Journal Name

ARTICLE TYPE

ELECTRONIC SUPPLEMENTARY INFORMATION

The aromatic nature of auracycles and diauracycles based on calculated ring-current strengths[†]

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Strengths of current-density vortices

Table S1 The net, diatropic, and paratropic ring-current strengths (in nA T^{-1}) of auracycles **1-4** at the DFT/BHandHLYP/def2-TZVP, 1C-X2C/BHandHLYP/def2-TZVP, and 2C-X2C/ωB97X-D/def2-TZVP levels of theory

Level of theory	Net	Diatropic	Paratropic
[Au(C$_5$H$_5$)] (**1**)			
QR-ECP	10.51	15.63	−5.11
1C-X2C	10.43	15.58	−5.15
2C-X2C	14.32	-	-
[Au(NC$_4$H$_4$)] (**2**)			
QR-ECP	7.41	13.06	−5.65
1C-X2C	7.24	12.25	−5.01
[Au(C$_6$H$_6$)]$^+$ (**3**)			
QR-ECP	3.82	11.92	−8.10
1C-X2C	7.55	14.21	−6.66
2C-X2C	3.90	-	-
[AuCl(C$_6$H$_6$)] (**3·Cl**)			
QR-ECP	4.21	12.08	−7.87
1C-X2C	4.29	12.15	−7.86
2C-X2C	4.25	-	-
[AuCl(C$_4$H$_4$)(NH$_3$)] (**4**)			
QR-ECP	−4.41	6.20	−10.61
1C-X2C	−4.51	6.17	−10.68
2C-X2C	−4.59	-	-

Table S2 The gold-gold distance (in pm) and the bond-current strength (in nA T^{-1}) of diauracycles **5–17**, calculated at the DFT/BHandHLYP/def2-TZVP level of theory with the GIMIC method, and at the DFT/ωB97X-D/def2-TZVP level of theory using numerical line integration of Ampère-Maxwell's law

Molecule	Au–Au distance	Net current (GIMIC)	Net current (Ampère-Maxwell's law)
[Au$_2$(NCH)$_2$] (**5**)	293.29	1.80	1.74
[Au$_2$(NHCH)$_2$] (**6**)	263.97	3.98	3.92
[Au$_2$Cl$_2$(NHCH)$_2$] (**7**)	244.83	11.11	9.73
[Au$_2$Cl$_2${(NH)$_2$CH}$_2$] (**8**)	250.23	10.40	9.34
[Au$_2${(NH)$_2$CH}$_2$]) (**9**)	273.64	2.69	2.53
[Au$_2${N(NH)CH}$_2$] (**10**)	279.49	1.97	1.82
[Au$_2$(N$_2$CH)$_2$] (**11**)^a	263.30	3.65	3.48
[Au$_2${NH(CH)$_2$}$_2$] (**12**)	250.01	9.88	10.07
[Au$_2${NH(CH)$_2$}$_2$] (**13**)	276.53	2.50	2.23
[Au$_2${S$_2$CC(CN)$_2$}$_2$]$^{2-}$ (**14**)	275.84	2.65	2.80
[Au$_2${N$_2$(CH)$_2$}$_2$] (**15**)	245.41	-^{b}	10.71
[Au$_2${(NH)$_2$(CH)$_2$}$_2$] (**16**)	284.77	3.33	3.17
[Au$_2$Cl$_2${N(NH)(CH)$_2$}$_2$] (**17**)	250.11	-^{b}	10.56

^{a} Triplet state
^{b} The value is not reliable because the plane cuts undesired vortexes

Table S3 The X–Au–X angle (in °) versus the ring-current strength (in nA T^{-1}) of molecules **1-18**

| Molecule	X–Au–X angle	Ring-current strength
[Au(C$_5$H$_5$)] (**1**)	103.1	10.51
[Au(NC$_4$H$_4$)] (**2**)	107.3	7.41
[Au(C$_6$H$_6$)]$^+$ (**3**)	83.0	3.82
[AuCl(C$_6$H$_6$)] (**3·Cl**)	90.8	4.21
[AuCl(C$_4$H$_4$)(NH$_3$)] (**4**)	80.5	−4.41
[Au$_2$(NCH)$_2$] (**5**)	130.9	12.43
[Au$_2$(NHCH)$_2$] (**6**)	142.1	−2.96
[Au$_2$Cl$_2$(NHCH)$_2$] (**7**)	147.0	−1.18
[Au$_2$Cl$_2${(NH)$_2$CH}$_2$] (**8**)	174.1	−3.02
[Au$_2${(NH)$_2$CH}$_2$]) (**9**)	169.0	−1.88
[Au$_2${N(NH)CH}$_2$] (**10**)	165.3	5.78
[Au$_2$(N$_2$CH)$_2$] (**11**)	170.1	11.12
[Au$_2${NH(CH)$_2$}$_2$] (**12**)	177.0	−1.69
[Au$_2${NH(CH)$_2$}$_2$] (**13**)	170.7	12.32
[Au$_2${S$_2$CC(CN)$_2$}$_2$]$^{2-}$ (**14**)	175.9	−1.97
[Au$_2${N$_2$(CH)$_2$}$_2$] (**15**)	164.0	−22.01
[Au$_2${(NH)$_2$(CH)$_2$}$_2$] (**16**)	172.6	13.83
[Au$_2$Cl$_2${N(NH)(CH)$_2$}$_2$] (**17**)	174.4	−0.44
[AuCl(C$_4$Ph$_4$)(phen)] (**18**)	81.1	−3.33

Molecular orbitals
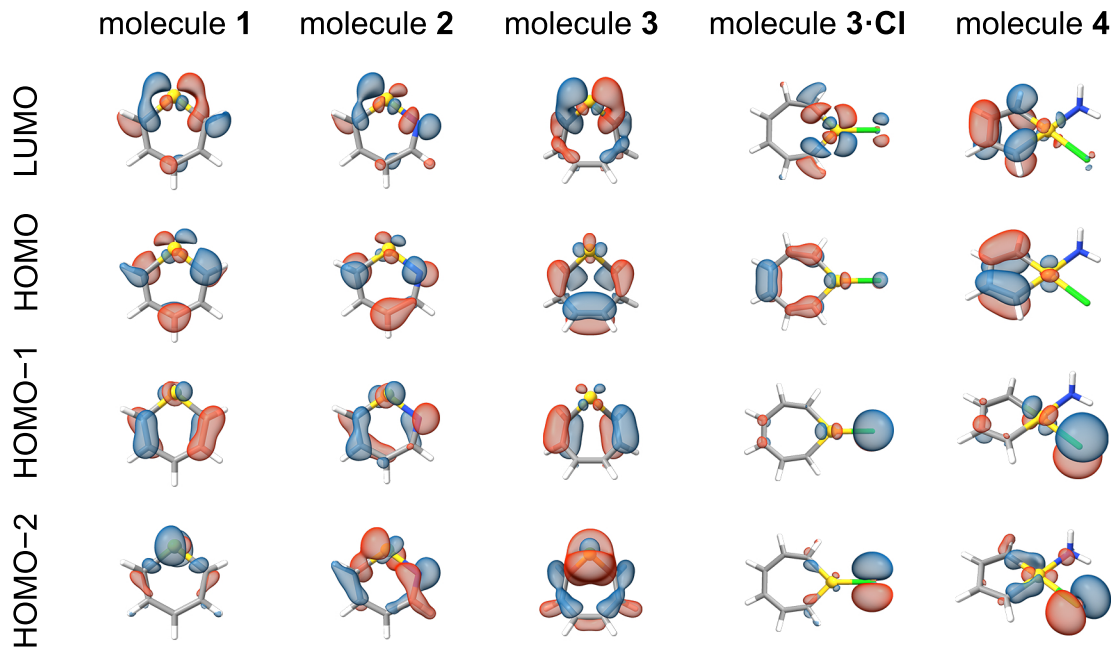
Fig. S1 Selected molecular orbitals of molecules **1-4**. Color code: C, grey; H, white; Au, yellow; Cl, green; N, blue.
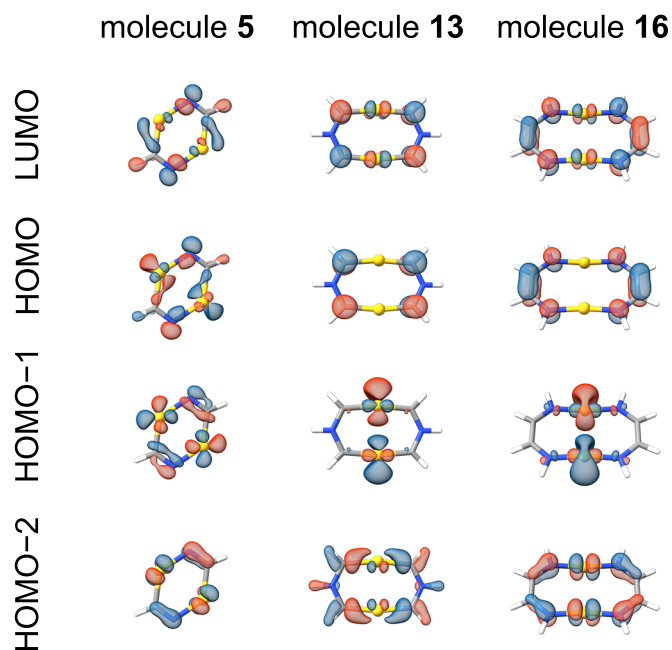
molecule **5**   molecule **13**   molecule **16**

Fig. S2 Selected molecular orbitals of molecules **5**, **13**, and **16**. Color code: C, grey; H, white; Au, yellow; N, blue.

Cartesian coordinates

[Au(C$_5$H$_5$)] (1, C$_2$)

Au	-0.0001014	1.8572693	-0.0007716
C	1.2354779	-0.6904050	0.1050386
C	1.5026496	0.6544633	0.1958480
C	-1.5027887	0.6543031	-0.1954919
C	-1.2354994	-0.6905425	-0.1050222
C	0.0000300	-1.3479206	-0.0000949
H	2.1264966	-1.3197276	0.0792924
H	2.4071462	1.0779947	-0.2468744
H	-2.4070419	1.0779858	0.2475329
H	-2.1264604	-1.3199478	-0.0792533
H	0.0000915	-2.4311316	-0.0002036

[Au{C(CH$_2$)CH$_2$CHCHCH}] (1a, C$_1$)

Au	-0.0645186	1.3992796	-1.3470696
C	1.3202580	-0.8376768	-0.3848650
C	1.5276172	0.6678500	-0.4430655
C	-1.5213658	0.6348541	-0.4127580
C	-1.2072452	-0.6724204	0.1114438
C	-0.0089907	-1.3135678	0.1531598
C	2.5599777	1.3438405	0.0610909
H	1.4538721	-1.2214062	-1.4051524
H	-1.9762885	1.3022490	0.3308542
H	-2.0391296	-1.1751404	0.6070324
H	0.0123866	-2.2894126	0.6281693
H	3.3702012	0.8020770	0.5461243
H	2.6334058	2.4216287	0.0093147
H	2.1266819	-1.2760703	0.2179724

[Au{C(CH$_3$)CHCHCHCH}] (1b, C$_1$)

Au	-0.0292876	1.8370158	-0.0503912

```
C      1.2203434     -0.6770134      0.0672901
C      1.5101733      0.6626584      0.1218695
C     -1.5370439      0.6402054     -0.1881881
C     -1.2574816     -0.7048745     -0.0946462
C     -0.0152563     -1.3459840     -0.0114082
C      2.7757704      1.2738617     -0.4193607
H      2.1096361     -1.3101933      0.0642798
H     -2.4174969      1.0641465      0.3007756
H     -2.1423098     -1.3416330     -0.0467198
H     -0.0028323     -2.4287187      0.0157018
H      3.0517497      2.2083849      0.0692458
H      3.5792523      0.5547309     -0.2263482
H      2.7440791      1.4327901     -1.5020451
```

[Au(NC$_4$H$_4$)] (2, C$_1$)

```
Au     0.0411865      1.7669461     -0.0989312
N      1.5409905      0.6108481      0.2079510
C      1.2392903     -0.6560887      0.1516919
C     -1.5355906      0.6640695     -0.1239063
C     -1.2541817     -0.6846814     -0.0896480
C     -0.0141078     -1.3186098      0.0495395
H      2.1242330     -1.2957218      0.0639608
H     -2.4497302      1.0982898      0.2757801
H     -2.1223941     -1.3425867     -0.1551008
H      0.0231579     -2.3981187     -0.0344627
```

[Au{C(CH$_2$)CH$_2$CHCHN}] (2a, C$_1$)

```
Au    -0.0068279      1.3867605     -1.3329175
N     -1.4251772      0.6095385     -0.3793602
C      1.3234367     -0.8913875     -0.4124888
C      1.5382228      0.5871498     -0.4254595
C     -1.1439727     -0.6138044      0.1092349
C      0.0271659     -1.3155641      0.2229971
C      2.5029031      1.3524834      0.0764963
H      1.3946224     -1.2415211     -1.4553096
H     -2.0449853     -1.0674198      0.5331778
H     -0.0092152     -2.2929466      0.6845118
H      3.3529188      0.8686654      0.5506006
H      2.4865763      2.4326785      0.0367255
H      2.1674828     -1.3307973      0.1331888
```

[Au{C(CH$_3$)CHCHCHN}] (2b, C$_1$)

```
Au    -0.0822094      1.7426002      0.0681587
N     -1.5843932      0.5882154     -0.2037751
C      1.2302781     -0.6698691      0.0626008
C      1.5304559      0.6763748      0.0593857
C     -1.2709617     -0.6790150     -0.1467017
C     -0.0083818     -1.3193434     -0.0531130
C      2.8090004      1.2813225     -0.4392195
H      2.0987813     -1.3259921      0.1460805
H     -2.1490764     -1.3264980     -0.0510748
H     -0.0298652     -2.3962079      0.0651776
H      3.0746073      2.2078359      0.0667959
H      3.6103567      0.5573833     -0.2572499
H      2.7782009      1.4644237     -1.5177858
```

[Au(C$_6$H$_6$)]$^+$ (3, C$_s$)

Au	0.8068578	2.0331328	1.9379091
C	0.1279888	-0.5619408	0.0597389
C	1.4850971	-0.5618634	0.0593101
C	2.3193226	0.6143349	-0.0688189
C	-0.7063051	0.6142342	-0.0684929
C	2.1129371	1.8181139	0.4762236
C	-0.5000130	1.8179438	0.4767165
H	-0.3767348	-1.5214473	0.0219350
H	1.9899158	-1.5213249	0.0213837
H	3.2222408	0.5271485	-0.6757146
H	-1.6093189	0.5268859	-0.6752245
H	2.6731631	2.7364240	0.3302923
H	-1.0601380	2.7363371	0.3309678

[Au{C(CH$_2$)CH$_2$CHCHCHCH}]$^+$ (3a, C$_1$)

Au	0.5594610	2.4873993	1.3330477
C	0.2101298	-0.5469910	0.2987221
C	1.5392360	-0.3699478	0.1791013
C	2.1810960	0.8255682	-0.4752008
C	-0.7854256	0.4233533	-0.1321141
C	2.2546392	2.0115717	0.4117996
C	-0.7681912	1.7395449	0.0887720
C	3.2301217	2.8369544	0.7728300
H	-0.1619540	-1.4911682	0.6831231
H	2.1982909	-1.1575381	0.5280225
H	1.6297668	1.1036696	-1.3806738
H	-1.6601999	0.0605262	-0.6773431
H	-1.4246056	2.5167567	-0.2930400
H	3.2097809	0.5933874	-0.7706135
H	4.2349154	2.6201769	0.4110264
H	3.1112499	3.7106778	1.4044807

[Au{C(CH$_3$)CHCHCHCHCH}]$^+$ (3b, C$_1$)

Au	0.8006407	2.0043155	1.9132780
C	0.1196058	-0.5618548	0.0479187
C	1.4744447	-0.5344014	0.0490207
C	2.3110017	0.6431587	-0.0856460
C	-0.7405049	0.5986936	-0.0662142
C	2.1620391	1.8545656	0.4651973
C	-0.5596461	1.7927397	0.5044252
C	2.9389327	3.1123474	0.2866914
H	-0.3664391	-1.5312157	0.0188122
H	1.9919249	-1.4879346	0.0202311
H	3.2010667	0.5403282	-0.7103842
H	-1.6439457	0.5026427	-0.6711532
H	-1.1412261	2.7023448	0.3917894
H	3.4119359	3.4490706	1.2104255
H	3.7250808	2.9082548	-0.4469344
H	2.3101838	3.9166181	-0.0984507

[AuCl(C$_6$H$_6$)] (3·Cl, C$_{2v}$)

Au	-2.1789005	-0.0024586	0.0000000
Cl	-4.4533235	0.0102502	0.0000000
C	1.6361342	0.6801353	0.0000000

```
C      1.6372373    -0.6801399     0.0000000
C      0.5283420    -1.5758749     0.0000000
C     -0.8079606    -1.3902396     0.0000000
C     -0.8102811     1.3877101     0.0000000
C      0.5258146     1.5740870     0.0000000
H      2.6094311     1.1595364     0.0000000
H      2.6113794    -1.1578497     0.0000000
H      0.7993256    -2.6318482     0.0000000
H     -1.4442405    -2.2792426     0.0000000
H     -1.4481031     2.2754137     0.0000000
H      0.7951451     2.6305208     0.0000000
```

$[AuCl(C_4H_4)(NH_3)]$ (4, C_1)

```
Au     0.7514889    -0.1296517     0.0000000
Cl     2.8347516    -1.1818154     0.0000000
N      1.8575824     1.7268759     0.0000000
C     -0.3166223    -1.8033443     0.0000000
C     -1.0864067     0.6611395     0.0000000
C     -1.6519007    -1.6294849     0.0000000
C     -2.0885498    -0.2416859     0.0000000
H     -2.3423574    -2.4681449     0.0000000
H     -3.1366550     0.0447118     0.0000000
H     -1.2460666     1.7367147     0.0000000
H      0.2148080    -2.7480383     0.0000000
H      1.6873619     2.2985660    -0.8229709
H      1.6873619     2.2985660     0.8229709
H      2.8352038     1.4355914     0.0000000
```

$[AuCl\{C(CH_2)CH_2CHCH\}(NH_3)]$ (4a, C_1)

```
Au     0.1116933     0.2037598     0.0041018
Cl     2.0255484    -1.1361524    -0.2345721
N      1.5394538     1.8342991     0.0554431
C     -1.2694523    -1.2272584     0.0053414
C     -1.5148860     1.3292660     0.1606482
C     -2.6584196    -0.7323058    -0.3410720
C     -2.6933512     0.7262007    -0.0469844
C     -0.9886522    -2.4765098     0.3781108
H     -3.4141145    -1.2952065     0.2189549
H     -3.6334032     1.2729319    -0.0195626
H     -1.4279636     2.3922116     0.3776566
H      1.4935570     2.4189373    -0.7746508
H      1.4663254     2.4343503     0.8721546
H      2.4431883     1.3608381     0.0673448
H      0.0142560    -2.7993145     0.6201261
H     -1.7924466    -3.2079427     0.4275173
H     -2.8608337    -0.9042482    -1.4062803
```

$[AuCl\{C(CH_3)CHCHCH\}(NH_3)]$ (4b, C_1)

```
Au     0.0884225     0.1238193     0.0000057
Cl     2.2378612    -0.8191499     0.0004489
N      1.1497375     2.0166599     0.0000085
C     -0.9850462    -1.5730457    -0.0000898
C     -1.7431537     0.9201933     0.0000243
C     -2.3189591    -1.3632656    -0.0001059
C     -2.7473763     0.0224236     0.0000026
```

```
C    -0.3010849   -2.8930727   -0.0000940
H    -3.0151501   -2.1987693   -0.0003198
H    -3.7949024    0.3116905    0.0003636
H    -1.8882159    1.9976362    0.0000263
H     0.9637828    2.5829249   -0.8232921
H     0.9637630    2.5829450    0.8232904
H     2.1335712    1.7467385    0.0000206
H    -1.0524659   -3.6886802   -0.0001435
H     0.3420487   -3.0084217   -0.8746326
H     0.3419862   -3.0084686    0.8744868
```

[Au$_2$(NCH)$_2$] (5, C$_{2h}$)

```
Au    1.2227506   -0.8095578    0.0000000
Au   -1.2227506    0.8095578    0.0000000
N    -0.4749027   -1.9292450    0.0000000
N     0.4749027    1.9292450    0.0000000
C     1.4872849    1.1929810    0.0000000
C    -1.4872849   -1.1929810    0.0000000
H     2.5010730    1.5982531    0.0000000
H    -2.5010730   -1.5982531    0.0000000
```

[Au$_2$(NHCH)$_2$] (6, C$_{2h}$)

```
Au    1.3191879   -0.0414348    0.0000000
Au   -1.3191879    0.0414348    0.0000000
N     0.5045285   -2.0016669    0.0000000
N    -0.5045285    2.0016669    0.0000000
C     0.7983281    1.8615270    0.0000000
C    -0.7983281   -1.8615270    0.0000000
H     0.8436025   -2.9654145    0.0000000
H    -0.8436025    2.9654145    0.0000000
H     1.3897740    2.7818285    0.0000000
H    -1.3897740   -2.7818285    0.0000000
```

[Au$_2$Cl$_2$(NHCH)$_2$] (7, C$_{2h}$)

```
Cl    3.5332908   -0.0813945    0.0000000
Cl   -3.5332908    0.0813945    0.0000000
Au    1.2236795   -0.0332743    0.0000000
C     0.7150121    1.8860448    0.0000000
N     0.5560745   -2.0665738    0.0000000
H     0.9364989   -3.0157638    0.0000000
C    -0.7150121   -1.8860448    0.0000000
Au   -1.2236795    0.0332743    0.0000000
N    -0.5560745    2.0665738    0.0000000
H    -0.9364989    3.0157638    0.0000000
H     1.4307143    2.7115742    0.0000000
H    -1.4307143   -2.7115742    0.0000000
```

[Au$_2$Cl$_2${(NH)$_2$CH}$_2$] (8, D$_{2h}$)

```
Au    0.0000000    1.2511642    0.0000000
Au    0.0000000   -1.2511642    0.0000000
N     1.9726546    1.1494745    0.0000000
N     1.9726546   -1.1494745    0.0000000
N    -1.9726546   -1.1494745    0.0000000
N    -1.9726546    1.1494745    0.0000000
```

```
C     2.6091858     0.0000000     0.0000000
C    -2.6091858     0.0000000     0.0000000
H     2.5265043     1.9964463     0.0000000
H    -2.5265043    -1.9964463     0.0000000
H     3.6993122     0.0000000     0.0000000
H     2.5265043    -1.9964463     0.0000000
H    -3.6993122     0.0000000     0.0000000
H    -2.5265043     1.9964463     0.0000000
Cl    0.0000000     3.5786994     0.0000000
Cl    0.0000000    -3.5786994     0.0000000
```

[Au$_2${(NH)$_2$CH}$_2$] (9, D$_{2h}$)

```
Au    0.0000000     1.3682168     0.0000000
Au    0.0000000    -1.3682168     0.0000000
N     1.9778999     1.1769801     0.0000000
N     1.9778999    -1.1769801     0.0000000
N    -1.9778999    -1.1769801     0.0000000
N    -1.9778999     1.1769801     0.0000000
C     2.5779802     0.0000000     0.0000000
C    -2.5779802     0.0000000     0.0000000
H     2.6307934     1.9484291     0.0000000
H    -2.6307934    -1.9484291     0.0000000
H     3.6691110     0.0000000     0.0000000
H     2.6307934    -1.9484291     0.0000000
H    -3.6691110     0.0000000     0.0000000
H    -2.6307934     1.9484291     0.0000000
```

Au$_2${N(NH)CH}$_2$ (10, C$_i$)

```
Au   -0.1616504     1.3863730    -0.0690891
Au    0.1616504    -1.3863730     0.0690891
N     2.0411209    -1.0984410    -0.2259407
N    -1.7852903    -1.2911037     0.0546014
N     1.7852903     1.2911037    -0.0546014
N    -2.0411209     1.0984410     0.2259407
C     2.4795453     0.1277010    -0.0395884
C    -2.4795453    -0.1277010     0.0395884
H     2.3971626     2.0976182     0.0826760
H    -2.3971626    -2.0976182    -0.0826760
H     3.5580808     0.2443859     0.1176886
H    -3.5580808    -0.2443859    -0.1176886
```

[Au$_2$(N$_2$CH)$_2$] (11, D$_{2h}$)

Triplet state optimized at the DFT/ωB97X-D/def2-TZVP level of theory.

MP2 calculation is not possible because the HF SCF calculation does not converge.

```
Au    0.0000000    -0.0000000     1.3164918
Au    0.0000000    -0.0000000    -1.3164918
N     1.9216174     0.0765404     1.1501187
N     1.9216174     0.0765404    -1.1501187
N    -1.9216174    -0.0765404    -1.1501187
N    -1.9216174    -0.0765404     1.1501187
C     2.5717588     0.1024889     0.0000000
C    -2.5717588    -0.1024889     0.0000000
H     3.6627176     0.1462106     0.0000000
H    -3.6627176    -0.1462106     0.0000000
```

[Au₂{NH(CH)₂)}₂] (12, C$_{2h}$)

Au	-1.1984824	-0.3554047	0.0000000
Au	1.1984824	0.3554047	0.0000000
N	-2.0047820	1.5284697	0.0000000
N	2.0047820	-1.5284697	0.0000000
C	-0.9992464	2.4320909	0.0000000
C	0.3236234	2.1356759	0.0000000
C	0.9992464	-2.4320909	0.0000000
C	-0.3236234	-2.1356759	0.0000000
H	-2.9393033	1.9055472	0.0000000
H	2.9393033	-1.9055472	0.0000000
H	-1.2615234	3.4939029	0.0000000
H	1.1399188	2.8611103	0.0000000
H	1.2615234	-3.4939029	0.0000000
H	-1.1399188	-2.8611103	0.0000000

[Au₂{NH(CH)₂}₂] (13, D$_{2h}$)

Au	0.0000000	1.3826533	0.0000000
Au	0.0000000	-1.3826533	0.0000000
N	2.5380601	0.0000000	0.0000000
N	-2.5380601	0.0000000	0.0000000
C	1.9448275	1.2248770	0.0000000
C	1.9448275	-1.2248770	0.0000000
C	-1.9448275	-1.2248770	0.0000000
C	-1.9448275	1.2248770	0.0000000
H	2.7049637	2.0092267	0.0000000
H	-2.7049637	-2.0092267	0.0000000
H	3.5586533	0.0000000	0.0000000
H	2.7049637	-2.0092267	0.0000000
H	-3.5586533	0.0000000	0.0000000
H	-2.7049637	2.0092267	0.0000000

[Au₂{S₂CC(CN)₂}₂]²⁻ (14, D₂)

Au	0.0000000	-1.3792085	0.0000000
Au	0.0000000	1.3792085	0.0000000
N	0.5842055	2.0721886	-5.8038917
N	0.5842055	-2.0721886	5.8038917
N	-0.5842055	2.0721886	5.8038917
N	-0.5842055	-2.0721886	-5.8038917
C	0.0000000	0.0000000	2.9531095
C	0.0000000	0.0000000	-2.9531095
C	0.0000000	0.0000000	4.3561182
C	0.0000000	0.0000000	-4.3561182
C	0.3240825	1.1524293	-5.1153733
C	0.3240825	-1.1524293	5.1153733
C	-0.3240825	1.1524293	5.1153733
C	-0.3240825	-1.1524293	-5.1153733
S	0.5304743	-1.4605275	2.1985358
S	-0.5304743	1.4605275	2.1985358
S	0.5304743	1.4605275	-2.1985358
S	-0.5304743	-1.4605275	-2.1985358

[Au₂{N₂(CH)₂}₂] (15, D₂)

Au	0.0000000	1.2270582	0.0000000
Au	0.0000000	-1.2270582	0.0000000

```
N     -0.3574908     1.4989398      1.8993482
N      0.3574908    -1.4989398      1.8993482
N     -0.3574908    -1.4989398     -1.8993482
N      0.3574908     1.4989398     -1.8993482
C     -0.2058925     0.7099454      2.8982111
C      0.2058925    -0.7099454      2.8982111
C     -0.2058925    -0.7099454     -2.8982111
C      0.2058925     0.7099454     -2.8982111
H     -0.3963290     1.1346388      3.8955095
H      0.3963290    -1.1346388      3.8955095
H     -0.3963290    -1.1346388     -3.8955095
H      0.3963290     1.1346388     -3.8955095
```

[Au$_2${(NH)$_2$(CH)$_2$}$_2$] (16, D$_{2h}$)

```
Au     0.0000000     1.4238396      0.0000000
Au     0.0000000    -1.4238396      0.0000000
N      0.0000000     1.5489889      1.9267781
N      0.0000000    -1.5489889      1.9267781
N      0.0000000    -1.5489889     -1.9267781
N      0.0000000     1.5489889     -1.9267781
C      0.0000000     0.6926740      2.9655493
C      0.0000000    -0.6926740      2.9655493
C      0.0000000    -0.6926740     -2.9655493
C      0.0000000     0.6926740     -2.9655493
H      0.0000000     1.1491246      3.9532168
H      0.0000000    -1.1491246      3.9532168
H      0.0000000    -1.1491246     -3.9532168
H      0.0000000     1.1491246     -3.9532168
H      0.0000000     2.5090655      2.2622705
H      0.0000000    -2.5090655      2.2622705
H      0.0000000    -2.5090655     -2.2622705
H      0.0000000     2.5090655     -2.2622705
```

[Au$_2$Cl$_2${NH(CH)$_2$N}$_2$] (17, C$_2$)

```
Au    -1.1911662     0.3807502      0.1836974
Au     1.1911662    -0.3807502      0.1836974
N     -1.7315717    -1.4325545     -0.5546320
N      1.7315717     1.4325545     -0.5546320
N      0.7681201    -2.0702191      1.0496890
N     -0.7681201     2.0702191      1.0496890
C     -1.2761425    -2.6012704     -0.2873178
C     -0.1909459    -2.8319938      0.6856968
C      1.2761425     2.6012704     -0.2873178
C      0.1909459     2.8319938      0.6856968
H     -1.7617467    -3.4735673     -0.7267246
H     -0.2530367    -3.8090594      1.1805729
H      1.7617467     3.4735673     -0.7267246
H      0.2530367     3.8090594      1.1805729
H     -2.5392127    -1.3988647     -1.1809345
H      2.5392127     1.3988647     -1.1809345
Cl    -3.3753166     1.0646821     -0.3543787
Cl     3.3753166    -1.0646821     -0.3543787
```

[AuCl(C$_4$Ph$_4$)(py)] (18, C$_1$)

```
Au    -0.9680932     1.6185802      0.7245894
```

```
N   -2.1503140    1.4950931    2.4894787
C   -0.3838922   -0.3073541    0.8110477
C    0.3516216   -0.7239971   -0.2571971
C    0.6364135    0.3165952   -1.2427729
C    0.1289379    1.5522239   -0.9570363
C   -0.8144538   -1.1380598    1.9304604
C   -0.4389530   -0.8187328    3.2449044
C   -0.9022233   -1.5711318    4.3192944
C   -1.7519600   -2.6570009    4.0986225
C   -2.1189104   -2.9946579    2.7955715
C   -1.6542645   -2.2424221    1.7195448
C    0.8067605   -2.1141545   -0.4146501
C    0.5590519   -2.8042273   -1.6096894
C    0.9629412   -4.1281890   -1.7559730
C    1.6311575   -4.7771309   -0.7178506
C    1.8911725   -4.0944063    0.4701326
C    1.4819361   -2.7724644    0.6213674
C    1.4686503    0.0631494   -2.4309036
C    1.0288483    0.4395677   -3.7063235
C    1.8241367    0.2068888   -4.8244535
C    3.0699785   -0.4043479   -4.6841532
C    3.5148020   -0.7842701   -3.4182779
C    2.7180080   -0.5583699   -2.2993301
C    0.4087549    2.7534923   -1.7360258
C    1.7393669    3.1646687   -1.9034120
C    2.0444968    4.2558145   -2.7105438
C    1.0247111    4.9495109   -3.3610372
C   -0.3019819    4.5523021   -3.1915539
C   -0.6112865    3.4697293   -2.3755456
C   -1.8490200    2.2416982    3.5623303
C   -2.5074583    2.0692637    4.7729160
C   -3.5169229    1.1177752    4.8693437
C   -3.8450960    0.3752520    3.7394319
C   -3.1370406    0.5875843    2.5656419
H    0.2227180    0.0266470    3.4114707
H   -0.5983064   -1.3146723    5.3287965
H   -2.1153218   -3.2425962    4.9358567
H   -2.7674353   -3.8459528    2.6177925
H   -1.9385029   -2.4979598    0.7028539
H    0.0444723   -2.2979148   -2.4203273
H    0.7601931   -4.6527035   -2.6833251
H    1.9512941   -5.8062494   -0.8358067
H    2.4184130   -4.5905068    1.2777443
H    1.6900065   -2.2358051    1.5415402
H    0.0599460    0.9171215   -3.8110152
H    1.4712664    0.5026940   -5.8063781
H    3.6896645   -0.5840829   -5.5554854
H    4.4832075   -1.2586293   -3.3020948
H    3.0661362   -0.8544249   -1.3147039
H    2.5275523    2.6118879   -1.4018838
H    3.0769311    4.5645816   -2.8328807
H    1.2612830    5.7987173   -3.9923837
H   -1.0982577    5.0950373   -3.6889696
H   -1.6416780    3.1633174   -2.2363409
H   -1.0746480    2.9858559    3.4213575
H   -2.2288783    2.6818148    5.6213273
```

```
H    -4.0435267     0.9635674     5.8037868
H    -3.3415686     0.0226161     1.6646621
H    -4.6340926    -0.3658997     3.7588087
Cl   -1.5807429     3.8752666     0.6576498
```

Magnetically induced current-density pathways

The MIC density strength is represented with a black ($1 \cdot 10^{-6}$ nA T^{-1}) – red – orange – yellow – white ($1 \cdot 10^{-1}$ nA T^{-1}) color scale.
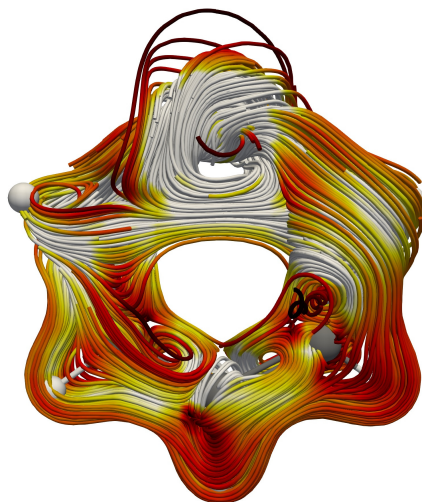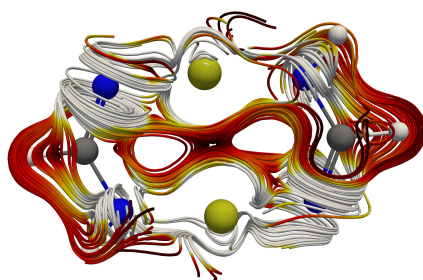

Fig. S3 The 3D streamline plot of the MIC density pathways of molecule [Au(C$_5$H$_5$)] (**1**). Color code: C, grey; H, white; Au, yellow.
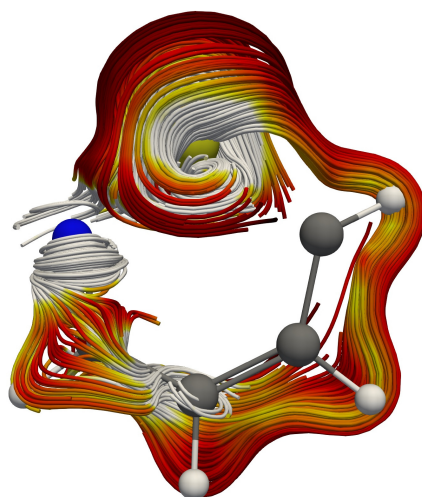
Fig. S4 The 3D streamline plot of the MIC density pathways of molecule [Au(NC$_4$H$_4$)] (**2**). Color code: C, grey; H, white; Au, yellow; N, blue.
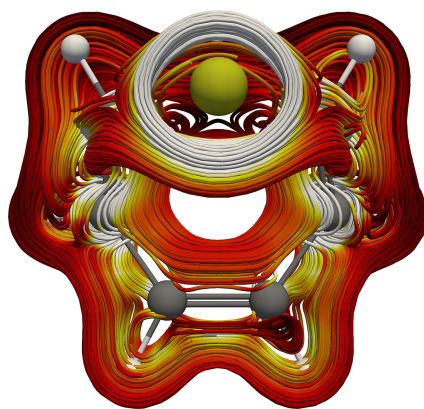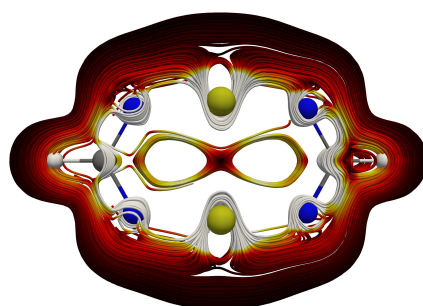
Fig. S5 The 3D streamline plot of the MIC density pathways of molecule $[Au(C_6H_6)]^+$ (**3**). Color code: C, grey; H, white; Au, yellow.
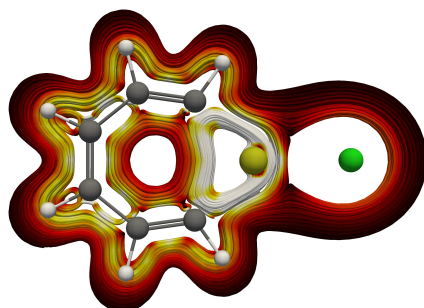
Fig. S6 The 3D streamline plot of the MIC density pathways of molecule $[AuCl(C_6H_6)]$ (**3·Cl**). Color code: C, grey; H, white; Au, yellow; Cl, green.
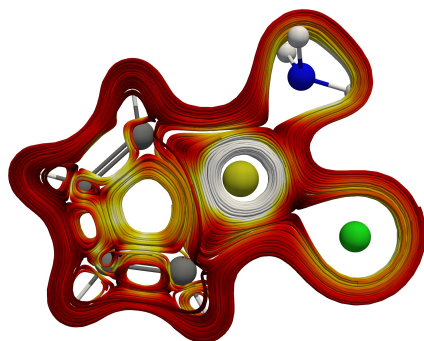
Fig. S7 The 3D streamline plot of the MIC density pathways of molecule $[AuCl(C_4H_4)(NH_3)]$ (**4**). Color code: C, grey; H, white; Au, yellow; Cl, green; N, blue.
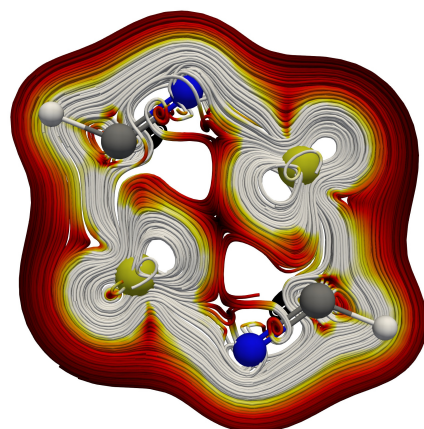
Fig. S8 The 3D streamline plot of the MIC density pathways of molecule $[Au_2(NCH)_2]$ (**5**). Color code: C, grey; H, white; Au, yellow; N, blue.
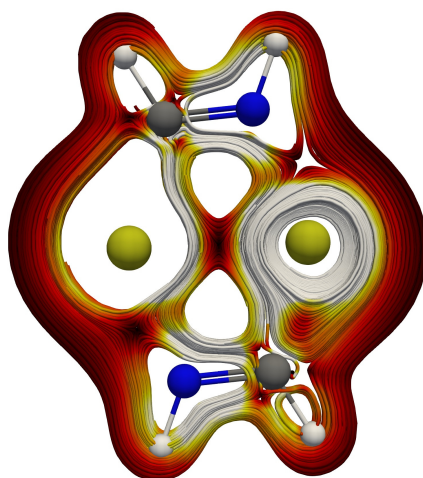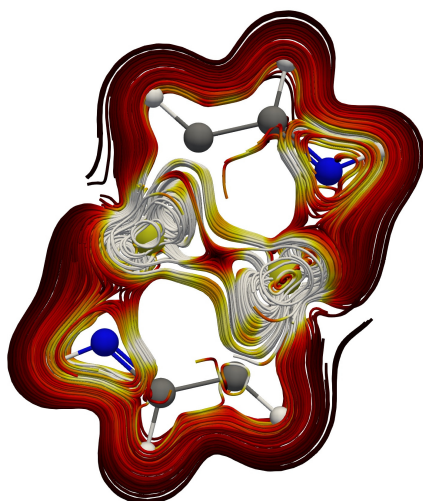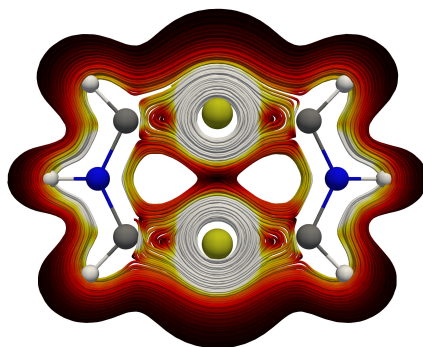
Fig. S9 The 3D streamline plot of the MIC density pathways of molecule [Au$_2$(NHCH)$_2$] (**6**). Color code: C, grey; H, white; Au, yellow; N, blue.
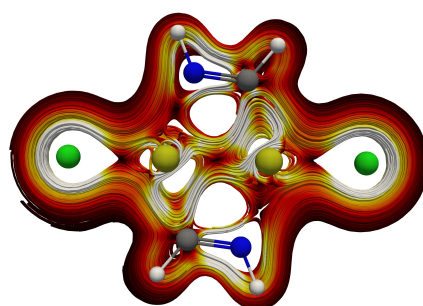
Fig. S10 The 3D streamline plot of the MIC density pathways of molecule [Au$_2$Cl$_2$(NHCH)$_2$] (**7**). Color code: C, grey; H, white; Au, yellow; Cl, green; N, blue.
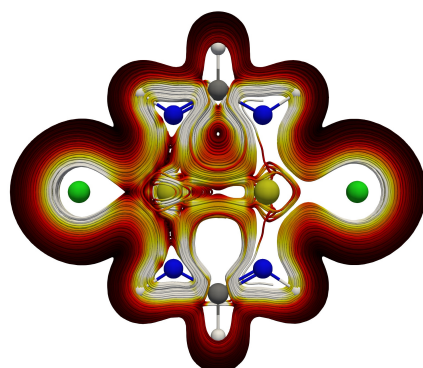
Fig. S11 The 3D streamline plot of the MIC density pathways of molecule [Au$_2$Cl$_2${(NH)$_2$CH}$_2$] (**8**). Color code: C, grey; H, white; Au, yellow; Cl, green; N, blue.
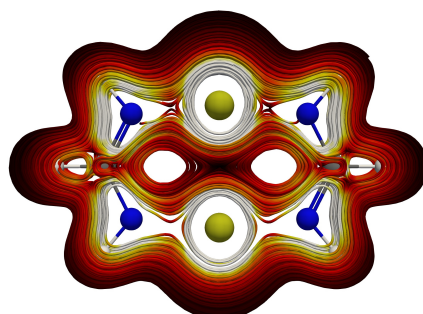
Fig. S12 The 3D streamline plot of the MIC density pathways of molecule [Au$_2${(NH)$_2$CH}$_2$] (**9**). Color code: C, grey; H, white; Au, yellow; N, blue.

Fig. S13 The 3D streamline plot of the MIC density pathways of molecule $[Au_2(NHNCH)_2]$ (**10**). Color code: C, grey; H, white; Au, yellow; N, blue.

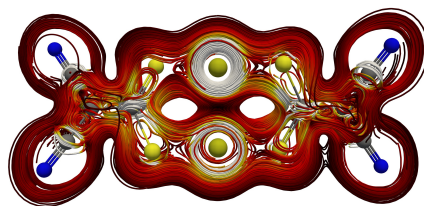Fig. S14 The 3D streamline plot of the MIC density pathways of molecule $[Au_2(N_2CH)_2]$ (**11**). Color code: C, grey; H, white; Au, yellow; N, blue.

Fig. S15 The 3D streamline plot of the MIC density pathways of molecule $[Au_2\{(CH)_2NH\}_2]$ (**12**). Color code: C, grey; H, white; Au, yellow; N, blue.

Fig. S16 The 3D streamline plot of the MIC density pathways of molecule $[Au_2\{(CH)_2NH\}_2]$ (**13**). Color code: C, grey; H, white; Au, yellow; N, blue.

Fig. S17 The 3D streamline plot of the MIC density pathways of molecule $[Au_2\{S_2CC(CN)_2\}_2]^{2-}$ (**14**). Color code: C, grey; H, white; Au, dark yellow; N, blue; S, light yellow.

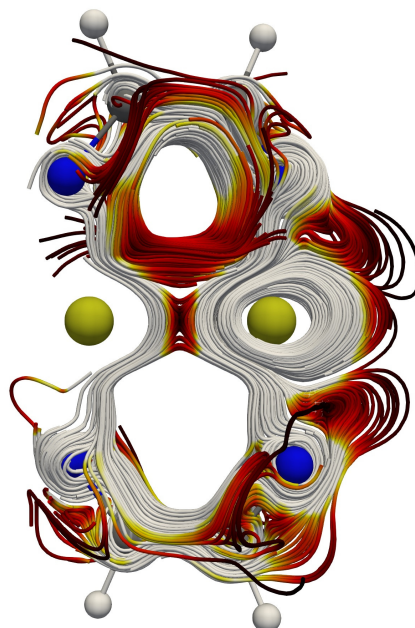Fig. S18 The 3D streamline plot of the MIC density pathways of molecule $[Au_2\{N_2(CH)_2\}_2]$ (**15**). Color code: C, grey; H, white; Au, yellow; N, blue.
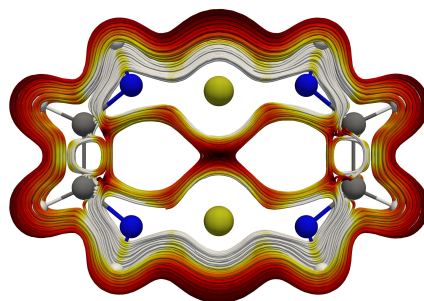

Fig. S19 The 3D streamline plot of the MIC density pathways of molecule $[Au_2\{(NH_2)(CH_2)\}_2]$ (**16**). Color code: C, grey; H, white; Au, yellow; N, blue.

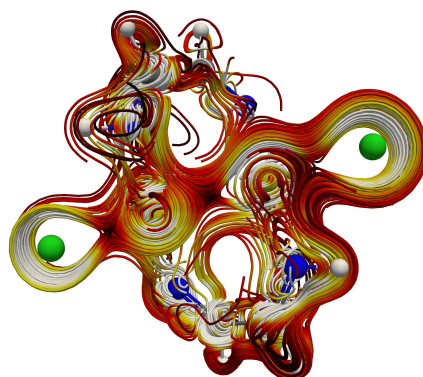Fig. S20 The 3D streamline plot of the MIC density pathways of molecule $[Au_2Cl_2\{(NH_2)(CH_2)\}_2]$ (**17**). Color code: C, grey; H, white; Au, yellow; Cl, green; N, blue.