Supplementary Information

Molecular recognition using receptor-free nanomechanical infrared spectroscopy based on a quantum cascade laser

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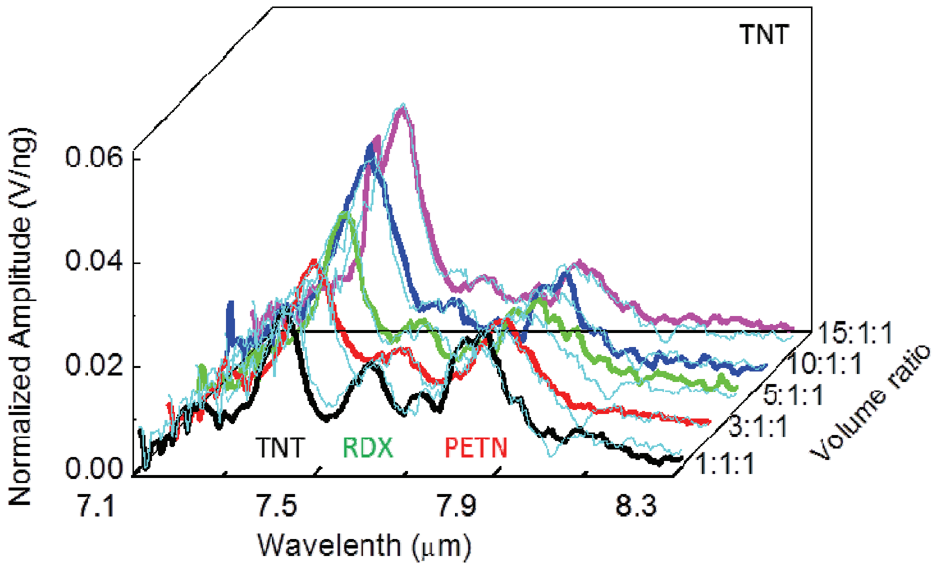
1. Fitting of the PCDS spectra of the ternary mixtures with linear superpositions of normalized PCDS spectra of individual explosive molecules



Supplementary Figure S1 | Normalized PCDS spectra of ternary mixtures of explosives (TNT:RDX:PETN) shown with increased volume ratio of the TNT sample solution from 1:1:1 (black), 3:1:1 (red), 5:1:1 (green), 10:1:1(blue) to 15:1:1 (magenta) and mathematically fitted IR spectra of the mixture (sky blue).

2. Theoretical prediction of maximum temperature rise at the cantilever free end as a function of incident IR beam radiation flux

In our PCDS setup, the temperature distribution within the microcantilever can be regarded as one-dimensional[1] since the Biot number is 3.61 x 10^{-5} using a constant convection heat transfer coefficient, h = 1000 $Wm^{-2}K^{-1}$. Assuming the incident IR beam radiation flux on the cantilever, q''_{rad}, is uniform over the entire cantilever, the steady state longitudinal temperature distribution, $T(x)$, of the cantilever is given by[2]

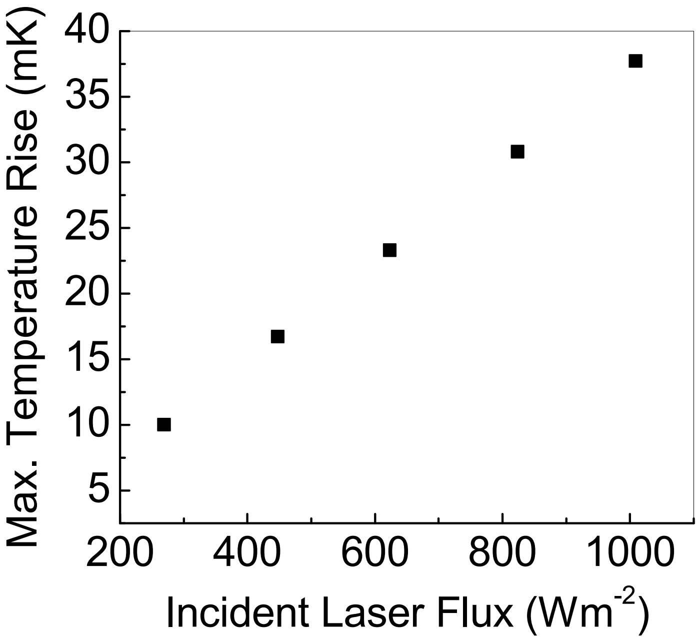
$$T(x) = T_0 + C_1(\cosh(\beta x) - 1) + C_2 \sinh(\beta x) \tag{1}$$

$$\beta = \sqrt{\frac{2(t_1 + t_2 + w)h}{w(\lambda_1 t_1 + \lambda_2 t_2)}} \tag{2}$$

$$C_1 = -\frac{A q''_{rad} w}{2(t_1 + t_2 + w)h} \tag{3}$$

$$C_2 = -C_1 \frac{(\lambda / h)\beta \sinh(\beta L) + \cosh(\beta L) - 1}{\sinh(\beta L) + (\lambda / h)\beta \cosh(\beta L)} \tag{4}$$

where, T_0 is the ambient temperature, t_1 and t_2 are thickness of the gold and silicon layer, respectively, w is the width of the cantilever, λ_1 and λ_2 are the thermal conductivity of the gold and silicon film, respectively, A is the spectral absorptivity of the cantilever, λ is the thermal conductivity of the bi-material cantilever, and L is the length of the cantilever. Maximum temperature rise at the cantilever free end, $T(L)- T_0$, is estimated with the spectral absorptivity[1], A = 0.125, at the IR wavelength of 7.57 μm and the measured IR beam radiation flux from the QCL. Figure S2 shows the estimated maximum temperature rise at the free end of the cantilever as a function of incident laser flux.



Supplementary Figure S2 | Calculated maximum temperature rise at the cantilever free end as a function of incident QCL laser flux.

References

1 Kwon, B., Wang, C., Park, K., Bhargava, R. & King, W. P. Thermomechanical sensitivity of microcantilevers in the mid-infrared spectral region. *Nanoscale Microscale Thermophys. Eng.* **15**, 16-28 (2011).

2 Rosenberger, M. R., Kwon, B., Cahill, D. G. & King, W. P. Impact of silicon nitride thickness on the infrared sensitivity of silicon nitride-aluminum microcantilevers. *Sens.Actuators A: Physical* **185**, 17-23 (2012).