# Supplementary Information

## Insight into the mechanism of boron-doping of carbon aerogel for enhancing the activity of low-temperature selective catalytic reduction of NO with $NH_3$

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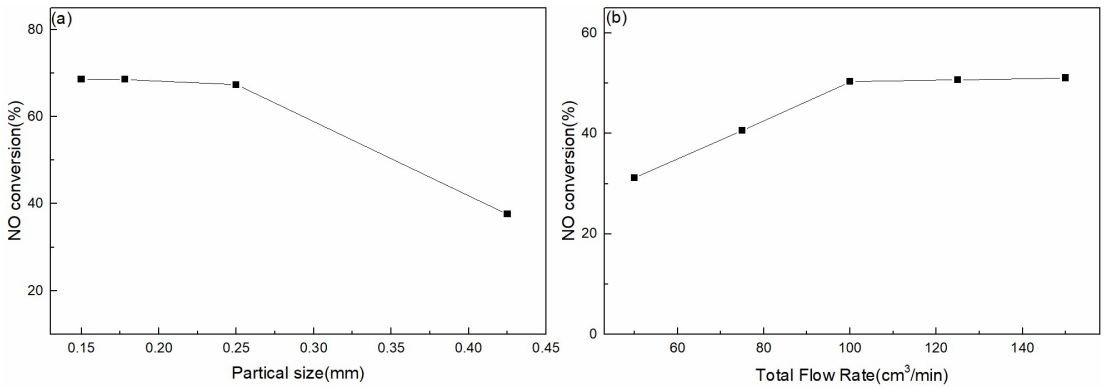


**Fig. S1.** (a) Eliminate internal diffusion by changing the catalyst pellets size (b) Eliminate external diffusion by changing the flow rate and volume of catalyst. Reaction conditions: [NO] = 500 ppm, [$NH_3$] = 500 ppm, [$O_2$] = 5%, $N_2$ balance, T = 200 ℃, GHSV = 2000 $h^{-1}$.

## S2. Mears Criterion for External Diffusion and Internal Diffusion

### Mears Criterion for External Diffusion (Fogler, p841; Mears, 1971)

If $\frac{-r_A'\rho_b Rn}{k_c C_{Ab}} < 0.15$, then external mass transfer effects can be neglected.

$-r_A'$ = reaction rate, kmol/kg-cat · s

n = reaction order

R = catalyst particle radius, m

$\rho_b$ = bulk density of catalyst bed, kg/$m^3$

=(1-ϕ) (ϕ= porosity or void fraction of packed bed)

$C_{Ab}$ = bulk gas concentration of A, kmol/$m^3$

$k_c$ = mass transfer coefficient, m/s

$\frac{-r_A'\rho_b Rn}{k_c C_{Ab}}$ = [1.33 x $10^{-7}$ kmol-$C_3$/kg-cat. s] [400 kg/$m^3$][ 1.3 x $10^{-5}$ m][1]/([ 8.306 m/s]*[ 0.005 kmol/$m^3$])=**1.148x$10^{-6}$ <0.15 {Mears for External Diffusion}**

### Weisz-Prater Criterion for Internal Diffusion (Fogler, p839)

If $C_{WP} = \frac{-r'_{A(obs)}\rho_c R^2}{D_e C_{As}} < 1$, then internal mass transfer effects can be neglected.

$-r'_{A(obs)}$ =observed reaction rate, kmol/kg-cat · s

R = catalyst particle radius, m

$\rho_c$ = solid catalyst density, kg/m$^3$; [$\rho_{c,\ anatase\ or\ rutile}$ = 4000 kg/m$^3$]

$D_e$ = effective gas-phase diffusivity, m$^2$/s **[Fogler, p815]**

$$= \frac{D_{AB}\varphi_p\sigma_c}{\tau}$$ where

$D_{AB}$ = gas-phase diffusivity m$^2$/s; $\varphi_p$= pellet porosity; $\sigma_c$=constriction factor; $\tau$ =tortuosity.

$C_{As}$ = gas concentration of A at the catalyst surface, kmol-A/m$^3$

$$C_{WP} = \frac{-r'_{A(obs)}\rho_c R^2}{D_e C_{As}}$$ = [1.33 x 10$^{-7}$ kmol-C$^3$/kg-cat . s] × [ 2.34×10$^5$ kg-cat/m$^3$] × [ 1.3 x 10$^{-5}$ m]$^2$ / ([5.76 x 10$^{-5}$ m$^2$/s] × [0.005 kmol-C3/m$^3$]) = **1.83 x 10$^{-5}$ < 1**

**{Weisz-Prater Criterion for Internal Diffusion}**

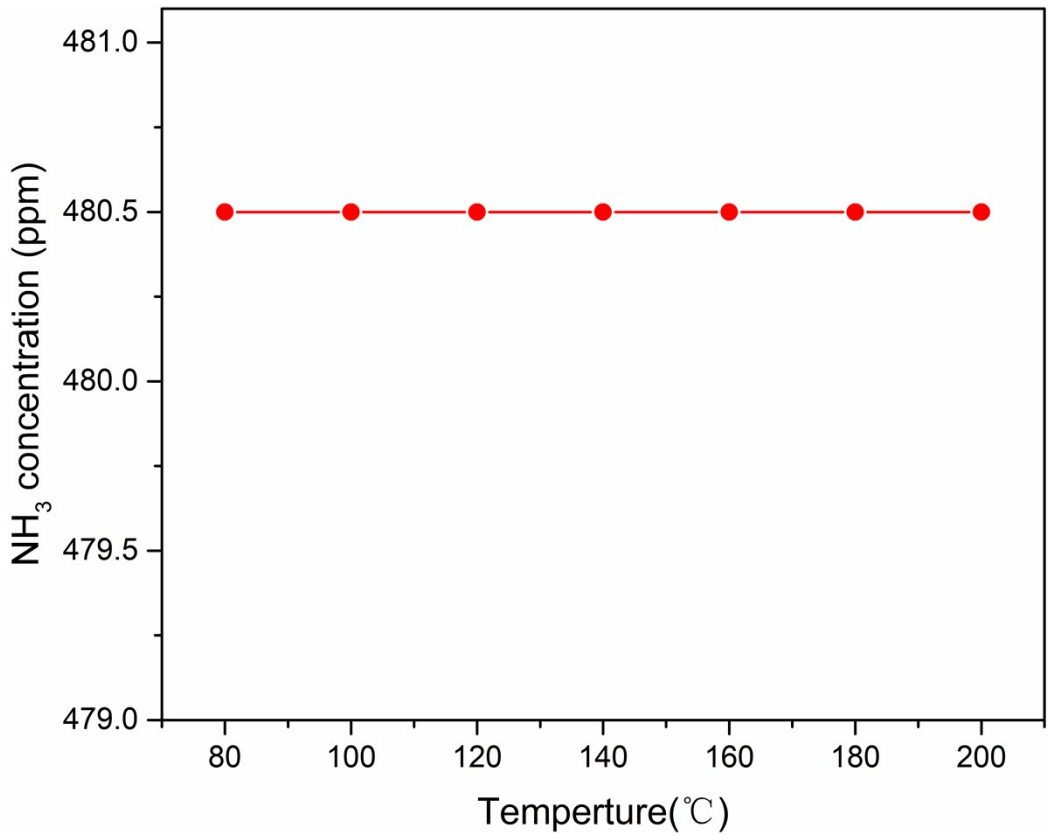


Fig. S3. $NH_3$ concentration curve of B-CA sample catalyst under $NH_3$+$O_2$. (reaction conditions: [$NH_3$] = 500 ppm, [$O_2$] = 5%, $N_2$ balance, GHSV = 2000 h$^{-1}$).

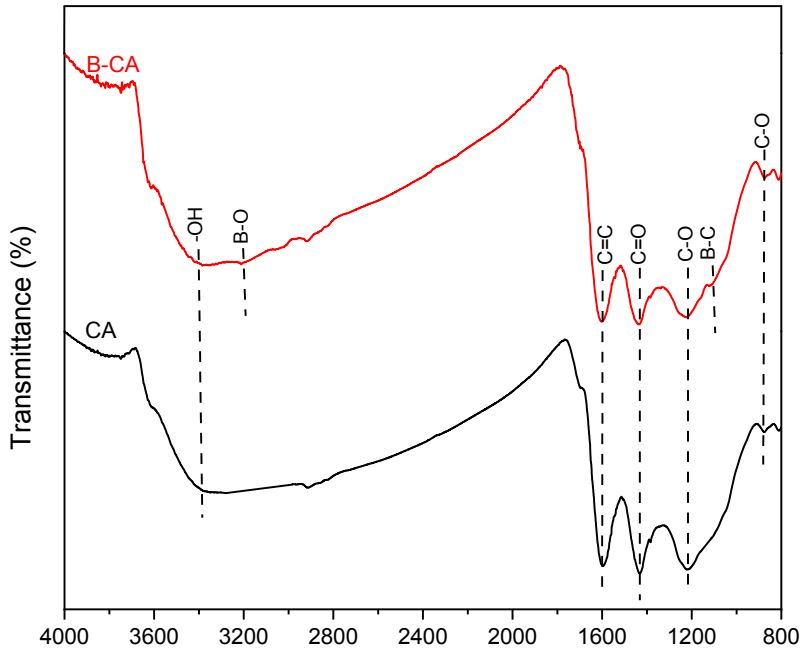


Fig. S4. FTIR spectra of CA and B-CA.

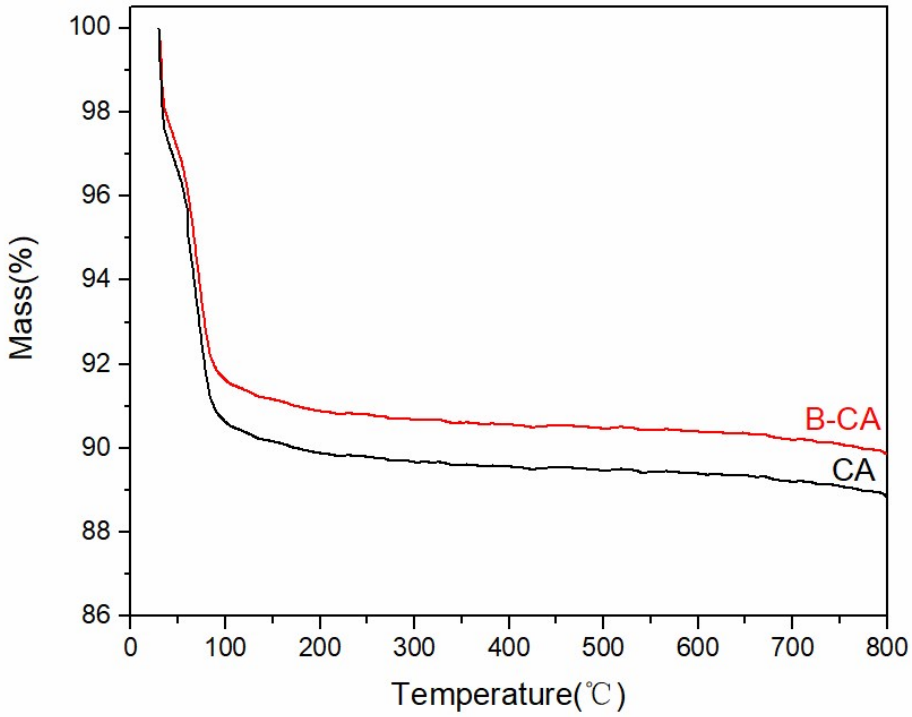


Fig. S5. The Thermogravimetry (TG) curves of sample B-CA and CA.

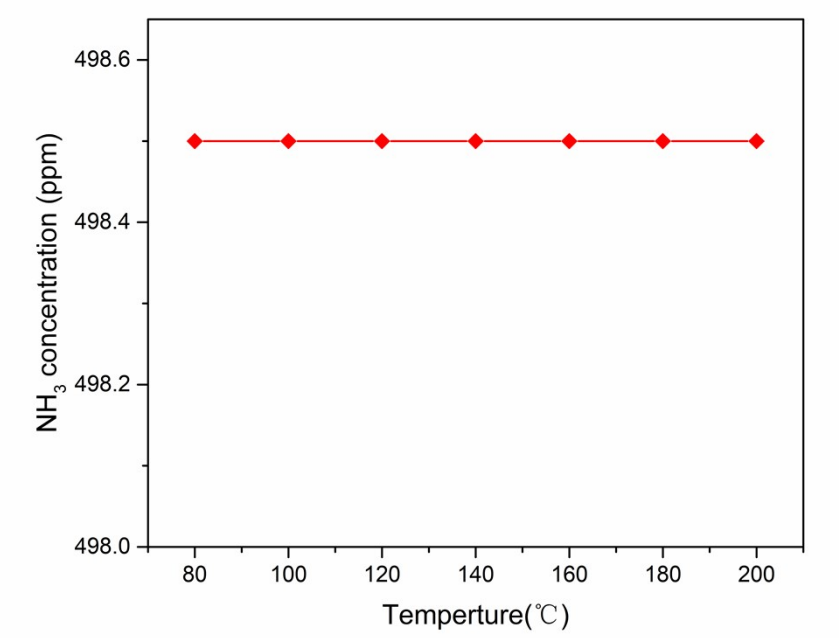


Fig. S6. $NH_3$ concentration curve of B-CA sample catalyst under $NH_3$+$O_2$. (reaction conditions: [$NH_3$] = 500 ppm, [$O_2$] = 5%, $N_2$ balance, GHSV = 2000 $h^{-1}$).

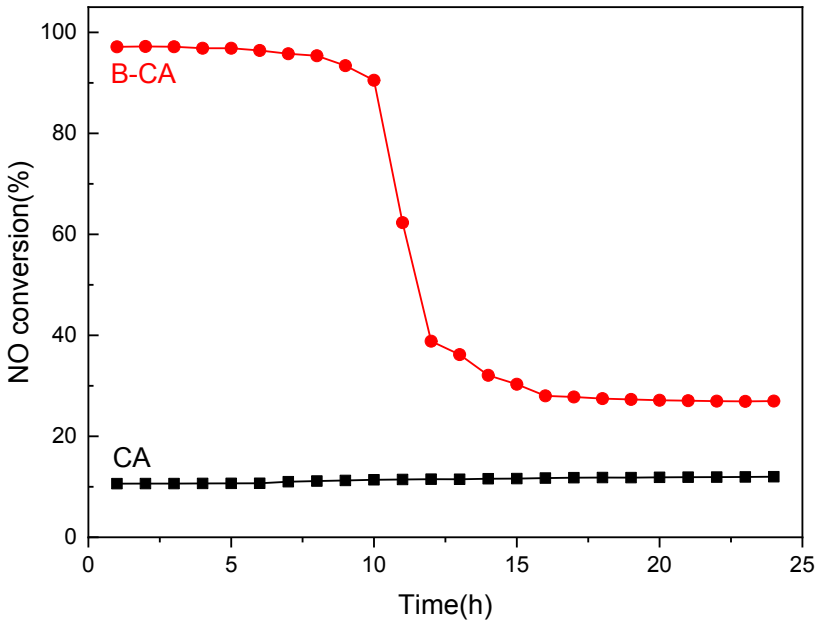


**Fig. S7.** Stability test of $NH_3$-SCR for the CA and B-CA sample.

**S8.** Archive entries for the calculations of the geometric model of stable adsorption of $NH_3$, NO, $O_2$ at different adsorption sites of BC3, BC2O, BCO2 on BCA.

BC3-$O_2$:

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Title Card Required

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| C | 3.23923800 | 4.90454400 | 0.06153500 |
| C | 5.33091400 | 3.59067400 | 0.06210600 |
| C | 7.42375400 | 2.27761600 | 0.06109200 |
| C | 9.52156500 | 0.95903300 | 0.05896800 |
| C | -0.20465600 | 6.28365500 | 0.04651400 |
| C | -1.00360700 | 5.08306800 | 0.02228700 |
| C | 1.85650100 | 4.97427100 | 0.04934700 |
| C | 1.08083600 | 3.75809500 | 0.02552700 |
| C | 3.93300200 | 3.66396500 | 0.05058800 |
| C | 3.16517300 | 2.44609600 | 0.02646600 |
| C | 6.01786400 | 2.35589500 | 0.05001700 |
| C | 5.25282400 | 1.13629800 | 0.02513000 |
| C | 8.10286200 | 1.04331400 | 0.04801100 |
| C | 7.34296300 | -0.17195100 | 0.02256200 |
| C | 10.16576400 | -0.27527400 | 0.04517500 |
| C | 9.43552700 | -1.46073600 | 0.02012900 |
| C | -2.38654300 | 5.11787700 | 0.00728800 |
| C | -3.16996700 | 3.93286000 | -0.01672900 |
| C | -0.32750700 | 3.81023900 | 0.01253900 |
| C | -1.09393900 | 2.60317200 | -0.00964600 |
| C | 1.75127200 | 2.49803600 | 0.01476200 |
| C | 0.98988500 | 1.28844400 | -0.00826000 |
| C | 3.83466000 | 1.18855000 | 0.01404200 |
| C | 3.07530200 | -0.01919200 | -0.01014800 |
| C | 5.92202700 | -0.12056500 | 0.01148500 |
| C | 5.16332500 | -1.32601400 | -0.01380800 |
| C | 8.01518300 | -1.43917100 | 0.00823100 |
| C | 7.24896800 | -2.62052300 | -0.01742500 |
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| C | -5.34335900 | 2.79226700 | -0.06566600 |
| C | -2.50620300 | 2.65408400 | -0.02280300 |
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| C | -1.18866100 | 0.13325100 | -0.03976400 |
| C | 1.65618500 | 0.03011600 | -0.01999300 |
| C | 0.89415300 | -1.17682300 | -0.04249900 |
| C | 3.74744000 | -1.27749600 | -0.02404100 |
| C | 2.98810100 | -2.48328600 | -0.04990000 |
| C | 5.83920700 | -2.59677600 | -0.02903500 |
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| C | -6.73970700 | 2.84236500 | -0.09836700 |

| | | | |
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| C | -2.60884600 | 0.18537500 | -0.04779600 |
| C | -3.38956600 | -1.01446900 | -0.04326500 |
| C | -0.52252700 | -1.12784300 | -0.04842400 |
| C | -1.28991300 | -2.34197800 | -0.07045600 |
| C | 1.57206600 | -2.43611100 | -0.05861400 |
| C | 0.81696500 | -3.64507000 | -0.08730800 |
| C | 3.66740500 | -3.75145600 | -0.06708200 |
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| C | -7.77367900 | -0.75651200 | -0.23923200 |
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| C | 1.50828200 | -4.91295200 | -0.10703600 |
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| C | -9.14970800 | -0.58343200 | -0.34515600 |
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| C | -4.82901700 | -3.57201800 | -0.17678900 |
| C | -2.71584300 | -4.77967200 | -0.13208800 |
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| H | 9.94630700 | -2.41988900 | 0.00942800 |
| H | 7.75922300 | -3.58089500 | -0.02866000 |
| H | 5.57964900 | -4.73854200 | -0.06822600 |
| H | 3.40714800 | -5.89760900 | -0.10957000 |
| H | 1.25866200 | -7.07482400 | -0.15222600 |
| H | -9.77682700 | -1.46770300 | -0.43029800 |
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| H | -5.30754100 | -4.55188500 | -0.19503200 |
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| H | -7.23061500 | 3.81326300 | -0.10297200 |
| H | -9.38605800 | 2.80218200 | -0.22355400 |
| H | -10.82873300 | 0.78472700 | -0.39858100 |
| H | -0.72015900 | 7.24082900 | 0.05427500 |
| H | 11.25164900 | -0.31380000 | 0.05403800 |

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| H | 8.00254600 | 3.19811000 | 0.08017600 |
| H | 10.10073300 | 1.87845100 | 0.07842100 |
| H | 1.73799700 | 7.14790900 | 0.07788100 |
| H | 3.81949400 | 5.82450800 | 0.07980400 |
| H | 5.90878600 | 4.51184800 | 0.08066600 |
| B | -5.65489500 | -2.26704900 | 0.09740600 |
| O | -6.06165500 | -2.66901100 | 1.55279600 |
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BC3-NO:

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| C | 5.33091400 | 3.59067400 | 0.06210600 |
| C | 7.42375400 | 2.27761600 | 0.06109200 |
| C | 9.52156500 | 0.95903300 | 0.05896800 |
| C | -0.20465600 | 6.28365500 | 0.04651400 |
| C | -1.00360700 | 5.08306800 | 0.02228700 |
| C | 1.85650100 | 4.97427100 | 0.04934700 |
| C | 1.08083600 | 3.75809500 | 0.02552700 |
| C | 3.93300200 | 3.66396500 | 0.05058800 |
| C | 3.16517300 | 2.44609600 | 0.02646600 |
| C | 6.01786400 | 2.35589500 | 0.05001700 |
| C | 5.25282400 | 1.13629800 | 0.02513000 |
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| C | 7.34296300 | -0.17195100 | 0.02256200 |
| C | 10.16576400 | -0.27527400 | 0.04517500 |
| C | 9.43552700 | -1.46073600 | 0.02012900 |
| C | -2.38654300 | 5.11787700 | 0.00728800 |
| C | -3.16996700 | 3.93286000 | -0.01672900 |
| C | -0.32750700 | 3.81023900 | 0.01253900 |
| C | -1.09393900 | 2.60317200 | -0.00964600 |
| C | 1.75127200 | 2.49803600 | 0.01476200 |
| C | 0.98988500 | 1.28844400 | -0.00826000 |
| C | 3.83466000 | 1.18855000 | 0.01404200 |
| C | 3.07530200 | -0.01919200 | -0.01014800 |
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| C | 7.24896800 | -2.62052300 | -0.01742500 |
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| C | -5.34335900 | 2.79226700 | -0.06566600 |
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| C | 1.65618500 | 0.03011600 | -0.01999300 |
| C | 0.89415300 | -1.17682300 | -0.04249900 |
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| C | 2.98810100 | -2.48328600 | -0.04990000 |
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| C | 5.06972400 | -3.77807200 | -0.05579600 |
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| C | -1.33696200 | -4.83437700 | -0.12829500 |
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| C | 0.72981900 | -6.12537200 | -0.13785700 |
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| C | -4.82901700 | -3.57201800 | -0.17678900 |
| C | -2.71584300 | -4.77967200 | -0.13208800 |
| C | -0.62518400 | -6.08685800 | -0.14882600 |
| H | 9.94630700 | -2.41988900 | 0.00942800 |
| H | 7.75922300 | -3.58089500 | -0.02866000 |
| H | 5.57964900 | -4.73854200 | -0.06822600 |
| H | 3.40714800 | -5.89760900 | -0.10957000 |
| H | 1.25866200 | -7.07482400 | -0.15222600 |
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| H | -5.30754100 | -4.55188500 | -0.19503200 |
| H | -3.28784300 | -5.70439100 | -0.15317400 |
| H | -1.20705200 | -7.00465000 | -0.17167000 |
| H | -2.89811000 | 6.07782200 | 0.01326000 |
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| H | -7.23061500 | 3.81326300 | -0.10297200 |
| H | -9.38605800 | 2.80218200 | -0.22355400 |
| H | -10.82873300 | 0.78472700 | -0.39858100 |
| H | -0.72015900 | 7.24082900 | 0.05427500 |
| H | 11.25164900 | -0.31380000 | 0.05403800 |
| H | 8.00254600 | 3.19811000 | 0.08017600 |
| H | 10.10073300 | 1.87845100 | 0.07842100 |
| H | 1.73799700 | 7.14790900 | 0.07788100 |
| H | 3.81949400 | 5.82450800 | 0.07980400 |
| H | 5.90878600 | 4.51184800 | 0.08066600 |
| B | -5.65489500 | -2.26704900 | 0.09740600 |
| O | -6.06165500 | -2.66901100 | 1.55279600 |
| O | -7.46225100 | -2.77121300 | 1.12257500 |

BC3-$NH_3$:

# opt freq ub3lyp/6-31g(d) scf=(maxcycle=500,xqc)

Title Card Required

0 2

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| C | -7.26592000 | 2.37243100 | 0.10935200 |
| C | -9.38742900 | 1.09288400 | 0.11822000 |
| C | 0.43190500 | 6.24356200 | 0.05772600 |
| C | 1.20985600 | 5.02955900 | 0.01484800 |
| C | -1.65235100 | 4.97036800 | 0.06660700 |
| C | -0.89842000 | 3.74090300 | 0.02373800 |
| C | -3.75160400 | 3.69630900 | 0.07557700 |
| C | -3.00599200 | 2.46529100 | 0.03272200 |
| C | -5.85914400 | 2.42510900 | 0.08456800 |
| C | -5.11652600 | 1.19263300 | 0.04165000 |
| C | -7.96759400 | 1.15077300 | 0.09334600 |
| C | -7.22974600 | -0.07772300 | 0.05055300 |
| C | -10.05341200 | -0.12965300 | 0.10148900 |
| C | -9.34483000 | -1.32787500 | 0.05992500 |
| C | 2.59267300 | 5.04112600 | -0.01060100 |
| C | 3.35756700 | 3.84298700 | -0.05278400 |
| C | 0.51016800 | 3.76857400 | -0.00167100 |
| C | 1.25462900 | 2.54883400 | -0.04403600 |
| C | -1.59120100 | 2.49262400 | 0.00725300 |

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| C | -5.80833200 | -0.05206500 | 0.02493000 |
| C | -5.07184100 | -1.27114700 | -0.01758900 |
| C | -7.92449500 | -1.33294000 | 0.03357800 |
| C | -7.17998700 | -2.52767500 | -0.00854200 |
| C | 4.75248700 | 3.85914200 | -0.07842500 |
| C | 5.51213200 | 2.66586900 | -0.12031900 |
| C | 2.66854900 | 2.57537800 | -0.06944900 |
| C | 3.41109700 | 1.35660400 | -0.11148300 |
| C | 0.56656100 | 1.29637000 | -0.06064000 |
| C | 1.30510500 | 0.07691700 | -0.10294300 |
| C | -1.54125600 | 0.02385600 | -0.05185300 |
| C | -0.80205500 | -1.19652000 | -0.09441400 |
| C | -3.65518800 | -1.24770000 | -0.04310800 |
| C | -2.91824900 | -2.46612500 | -0.08566600 |
| C | -5.76978800 | -2.52978200 | -0.03460700 |
| C | -5.02085400 | -3.72403300 | -0.07682200 |
| C | 6.91054600 | 2.68363800 | -0.14577900 |
| C | 7.66859000 | 1.49214300 | -0.18746800 |
| C | 4.83249600 | 1.39184800 | -0.13697100 |
| C | 5.57397900 | 0.17578800 | -0.17865400 |
| C | 2.72470600 | 0.10247200 | -0.12808000 |
| C | 3.47690400 | -1.11493200 | -0.16983100 |
| C | 0.61559700 | -1.17289400 | -0.11962400 |
| C | 1.35869300 | -2.39735700 | -0.16241400 |
| C | -1.50074800 | -2.44283700 | -0.11113200 |
| C | -0.76593600 | -3.66243400 | -0.15390200 |
| C | -3.61817000 | -3.72211300 | -0.10266600 |
| C | -2.86160100 | -4.92277800 | -0.14530500 |
| C | 9.08456900 | 1.54676200 | -0.21255200 |
| C | 9.84801500 | 0.38898600 | -0.25361900 |
| C | 7.00666800 | 0.22392300 | -0.20428800 |
| C | 7.80495000 | -0.97580600 | -0.24741000 |
| C | 4.89373200 | -1.07767000 | -0.19353900 |
| C | 2.78120000 | -2.37518200 | -0.18736900 |
| C | 3.50169900 | -3.63477800 | -0.23147500 |
| C | 0.64798400 | -3.63960300 | -0.17935700 |
| C | 1.37712600 | -4.88091100 | -0.22304900 |
| C | -1.47715200 | -4.91838900 | -0.17084900 |
| C | -0.71309600 | -6.14099100 | -0.21431800 |
| C | 9.21300700 | -0.85290100 | -0.27087400 |
| C | 7.19195900 | -2.25762900 | -0.26690700 |

| | | | |
|---|---|---|---|
| C | 4.90465300 | -3.66643200 | -0.25883200 |
| C | 2.75677100 | -4.84700400 | -0.24790300 |
| C | 0.64248600 | -6.12186000 | -0.23915400 |
| H | -9.87333500 | -2.27740900 | 0.04715600 |
| H | -7.70788900 | -3.47847600 | -0.02135700 |
| H | -5.54798600 | -4.67526300 | -0.08970400 |
| H | -3.39182600 | -5.87244200 | -0.15815800 |
| H | -1.25443200 | -7.08363100 | -0.22671100 |
| H | 9.80771900 | -1.76257900 | -0.30195700 |
| H | 7.87557100 | -3.10815900 | -0.30229500 |
| H | 5.35790600 | -4.65909000 | -0.29387500 |
| H | 3.31058400 | -5.78293500 | -0.28113800 |
| H | 1.20851400 | -7.04949000 | -0.27185400 |
| H | 3.12015000 | 5.99241900 | 0.00178000 |
| H | 5.27463600 | 4.81307800 | -0.06605900 |
| H | 7.42997100 | 3.63915200 | -0.13333700 |
| H | 9.56824800 | 2.52057000 | -0.19874200 |
| H | 10.93227900 | 0.44873500 | -0.27157900 |
| H | 0.96396200 | 7.19163200 | 0.07004000 |
| H | -11.13973200 | -0.14912300 | 0.12111500 |
| H | -7.82762100 | 3.30315900 | 0.14181500 |
| H | -9.94940800 | 2.02255700 | 0.15069200 |
| H | -1.49487300 | 7.14124200 | 0.11458900 |
| H | -3.59967900 | 5.85456500 | 0.12356900 |
| H | -5.71152900 | 4.57883600 | 0.13275500 |
| B | 5.69608200 | -2.38176800 | -0.24026200 |
| N | 5.88449900 | -2.93190800 | 3.47578100 |
| H | 6.15986000 | -2.96254000 | 2.49374400 |
| H | 5.79620900 | -1.94018900 | 3.69754900 |
| H | 4.93238000 | -3.29741800 | 3.49571500 |

BC2O-$O_2$:

# opt freq b3lyp/6-31g(d) scf=(maxcycle=500,xqc)

Title Card Required

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|---|---|---|---|
| C | 1.31407500 | 6.25479700 | 0.06872400 |
| C | 3.37347900 | 4.88059000 | 0.07691800 |
| C | 5.43521600 | 3.51310600 | 0.08522500 |
| C | 7.49486200 | 2.14279700 | 0.09354700 |
| C | 9.55737500 | 0.76937100 | 0.10193400 |
| C | -0.03909400 | 6.33587900 | 0.05036300 |
| C | -0.87042100 | 5.15247400 | 0.02003900 |
| C | 1.99950900 | 4.98047500 | 0.05865400 |
| C | 1.19056200 | 3.77950000 | 0.02816000 |
| C | 4.04983100 | 3.61877000 | 0.06660200 |

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|---|---|---|---|
| C | 3.25049200 | 2.41616200 | 0.03567800 |
| C | 6.09913500 | 2.25541500 | 0.07463900 |
| C | 5.30498800 | 1.05351200 | 0.04317600 |
| C | 8.14470300 | 0.88914300 | 0.08269900 |
| C | 7.35658100 | -0.30795200 | 0.05122000 |
| C | 10.17186300 | -0.48003400 | 0.09062800 |
| C | 9.41410200 | -1.64801400 | 0.06001700 |
| C | -2.24664400 | 5.21667400 | 0.00078500 |
| C | -3.06721100 | 4.04450500 | -0.02847100 |
| C | -0.20842400 | 3.86311100 | 0.00959000 |
| C | -1.00384200 | 2.67247000 | -0.01965900 |
| C | 1.84198300 | 2.50250400 | 0.01717600 |
| C | 1.05735000 | 1.31201200 | -0.01358300 |
| C | 3.89055100 | 1.14148600 | 0.02407200 |
| C | 3.10523600 | -0.04940700 | -0.00710200 |
| C | 5.94155500 | -0.22170800 | 0.03161500 |
| C | 5.15404600 | -1.41130600 | 0.00024600 |
| C | 7.99836200 | -1.59314800 | 0.03965900 |
| C | 7.20387000 | -2.75743700 | 0.00852400 |
| C | -4.45456400 | 4.10240900 | -0.05048500 |
| C | -5.26421700 | 2.93188900 | -0.07861800 |
| C | -2.41402300 | 2.75384400 | -0.03713800 |
| C | -3.19882700 | 1.56668400 | -0.06397100 |
| C | -0.35763100 | 1.39774900 | -0.03143800 |
| C | -1.13769200 | 0.21142600 | -0.06086100 |
| C | 1.69334200 | 0.03637800 | -0.02550300 |
| C | 0.90524200 | -1.15466900 | -0.05702600 |
| C | 3.74507000 | -1.32928900 | -0.01901300 |
| C | 2.95707100 | -2.51834600 | -0.05077400 |
| C | 5.79986000 | -2.70120300 | -0.01156000 |
| C | 4.99993500 | -3.86674900 | -0.04289200 |
| C | -6.65867200 | 2.98164500 | -0.10632300 |
| C | -7.45567200 | 1.81473100 | -0.13201400 |
| C | -4.62369500 | 1.63953600 | -0.08173300 |
| C | -5.39626000 | 0.45294200 | -0.10531500 |
| C | -2.54845500 | 0.30105600 | -0.07628200 |
| C | -3.34148300 | -0.88265100 | -0.10699700 |
| C | -0.50086500 | -1.06914800 | -0.07425700 |
| C | -1.28970000 | -2.26144300 | -0.10796700 |
| C | 1.54608100 | -2.43572500 | -0.06985500 |
| C | 0.75873000 | -3.62140300 | -0.10188800 |
| C | 3.60121300 | -3.80717500 | -0.06278100 |
| C | 2.78978200 | -4.97560900 | -0.09423100 |
| C | -8.87533900 | 1.90557000 | -0.16115500 |

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|---|---|---|---|
| C | -9.64982200 | 0.77005800 | -0.18513700 |
| C | -6.83557700 | 0.51843900 | -0.12510200 |
| C | -7.65992900 | -0.64950700 | -0.15112600 |
| C | -4.73589900 | -0.80988600 | -0.11543000 |
| C | -2.70109800 | -2.16884600 | -0.12559300 |
| C | -3.47077500 | -3.35652400 | -0.15756800 |
| C | -0.65567400 | -3.53495700 | -0.12148000 |
| C | -1.46015800 | -4.72139700 | -0.15304100 |
| C | 1.40450200 | -4.90834500 | -0.11366100 |
| C | 0.56937400 | -6.08454800 | -0.14471100 |
| C | -9.03772600 | -0.50209900 | -0.18049900 |
| C | -7.09463800 | -2.05923400 | -0.09775900 |
| C | -2.85500300 | -4.61039100 | -0.17156800 |
| C | -0.78792800 | -5.99598200 | -0.16307400 |
| H | 9.90350000 | -2.61824800 | 0.05145700 |
| H | 7.69355700 | -3.72850700 | -0.00011300 |
| H | 5.48941800 | -4.83792700 | -0.05163400 |
| H | 3.27773100 | -5.94772500 | -0.10272800 |
| H | 1.05461800 | -7.05730600 | -0.15261900 |
| H | -9.65893900 | -1.39390900 | -0.18819100 |
| H | -7.61539200 | -2.72171000 | -0.79574500 |
| H | -3.48371300 | -5.49523800 | -0.19184500 |
| H | -1.39566600 | -6.89679500 | -0.18519100 |
| H | -2.73602400 | 6.18828700 | 0.00815800 |
| H | -4.94606700 | 5.07287300 | -0.04618300 |
| H | -7.15455800 | 3.94988200 | -0.10774900 |
| H | -9.33480800 | 2.89095900 | -0.16416900 |
| H | -10.73343900 | 0.84489700 | -0.20635600 |
| H | -0.53168500 | 7.30509400 | 0.05844800 |
| H | 11.25632500 | -0.54426000 | 0.10592700 |
| H | 8.09881200 | 3.04690300 | 0.11735700 |
| H | 10.16019600 | 1.67336600 | 0.12590200 |
| H | 1.91837200 | 7.15832700 | 0.09168000 |
| H | 3.97493400 | 5.78674700 | 0.10003800 |
| H | 6.03782000 | 4.41819800 | 0.10884100 |
| B | -5.51674100 | -2.10800100 | -0.15703000 |
| O | -4.82807200 | -3.30756100 | -0.17945200 |
| O | -7.41264600 | -2.60315200 | 1.24890800 |
| O | -7.63791900 | -3.92225700 | 1.20534100 |

BC2O-NO:

# opt freq b3lyp/6-31g(d) scf=(maxcycle=500,xqc)

Title Card Required

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|---|---|---|---|
| C | -1.27880700 | 6.24287300 | 0.04625000 |

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|---|---|---|---|
| C | -3.34053900 | 4.88145900 | 0.03996900 |
| C | -5.40873400 | 3.53129200 | 0.03699900 |
| C | -7.47575000 | 2.17408200 | 0.03681700 |
| C | -9.54087500 | 0.80469300 | 0.03844300 |
| C | 0.07401600 | 6.31599000 | 0.04226600 |
| C | 0.89500500 | 5.12644200 | 0.02527300 |
| C | -1.96651700 | 4.97097900 | 0.03482500 |
| C | -1.16494000 | 3.76500400 | 0.01801900 |
| C | -4.02258700 | 3.62529400 | 0.03082800 |
| C | -3.22792600 | 2.41790500 | 0.01549600 |
| C | -6.08030900 | 2.27991700 | 0.03004600 |
| C | -5.28986100 | 1.07088900 | 0.01614700 |
| C | -8.13086600 | 0.92187900 | 0.03130300 |
| C | -7.34968100 | -0.27920400 | 0.01848600 |
| C | -10.16416800 | -0.44170600 | 0.03349700 |
| C | -9.40947200 | -1.61206000 | 0.02146500 |
| C | 2.26947300 | 5.18339500 | 0.02191500 |
| C | 3.07818700 | 4.00676500 | 0.00328700 |
| C | 0.23380500 | 3.83786100 | 0.01210500 |
| C | 1.02355800 | 2.64151000 | -0.00618600 |
| C | -1.81979300 | 2.49234300 | 0.00810400 |
| C | -1.03642300 | 1.29449500 | -0.00771200 |
| C | -3.87648200 | 1.14721400 | 0.00829100 |
| C | -3.09571900 | -0.04932200 | -0.00534100 |
| C | -5.93442900 | -0.20074000 | 0.01074400 |
| C | -5.15482100 | -1.39138200 | -0.00153600 |
| C | -7.99638300 | -1.55658500 | 0.01384300 |
| C | -7.20309800 | -2.72808000 | 0.00226500 |
| C | 4.46201400 | 4.07223900 | 0.00140200 |
| C | 5.26922000 | 2.90687000 | -0.02164600 |
| C | 2.43201700 | 2.71348600 | -0.01311600 |
| C | 3.21958700 | 1.52252600 | -0.03548200 |
| C | 0.37776500 | 1.36737200 | -0.01696000 |
| C | 1.15940100 | 0.17325800 | -0.03431000 |
| C | -1.68113000 | 0.02301000 | -0.01454900 |
| C | -0.89972600 | -1.17160500 | -0.02766700 |
| C | -3.74444100 | -1.31948300 | -0.00979100 |
| C | -2.96292000 | -2.51420900 | -0.02078100 |
| C | -5.80787400 | -2.67575900 | -0.00514500 |
| C | -5.01061900 | -3.85335000 | -0.01529100 |
| C | 6.65876400 | 2.99001700 | -0.01996100 |
| C | 7.47475700 | 1.84176400 | -0.05181900 |
| C | 4.64153700 | 1.60721700 | -0.04523900 |
| C | 5.42751000 | 0.42483200 | -0.07818500 |

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|---|---|---|---|
| C | 2.57722000 | 0.24630000 | -0.04691700 |
| C | 3.37173200 | -0.94477100 | -0.06774300 |
| C | 0.51377000 | -1.09885200 | -0.03883200 |
| C | 1.30334400 | -2.29764500 | -0.05064400 |
| C | -1.55658200 | -2.44263700 | -0.02970200 |
| C | -0.77161800 | -3.64131500 | -0.03821800 |
| C | -3.62345900 | -3.80207600 | -0.02236500 |
| C | -2.81926400 | -4.98181000 | -0.03008700 |
| C | 8.88948200 | 1.97648600 | -0.04443800 |
| C | 9.69838600 | 0.86578800 | -0.08326000 |
| C | 6.87488800 | 0.53518000 | -0.09242600 |
| C | 7.73777200 | -0.59802100 | -0.15097700 |
| C | 4.78802200 | -0.85514400 | -0.08766500 |
| C | 2.71406500 | -2.22671400 | -0.06506700 |
| C | 3.48966500 | -3.45891900 | -0.07085500 |
| C | 0.62778100 | -3.56903100 | -0.04747200 |
| C | 1.40922800 | -4.78381700 | -0.05205300 |
| C | -1.44308400 | -4.92803700 | -0.03676200 |
| C | -0.63258800 | -6.12365200 | -0.04173200 |
| C | 9.11536400 | -0.41453700 | -0.14209900 |
| C | 7.21083600 | -2.01067600 | -0.22603600 |
| C | 4.88339700 | -3.44214200 | -0.08677000 |
| C | 2.78118600 | -4.69987800 | -0.06033400 |
| C | 0.71988900 | -6.05225000 | -0.04805700 |
| H | -9.90093500 | -2.58135900 | 0.01793100 |
| H | -7.69803000 | -3.69686200 | -0.00058800 |
| H | -5.50843700 | -4.82037800 | -0.01682800 |
| H | -3.31811300 | -5.94824600 | -0.02961800 |
| H | -1.13903600 | -7.08545500 | -0.03944300 |
| H | 9.75850000 | -1.28982300 | -0.18336100 |
| H | 7.51993900 | -2.49420700 | -1.16485800 |
| H | 5.38208400 | -4.41179100 | -0.07676900 |
| H | 3.36993800 | -5.61473400 | -0.06196100 |
| H | 1.32132400 | -6.95791000 | -0.05083400 |
| H | 2.76710700 | 6.15072700 | 0.03322700 |
| H | 4.95097700 | 5.04385900 | 0.01710500 |
| H | 7.13205200 | 3.96911400 | 0.00493300 |
| H | 9.31593400 | 2.97588300 | -0.00802200 |
| H | 10.77991500 | 0.96870000 | -0.07471400 |
| H | 0.57474400 | 7.28099200 | 0.05172200 |
| H | -11.24879900 | -0.49977600 | 0.03925500 |
| H | -8.07577000 | 3.08091100 | 0.04707200 |
| H | -10.14170400 | 1.71061500 | 0.04811000 |
| H | -1.88041100 | 7.14835000 | 0.05891400 |

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|---|---|---|---|
| H | -3.93615300 | 5.79159700 | 0.05230800 |
| H | -6.00387900 | 4.44133700 | 0.04829000 |
| B | 5.61527700 | -2.13551200 | -0.12087100 |
| O | 8.06359900 | -3.96447800 | 0.57629200 |
| N | 7.78666100 | -2.82392800 | 0.89157100 |

$BC2O\text{-}NH_3$:

# opt freq b3lyp/6-31g(d) scf=(maxcycle=500,xqc)

Title Card Required

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|---|---|---|---|
| C | 0.99366100 | 6.24312300 | 0.09699700 |
| C | 3.09231700 | 4.92847700 | 0.10089900 |
| C | 5.19357400 | 3.62251900 | 0.10513900 |
| C | 7.29503100 | 2.31244000 | 0.10934400 |
| C | 9.39619500 | 0.99065300 | 0.11329900 |
| C | -0.36117300 | 6.28533100 | 0.07472700 |
| C | -1.15832500 | 5.07850500 | 0.03141500 |
| C | 1.71562700 | 4.98910400 | 0.07864000 |
| C | 0.94228300 | 3.76614200 | 0.03528100 |
| C | 3.80591100 | 3.68760000 | 0.08274400 |
| C | 3.03981600 | 2.46464700 | 0.03945700 |
| C | 5.89865000 | 2.38642300 | 0.08697400 |
| C | 5.13515600 | 1.16300400 | 0.04369300 |
| C | 7.98226400 | 1.07770900 | 0.09091500 |
| C | 7.22664400 | -0.14312400 | 0.04781800 |
| C | 10.04449000 | -0.24244700 | 0.09423600 |
| C | 9.32434100 | -1.43190800 | 0.05250600 |
| C | -2.53593700 | 5.10265000 | 0.00833200 |
| C | -3.32080300 | 3.90634200 | -0.03448000 |
| C | -0.45950600 | 3.80886400 | 0.01225000 |
| C | -1.21882700 | 2.59696300 | -0.03051800 |
| C | 1.63149700 | 2.50983800 | 0.01629300 |
| C | 0.87873800 | 1.29636100 | -0.02647700 |
| C | 3.72010900 | 1.21013000 | 0.02039400 |
| C | 2.96788300 | -0.00348800 | -0.02238300 |
| C | 5.80904400 | -0.09494700 | 0.02446600 |
| C | 5.05532600 | -1.30440100 | -0.01826400 |
| C | 7.90788700 | -1.41184800 | 0.02846300 |
| C | 7.14242500 | -2.59495900 | -0.01382600 |
| C | -4.71121300 | 3.92070000 | -0.05823700 |
| C | -5.47928400 | 2.72388800 | -0.10086900 |
| C | -2.62987200 | 2.63666600 | -0.05359800 |
| C | -3.38043700 | 1.42599700 | -0.09609900 |
| C | -0.53447000 | 1.34043300 | -0.04966600 |
| C | -1.28168800 | 0.12885900 | -0.09216000 |

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|---|---|---|---|
| C | 1.55385500 | 0.03940800 | -0.04571000 |
| C | 0.80215400 | -1.17331600 | -0.08836400 |
| C | 3.64548100 | -1.26348900 | -0.04160900 |
| C | 2.89216000 | -2.47263300 | -0.08426400 |
| C | 5.73922300 | -2.57269200 | -0.03754100 |
| C | 4.97178400 | -3.76109700 | -0.07992900 |
| C | -6.87835000 | 2.72281100 | -0.12578900 |
| C | -7.63329300 | 1.52759300 | -0.16865500 |
| C | -4.79616100 | 1.45661500 | -0.11940400 |
| C | -5.54072200 | 0.24004600 | -0.16201400 |
| C | -2.69319900 | 0.17462000 | -0.11490200 |
| C | -3.44841300 | -1.03000300 | -0.15694600 |
| C | -0.60730300 | -1.13156000 | -0.11152200 |
| C | -1.35991700 | -2.34668600 | -0.15435200 |
| C | 1.48195000 | -2.43262500 | -0.10760700 |
| C | 0.72993800 | -3.64283600 | -0.15024200 |
| C | 3.57488700 | -3.74084600 | -0.10356600 |
| C | 2.80075900 | -4.93603700 | -0.14622800 |
| C | -9.04953400 | 1.56795900 | -0.19485000 |
| C | -9.78541300 | 0.38894800 | -0.23867800 |
| C | -6.96035700 | 0.26001400 | -0.18645400 |
| C | -7.72680800 | -0.97224000 | -0.23128000 |
| C | -4.84953400 | -1.00593700 | -0.17802900 |
| C | -2.77197600 | -2.29609800 | -0.17702500 |
| C | -3.51329100 | -3.51255100 | -0.21989800 |
| C | -0.68194100 | -3.60018500 | -0.17355500 |
| C | -1.44932300 | -4.81266100 | -0.21663900 |
| C | 1.41654700 | -4.91213800 | -0.16957300 |
| C | 0.62046300 | -6.11503900 | -0.21288100 |
| C | -9.14286500 | -0.84683300 | -0.25679200 |
| C | -7.10635800 | -2.24794500 | -0.25113900 |
| C | -2.84327000 | -4.74657500 | -0.23913600 |
| C | -0.73796200 | -6.06751500 | -0.23528400 |
| H | 9.83909800 | -2.38863100 | 0.03795800 |
| H | 7.65626300 | -3.55356300 | -0.02841400 |
| H | 5.48917200 | -4.71804100 | -0.09438300 |
| H | 3.31971700 | -5.89209300 | -0.16062900 |
| H | 1.13661600 | -7.07164500 | -0.22730600 |
| H | -9.73564700 | -1.75769600 | -0.29038400 |
| H | -7.77345400 | -3.10878800 | -0.29372600 |
| H | -3.44040900 | -5.65281800 | -0.27371000 |
| H | -1.31854000 | -6.98571500 | -0.26782500 |
| H | -3.05397500 | 6.05922800 | 0.02289400 |
| H | -5.23350100 | 4.87492000 | -0.04407100 |

| | | | |
|---|---|---|---|
| H | -7.40828800 | 3.67304200 | -0.11242200 |
| H | -9.55132400 | 2.53196700 | -0.18044500 |
| H | -10.87114000 | 0.43000900 | -0.25858600 |
| H | -0.88167700 | 7.23982100 | 0.08922600 |
| H | 11.13067600 | -0.27414900 | 0.11231800 |
| H | 7.87342800 | 3.23271400 | 0.14201400 |
| H | 9.97596200 | 1.90936500 | 0.14596000 |
| H | 1.57154600 | 7.16354500 | 0.12956000 |
| H | 3.66661200 | 5.85196600 | 0.13352600 |
| H | 5.76801200 | 4.54558400 | 0.13778900 |
| B | -5.61284000 | -2.31772800 | -0.22557800 |
| O | -4.85299600 | -3.52206900 | -0.24236700 |
| N | -6.05727700 | -3.35011200 | 3.15790700 |
| H | -5.51829600 | -4.04272200 | 2.63849900 |
| H | -5.38522900 | -2.63606000 | 3.43882100 |
| H | -6.64978500 | -2.90259600 | 2.45772000 |

BCO2-$O_2$:

# opt freq ub3lyp/6-31g(d) scf=(maxcycle=500,xqc)

Title Card Required

0 2

| | | | |
|---|---|---|---|
| C | 1.12653300 | 6.25577900 | 0.06357300 |
| C | 3.21682500 | 4.91779300 | 0.08023900 |
| C | 5.30579800 | 3.58582700 | 0.07706000 |
| C | 7.39068200 | 2.25959100 | 0.05761100 |
| C | 9.48204000 | 0.93490100 | 0.02836700 |
| C | -0.22925600 | 6.31253000 | 0.03969000 |
| C | -1.03929800 | 5.11475000 | 0.02089900 |
| C | 1.83534500 | 4.99506300 | 0.06649200 |
| C | 1.05607600 | 3.78095100 | 0.05075400 |
| C | 3.90652000 | 3.67010000 | 0.07078600 |
| C | 3.13784000 | 2.45630100 | 0.04932300 |
| C | 5.98207500 | 2.34606500 | 0.05533500 |
| C | 5.21307000 | 1.13140400 | 0.02595100 |
| C | 8.06267400 | 1.02325800 | 0.02740500 |
| C | 7.29461100 | -0.18908600 | -0.00796500 |
| C | 10.11773700 | -0.30260400 | -0.00576000 |
| C | 9.38078300 | -1.48418100 | -0.04266900 |
| C | -2.42257700 | 5.15257900 | -0.01549300 |
| C | -3.21373500 | 3.96443400 | -0.03200300 |
| C | -0.35590100 | 3.84043800 | 0.03400500 |
| C | -1.11702800 | 2.63911400 | 0.02686800 |
| C | 1.72187200 | 2.51872000 | 0.04534700 |
| C | 0.96094800 | 1.31386800 | 0.02922100 |
| C | 3.79828000 | 1.19366800 | 0.02694200 |

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|---|---|---|---|
| C | 3.03379400 | -0.01244700 | -0.00132300 |
| C | 5.87452900 | -0.13112000 | -0.00719000 |
| C | 5.11094300 | -1.33392000 | -0.04413200 |
| C | 7.95965500 | -1.46042500 | -0.04537500 |
| C | 7.18841300 | -2.63831700 | -0.08582500 |
| C | -4.61676200 | 3.98457200 | -0.09683100 |
| C | -5.38269100 | 2.79431600 | -0.11998300 |
| C | -2.53392100 | 2.69527800 | 0.00436400 |
| C | -3.28638500 | 1.49345300 | 0.01022200 |
| C | -0.45097200 | 1.37486300 | 0.02741300 |
| C | -1.20905400 | 0.17215400 | 0.02000500 |
| C | 1.61794400 | 0.04746100 | 0.00567400 |
| C | 0.85359300 | -1.15569700 | -0.02265800 |
| C | 3.69391500 | -1.27782800 | -0.03980500 |
| C | 2.92765300 | -2.47916600 | -0.08346000 |
| C | 5.77772800 | -2.60979800 | -0.08837400 |
| C | 4.99895300 | -3.78574600 | -0.13743900 |
| C | -6.79264700 | 2.77715400 | -0.23008800 |
| C | -7.53887200 | 1.57949600 | -0.29672900 |
| C | -4.69795000 | 1.53646000 | -0.04466600 |
| C | -5.42957200 | 0.32418500 | -0.02414600 |
| C | -2.61960400 | 0.23487900 | 0.02335100 |
| C | -3.38512200 | -0.96061500 | 0.05287400 |
| C | -0.56109100 | -1.09700300 | -0.00479100 |
| C | -1.33312300 | -2.30213200 | -0.04350700 |
| C | 1.51385700 | -2.42166600 | -0.07511000 |
| C | 0.74334400 | -3.61958500 | -0.13722600 |
| C | 3.59199400 | -3.75366200 | -0.14046800 |
| C | 2.80361800 | -4.93017100 | -0.20434200 |
| C | -8.94608700 | 1.57593700 | -0.50827800 |
| C | -9.60736900 | 0.37213500 | -0.64868700 |
| C | -6.84712200 | 0.32546000 | -0.18669000 |
| C | -7.54825800 | -0.91079200 | -0.33712400 |
| C | -4.77611900 | -0.90987600 | 0.10491600 |
| C | -2.74317400 | -2.23768100 | -0.01025800 |
| C | -3.53010800 | -3.43039900 | -0.12752900 |
| C | -0.67203200 | -3.55848100 | -0.13089400 |
| C | -1.46162000 | -4.74767600 | -0.22571300 |
| C | 1.40958400 | -4.88985900 | -0.21048700 |
| C | 0.59546500 | -6.07330000 | -0.29162200 |
| C | -8.92357500 | -0.85809400 | -0.57763800 |
| C | -2.86358300 | -4.65861900 | -0.24012200 |
| C | -0.76735900 | -6.00444200 | -0.30393400 |
| H | 9.88837600 | -2.44463900 | -0.07028800 |

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|---|---|---|---|
| H | 7.69570400 | -3.59964200 | -0.11739000 |
| H | 5.50479900 | -4.74775400 | -0.17685900 |
| H | 3.30735700 | -5.89309700 | -0.25425100 |
| H | 1.09404500 | -7.03777500 | -0.34773600 |
| H | -9.45595100 | -1.79590900 | -0.69995100 |
| H | -3.46660300 | -5.55779000 | -0.32353400 |
| H | -1.35782600 | -6.91462200 | -0.37069400 |
| H | -2.92859500 | 6.11532100 | -0.03502200 |
| H | -5.12899100 | 4.94358200 | -0.13728500 |
| H | -7.32435700 | 3.72415000 | -0.29866000 |
| H | -9.47976700 | 2.51954000 | -0.57772500 |
| H | -10.68002200 | 0.36338100 | -0.82204300 |
| H | -0.73760100 | 7.27344100 | 0.03408300 |
| H | 11.20330400 | -0.34832800 | -0.00427700 |
| H | 7.97447400 | 3.17686100 | 0.08169100 |
| H | 10.06496600 | 1.85150900 | 0.05584500 |
| H | 1.71311400 | 7.17091800 | 0.07781000 |
| H | 3.80288300 | 5.83405800 | 0.09422500 |
| H | 5.89146400 | 4.50213600 | 0.09586200 |
| B | -5.61204800 | -2.23244200 | 0.32322400 |
| O | -4.86215200 | -3.40748600 | -0.17534200 |
| O | -6.94295800 | -2.10698200 | -0.29312400 |
| O | -5.91866900 | -2.45641900 | 1.79697800 |
| O | -4.80333300 | -2.62866400 | 2.50773600 |

BCO2-NO:

# opt freq b3lyp/6-31g(d) scf=(maxcycle=500,xqc)

Title Card Required

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|---|---|---|---|
| C | 1.05511100 | 6.26864600 | 0.07682200 |
| C | 3.15068600 | 4.94289900 | 0.08004100 |
| C | 5.24410500 | 3.62127100 | 0.08326800 |
| C | 7.33517700 | 2.29938500 | 0.08616600 |
| C | 9.43242000 | 0.97562500 | 0.08871300 |
| C | -0.30035500 | 6.31762200 | 0.05664700 |
| C | -1.10566500 | 5.11550000 | 0.01709200 |
| C | 1.77404400 | 5.01227100 | 0.05966600 |
| C | 0.99442100 | 3.79321700 | 0.01958000 |
| C | 3.85691500 | 3.69667000 | 0.06255200 |
| C | 3.08563100 | 2.47665200 | 0.02168800 |
| C | 5.93925100 | 2.37911400 | 0.06517900 |
| C | 5.17115800 | 1.15988200 | 0.02349200 |
| C | 8.01802900 | 1.06201700 | 0.06747000 |
| C | 7.25607600 | -0.15441800 | 0.02527000 |
| C | 10.07205300 | -0.25999700 | 0.06900000 |

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|---|---|---|---|
| C | 9.34352500 | -1.44656600 | 0.02780300 |
| C | -2.48527800 | 5.14672000 | -0.00375300 |
| C | -3.28161600 | 3.95533900 | -0.04205700 |
| C | -0.40675400 | 3.84536500 | -0.00084100 |
| C | -1.17173800 | 2.63807200 | -0.03919000 |
| C | 1.67782000 | 2.53199700 | 0.00083800 |
| C | 0.92141200 | 1.32308700 | -0.03858300 |
| C | 3.75674500 | 1.21635800 | 0.00219200 |
| C | 2.99932000 | 0.00693200 | -0.03860400 |
| C | 5.83746400 | -0.10047600 | 0.00352600 |
| C | 5.07721300 | -1.30820500 | -0.03843400 |
| C | 7.92855800 | -1.42596300 | 0.00496900 |
| C | 7.15656600 | -2.60799600 | -0.03720200 |
| C | -4.67551000 | 3.97256500 | -0.06533300 |
| C | -5.45373700 | 2.77626500 | -0.10308400 |
| C | -2.58214500 | 2.68796900 | -0.05865100 |
| C | -3.33119600 | 1.48146400 | -0.09438500 |
| C | -0.49201700 | 1.37808300 | -0.05874100 |
| C | -1.23936500 | 0.17217000 | -0.09763300 |
| C | 1.58516000 | 0.06091200 | -0.05910400 |
| C | 0.82602300 | -1.14848400 | -0.09908600 |
| C | 3.66717200 | -1.25818300 | -0.05954200 |
| C | 2.90356900 | -2.46497600 | -0.10168200 |
| C | 5.75533700 | -2.58294900 | -0.05960900 |
| C | 4.97656600 | -3.76613300 | -0.10287900 |
| C | -6.85602800 | 2.74456600 | -0.13164800 |
| C | -7.59887400 | 1.53355200 | -0.17638900 |
| C | -4.74932100 | 1.52038500 | -0.11401200 |
| C | -5.47009500 | 0.30686300 | -0.14600900 |
| C | -2.64893900 | 0.23013900 | -0.11546500 |
| C | -3.40089700 | -0.97240200 | -0.14720100 |
| C | -0.58118500 | -1.09551100 | -0.11756200 |
| C | -1.34483000 | -2.30773100 | -0.15649900 |
| C | 1.49508400 | -2.41510100 | -0.12159800 |
| C | 0.73024300 | -3.61948900 | -0.16519500 |
| C | 3.57922200 | -3.73827900 | -0.12485300 |
| C | 2.79224300 | -4.92508400 | -0.17027200 |
| C | -9.01950100 | 1.49539700 | -0.21732400 |
| C | -9.68142200 | 0.28517300 | -0.26938700 |
| C | -6.89119700 | 0.28756000 | -0.18449500 |
| C | -7.60135900 | -0.94784000 | -0.24126100 |
| C | -4.78977400 | -0.92610100 | -0.15005700 |
| C | -2.75310600 | -2.24811700 | -0.17019800 |
| C | -3.51971200 | -3.45045800 | -0.21539700 |

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|---|---|---|---|
| C | -0.68220000 | -3.56665400 | -0.18359900 |
| C | -1.46805800 | -4.76708900 | -0.23175300 |
| C | 1.40579100 | -4.89060000 | -0.19162900 |
| C | 0.59458300 | -6.08298300 | -0.24005600 |
| C | -8.98373300 | -0.94324600 | -0.28430800 |
| C | -2.86773100 | -4.68799600 | -0.25141500 |
| C | -0.76560000 | -6.02535600 | -0.26015400 |
| H | 9.85621900 | -2.40461700 | 0.01264400 |
| H | 7.66803100 | -3.56773000 | -0.05292400 |
| H | 5.48774800 | -4.72617700 | -0.11981900 |
| H | 3.30258700 | -5.88574400 | -0.18915800 |
| H | 1.09978300 | -7.04549500 | -0.26096300 |
| H | -9.51400700 | -1.88869700 | -0.32944300 |
| H | -3.46932300 | -5.59084900 | -0.29439400 |
| H | -1.35074300 | -6.94065800 | -0.29724300 |
| H | -2.99507000 | 6.10782300 | 0.00935900 |
| H | -5.19147000 | 4.93025500 | -0.05551200 |
| H | -7.40464900 | 3.68389400 | -0.12331400 |
| H | -9.57637900 | 2.42849700 | -0.20951000 |
| H | -10.76739800 | 0.26747000 | -0.30140900 |
| H | -0.81425800 | 7.27574200 | 0.07015300 |
| H | 11.15809200 | -0.30008100 | 0.08594100 |
| H | 7.91728100 | 3.21762400 | 0.11781600 |
| H | 10.01402600 | 1.89309400 | 0.12071100 |
| H | 1.63604300 | 7.18730400 | 0.10670200 |
| H | 3.73124800 | 5.86257100 | 0.11048300 |
| H | 5.82606200 | 4.53981100 | 0.11433700 |
| B | -5.57381500 | -2.21558400 | -0.17678500 |
| O | -4.88246300 | -3.42663100 | -0.26815200 |
| O | -6.95225300 | -2.16945300 | -0.26359500 |
| O | -4.15579700 | -2.98962900 | 2.51734100 |
| N | -5.14216800 | -2.39719100 | 2.38423700 |

BCO2-$NH_3$:

# opt freq ub3lyp/6-31g(d) scf=(maxcycle=500,xqc)

Title Card Required

0 2

| | | | |
|---|---|---|---|
| C | 1.00507200 | 6.22917200 | 0.03019700 |
| C | 3.11188700 | 4.91553400 | 0.04839600 |
| C | 5.21488100 | 3.60877700 | 0.05237800 |
| C | 7.31219000 | 2.30248800 | 0.04395600 |
| C | 9.41676300 | 0.99549200 | 0.02742400 |
| C | -0.35410400 | 6.27137700 | 0.01264100 |
| C | -1.14893100 | 5.06741600 | 0.00342100 |
| C | 1.72504700 | 4.97884400 | 0.03702500 |

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|---|---|---|---|
| C | 0.95923700 | 3.75970200 | 0.02910500 |
| C | 3.81401200 | 3.67913800 | 0.04622700 |
| C | 3.05473200 | 2.45615100 | 0.03403300 |
| C | 5.90633900 | 2.37543100 | 0.04100500 |
| C | 5.14775700 | 1.15049800 | 0.02287700 |
| C | 7.99768500 | 1.07029200 | 0.02591700 |
| C | 7.24411700 | -0.14857900 | 0.00337100 |
| C | 10.06604800 | -0.23541600 | 0.00621100 |
| C | 9.34104000 | -1.42497600 | -0.01767100 |
| C | -2.53887500 | 5.09076600 | -0.02140300 |
| C | -3.31837700 | 3.90081100 | -0.02886400 |
| C | -0.45340900 | 3.80539400 | 0.01632600 |
| C | -1.20795500 | 2.59573800 | 0.01430300 |
| C | 1.64134300 | 2.50382200 | 0.02973000 |
| C | 0.89047100 | 1.28930800 | 0.02099000 |
| C | 3.73025400 | 1.19816500 | 0.02238400 |
| C | 2.97952600 | -0.01444600 | 0.00528100 |
| C | 5.82107600 | -0.10452400 | 0.00301400 |
| C | 5.06884600 | -1.31531200 | -0.02072800 |
| C | 7.92144900 | -1.41299100 | -0.02014900 |
| C | 7.16110200 | -2.60000200 | -0.04693900 |
| C | -4.72581400 | 3.90885000 | -0.07101500 |
| C | -5.49041300 | 2.71308700 | -0.08214400 |
| C | -2.62110900 | 2.64007500 | -0.00056000 |
| C | -3.36695000 | 1.42680100 | 0.00792600 |
| C | -0.52508900 | 1.33653900 | 0.01891400 |
| C | -1.26839300 | 0.12793400 | 0.01745400 |
| C | 1.56001600 | 0.03154600 | 0.00966200 |
| C | 0.80721100 | -1.18009300 | -0.00655200 |
| C | 3.65334400 | -1.27338300 | -0.01824700 |
| C | 2.89781600 | -2.48585900 | -0.04724600 |
| C | 5.74985700 | -2.58690300 | -0.04968400 |
| C | 4.98673300 | -3.77037900 | -0.08335000 |
| C | -6.89637900 | 2.67808400 | -0.15138100 |
| C | -7.63435500 | 1.46184200 | -0.19620300 |
| C | -4.78372600 | 1.45861500 | -0.02557000 |
| C | -5.50023500 | 0.23902000 | 0.00105800 |
| C | -2.68362500 | 0.17876800 | 0.02187000 |
| C | -3.43552700 | -1.02532000 | 0.05507100 |
| C | -0.60486200 | -1.13458500 | 0.00759600 |
| C | -1.36459900 | -2.35219200 | -0.01676600 |
| C | 1.48314500 | -2.44278300 | -0.04111900 |
| C | 0.72865700 | -3.64926400 | -0.08517700 |
| C | 3.57518500 | -3.75407500 | -0.08660800 |

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|---|---|---|---|
| C | 2.80266800 | -4.93761600 | -0.13237100 |
| C | -9.04575800 | 1.42804300 | -0.34586700 |
| C | -9.70342400 | 0.21567800 | -0.44385900 |
| C | -6.92797800 | 0.21915900 | -0.11312600 |
| C | -7.62546000 | -1.01915900 | -0.22471400 |
| C | -4.82245300 | -0.98454400 | 0.09903700 |
| C | -2.77755000 | -2.30312300 | 0.01143700 |
| C | -3.53676000 | -3.50515900 | -0.08067100 |
| C | -0.69389900 | -3.60365400 | -0.07995100 |
| C | -1.46579200 | -4.80283000 | -0.15093000 |
| C | 1.40576500 | -4.91095700 | -0.13788000 |
| C | 0.60446400 | -6.10377200 | -0.19884400 |
| C | -9.00617500 | -1.00735800 | -0.39148800 |
| C | -2.87382400 | -4.72770700 | -0.15938600 |
| C | -0.75938800 | -6.05250400 | -0.20927600 |
| H | 9.85769700 | -2.38104600 | -0.03533400 |
| H | 7.67822000 | -3.55660700 | -0.06776100 |
| H | 5.50227100 | -4.72769900 | -0.11063800 |
| H | 3.31598100 | -5.89616200 | -0.16884500 |
| H | 1.11419600 | -7.06331500 | -0.24268000 |
| H | -9.52866900 | -1.95413700 | -0.48556200 |
| H | -3.46689400 | -5.63504900 | -0.23184500 |
| H | -1.33884700 | -6.97104300 | -0.26310500 |
| H | -3.05196500 | 6.05011100 | -0.03848300 |
| H | -5.24430700 | 4.86469500 | -0.10370900 |
| H | -7.44464200 | 3.61627800 | -0.20257000 |
| H | -9.59770900 | 2.36255400 | -0.40136400 |
| H | -10.78284800 | 0.19780900 | -0.57000900 |
| H | -0.87202600 | 7.22747100 | 0.00458900 |
| H | 11.15229400 | -0.26941100 | 0.00755500 |
| H | 7.88784500 | 3.22523100 | 0.05871300 |
| H | 9.99071900 | 1.91828500 | 0.04481600 |
| H | 1.58136400 | 7.15125200 | 0.03673700 |
| H | 3.68689600 | 5.83911900 | 0.05549100 |
| H | 5.79082400 | 4.53143900 | 0.06312000 |
| B | -5.62473200 | -2.30412600 | 0.25245300 |
| O | -4.90212500 | -3.49939600 | -0.09822700 |
| O | -6.98891200 | -2.23042400 | -0.18577400 |
| N | -5.85601700 | -2.56152500 | 2.03605600 |
| H | -6.38176900 | -1.79742200 | 2.46259500 |
| H | -4.96763500 | -2.65086100 | 2.53092200 |
| H | -6.38418500 | -3.42499800 | 2.17173900 |