# Supporting Information

## Complexes of glycolic acid with nitrogen isolated in argon matrices. II. Vibrational overtone excitations

Iwona Kosendiak, Jussi Ahokas, Justyna Krupa, Jan Lundell, Maria Wierzejewska

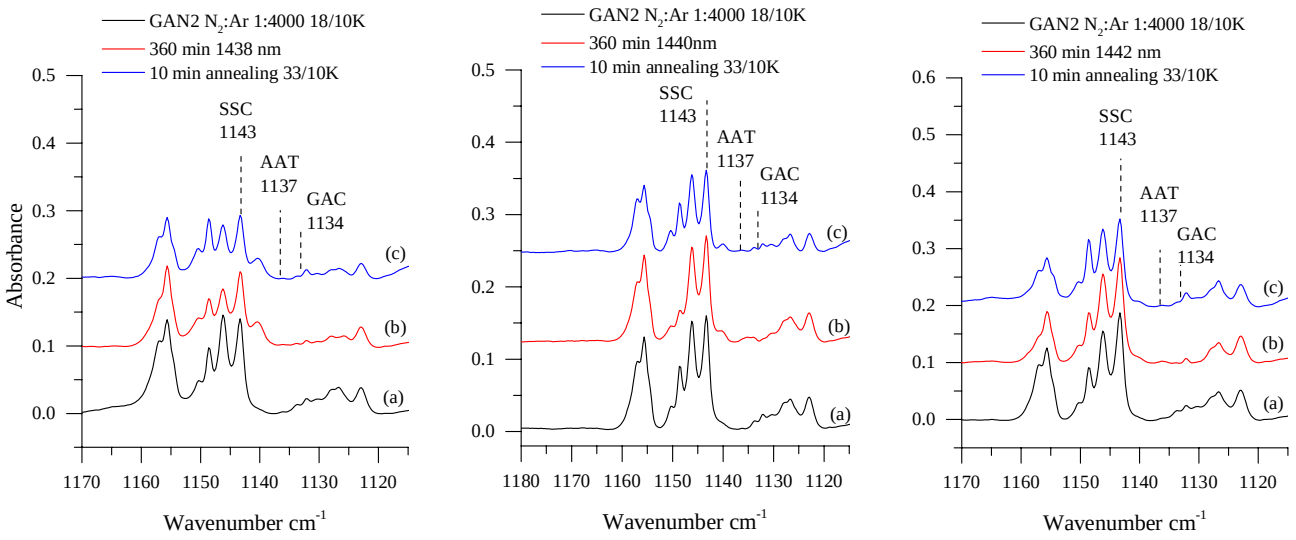


Figure S1. The δOH regions of the infrared spectra obtained for the 1:1 complex formed between SSC and $N_2$ (SSC1): (a) after co-deposition GA with $N_2$/Ar=1/4000 at 18 K (10 K for measurement); (b) upon 360 min irradiation at 1438, 1440 or 1442 nm; (c) upon annealing at 33 K/10 K. The perpendicular broken lines show position of the bands due to the GA monomer species.

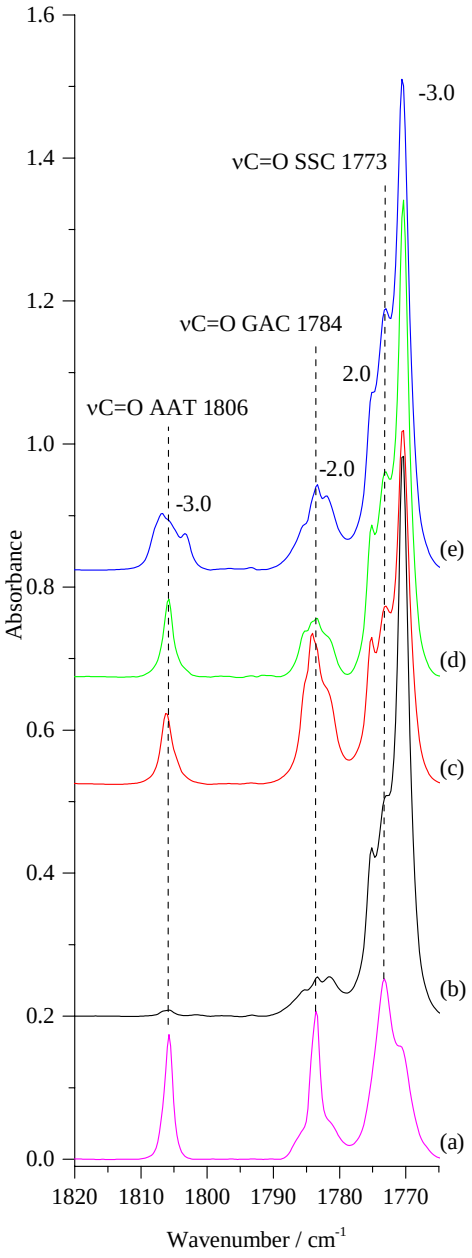


Figure S2. The νC=O region of the infrared spectra of SSC, GAC, AAT monomers and their complexes with nitrogen: (a) after deposition GA/Ar at 18 K/10 K and two subsequent irradiations at 1438 and 1400 nm (b) after co-deposition GA with $N_2$/Ar=1/4000 at 18 K/10 K; (c,d,e) upon 360 min irradiation at 1438, 1440 or 1442 nm, respectively. The perpendicular broken lines show position of the GA monomer species.

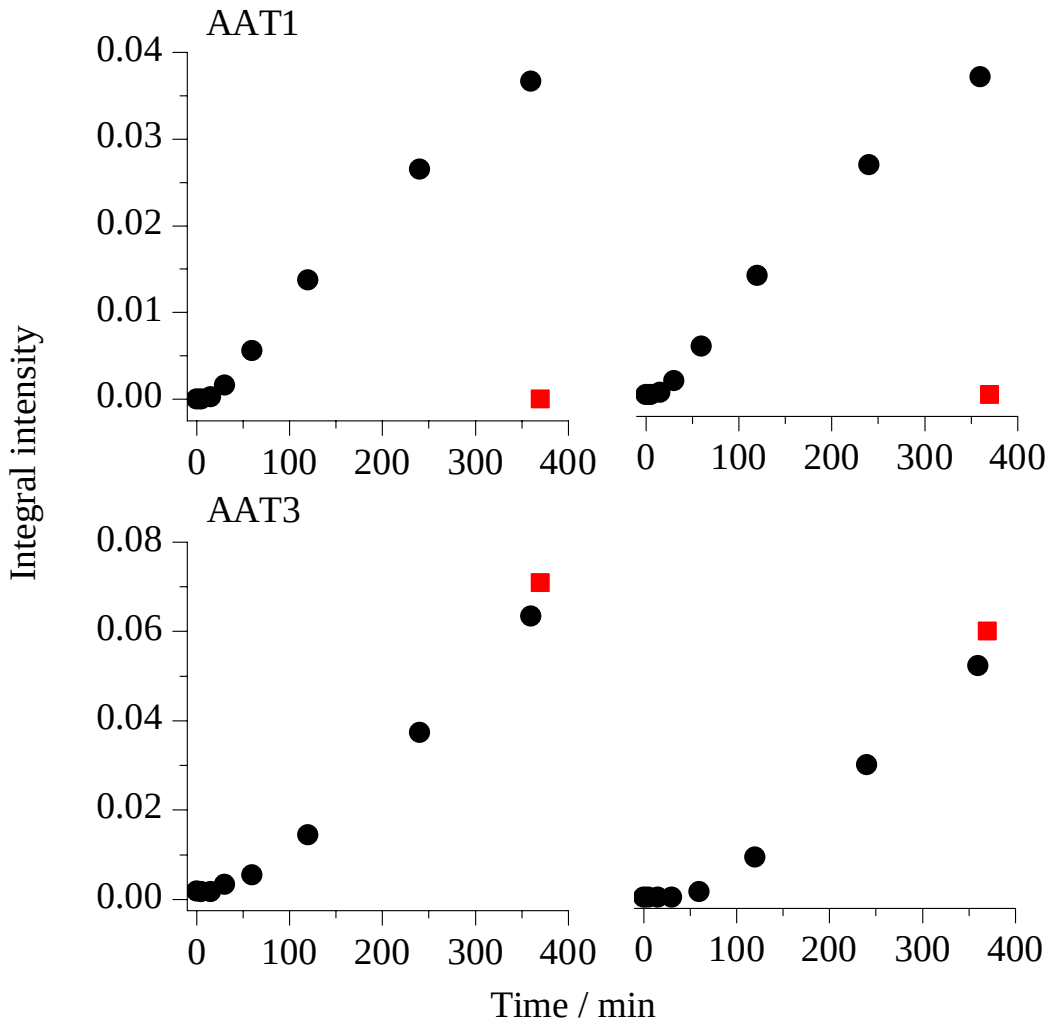


Figure S3. Plots of the integrated intensity of the selected bands of AAT1 ($\nu OH_A$ 3669.5 and $\nu OH_C$ 3475.5 $cm^{-1}$, $\lambda$=1440 nm) and AAT3 ($\nu OH_A$ 3664.5 and $\nu OH_C$ 3469.5 $cm^{-1}$, $\lambda$=1438 nm) versus time of irradiation. The last points (red squares) relate to the annealing at 33 K (10 K for measurement).

Table S1. The ⌾C=O shifts and intensities in GA complexes with nitrogen at different levels of theory.

| | | SSC1 | SSC2 | SSC3 |
|---|---|---|---|---|
| | | νC=O | νC=O | νC=O |
| MP2 | 6-311++G(2d,2p) | -5(246) | 1(274) | -1(249) |
| B3LYPD3 | 6-311++G(2d,2p) | -6(297) | 1(338) | 0(301) |
| | aug-cc-pVDZ | -7(284) | 0(326) | -2(289) |
| | aug-cc-pVTZ | -6(289) | 1(332) | 0(294) |
| | aug-cc-pVQZ | -8(290) | 0(333) | -2(295) |
| | | GAC1 | GAC2 | GAC3 |
| | | νC=O | νC=O | νC=O |
| MP2 | 6-311++G(2d,2p) | -4(243) | -4(267) | 1(245) |
| B3LYPD3 | 6-311++G(2d,2p) | -5(297) | -4(325) | 1(301) |
| | aug-cc-pVDZ | -5(281) | -4(310) | 1(285) |
| | aug-cc-pVTZ | -6(289) | -4(320) | 2(293) |
| | aug-cc-pVQZ | -6(290) | -4(320) | 2(294) |
| | | AAT1 | AAT2 | AAT3 |
| | | νC=O | νC=O | νC=O |
| MP2 | 6-311++G(2d,2p) | -4(276) | -2(247) | 0(258) |
| B3LYPD3 | 6-311++G(2d,2p) | -5(320) | -2(295) | -1(295) |
| | aug-cc-pVDZ | -5(306) | -1(281) | -1(281) |
| | aug-cc-pVTZ | -5(319) | -1(292) | -1(292) |
| | aug-cc-pVQZ | -5(319) | -1(292) | -1(293) |

Table S2. Experimental positions of the ⌾C=O bands and their shifts ($cm^{-1}$) observed for GA···$N_2$ complexes in argon matrices.

| Infrared | | Assignment | Raman [16] | |
|---|---|---|---|---|
| νC=O | ΔνC=O | | νC=O | ΔνC=O |
| 1805.5 | -0.5 | AAT3? | | |
| 1803.0 | -3.0 | AAT1 | 1810 | 0 |
| 1782.0 | -2.0 | GAC1 | 1787 | -1 |
| 1775.0 | 2.0 | SSC1? | | |
| 1770.0 | -3.0 | SSC1 | 1775 | -2 |

Experimental IR positions of SSC νC=O 1773.0 $cm^{-1}$, GAC: νC=O 1784.0 $cm^{-1}$, AAT: νC=O 1806.0 $cm^{-1}$.

Experimental Raman positions of SSC νC=O 1777.0 $cm^{-1}$, GAC: νC=O 1788.0 $cm^{-1}$, AAT: νC=O 1810.0 $cm^{-1}$ [12]