Supporting Information

Effects of Oxygen: Experimental and VTST/DFT Studies on Cumene Autoxidation with Air under an Atmosphere Pressure

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1 Saturated solubility of oxygen calculated by Hayduk’s semiempirical method and gas-liquid equilibrium theory

Here, a model for calculating the saturated solubility of oxygen was established based on the gas-liquid equilibrium theory. The gas-liquid equilibrium equations of oxygen, nitrogen and cumene were written as Equations S1 – S3. The sum of the molar fractions of the components in the gas phase was equal to 1, thus Equation S4 was given.

\[ p\varphi_1^vY_1 = H_1X_1y_1^* \]  
\[ p\varphi_2^vY_2 = H_2X_2y_2^* \]  
\[ p\varphi_3^vY_3 = P_3^Sx_3\gamma_3 \]  
\[ Y_1 + Y_2 + Y_3 = 1 \]

Where, \( p \) is the pressure of gas phase; \( H_1 \) and \( H_2 \) are Henry's coefficients of oxygen and nitrogen, respectively; \( \varphi_1^v \), \( \varphi_2^v \) and \( \varphi_3^v \) are fugacity coefficients of oxygen, nitrogen and cumene, respectively; \( \gamma_1^* \), \( \gamma_2^* \) and \( \gamma_3 \) are activity coefficients of oxygen, nitrogen and cumene, respectively; \( p_3^S \) is the saturated vapor pressure of cumene; \( Y_1 \), \( Y_2 \) and \( Y_3 \) are mole fractions of oxygen, nitrogen and cumene in the gas phase, respectively; \( X_1 \), \( X_2 \) and \( X_3 \) are mole fractions of oxygen, nitrogen and cumene in the liquid phase, respectively.

The reaction was carried out at a pressure of 1.0 bar and thus the gas was approximated as an ideal gas, therefore \( \varphi_1^v = \varphi_2^v = \varphi_3^v = 1 \). Cumene was the main component of the liquid phase, and the content of oxygen and nitrogen were very low. Thus, \( X_1 \rightarrow 0 \), \( X_2 \rightarrow 0 \), and \( X_3 \rightarrow 1 \) were obtained. Since \( X_1 \rightarrow 0 \) and \( X_2 \rightarrow 0 \), \( \gamma_3 \rightarrow 1 \) could be used.

As air was used as the oxidant in cumene autoxidation, dry air was feed into the gas phase continuously to eliminate the effects brought by the consumption of oxygen and to ensure the stability of the gas phase. To simplify the model, assumptions 1 and 2 were as follows.

Assumption 1: the reaction liquor had no weight loss caused by the flow air.

Assumption 2: changes in the compositions of the reaction liquor caused by cumene autoxidation had no effects on oxygen solubility.

As a result, when the ratio of nitrogen and oxygen in the reaction liquor was the same as that in the gas phase (\( \mu = Y_2/Y_1 \)), \( Y_1 = H_1X_1y_1^*/p \), \( Y_2 = \mu H_1X_1y_1^*/p \) and \( Y_3 = P_3^S/p \) were obtained. Equation S5 was then deduced to calculate the mole fraction of oxygen \((X_1)\) according to Equation
\[ X_1 = \frac{p - p_S}{(1 + \mu) \gamma_H^1} \]  

(S5)

The saturated vapor pressure of cumene at different temperature was calculated by Antoine equation (Equation S6) reported by Fu.

\[ \ln p_S^2 = 16.3170 - \frac{3605.723}{-53.131 + T} \]  

(S6)

Liang has reported that the Henry coefficient of oxygen in toluene was not a constant. Therefore, it may be inaccurate to calculate the oxygen solubility by the simple Henry’s Law, where Henry coefficient was a constant independent of temperature. To obtain the accurate solubility data of oxygen in cumene, the mole fraction of oxygen \( X_T \) in cumene under an oxygen partial pressure of 1.0 bar was calculated according to the semiempirical method (Equation S7) provided by Hayduk and his co-workers. The mole fraction of oxygen \( X_0 \) at the critical temperature \( T_C \) and the Hildebrand solubility parameter \( ^2\delta \) were calculated by Equations S8 and S9, respectively.

\[ \log(10^4 X_0) = 2.265 - 0.0655 \left( ^2\delta / \text{MPa}^{1/2} \right) \]  

(S8)

\[ ^2\delta = ^2\delta_0 + mT \]  

(S9)

Where, \( X_T \) is the mole fraction of oxygen dissolved in cumene at temperature \( T \) under an oxygen partial pressure of 1.0 bar; \(^2\delta_0\) is the Hildebrand solubility parameter of cumene, \(^2\delta_0 = 23.3 \) MPa\(^{1/2}\); \( m \) is a constant, \( m = -19.8 \times 10^{-3} \); \( T_C \) is the critical temperature of cumene, \( T_C = 631.05 \) K.

The saturated solubility of oxygen in cumene \( ([O_2]_T) = 2.23 \times 10^{-4} \text{g/(L•atm)} \) at 298.15 K under an oxygen partial pressure of 1.0 bar was obtained from Low’s report. This is to say, \( X_{298.15K} = 9.7675 \times 10^{-4} \). Subsequently, the mole fraction of oxygen \( X_T \) dissolved in cumene was calculated by Equation S10 and the results were listed in Table S1, showing a slight upward trend as the temperature increases.

\[ X_T = X_{298.15K} \times 10^{0.9242 \times \log\left( \frac{T}{298.15} \right)} \]  

(S10)

When \( \mu = 0 \), Equation 12 was derived from Equation 6. When air was used as the oxidant \((\mu = 3.7619)\), \( X_1 = X_T / (1 + \mu) \) could be given based on Equations S5 and S11. The mole concentration of oxygen \( ([O_2]_T) \) at a temperature of \( T \) was calculated by Equation S12.
\[ X_T = \frac{p - p^S}{y^2 N_1} \]  

(S11)

\[ [O_2]^p_T = X_T \times 10^3 \]  

(S12)

Where, \( V \) is the molecular volume of cumene, \( V = \Delta^\theta U/(\alpha^2 \delta)^2. \) \( \Delta^\theta U \) is the vaporization heat of cumene, which is equal to 45.171 \times 10^3 \text{ J/mol}.  

The calculations results were listed in Table S1.

| Entry | \( T \) (°C) | \( X_T \times 10^4 \) | \( P^i_3 \) (Pa) | \( P_{\text{oxygen}} \) (Pa) | \([O_2]^p_T \times 10^3 \) (mol/L) |
|-------|--------------|----------------|---------------|----------------|------------------|
| 1     | 70           | 10.83          | 6483.77       | 19916.66       | 12.84            |
| 2     | 80           | 10.86          | 9812.91       | 19217.54       | 12.13            |
| 3     | 90           | 10.89          | 14459.67      | 18241.72       | 11.27            |
| 4     | 100          | 10.92          | 20796.80      | 16910.92       | 10.22            |
| 5     | 110          | 10.96          | 29259.68      | 15133.72       | 8.94             |
| 6     | 120          | 10.99          | 40347.91      | 12805.19       | 7.40             |

2 Effects of \( \text{K}_2\text{CO}_3 \) on cumene autoxidation

![Graph showing conversion over time at 100 and 120 °C. General conditions: \( \text{K}_2\text{CO}_3 \) (0.5 mmol, 1.25 equiv.), CM (3 mL), air atmosphere.]

Control experiments with \( \text{K}_2\text{CO}_3 \) or without \( \text{K}_2\text{CO}_3 \) at 50, 100 and 120 °C were carried out and part of the results were depicted in Fig.S1. The reaction does not proceed at 50 °C no matter whether \( \text{K}_2\text{CO}_3 \) is added or not. Furthermore, it is unreasonable that the reaction of \( \text{CO}_3^2- \) with RH to form a tertiary carbon anion (\( \text{R}^- \)) with poor stability. The addition of \( \text{K}_2\text{CO}_3 \) at 120 °C has no apparent effect on the reaction rate as shown in Fig.S1. To be noted, the addition of \( \text{K}_2\text{CO}_3 \) at 100 °C promote the reaction rate, especially in 0 - 180 min, while has little promotion effects on the reaction rate in 180 - 420 min. Therefore, the addition of \( \text{K}_2\text{CO}_3 \) may promote the process in the radical initiation stage, but could not promote radical transfer process, which dominated the peroxidation rate. We deemed that \( \text{K}_2\text{CO}_2 \) was used to neutralize the organic acid to suppressing reaction such as \( \text{“H}^+ + \)
ROOH $\rightarrow$ RO$^+$ + H$_2$O$^*$, thus promoting the radical initiation process. The catalytic effect of K$_2$CO$_3$ needs to be further studied since no relevant evidence has been found so far.

3 Calculation results for $[\text{ROO}^*]/g(T)$ at 70-120 °C

Table S2: Calculation results for $[\text{ROO}^*]/g(T)$ at 70-120 °C

| Entry | $T$ (°C) | $[\text{ROO}^*]/g(T)$ |
|-------|----------|------------------------|
| 1     | 70       | 0.999716               |
| 2     | 80       | 0.999491               |
| 3     | 90       | 0.999099               |
| 4     | 100      | 0.998409               |
| 5     | 110      | 0.997158               |
| 6     | 120      | 0.994764               |

4. The conversion of cumene ($x$) over $t$

Figure S2: The conversion of cumene ($x$) over $t$. The data at 70, 80, 90, and 100 °C were obtained from our previous article.

5 Linear regression of ln(1-$x$) with $t$

Figure S3: Linear regression analysis of ln(1-$x$) with $t$
Table S3: Linear regression equations of ln(1-x) with t

| Temperature, °C | ln(1-x) = - K_1 t |
|-----------------|-------------------|
| 70              | ln(1-x) = -3.2157 \times 10^{-5} t - 0.00506 |
| 80              | ln(1-x) = -5.4056 \times 10^{-5} t - 0.00289 |
| 90              | ln(1-x) = -1.1691 \times 10^{-4} t + 0.00048 |
| 100             | ln(1-x) = -1.7270 \times 10^{-4} t - 0.00125 |
| 110             | ln(1-x) = -1.8613 \times 10^{-4} t - 0.0046 |
| 120             | ln(1-x) = -2.1521 \times 10^{-4} t - 0.00026 |
| 120\[^a\]       | ln(1-x) = -5.0566 \times 10^{-4} t + 0.0050 |

\[^a\] oxygen was used as the oxidant.

6 Curves of conversion and selectivity with time at 80, 100 and 120 °C

Figure S4: Curves of conversion and selectivity with time. (a) reacted at 80 °C with air as oxidant;
(b) reacted at 100 °C with air as oxidant; (c) reacted at 120 °C with air as oxidant; (d) reacted at 120 °C with oxygen as oxidant.

7 Reaction Rate for R· + O₂ calculated by VTST coupled with DFT calculations

Figure S5: Minimum energy path for the R· + O₂, calculated at B3LYP/6-311+G(d,p) level of theory.

Figure S6: The reaction rate for ROO → R· + O₂, calculated by VTST coupled with DFT calculations at 378.15K

8 DFT Calculations Results for the main processes for cumene autoxidation
Cartesian coordinates of optimized all stationary points together with their single-point (a.u.) in solution and the imaginary frequencies (cm⁻¹) of transition states.
Optimized structure for $O_2$, -150.366790

|     |        |        |        |
|-----|--------|--------|--------|
| O   | 0.00000000 | 0.00000000 | 0.60280400 |
| O   | 0.00000000 | 0.00000000 | -0.60280400 |

Optimized structure for $R \cdot O_2$, -349.472878

|     |        |        |        |
|-----|--------|--------|--------|
| C   | 0.06098200 | 9.88263200 | 0.10172600 |
| C   | 0.81049400 | 10.81459200 | 0.87637000 |
| C   | 0.42679700 | 12.14271900 | 0.98300400 |
| C   | -0.71698500 | 12.61085400 | 0.32779300 |
| C   | -1.47292800 | 11.71895400 | -0.44011600 |
| C   | -1.09859000 | 10.38873900 | -0.55377900 |
| H   | 1.70111100 | 10.48450000 | 1.39606600 |
| H   | 1.02240700 | 12.82351800 | 1.58189400 |
| H   | -1.01325600 | 13.64981600 | 0.41387500 |
| H   | -2.36232000 | 12.06847100 | -0.95366800 |
| H   | -1.70554800 | 9.72452300 | -1.15596900 |
| C   | 0.45120600 | 8.51406400 | -0.01174500 |
| C   | -0.35840200 | 7.55227500 | -0.83563200 |
| H   | 0.07772800 | 6.55266000 | -0.81690700 |
| H   | -1.39149500 | 7.46835600 | -0.47375000 |
| H   | -0.42424800 | 7.86394900 | -1.88621300 |
| C   | 1.67952600 | 8.00676500 | 0.69048600 |
| H   | 1.83262500 | 6.94382900 | 0.49929700 |
| H   | 2.58625700 | 8.53424000 | 0.36672200 |
| H   | 1.61692200 | 8.14065800 | 1.77832200 |

Optimized structure for $\{R \cdots O_2\}$, -499.839855

|     |        |        |        |
|-----|--------|--------|--------|
| C   | -0.71833000 | -1.29385800 | 0.44193800 |
| C   | 0.64826600 | -1.26618600 | 0.14482000 |
| C   | 1.23721000 | -0.12331500 | -0.37430700 |
| C   | 0.47971600 | 1.05765100 | -0.62308600 |
| C   | -0.90943500 | 0.99890100 | -0.31124200 |
| C   | -1.48781400 | -0.14945700 | 0.20764300 |
| H   | -1.17453800 | -2.18937800 | 0.84760100 |
| H   | 1.25684000 | -2.14681000 | 0.32103800 |
| H   | 2.29727800 | -0.13535800 | -0.59425000 |
| H   | -1.53320300 | 1.86738800 | -0.48127000 |
| H   | -2.54897500 | -0.15711900 | 0.43306000 |
| C   | 1.07999900 | 2.23657000 | -1.15964600 |
| C   | 0.25448600 | 3.46464500 | -1.42335900 |
| H   | -0.23373400 | 3.83616900 | -0.51322900 |
| H   | 0.86778300 | 4.27445500 | -1.82072500 |
| H   | -0.54820500 | 3.27292900 | -2.14762100 |
Optimized structure for vTS1, -499.841774, 91.82i

| Element | X          | Y          | Z          |
|---------|------------|------------|------------|
| C       | -0.77301700| -1.41906200| 0.34765000 |
| C       | 0.61703200 | -1.28972300| 0.31630700 |
| C       | 1.20308000 | -0.07473500| -0.00734600|
| C       | 0.41631100 | 1.06476400 | -0.30731700|
| C       | -0.99050000| 0.90856800 | -0.26386000|
| C       | -1.57044900| -0.31153800| 0.05377400 |
| H       | -1.22849600| -2.37000100| 0.59883200 |
| H       | 1.24564300 | -2.14228900| 0.54806500 |
| H       | 2.28267200 | 0.00073100 | -0.01515200|
| H       | -1.63372400| 1.74916500 | -0.48913700|
| H       | -2.65087200| -0.40141900| 0.07365400 |
| C       | 1.03091200 | 2.33099100 | -0.63087900|
| C       | 0.19191300 | 3.52812400 | -0.96239700|
| H       | -0.64923400| 3.65085200 | -0.27724500|
| H       | 0.79002300 | 4.43962700 | -0.92735500|
| H       | -0.22128600| 3.44472000 | -1.97831300|
| C       | 2.49472600 | 2.40123500 | -0.91460800|
| H       | 3.07743300 | 2.28595200 | 0.01465500 |
| H       | 2.82102400 | 1.60761100 | -1.59438600|
| H       | 2.76896500 | 3.36275600 | -1.35042000|
| O       | 1.30370700 | 3.07855700 | 1.66113800 |
| O       | 2.44639000 | 2.87439400 | 2.07776200 |

Optimized structure for ROO-, -499.866292

| Element | X          | Y          | Z          |
|---------|------------|------------|------------|
| C       | -0.80448200| -1.45879900| 0.08196900 |
| C       | 0.50545200 | -1.30633900| 0.53620800 |
| C       | 1.13022000 | -0.06449200| 0.46820200 |
| C       | 0.45418400 | 1.05217100 | -0.04329000|
| C       | -0.86058400| 0.88934300 | -0.48977300|
| C       | -1.48352000| -0.35786900| -0.43281300|
| H       | -1.29046500| -2.42657800| 0.13117100 |
| H       | 1.04249100 | -2.15512000| 0.94353500 |
| H       | 2.14659100 | 0.03957700 | 0.82852600 |
| H       | -1.41177900| 1.73119000 | -0.88882600|
| H       | -2.50245000| -0.46348600| -0.78785300|
Optimized structure for RH, -350.103655

C  0.13742400 -0.19351600 -0.00594700
C  -0.74995600 -1.27496100 -0.01866700
C  -2.13152100 -1.07775400 -0.01367800
C  -2.65272700  0.21398200  0.00431600
C  -1.78090300  1.30332000  0.01712300
C  -0.40249300  1.09982700  0.01204800
H  -0.35435800 -2.28599300 -0.03280700
H  -2.79786000 -1.93352400 -0.02392300
H  -3.72542500  0.37191100  0.00815500
H  -2.17542100  2.31362500  0.03105200
H   0.25750500  1.96094800  0.02230000
C   1.64174900 -0.42685700 -0.00980800
H   1.79327500 -1.51888200 -0.03588300
C   2.30801900  0.10056900  1.27428300
H   3.37581000 -0.13797900  1.27817500
H   2.20933000  1.18718800  1.35531400
H   1.85650400 -0.34381400  2.16503000
C   2.31339900  0.16235600 -1.26360400
H   3.38090400 -0.07795000 -1.27519200
H   1.86485700 -0.23681200 -2.17712200
H   2.21688700  1.25183900 -1.29149600

Optimized structure for {ROO--RH}, -849.970077

C  -1.49718600  0.93500200  0.44602900
C  -1.39781900  2.18702300  1.05377300
C  -0.75911500  3.23428900  0.39762100
C  -0.21508600  3.05606800 -0.88203200
C  -0.32627200  1.80020900 -1.48404200
C  -0.95890700  0.74583800 -0.82331300
H  -1.99268400  0.11752200  0.95730000
H  -1.81904100  2.34845400  2.03966200
"Optimized structure for TS1, -849.946341, 1766.35/
C  5.39021100  0.48850600  -0.94119400
C  4.97875300  -0.71183200  -0.36179600
C  3.71629900  -0.81583900   0.21575700
C  2.83388700   0.27413800   0.21886000
C  3.25564300  1.47038100  -0.36951700
C  4.52457800  1.57885800  -0.94061500
H  6.37445700  0.57130600  -1.38837300
| Atom | X  | Y  | Z               |
|------|----|----|-----------------|
| H    | 5.64225600 | -1.56961000 | -0.35879800    |
| H    | 3.40631800 | -1.75447600 | 0.65774300     |
| H    | 2.60080900 | 2.33214500  | -0.38705400    |
| H    | 4.83132500 | 2.51789200  | -1.38796800    |
| C    | 1.46954600 | 0.13751900  | 0.89535800     |
| C    | 0.47369100 | 1.23384400  | 0.52321700     |
| H    | 0.37610000 | 1.33246800  | -0.55946800    |
| H    | -0.50333800| 0.99279300  | 0.94203800     |
| H    | 0.78346700 | 2.19609800  | 0.93643600     |
| C    | 1.62679200 | 0.03673000  | 2.41867100     |
| C    | 2.28650800 | -0.79408500 | 2.68467700     |
| H    | 0.65483400 | -0.12608600 | 2.88779700     |
| H    | 2.05964700 | 0.95794300  | 2.80863700     |
| O    | 0.98737500 | -1.15597500 | 0.36990500     |
| O    | -0.20359800| -1.55648500 | 0.98253200     |
| C    | -2.93863800| -0.19802800 | -0.37522600    |
| C    | -3.63713100| -0.05601200 | 0.84177000     |
| C    | -4.35847800| 1.09577700  | 1.13268200     |
| C    | -4.40965300| 2.14668100  | 0.21506200     |
| C    | -3.72452600| 2.02931300  | -0.99291200    |
| C    | -2.99489200| 0.87850100  | -1.28089400    |
| H    | -3.60361200| -0.85074600 | 1.57686800     |
| H    | -4.88158400| 1.17558400  | 2.07924600     |
| H    | -4.97493700| 3.04383100  | 0.44028500     |
| H    | -3.58535700| 2.83598200  | -1.71702900    |
| H    | -2.47767600| 0.81426400  | -2.22939000    |
| C    | -2.15532600| -1.43103200 | -0.66494800    |
| H    | -1.13691000| -1.38704300 | 0.17352700     |
| C    | -1.45303000| -1.51353200 | -2.00976800    |
| H    | -0.82240800| -0.64516500 | -2.20848700    |
| H    | -0.81575900| -2.39923900 | -2.04731900    |
| H    | -2.18198000| -1.59549200 | -2.82712900    |
| C    | -2.80103600| -2.75122800 | -0.25757900    |
| H    | -2.08965800| -3.57267800 | -0.36484700    |
| H    | -3.15818200| -2.75189900 | 0.77297300     |
| H    | -3.66168500| -2.96223700 | -0.90557200    |

Optimized structure for {ROOH–R'}, 849.967875
H  -5.70897400  2.32861300  -0.87933100
H  -4.28394200  2.69685900  1.12397500
H  -2.54154100  1.06083600  1.72217000
H  -3.61569000  -1.31925000 -1.68696100
H  -5.35734000   0.30296500  -2.27335200
C  -1.88094100  -1.26979800  0.49330300
C  -1.52725000  -2.92095000  -0.58793100
H  -1.25192400  -1.79955600  -1.52295800
H  -0.68521000  -2.89602200  -0.24784200
H  -2.36363800  -2.96783000  -0.77898300
C  -2.29270900  -1.97306400  1.79550300
H  -1.50851300  -2.65724500  2.12267300
H  -2.47576200  -1.24511200  2.58758900
H  -3.21049800  -2.54336600  1.63301200
O  -0.73101200  -0.40063100  0.73845100
O   0.36202400  -1.18111200  1.30256900
C   3.20042100   0.66480100  -0.26869100
C   4.34033600   0.11027600  0.38211900
C   4.72651600  -1.20500080  0.17406800
C   4.00409400  -2.03620300  -0.68865300
C   2.88037500  -1.52059600  -1.34356300
C   2.48196200  -0.20570100  -1.14185800
H   4.92009900   0.72393900  1.05971500
H   5.59882500  -1.59175900  0.68997300
H   4.31035700  -3.06326400  -0.84828800
H   2.31342000  -2.15095700  -2.02048900
H   1.61590000   0.16693200  -1.67439200
C   2.79464800   2.01634500  -0.05788600
H   1.04184400  -1.05434500  0.61898100
C   1.56260200   2.55797000  -0.72613600
H   0.66893400   1.97596900  -0.46952500
H   1.37913600   3.59261100  -0.43385100
H   1.64612500   2.53523700  -1.82089900
C   3.57698800   2.91679400   0.85575400
H   3.18399700   3.93403600   0.83649400
H   3.54195400   2.57105700   1.89794200
H   4.63754100   2.96473600  0.58070400

Optimized structure for ROOH, -500.470546
C  -2.28417000   2.07782000   0.88060400
C  -1.38665600   2.96946300  1.46809800
C  -0.14276200   3.19771800  0.88638700
C   0.22716400   2.54737900  -0.29979900
C  -0.68371900   1.66203800  -0.88385900

S13
|   | C          | H          | O          |
|---|------------|------------|------------|
|   | -1.92689300 | 1.42434400 | -0.29563500 |
| H | -3.25177400 | 1.89652800 | 1.33489100  |
| H | -1.65488500 | 3.48814500 | 2.38183600  |
| H | 0.54334100  | 3.89665200 | 1.34789300  |
| H | -0.43426700 | 1.14496100 | -1.80136100 |
| H | -2.61565200 | 0.72962400 | -0.76343000 |
| C | 1.61580100  | 2.80085600 | -0.89306400 |
| C | 1.78842700  | 2.28264500 | -2.32134300 |
| H | 1.01227100  | 2.67597100 | -2.98139100 |
| H | 2.76352100  | 2.59007200 | -2.70172200 |
| H | 1.75454400  | 1.19153900 | -2.34976300 |
| C | 2.71004400  | 2.24254600 | 0.02835500  |
| H | 3.69900100  | 2.47217400 | -0.37113100 |
| H | 2.62864200  | 2.66882700 | 1.02948000  |
| H | 2.60760000  | 1.15756600 | 0.10692500  |
| O | 1.66465200  | 4.26429700 | -0.89617400 |
| O | 2.99009000  | 4.71372100 | -1.30376700 |
| H | 2.77775200  | 5.16023200 | -2.13562600 |

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