

This update to the ESI includes corrections to the previous version published on 11 January 2019.

## Update to Supporting Information

### Converting benzene into $\gamma$ -graphyne and its enhanced electrochemical oxygen evolution performance

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## List of Contents

### 1. CALCULATION

#### 1) Calculation of Gibbs free energy change

### 2. CHARACTERIZATIONS

#### 3) Figure S3 The crystal lattices of $\gamma$ -graphyne.

### 1. CALCULATION

#### 1) Calculation of Gibbs free energy change:

The mechanism is divided into 2 steps: the first is the destroy of C-H bond by mechanochemistry, the second is reaction between  $C_6$  fragments and  $CaC_2$ . Mechanochemistry is a powerful technology which could provide the driven force and energy input for the non-spontaneous first step. After the dehydrogenation of C-H, the second step is calculated to be spontaneous, as listed below.

Enthalpy change:

$$\Delta H = H_{\gamma\text{-graphyne}} - H_{C_6} + H_{Ca} - H_{CaC_2}$$

$$= \frac{6N}{N_A} (E_{C-C(\text{aromatic})} + E_{C-C} - E_{C-C(\text{aromatic})}) + \frac{3N}{N_A} (\Delta_f H_{Ca}^\theta - \Delta_f H_{CaC_2}^\theta)$$

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$$= \frac{6N}{N_A}(-332) + \frac{3N}{N_A}(0 + 63)$$

$$= -1614 \frac{N}{N_A} \text{ (kJ)}$$

Entropy change:

$$\Delta S = S_{\gamma\text{-graphyne}} - S_{C_6} + S_{Ca} - S_{CaC_2} + \Delta S_{\text{mix}}$$

$$= \frac{1}{N_A} \Delta_f S_{\gamma\text{-graphyne}}^\theta - \frac{N}{N_A} \Delta_f S_{C_6}^\theta + 3 \frac{N}{N_A} (\Delta_f S_{Ca}^\theta - \Delta_f S_{CaC_2}^\theta) + \Delta S_{\text{mix}}$$

$$= \frac{1}{N_A} \Delta_f S_{\gamma\text{-graphyne}}^\theta - \frac{N}{N_A} \Delta_f S_{C_6}^\theta + 3 \frac{N}{N_A} (42 - 70) + k \ln \frac{(3N+1)!}{3N!} - k \ln \frac{(N+3N)!}{(3N)! \cdot N!}$$

$$= \frac{1}{N_A} (\Delta_f S_{\gamma\text{-graphyne}}^\theta - \Delta_f S_{C_6}^\theta) - 84 \frac{N}{N_A} + k \ln(3N+1) - 9.5kN \text{ (J/K)}$$

Gibbs free energy change:

$$\Delta G = \Delta H - T\Delta S$$

$$= -1614000 \frac{N}{N_A} - \frac{T}{N_A} (\Delta_f S_{\gamma\text{-graphyne}}^\theta - \Delta_f S_{C_6}^\theta) + 84 \frac{NT}{N_A} - kT \ln(3N+1) + 9.5kNT$$

$$= -\frac{T}{N_A} (\Delta_f S_{\gamma\text{-graphyne}}^\theta - \Delta_f S_{C_6}^\theta) - kT \ln(3N+1) - \frac{N}{N_A} (1614000 - 84T - 9.5RT)$$

When  $T < 9903K$ ,  $\Delta G < 0$

## 2. CHARACTERIZATIONS

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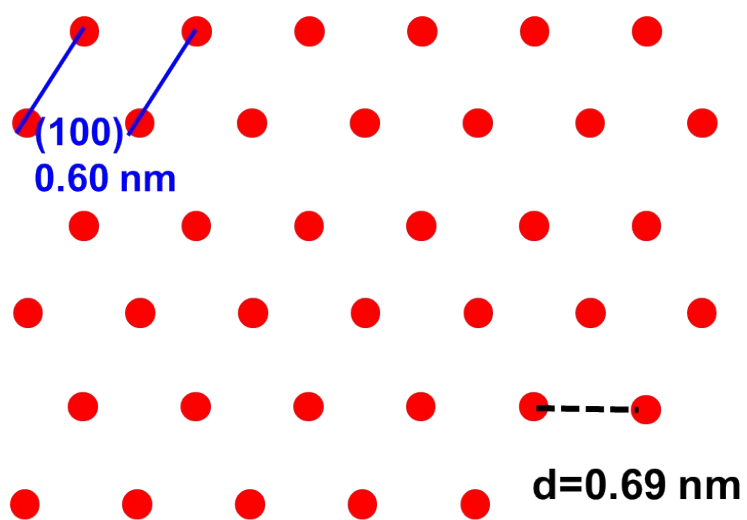


Figure S3 The crystal lattices of  $\gamma$ -graphyne.