Electronic supporting information to

Probing the Binding and Activation of Small Molecules by Gas-Phase Transition Metal Clusters via IR Spectroscopy

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Table S1 Experimental vibrational frequencies (in cm^{-1}) of anionic, neutral and cationic gold cluster complexes $Au_n(O_2)_m^{-/0/+}$

n	*m*	APES [a,1]	anionic [b, 2]	neutral [c,3]	cationic [d,4]
1	1			1213.6	
	2		911.9		
2	1	1360(70)			1467, 1756; 1503[e]
	2				1460, 1756; 1472[e]
	3				1443, 1759
3	1				1512
	2				1512
	3				1514
	4				1518, 1730
4	1	1360(80)	1078	1502	1488
	2			1508, 1573, 1650	1273, 1489, 1722
	3			1508, 1573, 1650	1261; 1487; 1717
	4				1236, 1493, 1714
5	1				1516
	2				1513
	3				1513
	4				1515, 1705
6	1	1330(100)	1081		1511
	2				1515, 1708
7	1			1063, 1528	1521
	2			1064, 1528	
8	1		1051, 1067, 1110		1463
	2				1446
9	1			1058	
10	1		1053		1068
	2				1069, 1530
11	1			1058	
	2			1058	
12	1		1053		1494
	2				1051, 1487
	3				1064, 1483
	4				1064
	5				1069
14	1		1069		
18	1		1061		
20	1		1068		
21	1			1069	
	3				1067, 1376
22	1				874, 1063, 1359

[a] vibrational data for the neutral species in the structure of the anion; [b] data from IR-MPD, original tabulated values are corrected by a factor of 1.0075 for the calibration of the IR laser frequency that had been initially erroneously ignored; estimated accuracy ±3 cm^{-1}, except for *n*=1 that is from Ne matrix IR spectroscopy Ref. [5], [c] data from IR-MPD with an estimated accuracy of ±3 cm^{-1}, except for *n*=1 that is from Ne matrix IR spectroscopy Ref. [5]; [d] data from IR-MPD with an estimated accuracy of ±10 cm^{-1}, reanalyzed original data; [e] Ref. [6] reports for $Au_2(O_2)_n^+$ (*n*=1,2) slightly higher values compared to Ref.[4b]. While the deviation for *n*=2 probably reflects the experimental (calibration) accuracy of IR-MPD using IR-FELs, the larger discrepancy for *n*=1 may be due to fragmentation of larger complexes affecting the shape and position of the depletion peak although the authors of ref. [6] took precautions to avoid such distortions.

References

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