

## Supporting Information

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### Design and Structural Characterization of all-metal aromaticity sandwich species $[\text{Bi}_3\text{Au}_3\text{Bi}_3]^{3-}$ : Insight from density functional theory

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This paper we wish to be considered for publication in *New Journal of Chemistry*.

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The complete results of CDA analysis

Table S1

**Table S1.** The complete results of CDA analysis

Orbital	Occ.	d	b	d - b	r
1	2.000000	0.000494	0.000000	0.000494	0.000614
2	2.000000	0.000362	-0.000007	0.000369	0.000511
3	2.000000	0.000397	-0.000004	0.000401	0.000056
4	2.000000	0.000513	0.000005	0.000508	0.000055
5	2.000000	0.000395	-0.000001	0.000396	0.000050
6	2.000000	0.000513	0.000003	0.000510	0.000059
7	2.000000	-0.000003	-0.000392	0.000388	-0.000775
8	2.000000	-0.000002	-0.000595	0.000593	-0.000113
9	2.000000	-0.000004	-0.000311	0.000307	-0.000683
10	2.000000	-0.000057	-0.000000	-0.000057	-0.000011
11	2.000000	-0.000021	-0.000000	-0.000021	0.000008
12	2.000000	-0.000088	-0.000002	-0.000086	-0.000045
13	2.000000	-0.000088	-0.000001	-0.000086	-0.000046
14	2.000000	-0.000063	-0.000001	-0.000063	0.000013
15	2.000000	-0.000065	-0.000001	-0.000064	0.000013
16	2.000000	-0.000029	0.000000	-0.000029	-0.000013
17	2.000000	-0.000006	-0.000000	-0.000006	0.000009
18	2.000000	-0.000028	0.000000	-0.000028	-0.000013
19	2.000000	-0.000006	-0.000000	-0.000006	0.000009
20	2.000000	-0.000050	-0.000000	-0.000049	-0.000023
21	2.000000	-0.000004	-0.000000	-0.000004	0.000018
22	2.000000	-0.000091	0.000002	-0.000093	-0.000124
23	2.000000	-0.000443	-0.000012	-0.000430	-0.000637

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24	2.000000	-0.000097	-0.000002	-0.000095	0.000025
25	2.000000	-0.000937	-0.000009	-0.000928	-0.000198
26	2.000000	-0.000097	-0.000000	-0.000097	0.000020
27	2.000000	-0.000954	-0.000012	-0.000942	-0.000190
28	2.000000	-0.000010	0.000976	-0.000986	0.001631
29	2.000000	-0.000014	0.001691	-0.001705	0.00593
30	2.000000	-0.000026	0.001052	-0.001078	0.001871
31	2.000000	-0.000013	-0.000100	0.000086	-0.000273
32	2.000000	-0.000001	0.000139	-0.000140	0.000012
33	2.000000	-0.000002	0.000130	-0.000132	0.000030
34	2.000000	-0.000000	0.000035	-0.000035	-0.000012
35	2.000000	-0.000000	0.000039	-0.000040	-0.000023
36	2.000000	-0.000000	0.000164	-0.000164	0.000004
37	2.000000	0.000064	0.000004	0.000061	0.000212
38	2.000000	0.000056	-0.000001	0.000057	-0.000087
39	2.000000	0.000044	0.000003	0.000041	0.000105
40	2.000000	0.000044	0.000001	0.000043	0.000108
41	2.000000	0.000022	-0.000003	0.000025	-0.000033
42	2.000000	0.000022	-0.000001	0.000024	-0.000036
43	2.000000	-0.000148	0.000001	-0.000149	0.000390
44	2.000000	-0.000080	0.000005	-0.000086	0.000325
45	2.000000	0.000007	0.000000	0.000006	0.000038
46	2.000000	0.000006	-0.000000	0.000007	0.000012
47	2.000000	0.000007	0.000000	0.000007	0.000039
48	2.000000	0.000006	0.000000	0.000006	0.000011
49	2.000000	0.000402	0.000009	0.000393	0.002056
50	2.000000	0.000330	0.000000	0.000330	-0.000354
51	2.000000	-0.000077	0.000003	-0.000080	0.000382
52	2.000000	-0.000076	0.000004	-0.000080	0.000382
53	2.000000	-0.000039	0.000002	-0.000041	0.000222
54	2.000000	-0.000038	0.000001	-0.000039	0.000224
55	2.000000	0.000003	0.000000	0.000003	0.000070
56	2.000000	-0.000014	0.000001	-0.000014	0.000037
57	2.000000	-0.000027	0.000007	-0.000034	0.000349
58	2.000000	0.000111	-0.000008	0.000119	0.000621
59	2.000000	-0.000028	0.000003	-0.000031	0.000354
60	2.000000	0.000116	-0.000000	0.000116	0.000633
61	2.000000	0.000391	0.000006	0.000385	0.001600
62	2.000000	0.000371	0.000030	0.000341	0.001525
63	2.000000	0.000003	0.000003	-0.000000	0.000310
64	2.000000	-0.000011	0.000000	-0.000011	0.000089
65	2.000000	0.000444	-0.000045	0.000489	-0.000538
66	2.000000	0.000458	-0.000003	0.000461	-0.000621
67	2.000000	-0.004256	-0.001431	-0.002825	0.101278

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68	2.000000	-0.014177	0.000303	-0.014480	0.021274
69	2.000000	0.020427	-0.001150	0.021577	0.065290
70	2.000000	0.019808	0.000137	0.019671	0.062713
71	2.000000	0.001284	0.000071	0.001213	-0.010213
72	2.000000	0.000915	-0.000876	0.001791	-0.008308
73	2.000000	0.010506	0.010401	0.000105	0.093579
74	2.000000	0.001963	0.008377	-0.006414	0.077167
75	2.000000	-0.002151	-0.008781	0.006630	0.035387
76	2.000000	-0.000025	0.007956	-0.007981	0.060570
77	2.000000	0.000046	0.008550	-0.008504	0.059382
78	2.000000	0.006566	0.016636	-0.010069	0.001963
79	2.000000	0.007565	0.043722	-0.036157	-0.052203
80	2.000000	-0.002950	0.029663	-0.032613	-0.043703
81	2.000000	0.000624	-0.003231	0.003854	0.022095
82	2.000000	-0.000008	0.018257	-0.018265	-0.002585
83	2.000000	0.000256	0.017453	-0.017197	-0.001804
84	2.000000	0.000811	0.019519	-0.018708	-0.005922
85	2.000000	-0.001709	-0.008545	0.006836	0.043960
86	2.000000	-0.001266	0.001040	-0.002306	-0.000557
87	2.000000	-0.000924	-0.000155	-0.000769	0.001830
88	.000000	0.000002	0.002381	-0.002378	-0.000108
89	2.000000	0.003753	-0.009643	0.013397	-0.009479
90	2.000000	0.003828	0.002160	0.001668	-0.054325
91	2.000000	-0.011252	-0.027586	0.016334	-0.347405
92	2.000000	0.009484	0.003108	0.006376	0.043627
93	2.000000	0.007994	0.000920	0.007074	0.047995
94	2.000000	-0.005040	0.094944	-0.099983	-0.032456
95	2.000000	0.018768	-0.008263	0.027031	0.173973
96	2.000000	0.009271	0.000098	0.009173	-0.165619
97	2.000000	0.010456	0.000136	0.010319	-0.165687
98	2.000000	0.001034	-0.276471	0.277505	-0.008006
99	2.000000	0.190247	0.002783	0.187464	-0.566505
sum	198	0.283695	-0.054713	0.338408	-0.551957

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