Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A.
This journal is © The Royal Society of Chemistry 2020

Electronic Supplementary Information

Efficient visible-light activation of molecular oxygen to produce hydrogen peroxide by P doped g-C_3N_4 hollow sphere

Xueming Dang[a], Ruying Yang[a], Zhe Wang[a], Siyi Wu[a], Huimin Zhao[a*]

[a] Key Laboratory of Industrial Ecology and Environmental Engineering (Ministry of Education, China), School of Environmental Science and Technology, Dalian University of Technology, Dalian 116024, China.

* To whom correspondence should be addressed. E-mail: zhaohuim@dlut.edu.cn; Tel: 86-411-84706800.

Table of Contents for Supporting Information

1. Preparation of SiO_2 sphere

Silica sphere were prepared via Stöber method with a little modification.[1] Briefly, 3.5 mL of aqueous ammonia (32 wt%) was added into an isopropanol solution containing 74.14 mL of isopropanol and 10 mL of ultrapure water. Sequentially, the mixture was stirred at 30 °C for 30 min before 5.6 mL of TEOS was added under vigorous stirring. Then the mixture was left stationary for 1 h to prepare uniform nonporous silica sphere. A mixture of TEOS (4.48 mL) and C_{18}TMOS (2.12 mL) was then added dropwise to the above solution under mild stirring. The mixed solution was further kept stationary at ambient temperature for 3 h. The white precipitate was obtained by centrifugation and dried at 70 °C for 6 h. Finally, the SiO_2 template was obtained after the calcination at 550 ℃ for 6 h in air.

2. Theoretical calculations

Geometry optimizations for all structures were carried out by using the DFT functional B3LYP with 6-31G (d) basis sets. Frequency calculations were done to confirm the stationary points at the same level. High accuracy energies in Table S3, Table S4 and Table S5 were calculated by using the PBE0 functional with 6-311G (d) basis sets. All calculations were performed in water using the Gaussian09 program. Basis set convergence tests were performed with respect to the choice of different basis set. The electron structures of the BCN and PCNHS were further calculated via an electron localization function (ELF) using Multiwfn.

3. Fabrication of samples coated FTO electrodes

The FTO glasses (1×1.5 cm^2) were firstly cleaned by washing with soap followed by sonication in isopropanol, acetone and water. Subsequently, the particles were dispersed in the ultrapure water (1 g L^{-1}) with addition of 0.05 g L^{-1} $Mg(NO_3)_2$. These samples were then coated on a fluoride tin oxide glass (FTO) through an electrophoresis method with a pure FTO as the counter electrode under the 5 V for 100 s.

4. Calculation processes for determining energy band structure of photocatalyst

The energy band structure of photocatalyst can be determined as follow: Firstly, the flat band (E_f) potential is obtained by fitting the Mott-Schottky plots. Secondly, the electric potential difference (ΔE) between the E_f and the valance band (VB) is measured by VB XPS. And the VB potential (E_{VB}) of photocatalyst can be calculated according to the equation (S1). Thirdly, the optical bandgap energy (E_g) is determined by transforming the plots of UV-vis absorption spectra. Then the conduction band potential (E_{CB}) is obtained from the equation (S2).

$$E_{VB} = E_f + \Delta E \quad \text{(S1)}$$

$$E_{CB} = E_{VB} - E_g \quad \text{(S2)}$$

5. XPS spectra of BCN and PCNHS-17

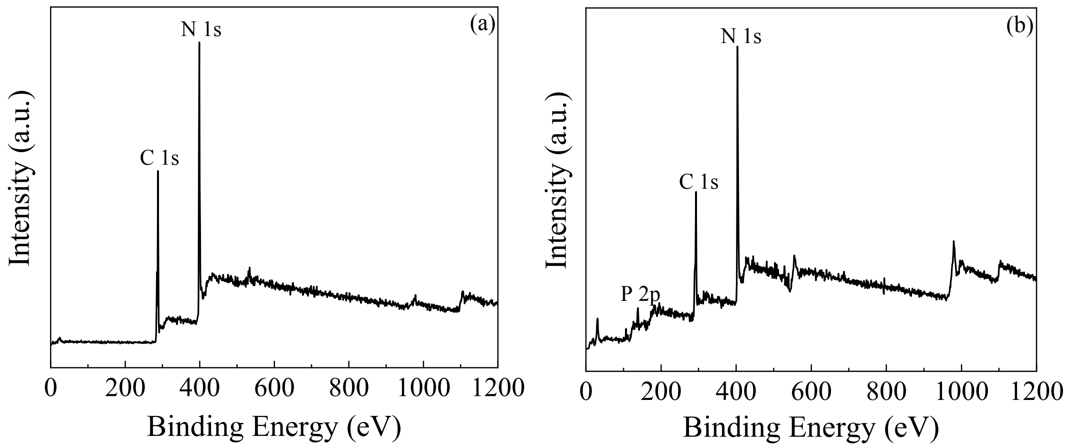


Fig. S1. XPS spectra of (a) BCN and (b) PCNHS-17.

6. XPS spectra of C 1s and N 1s of BCN

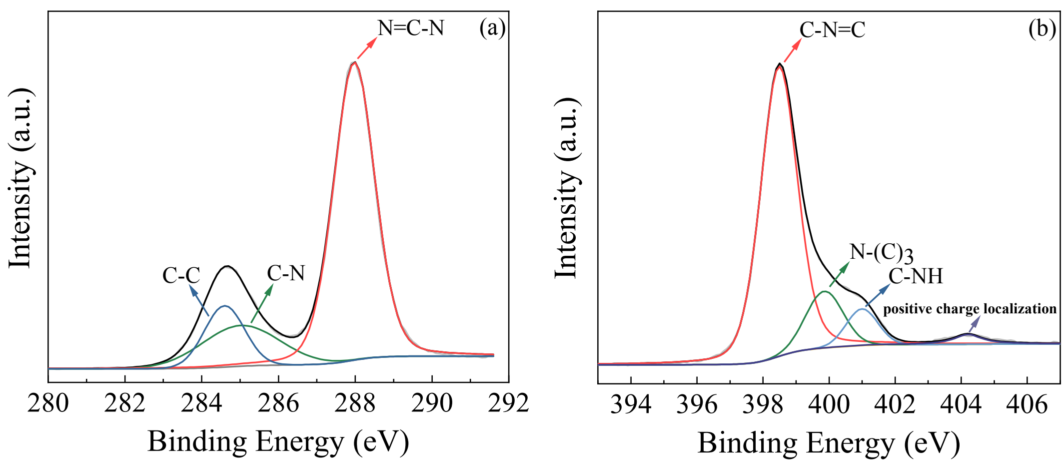


Fig. S2. XPS spectra of (a) C 1s and (b) N 1s of BCN.

7. Atomic concentrations of C, N, P and O elements in BCN and PCNHS-17

Table S1. Atomic concentrations (at%) of C, N, P and O elements in BCN and PCNHS-17.

	C (%)	N (%)	O (%)	P (%)	C/N
PCNHS-17	38.42	53.49	6.06	2.03	0.72
BCN	40.02	53.75	6.23	-	0.74

8. SEM of BCN and SiO_2 templates

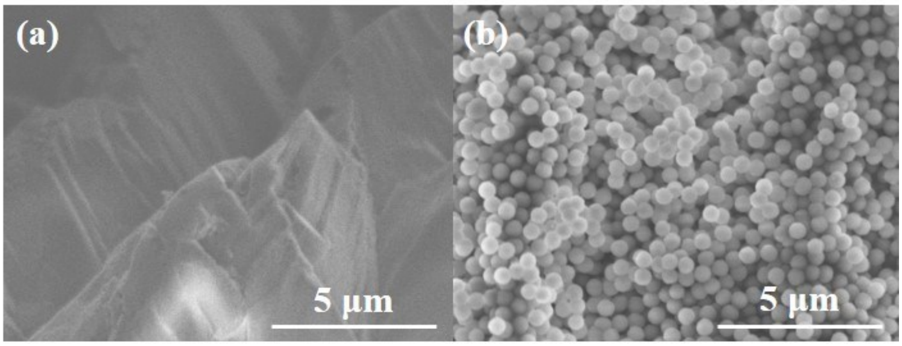


Fig. S3. SEM of (a) BCN and (b) SiO_2 templates.

9. Nitrogen adsorption-desorption isotherms of BCN and PCNHS-17

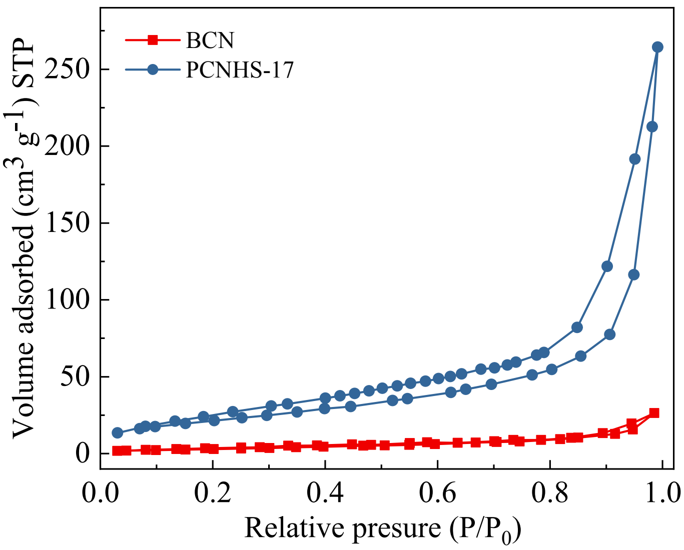


Fig. S4. Nitrogen adsorption-desorption isotherms of BCN and PCNHS-17.

10. Lowest unoccupied molecular orbital and highest occupied molecular orbital of BCN

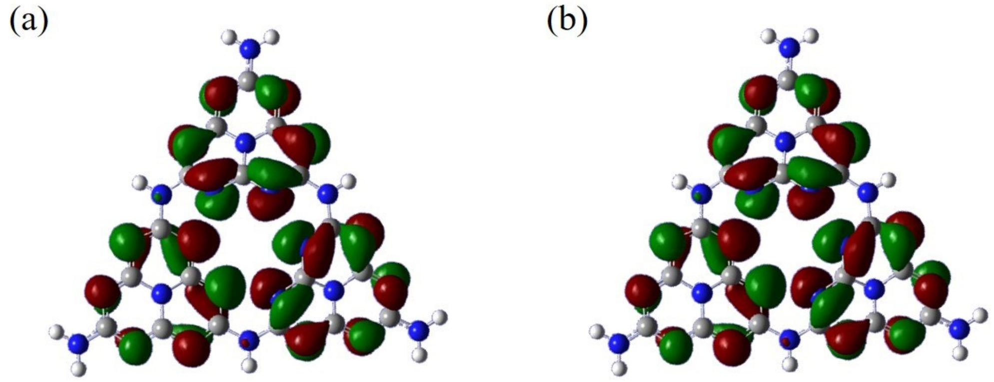


Fig. S5. (a) The lowest unoccupied molecular orbital (LUMO) and (b) the highest occupied molecular orbital (HOMO) of BCN. The isosurface is taken at a value of 0.002 e/Bohr3.

11. Lowest unoccupied molecular orbital and highest occupied molecular orbital of PCNHS-17

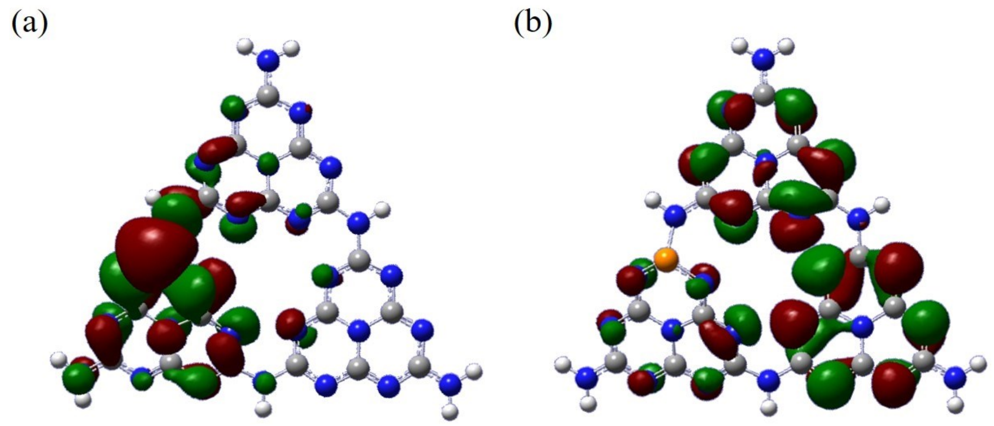


Fig. S6. (a) LUMO) and (b) HOMO of PCNHS-17. The isosurface is taken at a value of 0.002 e/Bohr3.

12. The effect of P precursor on H_2O_2 production

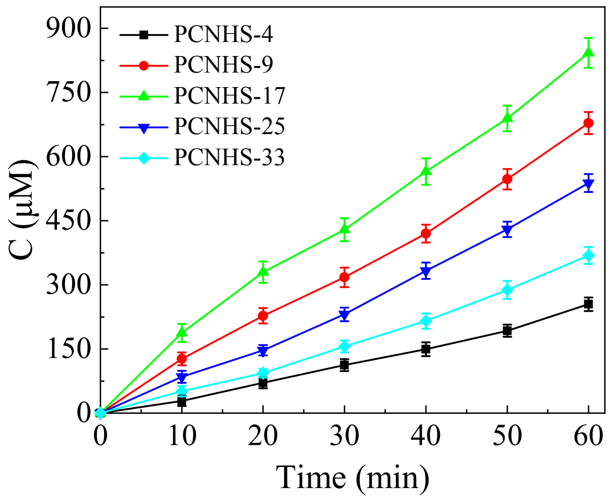


Fig. S7. The effect of P precursor on H_2O_2 production with isopropanol as hole sacrificial agent.

13. Comparison of photocatalytic H_2O_2 production by different g-C_3N_4 based photocatalysts

Table S2. Comparison of photocatalytic H_2O_2 production by different g-C_3N_4 based photocatalysts

Catalyst	Condition	Formed H_2O_2 (μmol h^{-1} g^{-1})	Ref.
PCNHS-17	H_2O (50 mL), catalyst (0.025 g, 0.5 g L^{-1}), O_2-equilibrated, Xe-lamp (λ≥420nm), 100 mW cm^{-2}, pH = 7, 25 °C.	174	This work
PCNHS-17	H_2O (50 mL), catalyst (0.025 g, 0.5 g L^{-1}), O_2-equilibrated, isopropanol (10 vol%), Xe-lamp (λ≥420nm), 100 mW cm^{-2}, pH = 7, 25 °C.	1684	This work
Ag@U-g-C_3N_4-NS	H_2O (100 mL), catalyst (0.1 g, 1 g L^{-1}), O_2-equilibrated, Xe-lamp (λ≥420nm), 100 mW cm^{-2}, pH = 3, 25 °C.	70	[2]
OCNs	H_2O (50 mL), catalyst (0.05g, 1 g L^{-1}); O_2-equilibrated; Xe-lamp (λ≥420nm), 35.2 mW cm^{-2}; pH = 7; 25 °C.	90	[3]
OCNs	H_2O (50 mL), catalyst (0.05g, 1 g L^{-1}); O_2-equilibrated; isopropanol (10 vol %); Xe-lamp (λ≥420nm), 35.2 mW cm^{-2}; pH=7; 25 °C.	1200	[3]
DCN	H_2O (60 mL), catalyst (0.05 g, 0.83 g L^{-1}), O_2-equilibrated, isopropanol (20 vol %), Xe-lamp (λ≥420nm), 100 mW cm^{-2}.	100	[4]
POCN	H_2O (200 mL), catalyst (0.2 g, 0.15 g of EDTA), O_2-equilibrated, High pressure sodium-lamp (λ ≥ 400nm), pH = 7, 30 °C.	2	[5]
AQ-C_3N_4	catalyst (0.5 g L^{-1}), O_2-equilibrated, 2-propanol (10 vol %), Xe-lamp (100 mW cm^{-2}), pH = 7.	361	[6]
3DOM g-$C_3N_4PW_{11}$	H_2O (100 mL), catalyst (0.1 g, 1 g L^{-1}); O_2-equilibrated; Xe-lamp (λ ≥ 320 nm); 25 ℃.	35	[7]
C-N-g-C_3N_4	H_2O (15 mL), catalyst (0.02 mg, 1.33 g L^{-1}); O_2-equilibrated; (700 nm≥ λ ≥ 420 nm).	49	[8]
IO CN-Cv	H_2O (20 mL), catalyst (0.02 mg, 1 g L^{-1}) O_2-equilibrated; ethanol (5 vol %); Xe-lamp (λ ≥ 420 nm).	325.4	[9]

g-C_3N_4/PDI-$BN_{0.2}$-$rGO_{0.05}$	H_2O (30 mL), catalyst (50 mg, 1.67 g L^{-1}); O_2 (1 atm), 2-PrOH (10 vol %), Xe- lamp ($\lambda \geq 420$ nm), 25 ℃.	2000	[10]
Au/C_3N_4	H_2O (30 mL), catalyst (40 mg, 1.33 g L^{-1}); O_2-equilibrated; isopropanol (10 vol %); Xe- lamp ($\lambda \geq 420$ nm).	816.75	[11]
g-C_3N_4/PDI/$rGO_{0.05}$	H_2O (50 mL), catalyst (250 mg, 5 g L^{-1}), O_2 (1 atm), Xe-lamp ($\lambda \geq 420$ nm), 13.1 mW cm^{-2}.	80	[12]
KPD-CN	H_2O (36 mL), catalyst (20 mg, 0.56 g L^{-1}), Xe-lamp ($\lambda \geq 420$ nm), 726.8 mW cm^{-2}).	500	[13]
CNK-OH	H_2O (5 mL), catalyst (10 mg, 2 g L^{-1}), O_2-equilibrated; Xe-lamp ($\lambda > 400$ nm).	78	[14]
CNK-OH	H_2O (5 mL), catalyst (10 mg, 2 g L^{-1}), O_2-equilibrated; isopropanol (1000 μmol), Xe-lamp ($\lambda > 400$ nm).	1020	[14]
g-C_3N_4/BDI_{50}	H_2O (30 mL), catalyst (50 mg, 1.67 g L^{-1}), Xe-lamp ($\lambda > 420$ nm), 25 ℃.	20	[15]
$Bi_4O_5Br_2$/g-C_3N_4	H_2O (50 mL), catalyst (50 mg, 1 g L^{-1}), Xe-lamp ($\lambda > 420$ nm).	124	[16]

14. The photocatalytic H_2O_2 production by BCN, CNHS, PBCN and PCNHS-17

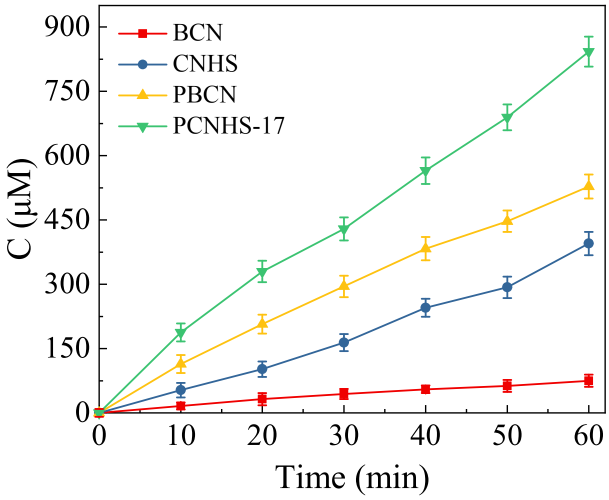


Fig. S8. The photocatalytic H_2O_2 production by BCN, CNHS, PBCN and PCNHS-17 with isopropanol as hole sacrificial agent.

15. XRD pattern of PCNHS-17 after photocatalytic H_2O_2 production process

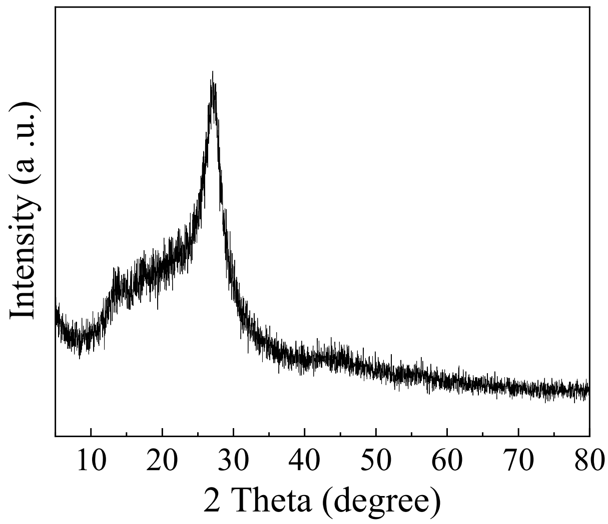


Fig. S9. XRD pattern of PCNHS-17 after the photocatalytic H_2O_2 production process.

16. FT-IR spectrum of PCNHS-17 after photocatalytic H_2O_2 production process

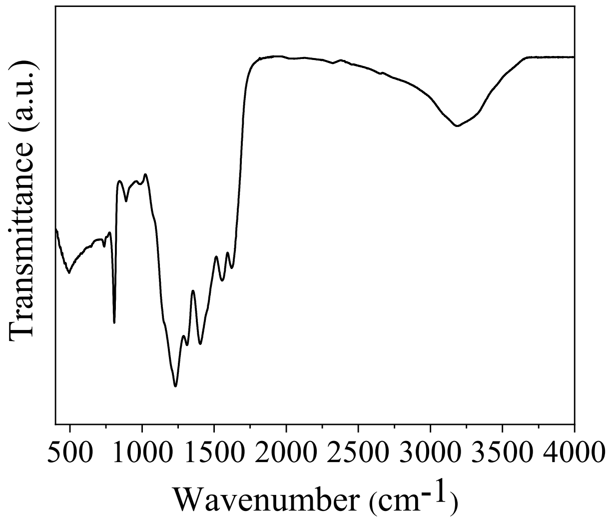


Fig. S10. FT-IR spectrum of PCNHS-17 after the photocatalytic H_2O_2 production process.

17. XPS spectra of PCNHS-17 after photocatalytic H_2O_2 production process

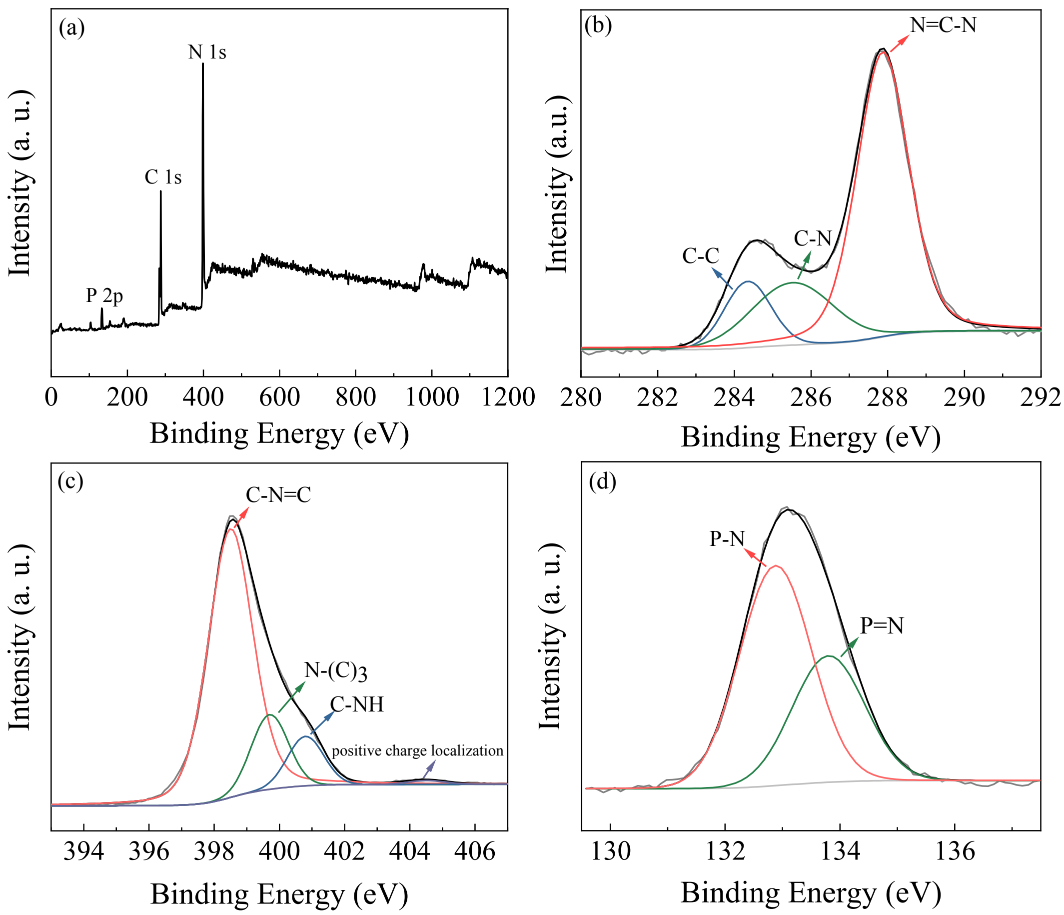


Fig. S11. XPS spectra of (a) PCNHS-17, (b) C 1s, (c) N 1s and (d) P 2p after photocatalytic H_2O_2 production.

18. LSV curves and Koutecky-Levich plots of BCN

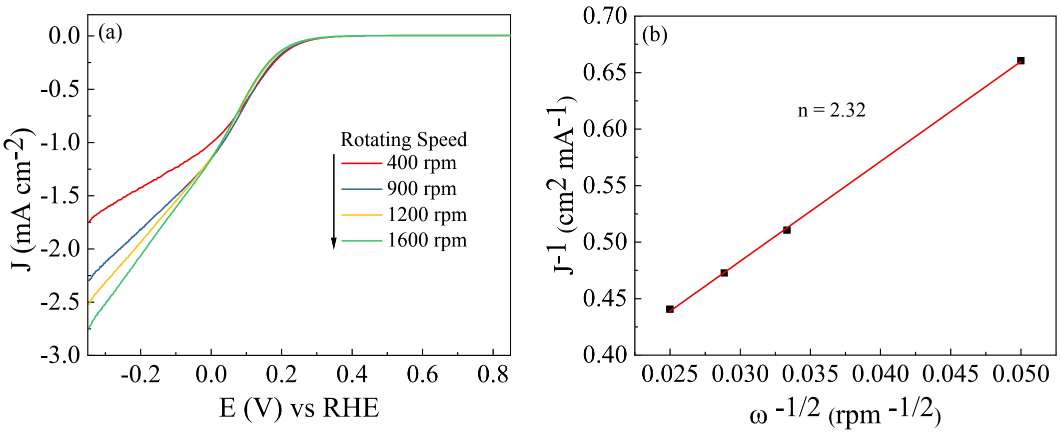


Fig. S12. (a) LSV curves of BCN measured on a RDE at different rotating speeds; (b) Koutecky-Levich plots of the data obtained at the constant electrode potential (0 V vs. SCE).

19. LSV curves and Koutecky-Levich plots of CNHS

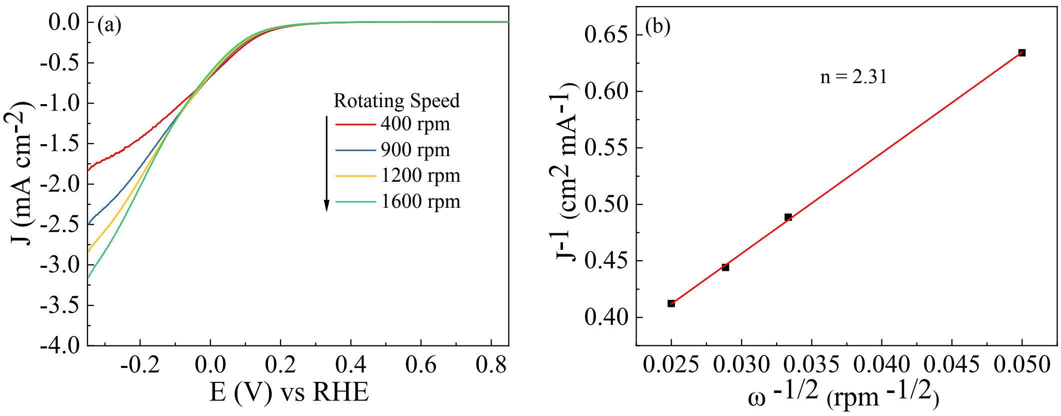
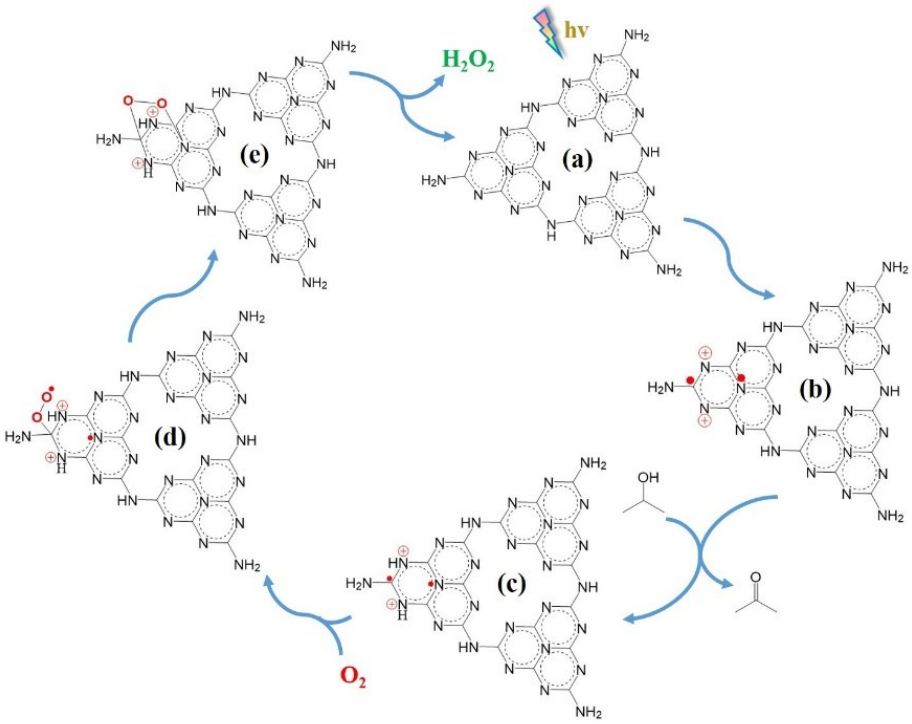


Fig. S13. (a) LSV curves of CNHS measured on a RDE at different rotating speeds; (b) Koutecky-Levich plots of the data obtained at the constant electrode potential (0 V vs. SCE).

20. Mechanism of photocatalytic O_2 reduction to generate H_2O_2 in BCN system



Scheme S1. The mechanism of photocatalytic O_2 reduction to generate H_2O_2 in BCN system.

21. The energy of b→c

The isopropanol is used as a hole trapping and acetone is its corresponding oxidation product in the photocatalytic H_2O_2 production.[3,17] Thus, the energy change form intermediate (b) to intermediate (c) is calculated based on the equation (S3).

Table S3. The energy of b→c

	b	c	acetone	isopropanol	ΔE (kcal mol^{-1})
PCNHS	-2471.0131	-2472.2243	-192.9604	-194.2518	50.3263
BCN	-2167.9130	-2169.1067			61.3077

$$\Delta E(b\rightarrow c) = E(c) + E(acetone) - E(b) - E(isopropanol) \qquad (S3)$$

22. The energy of d→e

Table S4. The energy of d→e

	d	e	ΔE (kcal mol^{-1})
PCNHS	-2622.4363	-2622.4240	7.7184
BCN	-2319.3782	-2319.3629	9.6009

$$\Delta E(d\rightarrow e) = E(e) - E(d) \qquad (S4)$$

23. The energy of e→a

Table S5. The energy of e→a

	e	a	H_2O_2	ΔE (kcal mol^{-1})
PCNHS	-2622.4240	-2471.1061	-151.4297	-70.1556
BCN	-2319.3629	-2168.0033		-43.9878

$$\Delta E(e\rightarrow a) = E(a) + E(H_2O_2) - E(e) \qquad (S5)$$

24. Basis set convergence tests

Basis set convergence tests have been performed for BCN and PCNHS. The results of these calculations are summarized in Table S6, which show the reaction energy differences are converged within 4%, indicating the 6-311G (d) results are well converged.[18,19]

Table S6. The reaction energy basis set convergence test.

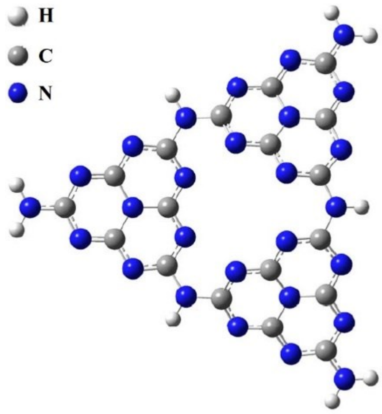
Basis Set	ΔE(b→c) (kcal mol^{-1})		ΔE(d→e) (kcal mol^{-1})		ΔE(e→a) (kcal mol^{-1})	
	BCN	PCNHS	BCN	PCNHS	BCN	PCNHS
6-31G	63.5668	52.2088	9.9147	7.9694	-44.7415	-72.2264
6-311G	61.3077	50.3263	9.6009	7.7184	-43.9878	-70.1556

1. J.H. Sun, J.S. Zhang, M.W. Zhang, M. Antonietti, X.Z. Fu, X.C. Wang, *Nat. Commun.*, 2012, **3**, 1-7.
2. J.S. Cai, J.Y. Huang, S.C. Wang, J. Iocozzia, Z.T. Sun, J.Y. Sun, Y.K. Yang, Y.K. Lai, Z.Q. Lin, *Adv. Mater.*, 2019, **31**, 1-11.
3. Z. Wei, M.L. Liu, Z.J. Zhang, W.Q. Yao, H.W. Tan, Y.F. Zhu, *Energ. Environ. Sci.*, 2018, **11**, 2581-2589.
4. L. Shi, L.Q. Yang, W. Zhou, Y.Y. Liu, L.S. Yin, X. Hai, H. Song, J.H. Ye, *Small*, 2018, **14**, 1-9.
5. J. Bai, Y.Z. Sun, M.Y. Li, L.N. Yang, J. Li, *Diam. Relat. Mater.*, 2018, **87**, 1-9.
6. H.I. Kim, Y. Choi, S. Hu, W. Choi, J.H. Kim, *Appl. Catal. B: Environ.*, 2018, **229**, 121-129.
7. S. Zhao, X. Zhao, H. Zhang, J. Li, Y.F. Zhu, *Nano Energy*, 2017, **35**, 405-414.
8. Y.J. Fu, C.A. Liu, M.L. Zhang, C. Zhu, H. Li, H.B. Wang, Y.X. Song, H. Huang, Y. Liu, Z.H. Kang, *Adv. Energ. Mater.*, 2018, **8**, 1-9.
9. J.Y. Lei, B. Chen, W.J. Lv, L. Zhou, L.Z. Wang, Y.D. Liu, J.L. Zhang, *ACS Sustain. Chem. Eng.*, 2019, **7**, 16467-16473.
10. Y. Kofuji, Y. Isobe, Y. Shiraishi, H. Sakamoto, S. Ichikawa, S. Tanaka, T. Hirai, *Chemcatchem*,

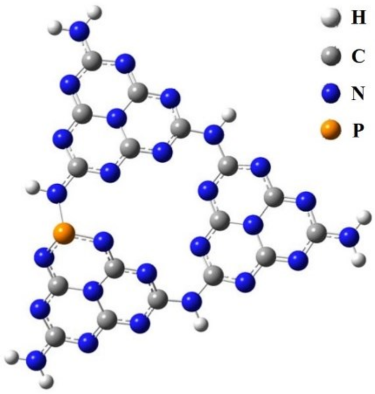
2018, **10**, 2070-2077.

11. S.J. Jiang, C.B. Xiong, S.Q. Song, B. Cheng, *ACS Sustain. Chem. Eng.*, 2019, **7**, 2018-2026.
12. Y. Kofuji, Y. Isobe, Y. Shiraishi, H. Sakamoto, S. Tanaka, S. Ichikawa, T. Hirai, *J. Am. Chem. Soc.*, 2016, **138**, 10019-10025.
13. G.H. Moon, M. Fujitsuka, S. Kim, T. Majima, X.C. Wang, W. Choi, *ACS Catal.*, 2017, **7**, 2886-2895.
14. Y.X. Li, S.X. Ouyang, H. Xu, X. Wang, Y.P. Bi, Y.F. Zhang, J.H. Ye, *J. Am. Chem. Soc.*, 2016, **138**, 13289-13297.
15. Y. Kofuji, S. Ohkita, Y. Shiraishi, H. Sakamoto, S. Tanaka, S. Ichikawa, T. Hirai, *ACS Catal.*, 2016, **6**, 7021-7029.
16. X. Zhao, Y. You, S. Huang, Y. Wu, Y. Ma, G. Zhang, Z. Zhang, *Appl. Catal. B: Environ.*, 2020, 119251.
17. J.Z. Zhang, C.Y. Yu, J.Y. Lang, Y.F. Zhou, B.X. Zhou, Y.H. Hu, M.C. Long, *Appl. Catal. B: Environ.*, 2020, **277**, 119225.
18. D. Krepel, L. Kalikhman-Razvozov, O. Hod, *J. Phys. Chem. C*, 2014, **118**, 21110-21118.
19. N. Myllys, J. Elm, T. Kurtén, *Comput. Theor. Chem.*, 2016, **1098**, 1-12.

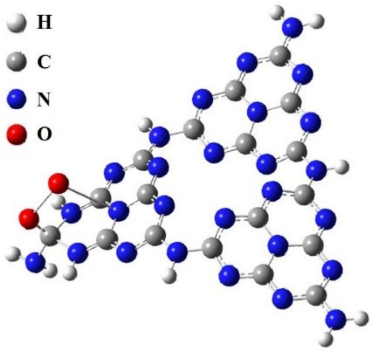
Cartesian Coordinates (in Å)



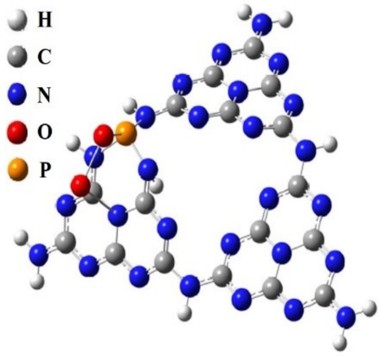
	BCN				a (54 atom)		
N	4.003885	-2.218804	0.40354	C	-6.634015	-0.010477	0.138901
C	3.193743	-1.23791	0.833662	H	-2.481252	4.298862	-0.308829
N	3.805257	0.005995	0.951947	N	4.104383	4.452102	-0.282026
N	1.896185	-1.328445	1.118337	C	3.39574	5.554539	-0.626492
C	1.27512	-2.419353	0.685963	N	2.046572	5.679566	-0.689712
N	-0.047605	-2.496452	0.723941	C	1.337367	4.629687	-0.315046
N	2.013374	-3.469984	0.140691	N	-0.001548	4.613035	-0.401009
C	3.418371	-3.383455	0.097322	N	2.002316	3.476227	0.14125
N	4.118618	-4.439938	-0.28008	C	3.407506	3.393833	0.096598
C	3.41347	-5.544714	-0.624266	N	3.996577	2.231001	0.402725
N	2.064726	-5.67377	-0.688573	C	3.189759	1.248091	0.834405
C	1.352113	-4.625702	-0.315316	N	1.892346	1.335249	1.121264
N	0.01322	-4.613006	-0.402414	C	1.267613	2.423867	0.688143
C	-0.598929	-3.517322	0.061407	N	-0.055345	2.497052	0.726862
N	-2.012913	1.148801	-0.52503	C	-0.610092	3.515812	0.06386
C	-2.704055	2.253198	-0.231003	H	4.786485	0.007707	0.693461
N	-1.978802	3.433549	-0.1491	N	-7.966963	-0.012609	0.239068
N	-4.024264	2.361328	-0.036089	H	-8.472882	0.859958	0.284899
C	-4.720941	1.215467	-0.032448	H	-8.470206	-0.886764	0.284084
N	-6.035943	1.205128	0.100409	N	4.106136	6.636851	-0.959547
N	-4.028509	-0.00618	-0.136851	H	3.635384	7.485673	-1.237616
C	-2.657727	-0.003869	-0.407381	H	5.115189	6.604989	-0.944572
N	-2.009314	-1.154381	-0.526488	N	4.127301	-6.625266	-0.955699
C	-2.69684	-2.261217	-0.233206	H	5.136246	-6.590336	-0.940342
N	-4.016661	-2.373714	-0.038201	H	3.65924	-7.475495	-1.234021
C	-4.71702	-1.230122	-0.033537	N	-1.967787	-3.439295	-0.152134
N	-6.032058	-1.224115	0.099384	H	-2.467605	-4.306162	-0.311701



PCNHS				a (54 atom)			
N	-3.610444	2.956613	0.344561	C	6.683136	-0.86244	0.228995
C	-2.997712	1.809308	0.681812	H	1.995038	-4.586836	-0.238435
N	-3.844813	0.741198	0.892234	N	-4.530666	-3.95769	-0.548384
N	-1.687184	1.592256	0.808149	C	-3.90896	-5.083073	-0.958462
C	-0.883631	2.584348	0.443746	N	-2.583412	-5.331055	-0.922655
N	0.430699	2.422194	0.459599	C	-1.814548	-4.391375	-0.398749
N	-1.423251	3.799864	0.01432	N	-0.482448	-4.54275	-0.440766
C	-2.819155	3.985128	0.020166	N	-2.380367	-3.218886	0.153567
N	-3.318022	5.166704	-0.302507	C	-3.796896	-3.00726	0.008771
C	-2.428013	6.136299	-0.621978	N	-4.364569	-1.861578	0.378456
N	-1.079045	6.023499	-0.689681	N	-1.959974	-1.216183	1.444901
C	-0.566267	4.845229	-0.380995	C	-1.515352	-2.293087	0.811009
N	0.750355	4.60926	-0.472055	N	-0.203402	-2.506754	0.774109
C	1.161998	3.393496	-0.092119	C	0.241355	-3.551959	0.07632
N	1.959758	-1.416406	-0.5166	H	-4.830251	0.991344	0.847864
C	2.495463	-2.594365	-0.184537	N	8.001865	-1.03274	0.367917
N	1.617545	-3.657791	-0.093758	H	8.387063	-1.962827	0.444888
N	3.787248	-2.872497	0.036775	H	8.615517	-0.231584	0.399211
C	4.629368	-1.830191	0.033243	N	-4.687658	-6.04668	-1.464447
N	5.930643	-1.989249	0.205101	H	-4.277673	-6.908122	-1.794668
N	4.108639	-0.531499	-0.123196	H	-5.686358	-5.911802	-1.52334
C	2.757525	-0.360803	-0.433769	N	-2.93728	7.337664	-0.913617
N	2.276931	0.858753	-0.623336	H	-3.935917	7.484256	-0.888918
C	3.089831	1.872199	-0.320755	H	-2.324869	8.098976	-1.168025
N	4.405871	1.818621	-0.07843	N	2.511887	3.131197	-0.271641
C	4.949953	0.59388	-0.030087	H	3.127957	3.929447	-0.371422
N	6.248892	0.418566	0.140189	P	-3.553576	-0.882485	1.405703



		BCN				e (58 atoms)	
N	3.716016	2.125247	0.259913	H	-5.34121100	0.34946600	-0.214716
C	2.444327	2.000427	0.686813	N	-1.81997500	5.91816700	-0.263183
N	1.757051	3.19507	0.823652	C	-3.14347700	5.94338700	-0.555829
N	1.806104	0.865313	0.953393	N	-3.996682	4.889927	-0.599378
C	2.363824	-0.252632	0.510295	C	-3.50213	3.713719	-0.257339
N	1.686258	-1.388305	0.544299	N	-4.232792	2.590448	-0.328573
N	3.646544	-0.221419	-0.050238	N	-2.157064	3.623352	0.147727
C	4.3382	0.993838	-0.058332	C	-1.312338	4.748331	0.083694
N	5.592597	0.966059	-0.474111	N	-0.00652	4.590973	0.34064
C	6.49596	-0.262267	-0.521757	C	0.375903	3.372808	0.751295
N	5.473133	-1.377479	-0.87888	N	-0.402745	2.338067	1.054958
C	4.214345	-1.423277	-0.485688	C	-1.66952	2.422981	0.664288
N	3.47144	-2.527643	-0.568657	N	-2.459151	1.360605	0.717421
C	2.213901	-2.423068	-0.112371	C	-3.639458	1.470759	0.10006
N	1.388499	-3.510392	-0.322533	H	1.827681	-4.407206	-0.495869
N	-2.469658	-1.007159	-0.549525	H	2.293986	4.018175	0.570586
C	-3.75989	-0.969904	-0.202701	N	-4.766653	-6.604171	0.337687
N	-4.336452	0.287956	-0.098864	H	-5.771616	-6.543349	0.41478
N	-4.57218	-2.008456	0.026863	H	-4.315829	-7.507319	0.362771
C	-4.004058	-3.2232	0.014079	N	-3.662639	7.138246	-0.853463
N	-4.717469	-4.322703	0.182223	H	-3.076897	7.960695	-0.849598
N	-2.608601	-3.323435	-0.145736	O	7.136426	-0.507739	0.572365
C	-1.864066	-2.182204	-0.453766	H	6.090486	1.849875	-0.458826
N	-0.551996	-2.282052	-0.628448	H	5.881946	-2.269726	-1.138833
C	-0.00252	-3.465318	-0.348898	N	7.365614	-0.028796	-1.649268
N	-0.628133	-4.624283	-0.118627	H	8.142924	-0.68268	-1.603777
C	-1.968085	-4.574376	-0.060302	H	6.882935	-0.139748	-2.538808
N	-2.693944	-5.664669	0.109278	H	-4.640422	7.22031	-1.091716
C	-4.035942	-5.493805	0.201183	O	5.61507	-0.644133	2.119593



	PCNHS				e (58 atoms)		
N	-0.691283	3.803408	-2.156361	N	-5.047051	-1.068234	-2.914118
C	-0.770855	2.610502	-1.522741	C	-5.023672	-2.145278	-3.738903
N	-1.994860	2.032980	-1.476421	N	-3.983025	-2.973394	-3.931035
N	0.253182	1.929607	-0.963786	C	-2.874739	-2.725092	-3.245196
C	1.471722	2.361065	-1.245358	N	-1.807718	-3.504112	-3.418174
N	2.546174	1.643548	-0.914434	N	-2.810262	-1.618407	-2.357430
N	1.650343	3.558683	-1.952059	C	-3.949165	-0.818940	-2.236818
C	0.523491	4.312698	-2.337226	N	-3.932038	0.224754	-1.382838
N	0.702336	5.509966	-2.883112	N	-1.557219	-0.528548	-0.611965
C	1.978102	5.924578	-3.036313	C	-1.645659	-1.452512	-1.518282
N	3.108882	5.226715	-2.761935	N	-0.644687	-2.329017	-1.688537
C	2.945483	4.025204	-2.237130	C	-0.738787	-3.221792	-2.659964
N	3.987382	3.207380	-2.024406	H	-2.728025	2.623216	-1.863987
C	3.699807	2.033375	-1.455822	N	7.067454	-5.413007	-1.769780
N	1.895066	-2.278451	-2.699241	H	6.896046	-6.394642	-1.931677
C	1.691572	-3.5981	-2.710096	H	7.994987	-5.099961	-1.522832
N	0.387028	-4.005206	-2.908009	N	-6.144267	-2.394647	-4.422044
N	2.609546	-4.567215	-2.585075	H	-6.186656	-3.180958	-5.054144
C	3.860305	-4.170286	-2.312637	H	-6.951373	-1.798427	-4.310291
N	4.851698	-5.037675	-2.193852	N	2.15252	7.156247	-3.532304
N	4.116961	-2.800146	-2.113516	H	1.35267	7.724298	-3.769796
C	3.103011	-1.867480	-2.344206	H	3.084273	7.513691	-3.683483
N	3.352632	-0.576274	-2.200593	N	4.737065	1.097428	-1.428422
C	4.550591	-0.242761	-1.713843	H	5.686590	1.448497	-1.472125
N	5.598966	-1.051384	-1.503454	P	-2.587307	0.740062	-0.349289
C	5.401684	-2.354872	-1.745359	H	-4.837567	0.680498	-1.305453
N	6.380018	-3.236624	-1.624327	H	-1.266797	-0.696076	-1.554085
C	6.065979	-4.531953	-1.868562	O	-3.312505	-0.176729	1.161233
H	0.236421	-4.927486	-3.298662	O	-4.137036	-1.900639	0.418918