Electronic Supplementary Material (ESI) for CrystEngComm.

The interplay of noncovalent interactions determining the antiparallel conformation of (isocyanide)gold(I) dimers

Jorge Echeverría

Departament de Química Inorgànica i Orgànica and Institut de Química Teòrica i Computacional IQTC-UB,
Universitat de Barcelona, Martí i Franquès 1-11, 08028 Barcelona (Spain).
e-mail: jorge.echeverria@qi.ub.es

ELECTRONIC SUPPLEMENTARY INFORMATION

Table S1. Cartesian coordinates of optimized dimers.

$[Cl\text{-}Au\text{-}CN\text{-}H]_2$

C	5.414768	5.809373	5.537919
N	5.844085	4.787944	5.840123
H	6.208104	4.049921	6.439349
Au	4.713942	7.603249	5.412034
Cl	3.941955	9.715785	5.688200
Au	5.868157	5.900081	9.030380
Cl	6.640147	3.787476	8.753733
C	5.167547	7.694131	8.905181
N	4.738302	8.715629	8.603095
H	4.374580	9.454127	8.004453

$[Cl\text{-}Au\text{-}CN\text{-}CH_3]_2$

C	6.993527	5.361377	5.677714
N	8.063541	5.497328	6.066221
C	9.396543	5.585345	6.537616
H	10.069552	5.278837	5.740374
Au	5.202252	5.073263	5.013277
Cl	3.121476	4.700006	4.227907
H	9.514538	4.902468	7.375483
H	9.601898	6.609997	6.841144
Au	7.219006	1.835392	5.207103
Cl	9.300001	2.208788	5.991806
C	5.427542	1.547289	4.543200
N	4.357426	1.411343	4.154970
C	3.024329	1.323255	3.683859
H	2.818729	0.298426	3.381092
H	2.906321	2.005561	2.845527
H	2.351510	1.630453	4.480996

$[Cl\text{-}Au\text{-}CN\text{-}C(CH_3)_3]_2$

C	7.314108	5.456151	5.784958
N	8.366144	5.676884	6.184298
C	9.698777	5.918828	6.681540
C	10.676406	5.449653	5.615848
Au	5.534321	5.122159	5.108362
Cl	3.445300	4.803057	4.315412
C	9.859287	5.123435	7.967269
C	9.827752	7.412873	6.933422
Au	6.890017	1.785076	5.108533
Cl	8.980914	2.105552	5.895800
C	5.108666	1.450310	4.436475
N	4.055796	1.229110	4.039599
C	2.722262	0.986958	3.544916
C	2.591064	-0.507905	3.298996
C	2.561341	1.777515	2.256254
C	1.746443	1.461469	4.609872

H	1.554702	1.620728	1.868857
H	2.709472	2.840281	2.441458
H	3.278469	1.443208	1.506382
H	1.589633	-0.718907	2.924592
H	3.316525	-0.845687	2.559099
H	2.741673	-1.068413	4.221484
H	0.728960	1.302935	4.252717
H	1.881791	0.900361	5.534620
H	1.891466	2.521533	4.812079
H	11.693293	5.607610	5.974938
H	10.532525	4.390306	5.409129
H	10.541678	6.014423	4.693243
H	10.865433	5.279706	8.356162
H	9.141180	5.454141	8.717798
H	9.712410	4.061243	7.777799
H	10.828513	7.623755	7.309689
H	9.677359	7.976788	6.012978
H	9.101083	7.746816	7.673877

$[Cl\text{-}Au\text{-}CN\text{-}CF_3]_2$

C	7.420410	5.522654	5.867312
N	8.465143	5.802405	6.268960
C	9.789337	5.962660	6.740030
F	10.639779	5.573210	5.812017
Au	5.692666	5.058255	5.195227
Cl	3.666868	4.508438	4.396990
F	9.960687	5.247301	7.833119
F	9.998687	7.241211	7.016574
Au	6.728446	1.849751	5.025835
Cl	8.754159	2.399417	5.824311
C	5.000704	1.385687	4.353631
N	3.955964	1.106111	3.951849
C	2.631724	0.946347	3.481069
F	2.421692	-0.332280	3.204757
F	2.460501	1.661546	2.387602
F	1.781421	1.336414	4.409005

Table S2. Cartesian coordinates of crystallographic (CSD) dimers.

EMUKOM

Au	1.388	-11.412	-10.209
Au	1.378	-14.800	-10.159
C	3.326	-11.279	-9.948
C	-0.559	-14.933	-10.419
C	5.878	-11.087	-9.648
C	-3.111	-15.125	-10.719
C	6.461	-12.472	-9.391
C	-3.694	-13.740	-10.976
C	7.975	-12.356	-9.217
C	-5.209	-13.856	-11.150

C	8.630	-11.682	-10.407
C	-5.863	-14.530	-9.961
C	7.997	-10.318	-10.684
C	-5.230	-15.894	-9.684
C	6.488	-10.424	-10.877
C	-3.722	-15.788	-9.490
Cl	-0.852	-11.503	-10.483
Cl	3.619	-14.709	-9.885
H	6.066	-10.524	-8.869
H	-3.299	-15.688	-11.499
H	6.258	-13.058	-10.137
H	-3.491	-13.153	-10.231
H	6.066	-12.852	-8.590
H	-3.299	-13.360	-11.777
H	8.167	-11.845	-8.415
H	-5.401	-14.367	-11.952
H	8.354	-13.242	-9.105
H	-5.587	-12.970	-11.262
H	9.577	-11.568	-10.231
H	-6.810	-14.644	-10.136
H	8.535	-12.246	-11.188
H	-5.768	-13.966	-9.179
H	8.396	-9.937	-11.481
H	-5.629	-16.275	-8.886
H	8.184	-9.722	-9.942
H	-5.417	-16.490	-10.425
H	6.109	-9.540	-11.000
H	-3.342	-16.672	-9.368
H	6.295	-10.951	-11.669
H	-3.528	-15.260	-8.698
N	4.437	-11.177	-9.812
N	-1.670	-15.035	-10.556

EMUKUS

Au	0.296	9.967	15.246
Au	0.618	6.758	13.922
Br	2.660	10.032	15.052
Br	-1.746	6.693	14.116
C	-1.662	9.962	15.453
C	2.575	6.763	13.715
C	5.119	6.747	13.481
C	-4.205	9.978	15.687
C	5.673	8.140	13.785
C	-4.759	8.584	15.383
C	7.196	8.139	13.668
C	-6.282	8.586	15.500
C	7.826	7.086	14.564
C	-6.912	9.638	14.603
C	7.240	5.708	14.293
C	-6.326	11.017	14.875
C	5.724	5.689	14.418
C	-4.810	11.036	14.750
H	5.358	6.510	12.540

H -4.445 10.215 16.628
H 5.409 8.410 14.700
H -4.496 8.315 14.467
H 5.291 8.796 13.150
H -4.377 7.929 16.018
H 7.543 9.032 13.917
H -6.629 7.693 15.251
H 7.452 7.963 12.728
H -6.538 8.761 16.440
H 8.803 7.065 14.408
H -7.889 9.660 14.760
H 7.673 7.328 15.512
H -6.759 9.397 13.656
H 7.626 5.060 14.933
H -6.713 11.665 14.234
H 7.496 5.422 13.381
H -6.582 11.303 15.787
H 5.380 4.793 14.177
H -4.466 11.932 14.991
H 5.463 5.880 15.354
H -4.549 10.845 13.814
N -2.768 9.980 15.565
N 3.681 6.745 13.603

EMULAZ

Au -27.726 -4.107 -20.913
Au -28.261 -7.686 -20.058
C -25.784 -3.956 -20.820
C -30.203 -7.838 -20.151
C -23.207 -3.745 -20.668
C -32.780 -8.049 -20.302
C -22.824 -2.872 -19.484
C -33.163 -8.922 -21.487
C -21.296 -2.787 -19.366
C -34.691 -9.007 -21.605
C -20.675 -4.156 -19.264
C -35.312 -7.638 -21.707
C -21.063 -5.045 -20.451
C -34.924 -6.749 -20.520
C -22.590 -5.147 -20.588
C -33.397 -6.647 -20.383
H -22.872 -3.305 -21.502
H -33.116 -8.489 -19.469
H -23.200 -3.255 -18.652
H -32.787 -8.539 -22.319
H -23.199 -1.964 -19.604
H -32.788 -9.830 -21.367
H -20.930 -2.320 -20.159
H -35.057 -9.473 -20.811
H -21.057 -2.258 -18.565
H -34.931 -9.535 -22.406
H -20.969 -4.586 -18.424
H -35.018 -7.208 -22.547

H	-19.690	-4.066	-19.233
H	-36.297	-7.728	-21.737
H	-20.685	-5.950	-20.320
H	-35.302	-5.844	-20.651
H	-20.684	-4.669	-21.283
H	-35.304	-7.124	-19.688
H	-22.817	-5.657	-21.405
H	-33.170	-6.137	-19.566
H	-22.963	-5.630	-19.809
H	-33.024	-6.164	-21.162
I	-30.250	-4.242	-21.065
I	-25.737	-7.551	-19.906
N	-24.657	-3.841	-20.760
N	-31.330	-7.953	-20.210

PUJPEP01

Au	19.450	0.378	16.444
Au	19.417	3.567	15.613
C	17.496	3.516	15.498
C	21.370	0.428	16.558
C	14.904	3.312	15.588
C	23.963	0.632	16.468
C	14.642	2.759	16.998
C	24.225	1.185	15.059
C	14.484	2.295	14.503
C	24.383	1.649	17.553
C	14.265	4.668	15.400
C	24.602	-0.723	16.656
H	15.073	1.895	17.091
H	23.794	2.049	14.965
H	13.688	2.661	17.135
H	25.179	1.283	14.922
H	23.864	0.571	14.399
H	15.003	3.373	17.658
H	14.914	1.445	14.672
H	23.952	2.499	17.384
H	14.755	2.628	13.630
H	24.112	1.316	18.426
H	13.521	2.184	14.520
H	25.345	1.760	17.536
H	14.449	4.990	14.505
H	24.417	-1.046	17.551
H	14.628	5.289	16.051
H	24.238	-1.345	16.005
H	13.305	4.592	15.526
H	25.561	-0.648	16.530
N	16.863	-0.653	15.880
N	22.004	4.597	16.177
N	16.363	3.481	15.501
N	22.504	0.464	16.556
O	17.393	0.457	16.321
O	21.474	3.488	15.736
O	15.635	-0.674	15.800

O 23.231 4.618 16.257
O 17.577 -1.592 15.628
O 21.289 5.536 16.429

LOTSAO

Au -13.694 11.278 2.893
Au -13.573 8.200 3.870
C -18.205 11.326 3.213
C -9.062 8.152 3.550
C -18.485 10.779 4.601
C -8.782 8.700 2.161
C -18.732 10.399 2.102
C -8.535 9.079 4.661
C -18.724 12.751 3.028
C -8.543 6.727 3.735
C -15.597 11.323 2.992
C -11.670 8.155 3.771
H -18.131 11.397 5.275
H -9.136 8.081 1.488
H -18.055 9.904 4.701
H -9.213 9.574 2.061
H -19.453 10.682 4.725
H -7.815 8.796 2.038
H -18.388 9.492 2.243
H -8.879 9.986 4.519
H -18.434 10.730 1.230
H -8.833 8.748 5.533
H -19.713 10.383 2.128
H -7.554 9.095 4.635
H -8.893 6.156 3.019
H -18.374 13.322 3.744
H -19.702 12.750 3.062
H -7.565 6.729 3.701
H -18.428 13.097 2.161
H -8.839 6.381 4.602
N -16.737 11.373 3.064
N -10.530 8.105 3.699
N -11.041 12.188 3.432
N -16.226 7.290 3.331
O -11.721 13.123 3.829
O -15.546 6.355 2.934
O -9.828 12.119 3.535
O -17.439 7.360 3.228
O -11.663 11.172 2.847
O -15.604 8.306 3.916