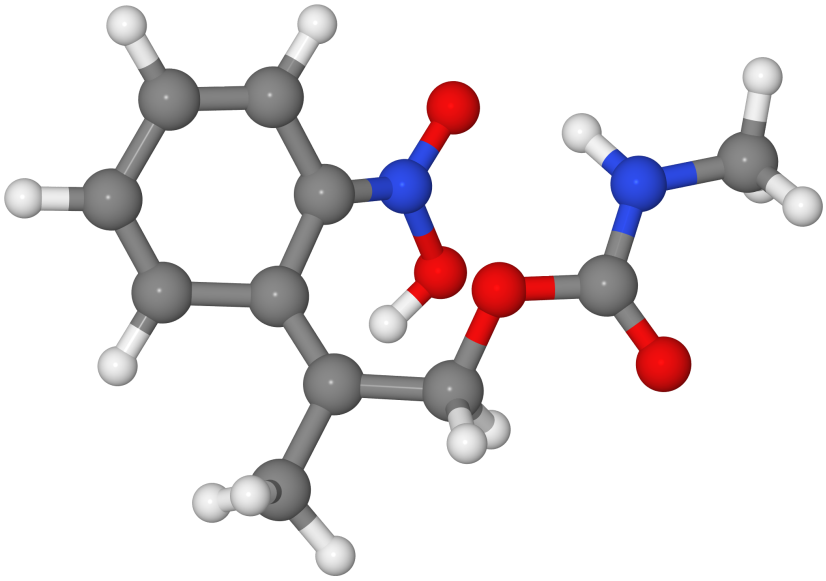
### S7.1. Cartesian Co-ordinates (XYZ format)

31

| | | | |
|---|---|---|---|
| C | -1.37003 | -0.24591 | -2.92637 |
| C | -0.03523 | -0.44910 | -2.62879 |
| C | 0.43728 | -0.69207 | -1.32438 |
| C | -0.56868 | -0.66476 | -0.31780 |
| C | -1.92211 | -0.47565 | -0.61032 |
| C | -2.32448 | -0.26436 | -1.91256 |
| H | -1.67580 | -0.08411 | -3.95403 |
| H | 0.69455 | -0.45495 | -3.43185 |
| H | -2.63567 | -0.49645 | 0.20512 |
| H | -3.37350 | -0.11528 | -2.14029 |
| N | -0.23976 | -0.85202 | 1.03782 |
| O | -0.32027 | -1.92524 | 1.62380 |
| O | 0.25286 | 0.21942 | 1.73035 |
| C | 1.85139 | -0.98134 | -1.10815 |
| C | 2.81974 | 0.10549 | -1.47077 |
| H | 2.54958 | 1.06492 | -1.01759 |
| H | 3.83072 | -0.14617 | -1.13814 |
| H | 2.87223 | 0.28892 | -2.56217 |

| | | | |
|---|---|---|---|
| C | 2.31262 | -2.37641 | -1.36489 |
| H | 3.39072 | -2.45606 | -1.20627 |
| H | 2.08749 | -2.68792 | -2.39878 |
| O | 1.65750 | -3.39361 | -0.58819 |
| C | 2.03417 | -3.46455 | 0.70849 |
| O | 2.93514 | -2.81829 | 1.19520 |
| N | 1.29302 | -4.38991 | 1.36346 |
| H | 0.50471 | -4.76909 | 0.86797 |
| C | 1.37230 | -4.53472 | 2.80024 |
| H | 0.76842 | -3.78381 | 3.31883 |
| H | 1.03058 | -5.53277 | 3.07877 |
| H | 2.41018 | -4.41783 | 3.11052 |
| H | 0.85894 | 0.66873 | 1.11947 |

## S8. CALCULATIONS ON NPPOC (H-TRANSFER; RELAXED; $S_0$)



| | | |
|---|---|---|
| Route | : # opt freq wb97xd/6-311++g(d,p) geom=connectivity int=ultrafine | |
| SMILES | : C[C](COC(=O)NC)c1ccccc1N(O)[O] | |
| Formula | : $C_{11}H_{14}N_2O_4$ | |
| Charge | : 0 | |
| Multiplicity | : 1 | |
| Dipole | : 11.4262 | Debye |
| Energy | : -837.82704857 | a.u. |
| Gibbs Energy | : -837.62365900 | a.u. |
| Number of imaginary frequencies | : 0 | |

### S8.1. Cartesian Co-ordinates (XYZ format)

31

| | | | |
|---|---|---|---|
| C | -1.74821103 | 0.07536200 | -2.60442400 |
| C | -0.64334601 | 0.75014299 | -2.23560095 |
| C | 0.29156899 | 0.18432100 | -1.25830996 |
| C | -0.32564399 | -0.84674001 | -0.40605500 |
| C | -1.39575195 | -1.65619397 | -0.94354600 |
| C | -2.07927489 | -1.20317698 | -2.01143003 |
| H | -2.39286089 | 0.47840601 | -3.37705803 |
| H | -0.39095399 | 1.67766905 | -2.73311496 |
| H | -1.66308498 | -2.56701303 | -0.42517900 |
| H | -2.90983391 | -1.77434897 | -2.40834999 |
| N | -0.02206800 | -1.01659298 | 0.86772799 |
| O | -0.37459999 | -1.94729805 | 1.59739900 |
| O | 0.77788699 | -0.08510800 | 1.51496696 |
| C | 1.61843896 | 0.48779100 | -1.30015600 |
| C | 2.15111589 | 1.60698903 | -2.15882111 |
| H | 1.48134398 | 2.46618891 | -2.19785595 |
| H | 3.11283302 | 1.95584595 | -1.77328098 |
| H | 2.32071495 | 1.26183999 | -3.18472004 |
| C | 2.73313189 | -0.26681301 | -0.62873399 |
| H | 3.10654998 | 0.27825499 | 0.24966601 |

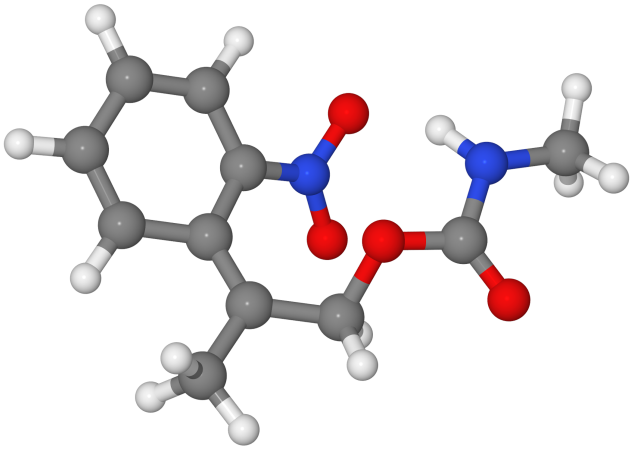
| | | | |
|---|---|---|---|
| H | 3.57120609 | -0.32118401 | -1.33219695 |
| O | 2.34995508 | -1.57253397 | -0.25256100 |
| C | 3.16068292 | -2.17534208 | 0.66173899 |
| O | 4.28729916 | -1.80404603 | 0.89442003 |
| N | 2.52863407 | -3.23090196 | 1.21963704 |
| H | 1.51847696 | -3.21577191 | 1.17848599 |
| C | 3.15436912 | -3.95052099 | 2.31087303 |
| H | 3.12964392 | -3.38177896 | 3.24585104 |
| H | 2.63115597 | -4.89623499 | 2.45303702 |
| H | 4.19432402 | -4.15623522 | 2.05868793 |
| H | 0.80689901 | 0.68636900 | 0.92788100 |

### S8.2. Frequencies

| Mode | IR frequency | IR intensity | Raman intensity |
|---|---|---|---|
| 1 | 34.62730000 | 0.31180000 | 0.00000000 |
| 2 | 46.75080000 | 3.68750000 | 0.00000000 |
| 3 | 69.75420000 | 2.92330000 | 0.00000000 |
| 4 | 94.11940000 | 0.62470000 | 0.00000000 |
| 5 | 101.82490000 | 1.35760000 | 0.00000000 |
| 6 | 109.34970000 | 19.40240000 | 0.00000000 |
| 7 | 130.92630000 | 1.36100000 | 0.00000000 |
| 8 | 139.40800000 | 1.18020000 | 0.00000000 |
| 9 | 143.73380000 | 1.44730000 | 0.00000000 |
| 10 | 162.66140000 | 3.72500000 | 0.00000000 |
| 11 | 212.95630000 | 2.67810000 | 0.00000000 |
| 12 | 218.09650000 | 5.16600000 | 0.00000000 |
| 13 | 242.24620000 | 1.92610000 | 0.00000000 |
| 14 | 286.49500000 | 3.70240000 | 0.00000000 |
| 15 | 290.31600000 | 9.92170000 | 0.00000000 |
| 16 | 340.61720000 | 2.94660000 | 0.00000000 |
| 17 | 367.09520000 | 47.09960000 | 0.00000000 |
| 18 | 396.21240000 | 15.72550000 | 0.00000000 |
| 19 | 418.75980000 | 47.65930000 | 0.00000000 |
| 20 | 435.93160000 | 4.99780000 | 0.00000000 |
| 21 | 471.82860000 | 8.12700000 | 0.00000000 |
| 22 | 492.39280000 | 25.01030000 | 0.00000000 |
| 23 | 550.40000000 | 38.18270000 | 0.00000000 |
| 24 | 563.29190000 | 55.30780000 | 0.00000000 |
| 25 | 579.66930000 | 7.34640000 | 0.00000000 |
| 26 | 585.61120000 | 17.31650000 | 0.00000000 |
| 27 | 619.20690000 | 6.83260000 | 0.00000000 |
| 28 | 644.60530000 | 6.17180000 | 0.00000000 |
| 29 | 702.04640000 | 25.60440000 | 0.00000000 |
| 30 | 733.29000000 | 9.63030000 | 0.00000000 |
| 31 | 751.14710000 | 32.51280000 | 0.00000000 |
| 32 | 759.93720000 | 19.52320000 | 0.00000000 |
| 33 | 798.00590000 | 5.39070000 | 0.00000000 |
| 34 | 822.73490000 | 8.37000000 | 0.00000000 |
| 35 | 832.53800000 | 23.99780000 | 0.00000000 |
| 36 | 932.34520000 | 17.73150000 | 0.00000000 |
| 37 | 959.54180000 | 7.18000000 | 0.00000000 |
| 38 | 987.31900000 | 34.60030000 | 0.00000000 |
| 39 | 993.54360000 | 4.55130000 | 0.00000000 |
| 40 | 1000.91080000 | 14.93530000 | 0.00000000 |
| 41 | 1005.75000000 | 0.81560000 | 0.00000000 |
| 42 | 1025.71950000 | 38.59420000 | 0.00000000 |
| 43 | 1063.43310000 | 14.49030000 | 0.00000000 |
| 44 | 1070.08960000 | 15.37270000 | 0.00000000 |
| 45 | 1096.60090000 | 4.06150000 | 0.00000000 |
| 46 | 1138.27960000 | 14.57620000 | 0.00000000 |
| 47 | 1153.24640000 | 15.49640000 | 0.00000000 |
| 48 | 1183.58710000 | 10.85470000 | 0.00000000 |
| 49 | 1195.14590000 | 92.93310000 | 0.00000000 |
| 50 | 1204.04770000 | 15.16680000 | 0.00000000 |
| 51 | 1221.76470000 | 23.11590000 | 0.00000000 |
| 52 | 1255.65870000 | 10.10970000 | 0.00000000 |
| 53 | 1289.18710000 | 198.12380000 | 0.00000000 |
| 54 | 1300.10270000 | 2.26720000 | 0.00000000 |
| 55 | 1326.84230000 | 299.71940000 | 0.00000000 |
| 56 | 1343.73110000 | 29.15070000 | 0.00000000 |
| 57 | 1398.68020000 | 30.95810000 | 0.00000000 |
| 58 | 1414.47140000 | 2.16090000 | 0.00000000 |
| 59 | 1418.92540000 | 7.30440000 | 0.00000000 |
| 60 | 1442.61920000 | 32.75010000 | 0.00000000 |

| | | | |
|---|---|---|---|
| 61 | 1465.44970000 | 11.29290000 | 0.00000000 |
| 62 | 1475.09690000 | 0.94880000 | 0.00000000 |
| 63 | 1484.71020000 | 28.23630000 | 0.00000000 |
| 64 | 1485.95330000 | 10.16550000 | 0.00000000 |
| 65 | 1495.66200000 | 20.58370000 | 0.00000000 |
| 66 | 1505.63060000 | 11.15460000 | 0.00000000 |
| 67 | 1512.78420000 | 10.05000000 | 0.00000000 |
| 68 | 1591.42260000 | 248.91230000 | 0.00000000 |
| 69 | 1615.09900000 | 41.79760000 | 0.00000000 |
| 70 | 1655.87060000 | 28.45490000 | 0.00000000 |
| 71 | 1675.19270000 | 647.16300000 | 0.00000000 |
| 72 | 1707.93970000 | 4.85100000 | 0.00000000 |
| 73 | 1831.22930000 | 384.28860000 | 0.00000000 |
| 74 | 3019.40160000 | 12.60520000 | 0.00000000 |
| 75 | 3040.29400000 | 25.08450000 | 0.00000000 |
| 76 | 3045.20070000 | 51.10800000 | 0.00000000 |
| 77 | 3068.95120000 | 12.85120000 | 0.00000000 |
| 78 | 3106.20900000 | 10.28800000 | 0.00000000 |
| 79 | 3125.12850000 | 22.18460000 | 0.00000000 |
| 80 | 3142.60920000 | 11.86580000 | 0.00000000 |
| 81 | 3162.05000000 | 8.71740000 | 0.00000000 |
| 82 | 3195.81840000 | 6.60720000 | 0.00000000 |
| 83 | 3210.75250000 | 7.39350000 | 0.00000000 |
| 84 | 3224.57250000 | 10.62090000 | 0.00000000 |
| 85 | 3240.19260000 | 5.32310000 | 0.00000000 |
| 86 | 3614.42810000 | 102.54770000 | 0.00000000 |
| 87 | 3729.40110000 | 18.03030000 | 0.00000000 |

## S9. CALCULATIONS ON NPPOC (AFTER LOSS OF $H^+$; $S_0$)



| | | |
|---|---|---|
| Route | : # opt freq wb97xd/6-311++g(d,p) geom=connectivity int=ultrafine | |
| SMILES | : C[C](COC(=O)NC)c1ccccc1N(=O)=O | |
| Formula | : $C_{11}H_{13}N_2O_4^{1-}$ | |
| Charge | : -1 | |
| Multiplicity | : 1 | |
| Energy | : -837.31174759 | a.u. |
| Gibbs Energy | : -837.11966100 | a.u. |
| Number of imaginary frequencies | : 0 | |

### S9.1. Cartesian Co-ordinates (XYZ format)

30

| | | | |
|---|---|---|---|
| C | -3.73561001 | -0.59105700 | -0.67162502 |
| C | -3.08367801 | 0.50276101 | -0.20201400 |
| C | -1.65233803 | 0.50014198 | 0.09228000 |
| C | -1.10536301 | -0.85204899 | 0.19738400 |
| C | -1.77862000 | -1.94854605 | -0.39269000 |
| C | -3.06228399 | -1.83776402 | -0.84478998 |
| H | -4.79218292 | -0.51539099 | -0.91597497 |
| H | -3.63261700 | 1.43077803 | -0.09381000 |
| H | -1.25726104 | -2.89703989 | -0.40728399 |
| H | -3.58168602 | -2.69565296 | -1.25642896 |
| N | 0.04816900 | -1.14442098 | 0.90851498 |
| O | 0.68758500 | -2.20472693 | 0.64957798 |
| O | 0.44773000 | -0.37899300 | 1.80402994 |
| C | -0.96248001 | 1.68568206 | 0.11472600 |
| C | -1.69974005 | 3.00270510 | 0.01213800 |
| H | -2.49738503 | 3.09855604 | 0.75869000 |
| H | -1.01620102 | 3.84118104 | 0.17294100 |
| H | -2.16475892 | 3.15005207 | -0.97360301 |
| C | 0.52361202 | 1.80033195 | 0.17143200 |
| H | 0.90908301 | 1.63708699 | 1.18703794 |
| H | 0.84674799 | 2.78362298 | -0.18094000 |
| O | 1.13551795 | 0.79592001 | -0.66407800 |
| C | 2.46122789 | 0.64139199 | -0.51564503 |
| O | 3.23136592 | 1.53554904 | -0.22336400 |
| N | 2.82106709 | -0.64592999 | -0.78144401 |
| H | 2.09518194 | -1.32709396 | -0.56756699 |

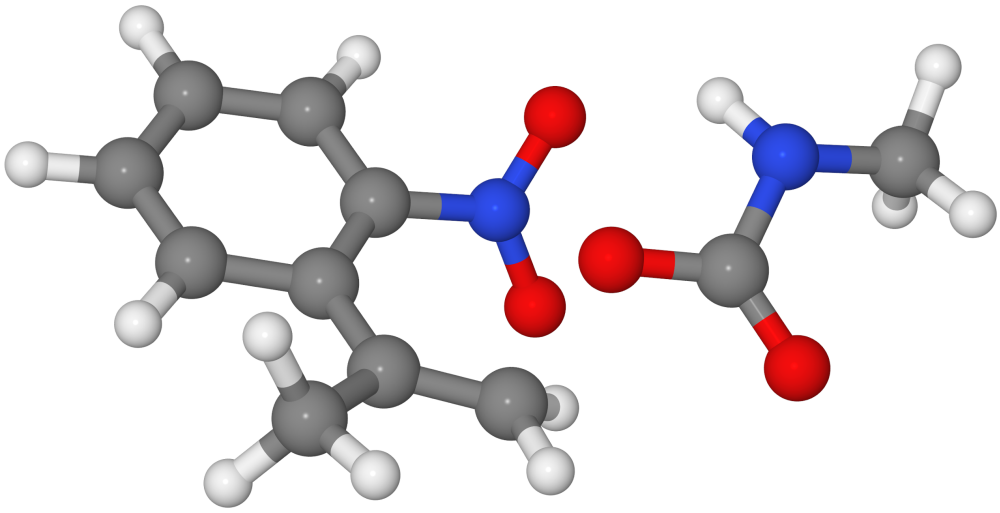
| | | | |
|---|---|---|---|
| C | 4.18183184 | -1.05104995 | -0.51062900 |
| H | 4.41067791 | -1.05109406 | 0.56187803 |
| H | 4.33331394 | -2.05785394 | -0.90460300 |
| H | 4.87511921 | -0.36927000 | -1.00592196 |

### S9.2. Frequencies

| Mode | IR frequency | IR intensity | Raman intensity |
|---|---|---|---|
| 1 | 46.98430000 | 1.68740000 | 0.00000000 |
| 2 | 58.46050000 | 3.09140000 | 0.00000000 |
| 3 | 66.23500000 | 4.76870000 | 0.00000000 |
| 4 | 102.89480000 | 0.53930000 | 0.00000000 |
| 5 | 109.28100000 | 0.86360000 | 0.00000000 |
| 6 | 121.45630000 | 8.36330000 | 0.00000000 |
| 7 | 142.82790000 | 4.27750000 | 0.00000000 |
| 8 | 153.88550000 | 5.13240000 | 0.00000000 |
| 9 | 163.27960000 | 2.56260000 | 0.00000000 |
| 10 | 177.23620000 | 1.25650000 | 0.00000000 |
| 11 | 221.70930000 | 3.28330000 | 0.00000000 |
| 12 | 241.00320000 | 1.44650000 | 0.00000000 |
| 13 | 273.09690000 | 9.77600000 | 0.00000000 |
| 14 | 292.55650000 | 6.40700000 | 0.00000000 |
| 15 | 303.60960000 | 1.51350000 | 0.00000000 |
| 16 | 357.73440000 | 2.60740000 | 0.00000000 |
| 17 | 370.61340000 | 16.33210000 | 0.00000000 |
| 18 | 417.83970000 | 19.56920000 | 0.00000000 |
| 19 | 425.28420000 | 2.35490000 | 0.00000000 |
| 20 | 482.04470000 | 2.45490000 | 0.00000000 |
| 21 | 502.86330000 | 32.89770000 | 0.00000000 |
| 22 | 576.61440000 | 2.36280000 | 0.00000000 |
| 23 | 578.52260000 | 1.78960000 | 0.00000000 |
| 24 | 590.06780000 | 11.09430000 | 0.00000000 |
| 25 | 649.47120000 | 78.95900000 | 0.00000000 |
| 26 | 676.97180000 | 34.75870000 | 0.00000000 |
| 27 | 711.53960000 | 31.83850000 | 0.00000000 |
| 28 | 728.05120000 | 53.42250000 | 0.00000000 |
| 29 | 753.69900000 | 12.31930000 | 0.00000000 |
| 30 | 775.21290000 | 18.97200000 | 0.00000000 |
| 31 | 784.03900000 | 5.37910000 | 0.00000000 |
| 32 | 803.44140000 | 12.24150000 | 0.00000000 |
| 33 | 832.50660000 | 22.66940000 | 0.00000000 |
| 34 | 864.69740000 | 5.18930000 | 0.00000000 |
| 35 | 946.99630000 | 15.99940000 | 0.00000000 |
| 36 | 974.26520000 | 10.79610000 | 0.00000000 |
| 37 | 975.22190000 | 2.30050000 | 0.00000000 |
| 38 | 978.60560000 | 2.00250000 | 0.00000000 |
| 39 | 991.46240000 | 10.56810000 | 0.00000000 |
| 40 | 1024.78310000 | 77.23900000 | 0.00000000 |
| 41 | 1037.78210000 | 20.73050000 | 0.00000000 |
| 42 | 1048.77220000 | 12.97970000 | 0.00000000 |
| 43 | 1084.36790000 | 6.67450000 | 0.00000000 |
| 44 | 1116.38320000 | 18.91130000 | 0.00000000 |
| 45 | 1150.22850000 | 13.08070000 | 0.00000000 |
| 46 | 1170.07820000 | 14.05690000 | 0.00000000 |
| 47 | 1190.58560000 | 59.39310000 | 0.00000000 |
| 48 | 1198.00300000 | 84.31730000 | 0.00000000 |
| 49 | 1202.55020000 | 5.69740000 | 0.00000000 |
| 50 | 1240.72360000 | 54.04840000 | 0.00000000 |
| 51 | 1265.31670000 | 305.78830000 | 0.00000000 |
| 52 | 1275.78850000 | 59.00980000 | 0.00000000 |
| 53 | 1319.92640000 | 38.68630000 | 0.00000000 |
| 54 | 1327.55670000 | 1119.55060000 | 0.00000000 |
| 55 | 1401.16270000 | 224.90480000 | 0.00000000 |
| 56 | 1408.41660000 | 3.62900000 | 0.00000000 |
| 57 | 1428.36170000 | 35.35870000 | 0.00000000 |
| 58 | 1438.79450000 | 200.90880000 | 0.00000000 |
| 59 | 1455.14180000 | 82.42190000 | 0.00000000 |
| 60 | 1462.95150000 | 62.46390000 | 0.00000000 |

| | | | |
|---|---|---|---|
| 61 | 1485.44230000 | 33.65850000 | 0.00000000 |
| 62 | 1490.64670000 | 9.40080000 | 0.00000000 |
| 63 | 1493.19800000 | 2.54460000 | 0.00000000 |
| 64 | 1500.13180000 | 19.02300000 | 0.00000000 |
| 65 | 1511.85160000 | 4.89180000 | 0.00000000 |
| 66 | 1514.81950000 | 19.33620000 | 0.00000000 |
| 67 | 1569.50930000 | 53.64440000 | 0.00000000 |
| 68 | 1601.39030000 | 244.70060000 | 0.00000000 |
| 69 | 1610.23700000 | 86.92050000 | 0.00000000 |
| 70 | 1674.49300000 | 95.78260000 | 0.00000000 |
| 71 | 1792.01630000 | 456.07470000 | 0.00000000 |
| 72 | 2986.41730000 | 151.23080000 | 0.00000000 |
| 73 | 3013.41020000 | 32.22700000 | 0.00000000 |
| 74 | 3024.31470000 | 82.54030000 | 0.00000000 |
| 75 | 3041.60700000 | 54.28990000 | 0.00000000 |
| 76 | 3081.52290000 | 20.79150000 | 0.00000000 |
| 77 | 3097.53060000 | 53.97730000 | 0.00000000 |
| 78 | 3099.90520000 | 42.90470000 | 0.00000000 |
| 79 | 3138.07380000 | 22.01210000 | 0.00000000 |
| 80 | 3154.42940000 | 32.45730000 | 0.00000000 |
| 81 | 3189.97700000 | 29.77970000 | 0.00000000 |
| 82 | 3205.18250000 | 30.41750000 | 0.00000000 |
| 83 | 3227.01860000 | 12.54300000 | 0.00000000 |
| 84 | 3501.56360000 | 269.89310000 | 0.00000000 |

## S10. CALCULATIONS ON NPPOC (DISSOCIATED; $S_0$)



Route : # opt=modredundant wb97xd/6-311++g(d,p) geom=connectivity int=ultrafine
SMILES : CC(COC(=O)NC)c1ccccc1N(=O)=O
Formula : $C_{11}H_{13}N_2O_4$
Charge : -1
Multiplicity : 1
Energy : -837.291387427 a.u.

### S10.1. Cartesian Co-ordinates (XYZ format)

30

| | | | |
|---|---|---|---|
| C | -3.97369500 | -0.24938000 | -0.54895000 |
| C | -3.10464200 | 0.76240400 | -0.21512700 |
| C | -1.73967300 | 0.56335400 | 0.17312100 |
| C | -1.39324100 | -0.82335300 | 0.22587200 |
| C | -2.25842700 | -1.84543300 | -0.16506000 |
| C | -3.55730500 | -1.58415400 | -0.54684600 |
| H | -4.99435400 | 0.00175500 | -0.82298400 |
| H | -3.47513700 | 1.77776000 | -0.24901500 |
| H | -1.88242900 | -2.86078000 | -0.13837500 |
| H | -4.22791000 | -2.38969600 | -0.82106900 |
| N | -0.11897500 | -1.33306900 | 0.70901500 |
| O | 0.44228800 | -2.20251300 | 0.05081700 |
| O | 0.29526600 | -0.94013100 | 1.78800600 |
| C | -0.90137200 | 1.71902800 | 0.30432600 |
| C | -1.42428000 | 3.02506300 | -0.26267600 |
| H | -2.25199200 | 3.45252500 | 0.32127800 |
| H | -0.62395800 | 3.76828200 | -0.26620100 |
| H | -1.78079900 | 2.92538400 | -1.29763800 |
| C | 0.43207200 | 1.69671400 | 0.69919300 |
| H | 0.78920400 | 0.99243500 | 1.43480500 |
| H | 0.96824700 | 2.63806300 | 0.70097600 |
| O | 1.44783100 | 0.84596900 | -0.66259500 |
| C | 2.68210100 | 0.60363900 | -0.37057300 |

| | | | |
|---|---|---|---|
| O | 3.42312600 | 1.29060200 | 0.33437400 |
| N | 3.15511700 | -0.57401300 | -0.96170900 |
| H | 2.40259900 | -1.21843400 | -1.15562700 |
| C | 4.37690600 | -1.16099200 | -0.46145900 |
| H | 4.27570800 | -1.56665500 | 0.55526000 |
| H | 4.69354200 | -1.96631400 | -1.13130800 |
| H | 5.15552800 | -0.39750400 | -0.43698500 |