Primary amino-functionalized N-Heterocyclic carbene ligands as support for Au(I)···Au(I) interactions: structural, electrochemical, spectroscopic and computational studies of the dinuclear $[Au_2(NH_2(CH_2)_2imMe)_2][NO_3]_2$

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Supplementary Information

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X-ray structure of $[5][NO_3]_2 \cdot 2CH_3OH$

Table S1. Full list of the bond lengths (Å) for $[C_{12}H_{22}Au_2N_6][NO_3]_2 \cdot 2CH_3OH$ (See Figure 1 for atom labelling).

Au(1)-C(1)	2.006(16)	N(7)-H(7A)	0.8600
Au(1)-N(7)	2.089(17)	N(7)-H(7B)	0.8600
Au(1)-Au(1)_1	3.2332(17)	C(8)-C(9)	1.49(3)
C(1)-N(2)	1.31(2)	C(8)-H(8A)	0.9700
C(1)-N(5)	1.33(3)	C(8)-H(8B)	0.9700
N(2)-C(3)	1.37(3)	C(9)-N(5)_1	1.43(3)
N(2)-C(6)	1.49(3)	C(9)-H(9A)	0.9700
C(3)-C(4)	1.30(3)	C(9)-H(9B)	0.9700
C(3)-H(3)	0.9300	N(10)-O(12)	1.19(2)
C(4)-N(5)	1.42(3)	N(10)-O(11)	1.20(2)
C(4)-H(4)	0.9300	N(10)-O(13)	1.28(3)
N(5)-C(9)_1	1.43(3)	O(20)-C(21)	1.37(5)
C(6)-H(6A)	0.9600	O(20)-H(20)	0.8200
C(6)-H(6B)	0.9600	C(21)-H(21A)	0.9600
C(6)-H(6C)	0.9600	C(21)-H(21B)	0.9600
N(7)-C(8)	1.46(3)	C(21)-H(21C)	0.9600

Table S2. Full list of the angles (°) for $[C_{12}H_{22}Au_2N_6][NO_3]_2 \cdot 2CH_3OH$ (See Figure 1 for atom labelling).

C(1)-Au(1)-N(7)	174.5(7)	C(8)-N(7)-Au(1)	118.7(13)
C(1)-Au(1)-Au(1)_1	93.6(5)	C(8)-N(7)-H(7A)	120.0
N(7)-Au(1)-Au(1)_1	91.9(5)	Au(1)-N(7)-H(7A)	50.3
N(2)-C(1)-N(5)	106.5(15)	C(8)-N(7)-H(7B)	120.0
N(2)-C(1)-Au(1)	126.5(14)	Au(1)-N(7)-H(7B)	99.2
N(5)-C(1)-Au(1)	126.8(15)	H(7A)-N(7)-H(7B)	120.0
C(1)-N(2)-C(3)	110.8(18)	N(7)-C(8)-C(9)	112.3(18)
C(1)-N(2)-C(6)	126.4(16)	N(7)-C(8)-H(8A)	109.1
C(3)-N(2)-C(6)	122.7(18)	C(9)-C(8)-H(8A)	109.1
C(4)-C(3)-N(2)	107(2)	N(7)-C(8)-H(8B)	109.1
C(4)-C(3)-H(3)	126.3	C(9)-C(8)-H(8B)	109.1
N(2)-C(3)-H(3)	126.3	H(8A)-C(8)-H(8B)	107.9
C(3)-C(4)-N(5)	107(2)	N(5)_1-C(9)-C(8)	114.5(17)
C(3)-C(4)-H(4)	126.6	N(5)_1-C(9)-H(9A)	108.6
N(5)-C(4)-H(4)	126.6	C(8)-C(9)-H(9A)	108.6
C(1)-N(5)-C(4)	108.3(19)	N(5)_1-C(9)-H(9B)	108.6
C(1)-N(5)-C(9)_1	125.2(18)	C(8)-C(9)-H(9B)	108.6
C(4)-N(5)-C(9)_1	126.5(19)	H(9A)-C(9)-H(9B)	107.6
N(2)-C(6)-H(6A)	109.5	O(12)-N(10)-O(11)	126(2)
N(2)-C(6)-H(6B)	109.5	O(12)-N(10)-O(13)	117(2)
H(6A)-C(6)-H(6B)	109.5	O(11)-N(10)-O(13)	117(2)
N(2)-C(6)-H(6C)	109.5	C(21)-O(20)-H(20)	109.5
H(6A)-C(6)-H(6C)	109.5	O(20)-C(21)-H(21A)	109.5
H(6B)-C(6)-H(6C)	109.5	O(20)-C(21)-H(21B)	109.5

H(21A)-C(21)-H(21B)	109.5
O(20)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5

Electrochemical Studies

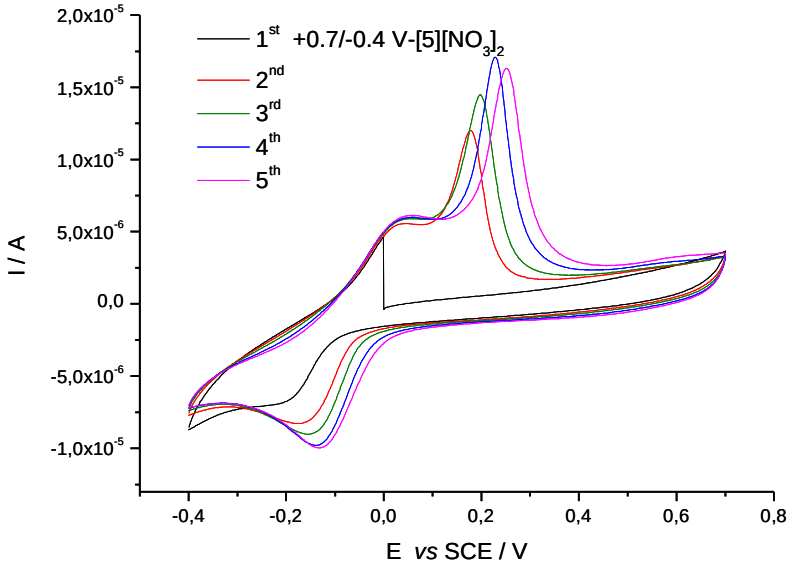


Fig. 1S CVs of **[5][NO$_3$]$_2$** in the potential range +0.7/-0.4 V showing 1 to 5 successive scans.

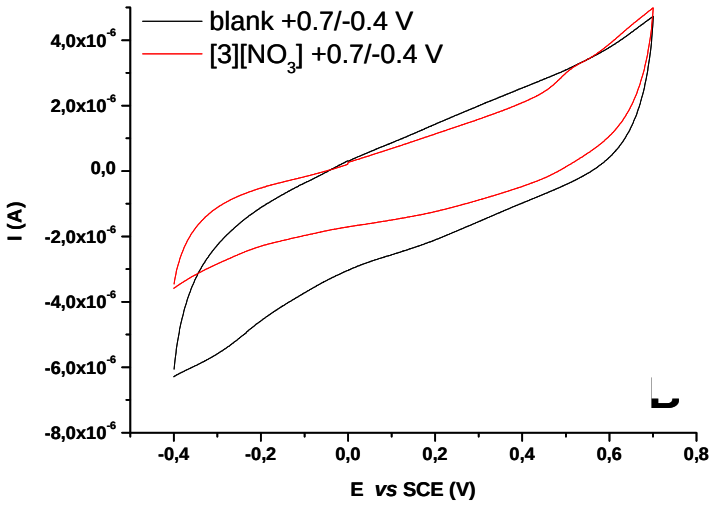
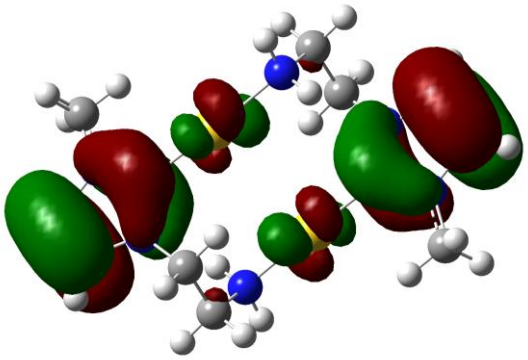


Fig. 2S CVs of **[3][NO$_3$]** and blank; scan rate 100 mV s^{-1}.

Density Functional Theory calculations

HOMO-1



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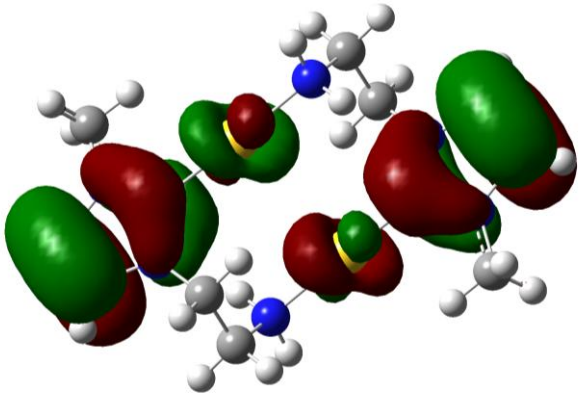
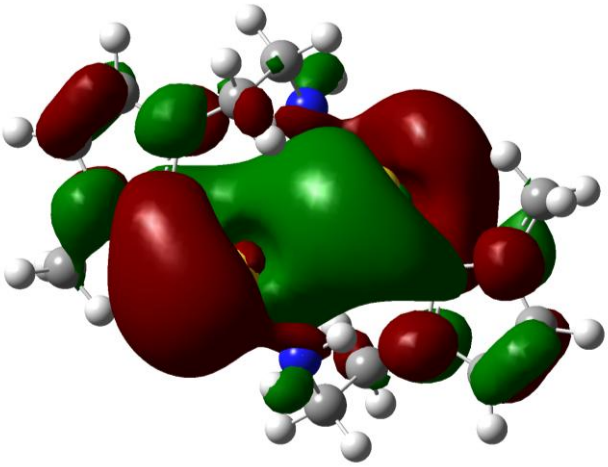


LUMO+1



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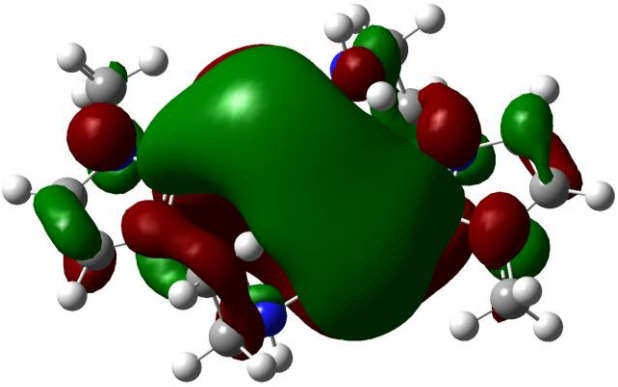

Fig. 3S Schematic description of the frontier molecular orbitals of **[5]**$^{2+}$.