

Electronic Supporting information for manuscript:

Synthesis, X-ray characterization, and DFT calculations of gold-nucleobase complexes: On the importance of regium bonds and anion- π interactions

Jordi Buils,^{a,b} Angel Terron,^a Miquel Barceló-Oliver,^a Juan Jesús Fiol,^a Angel García-Raso,^a Rosa M. Gomila^a and Antonio Frontera^{*a}

Table of contents:

Table S1	Page 2
Table S2	Page 3
Table S3	Page 5

Table S1. QTAIM parameters (a.u.) and delocalization index (DI) for the BCPs included in the manuscript

Figure	Interaction	ρ	$\nabla^2\rho$	H(r)	V(r)	G(r)	DI
9a	RgB	0.0073	0.0246	0.0012	-0.0038	0.0050	0.0975
9a	HB	0.0105	0.0388	0.0023	-0.0050	0.0074	0.0444
9a	HB	0.0070	0.0278	0.0016	-0.0038	0.0054	0.0302
11a	CH $\cdots$ Cl	0.0047	0.0140	0.0007	-0.0021	0.0028	0.0217
11a	CH $\cdots$ Cl	0.0032	0.0117	0.0007	-0.0015	0.0022	0.0066
11a	CH $\cdots$ Cl	0.0041	0.0137	0.0008	-0.0019	0.0026	0.0203
11a	CH $\cdots$ Cl	0.0040	0.0127	0.0007	-0.0018	0.0025	0.0174
11a	anion- π	0.0072	0.0254	0.0014	-0.0036	-0.0036	0.0542
11a	anion- π	0.0068	0.0198	0.0008	-0.0034	-0.0034	0.0469
11a	anion- π	0.0066	0.0227	0.0012	-0.0032	-0.0032	0.0519
11a	HB	0.0188	0.0582	0.0021	-0.0104	-0.0104	0.0081
11b	anion- π	0.0068	0.0255	0.0014	-0.0035	0.0049	0.1366
11b	anion- π	0.0063	0.0251	0.0014	-0.0035	0.0049	0.0445
11b	anion- π	0.0051	0.0180	0.0011	-0.0024	0.0034	0.0477
11b	HB	0.0243	0.0736	0.0015	-0.0154	0.0169	0.1388
11b	HB	0.0063	0.0178	0.0009	-0.0026	0.0035	0.0497

Table S2. Result of the CSD search for chlorine. Distances in Å and angles in degrees

Refcode	d	α_1	α_2	α_3	mean angle X $\cdots$ Au-Cl
AVATUN	3.54	113.159	72.181	68.908	84.749
AVATUN	3.56	69.585	78.963	111.915	86.821
AVATUN	3.68	102.83	92.101	76.413	90.448
AVATUN	3.48	84.401	101.357	97.614	94.457
AVATUN	3.58	82.133	75.909	96.009	84.684
BEDKAA	3.49	72.951	74.495	103.986	83.811
BEDKAA	3.83	93.681	107.198	74.969	91.949
BEDXUH	3.51	84.01	91.751	97.883	91.215
BEDXUH	3.56	82.257	103.597	96.366	94.073
BEDYES	3.69	83.925	86.892	97.669	89.495
BIRCUA	3.48	80.298	102.004	79.357	87.220
BUVVIY	3.66	91.985	84.592	90.997	89.191
BUWVUM	3.41	84.135	96.286	87.918	89.446
BUWVUM	3.43	98.257	83.574	86.138	89.323
BUWVUM01	3.32	87.4	85.827	94.84	89.356
BUWVUM01	3.36	85.618	97.657	84.737	89.337
DEDYUG	3.85	87.007	80.438	92.456	86.634
DIWYIU	3.87	89.243	87.779	69.941	82.321
DOYPOY	3.58	80.725	87.464	98.996	89.062
DUCYEI	3.77	87.132	88.385	92.705	89.407
DUCYIM	3.79	85.893	89.136	93.03	89.353
EHENOX	3.66	83.267	90.905	95.118	89.763
EHENOX	3.30	88.815	95.314	92.824	92.318
EHENUD	3.39	92.863	77.204	87.658	85.908
EHENUD	3.53	83.978	92.74	95.843	90.854
EHEPAL	3.22	82.282	93.32	82.649	86.084

EHEPAL	3.75	70.528	114.144	90.75	91.807
EHEPEP	3.38	89.486	88.176	91.746	89.803
EHEPEP	3.43	90.522	92.487	88.235	90.415
EHEPIT	3.47	92.959	92.476	86.787	90.741
EHEPIT	3.55	90.517	95.258	84.768	90.181
EHEXIA	3.85	73.932	89.326	109.645	90.968
EHEXIA	3.47	85.552	98.513	90.767	91.611
EHEXIA	3.74	93.946	101.175	83.343	92.821
EHEXIA	3.60	102.827	88.848	79.602	90.426
EHEXOG	3.76	78.412	91.09	102.535	90.679
EHEXOG	3.80	101.516	90.752	77.436	89.901
ELUVAK	3.67	99.882	86.826	80.201	88.970
ELUVAK	3.87	71.445	89.363	108.503	89.770
ESITIM	3.28	91.121	85.995	91.785	89.634
ESITIM	3.41	80.213	87.462	94.967	87.547
FAHCIE	3.50	80.347	80.581	97.446	86.125
FAJWAS	3.68	93.348	97.713	80.653	90.571
FEDTUF	3.54	86.179	82.929	94.643	87.917
FEYTEI	3.39	94.575	85.151	99.911	93.212
FEYTEI	3.40	93.58	85.936	99.865	93.127
GOXCAX	3.50	92.061	93.344	86.726	90.710
GOXCUR	3.59	96.369	102.298	80.279	92.982
HAFFEA	3.88	84.606	89.938	91.223	88.589
HAFFIE	3.40	73.163	103.855	83.146	86.721
HIHCIK	3.66	82.254	90.867	96.066	89.729
HOSHUI	3.79	90.006	85.454	89.89	88.450
HOSHUU	3.44	89.531	89.817	84.536	87.961
IJOTAF	3.58	94.907	88.439	80.61	87.985
KILFIV	3.53	94.598	91.798	85.019	90.472
KILFIV	3.43	86.122	85.743	94.271	88.712
KOXQEV	3.82	73.829	92.495	92.298	86.207
KUFNAB	3.70	71.774	91.71	110.162	91.215
LABMEK	3.56	85.554	91.907	88.331	88.597
MAJDAC	3.56	85.679	92.419	92.438	90.179
MAJDAC01	3.48	92.868	87.582	93.165	91.205
MESSUC	3.30	81.452	98.693	93.469	91.205
MIYYOL	3.60	91.87	87.52	87.459	88.950
MIYZAY	3.79	99.322	91.345	79.716	90.128
MIYZEC	3.64	85.376	82.429	91.544	86.450
MOCFER	3.52	95.051	85.453	82.351	87.618
MOCFUH	3.53	80.962	81.31	96.63	86.301
MUPHIP	3.72	73.351	78.722	106.398	86.157
NEVYOG	3.65	79.992	84.843	96.136	86.990
NOKMOR	3.36	86.966	86.672	95.853	89.830
NOKMOR	3.48	92.844	94.532	84.299	90.558
NOKMUX	3.35	87.847	90.103	93.143	90.364
NOKMUX	3.39	92.109	91.502	86.835	90.149
NOKNAE	3.46	86.391	89.391	96.546	90.776
NOKNAE	3.73	94.947	95.455	82.042	90.815
NUFYUL	3.55	91.357	79.753	88.174	86.428
OJELIA	3.50	84.299	87.779	95.723	89.267
PYAUCL10	3.64	79.477	89.898	98.496	89.290
PYAUCL10	3.65	106.867	87.182	75.203	89.751

QAWDEA	3.63	76.83	96.311	85.089	86.077
QIHVOS	3.86	75.875	109.152	72.237	85.755
RADLAJ	3.61	100.719	86.85	76.33	87.966
RIMFIF	3.34	88.132	90.815	105.717	94.888
RIMFIF	3.60	96.488	84.473	77.263	86.075
RIMFIF	3.31	92.581	86.911	103.168	94.220
RIMFIF	3.62	85.022	95.411	79.136	86.523
SASREM	3.41	92.525	87.443	87.966	89.311
SASREM01	3.42	92.418	87.256	87.841	89.172
SASRIQ	3.79	82.229	90.15	95.002	89.127
SASRIQ	3.72	78.363	76.609	104.709	86.560
SEVXID	3.50	84.837	96.701	95.692	92.410
SEVXID	3.74	105.703	103.189	73.595	94.162
SEVXID	3.34	91.868	97.719	88.825	92.804
SEVXID	3.48	99.352	92.207	79.779	90.446
SOVROM	3.80	68.885	114.155	102.317	95.119
SOVROM	3.45	80.695	96.336	88.762	88.598
SOVROM	3.54	79.565	98.525	79.922	86.004
SOVROM	3.80	105.857	75.837	74.571	85.422
SOVROM	3.86	103.977	78.468	67.744	83.396
SUYXAN	3.64	68.623	111.462	79.604	86.563
TIGMIH	3.96	76.029	65.895	99.382	80.435
UQIBEC	3.55	89.818	87.794	91.823	89.812
VANPUY	3.36	92.654	85.35	91.981	89.995
VANPUY	3.90	79.211	101.357	96.046	92.205
VOYNUU	3.67	84.684	83.412	90.012	86.036
VOYPAC	3.63	85.19	85.192	90.76	87.047
WEFQAD	3.49	89.998	87.274	92.141	89.804
WEFQAD	3.58	97.971	87.346	79.942	88.420
WEFQEH	3.37	77.909	102.201	95.847	91.986
WEFQEH	3.43	94.954	84.8	91.465	90.406
WEFQIL	3.40	90.265	90.511	89.695	90.157
WEFQIL	3.41	91.127	89.622	90.121	90.290
WEFQOR	3.37	79.649	89.231	89.846	86.242
WEFQOR	3.48	92.777	86.412	94.689	91.293
WEFREI	3.49	84.835	92.77	89.339	88.981
WEFREI	3.57	87.301	92.063	87.55	88.971
WEFREI	2.93	89.292	93.186	89.07	90.516
WEFREI	3.10	84.334	96.376	90.328	90.346
WIRGAH	3.29	85.93	94.052	91.954	90.645
WONZUX	3.52	86.154	92.709	92.284	90.382
WUJKUK	3.68	87.846	89.222	89.814	88.961
XIMWOI	3.69	79.662	87.111	99.17	88.648
YIDMAA	3.66	92.941	86.276	84.989	88.069
ZUHNAT	3.51	101.286	84.597	74.652	86.845
ZUHNIB	3.36	86.453	85.102	87.41	86.322
ZUHNOH	3.47	91.047	75.189	98.81	88.349

Table S3. Result of the CSD search for Bromine. Distances in Å and angles in degrees

Refcode	d	α_1	α_2	α_3	mean angle $X\cdots Au-Br$
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BUWTIY	3.484	83.487	93.719	86.517	87.908
BUWTIY	3.569	91.189	83.623	93.588	89.467
FEYKIG	3.556	89.073	90.288	88.679	89.347
UZIMEW	3.519	84.457	89.345	93.781	89.194
UZIMEW	3.594	87.678	88.174	92.082	89.311
WEFQUX	3.419	91.661	91.079	91.12	91.287
WEFQUX	3.929	81.977	99.608	95.297	92.294
WEFQUX	3.475	94.239	88.454	90.385	91.026
WEFQUX	3.877	92.578	102.668	83.16	92.802
WEFRAE	3.542	91.597	93.795	87.278	90.890
WEFRAE	3.588	89.374	86.236	92.666	89.425
WIRFUA	3.488	92.798	87.196	91.706	90.567
WOQME U	3.547	92.934	86.716	89.711	89.787
WOQME U	3.539	85.352	94.959	86.896	89.069