Physical Chemistry Chemical Physics

Supplementary data for the paper titled:

Noble Gas-Metal Chemical Bonding: The Microwave Spectra, Structures and Hyperfine Constants of Ar-AuF and Ar-AuBr.

by

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No. of Tables = 3

Table 1

Observed transition frequencies (in MHz) of Ar-AuF

J'-J''	F'-F''	Ar-AuF	obs-calc
2-1	$\frac{1}{2}$-$\frac{1}{2}$	7101.3306	-0.7[a]
	$\frac{5}{2}$-$\frac{3}{2}$	7108.2648	1.1
	$\frac{7}{2}$-$\frac{5}{2}$	7108.3723	-0.1
	$\frac{3}{2}$-$\frac{3}{2}$	7166.7472	-0.3
3-2	$\frac{5}{2}$-$\frac{3}{2}$	10635.5398	0.6
	$\frac{3}{2}$-$\frac{1}{2}$	10635.9298	-0.4
	$\frac{7}{2}$-$\frac{5}{2}$	10655.8307	-0.2
	$\frac{9}{2}$-$\frac{7}{2}$	10655.8763	0.5
4-3	$\frac{7}{2}$-$\frac{5}{2}$	14195.5243	0.3
	$\frac{5}{2}$-$\frac{3}{2}$	14195.6317	-1.0
	$\frac{9}{2}$-$\frac{7}{2}$	14205.0294	0.7
	$\frac{11}{2}$-$\frac{9}{2}$	14205.0515	0.0
5-4	$\frac{9}{2}$-$\frac{7}{2}$	17749.2071	1.3
	$\frac{7}{2}$-$\frac{5}{2}$	17749.2484	-2.2
	$\frac{11}{2}$-$\frac{9}{2}$	17754.8219	-0.6
	$\frac{13}{2}$-$\frac{11}{2}$	17754.8363	0.7
6-5	$\frac{11}{2}$-$\frac{9}{2}$	21301.1151	-2.7
	$\frac{9}{2}$-$\frac{7}{2}$	21301.1428	2.3
	$\frac{13}{2}$-$\frac{11}{2}$	21304.8620	4.9
	$\frac{15}{2}$-$\frac{13}{2}$	21304.8620	-3.4

[a] Residuals in kHz.

Table 2

Observed transition frequencies (in MHz) of Ar-Au^{79}Br and Ar-Au^{81}Br in the ground vibrational state.

J'-J''	F_1'-F_1''	F'-F''	Ar-Au^{79}Br	obs-calc	Ar-Au^{81}Br	obs-calc
5-4	$\frac{11}{2}$-$\frac{9}{2}$	5-4	7746.2400	0.5[a]	7647.8863	0.1[a]
	$\frac{13}{2}$-$\frac{11}{2}$	6-5	7749.4942	0.0	7651.5101	0.2
	$\frac{11}{2}$-$\frac{9}{2}$	4-3			7652.0173	-0.3
	$\frac{13}{2}$-$\frac{11}{2}$	7-6	7751.3235	0.6	7653.3238	0.6
	$\frac{13}{2}$-$\frac{11}{2}$	5-4	7751.5425	-1.0		
	$\frac{13}{2}$-$\frac{11}{2}$	8-7	7752.1061	0.1	7654.0623	0.6
	$\frac{11}{2}$-$\frac{9}{2}$	7-6	7752.8443	0.1	7654.7668	0.0
	$\frac{9}{2}$-$\frac{7}{2}$	6-5	7754.5909	0.3	7656.6773	0.4
	$\frac{9}{2}$-$\frac{7}{2}$	4-3	7755.0011	-0.2		
	$\frac{9}{2}$-$\frac{7}{2}$	5-4	7755.1091	-0.7	7655.8858	-0.1
	$\frac{11}{2}$-$\frac{9}{2}$	6-5	7755.4487	0.4	7656.1046	-0.3
	$\frac{7}{2}$-$\frac{5}{2}$	5-4	7762.0838	0.2	7663.0210	-0.1
6-5	$\frac{13}{2}$-$\frac{11}{2}$	6-5	9299.0298	-0.3	9180.9873	0.0
	$\frac{15}{2}$-$\frac{13}{2}$	7-6	9301.0066	0.2	9183.2172	0.3
	$\frac{13}{2}$-$\frac{11}{2}$	5-4	9301.3437	-0.1	9183.4515	-1.0
	$\frac{15}{2}$-$\frac{13}{2}$	6-5	9302.3939	-0.4	9184.7860	-1.1
	$\frac{15}{2}$-$\frac{13}{2}$	8-7	9302.4845	0.0	9184.7014	0.8
	$\frac{15}{2}$-$\frac{13}{2}$	9-8	9302.9727	-0.3	9185.1610	0.1
	$\frac{9}{2}$-$\frac{7}{2}$	4-3			9185.3381	0.2
	$\frac{13}{2}$-$\frac{11}{2}$	8-7	9303.4314	-0.1	9185.5990	0.3
	$\frac{13}{2}$-$\frac{11}{2}$	7-6	9304.3756	0.0	9186.0055	0.6
	$\frac{11}{2}$-$\frac{9}{2}$	5-4	9304.9223	-0.2	9186.4327	-0.2
	$\frac{11}{2}$-$\frac{9}{2}$	6-5			9186.6222	0.1
	$\frac{11}{2}$-$\frac{9}{2}$	7-6	9305.6789	0.3	9187.6635	0.1
	$\frac{11}{2}$-$\frac{9}{2}$	4-3			9187.9015	-0.6
	$\frac{9}{2}$-$\frac{7}{2}$	5-4			9188.4307	0.4
	$\frac{9}{2}$-$\frac{7}{2}$	6-5	9309.5325	-0.5	9191.1067	-0.3
7-6	$\frac{15}{2}$-$\frac{13}{2}$	7-6	10850.9385	0.2	10713.2159	0.4
	$\frac{17}{2}$-$\frac{15}{2}$	8-7	10852.2276	0.1	10714.6896	-0.4
	$\frac{15}{2}$-$\frac{13}{2}$	6-5	10852.4070	-0.5	10714.8137	-1.2
	$\frac{17}{2}$-$\frac{15}{2}$	7-6	10853.1928	-0.4	10715.8074	-0.8
	$\frac{17}{2}$-$\frac{15}{2}$	9-8	10853.4121	0.0	10715.8843	0.6
	$\frac{17}{2}$-$\frac{15}{2}$	10-9	10853.7373	-0.3	10716.1901	-0.2
	$\frac{15}{2}$-$\frac{13}{2}$	9-8	10854.0423	0.5	10716.4806	0.0
	$\frac{15}{2}$-$\frac{13}{2}$	8-7	10854.3933	0.6	10716.5857	0.0

[a] Residuals in kHz.

Table 2 (Continued)

Observed transition frequencies (in MHz) of Ar-Au^{79}Br and Ar-Au^{81}Br in the ground vibrational state.

J'-J''	F_1'-F_1''	F'-F''	Ar-Au^{79}Br	obs-calc	Ar-Au^{81}Br	obs-calc
	$\frac{13}{2}$-$\frac{11}{2}$	6-5			10717.1172	0.3[a]
	$\frac{11}{2}$-$\frac{9}{2}$	4-3			10717.2617	-1.1
	$\frac{11}{2}$-$\frac{9}{2}$	5-4	10854.5522	0.5[a]	10716.5037	0.3
	$\frac{13}{2}$-$\frac{11}{2}$	7-6	10855.5952	0.3	10717.3955	0.3
	$\frac{13}{2}$-$\frac{11}{2}$	8-7	10856.1290	0.3	10718.3004	0.0
	$\frac{11}{2}$-$\frac{9}{2}$	6-5			10718.6729	0.4
	$\frac{11}{2}$-$\frac{9}{2}$	7-6	10858.3489	0.2	10720.3901	-0.3
8-7	$\frac{17}{2}$-$\frac{15}{2}$	8-7	12402.3633	0.5	12244.9644	0.3
	$\frac{19}{2}$-$\frac{17}{2}$	9-8	12403.2493	0.1	12245.9894	-0.8
	$\frac{17}{2}$-$\frac{15}{2}$	7-6	12403.3529	-1.2	12246.0624	-0.3
	$\frac{19}{2}$-$\frac{17}{2}$	8-7	12403.9411	-1.1	12246.8055	-0.9
	$\frac{19}{2}$-$\frac{17}{2}$	10-9	12404.2104	0.9	12246.9604	1.3
	$\frac{19}{2}$-$\frac{17}{2}$	11-10	12404.4379	0.6	12247.1731	-0.5
	$\frac{17}{2}$-$\frac{15}{2}$	10-9	12404.6497	0.2	12247.3795	3.4
	$\frac{17}{2}$-$\frac{15}{2}$	9-8	12404.7764	0.5	12247.3795	0.2
	$\frac{13}{2}$-$\frac{11}{2}$	6-5			12247.5030	0.3
	$\frac{15}{2}$-$\frac{13}{2}$	7-6	12405.5234	0.9	12247.8837	1.3
	$\frac{13}{2}$-$\frac{11}{2}$	5-4	12405.6504	-1.0	12247.9734	-1.0
	$\frac{15}{2}$-$\frac{13}{2}$	8-7	12405.9567	-0.4	12248.1872	0.7
	$\frac{15}{2}$-$\frac{13}{2}$	6-5	12406.1025	-1.2	12248.4042	-2.2
	$\frac{15}{2}$-$\frac{13}{2}$	9-8	12406.4458	0.2	12248.9098	0.4
	$\frac{13}{2}$-$\frac{11}{2}$	7-6			12249.1104	0.6
	$\frac{13}{2}$-$\frac{11}{2}$	8-7	12407.8418	0.4	12250.2803	-0.1

[a] Residuals in kHz.

Table 3

Correlation Coefficients From Least Squares Fit: Ar-AuF

B_0	1.00			
D_J	-0.92	1.00		
eQq(Au)	0.15	-0.16	1.00	

Correlation Coefficients From Least Squares Fit: Ar-Au^{79}Br

B_0	1.00				
D_J	-0.96	1.00			
C_I(Br)	-0.28	0.19	1.00		
eQq(Au)	0.12	-0.08	-0.48	1.00	
eQq(Br)	-0.18	0.12	0.68	-0.53	1.00

Correlation Coefficients From Least Squares Fit: Ar-Au^{81}Br

B_0	1.00				
D_J	-0.96	1.00			
C_I(Br)	-0.26	0.20	1.00		
eQq(Au)	0.05	-0.04	-0.40	1.00	
eQq(Br)	-0.23	0.17	0.75	-0.45	1.00