SUPPORTING INFORMATION

D_{5h} H©$Cu_5H_5^-$: a covalently bonded planar pentacoordinate hydrogen star

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Supporting Information

Scheme S1. The idea of designing **1** by stepwise replacing Li in H©$Li_5H_5^-$ with Cu.

Table S1. The lowest vibrational frequency at nine classical theoretical levels for the global-minimum structure **1** (D_{5h}, $^1A_1'$) of H©$Cu_5H_5^-$ cluster.

Table S2. Composition analysis of canonical molecular orbitals (CMOs) for the GM (**1**) structure of H©$Cu_5H_5^-$ at the PBE0/def2-TZVPP level.

Table S3. Energy components of IQA for the D_{5h} H©$Cu_5H_5^-$ and Cu_5H_5 systems at the PBE0/TZ2P level; V_{IQA}^{int}, V_C^{int}, and V_{XC}^{int} are the interatomic IQA interaction energy, the coulombic and exchange-correlation energy components, respectively, in kcal mol^{-1}.

Table S4. The EDA results of **1** using H and Cu_5H_5 in different charge and electronic states as interacting fragments at the PBE0/TZ2P-ZORA level. All energy values are in kcal mol^{-1}.

Table S5. The EDA–NOCV results of **1** using H and $Cu_5H_5^-$ as interacting fragments at the PBE0/TZ2P-ZORA level. All energy values are in kcal mol^{-1}.

Figure S1. Optimized structures for the top 20 low-lying isomers of $Cu_5H_6^-$ at the PBE0-D3(BJ)/def2-TZVPP level. Relative energies are listed in kcal mol^{-1} at both the single-point CCSD(T)/def2-TZVPP//PBE0-D3(BJ)/def2-TZVPP levels, with zero-point energy (ZPE) corrections at PBE0-D3(BJ)/def2-TZVPP.

Figure S2. Optimized structures of two low-lying isomers of $M_5H_6^-$ (M = Ag, Au) at the PBE0-D3(BJ)/def2-TZVPP level. Relative energies are listed in kcal mol^{-1} at the single-point CCSD(T)/def2-TZVPP//PBE0-D3(BJ)/def2-TZVPP level, with zero-point energy (ZPE) corrections at PBE0-D3(BJ)/def2-TZVPP.

Figure S3. The Wiberg bond indices (WBIs, blue colour) and natural atomic charges (|e|, red colour) of **1** and $H©Li_5H_5^-$ at the PBE0-D3(BJ)/def2-TZVPP level are shown.

Figure S4. Calculated RMSDs of **1** during the BOMD simulations for 50 ps at PBE0/def2-SVP level, at the temperatures of 4, 300, 400 and 600 K.

Figure S5. (a) 2D plot of ELF of ppH $H©Cu_5H_5^-$. (b) Plot of the Laplacian of electron density, bond paths and critical points. The red dashed lines denote the areas of charge concentration ($\nabla^2\rho(r) < 0$) and the blue area is vice versa. The brown sticks between the atoms represent bond paths. The brown and yellow dots are bond and ring critical points, respectively.

Figure S6. Calculated AIM charges (in |e|) of **1** at the PBE0-D3(BJ)/def2-TZVPP level.

Figure S7. B^{ind}_z isolines (left panel) and GIMIC current-density maps of **1** (right panel) at the BHandHLYP/def2-TZVP level.

Figure S8. The canonical molecular orbital energy diagram of **1**.

Cartesian coordinates of the top 20 low-lying isomers of $Cu_5H_6^-$ at the PBE0-D3(BJ)/def2-TZVPP level.

Scheme S1. The idea of designing **1** by stepwise replacing Li in H©$Li_5H_5^-$ with Cu.

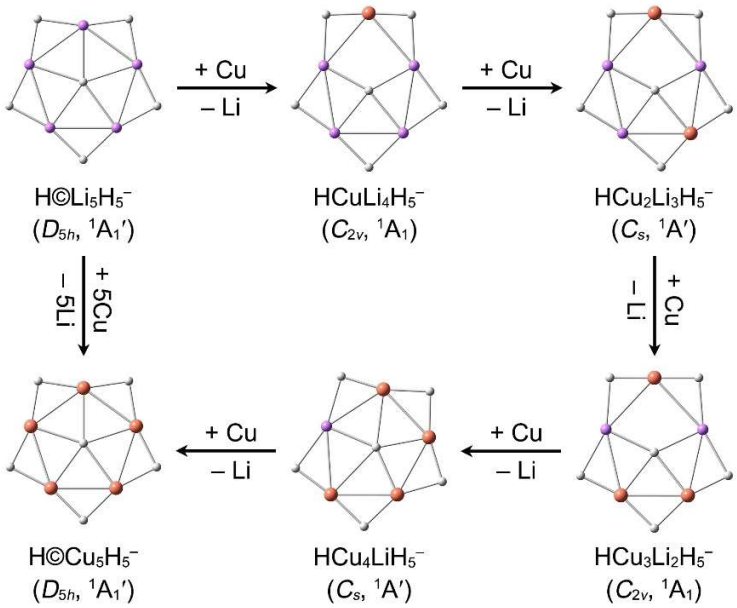
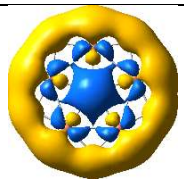
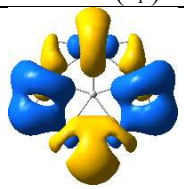
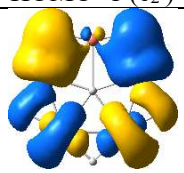
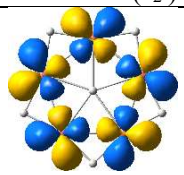
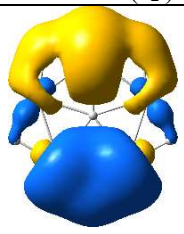
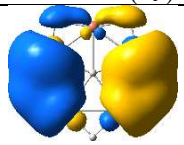
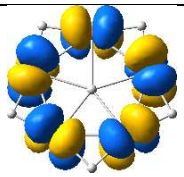
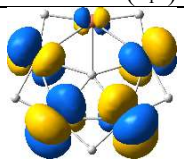
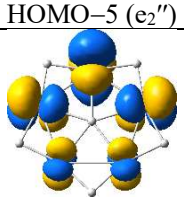
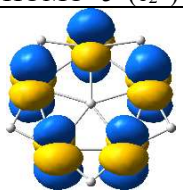
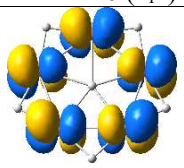
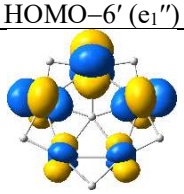
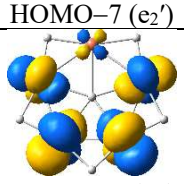


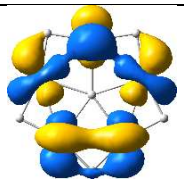
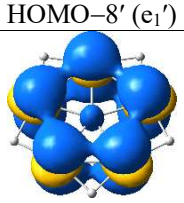
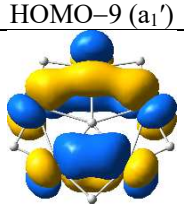
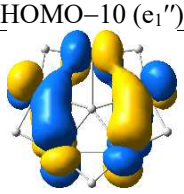
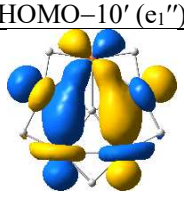
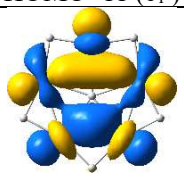
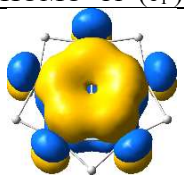
Table S1. The lowest vibrational frequency at nine classical theoretical levels for the global-minimum structure **1** (D_{5h}, $^1A_1'$) of H©$Cu_5H_5^-$ cluster.

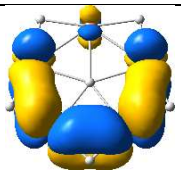
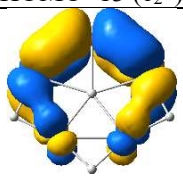
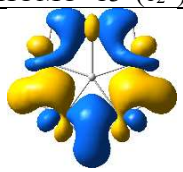
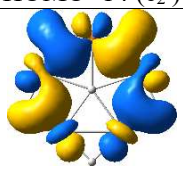
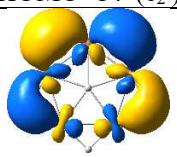
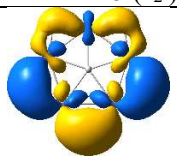
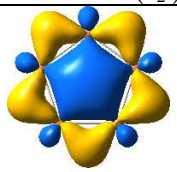
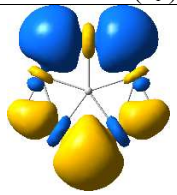
	Theoretical level	Lowest vibrational frequency (cm^{-1})
1	PBE0-D3(BJ)/def2-TZVPP	39.3
2	BP86-D3(BJ)/def2-TZVPP	46.7
3	B3LYP-D3(BJ)/def2-TZVPP	45.9
4	B2PLYP-D3(BJ)/def2-TZVPP	31.9
5	B3PW91-D3(BJ)/def2-TZVPP	47.4
6	TPSS-D3(BJ)/def2-TZVPP	45.2
7	ωB97X-D/def2-TZVPP	29.8
8	TPSSh/def2-TZVPP	37.1
9	CCSD/def2-TZVP	25.8

Table S2. Composition analysis of canonical molecular orbitals (CMOs) for the GM (**1**) structure of H©$Cu_5H_5^-$ at the PBE0/def2-TZVPP level. (^{a}H represents the H atom at the periphery.)

CMO	H (%)	H^a_5 (%)	Cu_5 (%)	
	s	s	s/p/d	total
 HOMO (a_1')	**21.44**	**22.86**	5.89/18.87/**29.20**	**53.96**
 HOMO–1 (e_2')	0.00	16.02	3.89/3.64/**73.69**	**81.22**
 HOMO–1′ (e_2')	0.00	16.02	4.21/4.73/**73.77**	**82.71**
 HOMO–2 (a_2')	0.00	0.00	0.00/0.00/**99.86**	**99.86**
 HOMO–3 (e_1')	0.00	17.51	19.41/2.28/**58.16**	**79.85**
 HOMO–3′ (e_1')	0.00	17.51	19.41/2.69/**58.66**	**80.76**

CMO	H (%)	H^a_5 (%)	Cu_5 (%)	
	s	s	s/p/d	total
 HOMO–4 (a_1'')	0.00	0.00	0.00/0.00/**99.99**	**99.99**
 HOMO–5 (e_2'')	0.00	0.00	0.00/0.00/**99.92**	**99.92**
 HOMO–5′ (e_2'')	0.00	0.00	0.00/0.00/**99.69**	**99.69**
 HOMO–6 (e_1'')	0.00	0.00	0.00/0.00/**99.25**	**99.25**
 HOMO–6′ (e_1'')	0.00	0.00	0.00/0.00/**99.25**	**99.25**
 HOMO–7 (e_2')	0.00	0.00	0.00/0.00/**98.95**	**98.95**
 HOMO–7′ (e_2')	0.00	0.00	0.00/0.00/**98.96**	**98.96**
 HOMO–8 (e_1')	0.00	0.00	0.00/0.00/**98.30**	**98.30**

CMO	H (%)	H^a_5 (%)	Cu_5 (%)	
	s	s	s/p/d	total
 HOMO−8′ (e_1')	0.00	0.00	0.00/0.00/**97.71**	**97.71**
 HOMO−9 (a_1')	2.59	0.00	9.54/0.00/**83.72**	**93.26**
 HOMO−10 (e_1'')	0.00	0.00	0.00/0.00/**99.66**	**99.66**
 HOMO−10′ (e_1'')	0.00	0.00	0.00/0.00/**99.65**	**99.65**
 HOMO−11 (e_1')	0.00	0.00	0.00/0.00/**97.82**	**97.82**
 HOMO−11′ (e_1')	0.00	0.00	0.00/0.00/**98.46**	**98.46**
 HOMO−12 (a_2'')	0.00	0.00	0.00/0.00/**99.25**	**99.25**

CMO	H (%)	H^{a}_{5} (%)	Cu_5 (%)	
	s	s	s/p/d	total
 HOMO−13 (e_2'')	0.00	0.00	0.00/0.00/**99.68**	**99.68**
 HOMO−13′ (e_2'')	0.00	0.00	0.00/0.00/**99.90**	**99.90**
 HOMO−14 (e_2')	0.00	16.42	0.63/4.95/**75.66**	**81.24**
 HOMO−14′ (e_2')	0.00	16.41	1.15/4.39/**76.34**	**81.88**
 HOMO−15 (e_2')	0.00	**43.21**	1.01/6.00/**46.79**	**53.80**
 HOMO−15′ (e_2')	0.00	**43.20**	0.56/6.67/**46.77**	**54.00**
 HOMO−16 (a_1')	**25.90**	5.62	0.00/4.17/**61.82**	**65.99**
 HOMO−17 (e_1')	0.00	**44.16**	11.53/1.82/**37.20**	**50.55**

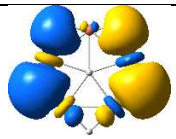
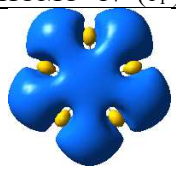
CMO	H (%)	H^{a}_{5} (%)	Cu_5 (%)	
	s	s	s/p/d	total
 HOMO−17′ (e_1′)	0.00	**44.16**	12.49/1.16/**38.31**	**51.96**
 HOMO−18 (a_1′)	16.21	**32.41**	**24.38**/1.91/19.09	**45.38**

Table S3. Energy components of IQA for the D_{5h} H©$Cu_5H_5^-$ and Cu_5H_5 systems at the PBE0/TZ2P level; V_{IQA}^{int}, V_{C}^{int}, and V_{XC}^{int} are the interatomic IQA interaction energy, the coulombic and exchange-correlation energy components, respectively, in kcal mol^{-1}.

	$HCu_5H_5^-$	Cu_5H_5
V_{IQA}^{int} (H–Cu)	–51.23	—
V_{C}^{int} (H–Cu)	–17.91 (34.96%)	—
V_{XC}^{int} (H–Cu)	–33.32 (65.04%)	—
V_{IQA}^{int} (Cu–Cu)	–19.51	–12.53
V_{C}^{int} (Cu–Cu)	22.04 (34.66%)	24.97 (39.97%)
V_{XC}^{int} (Cu–Cu)	–41.55 (65.34%)	–37.50 (60.03%)
V_{IQA}^{int} (H^a–Cu)	–101.78	–108.49
V_{C}^{int} (H^a–Cu)	–24.05 (23.63%)	–26.05 (24.01%)
V_{XC}^{int} (H^a–Cu)	–77.73 (76.37%)	–82.44 (75.99%)

[a]The H atom at the periphery.

Table S4. The EDA results of **1** using H and Cu_5H_5 in different charge and electronic states as interacting fragments at the PBE0/TZ2P-ZORA level. All energy values are in kcal mol^{-1}.

Energy Term	H (D, $1s^1$) + $Cu_5H_5^-$ (D)	H^- (S, $1s^2$) + Cu_5H_5 (S)	H^+ (S, $1s^0$) + $Cu_5H_5^{2-}$ (S)
ΔE_{int}	–72.78	–85.32	–466.01
ΔE_{Pauli}	96.01	370.47	0.02
ΔE_{elstat}	–81.63 (48.36%)	–312.73 (68.61%)	–252.39 (54.16%)
ΔE_{orb}	**–87.16** (51.64%)	–143.06 (31.39%)	–213.64 (45.84%)

Table S5. The EDA–NOCV results of **1** using H and $Cu_5H_5^-$ as interacting fragments at the PBE0/TZ2P-ZORA level. All energy values are in kcal mol^{-1}.

Energy Term	Interaction	H (D, $1s^1$) + $Cu_5H_5^-$(D)
ΔE_{int}		−72.78
ΔE_{Pauli}		96.01
ΔE_{elstat}[a]		−81.63 (48.36%)
ΔE_{orb}[a]		−87.16 (51.64%)
$\Delta E_{orb(1)}$[b]	$Cu_5H_5^-$→H σ donation	−79.65 (91.38%)
$\Delta E_{orb(rest)}$[b]		−7.51 (8.62%)

a. The percentage contribution with respect to the total attraction is given in parentheses; *b*. the percentage contribution with respect to the total orbital interaction is given in parentheses.

Figure S1. Optimized structures for the top 20 low-lying isomers of $Cu_5H_6^-$ at the PBE0-D3(BJ)/def2-TZVPP level. Relative energies are listed in kcal mol^{-1} at both the single-point CCSD(T)/def2-TZVPP//PBE0-D3(BJ)/def2-TZVPP levels, with zero-point energy (ZPE) corrections at PBE0-D3(BJ)/def2-TZVPP. (The most stable triplet structure is higher 61.03 kcal mol^{-1} in energy than **1**, so it is not listed.)

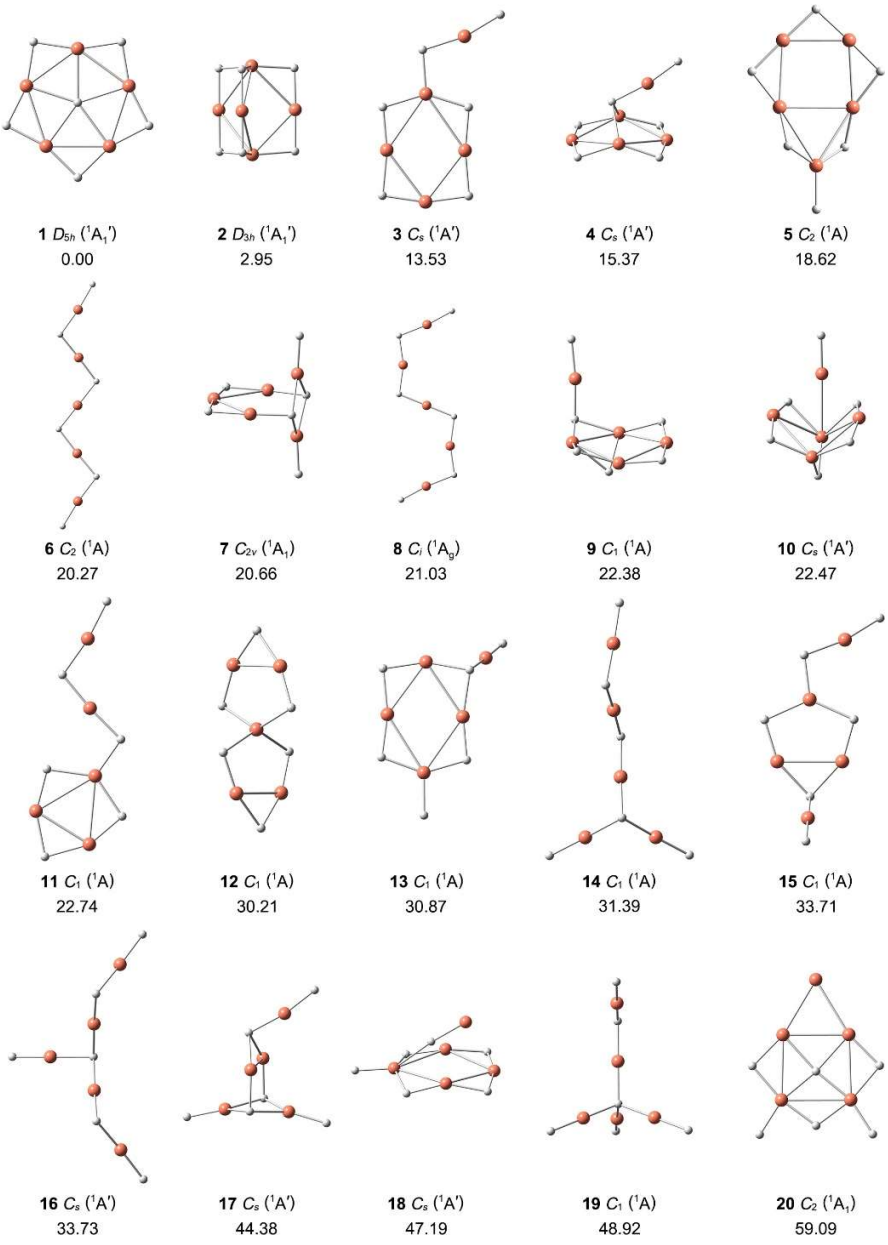


Figure S2. Optimized structures of two low-lying isomers of $M_5H_6^-$ (M = Ag, Au) at the PBE0-D3(BJ)/def2-TZVPP level. Relative energies are listed in kcal mol^{-1} at the single-point CCSD(T)/def2-TZVPP//PBE0-D3(BJ)/def2-TZVPP level, with zero-point energy (ZPE) corrections at PBE0-D3(BJ)/def2-TZVPP.

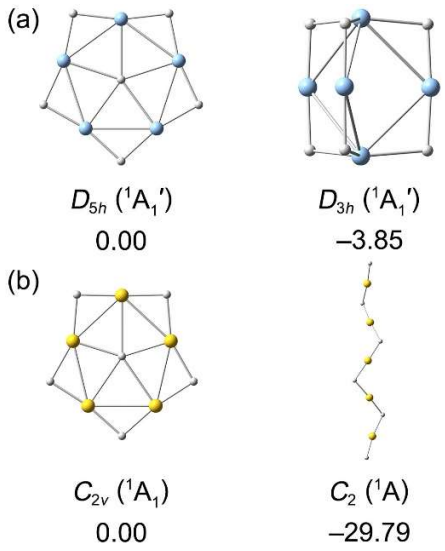
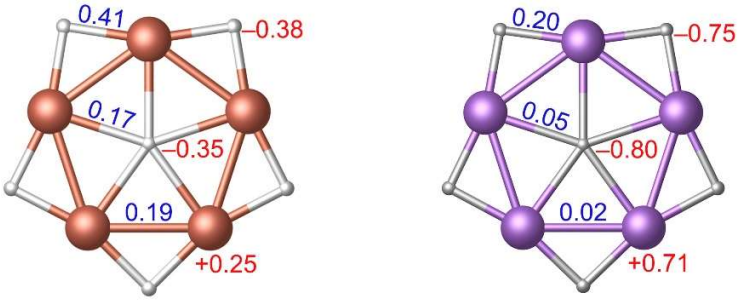


Figure S3. The Wiberg bond indices (WBIs, blue colour) and natural atomic charges (|e|, red colour) of **1** and H©$Li_5H_5^-$ at the PBE0-D3(BJ)/def2-TZVPP level are shown.



1 H©$Cu_5H_5^-$ (D_{5h}, $^1A_1'$) H©$Li_5H_5^-$ (D_{5h}, $^1A_1'$)

Figure S4. Calculated RMSDs of **1** during the BOMD simulations for 50 ps at PBE0/def2-SVP level, at the temperatures of 4, 300, 400 and 600 K.

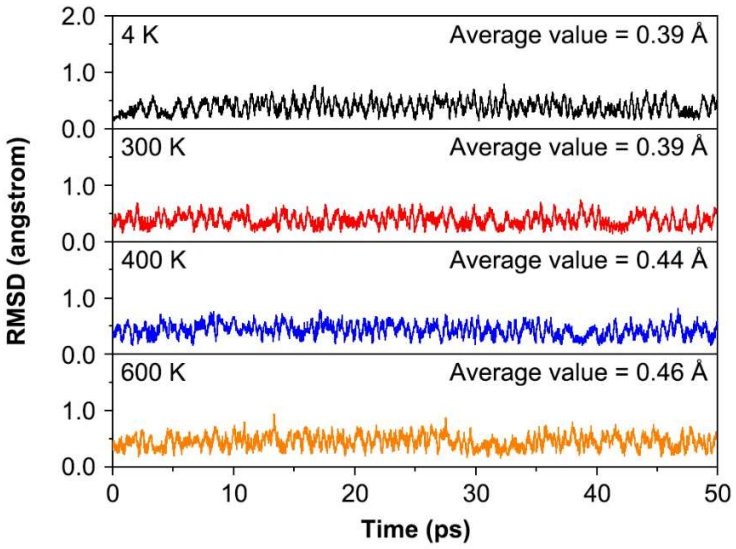


Figure S5. (a) 2D plot of ELF of ppH H©$Cu_5H_5^-$. (b) Plot of the Laplacian of electron density, bond paths and critical points. The red dashed lines denote the areas of charge concentration ($\nabla^2\rho(r) < 0$) and the blue area is vice versa. The brown sticks between the atoms represent bond paths. The brown and yellow dots are bond and ring critical points, respectively.

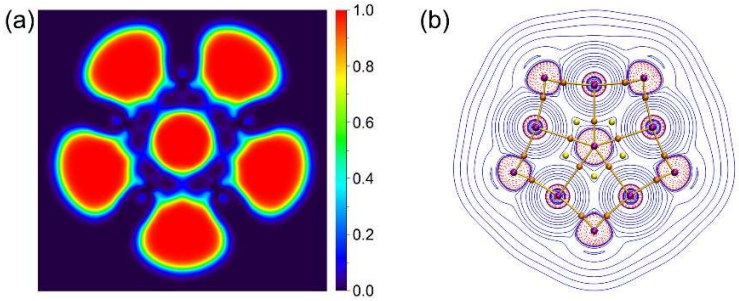
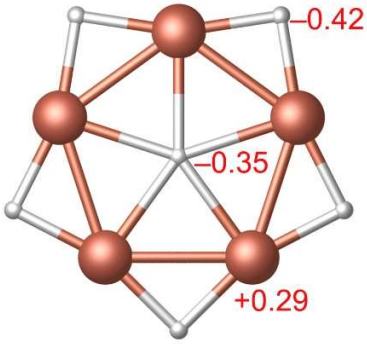


Figure S6. Calculated AIM charges (in |e|) of **1** at the PBE0-D3(BJ)/def2-TZVPP level.



1 H©$Cu_5H_5^-$ (D_{5h}, $^1A_1'$)

Figure S7. B^{ind}_z isolines (left panel) and GIMIC current-density maps of **1** (right panel) at the BHandHLYP/def2-TZVP level.

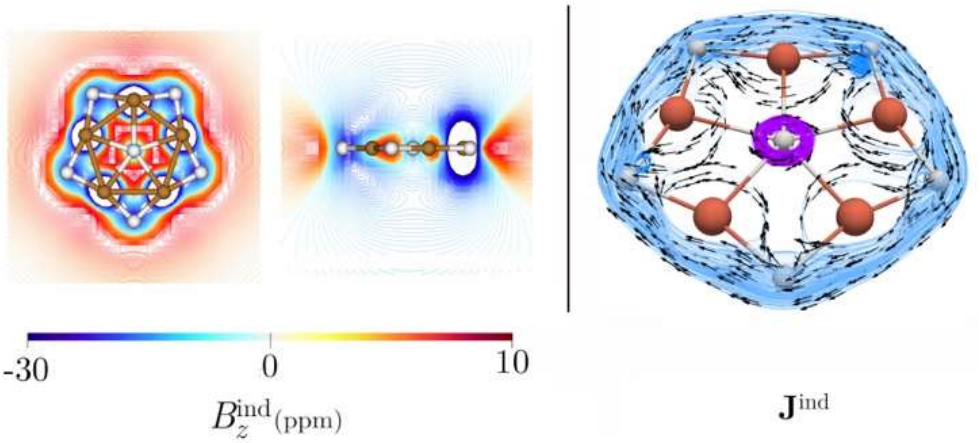
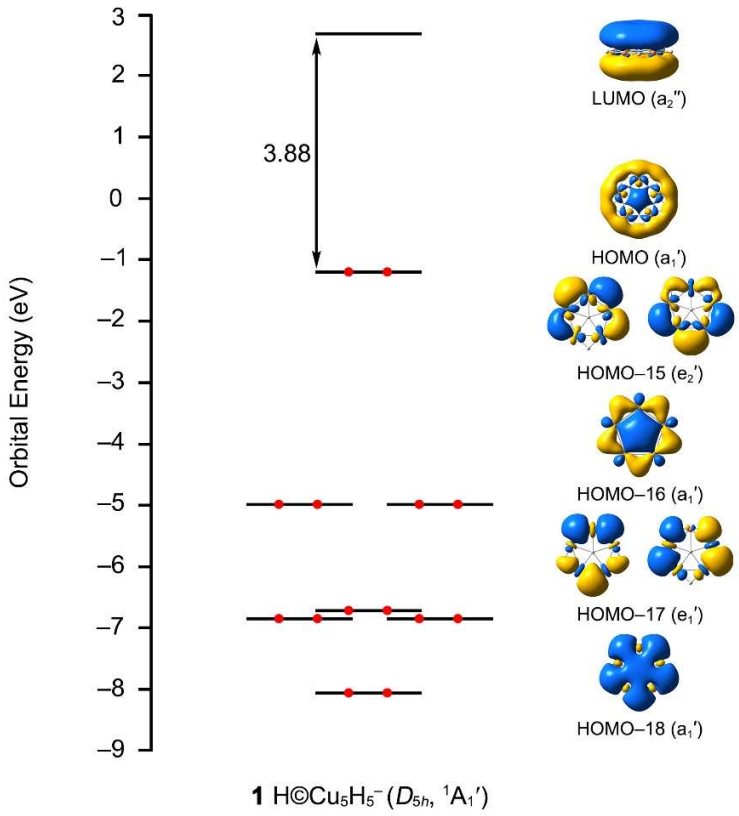


Figure S8. The canonical molecular orbital energy diagram of **1**.



Cartesian coordinates of the top 20 low-lying isomers of $Cu_5H_6^-$ at the PBE0-D3(BJ)/def2-TZVPP level.

1 $HCu_5H_5^-$ (D_{5h}, $^1A_1'$)

Cu	0.00000000	2.00998100	0.00000000
Cu	-1.91160600	0.62111800	0.00000000
Cu	-1.18143700	-1.62610900	0.00000000
Cu	1.18143700	-1.62610900	0.00000000
Cu	1.91160600	0.62111800	0.00000000
H	0.00000000	0.00000000	0.00000000
H	2.65840500	-0.86376800	0.00000000
H	1.64298500	2.26137400	0.00000000
H	-1.64298500	2.26137400	0.00000000
H	-2.65840500	-0.86376800	0.00000000
H	0.00000000	-2.79521200	0.00000000

2 (D_{3h}, $^1A_1'$)

Cu	0.00000000	1.74550081	0.00000000
Cu	1.51164804	-0.87275040	0.00000000
Cu	0.00000000	0.00000000	1.71584600
Cu	-0.00000000	0.00000000	-1.71584600
Cu	-1.51164804	-0.87275040	0.00000000
H	0.00000000	1.72391181	-1.60942100
H	1.49295142	-0.86195590	-1.60942100
H	-1.49295142	-0.86195590	1.60942100
H	-1.49295142	-0.86195590	-1.60942100
H	0.00000000	1.72391181	1.60942100
H	1.49295142	-0.86195590	1.60942100

3 (C_s, $^1A'$)

Cu	0.20250272	3.49274928	0.00000000
Cu	1.35632941	-0.56070669	0.00000000
Cu	-1.42812988	-1.32289205	0.00000000
Cu	-0.59734494	1.05931998	0.00000000
Cu	0.46706904	-2.78096836	0.00000000
H	1.26453312	4.61996506	0.00000000
H	1.94472810	-2.14622375	0.00000000
H	-1.15200105	2.59981790	0.00000000
H	-1.12976357	-2.98324377	0.00000000

H	1.05403922	1.00619715	0.00000000
H	-1.99390019	0.16592479	0.00000000

4 (C_s, ^{1}A′)

Cu	0.23149746	2.19958109	0.00000000
Cu	-1.27611267	-1.25010256	0.00000000
Cu	-0.11921435	0.31127134	1.40476700
Cu	1.26653644	-1.54245613	0.00000000
Cu	-0.11921435	0.31127134	-1.40476700
H	-1.22883419	-0.95983739	1.60625300
H	1.65224260	-3.03730704	0.00000000
H	1.11032424	0.07768407	0.00000000
H	0.08690901	2.01095550	-1.61185400
H	-1.22883419	-0.95983739	-1.60625300
H	0.08690901	2.01095550	1.61185400

5 (C_2, ^{1}A)

Cu	-0.17266102	-1.36499824	0.52165013
Cu	0.20893690	-1.17200171	-1.88978287
Cu	-0.20893690	1.17200171	-1.88978287
Cu	0.17266102	1.36499824	0.52165013
Cu	0.00000000	0.00000000	2.61519813
H	-0.36569243	2.27931958	-0.76908487
H	0.92002026	1.19574550	1.93094613
H	-0.92002026	-1.19574550	1.93094613
H	0.36569243	-2.27931958	-0.76908487
H	0.00000000	0.00000000	-3.00679987
H	0.00000000	0.00000000	4.19403113

6 (C_2, ^{1}A)

Cu	-0.02331234	2.51215384	-0.02234524
Cu	0.02750244	5.02528557	-0.02647124
Cu	0.02331234	-2.51215384	-0.02234524
Cu	-0.02750244	-5.02528557	-0.02647124
Cu	0.00000000	0.00000000	0.09530776
H	0.74709914	-6.34327946	0.09861776
H	-0.98210549	-3.72822689	-0.18126724
H	0.98568577	-1.25000522	0.11636476
H	-0.98568577	1.25000522	0.11636476
H	0.98210549	3.72822689	-0.18126724
H	-0.74709914	6.34327946	0.09861776

7 (C_{2v}, $^1A_1$)

Cu	0.00000000	1.57795200	0.25739785
Cu	0.00000000	0.00000000	2.04667785
Cu	0.00000000	-1.57795200	0.25739785
Cu	-1.26618800	0.00000000	-1.25456615
Cu	1.26618800	0.00000000	-1.25456615
H	2.81608700	-0.00000000	-1.33628615
H	0.00000000	-1.62092800	1.90836285
H	-2.81608700	-0.00000000	-1.33628615
H	-0.00000000	1.62092800	1.90836285
H	0.00000000	-1.31650200	-1.33102515
H	-0.00000000	1.31650200	-1.33102515

8 (C_i, ^1A_g)

Cu	-4.32224395	-0.50380939	0.00151989
Cu	-2.30919009	1.00653679	-0.00202234
Cu	0.00000000	0.00000000	0.00000000
Cu	2.30919009	-1.00653679	0.00202234
Cu	4.32224395	0.50380939	-0.00151989
H	0.76567512	-1.39182791	0.07619934
H	-3.89298310	1.05437666	0.07306757
H	-0.76567512	1.39182791	-0.07619934
H	-4.90268782	-1.92233146	-0.05735384
H	3.89298310	-1.05437666	-0.07306757
H	4.90268782	1.92233146	0.05735384

9 (C_1, ^1A)

Cu	-0.18472900	-0.94640800	0.82058900
Cu	1.51307500	1.19799100	-0.31035800
Cu	1.87249600	-1.15197300	-0.32369700
Cu	-0.69966300	1.30829800	0.40976900
Cu	-2.47573200	-0.40330500	-0.56863100
H	-3.43041000	-0.83318000	-1.70813700
H	0.22567500	2.30960800	-0.53327700
H	2.70318700	0.14748800	-0.87942800
H	-1.70818800	0.00187200	0.81806400
H	0.74620700	0.46166300	1.32763700
H	0.72556800	-2.22094600	0.17264700

10 (C_s, $^1A'$)

Cu	-0.07918374	-0.39720307	1.66803300
Cu	1.89599528	-0.29580724	0.00000000
Cu	-1.81441833	-0.26618501	0.00000000
Cu	-0.07918374	-0.39720307	-1.66803300
Cu	0.05885165	1.38151393	0.00000000
H	-1.55298248	-1.06131014	-1.54396600
H	-1.55298248	-1.06131014	1.54396600
H	1.14875816	0.66225940	1.33947300
H	1.14875816	0.66225940	-1.33947300
H	-1.57718875	1.54899050	0.00000000
H	2.90586484	-1.47923965	0.00000000

11 (C_1, ^{1}A)

Cu	-0.69605299	-0.64472603	0.00000000
Cu	4.27374700	0.17017307	0.00000000
Cu	-3.20948499	-0.69705908	0.00000000
Cu	-2.21630803	1.37921494	0.00000000
Cu	1.75259400	-0.18601198	0.00000000
H	5.71461901	-0.37438690	0.00000000
H	-3.84466002	0.87181991	0.00000000
H	-0.64539102	1.14428297	0.00000000
H	-2.05790896	-1.78706706	0.00000000
H	0.74070303	-1.43509600	0.00000000
H	2.86228298	0.95431005	0.00000000

12 (C_1, ^{1}A)

Cu	-0.00102100	-0.06028900	0.00322400
Cu	-2.26971500	-0.08622800	1.14583400
Cu	-2.26055600	0.09653200	-1.15176900
Cu	2.22559400	1.17483400	0.09271800
Cu	2.30578100	-1.12207800	-0.09011200
H	-0.81043400	-0.22706100	1.68979800
H	0.86004800	-1.72089200	-0.12741100
H	3.50696000	0.06991300	-0.00666200
H	0.74289000	1.66936700	0.14461000
H	-0.79599300	0.04269400	-1.69706900
H	-3.50588200	0.08562600	-0.00023700

13 (C_1, ^{1}A)

Cu	-1.07224800	1.23803100	-0.29129500
Cu	2.39177300	-0.89360400	0.10851700

Cu	1.26784700	1.37432600	0.22505600
Cu	-0.07460900	-0.98073100	-0.38960600
Cu	-2.59236600	-0.67283500	0.31649800
H	-3.65540800	-1.08614200	1.33669300
H	-1.58376700	-0.21999100	-0.89846900
H	-0.06857500	2.41819400	0.09267400
H	2.70840200	0.69998600	0.41099700
H	3.71971700	-1.74065600	0.19931500
H	1.18814900	-1.96181300	-0.24713300

14 (C_1, ^{1}A)

Cu	-4.35376600	0.02664800	0.14444400
Cu	-1.85725700	-0.05303600	-0.10273900
Cu	0.63879500	0.09518100	-0.23360800
Cu	2.71910400	-1.31364200	0.08951700
Cu	2.86539100	1.24212100	0.12160500
H	1.94716400	0.00334500	0.76244100
H	-3.00559500	-0.38125600	0.94140700
H	-5.71170800	0.36561300	-0.48292900
H	3.40079000	-2.60450000	-0.35606900
H	-0.66653000	0.23304800	-1.12708700
H	3.68013300	2.46284700	-0.29511900

15 (C_1, ^{1}A)

Cu	-0.69306800	-1.06608300	-0.33670000
Cu	-1.15313400	1.22676700	-0.26510200
Cu	3.64890800	-0.28048800	0.08559600
Cu	-3.10442700	-0.36649500	0.30495300
Cu	1.22338900	0.49715100	0.18156500
H	2.73757000	0.99522600	0.49025700
H	4.74384600	-1.31385700	-0.26180900
H	0.83615600	-1.20727300	0.03544400
H	0.19044800	1.94270300	0.14245000
H	-2.06583200	-0.12272900	-0.92086000
H	-4.17056200	-0.60878900	1.37548300

16 (C_s, ^{1}A′)

Cu	-0.12476279	2.14824825	0.00000000
Cu	0.16837306	-0.02657793	1.26563500
Cu	-0.09743284	-1.04639101	3.52635000
Cu	-0.09743284	-1.04639101	-3.52635000

Cu	0.16837306	-0.02657793	-1.26563500
H	0.24755737	3.62669593	0.00000000
H	-1.04889248	-1.44843992	4.65889500
H	1.03017149	-0.68532236	-2.41893100
H	-1.04889248	-1.44843992	-4.65889500
H	1.03017149	-0.68532236	2.41893100
H	-0.70652684	0.57382787	0.00000000

17 (C_s, ^{1}A′)

Cu	0.35508600	0.18887400	-1.19035000
Cu	0.35508600	2.49824800	0.00000000
Cu	-1.62020500	-0.82912500	0.00000000
Cu	0.35508600	0.18887400	1.19035000
Cu	0.59633300	-2.01439400	0.00000000
H	1.21504000	1.11605700	0.00000000
H	-0.22968100	3.91760200	0.00000000
H	1.74576300	-3.04870900	0.00000000
H	-0.40498500	-1.23054600	1.36790600
H	-3.12132900	-0.46566000	0.00000000
H	-0.40498500	-1.23054600	-1.36790600

18 (C_s, ^{1}A′)

Cu	-0.90284512	-1.69227121	0.00000000
Cu	1.53715563	-1.02314351	0.00000000
Cu	0.02491574	2.20809552	0.00000000
Cu	-0.30757030	0.16776424	1.37787300
Cu	-0.30757030	0.16776424	-1.37787300
H	-0.33530310	1.78131565	-1.58051400
H	0.23870011	3.76298163	0.00000000
H	-0.88619125	-1.42514197	-1.59898200
H	-0.88619125	-1.42514197	1.59898200
H	0.92580466	0.50660182	0.00000000
H	-0.33530310	1.78131565	1.58051400

19 (C_1, ^{1}A)

Cu	-1.76387900	0.06149700	-1.31395600
Cu	-1.11628800	-1.38812700	0.85840100
Cu	-1.07803100	1.33197000	0.95305900
Cu	0.74986800	-0.00499200	-0.48918400
Cu	3.19845700	-0.00068300	-0.02857800
H	2.13476300	-0.00795100	-1.24969600

H	-2.61500200	0.11925500	-2.57518000
H	-1.35362000	2.57679200	1.78484200
H	-1.42341100	-2.68091000	1.60140200
H	-0.79701400	-0.00230200	0.03201900
H	4.34057900	0.00482000	0.99411100

20 (C_2, $^1A_1$)

Cu	0.00000000	0.00000000	2.71918023
Cu	0.00000000	1.30355200	-1.81685177
Cu	0.00000000	1.23919200	0.64373523
Cu	0.00000000	-1.23919200	0.64373523
Cu	0.00000000	-1.30355200	-1.81685177
H	0.00000000	2.39651900	-0.53021777
H	0.00000000	-2.39651900	-0.53021777
H	0.00000000	0.00000000	-2.78490877
H	0.00000000	2.12896100	-3.11567877
H	0.00000000	0.00000000	-0.73876577
H	0.00000000	-2.12896100	-3.11567877