Intriguing Gold Trifluoride – Molecular Structure of Monomers and Dimers: An Electron Diffraction and Quantum Chemical Study

Balázs Réffy, Mária Kolonits, Axel Schulz, Thomas M. Klapötke and Magdolna Hargittai

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Supporting Information

Symmetry Coordinates for the Ground State Geometry of AuF_3 (C_{2v}) and Au_2F_6 (D_{2h}) [a]

AuF_3

$S_1(A_1)=\Delta r_{1,2}$

$S_2(A_1)=1/\sqrt{2}\,(\Delta r_{1,3}+\Delta r_{1,4})$

$S_3(A_1)=1/\sqrt{6}\,(2\cdot\alpha_{4,1,3}-\alpha_{2,1,4}-\alpha_{3,1,2})$

$S_4(B_2)=1/\sqrt{2}\,(-\Delta r_{1,3}+\Delta r_{1,4})$

$S_5(B_2)=1/\sqrt{2}\,(\alpha_{2,1,4}-\alpha_{3,1,2})$

$S_6(B_1)=\beta_{1,2,3,4}$

Au_2F_6

$S_1(A_g)=1/4(\Delta r_{2,6}+\Delta r_{2,5}+\Delta r_{1,8}+\Delta r_{1,7})$

$S_2(A_g)=1/4(\Delta r_{1,3}+\Delta r_{1,4}+\Delta r_{2,3}+\Delta r_{2,4})$

$S_3(A_g)=1/\sqrt{2}\,(\alpha_{5,2,6}+\alpha_{8,1,7})$

$S_4(A_g)=1/4(\alpha_{3,2,4}-\alpha_{2,4,1}+\alpha_{4,1,3}-\alpha_{1,3,2})$

$S_5(A_u)=1/4(\beta_{1,3,2,5}+\beta_{1,4,2,6}+\beta_{2,3,1,7}+\beta_{2,4,1,8})$

$S_6(B_{1u})=1/4(\Delta r_{2,6}+\Delta r_{2,5}-\Delta r_{1,8}-\Delta r_{1,7})$

$S_7(B_{1u})=1/4(\Delta r_{1,3}+\Delta r_{1,4}-\Delta r_{2,3}-\Delta r_{2,4})$

$S_8(B_{1u})=1/\sqrt{2}\,(\alpha_{5,2,6}+\alpha_{8,1,7})$

$S_9(B_{2u})=1/4(\Delta r_{2,6}-\Delta r_{2,5}+\Delta r_{1,8}-\Delta r_{1,7})$

$S_{10}(B_{2u})=1/4(\Delta r_{1,3}-\Delta r_{1,4}+\Delta r_{2,3}-\Delta r_{2,4})$

$S_{11}(B_{2u})=1/4(\alpha_{3,2,5}-\alpha_{4,2,6}+\alpha_{3,1,7}-\alpha_{4,1,8})$

$S_{12}(B_{3u})=\beta_{3,2,4,1}$

$S_{13}(B_{3u})=(\beta_{1,3,2,5}-\beta_{1,4,2,6}-\beta_{2,3,1,7}+\beta_{2,4,1,8})$

$S_{14}(B_{1g})=(\beta_{1,3,2,5}+\beta_{1,4,2,6}-\beta_{2,3,1,7}-\beta_{2,4,1,8})$

$S_{15}(B_{2g})=(-\beta_{1,3,2,5}+\beta_{1,4,2,6}-\beta_{2,3,1,7}+\beta_{2,4,1,8})$

$S_{16}(B_{3g})=1/4(-\Delta r_{2,6}+\Delta r_{2,5}+\Delta r_{1,8}-\Delta r_{1,7})$

$S_{17}(B_{3g})=1/4(-\Delta r_{1,3}+\Delta r_{1,4}+\Delta r_{2,3}-\Delta r_{2,4})$

$S_{18}(B_{3g})=1/4(-\alpha_{3,2,5}+\alpha_{4,2,6}+\alpha_{3,1,7}-\alpha_{4,1,8})$

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[a] For numbering of atoms see Figure 3 in paper.

Elements of the F-Matrix of AuF_3 and Au_2F_6 (Stretching Force Constants in mdyn/Å, Stretch-Bend Interactions in mdyn/rad, Bending Force Constants in mdyn Å/rad^2) [a]

AuF_3

		1	2	3
A_1	1	4.044		
	2	0.094	3.578	
	3	-0.053	0.034	0.500

		4
B_1	4	0.549

		5	6
B_2	5	3.879	
	6	0.036	0.214

Au_2F_6

		1	2	3	4
A_g	1	4.208			
	2	0.020	2.161		
	3	-0.010	0.010	0.860	
	4	0.031	-0.032	-0.124	0.730

		5
A_u	5	0.657

		6	7	8
B_{1u}	6	4.142		
	7	0.139	1.955	
	8	-0.003	0.066	0.864

		9	10	11
B_{2u}	9	3.966		
	10	-0.090	2.191	
	11	0.103	-0.211	0.760

		12	13
B_{3u}	12	2.729	
	13	0.781	1.394

		14
B_{1g}	14	0.504

[a] Numbering of columns and rows corresponds to the symmetry coordinates.

		15
B_{2g}	15	0.698

		16	17	18
B_{3g}	16	3.945		
	17	-0.001	1.603	
	18	0.072	-0.174	0.733

Total Experimental Intensities for Gold Trifluoride
Temperature= 600 K
Camera range= 19 cm

s_{min}=9.0000 s_{max}=29.5000 step size=.2500

				.5728	.5673	.5690	.5755
.5861	.5939	.5955	.5940	.5882	.5811	.5734	.5685
.5684	.5717	.5768	.5794	.5780	.5747	.5703	.5664
.5659	.5663	.5681	.5684	.5669	.5629	.5596	.5565
.5550	.5567	.5569	.5562	.5538	.5507	.5479	.5463
.5457	.5452	.5459	.5464	.5456	.5439	.5422	.5410
.5399	.5389	.5387	.5389	.5381	.5374	.5366	.5366
.5361	.5365	.5370	.5372	.5371	.5364	.5351	.5340
.5335	.5334	.5337	.5337	.5339	.5345	.5345	.5347
.5353	.5355	.5359	.5359	.5355	.5352	.5347	.5343
.5340	.5346	.5356	.5365	.5376	.5381	.5381	

Camera range= 50 cm

s_{min}=2.0000 s_{max}=14.0000 step size=.1250

.1856	.2000	.2160	.2376	.2622	.2923	.3245	.356
.3849	.4138	.4367	.4580	.4810	.5024	.5302	.560
.5927	.6237	.6495	.6658	.6713	.6661	.6539	.637
.6183	.6033	.5936	.5876	.5892	.5945	.6056	.619
.6376	.6570	.6774	.6989	.7216	.7436	.7608	.775
.7811	.7826	.7764	.7664	.7543	.7449	.7373	.733
.7333	.7384	.7407	.7446	.7446	.7443	.7416	.738
.7339	.7308	.7311	.7318	.7360	.7418	.7491	.756
.7638	.7697	.7748	.7764	.7774	.7772	.7744	.770
.7671	.7625	.7579	.7524	.7485	.7456	.7447	.743
.7459	.7483	.7514	.7549	.7579	.7610	.7618	.761
.7608	.7596	.7561	.7529	.7514	.7493	.7483	.747
.7485							

Temperature= 1094 K
Camera range= 19 cm

s_{min}=9.0000 s_{max}=29.5000 step size=.2500

				.5096	.5078	.5086	.5105
.5149	.5193	.5216	.5217	.5200	.5181	.5159	.5137
.5127	.5113	.5106	.5103	.5102	.5108	.5111	.5110
.5096	.5089	.5082	.5067	.5055	.5043	.5033	.5022
.5013	.5005	.4987	.4984	.4971	.4968	.4956	.4948
.4941	.4940	.4933	.4940	.4930	.4930	.4927	.4915
.4911	.4901	.4902	.4897	.4888	.4884	.4896	.4899
.4898	.4906	.4908	.4906	.4903	.4894	.4895	.4894
.4894	.4898	.4899	.4905	.4911	.4919	.4924	.4931
.4932	.4929	.4932	.4931	.4933	.4934	.4934	.4940
.4940	.4947	.4951	.4963	.4962	.4975	.4973	

Camera range= 50 cm

s_{min}=2.0000 s_{max}=14.0000 step size=.1250

.1228	.1299	.1387	.1476	.1593	.1707	.1839	.1981
.2126	.2300	.2471	.2657	.2834	.3004	.3171	.3310
.3428	.3527	.3597	.3652	.3681	.3694	.3704	.3711
.3715	.3711	.3714	.3718	.3730	.3739	.3760	.3801
.3844	.3902	.3957	.4038	.4123	.4194	.4262	.4336
.4382	.4427	.4461	.4473	.4482	.4472	.4452	.4439
.4426	.4404	.4390	.4368	.4357	.4343	.4323	.4323
.4302	.4311	.4311	.4325	.4333	.4354	.4363	.4391
.4417	.4428	.4452	.4462	.4465	.4471	.4473	.4467
.4454	.4439	.4430	.4415	.4404	.4389	.4381	.4377
.4358	.4359	.4353	.4344	.4336	.4337	.4335	.4343
.4332	.4335	.4333	.4338	.4333	.4324	.4323	.4315
.4208							