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Gold oxyfluorides, $Au(OF)_n$ (n = 1−6): Novel superhalogens with oxyfluoride ligands

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Supplementary Materials submitted to NJC

AuOF

Cartesian coordinates (in Å)

Au	0.000000000	0.422073000	0.000000000
F	-0.549420000	-2.357688000	0.000000000
O	0.618097000	-1.515572000	0.000000000

Frequency (cm^{-1})	IR Intensity (a.u.)
213.025	4.1879
469.3106	9.0566
873.0745	102.2588

$Au(OF)_2$

Cartesian coordinates (in Å)

Au	0.000000000	0.000000000	0.000000000
O	0.000000000	1.966150000	0.000000000
O	0.000000000	-1.966150000	0.000000000
F	-1.317489000	-2.491167000	0.000000000
F	1.317489000	2.491167000	0.000000000

Frequency (cm^{-1})	IR Intensity (a.u.)
53.5	1.8
81.3	1.8
176.1	1.7
213.5	0

297.9	0.5
509.5	0
577.0	25.4
882.2	552.5
918.6	0

$Au(OF)_3$

Cartesian coordinates (in Å)

Au	0.120703000	-0.077370000	-0.102434000
O	2.066115000	-0.043854000	-0.483897000
O	-0.626456000	1.803275000	0.038622000
O	-1.756762000	-0.723388000	0.192167000
F	2.811793000	0.104953000	0.723437000
F	-2.018634000	1.792382000	0.191892000
F	-1.570795000	-2.139113000	0.208798000

Frequency (cm^{-1})	IR Intensity (a.u.)
30.8	1.2
67.2	0
75.6	1.9
95.9	0.5
142.4	0.3
155.4	1.7
232.7	1.3
272.8	1.7
285.4	8.3
509.1	0.3
537.2	9.8

579.2	57.0
908.5	163.3
916.8	70.3
949.5	116.1

$Au(OF)_4$

Cartesian coordinates (in Å)

Au	0.000000000	0.000000000	0.000150000
O	0.946639000	1.787087000	-0.000437000
O	-1.753596000	1.005171000	-0.000177000
O	-0.946639000	-1.787087000	-0.000437000
O	1.753596000	-1.005171000	-0.000177000
F	2.832196000	-0.105668000	0.000829000
F	0.000000000	2.822503000	-0.000943000
F	-2.832196000	0.105668000	0.000829000
F	0.000000000	-2.822503000	-0.000943000

Frequency (cm^{-1})	IR Intensity (a.u.)
25.0	0
36.4	0
81.4	1.3
114.4	3.8
131.5	1.0
132.7	0
136.5	0
151.8	0.6
208.4	4.0
234.8	0

242.0	0
289.4	10.9
299.5	1.0
436.0	0
520.2	0
547.8	20.9
564.6	2.6
897.5	0
909.0	823.7
922.6	649.3
970.7	0

$Au(OF)_5$

Cartesian coordinates (in Å)

Au	0.139457000	0.003823000	0.014702000
O	0.918401000	-1.889491000	0.225085000
O	2.005772000	0.736502000	-0.014793000
O	-0.941110000	-0.556292000	-1.693261000
O	-0.547286000	1.936070000	-0.014783000
O	-1.523714000	-0.795192000	0.919706000
F	2.031974000	2.132862000	-0.064790000
F	-2.143514000	-1.161102000	-1.403421000
F	-1.942903000	1.945698000	-0.196129000
F	-1.343323000	-0.581099000	2.287884000
F	2.251815000	-1.864666000	-0.238776000

Frequency (cm^{-1})	IR Intensity (a.u.)
21.0	0

32.6	0.2
42.9	0
65.4	0
91.9	0.2
101.1	0.5
116.5	0
122.9	0.2
133.6	0.3
151.0	0.4
171.2	1.3
191.1	0.3
228.8	0.2
247.1	0.5
248.1	0.3
286.0	3.0
296.9	6.8
460.9	1.2
491.6	1.1
518.0	3.9
550.2	38.1
567.2	36.2
943.5	64.2
953.7	199.0
969.9	187.7
973.1	147.7
997.6	98.9

$Au(OF)_6$

Cartesian coordinates (in Å)

Au	0.097043000	-0.055902000	-0.044383000
O	-1.270989000	0.589721000	1.514272000
O	-1.216659000	1.569586000	-0.582095000
O	1.274217000	-0.218556000	-1.713960000
O	1.090020000	-1.635099000	0.799105000
O	1.294964000	1.310449000	0.940328000
O	-0.935307000	-1.518016000	-1.081315000
F	-2.384489000	-0.191403000	1.682035000
F	2.084147000	-1.140297000	1.646849000
F	2.618983000	-0.234240000	-1.357069000
F	-2.280169000	1.134792000	-1.338054000
F	-2.187245000	-1.736775000	-0.467996000
F	1.086958000	2.571432000	0.333747000

Frequency (cm^{-1})	IR Intensity (a.u.)
16.2	0
30.9	0
39.2	0
45.7	0.1
54.6	0
80.8	0
100.2	0
111.0	0
113.4	0.4
133.1	0.1

140.4	0.6
150.5	0.7
154.6	0.1
171.9	0.3
188.5	0.1
199.1	0
241.5	0
243.8	0.9
254.6	0.2
267.6	6.1
291.2	4.2
379.9	0.4
435.4	7.9
486.4	3.8
503.8	7.6
531.8	24.5
555.1	29.0
936.8	35.4
944.3	62.8
951.2	134.0
965.2	346.1
981.1	151.4
1026.8	138.8