

Electronic Supporting Information

Identification of the preferential CO and SO₂ adsorption sites within NOTT-401

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S1. Experimental Details

Chemicals: Scandium triflate ($[\text{Sc}(\text{SO}_3\text{CF}_3)_3] \cdot x\text{H}_2\text{O}$), thiophene-2,5-dicarboxylic acid (H_2TDA), *N,N*-dimethylformamide (DMF) and tetrahydrofuran (THF) were purchased from Sigma-Aldrich and used as received.

NOTT-401 synthesis: NOTT-401 was synthesized according to the procedure previously reported.¹ Briefly, scandium triflate (0.057 g, 0.116 mmol) and H_2TDA , (0.01 g, 0.058 mmol) were dispersed in THF (4.0 mL), DMF (3.0 mL), H_2O (1.0 mL) and HCl (36.5 %, 100 μL) and sealed in a pressure tube. The clear solution was heated at 363 K in an oil bath for 72 h. The tube was cooled to room temperature, the crystalline product was separated by filtration, washed with DMF (5.00 ml) and dried in air.

Sample activation: Before the adsorption experiments, the sample was acetone-exchanged to remove any uncoordinated solvents (water and DMF) from the pores. The sample was activated at 453 K for 2 h (with a heating ramp of 5 K min^{-1}) under vacuum (10^{-6} bar) to afford the fully desolvated sample.

S2. Bulk Powder PXRD

Powder X-Ray Diffraction Patterns (PXRD) were collected on a Rigaku Diffractometer, Ultima IV with a $\text{Cu-K}\alpha_1$ radiation ($\lambda = 1.5406 \text{ \AA}$) using a nickel filter. Patterns were recorded in the $2\text{--}30^\circ$ 2θ range with a step scan of 0.02° and a scan rate of $0.08^\circ \text{ min}^{-1}$.

S3. Thermogravimetric Analysis

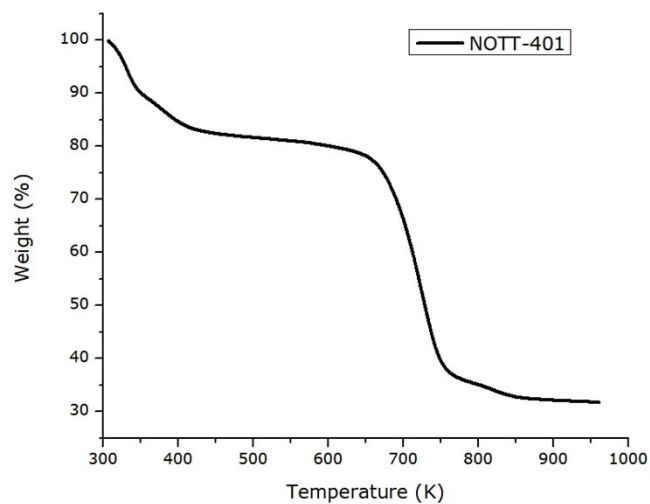


Figure S1. TGA trace of as synthesized NOTT-401.

S4. Adsorption Isotherms of N₂ and SO₂

N₂ isotherms (up to $P/P_0 = 1$ and 77 K) were recorded on a Quantachrome Autosorb MP-1 equipment under high vacuum in a clean system with a diaphragm pumping system. SO₂ isotherms were recorded at 298 K and up to 1 bar with the aid of a Dynamic Gravimetric Gas/Vapour Sorption Analyser, DVS Vacuum (Surface Measurements Systems Ltd.). Ultra-pure grade (99.9995%) N₂ and SO₂ were purchased from PRAXAIR.

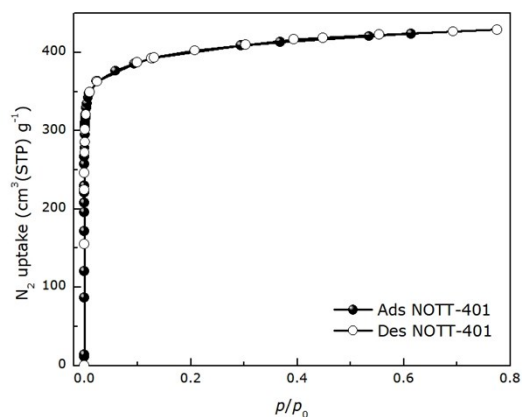


Figure S2. N₂ adsorption isotherm at 77 K of as activated NOTT-401.

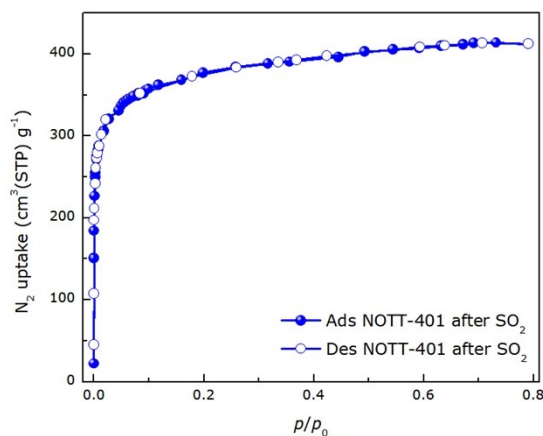


Figure S3. N₂ adsorption isotherm at 77 K of NOTT-401 after SO₂ adsorption-desorption experiment.

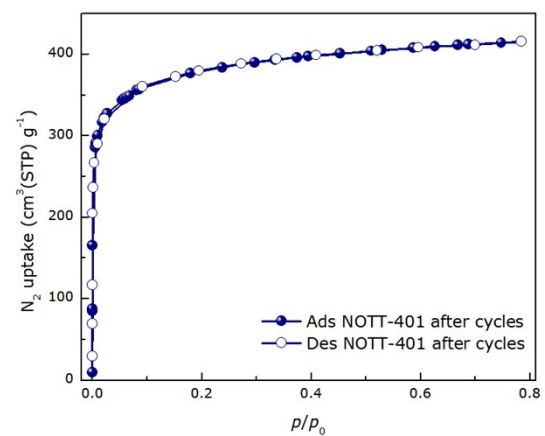


Figure S4. N_2 adsorption isotherm at 77 K of NOTT-401 after 50 SO_2 adsorption/desorption cycles.

S5. Isothermic Heat of Adsorption of SO₂

The heat of adsorption of SO₂, ΔH , was calculated by the isosteric method for NOTT-401, using the corresponding adsorption isotherms at three different temperatures (**Figure S5A**, C, E). A virial-type equation was used to fit the adsorption isotherms:

$$\ln\left(\frac{n}{p}\right) = A_0 + A_1n + A_2n^2 + \dots \quad \text{Eq. S5.1}$$

where p is the pressure, n is the amount adsorbed and A_0, A_1, \dots are the virial coefficients (A_2 and higher terms can be ignored at lower coverage values). A plot of $\ln(n/p)$ versus n should give a straight line at low surface coverage (**Figure S5B**, D, F).

The obtained values and their average ($-39.1 \text{ kJ mol}^{-1}$) are reported on **Table S1**.

Table S1. Calculated heats of adsorption at three different temperatures 298, 303 and 308 K.

T [K]	Calculated Q _{st} [kJ mol ⁻¹]
298 and 303	-45.1
303 and 308	-50.1
298 and 308	-38.8
Average=	-44.7

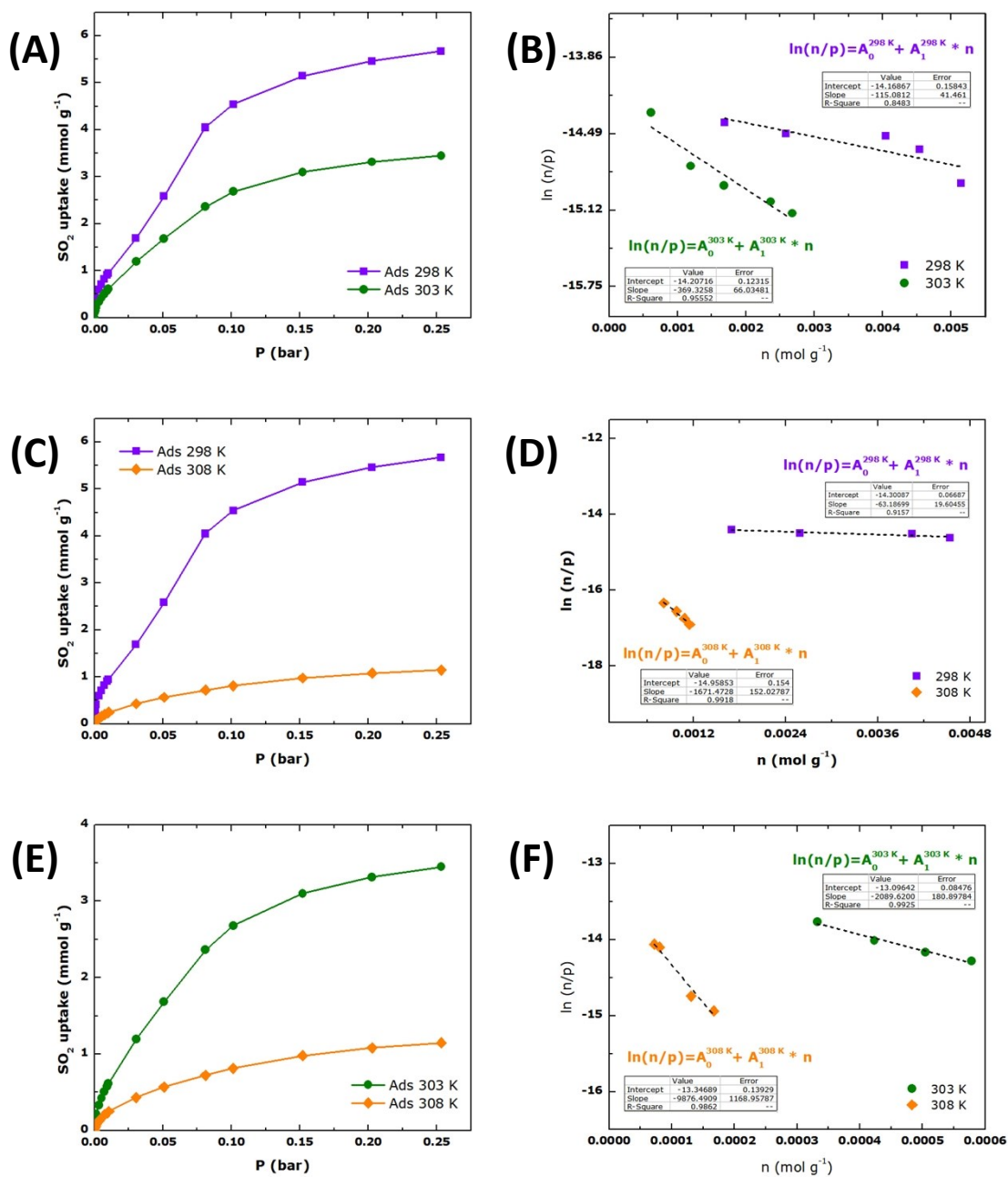


Figure S5. SO₂ adsorption isotherms at A) 298 and 303 K, C) 303 and 308 K, E) 298 and 308 K, for NOTT-401. Virial fitting plots at B) 298 and 303 K, D) 303 and 308 K, F) 298 and 308 K.

S6. SO₂ Cycling

Cycling SO₂ experiments on NOTT-401 were carried out by operating vacuum (1.7×10^{-6} Torr) for 30 minutes and 298 K. Then, we showed that the SO₂ capture capacity remains constant during 50 adsorption-desorption cycles (6.61 ± 0.15 mmol g⁻¹).

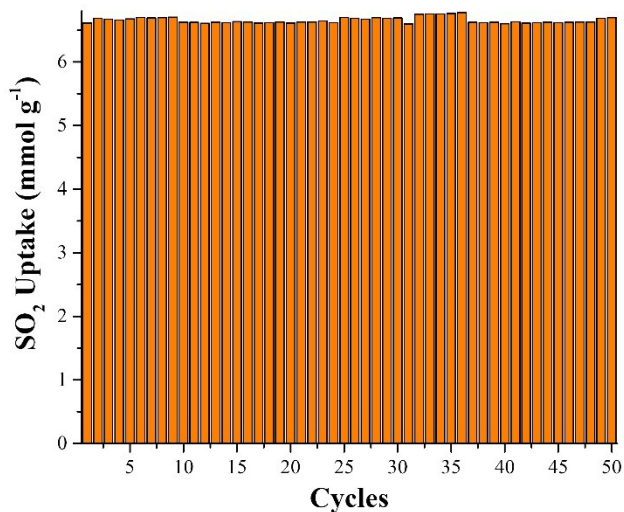


Figure S6. Adsorption-desorption cycles for SO₂ in NOTT-401 at 1 bar and 298 K. Re-activation of this sample was conducted by only operating vacuum (1.7×10^{-6} Torr) for 30 minutes at 298 K

S7. CO molecules per unit cell

From the saturated sample with an uptake of 2.24 mmol CO g⁻¹ (which corresponds to a 6.27 %w gain), it was estimated that 8.87 CO molecules were present in the unit cell.

The molecules of CO per unit cell were calculated using the following equation

$$\frac{28x}{28x + 928.22} = \%w$$

Where, 28 g mol⁻¹ and 928 g mol⁻¹ are the molar mass of carbon monoxide and one NOTT-401 unit cell, respectively

S8. FTIR Spectroscopy

FTIR spectra were measured (in-situ and at 298 K) using an FTIR Nicolet 6700 spectrophotometer (DTGS detector) with a 4 cm^{-1} resolution equipped with a diffuse reflectance vacuum chamber with CaF_2 windows in a similar way to a previously reported methodology.² FTIR spectra were collected on an activated sample of NOTT-401 (10–6 bar and 180 °C for 2 hours). Pulses of CO, with an increment of 0.06 bar, were measured.

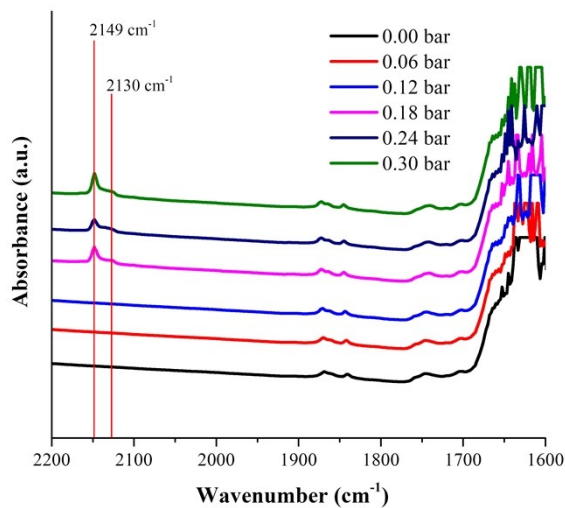


Figure S7. DRIFTS spectra of activated NOTT-401 at 298 K under a CO atmosphere at different CO pressures (from 0.00 bar to 0.30 bar), in the region between 2200 and 1600 cm^{-1} .

S9. Numerical details, cell parameters and atomic positions

For each structure we used the following k-point mesh 2x2x2, and the tolerances: 7, 7, 7, 9, 30, according to the CRYSTAL manual. For the IR analysis we moved 50 atoms: 8 atoms associated to μ_2 -OH groups, 32 atoms for CH groups, 8 sulfur atoms and the CO. In each unit cell there are 130 atoms. Cell parameters and atomic positions for each structure:

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#GEOMETRY INFORMATION FOR STRUCTURE I
LATTICE PARAMETERS (ANGSTROMS AND DEGREES)
PRIMITIVE CELL - VOLUME=3253.094931 DENSITY=0.961 g/cm^3
      A           B           C           ALPHA           BETA           GAMMA
      17.30964313  17.32440924  17.21437072  97.608384  97.548309 137.436689
*****
ATOM      X/A           Y/B           Z/C
*****
21 SC    -2.109026076256E-01  4.876570531111E-01  -1.863339861316E-01
21 SC     1.695419305687E-01  -2.597966221067E-02  -3.170187534469E-01
21 SC     4.851553508850E-01  1.731385798583E-01  -3.045039486452E-01
21 SC    -2.552537619849E-02  -2.089164427374E-01  -1.969550656114E-01
21 SC     2.094808526821E-01  -4.854061409819E-01  1.832245001032E-01
21 SC    -1.712542006341E-01  2.794789007635E-02  3.140266647654E-01
21 SC    -4.860032937804E-01  -1.709827483647E-01  3.014545206258E-01
21 SC     2.516774414421E-02  2.117844423224E-01  1.946343107513E-01
16 S     -1.276938746915E-01  -1.424297276419E-01  2.046369084708E-02
16 S     3.362178666345E-01  -1.443651530653E-01  4.758591072120E-01
16 S     1.280348757212E-01  1.457380070023E-01  -2.219980943966E-02
16 S    -3.374282550316E-01  1.466735825100E-01  -4.787539752926E-01
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16 S     1.410243734671E-01  -3.351603520715E-01  1.647310308437E-02
16 S    -1.464769131273E-01  -1.221052472363E-01  -4.830858148263E-01
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6 C	3.013570687268E-01	2.605554323908E-01	4.075489510177E-01
6 C	3.483361526503E-01	-1.058117797273E-01	9.142798329298E-02
1 H	-2.891263397280E-01	-4.306618265187E-01	4.486646154193E-02
1 H	2.386659297079E-02	-3.424643049876E-01	4.634486792173E-01
1 H	2.686545617622E-01	3.018513709541E-01	-1.678209342245E-01
1 H	-3.530628782839E-02	4.486368619418E-01	-3.495643781573E-01
1 H	4.450035137397E-01	2.941397501130E-01	4.776111120250E-01
1 H	3.109190571430E-01	-3.259465514690E-02	2.185826779609E-02
1 H	-3.435626794850E-01	-3.077524513922E-01	-3.678082232403E-01
1 H	-4.413954116181E-01	2.479844215833E-02	-1.359305651236E-01
1 H	2.813878300481E-01	4.292698899690E-01	-5.135356161509E-02
1 H	-2.543429536443E-02	3.453965259580E-01	-4.678156781955E-01
1 H	-2.689906421862E-01	-3.001765433009E-01	1.652439208538E-01
1 H	3.421789173826E-02	-4.451498069027E-01	3.451724348211E-01
1 H	-4.464847957656E-01	-2.919927460025E-01	-4.802953523942E-01
1 H	-3.130275538539E-01	3.456171056022E-02	-2.338576986143E-02
1 H	3.422041138886E-01	3.104833495769E-01	3.656297171837E-01
1 H	4.395638190102E-01	-2.304874428974E-02	1.338588226882E-01

6 C -4.736568031353E-01 -3.266865023435E-01 1.020741746225E-01
 8 O -4.985577448504E-01 -4.083814379378E-01 7.565031836660E-02

#GEOMETRY INFORMATION FOR STRUCTURE II

LATTICE PARAMETERS (ANGSTROMS AND DEGREES)

PRIMITIVE CELL - VOLUME=3288.008138 DENSITY=0.951 g/cm³

A B C ALPHA BETA GAMMA
 16.91623083 16.93353332 17.64360801 97.804245 97.848304 135.751199

ATOM X/A Y/B Z/C

21 SC -1.749606215696E-01 -4.919677766995E-01 -1.993055319732E-01
 21 SC 2.083482055900E-01 2.344212964980E-02 -3.011281241393E-01
 21 SC -4.870111728235E-01 2.053878998721E-01 -3.085640589553E-01
 21 SC 1.635104503558E-02 -1.792333463871E-01 -1.914800158018E-01
 21 SC 1.774529347016E-01 4.924465991013E-01 1.993019351971E-01
 21 SC -2.067989007972E-01 -2.332571558316E-02 2.998396251613E-01
 21 SC 4.896461954149E-01 -2.050862893383E-01 3.093564045044E-01
 21 SC -1.224657205293E-02 1.803543582841E-01 1.913418574739E-01
 16 S -1.174968521638E-01 -1.425051111374E-01 1.790029235468E-02
 16 S 3.411943958184E-01 -1.385062759165E-01 4.840833827662E-01
 16 S 1.212590657164E-01 1.438224507247E-01 -1.782824847402E-02
 16 S -3.366037470643E-01 1.373745510068E-01 -4.807076790118E-01
 16 S 1.409266210131E-01 1.206106934337E-01 4.787970710065E-01
 16 S 1.425370277720E-01 -3.384416009318E-01 2.189242878720E-02
 16 S -1.391457041589E-01 -1.230737835890E-01 -4.807348943876E-01
 16 S -1.407592855488E-01 3.400207855987E-01 -1.962425436684E-02
 8 O -1.057076901013E-01 -3.621330535433E-01 -2.545209474391E-01
 8 O 3.935309662616E-01 1.481912175552E-01 -2.453356158052E-01
 8 O 1.483137580985E-01 -1.043226698646E-01 -2.456281715480E-01
 8 O -3.586176934704E-01 3.915293663607E-01 -2.549159650003E-01
 8 O 1.101367186849E-01 3.633576037102E-01 2.547020286035E-01
 8 O -3.916454835246E-01 -1.448839947714E-01 2.447685375707E-01
 8 O -1.439762887226E-01 1.063791345774E-01 2.457739920382E-01
 8 O 3.617004258189E-01 -3.905429795039E-01 2.521143384484E-01
 1 H -1.478940829375E-01 -3.897022832011E-01 -3.112227981084E-01
 1 H 4.225160901802E-01 1.615799721863E-01 -1.889123347927E-01
 1 H 1.694762823317E-01 -1.434501133460E-01 -2.565240160503E-01
 1 H -3.872463020334E-01 4.226121366080E-01 -2.417103391687E-01
 1 H 1.531095908993E-01 3.905834718171E-01 3.110788184996E-01
 1 H -4.205336147585E-01 -1.573261674257E-01 1.885710575779E-01
 1 H -1.644487780105E-01 1.461574201947E-01 2.567859449298E-01
 1 H 3.906292517107E-01 -4.212117236101E-01 2.386222849425E-01
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 8 O 1.983169863874E-01 -8.480411444333E-02 -3.922132359646E-01
 8 O 2.182887565876E-01 1.233014410115E-01 -2.033651939450E-01
 8 O -1.715129605168E-01 4.223476040149E-01 -2.978331762381E-01
 8 O 4.260349092710E-01 2.194783339356E-01 -3.961103205453E-01
 8 O 1.204913404663E-01 -1.786186139270E-01 -1.062032657920E-01
 8 O -9.431169435445E-02 -1.978947533405E-01 -2.886880288787E-01
 8 O -4.086144668970E-01 1.930824849529E-01 -2.107064402929E-01
 8 O 1.931710398705E-01 4.114025751039E-01 1.065454968721E-01
 8 O -1.947326587683E-01 8.563138543818E-02 3.923916475679E-01
 8 O -2.208416539749E-01 -1.251328872774E-01 2.002190705255E-01
 8 O 1.760991911055E-01 -4.208691455981E-01 2.986577000099E-01
 8 O -4.249525693799E-01 -2.231112493857E-01 3.938813366988E-01
 8 O -1.152173708005E-01 1.800175607371E-01 1.055222363656E-01
 8 O 9.744674565013E-02 1.983126038283E-01 2.882435998248E-01
 8 O 4.067979421015E-01 -1.918073906018E-01 2.161169700706E-01
 8 O 1.617535130197E-03 -3.718358108830E-01 -1.208428036004E-01
 8 O 2.503637841566E-01 1.223518718130E-01 -3.786731435675E-01
 8 O 2.883186465464E-02 -7.717097038375E-02 -3.537279181719E-01
 8 O -2.216303161929E-01 3.809551234906E-01 -1.474255109352E-01
 8 O 3.882998944212E-01 2.593047486317E-02 -3.837839960301E-01
 8 O -8.463098995114E-02 -2.278381080287E-01 -1.138927548018E-01
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 8 O -3.647100400527E-01 2.430741980092E-01 -3.612864659371E-01
 8 O 2.702335369717E-04 3.731074315193E-01 1.228031467892E-01
 8 O -2.484989219242E-01 -1.232680297544E-01 3.768372566781E-01
 8 O -2.782137271997E-02 7.399607865561E-02 3.509172485967E-01
 8 O 2.232236591716E-01 -3.806167830448E-01 1.476110056663E-01

8 O	-3.841972106786E-01	-2.658885974603E-02	3.867142402363E-01
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6 C	-2.534454074340E-01	3.189523070287E-01	-3.519297059582E-01
6 C	3.247946270423E-01	1.785111504990E-01	-4.162853947289E-01
6 C	9.778570682785E-02	-2.599549297632E-01	-8.508820647054E-02
6 C	-7.295943509748E-02	-1.512896786040E-01	-3.441271053819E-01
6 C	-3.057987819436E-01	2.700017934289E-01	-1.560417492362E-01
6 C	1.528863756360E-01	3.108068636532E-01	8.272514449203E-02
6 C	-2.712198617464E-01	6.914337755909E-02	4.168438315539E-01
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6 C	2.581286597885E-01	-3.191710693439E-01	3.545705513773E-01
6 C	-3.230817045665E-01	-1.808317658788E-01	4.141374536571E-01
6 C	-9.406688484463E-02	2.611623880736E-01	8.542296998387E-02
6 C	7.470452900099E-02	1.494855107754E-01	3.424987147333E-01
6 C	3.066370696164E-01	-2.687573896965E-01	1.587100949189E-01
6 C	-1.807487033529E-01	-2.849191140768E-01	-1.751139421260E-02
6 C	2.337961001030E-01	-1.643724521879E-01	-4.825791706167E-01
6 C	1.876897404463E-01	1.835939394536E-01	-9.340935903357E-02
6 C	-2.212670725541E-01	2.817335272831E-01	-4.078553470522E-01
6 C	2.883545589021E-01	1.944626364116E-01	-4.871632944463E-01
6 C	1.853257178928E-01	-2.258516890849E-01	-1.481084445850E-02
6 C	-1.698002624304E-01	-1.832478874820E-01	-4.019382227908E-01
6 C	-2.800401017210E-01	2.311078620685E-01	-9.813413004271E-02
6 C	1.792363504592E-01	2.839495100249E-01	1.455878342310E-02
6 C	-2.295720187802E-01	1.647737867975E-01	4.840790207648E-01
6 C	-1.899261113173E-01	-1.851060137446E-01	9.029127780135E-02
6 C	2.255956128621E-01	-2.816535206947E-01	4.098226879216E-01
6 C	-2.865562814327E-01	-1.970150226721E-01	4.848393452696E-01
6 C	-1.811541157262E-01	2.268371206528E-01	1.479810904827E-02
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6 C	2.826032139788E-01	-2.298089084091E-01	9.968664270612E-02
6 C	-2.513503314103E-01	-3.571595434031E-01	2.450630932268E-02
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6 C	2.484734025481E-01	2.961627960402E-01	-9.226284616288E-02
6 C	-1.102894010532E-01	3.435504386678E-01	-4.119311328793E-01
6 C	3.531234529470E-01	2.591045544925E-01	4.657412790038E-01
6 C	2.992059703018E-01	-1.147459847592E-01	3.028678617406E-02
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6 C	2.435201950740E-01	3.533025683761E-01	-3.084967751248E-02
6 C	-1.150194336594E-01	2.768824773506E-01	-4.734699857485E-01
6 C	-2.565938564232E-01	-3.003138687460E-01	8.590393198224E-02
6 C	1.142877460316E-01	-3.420167002326E-01	4.1213477393872E-01
6 C	-3.515695279782E-01	-2.616809983486E-01	-4.681388866229E-01
6 C	-2.933510584814E-01	1.151085304243E-01	-3.198114264604E-02
6 C	2.865977792998E-01	2.518580016603E-01	4.017583409194E-01
6 C	3.549804134458E-01	-1.170563740201E-01	9.527122492536E-02
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1 H	4.128002587516E-02	-3.059851531489E-01	4.854167481214E-01
1 H	2.942012153198E-01	3.350038466683E-01	-1.350808417162E-01
1 H	-2.866916478507E-02	4.339307739397E-01	-3.712723492466E-01
1 H	4.455829051069E-01	3.096490272718E-01	4.775269311054E-01
1 H	3.401143101937E-01	-3.467161488897E-02	1.653548026129E-02
1 H	-3.196102865982E-01	-2.983879830671E-01	-3.595641208276E-01
1 H	-4.386262152066E-01	3.926956374588E-02	-1.403026807681E-01
1 H	2.842865304848E-01	4.418813930564E-01	-2.017761170785E-02
1 H	-3.755390493871E-02	3.087974967241E-01	-4.867139269773E-01
1 H	-3.068093409840E-01	-3.412936460888E-01	1.263297381906E-01
1 H	3.250274994589E-02	-4.314189222548E-01	3.703474659277E-01
1 H	-4.440927967405E-01	-3.123005463716E-01	-4.801945688630E-01
1 H	-3.325908446333E-01	3.460536233289E-02	-1.977730484559E-02
1 H	3.207562008917E-01	2.960327531984E-01	3.574568854638E-01
1 H	4.447023076280E-01	-3.912428069857E-02	1.384305047232E-01
8 O	4.462434122059E-01	-2.446452281470E-01	4.680855328969E-02
6 C	3.674149630673E-01	-3.438466781575E-01	1.003826926132E-02

S10. Theoretical IR spectra for structures I and II of NOTT-401 \cdots CO

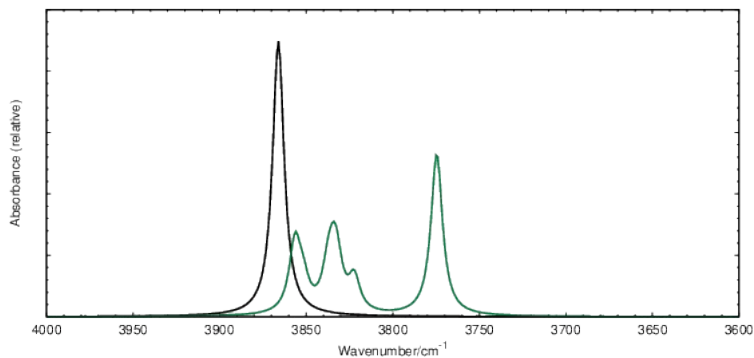


Figure S8. Theoretical IR for NOTT-401 (black) and structure I of NOTT-401 \cdots CO (green).

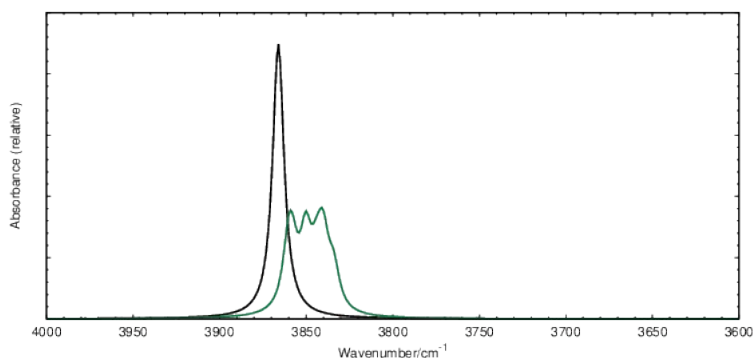


Figure S9. Theoretical IR for NOTT-401 (black) and structure II of NOTT-401 \cdots CO (green).

S11. References

- 1 I. A. Ibarra, S. Yang, X. Lin, A. J. Blake, P. J. Rizkallah, H. Nowell, D. R. Allan, N. R. Champness, P. Hubberstey and M. Schröder, Highly porous and robust scandium-based metal-organic frameworks for hydrogen storage, *Chem. Commun.*, 2011, **47**, 8304–8306.
- 2 B. Landeros-Rivera, I. A. Ibarra, M. L. Díaz-Ramírez, R. Vargas, H. A. Lara-García, J. Garza and A. Martínez, A detailed description of the CO molecule adsorbed in InOF-1, *Phys. Chem. Chem. Phys.*, 2020, **22**, 7969–7974.