

Dynamics and magnetic properties of an NO molecule encapsulated in an open-cage fullerene derivative evidenced by low temperature heat capacity

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Experimental

1. Sample preparation

1, (NO)**@1**, **2** and (NO)**@2** were synthesized according to the literature methods.¹⁻³

Preparation of **1**

Compound **1** was dissolved in a 1:1 mixed solvent system consisting of chloroform and hexane. The microcrystals were obtained by slow evaporation at 5 °C over few days. After filtration, the crystalline sample was washed with chloroform/hexane (1:1) and dried under vacuum at 120 °C for 24 hours. CHN elemental analyses found: C 82.66 %, H 3.16 %, N 3.03 %, calculated for $C_{82}H_{28}N_2O_4S(H_2O)_{2.6}(N_2)_{0.29}$: C 82.61 %, H 2.81 %, N 3.03 %

Preparation of (NO)**@1**

(NO)**@1** was crystallized in the similar manner with that of **1**. The sample was dried under vacuum at room temperature for 15 min.

CHN elemental analyses found: C 80.29%, H 3.54%, N 3.00%, calculated for $C_{82}H_{28}N_2O_4S(NO)_{0.63}(N_2)_{0.06}(H_2O)_{3.95}(C_6H_{14})_{0.66}$: C 80.30%, H 3.54%, N 2.99%

Preparation of **2**

Compound **2** was dissolved in chloroform. The microcrystals were obtained by slow evaporation at 5 °C over a day. After filtration, the crystalline sample was washed with chloroform and dried under vacuum for an hour. CHN elemental analyses found: C 80.77%, H 3.81%, N 2.31%, calculated for $C_{82}H_{32}N_2O_4S(H_2O)_{4.33}$: C 80.78%, H 3.36%, N 2.29%

Preparation of (NO)**@2**

(NO)**@2** was crystallized in the similar manner with that of **2**. The sample was dried under vacuum at room temperature for 2 hours.

CHN elemental analyses found: C 77.01%, H 3.18%, N 3.16%, calculated for $C_{82}H_{32}N_2O_4S(NO)_{0.80}(N_2)_{0.06}(H_2O)_{0.91}(CHCl_3)_{0.99}$: C 77.01%, H 2.72%, N 3.16%

2. Heat capacity measurements

Heat capacities were acquired by relaxation calorimeter using Quantum Design Physical Property Measurement System (PPMS) with heat capacity measurement option. ^3He option was used between 0.35 and 10 K and ^4He option was used above 10 K. Sample masses were measured by using ultra microbalance Sartorius MSA2.7S0TRDM. The samples were pressed into pellet and attached to a sample platform using Apiezon N grease. Buoyancies of the samples were corrected using the sample densities (Table S1).

Table S1. Buoyancy corrected sample masses used for heat capacity measurements.

	^3He	^4He
1	0.6417 mg	0.7848 mg
2	0.6888 mg	0.9423 mg
(NO)@1	0.5528 mg	0.8058 mg
(NO)@2	0.5035 mg	1.4029 mg

The lattice heat capacities for (NO)@1 and (NO)@2 were estimated by a fit for C_p in the temperature range from 2 to 5 K using following equation:

$$C_p = ET^{-2} + C_3T^3 + C_5T^5 + C_7T^7 + C_9T^9 \quad \text{Eq. S1}$$

where the first term is the high temperature side of the Schottky contribution, and the letter term is the lattice contribution. The optimized parameters for (NO)@1 and (NO)@2 are shown in Table S2. Removal of the ET^{-2} from the Eq. S1 affords the lattice heat capacities.

Table S2. Fitting parameters for Eq. S1.

	E	C_3	C_5	C_7	C_9
(NO)@1	0.5738	0.0517	3.55867E-4	-3.28178E-5	4.71265E-7
(NO)@2	0.53727	0.03555	0.00143	-8.20906E-5	1.39563E-6

Table S3. Fitting parameters for low temperature side of the ΔC_p (blue curve in Fig. 2b) using $C_{\text{sch,low}} = A(B/T)^2 e^{-B/T}$.

	A	B
(NO)@1	0.31209	4.63632
(NO)@2	0.26765	4.44698

3. Theoretical calculations

The calculations were conducted with the ORCA 4.2.⁴ The molecular coordinates were obtained from their crystal structures with slight modification, where the tert-butyl groups were replaced by the hydrogens. All the geometry optimizations and the frequency calculations were conducted at the UB3LYP-D3BJ⁵⁻⁸/Def2-SVP⁹ with RIJCOSX approximation using Def2/J¹⁰ auxiliary basis set for speeding up the calculations.

For calculating *g*-factors, the molecular coordinates were reoriented as the NO axis being parallel to *z*-axis. Def2-TZVP⁹ and Def2-SVP⁹ basis sets were applied for NO units and cage molecules, respectively. Example of the input files used for calculations were summarized in the next pages. The initial orbitals for the complete-active space self-consistent field (CASSCF) calculations were obtained from the quasi-restricted orbitals (QRO) at UBP86¹¹ level with RI approximation (input #1), followed by the SCF iteration without changing QRO using "NOITER" command (input #2). Because the orbital hybridization among the $2\pi^*$ -orbitals of the NO units and the orbitals of the cage molecules are weak, it is easy to recognize $2\pi^*$ -orbitals from the molecular orbitals. Therefore, we selected the two $2\pi^*$ -orbitals of the NO as the active orbitals. (1,2)-CASSCF calculations with the RI approximation using Def2-TZVP/c¹² for the NO units and Def2-SVP/c for the cages, and N-electron valence perturbation theory (NEVPT2) were applied to consider static and dynamic electron correlation. Spin-orbit coupling (SOC) calculations based on quasi-degenerated perturbation theory (QDPT) afforded SOC energies and *g*-factors (input #3).

#1. Calculation of unrestricted natural orbitals

! uks bp86 def2-svp def2/j ri uno pal16

%scf maxiter 999 end

*xyz 0 2

```
O 0.00000 -0.00000 0.00000 newgto "def2-tzvp" end
N -0.00000 0.00000 1.15045 newgto "def2-tzvp" end
C -3.29075 -0.48076 4.73507
C -2.99548 0.81528 4.83282
C -2.71248 1.72417 3.66344
C -1.22549 2.12548 3.54527
C -0.19145 1.60917 4.32941
C -0.05265 0.62155 5.46795
C 1.37780 -0.04380 5.30973
C 2.00883 0.64008 4.15467
C 2.90662 0.20080 3.18840
C 2.82058 -1.94074 1.73389
C 1.79941 -2.88024 1.66393
C 0.69732 -3.20277 2.70957
C -0.55950 -3.25674 1.78367
C -1.82211 -2.69417 1.98137
C -2.29936 -2.31245 3.33739
C -3.41253 -1.22375 3.43206
S 3.51589 -1.46388 3.30293
N -4.76484 -3.21641 2.96536
O -0.76764 0.36661 6.40036
O -1.83809 -2.79373 4.35543
N -3.00101 3.95130 4.61301
C -3.30158 -0.30317 2.23730
C -2.81031 1.83026 1.14443
O 1.80017 -0.89509 6.04561
C -3.28674 -0.95770 0.94975
O -0.89849 2.90022 2.34273
O 0.64660 -2.21756 3.68512
C -1.28001 3.31084 -0.09004
C -3.70591 5.05381 4.87513
C 0.11944 3.66033 -0.27192
C -3.56062 2.99249 3.87282
C -1.77810 2.86442 1.16231
C -3.20971 1.27392 -0.07945
C -3.03998 1.04766 2.33766
O 0.97019 3.59658 0.81558
C -2.67593 1.72307 -1.34289
C 1.48736 2.60028 2.83085
C -1.72046 2.72881 -1.34767
C -3.44058 -0.15303 -0.18116
C -2.57946 -2.23233 0.82241
C 0.44369 3.27590 2.11685
C -5.95422 -1.25620 3.67420
C -4.77300 -1.94294 3.36192
C 2.65539 2.38912 -0.51374
C -2.17848 -2.62936 -0.46911
C -3.02967 -0.57803 -1.50265
C -7.16673 -1.93501 3.56223
C 1.16291 1.75191 3.85396
C -0.58300 2.63216 -2.25582
C -5.00962 5.25530 4.41295
C 3.23874 1.05432 -0.52700
C -0.43682 1.51302 -0.08364
C 2.53716 2.24361 1.91180
C -7.15866 -3.27034 3.14786
C -4.86637 3.09186 3.37362
C 3.09638 0.94405 1.94976
C -5.92801 -3.86546 2.86267
C -2.55283 0.57908 -2.23221
C 2.85445 0.46451 -1.79801
C 2.82594 -1.71294 -0.70598
C 2.27014 2.94919 0.68928
C -0.91445 -3.29537 -0.65704
C 0.56723 3.18521 -1.56959
C 0.86426 0.87198 -3.21427
C 3.38327 0.28439 0.66043
C -5.59951 4.24669 3.64742
C -0.10888 -3.51752 0.45580
C 3.18996 -1.17451 0.54762
C 1.96065 1.37408 -2.50380
C 1.81962 2.56171 -1.68916
C 1.31219 -3.27126 0.38080
C -1.44975 0.46632 -3.08369
C -0.78143 -0.81721 -3.23060
C -2.40302 -1.80940 -1.64602
C 1.54355 -1.43801 -2.67097
C -1.25676 -1.93907 -2.53522
C -0.32501 -2.85953 -1.91245
C 1.88214 -2.80377 -0.79652
C 2.64849 -0.90129 -1.88669
C 1.05328 -2.61094 -1.97600
C 0.65012 -0.56571 -3.30260
C -3.43690 -1.07381 5.63910
H -2.90575 1.27871 5.81438
H 0.86522 -4.20723 3.14895
H -0.00023 -2.50122 4.35538
H -3.20805 5.81716 5.48425
H -5.91013 -0.21542 4.00017
H -8.10743 -1.43012 3.79665
H -5.54457 6.17768 4.64858
H -8.08503 -3.83996 3.04741
H -5.29121 2.28325 2.77679
H -5.87562 -4.91028 2.53656
H -6.61809 4.35801 3.26702
*
```

#2. Construction of initial orbitals for CASSCF calculation

! uks bp86 def2-svp def2/j ri moread noiter

%moinp "NO@|a_uno.qro" # Name of .qro file from previous calculation

*xyz 0 2

```
O 0.00000 -0.00000 0.00000 newgto "def2-tzvp" end
N -0.00000 0.00000 1.15045 newgto "def2-tzvp" end
C -3.29075 -0.48076 4.73507
C -2.99548 0.81528 4.83282
C -2.71248 1.72417 3.66344
C -1.22549 2.12548 3.54527
C -0.19145 1.60917 4.32941
C -0.05265 0.62155 5.46795
C 1.37780 -0.04380 5.30973
C 2.00883 0.64008 4.15467
C 2.90662 0.20080 3.18840
C 2.82058 -1.94074 1.73389
C 1.79941 -2.88024 1.66393
C 0.69732 -3.20277 2.70957
C -0.55950 -3.25674 1.78367
C -1.82211 -2.69417 1.98137
C -2.29936 -2.31245 3.33739
C -3.41253 -1.22375 3.43206
S 3.51589 -1.46388 3.30293
N -4.76484 -3.21641 2.96536
O -0.76764 0.36661 6.40036
O -1.83809 -2.79373 4.35543
N -3.00101 3.95130 4.61301
C -3.30158 -0.30317 2.23730
C -2.81031 1.83026 1.14443
O 1.80017 -0.89509 6.04561
C -3.28674 -0.95770 0.94975
O -0.89849 2.90022 2.34273
O 0.64660 -2.21756 3.68512
C -1.28001 3.31084 -0.09004
C -3.70591 5.05381 4.87513
C 0.11944 3.66033 -0.27192
C -3.56062 2.99249 3.87282
C -1.77810 2.86442 1.16231
C -3.20971 1.27392 -0.07945
C -3.03998 1.04766 2.33766
O 0.97019 3.59658 0.81558
C -2.67593 1.72307 -1.34289
C 1.48736 2.60028 2.83085
C -1.72046 2.72881 -1.34767
C -3.44058 -0.15303 -0.18116
C -2.57946 -2.23233 0.82241
C 0.44369 3.27590 2.11685
C -5.95422 -1.25620 3.67420
C -4.77300 -1.94294 3.36192
C 2.65539 2.38912 -0.51374
C -2.17848 -2.62936 -0.46911
C -3.02967 -0.57803 -1.50265
C -7.16673 -1.93501 3.56223
C 1.16291 1.75191 3.85396
C -0.58300 2.63216 -2.25582
C -5.00962 5.25530 4.41295
C 3.23874 1.05432 -0.52700
C -0.43682 1.51302 -0.08364
C 2.53716 2.24361 1.91180
C -7.15866 -3.27034 3.14786
C -4.86637 3.09186 3.37362
C 3.09638 0.94405 1.94976
C -5.92801 -3.86546 2.86267
C -2.55283 0.57908 -2.23221
C 2.85445 0.46451 -1.79801
C 2.82594 -1.71294 -0.70598
C 2.27014 2.94919 0.68928
C -0.91445 -3.29537 -0.65704
C 0.56723 3.18521 -1.56959
C 0.86426 0.87198 -3.21427
C 3.38327 0.28439 0.66043
C -5.59951 4.24669 3.64742
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C 3.18996 -1.17451 0.54762
C 1.96065 1.37408 -2.50380
C 1.81962 2.56171 -1.68916
C 1.31219 -3.27126 0.38080
C -1.44975 0.46632 -3.08369
C -0.78143 -0.81721 -3.23060
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C 1.54355 -1.43801 -2.67097
C -1.25676 -1.93907 -2.53522
C -0.32501 -2.85953 -1.91245
C 1.88214 -2.80377 -0.79652
C 2.64849 -0.90129 -1.88669
C 1.05328 -2.61094 -1.97600
C 0.65012 -0.56571 -3.30260
C -3.43690 -1.07381 5.63910
H -2.90575 1.27871 5.81438
H 0.86522 -4.20723 3.14895
H -0.00023 -2.50122 4.35538
H -3.20805 5.81716 5.48425
H -5.91013 -0.21542 4.00017
H -8.10743 -1.43012 3.79665
H -5.54457 6.17768 4.64858
H -8.08503 -3.83996 3.04741
H -5.29121 2.28325 2.77679
H -5.87562 -4.91028 2.53656
H -6.61809 4.35801 3.26702
*
```

#3. CASSCF/NEVPT2 and SOC calculation

```
! def2-svp def2-svp/c moread ri-nevpt2 pal8
%moinp "NO@!a_gro.gbw" #Name of .gbw file from previous calculation
%maxcore 7000

%casscf
trafostep ri
nel 1
norb 2
mult 2
nroots 2
rel
dosoc true
gtensor true
end
end

*xyz 0 2
O 0.00000 -0.00000 0.00000 newgto "def2-tzvp" end newauxcgo "def2-tzvp/c" end
N -0.00000 0.00000 1.15045 newgto "def2-tzvp" end newauxcgo "def2-tzvp/c" end
C -3.29075 -0.48076 4.73507
C -2.99548 0.81528 4.83282
C -2.71248 1.72417 3.66344
C -1.22549 2.12548 3.54527
C -0.19145 1.60917 4.32941
C -0.05265 0.62155 5.46795
C 1.37780 -0.04380 5.30973
C 2.00883 0.64008 4.15467
C 2.90662 0.20080 3.18840
C 2.82058 -1.94074 1.73389
C 1.79941 -2.88024 1.66393
C 0.69732 -3.20277 2.70957
C -0.55950 -3.25674 1.78367
C -1.82211 -2.69417 1.98137
C -2.29936 -2.31245 3.33739
C -3.41253 -1.22375 3.43206
S 3.51589 -1.46388 3.30293
N -4.76484 -3.21641 2.96536
O -0.76764 0.36661 6.40036
O -1.83809 -2.79373 4.35543
N -3.00101 3.95130 4.61301
C -3.30158 -0.30317 2.23730
C -2.81031 1.83026 1.14443
O 1.80017 -0.89509 6.04561
C -3.28674 -0.95770 0.94975
C -0.89849 2.90022 2.34273
O 0.64660 -2.21756 3.68512
C -1.28001 3.31084 -0.09004
C -3.70591 5.05381 4.87513
C 0.11944 3.66033 -0.27192
C -3.56062 2.99249 3.87282
C -1.77810 2.86442 1.16231
C -3.20971 1.27392 -0.07945
C -3.03998 1.04766 2.33766
C 0.97019 3.59658 0.81558
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C 1.48736 2.60028 2.83085
C -1.72046 2.72881 -1.34767
C -3.44058 -0.15303 -0.18116
C -2.57946 -2.23233 0.82241
C 0.44369 3.27590 2.11685
C -5.95422 -1.25620 3.67420
C -4.77300 -1.94294 3.36192
C 2.65539 2.38912 -0.51374
C -2.17848 -2.62936 -0.46911
C -3.02967 -0.57803 -1.50265
C -7.16673 -1.93501 3.56223
C 1.16291 1.75191 3.85396
C -0.58300 2.63216 -2.25582
C -5.00962 5.25530 4.41295
C 3.23874 1.05432 -0.52700
C -0.43682 1.51302 -0.08364
C 2.53716 2.24361 1.91180
C -7.15866 -3.27034 3.14786
C -4.86637 3.09186 3.37362
C 3.09638 0.94405 1.94976
C -5.92801 -3.86546 2.86267
C -2.55283 0.57908 -2.23221
C 2.85445 0.46451 -1.79801
C 2.82594 -1.71294 -0.70598
C 2.27014 2.94919 0.68928
C -0.91445 -3.29537 -0.65704
C 0.56723 3.18521 -1.56959
C 0.86426 0.87198 -3.21427
C 3.38327 0.28439 0.66043
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C 3.18996 -1.17451 0.54762
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C 1.91962 2.56171 -1.68916
C 1.31219 -3.27126 0.38080
C -1.44975 0.46632 -3.08369
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C 1.54355 -1.43801 -2.67097
C -1.25676 -1.93907 -2.53522
C -0.32501 -2.85953 -1.91245
C 1.88214 -2.80377 -0.79652
C 2.64849 -0.90129 -1.88669
C 1.05328 -2.61094 -1.97600
C 0.65012 -0.56571 -3.30260
H -3.43690 -1.07381 5.63910
H -2.90575 1.27871 5.81438
H 0.86522 -4.20723 3.14895
H -0.00023 -2.50122 4.35538
H -3.20805 5.81716 5.48425
H -5.91013 -0.21542 4.00017
```

```
H -8.10743 -1.43012 3.79665
H -5.54457 6.17768 4.64858
H -8.08503 -3.83996 3.04741
H -5.29121 2.28325 2.77679
H -5.87562 -4.91028 2.53656
H -6.61809 4.35801 3.26702*
```

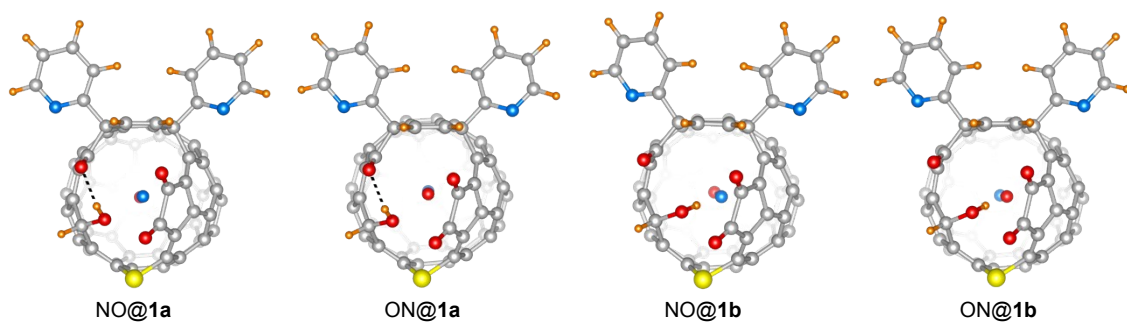


Figure S1. Optimized geometries around the hydroxy group of **1** series.

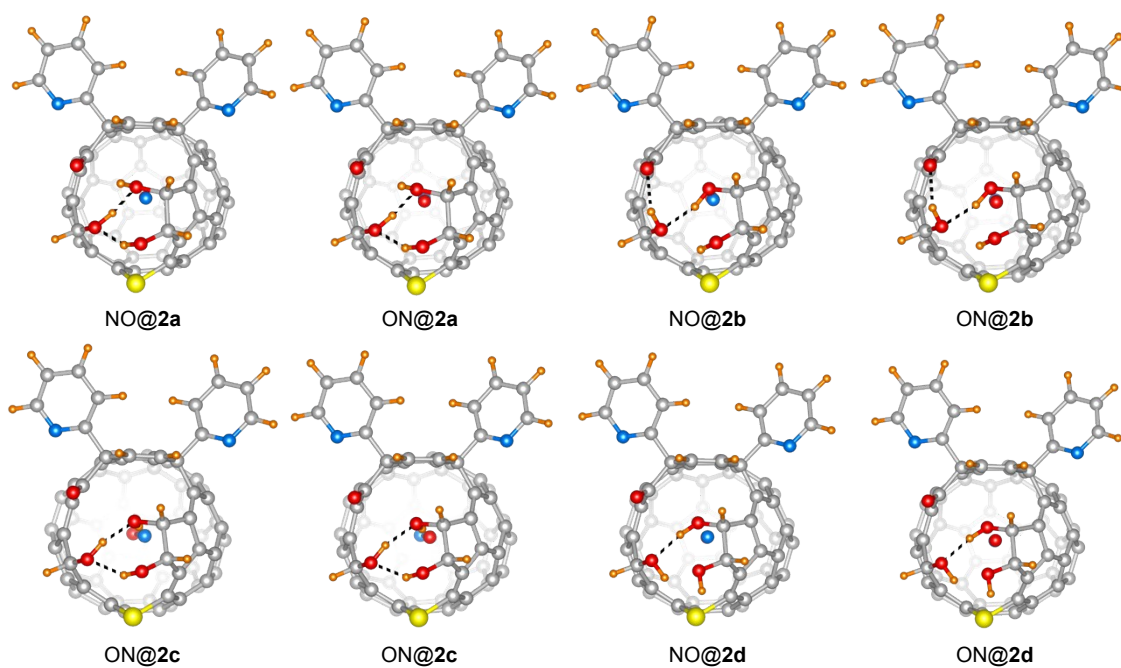


Figure S2. Optimized geometries around the hydroxy groups of **2** series.

Table S4. Total electronic energy including zero-point energies of the series of NO@1.

	Electronic energy + zero-point energy / Eh	$E_{O-up} - E_{N-up}$ / cm^{-1}	ΔE / kcal mol^{-1}
NO@1a	-3760.66838973	1.80	0
ON@1a	-3760.66838153		0.0052
NO@1b	-3760.65931997	178.01	5.7140
ON@1b	-3760.65851083		6.2237

Table S5. Total electronic energy including zero-point energies of the series of NO@2.

	Electronic energy + zero-point energy / Eh	$E_{O-up} - E_{N-up}$ / cm^{-1}	ΔE / kcal mol^{-1}
NO@2a	-3763.02500604	30.33	0.3429
ON@2a	-3763.02486819		0.4297
NO@2b	-3763.02475723	-174.48	0.4996
ON@2b	-3763.02555030		0
ON@2c	-3763.02121401	256.20	2.7319
ON@2c	-3763.02004945		3.4655
NO@2d	-3763.01514235	-1.36	6.5570
ON@2d	-3763.01514852		6.5531

Table S6. Theoretical g -values for NO molecules caged in 2c and 2d.

	NO@2c	ON@2c	NO@2d	ON@2d
g_{\parallel}	1.506	1.224	0.404	0.483
g_{\perp}	1.939	1.843	1.188	1.292

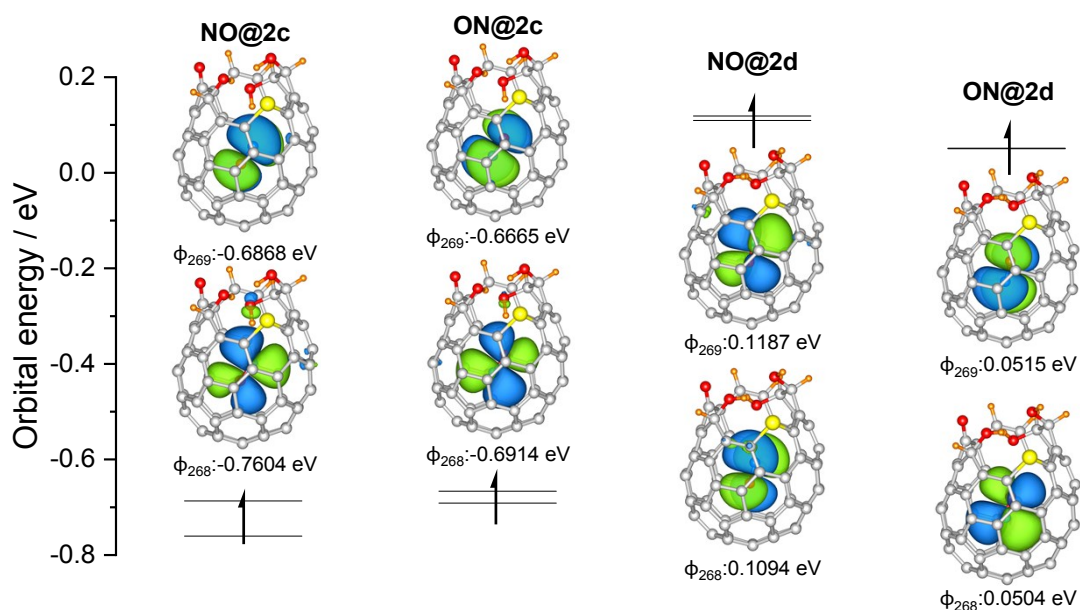


Figure S3. CASSCF orbital energy and electron density map (isovalue = 0.01) for NO molecules caged in **2c** and **2d**.

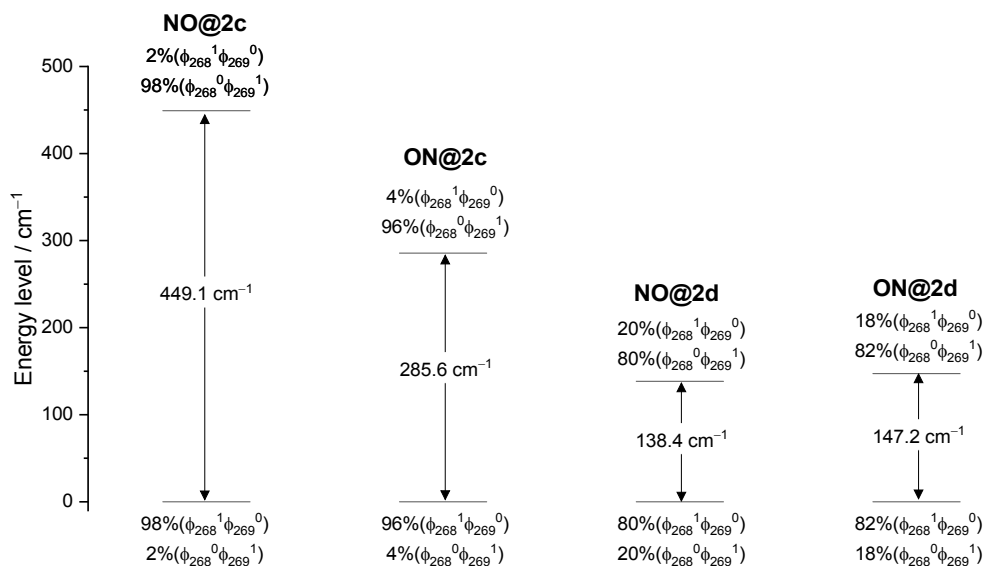


Figure S4. Energy levels and compositions of the ground and first-excited states of NO molecules caged in **2c** and **2d**.

Optimized geometries of the present compounds are summarized below.

NO@1a			C -1.77810	2.86442	1.16231	C -5.59951	4.24669	3.64742
O 0.00000	0.00000	0.00000	C -3.20971	1.27392	-0.07945	C -0.10888	-3.51752	0.45580
N 0.00000	0.00000	1.15045	C -3.03998	1.04766	2.33766	C 3.18996	-1.17451	0.54762
C -3.29075	-0.48076	4.73507	C 0.97019	3.59658	0.81558	C 1.96065	1.37408	-2.50380
C -2.99548	0.81528	4.83282	C -2.67593	1.72307	-1.34289	C 1.81962	2.56171	-1.68916
C -2.71248	1.72417	3.66344	C 1.48736	2.60028	2.83085	C 1.31219	-3.27126	0.38080
C -1.22549	2.12548	3.54527	C -1.72046	2.72881	-1.34767	C -1.44975	0.46632	-3.08369
C -0.19145	1.60917	4.32941	C -3.44058	-0.15303	-0.18116	C -0.78143	-0.81721	-3.23060
C -0.05265	0.62155	5.46795	C -2.57946	-2.23233	0.82241	C -2.40302	-1.80940	-1.64602
C 1.37780	-0.04380	5.30973	C 0.44369	3.27590	2.11685	C 1.54355	-1.43801	-2.67097
C 2.00883	0.64008	4.15467	C -5.95422	-1.25620	3.67420	C -1.25676	-1.93907	-2.53522
C 2.90662	0.20080	3.18840	C -4.77300	-1.94294	3.36192	C -0.32501	-2.85953	-1.91245
C 2.82058	-1.94074	1.73389	C 2.65539	2.38912	-0.51374	C 1.88214	-2.80377	-0.79652
C 1.79941	-2.88024	1.66393	C -2.17848	-2.62936	-0.46911	C 2.64849	-0.90129	-1.88669
C 0.69732	-3.20277	2.70957	C -3.02967	-0.57803	-1.50265	C 1.05328	-2.61094	-1.97600
C -0.55950	-3.25674	1.78367	C -7.16673	-1.93501	3.56223	C 0.65012	-0.56571	-3.30260
C -1.82211	-2.69417	1.98137	C 1.16291	1.75191	3.85396	H -3.43690	-1.07381	5.63910
C -2.29936	-2.31245	3.33739	C -0.58300	2.63216	-2.25582	H -2.90575	1.27871	5.81438
C -3.41253	-1.22375	3.43206	C -5.00962	5.25530	4.41295	H 0.86522	-4.20723	3.14895
S 3.51589	-1.46388	3.30293	C 3.23874	1.05432	-0.52700	H -0.00023	-2.50122	4.35538
N -4.76484	-3.21641	2.96536	C -0.43682	1.51302	-3.08364	H -3.20805	5.81716	5.48425
O -0.76764	0.36661	6.40036	C 2.53716	2.24361	1.91180	H -5.91013	-0.21542	4.00017
O -1.83809	-2.79373	4.35543	C -7.15866	-3.27034	3.14786	H -8.10743	-1.43012	3.79665
N -3.00101	3.95130	4.61301	C -4.86637	3.09186	3.37362	H -5.54457	6.17768	4.64858
C -3.30158	-0.30317	2.23730	C 3.09638	0.94405	1.94976	H -8.08503	-3.83996	3.04741
C -2.81031	1.83026	1.14443	C -5.92801	-3.86546	2.86267	H -5.29121	2.28325	2.77679
O 1.80017	-0.89509	6.04561	C -2.55283	0.57908	-2.23221	H -5.87562	-4.91028	2.53656
C -3.28674	-0.95770	0.94975	C 2.85445	0.46451	-1.79801	H -6.61809	4.35801	3.26702
C -0.89849	2.90022	2.34273	C 2.82594	-1.71294	-0.70598			
O 0.64660	-2.21756	3.68512	C 2.27014	2.94919	0.68928			
C -1.28001	3.31084	-0.09004	C -0.91445	-3.29537	-0.65704			
C -3.70591	5.05381	4.87513	C 0.56723	3.18521	-1.56959			
C 0.11944	3.66033	-0.27192	C 0.86426	0.87198	-3.21427			
C -3.56062	2.99249	3.87282	C 3.38327	0.28439	0.66043			

ON@1a	C -3.11700	1.16147	2.01216	C 1.79826	2.20316	-2.08244		
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O 0.00000	0.00000	1.14865	C -2.67210	1.25564	-1.71873	C -1.35094	-0.21496	-3.20275
C -3.36994	0.03115	4.62049	C 1.32070	2.96016	2.36177	C -0.63519	-1.47846	-3.12390
C -3.13925	1.33952	4.51220	C -1.75363	2.28543	-1.86356	C -2.26983	-2.26868	-1.44247
C -2.86476	2.06052	3.21714	C -3.40340	-0.44027	-0.28716	C 1.68932	-1.91092	-2.41103
C -1.39468	2.50913	3.07395	C -2.50978	-2.30360	1.05586	C -1.09303	-2.49270	-2.26994
C -0.37057	2.17157	3.96092	C 0.27901	3.47351	1.52058	C -0.15143	-3.26642	-1.48419
C -0.23410	1.40172	5.25635	C -5.98459	-0.98215	3.73753	C 2.01394	-2.94670	-0.33336
C 1.21253	0.75372	5.23853	C -4.79059	-1.66814	3.47651	C 2.74795	-1.21296	-1.69355
C 1.85882	1.25809	4.00122	C 2.60006	2.25303	-0.87227	C 1.21806	-2.97641	-1.55019
C 2.79795	0.69797	3.14183	C -2.05646	-2.88502	-0.14536	C 0.78807	-1.18599	-3.19839
C 2.83577	-1.65505	2.05069	C -2.94042	-1.05451	-1.51350	H -3.50730	-0.41567	5.60638
C 1.85389	-2.63645	2.10453	C -7.18163	-1.69662	3.70931	H -3.09173	1.95625	5.40854
C 0.73172	-2.83894	3.15919	C 0.99259	2.27954	3.50212	H 0.92317	-3.75690	3.75134
C -0.49127	-3.08839	2.22044	C -0.58591	2.08871	-2.71529	H -0.03822	-1.92614	4.66365
C -1.77754	-2.55146	2.29304	C -5.36594	5.53206	3.24986	H -3.58507	6.42691	4.10646
C -2.30959	-1.98063	3.55811	C 3.22596	0.95601	-0.65232	H -5.96309	0.08562	3.96207
C -3.44539	-0.91563	3.45305	C -0.37545	0.85729	-3.34664	H -8.13110	-1.19269	3.90757
S 3.45619	-0.90267	3.54156	C 2.40760	2.49479	1.54027	H -5.95545	6.45052	3.29037
N -4.75652	-2.97425	3.20728	C -7.14621	-3.06500	3.42644	H -8.05927	-3.66340	3.39591
O -0.95813	1.30608	6.21179	C -5.10302	3.20250	2.71785	H -5.48365	2.25649	2.32908
O -1.87823	-2.29447	4.65202	C 3.00491	1.23890	1.80470	H -5.83024	-4.72691	2.96180
N -3.27328	4.42747	3.67031	C -5.90449	-3.65644	3.18395	H -6.93497	4.30546	2.38850
C -3.32800	-0.19774	2.12654	C -2.48253	-0.01091	-2.40789			
C -2.88282	1.75379	0.71482	C 2.90479	0.15620	-1.82170			
O 1.63077	0.04036	6.11085	C 2.91460	-1.81840	-0.39322			
C -3.25725	-1.04915	0.96139	C 2.15814	2.98444	0.21302			
C -1.05566	3.08796	1.76936	C -0.76551	-3.52380	-0.19186			
O 0.61305	-1.71986	3.97058	C 0.52236	2.78937	-2.09818			
C -1.37341	3.07995	-0.70660	C 0.95006	0.25432	-3.33820			
C -4.04391	5.51766	3.70157	C 3.35665	0.39201	0.64779			
C 0.01809	3.45050	-0.90722	C -5.90471	4.34283	2.75149			
C -3.78353	3.29600	3.18273	C 0.01104	-3.53645	0.96318			
C -1.89356	2.82210	0.58895	C 3.21735	-1.07292	0.76750			
C -3.22493	0.99269	-0.41173	C 2.00513	0.90603	-2.68958			

NO@Ib			C 3.40024	-0.46352	1.90355	C -1.96332	-2.88555	-0.79716
O 0.00000	0.00000	0.00000	C -0.59260	-3.43904	1.62917	C -1.48244	3.22236	0.16498
N 0.00000	0.00000	1.14753	C 2.43970	-1.80822	-1.47311	C 0.82642	-0.93303	-3.12951
C 3.93202	1.48332	3.92507	C -0.80544	-2.14351	3.52520	C 0.04940	0.27648	-3.35203
C 3.75543	0.21519	4.29435	C 1.57961	-2.83993	-1.12774	C 1.86494	1.60067	-2.31344
C 3.37750	-0.90825	3.36302	C 3.27052	0.27406	-0.81486	C -2.16472	0.89264	-2.44965
C 1.94346	-1.42248	3.61099	C 2.49662	2.48299	-0.05081	C 0.56333	1.52231	-2.96129
C 1.03862	-0.84411	4.50539	C 0.13827	-2.88236	2.73800	C -0.29738	2.49932	-2.32214
C 1.02993	0.28844	5.51735	C 6.41151	2.11833	2.55496	C -2.23639	2.54322	-0.78605
C -0.44334	0.87463	5.51255	C 5.18907	2.61652	2.08507	C -3.05983	0.45574	-1.38577
C -1.21711	-0.01370	4.60380	C -2.57684	-2.54704	0.47509	C -1.63851	2.18641	-2.06464
C -2.29751	0.22700	3.76137	C 1.81448	2.61662	-1.27804	C -1.34686	-0.04085	-3.09673
C -2.62432	2.08853	1.97823	C 2.59336	0.43947	-2.08621	H 4.14982	2.24548	4.67550
C -1.67945	3.02198	1.56272	C 7.59053	2.70547	2.09381	H 3.83091	-0.05795	5.34552
C -0.36700	3.41783	2.31603	C -0.36513	-1.12664	4.32778	H -0.45144	4.33585	2.91584
C 0.62829	3.54774	1.12646	C 0.29118	-2.95378	-1.80225	H 0.11709	1.58404	2.66771
C 1.95565	3.12364	1.13436	C 6.14393	-4.06399	4.19100	H 4.55520	-4.68712	5.53124
C 2.75138	3.08015	2.39766	C -3.24752	-1.25893	0.36134	H 6.42922	1.29025	3.26518
C 3.85133	1.97141	2.50622	C -0.08856	-2.00405	-2.75800	H 8.56078	2.34012	2.43999
S -2.95306	1.87817	3.71409	C -2.02621	-1.98633	2.77769	H 6.81039	-4.88819	4.45375
N 5.11381	3.62819	1.21806	C 7.51028	3.76556	1.18762	H 8.40736	4.25537	0.80322
O 1.86615	0.66894	6.29140	C 5.62398	-2.06831	2.95486	H 5.87781	-1.29334	2.22910
O 2.58269	3.87145	3.29266	C -2.66011	-0.72070	2.71549	H 6.13158	5.01956	0.07349
N 4.02757	-2.96941	4.50350	C 6.24232	4.19036	0.78174	H 7.49215	-3.14238	2.76259
C 3.56108	0.85635	1.52659	C 2.07288	-0.84723	-2.50141			
C 3.02409	-1.45967	0.92586	C -3.14893	-0.88145	-1.03905			
O -0.79944	1.81168	6.17294	C -3.06917	1.45087	-0.33972			
C 3.28463	1.26700	0.16633	C -1.93680	-2.87674	1.65430			
C 1.46324	-2.40566	2.63313	C 0.48968	3.18171	-1.30577			
O 0.04805	2.39893	3.19021	C -0.66766	-3.42634	-0.82397			
C 1.42330	-3.21039	0.26975	C -1.43506	-1.44891	-2.73403			
C 4.88612	-3.95149	4.78889	C -3.22632	-0.30312	1.41522			
C 0.04573	-3.65005	0.42177	C 6.51742	-3.09601	3.25475			
C 4.38120	-2.05073	3.60376	C -0.09970	3.54828	-0.09634			
C 2.10286	-2.52653	1.31237	C -3.16189	1.12167	1.03143			
C 3.15637	-1.11728	-0.42822	C -2.33998	-1.86386	-1.75049			

ON@Ib	C 3.22817	0.69545	2.16903	C -0.66731	-3.31755	-1.10026		
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O 0.00000	0.00000	1.14896	C 3.04725	-0.64375	-1.33947	C 1.32983	-0.29999	-3.08464
C 2.86182	2.53801	4.32194	C -0.14163	-2.53118	3.33530	C 0.17285	0.55107	-3.31589
C 3.15309	1.27045	4.61198	C 2.61579	-1.94349	-1.12049	C 1.29247	2.36691	-2.06022
C 3.28173	0.16258	3.59782	C 2.99530	1.54024	-0.51069	C -2.16303	0.23544	-2.58049
C 2.12940	-0.85987	3.69458	C 1.40451	3.23992	0.29025	C 0.15801	1.86464	-2.82238
C 1.01924	-0.72380	4.53316	C 1.05688	-2.80896	2.59879	C -1.04380	2.40264	-2.21384
C 0.52447	0.24517	5.59336	C 5.00406	4.14352	3.19553	C -2.95108	1.61004	-0.85221
C -1.05806	0.24216	5.49215	C 3.71216	4.19472	2.65518	C -2.89489	-0.58134	-1.62066
C -1.38556	-0.79327	4.47536	C -1.44097	-3.32732	0.12888	C -2.18417	1.59837	-2.08951
C -2.42255	-0.90388	3.55496	C 0.80086	3.20807	-0.98422	C -1.01649	-0.27770	-3.19792
C -3.31496	0.83392	1.84308	C 2.38613	1.54213	-1.82649	H 2.73063	3.26621	5.12446
C -2.76494	2.07953	1.55668	C 5.90250	5.15980	2.86825	H 3.26142	0.96328	5.65083
C -1.74893	2.87706	2.43924	C -0.16374	-1.48859	4.22089	H -2.21050	3.65374	3.06647
C -0.79675	3.44940	1.34972	C 1.50753	-2.47175	-1.90853	H -0.62270	1.34417	2.76284
C 0.58991	3.54198	1.45374	C 6.96418	-1.80090	4.53511	H 5.63892	-3.04665	5.71863
C 1.26439	3.69722	2.77767	C -2.53642	-2.37271	0.01980	H 5.28951	3.32332	3.85610
C 2.69088	3.06957	2.92682	C 0.86059	-1.65822	-2.84629	H 6.91811	5.14941	3.27211
S -3.64739	0.38327	3.53231	C -1.28372	-2.77885	2.49388	H 7.87103	-2.33629	4.82397
N 3.31317	5.17651	1.84430	C 5.48294	6.18834	2.02108	H 6.15223	7.00463	1.74155
O 1.10688	0.85066	6.45198	C 5.81949	-0.06474	3.32785	H 5.81269	0.79196	2.65128
O 0.75560	4.29631	3.69300	C -2.33944	-1.83619	2.43788	H 3.80009	6.93603	0.87036
N 4.57756	-1.58336	4.70998	C 4.17288	6.14929	1.53634	H 7.96116	-0.36233	3.25312
C 2.90259	2.00555	1.87260	C 2.41207	0.19052	-2.34747			
C 3.31184	-0.29078	1.11549	C -2.49884	-1.87949	-1.34733			
O -1.77866	0.92461	6.16732	C -3.34118	0.25648	-0.53252			
C 2.57550	2.38855	0.51572	C -0.79852	-3.48616	1.34177			
C 2.11309	-1.87282	2.63287	C -0.63459	3.24583	-1.10049			
O -1.04376	2.02569	3.30753	C 0.73577	-3.33863	-1.04091			
C 2.52295	-2.45178	0.23888	C -0.59437	-1.64230	-2.91207			
C 5.71934	-2.19650	5.03121	C -2.94018	-1.56028	1.11610			
C 1.40213	-3.37826	0.24957	C 7.00986	-0.70807	3.66535			
C 4.62075	-0.54516	3.87390	C -1.39325	3.27558	0.06906			
C 2.83300	-1.64843	1.36834	C -3.39005	-0.18782	0.80824			
C 3.38767	0.17983	-0.20409	C -1.33816	-2.43652	-2.03215			

NO@2a	C 2.09968	-0.77349	4.16276	C 2.48861	-2.25678	0.70280		
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O 0.00000	0.00000	0.00000	C -0.67231	2.99113	-1.48774	C 2.97800	0.24841	-1.87402
S 1.46353	-3.36041	3.47928	C -1.34549	-2.71522	-1.71396	C 0.59340	1.09711	-3.18949
O -0.70846	0.24939	4.65666	C -0.86019	-3.37279	-0.51363	C 2.15502	-0.71380	-2.57462
O -1.32410	-2.16226	4.13560	C -2.60335	1.68065	-1.44815	C 1.36136	2.01695	-2.46450
O -3.37267	-0.27409	4.59616	C 1.37434	-0.62805	5.49806	C 3.71327	0.34466	0.46345
O 0.64951	-1.67550	6.03738	C 0.99252	-2.71291	-1.74591	C 2.89515	-1.72330	-0.55484
N -5.47588	1.58771	3.07052	C 1.63164	2.74805	2.09536	C -0.79949	5.82415	2.95129
C -4.51061	2.43438	3.43161	C 0.90424	2.51767	3.34909	C 0.65222	7.46254	3.94776
C -3.21403	0.29819	3.54034	C 2.13399	-1.93219	-1.77485	C -0.44039	7.16066	3.13271
C -6.72361	2.04707	2.94777	C -0.53137	3.31211	0.97979	N 0.99005	5.12373	4.38613
C -2.36217	2.29652	2.24856	C -2.45659	-0.60490	-2.34770	H -1.36124	0.04984	5.34706
C -2.90455	1.75735	1.02516	C 3.46345	-0.24151	1.75026	H -0.99445	-1.25219	3.97336
C -3.07577	1.87033	3.50815	C -1.87793	-2.70297	3.00131	H 0.10031	-2.11214	5.35974
C -6.05850	4.26888	3.55411	C -1.28532	3.15348	-0.19174	H -7.48481	1.31710	2.64953
C -4.75501	3.79166	3.68439	C 2.86462	-1.51128	1.91946	H -6.28270	5.32193	3.74241
C -3.37166	0.37178	1.01672	C 0.52884	-3.29142	1.95780	H -3.93361	4.45017	3.97261
C -1.19146	3.02496	2.23365	C 3.08157	0.83940	2.62583	H -8.10426	3.71122	3.06481
C -2.49015	2.34825	-0.17025	C 1.33043	6.40228	4.55637	H -2.92967	2.25267	5.68437
C -0.40454	3.33513	3.49642	C 0.71197	2.97358	-1.57480	H -0.79606	3.42184	5.67137
C -3.11063	-1.65532	-0.35813	C -1.35372	-0.23857	-3.13392	H 0.32645	1.23608	6.15628
C -2.73618	-1.75482	2.08968	C 2.71384	2.33604	-0.57749	H 2.14952	-0.36646	6.24090
C -7.06984	3.38033	3.17817	C 0.92781	3.27583	0.91327	H -2.52953	-3.53836	3.31643
C -2.67128	-2.32616	0.77703	C 2.59090	1.59700	-1.82348	H 2.18714	6.59609	5.21232
C -3.46728	-0.26565	-0.23553	C -2.46167	-1.87110	-1.64123	H -1.64719	5.55195	2.32168
C 1.28155	-3.10949	0.71594	C 1.00181	-0.29867	-3.25124	H 0.97276	8.49343	4.11298
C -2.39733	2.41143	4.74332	C -0.19927	-1.12153	-3.21426	H -1.00660	7.95570	2.64074
C 2.32326	0.57396	3.73311	C -0.19301	-2.32401	-2.49905			
C -3.15771	-0.42489	2.22837	C 1.51405	3.13114	-0.37216			
C -1.53285	-3.20999	0.68817	C -0.86055	1.13015	-3.10464			
C -0.85816	-3.24137	1.94345	C 2.26909	-1.78196	3.23142			
C -1.22468	3.05013	4.73737	C 2.80942	2.00836	1.84376			
C -0.04282	4.83318	3.59097	C 0.58354	-3.30798	-0.49541			
C -3.08800	0.37971	-1.47966	C 3.48805	-0.39979	-0.67762			
C 0.51395	0.67593	5.22838	C 3.31204	1.74536	0.51830			

ON@2a	C 1.89586	-0.90695	4.13884	C 1.88430	-2.74786	0.83309		
O 0.00000	0.00000	1.14885	C 1.60709	1.44067	3.93144	C -1.03999	2.07843	-2.55359
N 0.00000	0.00000	0.00000	C -0.03431	2.85973	-1.85159	C 2.89040	-0.66462	-1.96102
S 0.67565	-3.33014	3.69275	C -1.99116	-2.53820	-1.55516	C 0.74178	0.58138	-3.36374
O -0.59920	0.76893	4.51859	C -1.64991	-3.17577	-0.29598	C 1.85967	-1.47362	-2.57474
O -1.76199	-1.47590	4.22076	C -2.21231	2.03206	-1.70318	C 1.70985	1.36430	-2.72239
O -3.31517	0.86356	4.49122	C 1.24208	-0.47929	5.45055	C 3.66379	-0.52661	0.36172
O 0.30625	-1.28060	6.07951	C 0.28561	-3.07129	-1.57259	C 2.38135	-2.43709	-0.46629
N -4.96297	3.01293	2.78743	C 2.20725	2.42491	1.75245	C 0.55785	6.03853	2.30812
C -3.82390	3.64419	3.07529	C 1.46544	2.48095	3.01763	C 2.35325	7.38606	3.17194
C -3.04893	1.28574	3.38732	C 1.57417	-2.57715	-1.66645	C 1.21414	7.26876	2.37333
C -6.07397	3.73373	2.61689	C 0.21289	3.36298	0.57744	N 2.15224	5.08117	3.82249
C -1.78219	2.90993	1.92267	C -2.60279	-0.29793	-2.38759	H -1.27087	0.79205	5.21929
C -2.45130	2.39906	0.75117	C 3.30862	-0.92162	1.69600	H -1.23653	-0.68290	3.98005
C -2.55552	2.77505	3.21162	C -2.43926	-1.97629	3.13578	H -0.33794	-1.64058	5.44173
C -4.90804	5.78858	3.02277	C -0.57480	3.27298	-0.57914	H -6.98685	3.17436	2.38236
C -3.74674	5.03837	3.20275	C 2.44022	-2.00129	1.97814	H -4.88209	6.87745	3.11430
C -3.22316	1.16272	0.86700	C -0.24175	-3.18673	2.16583	H -2.79185	5.51382	3.43422
C -0.47669	3.34878	1.84810	C 3.19505	0.29309	2.46566	H -7.03456	5.67406	2.57510
C -1.93067	2.76824	-0.49084	C 2.77676	6.25841	3.88164	H -2.29349	3.30965	5.34453
C 0.37889	3.58471	3.08216	C 1.30878	2.52102	-1.92892	H 0.05002	3.95434	5.23766
C -3.45051	-0.98632	-0.31444	C -1.45707	-0.26526	-3.19685	H 0.65496	1.62644	5.92776
C -3.07463	-0.94492	2.13538	C 3.12749	1.53716	-0.86441	H 2.06720	-0.33454	6.17127
C -6.10189	5.12597	2.72385	C 1.62476	2.99022	0.52267	H -3.25740	-2.61188	3.52102
C -3.15871	-1.63280	0.88086	C 2.82099	0.73542	-2.03764	H 3.66051	6.31017	4.52831
C -3.47938	0.45311	-0.32239	C -2.88556	-1.45974	-1.56772	H -0.33443	5.91104	1.69439
C 0.51428	-3.29662	0.91735	C 0.82095	-0.87018	-3.29341	H 2.90156	8.32749	3.24851
C -1.75307	3.25633	4.39619	C -0.53488	-1.39105	-3.18827	H 0.84011	8.12440	1.80521
C 2.41339	0.30924	3.58837	C -0.79166	-2.49295	-2.36558			
C -3.18076	0.45257	2.14831	C 2.14366	2.60042	-0.74080			
C -2.25055	-2.75544	0.88111	C -0.66521	0.95175	-3.29112			
C -1.58152	-2.82380	2.13806	C 1.81809	-2.00815	3.30549			
C -0.46599	3.60729	4.33900	C 3.18229	1.41690	1.57734			
C 1.07344	4.96323	3.04399	C -0.22904	-3.44025	-0.27476			
C -2.98122	0.87905	-1.61801	C 3.25811	-1.30054	-0.70725			
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O 0.00000	0.00000	0.00000	C -2.73058	1.12793	-1.62610	C 1.64273	2.47020	-1.81553
S 3.31594	-0.70416	3.75161	C 1.49179	-2.76786	-1.50409	C -0.36689	0.99281	-3.20060
O -0.73928	-0.28995	4.18326	C 2.23104	-2.72131	-0.25343	C 1.97654	1.21701	-2.45658
O 0.72461	-2.51712	4.37885	C -2.80209	-1.20171	-1.51687	C -0.70053	2.17613	-2.53005
O -1.92538	-2.81193	4.61654	C 0.93358	0.83303	5.52159	C 1.86343	3.20473	0.51403
O 1.35199	-0.35831	6.09708	C 2.85797	-0.86937	-1.50449	C 3.10185	1.28723	-0.36508
N -4.62252	-3.43743	3.03955	C -1.39445	3.00653	1.97197	C -5.39686	2.70956	2.66671
C -4.74236	-2.14640	3.35410	C -1.70470	2.32822	3.22918	C -6.00275	4.86566	3.54128
C -2.26531	-2.36102	3.53648	C 2.89796	0.51063	-1.57487	C -6.32533	3.74558	2.77249
C -5.72805	-4.17626	2.91507	C -3.03513	1.50758	0.81982	N -3.86844	3.90004	4.08009
C -3.32673	-0.53755	2.14426	C -0.82825	-2.45273	-2.28505	H -0.07536	-0.98137	4.36122
C -3.15786	-1.32593	0.94855	C 2.11806	2.71060	1.83784	H -0.11342	-2.85552	4.77176
C -3.43721	-1.32485	3.43508	C 0.90895	-3.18941	3.17141	H 1.64762	-0.98709	5.41703
C -7.13901	-2.30570	3.42218	C -3.28338	0.76524	-0.34305	H -5.58221	-5.23127	2.65707
C -5.98660	-1.53232	3.55477	C 2.77570	1.48214	2.08625	H -8.12509	-1.85794	3.57111
C -2.32507	-2.52388	1.00823	C 2.79538	-1.47365	2.22921	H -6.03746	-0.47210	3.80773
C -3.24576	0.83851	2.08581	C 0.97460	3.07932	2.64082	H -7.88855	-4.30136	2.98331
C -3.33595	-0.68029	-0.27809	C -4.75904	4.88864	4.17910	H -3.65867	-0.91867	5.59671
C -3.11910	1.70533	3.32408	C -1.90329	2.23818	-1.70712	H -3.45856	1.50436	5.49802
C -0.47376	-3.55679	-0.24989	C -0.43227	-1.36483	-3.07693	H -1.24218	0.78643	5.89414
C -0.31107	-3.28149	2.20117	C -0.27242	3.52637	-0.66229	H 1.01554	1.61200	6.30074
C -7.01251	-3.65919	3.09624	C -2.16188	2.68163	0.75633	H 1.21974	-4.23256	3.38195
C 0.26378	-3.58421	0.92610	C 0.32335	2.94890	-1.85647	H -4.46992	5.74540	4.79919
C -1.80919	-3.01670	-0.20686	C 0.15297	-3.18276	-1.50581	H -5.61423	1.81994	2.07452
C 3.17482	-0.79055	0.98577	C 1.00398	0.50458	-3.16818	H -6.69629	5.70245	3.64808
C -3.49511	-0.41964	4.63923	C 0.96277	-0.94884	-3.08863	H -7.28717	3.67948	2.25758
C 0.67886	2.35248	3.76388	C 1.89700	-1.62635	-2.29690			
C -1.61912	-2.79639	2.26172	C -1.62963	3.02439	-0.51502			
C 1.64231	-3.15540	0.92202	C -1.25069	-0.16279	-3.12744			
C 1.97224	-2.59120	2.19844	C 2.56457	0.88901	3.40591			
C -3.37787	0.90859	4.58590	C -0.08615	3.51365	1.77714			
C -4.16970	2.83535	3.33292	C 3.01456	-1.50762	-0.21830			
C -2.04019	-2.36166	-1.48152	C 2.39594	2.54270	-0.57437			
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ON@2b	C 1.55316	1.42610	4.16279	C 3.23054	0.67045	0.86889		
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S 3.26355	-0.67443	3.72142	C 1.54712	-2.81924	-1.53825	C -0.25359	0.92082	-3.33966
O -0.78615	-0.22958	4.02626	C 2.25741	-2.75418	-0.27205	C 2.07283	1.14708	-2.54684
O 0.64707	-2.46465	4.31939	C -2.73484	-1.23523	-1.67390	C -0.59587	2.11698	-2.69682
O -2.00194	-2.74171	4.50546	C 0.84858	0.90022	5.40701	C 1.90395	3.18569	0.38573
O 1.25071	-0.28104	6.01366	C 2.92177	-0.92695	-1.53970	C 3.15167	1.24810	-0.43226
N -4.67267	-3.38497	2.89024	C -1.38586	3.03078	1.77431	C -5.40466	2.75310	2.38219
C -4.78950	-2.08504	3.16648	C -1.72720	2.37539	3.03529	C -6.03011	4.92004	3.21541
C -2.31781	-2.31375	3.40850	C 2.97043	0.45162	-1.63271	C -6.33471	3.79077	2.45282
C -5.78113	-4.11787	2.75664	C -3.00439	1.51580	0.61186	N -3.91004	3.96034	3.81724
C -3.33438	-0.50726	1.96283	C -0.75194	-2.50730	-2.37664	H -0.14358	-0.93101	4.24098
C -3.14498	-1.31750	0.78500	C 2.12681	2.71370	1.72327	H -0.20221	-2.79217	4.69796
C -3.48022	-1.27202	3.26334	C 0.85720	-3.16065	3.12855	H 1.54376	-0.92857	5.35035
C -7.18845	-2.22279	3.17542	C -3.22971	0.75386	-0.54316	H -5.63796	-5.18078	2.53167
C -6.03308	-1.45563	3.31773	C 2.77364	1.48723	2.00748	H -8.17404	-1.76313	3.28641
C -2.32297	-2.52064	0.88301	C 2.77135	-1.46671	2.20141	H -6.08138	-0.38848	3.54032
C -3.24473	0.86796	1.88335	C 0.96825	3.10263	2.49423	H -7.94370	-4.22356	2.77100
C -3.29151	-0.69050	-0.45541	C -4.80207	4.95037	3.88270	H -3.74669	-0.82831	5.41243
C -3.14457	1.75569	3.10912	C -1.81606	2.19896	-1.90221	H -3.53333	1.59174	5.27767
C -0.44956	-3.58095	-0.31674	C -0.33325	-1.43468	-3.17767	H -1.33505	0.85396	5.72068
C -0.34179	-3.26824	2.13325	C -0.20285	3.49767	-0.84331	H 0.91063	1.69159	6.17530
C -7.06530	-3.58573	2.88993	C -2.12649	2.68661	0.54747	H 1.16144	-4.19950	3.36717
C 0.26049	-3.59143	0.87624	C 0.41617	2.89641	-2.01348	H -4.52724	5.81476	4.49870
C -1.78277	-3.03478	-0.31273	C 0.20730	-3.22888	-1.56347	H -5.60848	1.85651	1.79573
C 3.18325	-0.80678	0.95564	C 1.11339	0.42684	-3.26797	H -6.72572	5.75807	3.29565
C -3.55986	-0.34627	4.45050	C 1.06319	-1.02489	-3.16485	H -7.28401	3.71861	1.91591
C 0.64409	2.39616	3.62250	C 1.97539	-1.69311	-2.34072			
C -1.64888	-2.77851	2.15669	C -1.56516	3.00445	-0.71779			
C 1.63964	-3.16561	0.89631	C -1.14387	-0.22980	-3.26690			
C 1.94254	-2.58055	2.16997	C 2.52919	0.91666	3.33142			
C -3.43404	0.98031	4.37782	C -0.07075	3.52702	1.59986			
C -4.19390	2.88653	3.07630	C 3.04597	-1.54363	-0.23947			
C -1.98112	-2.39868	-1.60249	C 2.45745	2.50322	-0.67888			
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3.15398	-1.75378	3.54495	1.78071	-1.92547	-2.22537	-0.12148	2.15184	-2.69745
-0.92629	-1.65142	3.65897	2.42207	-2.29186	-0.97552	2.14876	2.15407	-1.72749
0.59726	-3.74473	3.33655	-2.57249	-0.53185	-2.08164	-0.55809	3.02707	-1.69484
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1.00682	-2.29939	5.68171	3.05547	-0.11385	-1.47189	3.12201	1.52898	0.34757
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-3.41512	-1.17504	1.52068	-0.48647	-1.40699	-3.04651	-0.60211	-1.09837	2.92828
-3.11180	-1.50344	0.14941	1.91404	2.08285	2.81700	-0.10586	-3.07224	3.47595
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-6.17001	-2.65526	2.39827	2.61842	0.86222	2.68411	-8.29722	-3.00212	2.21041
-2.22939	-2.63603	-0.12265	2.76516	-1.95528	1.81638	-6.26130	-1.83945	3.11681
-3.37963	0.13808	1.94651	0.69580	2.12015	3.59521	-7.97808	-4.87501	0.54837
-3.22358	-0.47719	-0.79164	-5.17724	3.21109	5.16438	-3.98836	-2.73840	4.58090
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-0.23540	-3.12950	-1.47634	-0.08495	-0.10689	-3.38971	-1.63587	-1.29575	5.54245
-0.27676	-3.69879	0.94127	-0.33056	3.65648	0.55264	0.50936	-0.54168	6.48517
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3.19968	-0.88300	0.91306	1.26474	1.70880	-2.71759	-7.11837	4.10803	4.81409
-3.77915	-1.93233	3.87415	1.28589	0.31542	-3.14176	-7.55993	2.63757	2.80998
0.35807	1.03621	4.36421	2.18922	-0.57412	-2.55023			
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1.76094	-3.09862	-0.06293	-0.95266	1.02474	-3.09948			
1.97799	-2.99768	1.34596	2.34629	-0.16107	3.69432			
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C -3.12006	-1.48002	0.23856	C 1.92520	2.16241	2.78025	H -0.11647	-2.96745	3.61053
C -3.62852	-2.25875	2.55381	C 0.85527	-3.84605	2.15551	H 1.20817	-2.59350	4.95629
C -7.30916	-3.20778	2.04359	C -3.22831	0.91072	-0.33882	H -5.66394	-5.45737	0.09520
C -6.17913	-2.54818	2.52835	C 2.62477	0.93580	2.68484	H -8.30812	-2.89236	2.35568
C -2.24299	-2.62453	0.00048	C 2.76220	-1.90757	1.90659	H -6.26560	-1.70983	3.22109
C -3.37982	0.21894	1.98318	C 0.70907	2.23022	3.55947	H -7.99991	-4.81733	0.75253
C -3.22876	-0.48367	-0.73451	C -5.15452	3.38623	5.12742	H -3.99373	-2.57190	4.70785
C -3.36905	0.64579	3.43977	C -1.81190	2.75929	-1.05441	H -3.82511	-0.24339	5.41032
C -0.25417	-3.16937	-1.34102	C -0.09476	-0.20949	-3.34938	H -1.63336	-1.10946	5.62216
C -0.29223	-3.66080	1.09400	C -0.31605	3.67659	0.47300	H 0.51977	-0.33632	6.53449
C -7.14308	-4.27329	1.15561	C -2.27026	2.40120	1.39466	H 1.19559	-4.89346	2.05150
C 0.38845	-3.53088	-0.16351	C 0.38779	3.51721	-0.78967	H -4.92674	4.01701	5.99462
C -1.61218	-2.69807	-1.25566	C 0.44810	-2.41538	-2.36642	H -5.79648	1.09208	2.14193
C 3.19821	-0.86548	0.96950	C 1.26439	1.62063	-2.73734	H -7.09052	4.28692	4.75832
C -3.78256	-1.78919	3.97586	C 1.27833	0.21446	-3.11744	H -7.54070	2.77746	2.78553
C 0.36850	1.17310	4.36341	C 2.17907	-0.66008	-2.50015			
C -1.63255	-3.26779	1.16880	C -1.65924	3.13373	0.34278			
C 1.74590	-3.10302	0.06665	C -0.95664	0.93466	-3.09321			
C 1.96796	-2.95958	1.47116	C 2.35000	-0.05381	3.72747			
C -3.68175	-0.51539	4.36166	C -0.30543	2.89470	2.79103			
C -4.45394	1.70237	3.73110	C 3.14386	-1.17508	-0.40548			
C -1.77346	-1.68205	-2.28026	C 2.37961	2.76887	0.46641			
C -0.87556	-0.72304	4.93758	C 0.35914	3.50317	1.66576			

NO@2d			1.71552	1.27401	4.19358		3.24033	0.75706	0.77680
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0.00000	0.00000	0.00000	-2.81511	1.14152	-1.53636		1.51639	2.59097	-1.83469
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-4.54302	-3.52337	2.84868	-1.39512	2.92399	2.07509		-5.37153	2.52464	2.91766
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2.12856	-2.57572	1.98269	2.66270	0.84373	3.28925				
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ON@2d			1.76821	1.31157	4.15858	3.25243	0.76318	0.73061
0.00000	0.00000	1.14803	-0.52692	1.90398	4.12524	-2.51946	-0.06225	-2.29507
0.00000	0.00000	0.00000	-2.82676	1.12932	-1.52049	1.50130	2.57390	-1.87916
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0.98981	-2.52854	4.22986	-2.84234	-1.20390	-1.46324	-0.86563	2.24439	-2.49064
-1.81410	-3.04203	4.57552	1.16178	0.74520	5.43392	1.81565	3.25128	0.45678
1.58682	-0.49892	5.92020	2.80754	-0.74246	-1.71675	3.05899	1.39194	-0.53391
-4.51304	-3.49473	2.92668	-1.36619	2.94216	2.05854	-5.33052	2.56013	2.94978
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-3.17687	0.74643	2.19978	1.02671	3.04071	2.61499	-7.77402	-4.37229	3.03525
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-6.88908	-3.74497	3.16206	-2.18526	2.63906	0.87074	1.47177	-4.21627	3.18946
0.38758	-3.54327	0.79184	0.17183	3.02278	-1.84531	-4.30606	5.60560	5.02342
-1.74554	-3.01933	-0.23644	0.15550	-3.10993	-1.62806	-5.57385	1.66648	2.37355
3.26469	-0.71568	0.75114	0.84279	0.62742	-3.24913	-6.59894	5.53856	4.01255
-3.29137	-0.57989	4.72687	0.83790	-0.82857	-3.20545	-7.25362	3.50813	2.66151
0.79655	2.27300	3.72511	1.82424	-1.50339	-2.47784			
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2.14917	-2.55870	1.97874	2.70540	0.87357	3.24769			
-3.19422	0.75093	4.70678	-0.08001	3.48014	1.81584			
-4.06518	2.70013	3.53727	3.04817	-1.40871	-0.45853			
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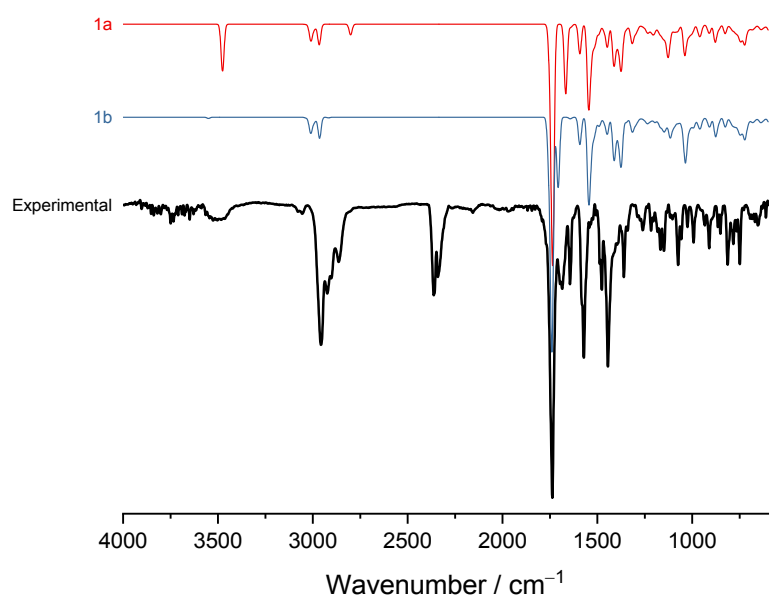


Figure S5. Experimental and simulated IR spectra for **1**.

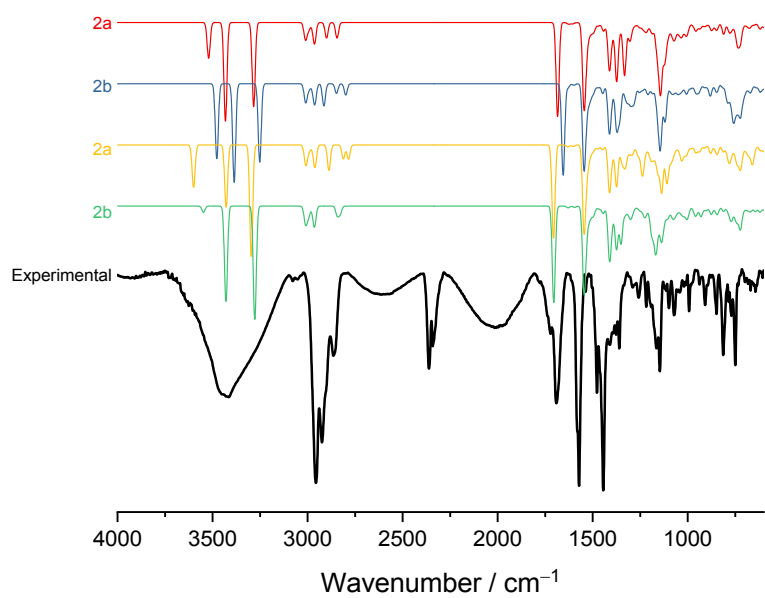


Figure S6. Experimental and simulated IR spectra for **2**.

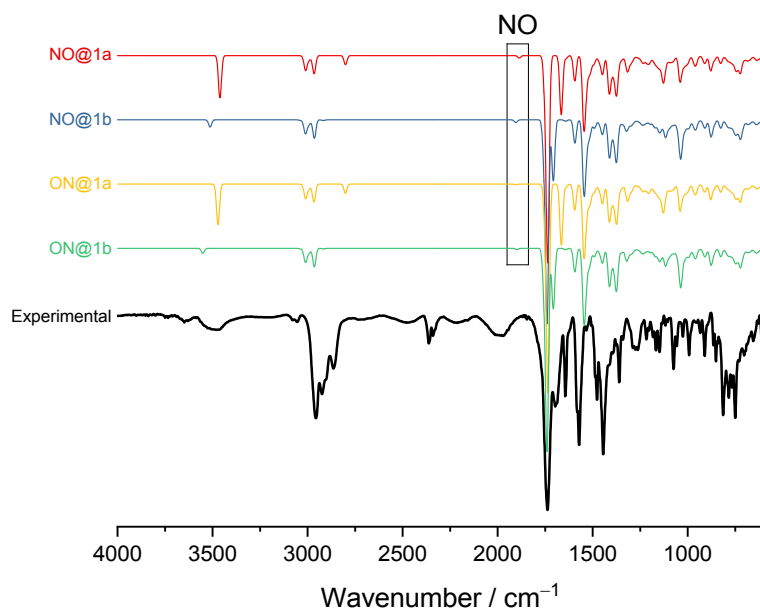


Figure S7. Experimental and simulated IR spectra for (NO)@1.

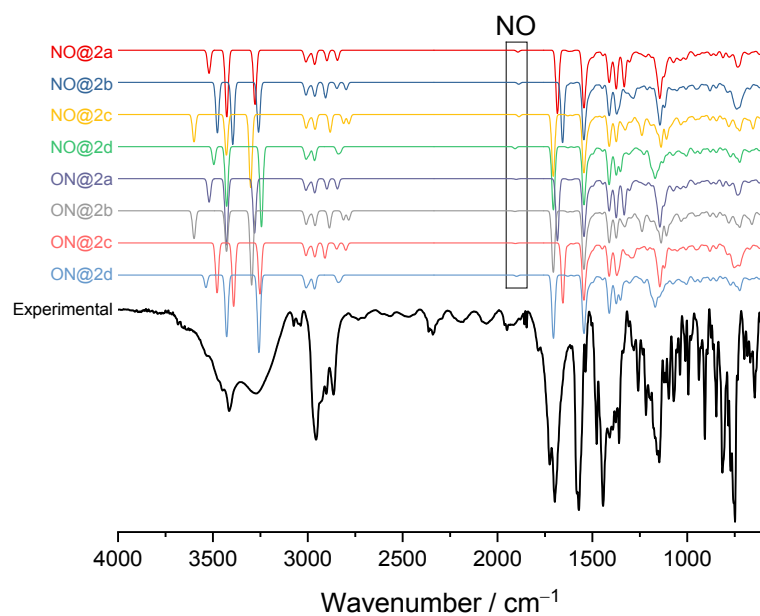


Figure S8. Experimental and simulated IR spectra for (NO)@2.

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