Supporting Information

![FTIR spectra figure]

**Figure S1.** FTIR spectra in the range of $\nu$(NO$_2$) for 2,4-dinitroaniline 1 dissolved in THF in different concentrations at room temperature. A certain weight of 1 given was mixed with 10 cm$^3$ THF for FTIR measurements.

![Scheme S1]

**Scheme S1.** Chlorodinitro and mononitro substrates used for FTIR measurements.
(a) Chloro-2,4-dinitrobenzene 5

(b) 2-Chloronitrobenzene (2CNB)

(Figure S2 on pp. 2 & 3)
Figure S2. High-pressure FTIR spectra in the range of $\nu$(NO$_2$) for (a) 5, (b) 2-chloronitrobenzene (2CNB) and (c) 4-chloronitrobenzene (4CNB) dissolved in THF measured in ATR mode at 323 K at 4 MPa of H$_2$ and different CO$_2$ pressures given.
Figure S3. The optimized structures of 5 (a) and CO$_2$-coordinated clusters of 5 with five CO$_2$ molecules. The bonding distances of NO of nitro groups are given in Å.