

Supporting Information

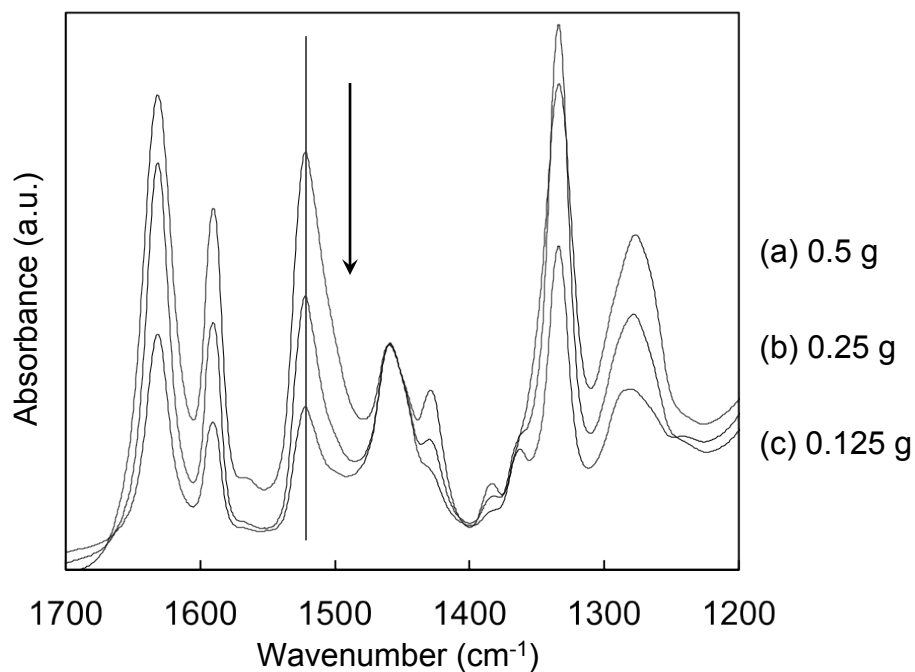
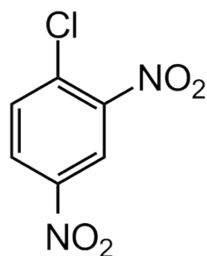
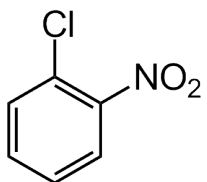


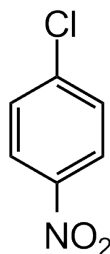
Figure S1. FTIR spectra in the range of $\nu(\text{NO}_2)$ for 2,4-dinitroaniline **1** dissolved in THF in different concentrations at room temperature. A certain weight of **1** given was mixed with 10 cm^3 THF for FTIR measurements.



5: Chloro-2,4-dinitrobenzene

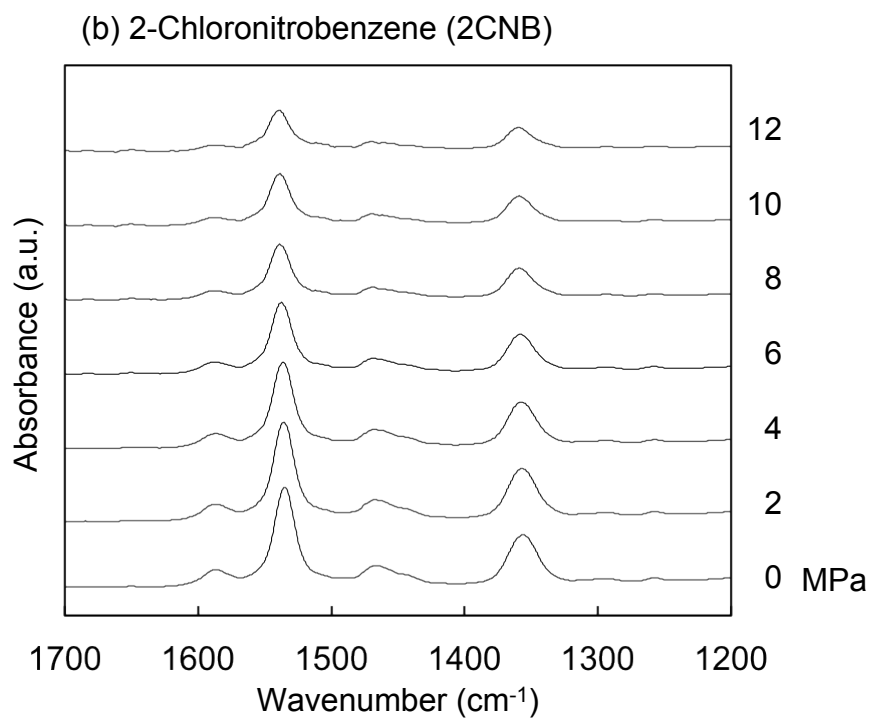
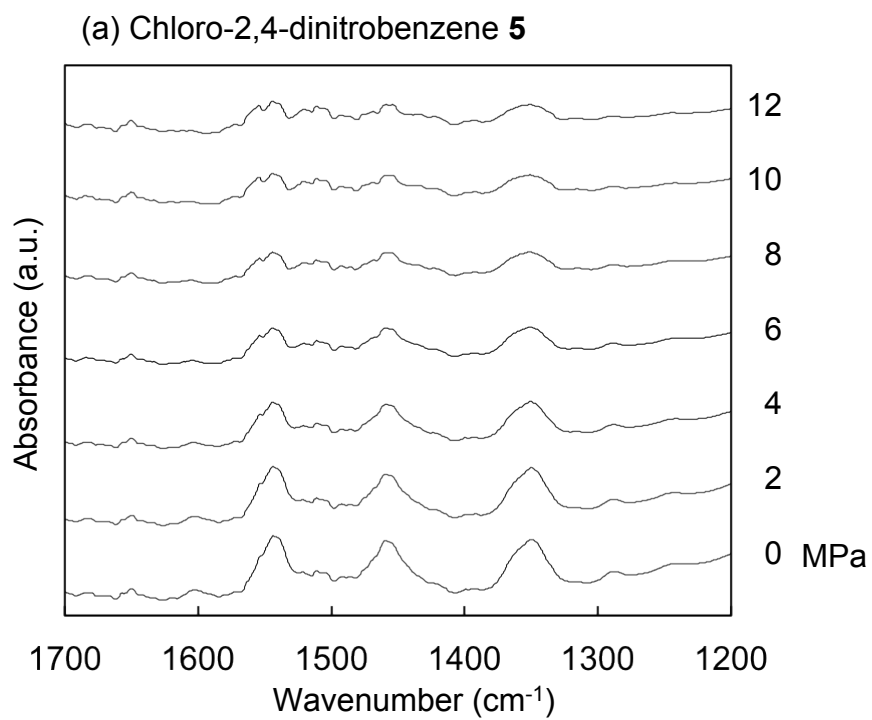


2CNB: 2-Chloronitrobenzene



4CNB: 4-Chloronitrobenzene

Scheme S1. Chlorodinitro and mononitro substrates used for FTIR measurements.



(Figure S2 on pp. 2 & 3)

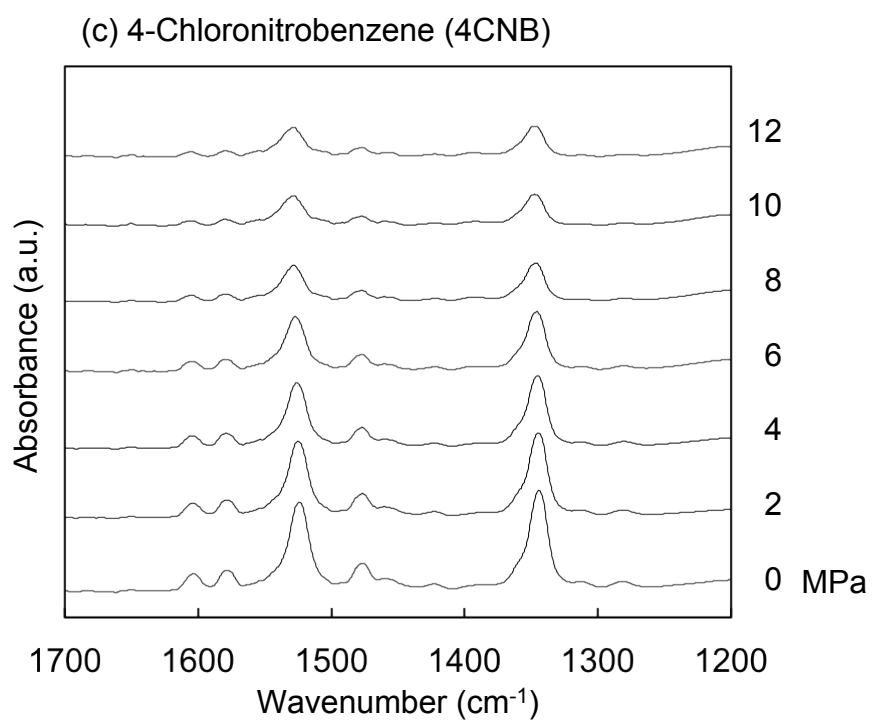
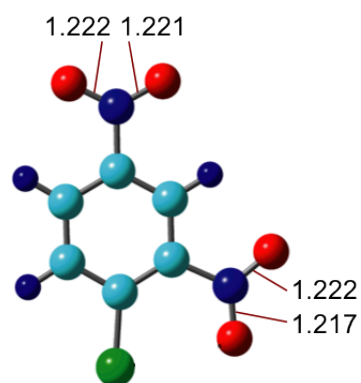


Figure S2. High-pressure FTIR spectra in the range of $\nu(\text{NO}_2)$ for (a) **5**, (b) 2-chloronitrobenzene (2CNB) and (c) 4-chloronitrobenzene (4CNB) dissolved in THF measured in ATR mode at 323 K at 4 MPa of H_2 and different CO_2 pressures given.

(a) Chloro-2,4-dinitrobenzene **5**



(b) Cluster of **5** with five CO₂

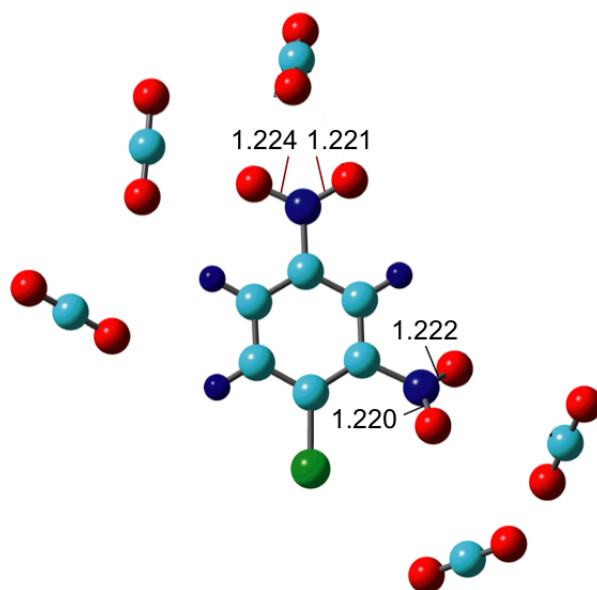


Figure S3. The optimized structures of **5** (a) and CO₂-coordinated clusters of **5** with five CO₂ molecules. The bonding distances of NO of nitro groups are given in Å.