Electronic Supplementary Material (ESI) for Dalton Transactions

Electronic Supplementary Information

The first crystallographic example of a face-sharing fluoroaluminate anion $Al_2F_9^{3-}$

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Experimental Section

Synthesis of [C_{18}MIm]Cl. Equimolar amounts of 1-Methylimidazole (Aldrich, 99%) and 1-chlorooctadecane (Wako Chemicals, 95%) were mixed in acetonitrile dehydrated (Wako Pure Chemical Industries, water content < 50 ppm) in a high-pressure vessel made of Pyrex glass under a dry argon atmosphere. The high-pressure vessel was sealed with an airtight cap. The reaction mixture was stirred at 90 °C for three days. After elimination of the solvent under vacuum, the obtained solid was purified by dissolving in acetonitrile dehydrated and then precipitated from the solution by addition ethyl acetate dehydrated (Wako Pure Chemical Industries, water content < 50 ppm) under a dry argon atmosphere. The final product was dried under vacuum at 80 °C for three days.

Synthesis of [C_{18}MIm][AlF_4]. Anhydrous $AlCl_3$ (Wako Chemicals, 1.322 g, 9.92 mmol) was slowly added onto [C_{18}MIm]Cl (3.680 g, 9.92 mmol) in a PFA (Tetrafluoroehylene-perfluoroalkylvinylether copolymer) reactor under a dry Ar atmosphere. After vigorous agitation at 50 °C overnight, a large excess of anhydrous hydrogen fluoride (dried over K_2NiF_6, Daikin industries Co., Ltd., purity > 99 %) was distilled onto [C_{18}MIm][$AlCl_4$] at −196 °C and the reaction proceeded upon warming up to room temperature. Residual HF and byproduct HCl were eliminated from the reactor by evacuation through a chemical trap using a rotary pump. The final product was obtained by slowly warming up the reactor under vacuum to 90 °C. Anal. Calcd. for $C_{22}H_{43}N_2F_4Al_1$: C, 60.27; H, 9.82; N, 6.39; F, 17.35. Found: C, 59.96; H, 9.72; N,

6.37; F, 17.55 (by Elemental Analysis Center of Institute for Chemical Research, Kyoto University). Raman (frequency/cm^{-1}): 633 (AlF_4^-, ν_1) (see ref. [7] for the assignment of Raman spectrum).

Crystal growth and X-ray crystallography. Single crystals of $[C_{18}MIm]_3[Al_2F_9](CH_2Cl_2)_{1.754}$ were grown by slow evaporation of the solvent from a CH_2Cl_2 solution of $[C_{18}MIm][AlF_4]$. Translucent crystals were obtained after pumping off the remaining solvent under vacuum for 3 h. The $[C_{18}MIm]_3[Al_2F_9](CH_2Cl_2)_{1.754}$ crystal was transferred into a quartz capillary (0.5 mm o.d., dried under a vacuum at 500 °C) under a dry Ar atmosphere, and centered on the X-ray diffractometer (R-axis Rapid II, Rigaku controlled by the program RAPID AUTO 2.40)[1] equipped with an imaging plate area detector and graphite-monochromated Mo-Kα radiation (0.71073 Å). The capillary was tentatively plugged with vacuum grease and sealed using an oxygen burner. The measurements consisted of 20 ω scans (130–190°, 3°/frame) at the fixed φ (30°) and χ (45°) angles and 54 ω scans (0°–162°, 3°/frame) at the fixed φ (180°) and χ (45°) angles. The exposure time was 600 s deg^{-1}. Integration, scaling and absorption corrections were performed using RAPID AUTO 2.40. The structure was solved using SIR-92[2] and refined by SHELXL-97[3] linked to Win-GX.[4] Anisotropic displacement factors were introduced for all atoms except for hydrogen.

Calculations. The Gaussian 03 program[5] was used for quantum mechanical calculations. Three calculation methods (B3LYP, PBE1PBE and MP2) combined with

cc-pVTZ and aug-ccpVTZ basis sets were used. Vibrational frequencies and intensities were calculated for the optimized geometries (see the end of this ESI for the detailed data). The NBO analyses were performed for the B3LYP, PBE1PBE and MP2 optimized local minima.[6]

Table S1 Summary of crystal data and refinement results for $[C_{18}MIm]_3[Al_2F_9](CH_2Cl_2)_{1.754}$.

	$[C_{18}MIm]_3[Al_2F_9](CH_2Cl_2)_{1.754}$
Formula	$C_{67.75}H_{132.51}N_6F_9Al_2Cl_{3.51}$
M	1380.67
Crystal size/mm	0.40 × 0.30 × 0.10
T/°C	–100
Crystal system	Triclinic
Space group	P–1
a/Å	8.8125(6)
b/Å	14.8052(10)
c/Å	30.847(2)
α/°	96.083(2)
β/°	99.426(2)
γ/°	90.012(2)
V/Å^3	3947.3(5)
Z	2
D_c/g cm^{-3}	1.162
F(000)	1495
μ/mm^{-1}	0.217
λ/Å	0.71073
Reflns collected/unique	28593/12675
$R_1(F_o)^a$	0.0702
$wR_2(F_o^2)^b$	0.1752
R_{int}	0.0627

[a] $R_1 = \sum||F_o| - |F_c||/\sum|F_o|$ for $I > 2\sigma(I)$.

[b] $wR_2 = \{\sum[w(F_o^2 - F_c^2)^2]/\sum[w(F_o^2)^2]\}^{1/2}$ for $I > 2\sigma(I)$.

Table S2 Bond lengths (Å) and angles (°) for $Al_2F_9^{3-}$ in $[C_{18}MIm]_3[Al_2F_9](CH_2Cl_2)_{1.754}$. The atom numbering schemes are shown in Fig. 1.

Al1–F1	1.723(3)	Al1–F2	1.723(2)	Al1–F3	1.727(2)
Al2–F7	1.744(2)	Al2–F8	1.740(2)	Al2–F9	1.750(2)
Al1–F4	1.928(2)	Al1–F5	1.959(3)	Al1–F6	1.902(3)
Al2–F4	1.878(2)	Al2–F5	1.874(2)	Al2–F6	1.898(3)
F1–Al1–F2	98.20(13)	F2–Al1–F3	99.81(13)	F1–Al1–F3	98.32(13)
F7–Al2–F8	97.77(12)	F8–Al2–F9	94.24(12)	F7–Al2–F9	96.74(12)
F1–Al1–F4	90.02(11)	F1–Al1–F5	91.97(11)	F1–Al1–F6	161.99(13)
F2–Al1–F4	93.11(11)	F2–Al1–F5	164.12(13)	F2–Al1–F6	92.86(12)
F3–Al1–F4	163.41(13)	F3–Al1–F5	90.69(11)	F3–Al1–F6	93.72(12)
F7–Al2–F4	91.82(12)	F7–Al2–F5	92.51(12)	F7–Al2–F6	165.31(13)
F8–Al2–F4	167.74(13)	F8–Al2–F5	94.07(11)	F8–Al2–F6	92.83(12)
F9–Al2–F4	92.20(11)	F9–Al2–F5	166.61(13)	F9–Al2–F6	92.57(11)
F4–Al1–F5	74.63(10)	F5–Al1–F6	74.47(10)	F4–Al1–F6	75.16(10)
F4–Al2–F5	77.81(10)	F5–Al2–F6	76.55(10)	F4–Al2–F6	76.44(11)
Al1–F4–Al2	89.78(10)	Al1–F5–Al2	88.97(10)	Al1–F6–Al2	90.00(11)

Table S3 The C−H···F interaction geometries (Å, °) of $Al_2F_9^{3-}$ in $[C_{18}MIm]_3[Al_2F_9](CH_2Cl_2)_{1.754}$.

D–H···*A*	*D*–H	H···*A*	*D*···*A*	∠*D*–H···*A*
C66–H66b^{i}···F1	0.970	2.130	3.085	167.71
C84–H84b^{ii}···F1	0.960	2.191	3.101	157.75
C24–H24a···F2	0.960	2.477	3.263	139.05
C35–H35^{i}···F2	0.930	2.142	3.012	155.20
C65–H65^{i}···F2	0.930	2.293	3.217	172.62
C34–H34^{ii}···F3	0.930	2.539	3.091	118.39
C92–H92b^{ii}···F3	0.970	2.122	3.089	174.56
C2–H2···F4	0.930	2.458	3.015	118.55
C24–H24a···F4	0.960	2.391	3.173	138.35
C62–H62^{iii}···F4	0.930	2.486	3.111	124.75
C66–H66a^{iii}···F4	0.970	2.582	3.363	137.68
C34–H34^{ii}···F5	0.930	2.557	3.487	178.32
C64–H64^{ii}···F5	0.930	2.476	3.296	147.19
C54–H54c^{ii}···F6	0.960	2.443	3.225	138.59
C4–H4^{iv}···F7	0.930	2.158	3.081	171.08
C62–H62^{iii}···F7	0.930	2.177	3.074	161.81
C24–H24b^{iv}···F8	0.960	2.340	2.961	121.79
C32–H32···F8	0.930	2.392	3.113	134.23
C54–H54a···F8	0.960	2.420	3.285	149.78
C91–H91b···F8	0.970	2.209	3.125	157.04
C2–H2···F9	0.930	1.982	2.900	169.15
C32–H32···F9	0.930	2.199	3.016	146.10
C36–H36a···F9	0.970	2.564	3.373	141.02
C91–H91b···F9	0.970	2.668	3.345	127.22

Symmetry codes: (i) $-x, 2-y, -z$; (ii) $1-x, 2-y, -z$; (iii) $x, -1+y, z$; (iv) $1+x, y, z$.

Table S4 Bond valence sum (*s*) calculations for AlF_4^-, AlF_6^{3-} and $Al_2F_9^{3-}$ (s = exp $[(r_o-r)/B]$, r_o = 1.550 Å, B = 0.37).[7]

Bond	*R*	*s*	Bond valence sum
	AlF_4^- (T_d)[8]		
Al−F1	1.660	0.733	
Al−F2	1.661	0.731	
Al−F3	1.656	0.741	
Al−F4	1.640	0.774	
Al			2.978
Al−F1	1.651	0.751	
Al−F2	1.646	0.761	
Al−F1’	1.651	0.751	
Al−F2’	1.646	0.761	
Al			3.024
	AlF_6^{3-} (O_h)[9]		
Al−F1	1.793	0.512	
Al−F2	1.822	0.473	
Al−F3	1.806	0.494	
Al−F1’	1.793	0.512	
Al−F2’	1.822	0.473	
Al−F3’	1.806	0.494	
Al			2.957
	$Al_2F_9^{3-}$ (D_{3h})		
Al1−F1	1.723	0.618	
Al1−F2	1.723	0.618	
Al1−F3	1.727	0.611	
Al1−F4	1.928	0.355	
Al1−F5	1.959	0.327	
Al1−F6	1.902	0.381	
Al1			2.911
Al2−F4	1.878	0.407	
Al2−F5	1.874	0.411	
Al2−F6	1.898	0.385	
Al2−F7	1.744	0.584	
Al2−F8	1.740	0.590	
Al2−F9	1.750	0.575	
Al2			2.952

Table S5 Calculated geometrical parameters (Å, °) for AlF_4^-, AlF_6^{3-} and $Al_2F_9^{3-}$ (see Fig. 3 for the atom naming scheme).

	B3LYP		PBE1PBE		MP2	
	cc-pVTZ	aug-cc-pVTZ	cc-pVTZ	aug-cc-pVTZ	cc-pVTZ	aug-cc-pVTZ
			AlF_4^- (T_d)			
Al−F	1.703	1.703	1.697	1.697	1.704	1.706
F−Al−F	109.5	109.5	109.5	109.5	109.5	109.5
			AlF_6^{3-} (O_h)			
Al−F	1.894	1.897	1.887	1.889	1.893	1.899
F−Al−F	90.0	90.0	90.0	90.0	90.0	90.0
			$Al_2F_9^{3-}$ (D_{3h})			
Al−F_t	1.789	1.795	1.784	1.788	1.790	1.797
Al−F_b	1.956	1.948	1.945	1.937	1.950	1.944
F_t−Al−F_t	96.3	96.1	96.2	96.1	96.2	96.2
F_b−Al−F_b	74.9	75.0	75.1	75.2	75.1	75.0
F_t−Al−F_b (*cis*)	93.5	93.6	93.5	93.5	93.5	93.5
F_t−Al−F_b (*trans*)	165.3	165.5	165.5	165.6	165.5	165.5
Al−F_b−Al	90.8	90.7	90.5	90.4	90.6	90.6
F_{t2}−Al−F_b	91.6	92.1	91.6	92.1	91.6	92.0
Al−F_b−Al	108.1	108.0	107.8	108.0	107.8	107.7

Table S6 Natural bond orbital (NBO) charges, valencies and bond orders for AlF_4^-, AlF_6^{3-} and $Al_2F_9^{3-}$ (see Fig. 3 for the definition of F_t and F_b).

	B3LYP				PBE1PBE				MP2			
	cc-pVTZ		aug-cc-pVTZ		cc-pVTZ		aug-cc-pVTZ		cc-pVTZ		aug-cc-pVTZ	
	Charges [Valencies]											
	AlF_4^- (T_d)											
Al	2.063	[2.065]	2.157	[1.769]	2.062	[2.007]	2.149	[1.780]	2.025	[2.157]	2.108	[1.992]
F	−0.766	[0.516]	−0.789	[0.442]	−0.766	[0.502]	−0.787	[0.445]	−0.756	[0.539]	−0.777	[0.498]
	AlF_6^{3-} (O_h)											
Al	1.973	[2.190]	2.112	[2.200]	1.969	[2.212]	2.096	[2.213]	1.932	[2.393]	2.049	[2.257]
F	−0.829	[0.365]	−0.852	[0.367]	−0.828	[0.369]	−0.849	[0.369]	−0.822	[0.399]	−0.842	[0.376]
	$Al_2F_9^{3-}$ (D_{3h})											
Al	1.987	[2.204]	2.094	[1.990]	1.976	[1.971]	2.073	[2.021]	1.939	[2.347]	2.024	[2.104]
F_t	−0.795	[0.434]	−0.821	[0.387]	−0.793	[0.379]	−0.818	[0.391]	−0.786	[0.469]	−0.808	[0.415]
F_b	−0.735	[0.601]	−0.753	[0.553]	−0.731	[0.555]	−0.747	[0.565]	−0.720	[0.627]	−0.734	[0.572]
	Bond orders											
	AlF_4^- (T_d)											
Al−F	0.516		0.442		0.502		0.445		0.539		0.498	
	AlF_6^{3-} (O_h)											
Al−F	0.365		0.367		0.369		0.369		0.399		0.376	
	$Al_2F_9^{3-}$ (D_{3h})											
Al−F_t	0.434		0.387		0.379		0.391		0.469		0.415	
Al−F_b	0.301		0.277		0.278		0.282		0.314		0.286	

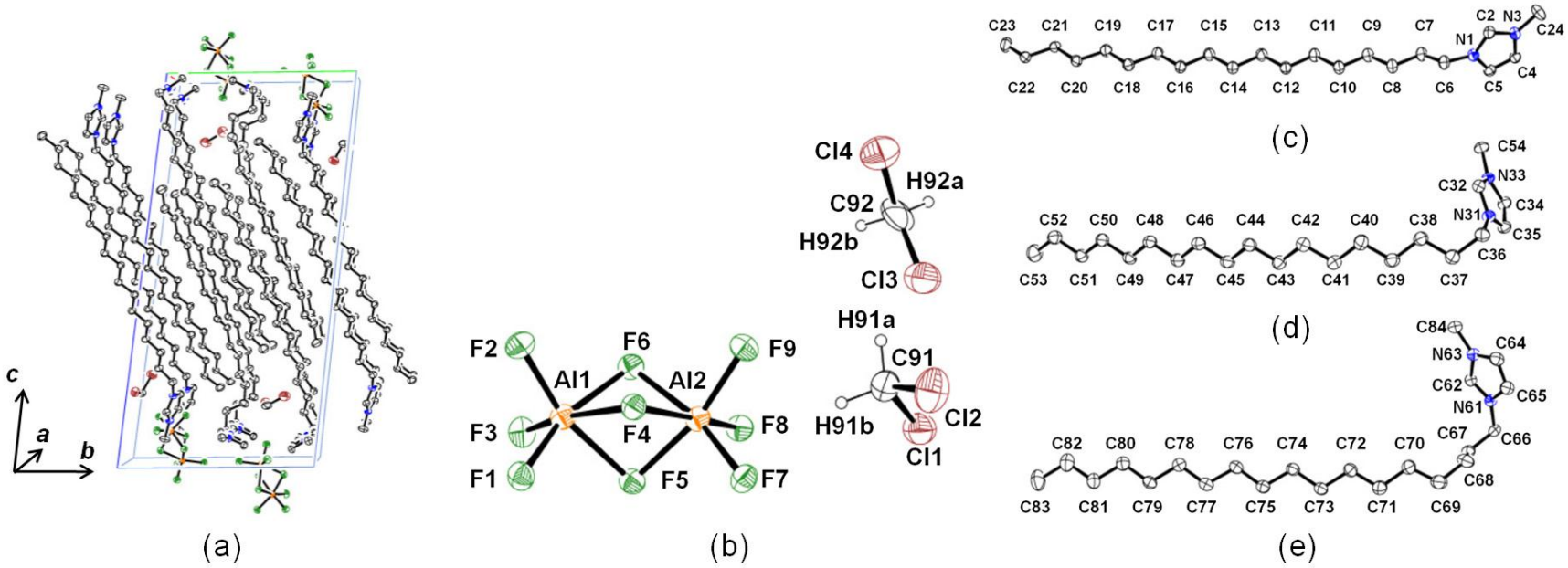

Fig. S1 Crystal structure of $[C_{18}MIm_3][Al_2F_9](CH_2Cl_2)_{1.754}$ at –100 °C. (a) Packing diagram, (b) atom numbering for $[Al_2F_9]^{3-}$ and CH_2Cl_2, (c) atom numbering scheme for Cation 1, (d) atom numbering shceme for Cation 2, (e) atom numberingscheme for Cation 3. The displacement ellipsoids are shown with 30% probability. Hydrogen atoms are omitted for clarity.

Calculated frequencies and vibrational modes of AlF_4^-, AlF_6^{3-} and $Al_2F_9^{3-}$ from Gaussian result files at B3LYP/cc-pVTZ level.

AlF_4^- (T_d)

	1			2			3		
	E			E			T2		
Frequencies --	196.6476			196.6476			302.2329		
Red. masses --	18.9984			18.9984			20.2484		
Frc consts --	0.4329			0.4329			1.0897		
IR Inten --	0.0000			0.0000			36.7147		
Raman Activ --	0.1803			0.1803			0.3170		
Depolar (P) --	0.7500			0.7500			0.7500		
Depolar (U) --	0.8571			0.8571			0.8571		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 13	0.00	0.00	0.00	0.00	0.00	0.00	-0.01	0.06	-0.39
2 9	-0.10	0.39	-0.29	0.40	-0.11	-0.28	-0.26	-0.33	0.18
3 9	0.10	-0.39	-0.29	-0.40	0.11	-0.28	0.35	0.28	0.10
4 9	-0.10	-0.39	0.29	0.40	0.11	0.28	0.27	-0.32	0.19
5 9	0.10	0.39	0.29	-0.40	-0.11	0.28	-0.35	0.29	0.09

	4			5			6		
	T2			T2			A1		
Frequencies --	302.2329			302.2329			607.9132		
Red. masses --	20.2484			20.2484			18.9984		
Frc consts --	1.0897			1.0897			4.1367		
IR Inten --	36.7147			36.7147			0.0000		
Raman Activ --	0.3170			0.3170			3.6049		
Depolar (P) --	0.7500			0.7500			0.0000		
Depolar (U) --	0.8571			0.8571			0.0000		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 13	-0.01	0.39	0.06	0.40	0.01	-0.01	0.00	0.00	0.00
2 9	0.35	-0.10	0.28	-0.14	0.30	0.32	0.29	0.29	0.29
3 9	0.27	-0.19	-0.32	-0.13	0.31	-0.32	-0.29	-0.29	0.29
4 9	-0.35	-0.09	0.29	-0.14	-0.32	-0.30	0.29	-0.29	-0.29
5 9	-0.26	-0.17	-0.33	-0.15	-0.31	0.30	-0.29	0.29	-0.29

	7			8			9		
	T2			T2			T2		
Frequencies --	786.0216			786.0216			786.0216		
Red. masses --	22.5264			22.5264			22.5264		
Frc consts --	8.1999			8.1999			8.1999		
IR Inten --	180.3951			180.3951			180.3951		
Raman Activ --	0.1960			0.1960			0.1960		
Depolar (P) --	0.7500			0.7500			0.7500		
Depolar (U) --	0.8571			0.8571			0.8571		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 13	0.01	0.24	0.62	0.01	0.62	-0.24	0.66	-0.01	-0.01
2 9	-0.27	-0.28	-0.30	-0.12	-0.15	-0.11	-0.23	-0.20	-0.20
3 9	0.11	0.10	-0.14	-0.27	-0.30	0.28	-0.24	-0.20	0.20
4 9	0.26	-0.27	-0.29	0.12	-0.14	-0.10	-0.24	0.21	0.21
5 9	-0.12	0.11	-0.15	0.26	-0.29	0.27	-0.24	0.21	-0.20

AlF_6^{3-} (O_h)

	1			2			3		
	T2U			T2U			T2U		
Frequencies --	168.8702			168.8702			168.8702		
Red. masses --	18.9984			18.9984			18.9984		
Frc consts --	0.3192			0.3192			0.3192		
IR Inten --	0.0000			0.0000			0.0000		
Raman Activ --	0.0000			0.0000			0.0000		
Depolar (P) --	0.0000			0.0000			0.0000		
Depolar (U) --	0.0000			0.0000			0.0000		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 13	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2 9	0.01	0.00	0.00	0.00	0.50	0.00	0.50	0.00	0.00
3 9	0.01	0.00	0.00	0.00	0.50	0.00	0.50	0.00	0.00
4 9	-0.01	0.00	0.50	0.00	0.00	0.00	-0.50	0.00	-0.01

5	9	-0.01	0.00	0.50	0.00	0.00	0.00	-0.50	0.00	-0.01
6	9	0.00	0.00	-0.50	0.00	-0.50	0.00	0.00	0.00	0.01
7	9	0.00	0.00	-0.50	0.00	-0.50	0.00	0.00	0.00	0.01

	4	5	6
	T2G	T2G	T2G
Frequencies --	272.5528	272.5528	272.5528
Red. masses --	18.9984	18.9984	18.9984
Frc consts --	0.8315	0.8315	0.8315
IR Inten --	0.0000	0.0000	0.0000
Raman Activ --	0.3304	0.3304	0.3304
Depolar (P) --	0.7500	0.7500	0.7500
Depolar (U) --	0.8571	0.8571	0.8571

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	13	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2	9	-0.01	-0.08	0.00	0.00	-0.49	0.00	-0.50	0.00	0.00
3	9	0.01	0.08	0.00	0.00	0.49	0.00	0.50	0.00	0.00
4	9	0.49	0.00	-0.08	-0.08	0.00	-0.49	-0.01	0.00	0.00
5	9	-0.49	0.00	0.08	0.08	0.00	0.49	0.01	0.00	0.00
6	9	0.00	-0.49	0.01	0.00	0.08	0.00	0.00	0.01	0.50
7	9	0.00	0.49	-0.01	0.00	-0.08	0.00	0.00	-0.01	-0.50

	7	8	9
	EG	EG	T1U
Frequencies --	275.3198	275.3198	332.7274
Red. masses --	18.9984	18.9984	19.1502
Frc consts --	0.8485	0.8485	1.2491
IR Inten --	0.0000	0.0000	0.0437
Raman Activ --	0.3521	0.3521	0.0000
Depolar (P) --	0.7500	0.7500	0.0000
Depolar (U) --	0.8571	0.8571	0.0000

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	13	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.14	0.00
2	9	0.00	0.00	0.40	0.00	0.00	-0.42	0.00	-0.32	0.00
3	9	0.00	0.00	-0.40	0.00	0.00	0.42	0.00	-0.32	0.00
4	9	0.00	0.16	0.00	0.00	0.55	0.00	0.00	0.54	0.00
5	9	0.00	-0.16	0.00	0.00	-0.55	0.00	0.00	0.54	0.00
6	9	0.56	0.00	0.00	0.14	0.00	0.00	0.00	-0.32	0.00
7	9	-0.56	0.00	0.00	-0.14	0.00	0.00	0.00	-0.32	0.00

	10	11	12
	T1U	T1U	A1G
Frequencies --	332.7274	332.7274	432.0972
Red. masses --	19.1502	19.1502	18.9984
Frc consts --	1.2491	1.2491	2.0899
IR Inten --	0.0437	0.0437	0.0000
Raman Activ --	0.0000	0.0000	1.7187
Depolar (P) --	0.0000	0.0000	0.0000
Depolar (U) --	0.0000	0.0000	0.0000

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	13	-0.14	0.00	0.00	0.00	0.00	0.14	0.00	0.00	0.00
2	9	0.32	0.00	0.00	0.00	0.00	0.54	0.00	0.00	-0.41
3	9	0.32	0.00	0.00	0.00	0.00	0.54	0.00	0.00	0.41
4	9	0.32	0.00	0.00	0.00	0.00	-0.32	0.00	-0.41	0.00
5	9	0.32	0.00	0.00	0.00	0.00	-0.32	0.00	0.41	0.00
6	9	-0.54	0.00	0.00	0.00	0.00	-0.32	0.41	0.00	0.00
7	9	-0.54	0.00	0.00	0.00	0.00	-0.32	-0.41	0.00	0.00

	13	14	15
	T1U	T1U	T1U
Frequencies --	504.7746	504.7746	504.7746
Red. masses --	24.7156	24.7156	24.7156
Frc consts --	3.7104	3.7104	3.7104
IR Inten --	277.0480	277.0480	277.0480
Raman Activ --	0.0000	0.0000	0.0000
Depolar (P) --	0.0000	0.0000	0.0000
Depolar (U) --	0.0000	0.0000	0.0000

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	13	0.00	0.00	0.85	0.01	0.85	0.00	0.85	-0.01	0.00
2	9	0.00	0.00	-0.32	0.00	-0.14	0.00	-0.14	0.00	0.00
3	9	0.00	0.00	-0.32	0.00	-0.14	0.00	-0.14	0.00	0.00

4	9	0.00	0.00	-0.14	0.00	-0.32	0.00	-0.14	0.00	0.00
5	9	0.00	0.00	-0.14	0.00	-0.32	0.00	-0.14	0.00	0.00
6	9	0.00	0.00	-0.14	0.00	-0.14	0.00	-0.32	0.00	0.00
7	9	0.00	0.00	-0.14	0.00	-0.14	0.00	-0.32	0.00	0.00

$Al_2F_9^{3-}$ (D_{3h})

	1	2	3
	A1"	E'	E'
Frequencies --	91.6157	123.9563	123.9569
Red. masses --	18.9984	19.0159	19.0159
Frc consts --	0.0940	0.1721	0.1722
IR Inten --	0.0000	0.6001	0.5992
Raman Activ --	0.0000	0.0002	0.0002
Depolar (P) --	0.7500	0.7500	0.7488
Depolar (U) --	0.8571	0.8571	0.8563

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	13	0.00	0.00	0.00	0.03	0.00	0.00	0.00	-0.03	0.00
2	9	-0.41	0.00	0.00	-0.10	0.00	0.00	0.00	0.23	0.43
3	9	0.20	0.35	0.00	-0.19	0.06	-0.37	-0.06	0.13	-0.21
4	9	0.20	-0.35	0.00	-0.19	-0.06	0.37	0.06	0.13	-0.21
5	13	0.00	0.00	0.00	0.03	0.00	0.00	0.00	-0.03	0.00
6	9	0.00	0.00	0.00	0.35	0.00	0.00	0.00	-0.23	0.00
7	9	0.00	0.00	0.00	0.26	0.05	0.00	-0.05	-0.32	0.00
8	9	0.00	0.00	0.00	0.26	-0.05	0.00	0.05	-0.32	0.00
9	9	0.41	0.00	0.00	-0.10	0.00	0.00	0.00	0.23	-0.43
10	9	-0.20	-0.35	0.00	-0.19	0.06	0.37	-0.06	0.13	0.21
11	9	-0.20	0.35	0.00	-0.19	-0.06	-0.37	0.06	0.13	0.21

	4	5	6
	E"	E"	A2'
Frequencies --	159.3929	159.4288	170.0381
Red. masses --	20.6592	20.6589	18.9984
Frc consts --	0.3092	0.3094	0.3236
IR Inten --	0.0000	0.0000	0.0000
Raman Activ --	0.3269	0.3246	0.0000
Depolar (P) --	0.7500	0.7500	0.7500
Depolar (U) --	0.8571	0.8571	0.8571

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	13	0.32	0.00	0.00	0.00	0.32	0.00	0.00	0.00	0.00
2	9	0.03	0.00	0.00	0.00	0.16	-0.36	-0.22	0.00	0.00
3	9	0.13	-0.05	-0.31	-0.05	0.07	0.18	0.11	0.19	0.00
4	9	0.13	0.05	0.31	0.05	0.07	0.18	0.11	-0.19	0.00
5	13	-0.32	0.00	0.00	0.00	-0.32	0.00	0.00	0.00	0.00
6	9	0.00	0.00	0.00	0.00	0.00	0.47	-0.49	0.00	0.00
7	9	0.00	0.00	0.40	0.00	0.00	-0.23	0.24	0.42	0.00
8	9	0.00	0.00	-0.40	0.00	0.00	-0.23	0.24	-0.42	0.00
9	9	-0.03	0.00	0.00	0.00	-0.16	-0.36	-0.22	0.00	0.00
10	9	-0.13	0.05	-0.31	0.05	-0.07	0.18	0.11	0.19	0.00
11	9	-0.13	-0.05	0.31	-0.05	-0.07	0.18	0.11	-0.19	0.00

	7	8	9
	A1'	E"	E"
Frequencies --	211.9720	215.6427	215.6438
Red. masses --	19.6014	19.0211	19.0211
Frc consts --	0.5189	0.5211	0.5211
IR Inten --	0.0000	0.0000	0.0000
Raman Activ --	0.7121	0.0088	0.0087
Depolar (P) --	0.3098	0.7500	0.7500
Depolar (U) --	0.4731	0.8571	0.8571

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	13	0.00	0.00	0.19	0.04	0.00	0.00	0.00	0.04	0.00
2	9	0.00	0.09	0.38	-0.36	0.00	0.00	0.00	0.23	0.31
3	9	0.08	-0.05	0.38	0.08	-0.26	0.27	-0.26	-0.21	-0.15
4	9	-0.08	-0.05	0.38	0.08	0.26	-0.27	0.26	-0.21	-0.15
5	13	0.00	0.00	-0.19	-0.04	0.00	0.00	0.00	-0.04	0.00
6	9	0.00	-0.03	0.00	0.00	0.00	0.00	0.00	0.00	0.32
7	9	-0.03	0.02	0.00	0.00	0.00	0.28	0.00	0.00	-0.16
8	9	0.03	0.02	0.00	0.00	0.00	-0.28	0.00	0.00	-0.16

9	9	0.00	0.09	-0.38	0.36	0.00	0.00	0.00	-0.23	0.31
10	9	0.08	-0.05	-0.38	-0.08	0.26	0.27	0.26	0.21	-0.15
11	9	-0.08	-0.05	-0.38	-0.08	-0.26	-0.27	-0.26	0.21	-0.15

	10	11	12
	E'	E'	A2"
Frequencies --	239.6916	239.6919	318.6257
Red. masses --	19.0249	19.0249	19.4647
Frc consts --	0.6440	0.6440	1.1643
IR Inten --	0.9808	0.9806	28.6380
Raman Activ --	0.1337	0.1337	0.0000
Depolar (P) --	0.7500	0.7500	0.7500
Depolar (U) --	0.8571	0.8571	0.8571

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	13	0.00	-0.04	0.00	-0.04	0.00	0.00	0.00	0.00	0.17
2	9	0.00	-0.13	-0.21	0.44	0.00	0.00	0.00	-0.26	-0.22
3	9	0.25	0.30	0.10	0.01	0.25	-0.18	-0.22	0.13	-0.22
4	9	-0.25	0.30	0.10	0.01	-0.25	0.18	0.22	0.13	-0.22
5	13	0.00	-0.04	0.00	-0.04	0.00	0.00	0.00	0.00	0.17
6	9	0.00	-0.35	0.00	-0.19	0.00	0.00	0.00	0.00	0.29
7	9	0.07	-0.23	0.00	-0.31	0.07	0.00	0.00	0.00	0.29
8	9	-0.07	-0.23	0.00	-0.31	-0.07	0.00	0.00	0.00	0.29
9	9	0.00	-0.13	0.21	0.44	0.00	0.00	0.00	0.26	-0.22
10	9	0.25	0.30	-0.10	0.01	0.25	0.18	0.22	-0.13	-0.22
11	9	-0.25	0.30	-0.10	0.01	-0.25	-0.18	-0.22	-0.13	-0.22

	13	14	15
	E"	E"	E'
Frequencies --	343.4547	343.4569	367.9868
Red. masses --	19.5293	19.5293	19.5018
Frc consts --	1.3573	1.3573	1.5559
IR Inten --	0.0000	0.0000	21.8243
Raman Activ --	0.0040	0.0039	0.2459
Depolar (P) --	0.7500	0.7500	0.7500
Depolar (U) --	0.8571	0.8571	0.8571

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	13	0.00	-0.18	0.00	-0.18	0.00	0.00	0.00	0.18	0.00
2	9	0.00	-0.15	0.18	0.30	0.00	0.00	0.00	0.32	-0.28
3	9	0.19	0.19	-0.09	-0.04	0.19	0.16	-0.23	-0.08	0.14
4	9	-0.19	0.19	-0.09	-0.04	-0.19	-0.16	0.23	-0.08	0.14
5	13	0.00	0.18	0.00	0.18	0.00	0.00	0.00	0.18	0.00
6	9	0.00	0.00	0.58	0.00	0.00	0.00	0.00	-0.37	0.00
7	9	0.00	0.00	-0.29	0.00	0.00	0.50	0.08	-0.23	0.00
8	9	0.00	0.00	-0.29	0.00	0.00	-0.50	-0.08	-0.23	0.00
9	9	0.00	0.15	0.18	-0.30	0.00	0.00	0.00	0.32	0.28
10	9	-0.19	-0.19	-0.09	0.04	-0.19	0.16	-0.23	-0.08	-0.14
11	9	0.19	-0.19	-0.09	0.04	0.19	-0.16	0.23	-0.08	-0.14

	16	17	18
	E'	E'	E'
Frequencies --	367.9871	379.2438	379.2440
Red. masses --	19.5019	19.0560	19.0560
Frc consts --	1.5559	1.6148	1.6148
IR Inten --	21.8255	0.1508	0.1509
Raman Activ --	0.2464	0.1205	0.1203
Depolar (P) --	0.7500	0.7500	0.7500
Depolar (U) --	0.8571	0.8571	0.8571

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	13	-0.18	0.00	0.00	-0.06	0.00	0.00	0.00	0.06	0.00
2	9	0.21	0.00	0.00	-0.01	0.00	0.00	0.00	-0.01	-0.11
3	9	-0.19	0.23	0.25	0.00	-0.01	0.09	0.01	0.01	0.05
4	9	-0.19	-0.23	-0.25	0.00	0.01	-0.09	-0.01	0.01	0.05
5	13	-0.18	0.00	0.00	-0.06	0.00	0.00	0.00	0.06	0.00
6	9	0.19	0.00	0.00	0.62	0.00	0.00	0.00	0.50	0.00
7	9	0.32	-0.08	0.00	-0.22	0.49	0.00	-0.49	-0.34	0.00
8	9	0.32	0.08	0.00	-0.22	-0.49	0.00	0.49	-0.34	0.00
9	9	0.21	0.00	0.00	-0.01	0.00	0.00	0.00	-0.01	0.11
10	9	-0.19	0.23	-0.25	0.00	-0.01	-0.09	0.01	0.01	-0.05
11	9	-0.19	-0.23	0.25	0.00	0.01	0.09	-0.01	0.01	-0.05

	19	20	21

		A1'			A2"			A1'		
Frequencies --		404.0948			448.3132			507.5114		
Red. masses --		20.5952			20.5404			19.0956		
Frc consts --		1.9814			2.4323			2.8978		
IR Inten --		0.0000			221.6424			0.0000		
Raman Activ --		1.8783			0.0000			2.4215		
Depolar (P) --		0.0002			0.7500			0.0034		
Depolar (U) --		0.0004			0.8571			0.0068		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	13	0.00	0.00	-0.32	0.00	0.00	0.31	0.00	0.00	0.08
2	9	0.00	0.36	-0.01	0.00	-0.20	0.07	0.00	-0.04	0.02
3	9	0.31	-0.18	-0.01	-0.17	0.10	0.07	-0.03	0.02	0.02
4	9	-0.31	-0.18	-0.01	0.17	0.10	0.07	0.03	0.02	0.02
5	13	0.00	0.00	0.32	0.00	0.00	0.31	0.00	0.00	-0.08
6	9	0.00	0.09	0.00	0.00	0.00	-0.43	0.00	0.57	0.00
7	9	0.08	-0.04	0.00	0.00	0.00	-0.43	0.49	-0.29	0.00
8	9	-0.08	-0.04	0.00	0.00	0.00	-0.43	-0.49	-0.29	0.00
9	9	0.00	0.36	0.01	0.00	0.20	0.07	0.00	-0.04	-0.02
10	9	0.31	-0.18	0.01	0.17	-0.10	0.07	-0.03	0.02	-0.02
11	9	-0.31	-0.18	0.01	-0.17	-0.10	0.07	0.03	0.02	-0.02

		22			23			24		
		?A			?A			?A		
Frequencies --		561.8863			576.3015			576.3150		
Red. masses --		21.7341			22.4214			22.4217		
Frc consts --		4.0429			4.3875			4.3877		
IR Inten --		478.2698			0.0000			0.0000		
Raman Activ --		0.0000			0.0155			0.0153		
Depolar (P) --		0.7500			0.7500			0.7500		
Depolar (U) --		0.8571			0.8571			0.8571		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	13	0.00	0.00	0.41	0.46	0.00	0.00	0.00	0.46	0.00
2	9	0.00	0.28	-0.18	-0.03	0.00	0.00	0.00	-0.38	0.21
3	9	0.24	-0.14	-0.18	-0.29	0.15	0.18	0.15	-0.12	-0.10
4	9	-0.24	-0.14	-0.18	-0.29	-0.15	-0.18	-0.15	-0.12	-0.10
5	13	0.00	0.00	0.41	-0.46	0.00	0.00	0.00	-0.46	0.00
6	9	0.00	0.00	-0.03	0.00	0.00	0.00	0.00	0.00	-0.02
7	9	0.00	0.00	-0.03	0.00	0.00	-0.02	0.00	0.00	0.01
8	9	0.00	0.00	-0.03	0.00	0.00	0.02	0.00	0.00	0.01
9	9	0.00	-0.28	-0.18	0.03	0.00	0.00	0.00	0.38	0.21
10	9	-0.24	0.14	-0.18	0.29	-0.15	0.18	-0.15	0.12	-0.10
11	9	0.24	0.14	-0.18	0.29	0.15	-0.18	0.15	0.12	-0.10

		25			26			27		
		E'			E'			A1'		
Frequencies --		630.3393			630.3399			638.9746		
Red. masses --		23.5638			23.5638			23.2394		
Frc consts --		5.5163			5.5163			5.5904		
IR Inten --		440.3312			440.2793			0.0000		
Raman Activ --		0.0547			0.0543			0.6879		
Depolar (P) --		0.7500			0.7498			0.0916		
Depolar (U) --		0.8571			0.8570			0.1678		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	13	0.53	0.00	0.00	0.00	0.53	0.00	0.00	0.00	0.52
2	9	-0.06	0.00	0.00	0.00	-0.32	0.14	0.00	0.21	-0.18
3	9	-0.25	0.11	0.12	0.11	-0.13	-0.07	0.19	-0.11	-0.18
4	9	-0.25	-0.11	-0.12	-0.11	-0.13	-0.07	-0.19	-0.11	-0.18
5	13	0.53	0.00	0.00	0.00	0.53	0.00	0.00	0.00	-0.52
6	9	-0.08	0.00	0.00	0.00	-0.17	0.00	0.00	-0.03	0.00
7	9	-0.15	0.04	0.00	0.04	-0.10	0.00	-0.02	0.01	0.00
8	9	-0.15	-0.04	0.00	-0.04	-0.10	0.00	0.02	0.01	0.00
9	9	-0.06	0.00	0.00	0.00	-0.32	-0.14	0.00	0.21	0.18
10	9	-0.25	0.11	-0.12	0.11	-0.13	0.07	0.19	-0.11	0.18
11	9	-0.25	-0.11	0.12	-0.11	-0.13	0.07	-0.19	-0.11	0.18

Calculated frequencies and vibrational modes of AlF_4^-, AlF_6^{3-} and $Al_2F_9^{3-}$ from Gaussian result files at PBE1PBE/cc-pVTZ level.

AlF_4^- (T_d)

	1	2	3
	E	E	T2
Frequencies --	196.9040	196.9040	302.7715
Red. masses --	18.9984	18.9984	20.2537
Frc consts --	0.4340	0.4340	1.0939
IR Inten --	0.0000	0.0000	37.4006
Raman Activ --	0.1732	0.1732	0.2983
Depolar (P) --	0.7500	0.7500	0.7500
Depolar (U) --	0.8571	0.8571	0.8571

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	13	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.28	-0.28
2	9	-0.38	0.05	0.33	-0.16	0.41	-0.25	0.01	-0.31	0.32
3	9	0.38	-0.05	0.33	0.16	-0.41	-0.25	0.44	0.12	-0.13
4	9	-0.38	-0.05	-0.33	-0.16	-0.41	0.25	-0.01	-0.32	0.32
5	9	0.38	0.05	-0.33	0.16	0.41	0.25	-0.44	0.11	-0.12

	4	5	6
	T2	T2	A1
Frequencies --	302.7715	302.7715	613.9544
Red. masses --	20.2537	20.2537	18.9984
Frc consts --	1.0939	1.0939	4.2193
IR Inten --	37.4006	37.4006	0.0000
Raman Activ --	0.2983	0.2983	3.4983
Depolar (P) --	0.7500	0.7500	0.0000
Depolar (U) --	0.8571	0.8571	0.0000

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	13	-0.10	0.27	0.28	0.38	0.07	0.07	0.00	0.00	0.00
2	9	0.46	0.04	0.03	-0.03	0.33	0.33	0.29	0.29	0.29
3	9	0.03	-0.39	-0.23	-0.14	0.22	-0.38	-0.29	-0.29	0.29
4	9	-0.39	0.20	0.19	-0.24	-0.27	-0.27	0.29	-0.29	-0.29
5	9	0.04	-0.23	-0.38	-0.13	-0.38	0.22	-0.29	0.29	-0.29

	7	8	9
	T2	T2	T2
Frequencies --	794.2485	794.2485	794.2485
Red. masses --	22.5199	22.5199	22.5199
Frc consts --	8.3701	8.3701	8.3701
IR Inten --	183.0626	183.0626	183.0626
Raman Activ --	0.2041	0.2041	0.2041
Depolar (P) --	0.7500	0.7500	0.7500
Depolar (U) --	0.8571	0.8571	0.8571

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	13	-0.01	0.52	-0.41	-0.08	0.41	0.52	0.66	0.05	0.06
2	9	-0.03	-0.06	-0.01	-0.26	-0.28	-0.29	-0.27	-0.24	-0.24
3	9	-0.29	-0.31	0.31	0.06	0.04	-0.08	-0.23	-0.21	0.20
4	9	0.04	-0.06	-0.02	0.31	-0.33	-0.33	-0.20	0.17	0.17
5	9	0.29	-0.31	0.31	-0.01	-0.01	-0.03	-0.24	0.20	-0.21

AlF_6^{3-} (O_h)

	1	2	3
	T2U	T2U	T2U
Frequencies --	171.5413	171.5413	171.5413
Red. masses --	18.9984	18.9984	18.9984
Frc consts --	0.3294	0.3294	0.3294
IR Inten --	0.0000	0.0000	0.0000
Raman Activ --	0.0000	0.0000	0.0000
Depolar (P) --	0.0000	0.0000	0.0000
Depolar (U) --	0.0000	0.0000	0.0000

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	13	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2	9	0.00	0.00	0.00	0.00	0.50	0.00	0.50	0.00	0.00
3	9	0.00	0.00	0.00	0.00	0.50	0.00	0.50	0.00	0.00
4	9	0.00	0.00	0.50	0.00	0.00	0.00	-0.50	0.00	0.00

5	9	0.00	0.00	0.50	0.00	0.00	0.00	-0.50	0.00	0.00
6	9	0.00	0.00	-0.50	0.00	-0.50	0.00	0.00	0.00	0.00
7	9	0.00	0.00	-0.50	0.00	-0.50	0.00	0.00	0.00	0.00

	4	5	6
	T2G	T2G	T2G
Frequencies --	274.7210	274.7210	274.7210
Red. masses --	18.9984	18.9984	18.9984
Frc consts --	0.8448	0.8448	0.8448
IR Inten --	0.0000	0.0000	0.0000
Raman Activ --	0.3243	0.3243	0.3243
Depolar (P) --	0.7500	0.7500	0.7500
Depolar (U) --	0.8571	0.8571	0.8571

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	13	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2	9	-0.50	0.00	0.00	0.00	0.00	0.00	0.00	-0.50	0.00
3	9	0.50	0.00	0.00	0.00	0.00	0.00	0.00	0.50	0.00
4	9	0.00	0.00	0.00	0.50	0.00	0.00	0.00	0.00	-0.50
5	9	0.00	0.00	0.00	-0.50	0.00	0.00	0.00	0.00	0.50
6	9	0.00	0.00	0.50	0.00	-0.50	0.00	0.00	0.00	0.00
7	9	0.00	0.00	-0.50	0.00	0.50	0.00	0.00	0.00	0.00

	7	8	9
	EG	EG	T1U
Frequencies --	282.1296	282.1296	335.5685
Red. masses --	18.9984	18.9984	19.1674
Frc consts --	0.8910	0.8910	1.2717
IR Inten --	0.0000	0.0000	0.0027
Raman Activ --	0.3420	0.3420	0.0000
Depolar (P) --	0.7500	0.7500	0.0000
Depolar (U) --	0.8571	0.8571	0.0000

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	13	0.00	0.00	0.00	0.00	0.00	0.00	-0.14	0.01	0.00
2	9	0.00	0.00	0.54	0.00	0.00	0.21	0.32	-0.03	0.00
3	9	0.00	0.00	-0.54	0.00	0.00	-0.21	0.32	-0.03	0.00
4	9	0.00	-0.45	0.00	0.00	0.36	0.00	0.32	0.05	0.00
5	9	0.00	0.45	0.00	0.00	-0.36	0.00	0.32	0.05	0.00
6	9	0.09	0.00	0.00	0.57	0.00	0.00	-0.53	-0.03	0.00
7	9	-0.09	0.00	0.00	-0.57	0.00	0.00	-0.53	-0.03	0.00

	10	11	12
	T1U	T1U	A1G
Frequencies --	335.5685	335.5685	437.1833
Red. masses --	19.1674	19.1674	18.9984
Frc consts --	1.2717	1.2717	2.1394
IR Inten --	0.0027	0.0027	0.0000
Raman Activ --	0.0000	0.0000	1.7191
Depolar (P) --	0.0000	0.0000	0.0000
Depolar (U) --	0.0000	0.0000	0.0000

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	13	0.01	0.14	0.00	0.00	0.00	0.15	0.00	0.00	0.00
2	9	-0.03	-0.32	0.00	0.00	0.00	0.53	0.00	0.00	-0.41
3	9	-0.03	-0.32	0.00	0.00	0.00	0.53	0.00	0.00	0.41
4	9	-0.03	0.53	0.00	0.00	0.00	-0.32	0.00	-0.41	0.00
5	9	-0.03	0.53	0.00	0.00	0.00	-0.32	0.00	0.41	0.00
6	9	0.05	-0.32	0.00	0.00	0.00	-0.32	0.41	0.00	0.00
7	9	0.05	-0.32	0.00	0.00	0.00	-0.32	-0.41	0.00	0.00

	13	14	15
	T1U	T1U	T1U
Frequencies --	514.5198	514.5198	514.5198
Red. masses --	24.6869	24.6869	24.6869
Frc consts --	3.8505	3.8505	3.8505
IR Inten --	283.0215	283.0215	283.0215
Raman Activ --	0.0000	0.0000	0.0000
Depolar (P) --	0.0000	0.0000	0.0000
Depolar (U) --	0.0000	0.0000	0.0000

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	13	0.00	0.00	0.84	0.84	0.00	0.00	0.00	0.84	0.00
2	9	0.00	0.00	-0.33	-0.14	0.00	0.00	0.00	-0.14	0.00
3	9	0.00	0.00	-0.33	-0.14	0.00	0.00	0.00	-0.14	0.00

4	9	0.00	0.00	-0.14	-0.14	0.00	0.00	0.00	-0.33	0.00
5	9	0.00	0.00	-0.14	-0.14	0.00	0.00	0.00	-0.33	0.00
6	9	0.00	0.00	-0.14	-0.33	0.00	0.00	0.00	-0.14	0.00
7	9	0.00	0.00	-0.14	-0.33	0.00	0.00	0.00	-0.14	0.00

$Al_2F_9^{3-}$ (D_{3h})

	1	2	3
	A1"	E'	E'
Frequencies --	92.9596	125.9255	125.9265
Red. masses --	18.9984	19.0179	19.0179
Frc consts --	0.0967	0.1777	0.1777
IR Inten --	0.0000	0.7421	0.7413
Raman Activ --	0.0000	0.0002	0.0002
Depolar (P) --	0.7500	0.7464	0.7500
Depolar (U) --	0.8571	0.8548	0.8571

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	13	0.00	0.00	0.00	0.00	-0.03	0.00	0.03	0.00	0.00
2	9	-0.41	0.00	0.00	0.00	0.23	0.43	-0.09	0.00	0.00
3	9	0.20	0.35	0.00	-0.06	0.13	-0.22	-0.19	0.06	-0.37
4	9	0.20	-0.35	0.00	0.06	0.13	-0.22	-0.19	-0.06	0.37
5	13	0.00	0.00	0.00	0.00	-0.03	0.00	0.03	0.00	0.00
6	9	0.00	0.00	0.00	0.00	-0.22	0.00	0.35	0.00	0.00
7	9	0.00	0.00	0.00	-0.05	-0.32	0.00	0.25	0.05	0.00
8	9	0.00	0.00	0.00	0.05	-0.32	0.00	0.25	-0.05	0.00
9	9	0.41	0.00	0.00	0.00	0.23	-0.43	-0.09	0.00	0.00
10	9	-0.20	-0.35	0.00	-0.06	0.13	0.22	-0.19	0.06	0.37
11	9	-0.20	0.35	0.00	0.06	0.13	0.22	-0.19	-0.06	-0.37

	4	5	6
	A2'	E"	E"
Frequencies --	173.2571	173.5173	173.5370
Red. masses --	18.9984	20.6144	20.6141
Frc consts --	0.3360	0.3657	0.3658
IR Inten --	0.0000	0.0000	0.0000
Raman Activ --	0.0000	0.3260	0.3244
Depolar (P) --	0.7500	0.7500	0.7500
Depolar (U) --	0.8571	0.8571	0.8571

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	13	0.00	0.00	0.00	0.00	0.32	0.00	0.32	0.00	0.00
2	9	-0.22	0.00	0.00	0.00	0.14	-0.40	0.07	0.00	0.00
3	9	0.11	0.19	0.00	-0.03	0.09	0.20	0.12	-0.03	-0.35
4	9	0.11	-0.19	0.00	0.03	0.09	0.20	0.12	0.03	0.35
5	13	0.00	0.00	0.00	0.00	-0.32	0.00	-0.32	0.00	0.00
6	9	-0.49	0.00	0.00	0.00	0.00	0.41	0.00	0.00	0.00
7	9	0.24	0.42	0.00	0.00	0.00	-0.20	0.00	0.00	0.35
8	9	0.24	-0.42	0.00	0.00	0.00	-0.20	0.00	0.00	-0.35
9	9	-0.22	0.00	0.00	0.00	-0.14	-0.40	-0.07	0.00	0.00
10	9	0.11	0.19	0.00	0.03	-0.09	0.20	-0.12	0.03	-0.35
11	9	0.11	-0.19	0.00	-0.03	-0.09	0.20	-0.12	-0.03	0.35

	7	8	9
	A1'	E"	E"
Frequencies --	214.2220	219.8105	219.8127
Red. masses --	19.5828	19.0866	19.0867
Frc consts --	0.5295	0.5433	0.5434
IR Inten --	0.0000	0.0000	0.0000
Raman Activ --	0.6687	0.0006	0.0006
Depolar (P) --	0.3222	0.7500	0.7500
Depolar (U) --	0.4874	0.8571	0.8571

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	13	0.00	0.00	0.19	0.00	0.07	0.00	0.07	0.00	0.00
2	9	0.00	0.10	0.38	0.00	0.25	0.26	-0.36	0.00	0.00
3	9	0.08	-0.05	0.38	-0.27	-0.21	-0.13	0.10	-0.27	0.23
4	9	-0.08	-0.05	0.38	0.27	-0.21	-0.13	0.10	0.27	-0.23
5	13	0.00	0.00	-0.19	0.00	-0.07	0.00	-0.07	0.00	0.00
6	9	0.00	-0.04	0.00	0.00	0.00	0.36	0.00	0.00	0.00
7	9	-0.03	0.02	0.00	0.00	0.00	-0.18	0.00	0.00	0.31
8	9	0.03	0.02	0.00	0.00	0.00	-0.18	0.00	0.00	-0.31

9	9	0.00	0.10	-0.38	0.00	-0.25	0.26	0.36	0.00	0.00
10	9	0.08	-0.05	-0.38	0.27	0.21	-0.13	-0.10	0.27	0.23
11	9	-0.08	-0.05	-0.38	-0.27	0.21	-0.13	-0.10	-0.27	-0.23

	10	11	12
	E'	E'	A2"
Frequencies --	243.0129	243.0138	320.6031
Red. masses --	19.0325	19.0325	19.4894
Frc consts --	0.6622	0.6622	1.1803
IR Inten --	1.4283	1.4281	31.3833
Raman Activ --	0.1367	0.1370	0.0000
Depolar (P) --	0.7500	0.7500	0.7500
Depolar (U) --	0.8571	0.8571	0.8571

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	13	0.00	-0.05	0.00	-0.05	0.00	0.00	0.00	0.00	0.18
2	9	0.00	-0.13	-0.20	0.44	0.00	0.00	0.00	-0.26	-0.22
3	9	0.25	0.30	0.10	0.01	0.25	-0.17	-0.22	0.13	-0.22
4	9	-0.25	0.30	0.10	0.01	-0.25	0.17	0.22	0.13	-0.22
5	13	0.00	-0.05	0.00	-0.05	0.00	0.00	0.00	0.00	0.18
6	9	0.00	-0.34	0.00	-0.20	0.00	0.00	0.00	0.00	0.28
7	9	0.06	-0.23	0.00	-0.30	0.06	0.00	0.00	0.00	0.28
8	9	-0.06	-0.23	0.00	-0.30	-0.06	0.00	0.00	0.00	0.28
9	9	0.00	-0.13	0.20	0.44	0.00	0.00	0.00	0.26	-0.22
10	9	0.25	0.30	-0.10	0.01	0.25	0.17	0.22	-0.13	-0.22
11	9	-0.25	0.30	-0.10	0.01	-0.25	-0.17	-0.22	-0.13	-0.22

	13	14	15
	E"	E"	E'
Frequencies --	347.6585	347.6594	374.0721
Red. masses --	19.4954	19.4954	19.5444
Frc consts --	1.3883	1.3883	1.6113
IR Inten --	0.0000	0.0000	20.3005
Raman Activ --	0.0005	0.0006	0.1442
Depolar (P) --	0.7500	0.7500	0.7500
Depolar (U) --	0.8571	0.8571	0.8571

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	13	0.00	-0.18	0.00	-0.18	0.00	0.00	-0.18	0.00	0.00
2	9	0.00	-0.14	0.18	0.30	0.00	0.00	0.19	0.00	0.00
3	9	0.19	0.19	-0.09	-0.03	0.19	0.15	-0.18	0.22	0.26
4	9	-0.19	0.19	-0.09	-0.03	-0.19	-0.15	-0.18	-0.22	-0.26
5	13	0.00	0.18	0.00	0.18	0.00	0.00	-0.18	0.00	0.00
6	9	0.00	0.00	0.59	0.00	0.00	0.00	0.35	0.00	0.00
7	9	0.00	0.00	-0.30	0.00	0.00	0.51	0.26	0.05	0.00
8	9	0.00	0.00	-0.30	0.00	0.00	-0.51	0.26	-0.05	0.00
9	9	0.00	0.14	0.18	-0.30	0.00	0.00	0.19	0.00	0.00
10	9	-0.19	-0.19	-0.09	0.03	-0.19	0.15	-0.18	0.22	-0.26
11	9	0.19	-0.19	-0.09	0.03	0.19	-0.15	-0.18	-0.22	0.26

	16	17	18
	E'	E'	E'
Frequencies --	374.0730	384.3668	384.3669
Red. masses --	19.5444	19.0044	19.0044
Frc consts --	1.6113	1.6542	1.6542
IR Inten --	20.2996	0.3422	0.3420
Raman Activ --	0.1446	0.2185	0.2181
Depolar (P) --	0.7500	0.7500	0.7500
Depolar (U) --	0.8571	0.8571	0.8571

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	13	0.00	-0.18	0.00	0.00	0.02	0.00	-0.02	0.00	0.00
2	9	0.00	-0.31	0.30	0.00	-0.09	-0.03	-0.06	0.00	0.00
3	9	0.22	0.07	-0.15	0.07	0.02	0.02	0.06	-0.07	0.03
4	9	-0.22	0.07	-0.15	-0.07	0.02	0.02	0.06	0.07	-0.03
5	13	0.00	-0.18	0.00	0.00	0.02	0.00	-0.02	0.00	0.00
6	9	0.00	0.23	0.00	0.00	0.58	0.00	0.55	0.00	0.00
7	9	0.05	0.32	0.00	-0.49	-0.27	0.00	-0.30	0.49	0.00
8	9	-0.05	0.32	0.00	0.49	-0.27	0.00	-0.30	-0.49	0.00
9	9	0.00	-0.31	-0.30	0.00	-0.09	0.03	-0.06	0.00	0.00
10	9	0.22	0.07	0.15	0.07	0.02	-0.02	0.06	-0.07	-0.03
11	9	-0.22	0.07	0.15	-0.07	0.02	-0.02	0.06	0.07	0.03

	19	20	21

		A1'			A2"			A1'		
Frequencies --		407.3099			457.4627			513.9357		
Red. masses --		20.5891			20.4220			19.0877		
Frc consts --		2.0125			2.5180			2.9705		
IR Inten --		0.0000			204.6418			0.0000		
Raman Activ --		1.6927			0.0000			2.4866		
Depolar (P) --		0.0004			0.7500			0.0018		
Depolar (U) --		0.0008			0.8571			0.0036		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	13	0.00	0.00	-0.32	0.00	0.00	0.30	0.00	0.00	0.07
2	9	0.00	0.36	-0.01	0.00	-0.20	0.07	0.00	-0.05	0.02
3	9	0.31	-0.18	-0.01	-0.17	0.10	0.07	-0.04	0.02	0.02
4	9	-0.31	-0.18	-0.01	0.17	0.10	0.07	0.04	0.02	0.02
5	13	0.00	0.00	0.32	0.00	0.00	0.30	0.00	0.00	-0.07
6	9	0.00	0.10	0.00	0.00	0.00	-0.43	0.00	0.57	0.00
7	9	0.08	-0.05	0.00	0.00	0.00	-0.43	0.49	-0.28	0.00
8	9	-0.08	-0.05	0.00	0.00	0.00	-0.43	-0.49	-0.28	0.00
9	9	0.00	0.36	0.01	0.00	0.20	0.07	0.00	-0.05	-0.02
10	9	0.31	-0.18	0.01	0.17	-0.10	0.07	-0.04	0.02	-0.02
11	9	-0.31	-0.18	0.01	-0.17	-0.10	0.07	0.04	0.02	-0.02

		22			23			24		
		A2"			E"			E"		
Frequencies --		570.1166			584.3856			584.3963		
Red. masses --		21.8371			22.4335			22.4337		
Frc consts --		4.1819			4.5138			4.5141		
IR Inten --		496.3510			0.0000			0.0000		
Raman Activ --		0.0000			0.0260			0.0257		
Depolar (P) --		0.7500			0.7500			0.7500		
Depolar (U) --		0.8571			0.8571			0.8571		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	13	0.00	0.00	0.42	0.00	0.46	0.00	0.46	0.00	0.00
2	9	0.00	0.27	-0.18	0.00	-0.38	0.21	-0.03	0.00	0.00
3	9	0.24	-0.14	-0.18	0.15	-0.12	-0.10	-0.29	0.15	0.18
4	9	-0.24	-0.14	-0.18	-0.15	-0.12	-0.10	-0.29	-0.15	-0.18
5	13	0.00	0.00	0.42	0.00	-0.46	0.00	-0.46	0.00	0.00
6	9	0.00	0.00	-0.04	0.00	0.00	-0.01	0.00	0.00	0.00
7	9	0.00	0.00	-0.04	0.00	0.00	0.01	0.00	0.00	-0.01
8	9	0.00	0.00	-0.04	0.00	0.00	0.01	0.00	0.00	0.01
9	9	0.00	-0.27	-0.18	0.00	0.38	0.21	0.03	0.00	0.00
10	9	-0.24	0.14	-0.18	-0.15	0.12	-0.10	0.29	-0.15	0.18
11	9	0.24	0.14	-0.18	0.15	0.12	-0.10	0.29	0.15	-0.18

		25			26			27		
		E'			E'			A1'		
Frequencies --		639.8209			639.8276			648.0572		
Red. masses --		23.5663			23.5663			23.2850		
Frc consts --		5.6840			5.6842			5.7617		
IR Inten --		447.4915			447.5160			0.0000		
Raman Activ --		0.0509			0.0507			0.6632		
Depolar (P) --		0.7500			0.7500			0.0778		
Depolar (U) --		0.8571			0.8571			0.1443		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	13	0.00	0.53	0.00	0.53	0.00	0.00	0.00	0.00	0.52
2	9	0.00	-0.32	0.14	-0.06	0.00	0.00	0.00	0.21	-0.18
3	9	0.11	-0.13	-0.07	-0.25	0.11	0.12	0.18	-0.11	-0.18
4	9	-0.11	-0.13	-0.07	-0.25	-0.11	-0.12	-0.18	-0.11	-0.18
5	13	0.00	0.53	0.00	0.53	0.00	0.00	0.00	0.00	-0.52
6	9	0.00	-0.18	0.00	-0.08	0.00	0.00	0.00	-0.02	0.00
7	9	0.04	-0.10	0.00	-0.15	0.04	0.00	-0.01	0.01	0.00
8	9	-0.04	-0.10	0.00	-0.15	-0.04	0.00	0.01	0.01	0.00
9	9	0.00	-0.32	-0.14	-0.06	0.00	0.00	0.00	0.21	0.18
10	9	0.11	-0.13	0.07	-0.25	0.11	-0.12	0.18	-0.11	0.18
11	9	-0.11	-0.13	0.07	-0.25	-0.11	0.12	-0.18	-0.11	0.18

Calculated frequencies and vibrational modes of AlF_4^-, AlF_6^{3-} and $Al_2F_9^{3-}$ from Gaussian result files at B3LYP/aug-cc-pVTZ level.

AlF_4^- (T_d)

	1			2			3		
	E			E			T2		
Frequencies --	193.1230			193.1230			300.4802		
Red. masses --	18.9984			18.9984			20.2545		
Frc consts --	0.4175			0.4175			1.0775		
IR Inten --	0.0000			0.0000			38.5851		
Raman Activ --	0.1665			0.1665			0.2176		
Depolar (P) --	0.7500			0.7500			0.7500		
Depolar (U) --	0.8571			0.8571			0.8571		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 13	0.00	0.00	0.00	0.00	0.00	0.00	0.00	-0.13	-0.37
2 9	0.00	-0.35	0.35	0.41	-0.21	-0.20	-0.39	-0.25	0.03
3 9	0.00	0.35	0.35	-0.41	0.21	-0.20	0.19	0.34	0.24
4 9	0.00	0.35	-0.35	0.41	0.21	0.20	0.39	-0.24	0.03
5 9	0.00	-0.35	-0.35	-0.41	-0.21	0.20	-0.19	0.34	0.23

	4			5			6		
	T2			T2			A1		
Frequencies --	300.4802			300.4802			603.0863		
Red. masses --	20.2545			20.2545			18.9984		
Frc consts --	1.0775			1.0775			4.0712		
IR Inten --	38.5851			38.5851			0.0000		
Raman Activ --	0.2176			0.2176			6.9159		
Depolar (P) --	0.7500			0.7500			0.0000		
Depolar (U) --	0.8571			0.8571			0.0000		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 13	0.00	0.37	-0.13	0.40	0.00	0.00	0.00	0.00	0.00
2 9	0.19	-0.24	0.34	-0.14	0.31	0.31	0.29	0.29	0.29
3 9	0.39	-0.03	-0.24	-0.14	0.31	-0.31	-0.29	-0.29	0.29
4 9	-0.19	-0.23	0.34	-0.14	-0.31	-0.31	0.29	-0.29	-0.29
5 9	-0.39	-0.03	-0.25	-0.14	-0.31	0.31	-0.29	0.29	-0.29

	7			8			9		
	T2			T2			T2		
Frequencies --	771.9515			771.9515			771.9515		
Red. masses --	22.5188			22.5188			22.5188		
Frc consts --	7.9063			7.9063			7.9063		
IR Inten --	209.6815			209.6815			209.6815		
Raman Activ --	0.4674			0.4674			0.4674		
Depolar (P) --	0.7500			0.7500			0.7500		
Depolar (U) --	0.8571			0.8571			0.8571		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 13	0.66	0.00	-0.01	0.00	-0.10	0.66	0.01	0.66	0.10
2 9	-0.23	-0.20	-0.20	-0.17	-0.17	-0.21	-0.23	-0.26	-0.24
3 9	-0.24	-0.21	0.21	0.23	0.24	-0.26	-0.18	-0.21	0.17
4 9	-0.24	0.21	0.21	0.17	-0.17	-0.20	0.23	-0.26	-0.24
5 9	-0.24	0.21	-0.20	-0.23	0.24	-0.26	0.17	-0.20	0.17

AlF_6^{3-} (O_h)

	1			2			3		
	T2U			T2U			T2U		
Frequencies --	160.9810			160.9810			160.9810		
Red. masses --	18.9984			18.9984			18.9984		
Frc consts --	0.2901			0.2901			0.2901		
IR Inten --	0.0000			0.0000			0.0000		
Raman Activ --	0.0000			0.0000			0.0000		
Depolar (P) --	0.0000			0.0000			0.0000		
Depolar (U) --	0.0000			0.0000			0.0000		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 13	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2 9	0.00	0.41	0.00	0.01	-0.29	0.00	0.50	0.00	0.00
3 9	0.00	0.41	0.00	0.01	-0.29	0.00	0.50	0.00	0.00
4 9	0.00	0.00	0.29	-0.01	0.00	0.41	-0.50	0.00	-0.01

5	9	0.00	0.00	0.29	-0.01	0.00	0.41	-0.50	0.00	-0.01
6	9	0.00	-0.41	-0.29	0.00	0.29	-0.41	0.00	0.00	0.01
7	9	0.00	-0.41	-0.29	0.00	0.29	-0.41	0.00	0.00	0.01

	4	5	6
	EG	EG	T2G
Frequencies --	244.0210	244.0210	259.8489
Red. masses --	18.9984	18.9984	18.9984
Frc consts --	0.6665	0.6665	0.7558
IR Inten --	0.0000	0.0000	0.0000
Raman Activ --	1.4998	1.4998	0.3029
Depolar (P) --	0.7500	0.7500	0.7500
Depolar (U) --	0.8571	0.8571	0.8571

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	13	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2	9	0.00	0.00	0.58	0.00	0.00	0.02	0.00	-0.50	0.00
3	9	0.00	0.00	-0.58	0.00	0.00	-0.02	0.00	0.50	0.00
4	9	0.00	-0.31	0.00	0.00	0.49	0.00	0.02	0.00	-0.50
5	9	0.00	0.31	0.00	0.00	-0.49	0.00	-0.02	0.00	0.50
6	9	0.27	0.00	0.00	0.51	0.00	0.00	0.00	-0.02	0.00
7	9	-0.27	0.00	0.00	-0.51	0.00	0.00	0.00	0.02	0.00

	7	8	9
	T2G	T2G	T1U
Frequencies --	259.8489	259.8489	320.8481
Red. masses --	18.9984	18.9984	19.1488
Frc consts --	0.7558	0.7558	1.1614
IR Inten --	0.0000	0.0000	0.8527
Raman Activ --	0.3029	0.3029	0.0000
Depolar (P) --	0.7500	0.7500	0.0000
Depolar (U) --	0.8571	0.8571	0.0000

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	13	0.00	0.00	0.00	0.00	0.00	0.00	-0.02	0.14	0.01
2	9	-0.50	0.00	0.00	-0.05	0.02	0.00	0.04	-0.31	0.04
3	9	0.50	0.00	0.00	0.05	-0.02	0.00	0.04	-0.31	0.04
4	9	-0.05	0.00	0.00	0.50	0.00	0.02	0.04	0.53	-0.02
5	9	0.05	0.00	0.00	-0.50	0.00	-0.02	0.04	0.53	-0.02
6	9	0.00	0.05	0.50	0.00	-0.50	0.05	-0.07	-0.31	-0.02
7	9	0.00	-0.05	-0.50	0.00	0.50	-0.05	-0.07	-0.31	-0.02

	10	11	12
	T1U	T1U	A1G
Frequencies --	320.8481	320.8481	423.1916
Red. masses --	19.1488	19.1488	18.9984
Frc consts --	1.1614	1.1614	2.0047
IR Inten --	0.8527	0.8527	0.0000
Raman Activ --	0.0000	0.0000	8.2364
Depolar (P) --	0.0000	0.0000	0.0000
Depolar (U) --	0.0000	0.0000	0.0000

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	13	-0.13	-0.02	0.05	0.05	0.00	0.13	0.00	0.00	0.00
2	9	0.29	0.05	0.19	-0.12	0.01	0.50	0.00	0.00	-0.41
3	9	0.29	0.05	0.19	-0.12	0.01	0.50	0.00	0.00	0.41
4	9	0.29	-0.08	-0.11	-0.12	-0.01	-0.30	0.00	-0.41	0.00
5	9	0.29	-0.08	-0.11	-0.12	-0.01	-0.30	0.00	0.41	0.00
6	9	-0.50	0.05	-0.11	0.20	0.01	-0.30	0.41	0.00	0.00
7	9	-0.50	0.05	-0.11	0.20	0.01	-0.30	-0.41	0.00	0.00

	13	14	15
	T1U	T1U	T1U
Frequencies --	462.7368	462.7368	462.7368
Red. masses --	24.7179	24.7179	24.7179
Frc consts --	3.1184	3.1184	3.1184
IR Inten --	390.1604	390.1604	390.1604
Raman Activ --	0.0000	0.0000	0.0000
Depolar (P) --	0.0000	0.0000	0.0000
Depolar (U) --	0.0000	0.0000	0.0000

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	13	0.85	-0.01	0.02	0.01	0.85	0.00	-0.02	0.00	0.85
2	9	-0.14	0.00	-0.01	0.00	-0.14	0.00	0.00	0.00	-0.32
3	9	-0.14	0.00	-0.01	0.00	-0.14	0.00	0.00	0.00	-0.32

4	9	-0.14	0.00	0.00	0.00	-0.32	0.00	0.00	0.00	-0.14
5	9	-0.14	0.00	0.00	0.00	-0.32	0.00	0.00	0.00	-0.14
6	9	-0.32	0.00	0.00	0.00	-0.14	0.00	0.01	0.00	-0.14
7	9	-0.32	0.00	0.00	0.00	-0.14	0.00	0.01	0.00	-0.14

$Al_2F_9^{3-}$ (D_{3h})

	1	2	3
	A1"	E'	E'
Frequencies --	89.0857	121.9832	121.9873
Red. masses --	18.9984	19.0177	19.0177
Frc consts --	0.0888	0.1667	0.1667
IR Inten --	0.0000	0.8177	0.8145
Raman Activ --	0.0000	0.0035	0.0034
Depolar (P) --	0.7500	0.7500	0.7500
Depolar (U) --	0.8571	0.8571	0.8571

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	13	0.00	0.00	0.00	0.03	0.00	0.00	0.00	-0.03	0.00
2	9	-0.41	0.00	0.00	-0.09	0.00	0.00	0.00	0.23	0.43
3	9	0.20	0.35	0.00	-0.19	0.06	-0.37	-0.06	0.13	-0.22
4	9	0.20	-0.35	0.00	-0.19	-0.06	0.37	0.06	0.13	-0.22
5	13	0.00	0.00	0.00	0.03	0.00	0.00	0.00	-0.03	0.00
6	9	0.00	0.00	0.00	0.34	0.00	0.00	0.00	-0.23	0.00
7	9	0.00	0.00	0.00	0.26	0.05	0.00	-0.05	-0.32	0.00
8	9	0.00	0.00	0.00	0.26	-0.05	0.00	0.05	-0.32	0.00
9	9	0.41	0.00	0.00	-0.09	0.00	0.00	0.00	0.23	-0.43
10	9	-0.20	-0.35	0.00	-0.19	0.06	0.37	-0.06	0.13	0.22
11	9	-0.20	0.35	0.00	-0.19	-0.06	-0.37	0.06	0.13	0.22

	4	5	6
	E"	E"	A2'
Frequencies --	160.0539	160.0864	165.3085
Red. masses --	20.6409	20.6406	18.9984
Frc consts --	0.3115	0.3117	0.3059
IR Inten --	0.0000	0.0000	0.0000
Raman Activ --	0.2799	0.2789	0.0000
Depolar (P) --	0.7500	0.7500	0.7500
Depolar (U) --	0.8571	0.8571	0.8571

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	13	0.32	0.00	0.00	0.00	0.32	0.00	0.00	0.00	0.00
2	9	0.05	0.00	0.00	0.00	0.15	-0.38	-0.22	0.00	0.00
3	9	0.13	-0.04	-0.33	-0.04	0.07	0.19	0.11	0.19	0.00
4	9	0.13	0.04	0.33	0.04	0.07	0.19	0.11	-0.19	0.00
5	13	-0.32	0.00	0.00	0.00	-0.32	0.00	0.00	0.00	0.00
6	9	0.00	0.00	0.00	0.00	0.00	0.44	-0.49	0.00	0.00
7	9	0.00	0.00	0.38	0.00	0.00	-0.22	0.24	0.42	0.00
8	9	0.00	0.00	-0.38	0.00	0.00	-0.22	0.24	-0.42	0.00
9	9	-0.05	0.00	0.00	0.00	-0.15	-0.38	-0.22	0.00	0.00
10	9	-0.13	0.04	-0.33	0.04	-0.07	0.19	0.11	0.19	0.00
11	9	-0.13	-0.04	0.33	-0.04	-0.07	0.19	0.11	-0.19	0.00

	7	8	9
	A1'	E"	E"
Frequencies --	208.4737	209.8474	209.8478
Red. masses --	19.5344	19.0483	19.0483
Frc consts --	0.5002	0.4942	0.4942
IR Inten --	0.0000	0.0000	0.0000
Raman Activ --	0.4376	0.0029	0.0030
Depolar (P) --	0.1417	0.7500	0.7500
Depolar (U) --	0.2483	0.8571	0.8571

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	13	0.00	0.00	0.18	0.00	0.06	0.00	0.06	0.00	0.00
2	9	0.00	0.10	0.38	0.00	0.24	0.29	-0.37	0.00	0.00
3	9	0.09	-0.05	0.38	-0.26	-0.21	-0.14	0.09	-0.26	0.25
4	9	-0.09	-0.05	0.38	0.26	-0.21	-0.14	0.09	0.26	-0.25
5	13	0.00	0.00	-0.18	0.00	-0.06	0.00	-0.06	0.00	0.00
6	9	0.00	-0.03	0.00	0.00	0.00	0.33	0.00	0.00	0.00
7	9	-0.03	0.02	0.00	0.00	0.00	-0.17	0.00	0.00	0.29
8	9	0.03	0.02	0.00	0.00	0.00	-0.17	0.00	0.00	-0.29

9	9	0.00	0.10	-0.38	0.00	-0.24	0.29	0.37	0.00	0.00
10	9	0.09	-0.05	-0.38	0.26	0.21	-0.14	-0.09	0.26	0.25
11	9	-0.09	-0.05	-0.38	-0.26	0.21	-0.14	-0.09	-0.26	-0.25

	10	11	12
	E'	E'	A2"
Frequencies --	232.0421	232.0429	307.9519
Red. masses --	19.0310	19.0310	19.5221
Frc consts --	0.6037	0.6037	1.0908
IR Inten --	1.7206	1.7208	38.1042
Raman Activ --	0.0117	0.0118	0.0000
Depolar (P) --	0.7500	0.7500	0.7500
Depolar (U) --	0.8571	0.8571	0.8571

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	13	0.00	-0.05	0.00	-0.05	0.00	0.00	0.00	0.00	0.18
2	9	0.00	-0.13	-0.20	0.44	0.00	0.00	0.00	-0.26	-0.22
3	9	0.25	0.30	0.10	0.01	0.25	-0.18	-0.23	0.13	-0.22
4	9	-0.25	0.30	0.10	0.01	-0.25	0.18	0.23	0.13	-0.22
5	13	0.00	-0.05	0.00	-0.05	0.00	0.00	0.00	0.00	0.18
6	9	0.00	-0.34	0.00	-0.20	0.00	0.00	0.00	0.00	0.28
7	9	0.06	-0.24	0.00	-0.31	0.06	0.00	0.00	0.00	0.28
8	9	-0.06	-0.24	0.00	-0.31	-0.06	0.00	0.00	0.00	0.28
9	9	0.00	-0.13	0.20	0.44	0.00	0.00	0.00	0.26	-0.22
10	9	0.25	0.30	-0.10	0.01	0.25	0.18	0.23	-0.13	-0.22
11	9	-0.25	0.30	-0.10	0.01	-0.25	-0.18	-0.23	-0.13	-0.22

	13	14	15
	E"	E"	E'
Frequencies --	336.9186	336.9204	357.8462
Red. masses --	19.5186	19.5187	19.4441
Frc consts --	1.3054	1.3054	1.4670
IR Inten --	0.0000	0.0000	15.7346
Raman Activ --	0.0005	0.0004	0.3357
Depolar (P) --	0.7500	0.7500	0.7500
Depolar (U) --	0.8571	0.8571	0.8571

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	13	0.00	-0.18	0.00	-0.18	0.00	0.00	0.00	0.17	0.00
2	9	0.00	-0.14	0.18	0.29	0.00	0.00	0.00	0.32	-0.29
3	9	0.19	0.19	-0.09	-0.03	0.19	0.16	-0.23	-0.07	0.14
4	9	-0.19	0.19	-0.09	-0.03	-0.19	-0.16	0.23	-0.07	0.14
5	13	0.00	0.18	0.00	0.18	0.00	0.00	0.00	0.17	0.00
6	9	0.00	0.00	0.59	0.00	0.00	0.00	0.00	-0.36	0.00
7	9	0.00	0.00	-0.30	0.00	0.00	0.51	0.07	-0.23	0.00
8	9	0.00	0.00	-0.30	0.00	0.00	-0.51	-0.07	-0.23	0.00
9	9	0.00	0.14	0.18	-0.29	0.00	0.00	0.00	0.32	0.29
10	9	-0.19	-0.19	-0.09	0.03	-0.19	0.16	-0.23	-0.07	-0.14
11	9	0.19	-0.19	-0.09	0.03	0.19	-0.16	0.23	-0.07	-0.14

	16	17	18
	E'	E'	E'
Frequencies --	357.8469	380.6479	380.6481
Red. masses --	19.4441	19.0632	19.0631
Frc consts --	1.4670	1.6274	1.6274
IR Inten --	15.7437	0.3135	0.3130
Raman Activ --	0.3364	0.1050	0.1046
Depolar (P) --	0.7500	0.7500	0.7500
Depolar (U) --	0.8571	0.8571	0.8571

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	13	-0.17	0.00	0.00	-0.06	0.00	0.00	0.00	0.06	0.00
2	9	0.21	0.00	0.00	-0.01	0.00	0.00	0.00	-0.01	-0.10
3	9	-0.19	0.23	0.25	0.01	-0.01	0.09	0.01	0.01	0.05
4	9	-0.19	-0.23	-0.25	0.01	0.01	-0.09	-0.01	0.01	0.05
5	13	-0.17	0.00	0.00	-0.06	0.00	0.00	0.00	0.06	0.00
6	9	0.19	0.00	0.00	0.62	0.00	0.00	0.00	0.51	0.00
7	9	0.32	-0.07	0.00	-0.22	0.49	0.00	-0.49	-0.34	0.00
8	9	0.32	0.07	0.00	-0.22	-0.49	0.00	0.49	-0.34	0.00
9	9	0.21	0.00	0.00	-0.01	0.00	0.00	0.00	-0.01	0.10
10	9	-0.19	0.23	-0.25	0.01	-0.01	-0.09	0.01	0.01	-0.05
11	9	-0.19	-0.23	0.25	0.01	0.01	0.09	-0.01	0.01	-0.05

	19	20	21

		A1'			A2"			A1'		
Frequencies --		397.8096			446.0306			512.4376		
Red. masses --		20.5896			20.6093			19.1019		
Frc consts --		1.9198			2.4157			2.9554		
IR Inten --		0.0000			261.4174			0.0000		
Raman Activ --		2.4996			0.0000			2.2592		
Depolar (P) --		0.0080			0.7500			0.0075		
Depolar (U) --		0.0158			0.8571			0.0148		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	13	0.00	0.00	-0.32	0.00	0.00	0.32	0.00	0.00	0.08
2	9	0.00	0.36	-0.02	0.00	-0.18	0.07	0.00	-0.03	0.01
3	9	0.31	-0.18	-0.02	-0.16	0.09	0.07	-0.03	0.02	0.01
4	9	-0.31	-0.18	-0.02	0.16	0.09	0.07	0.03	0.02	0.01
5	13	0.00	0.00	0.32	0.00	0.00	0.32	0.00	0.00	-0.08
6	9	0.00	0.08	0.00	0.00	0.00	-0.44	0.00	0.57	0.00
7	9	0.07	-0.04	0.00	0.00	0.00	-0.44	0.49	-0.29	0.00
8	9	-0.07	-0.04	0.00	0.00	0.00	-0.44	-0.49	-0.29	0.00
9	9	0.00	0.36	0.02	0.00	0.18	0.07	0.00	-0.03	-0.01
10	9	0.31	-0.18	0.02	0.16	-0.09	0.07	-0.03	0.02	-0.01
11	9	-0.31	-0.18	0.02	-0.16	-0.09	0.07	0.03	0.02	-0.01

		22			23			24		
		?A			?A			?A		
Frequencies --		540.3282			548.6512			548.6777		
Red. masses --		21.5869			22.4268			22.4273		
Frc consts --		3.7133			3.9775			3.9780		
IR Inten --		539.0829			0.0000			0.0001		
Raman Activ --		0.0000			0.7015			0.6963		
Depolar (P) --		0.7500			0.7500			0.7500		
Depolar (U) --		0.8571			0.8571			0.8571		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	13	0.00	0.00	0.40	0.46	0.00	0.00	0.00	0.46	0.00
2	9	0.00	0.28	-0.18	-0.03	0.00	0.00	0.00	-0.38	0.21
3	9	0.24	-0.14	-0.18	-0.29	0.15	0.18	0.15	-0.11	-0.10
4	9	-0.24	-0.14	-0.18	-0.29	-0.15	-0.18	-0.15	-0.11	-0.10
5	13	0.00	0.00	0.40	-0.46	0.00	0.00	0.00	-0.46	0.00
6	9	0.00	0.00	-0.02	0.00	0.00	0.00	0.00	0.00	-0.01
7	9	0.00	0.00	-0.02	0.00	0.00	-0.01	0.00	0.00	0.00
8	9	0.00	0.00	-0.02	0.00	0.00	0.01	0.00	0.00	0.00
9	9	0.00	-0.28	-0.18	0.03	0.00	0.00	0.00	0.38	0.21
10	9	-0.24	0.14	-0.18	0.29	-0.15	0.18	-0.15	0.11	-0.10
11	9	0.24	0.14	-0.18	0.29	0.15	-0.18	0.15	0.11	-0.10

		25			26			27		
		E'			E'			A1'		
Frequencies --		605.7698			605.7896			624.1448		
Red. masses --		23.6254			23.6255			23.3319		
Frc consts --		5.1079			5.1083			5.3551		
IR Inten --		550.8383			550.6737			0.0000		
Raman Activ --		0.2873			0.2869			3.8723		
Depolar (P) --		0.7500			0.7500			0.0041		
Depolar (U) --		0.8571			0.8571			0.0081		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	13	0.54	0.00	0.00	0.00	0.54	0.00	0.00	0.00	0.52
2	9	-0.07	0.00	0.00	0.00	-0.31	0.14	0.00	0.21	-0.18
3	9	-0.25	0.11	0.12	0.11	-0.13	-0.07	0.18	-0.11	-0.18
4	9	-0.25	-0.11	-0.12	-0.11	-0.13	-0.07	-0.18	-0.11	-0.18
5	13	0.54	0.00	0.00	0.00	0.54	0.00	0.00	0.00	-0.52
6	9	-0.08	0.00	0.00	0.00	-0.19	0.00	0.00	-0.04	0.00
7	9	-0.16	0.05	0.00	0.05	-0.11	0.00	-0.03	0.02	0.00
8	9	-0.16	-0.05	0.00	-0.05	-0.11	0.00	0.03	0.02	0.00
9	9	-0.07	0.00	0.00	0.00	-0.31	-0.14	0.00	0.21	0.18
10	9	-0.25	0.11	-0.12	0.11	-0.13	0.07	0.18	-0.11	0.18
11	9	-0.25	-0.11	0.12	-0.11	-0.13	0.07	-0.18	-0.11	0.18

Calculated frequencies and vibrational modes of AlF_4^-, AlF_6^{3-} and $Al_2F_9^{3-}$ from Gaussian result files at PBE1PBE/aug-cc-pVTZ level.

AlF_4^- (T_d)

	1	2	3
	E	E	T2
Frequencies --	193.3965	193.3965	301.1345
Red. masses --	18.9984	18.9984	20.2596
Frc consts --	0.4187	0.4187	1.0824
IR Inten --	0.0000	0.0000	38.8463
Raman Activ --	0.1546	0.1546	0.1990
Depolar (P) --	0.7500	0.7500	0.7500
Depolar (U) --	0.8571	0.8571	0.8571

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	13	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.28	-0.28
2	9	-0.33	0.38	-0.05	-0.25	-0.16	0.41	0.00	-0.32	0.32
3	9	0.33	-0.38	-0.05	0.25	0.16	0.41	0.44	0.12	-0.12
4	9	-0.33	-0.38	0.05	-0.25	0.16	-0.41	0.00	-0.32	0.32
5	9	0.33	0.38	0.05	0.25	-0.16	-0.41	-0.44	0.12	-0.12

	4	5	6
	T2	T2	A1
Frequencies --	301.1345	301.1345	610.2675
Red. masses --	20.2596	20.2596	18.9984
Frc consts --	1.0824	1.0824	4.1688
IR Inten --	38.8463	38.8463	0.0000
Raman Activ --	0.1990	0.1990	6.6229
Depolar (P) --	0.7500	0.7500	0.0000
Depolar (U) --	0.8571	0.8571	0.0000

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	13	0.27	-0.21	-0.21	0.29	0.19	0.19	0.00	0.00	0.00
2	9	-0.42	0.12	0.12	0.19	0.31	0.31	0.29	0.29	0.29
3	9	-0.10	0.44	0.03	-0.10	0.01	-0.44	-0.29	-0.29	0.29
4	9	0.23	-0.29	-0.30	-0.40	-0.15	-0.15	0.29	-0.29	-0.29
5	9	-0.09	0.02	0.44	-0.10	-0.44	0.01	-0.29	0.29	-0.29

	7	8	9
	T2	T2	T2
Frequencies --	782.3679	782.3679	782.3679
Red. masses --	22.5125	22.5125	22.5125
Frc consts --	8.1189	8.1189	8.1189
IR Inten --	208.7916	208.7916	208.7916
Raman Activ --	0.4439	0.4439	0.4439
Depolar (P) --	0.7500	0.7500	0.7500
Depolar (U) --	0.8571	0.8571	0.8571

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	13	0.37	0.39	0.39	-0.02	-0.46	0.48	0.55	-0.27	-0.24
2	9	-0.37	-0.37	-0.37	0.00	0.02	-0.02	-0.04	0.00	0.00
3	9	-0.13	-0.13	0.09	0.30	0.32	-0.32	-0.19	-0.15	0.17
4	9	0.11	-0.15	-0.15	0.01	0.01	-0.03	-0.36	0.34	0.34
5	9	-0.13	0.10	-0.13	-0.28	0.31	-0.31	-0.21	0.19	-0.17

AlF_6^{3-} (O_h)

	1	2	3
	T2U	T2U	T2U
Frequencies --	164.4134	164.4134	164.4134
Red. masses --	18.9984	18.9984	18.9984
Frc consts --	0.3026	0.3026	0.3026
IR Inten --	0.0000	0.0000	0.0000
Raman Activ --	0.0000	0.0000	0.0000
Depolar (P) --	0.0000	0.0000	0.0000
Depolar (U) --	0.0000	0.0000	0.0000

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	13	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2	9	0.07	0.00	0.00	0.49	0.00	0.00	0.00	0.50	0.00
3	9	0.07	0.00	0.00	0.49	0.00	0.00	0.00	0.50	0.00
4	9	-0.07	0.00	0.49	-0.49	0.00	-0.07	0.00	0.00	0.00

5	9	-0.07	0.00	0.49	-0.49	0.00	-0.07	0.00	0.00	0.00
6	9	0.00	0.00	-0.49	0.00	0.00	0.07	0.00	-0.50	0.00
7	9	0.00	0.00	-0.49	0.00	0.00	0.07	0.00	-0.50	0.00

	4	5	6
	EG	EG	T2G
Frequencies --	253.9287	253.9287	263.0745
Red. masses --	18.9984	18.9984	18.9984
Frc consts --	0.7218	0.7218	0.7747
IR Inten --	0.0000	0.0000	0.0000
Raman Activ --	1.3311	1.3311	0.1530
Depolar (P) --	0.7500	0.7500	0.7500
Depolar (U) --	0.8571	0.8571	0.8571

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	13	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2	9	0.00	0.00	-0.48	0.00	0.00	0.32	0.00	-0.50	0.00
3	9	0.00	0.00	0.48	0.00	0.00	-0.32	0.00	0.50	0.00
4	9	0.00	0.52	0.00	0.00	0.25	0.00	0.02	0.00	-0.50
5	9	0.00	-0.52	0.00	0.00	-0.25	0.00	-0.02	0.00	0.50
6	9	0.04	0.00	0.00	0.58	0.00	0.00	0.00	-0.02	0.00
7	9	-0.04	0.00	0.00	-0.58	0.00	0.00	0.00	0.02	0.00

	7	8	9
	T2G	T2G	T1U
Frequencies --	263.0745	263.0745	324.9204
Red. masses --	18.9984	18.9984	19.1744
Frc consts --	0.7747	0.7747	1.1927
IR Inten --	0.0000	0.0000	0.3405
Raman Activ --	0.1530	0.1530	0.0000
Depolar (P) --	0.7500	0.7500	0.0000
Depolar (U) --	0.8571	0.8571	0.0000

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	13	0.00	0.00	0.00	0.00	0.00	0.00	-0.15	0.00	0.01
2	9	-0.50	0.00	0.00	0.00	0.02	0.00	0.32	0.00	0.03
3	9	0.50	0.00	0.00	0.00	-0.02	0.00	0.32	0.00	0.03
4	9	0.00	0.00	0.00	0.50	0.00	0.02	0.32	0.00	-0.02
5	9	0.00	0.00	0.00	-0.50	0.00	-0.02	0.32	0.00	-0.02
6	9	0.00	0.00	0.50	0.00	-0.50	0.00	-0.53	0.00	-0.02
7	9	0.00	0.00	-0.50	0.00	0.50	0.00	-0.53	0.00	-0.02

	10	11	12
	T1U	T1U	A1G
Frequencies --	324.9204	324.9204	429.6159
Red. masses --	19.1744	19.1744	18.9984
Frc consts --	1.1927	1.1927	2.0660
IR Inten --	0.3405	0.3405	0.0000
Raman Activ --	0.0000	0.0000	3.7696
Depolar (P) --	0.0000	0.0000	0.0000
Depolar (U) --	0.0000	0.0000	0.0000

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	13	0.00	0.15	0.00	0.01	0.00	0.15	0.00	0.00	0.00
2	9	0.00	-0.32	0.00	-0.02	0.00	0.53	0.00	0.00	-0.41
3	9	0.00	-0.32	0.00	-0.02	0.00	0.53	0.00	0.00	0.41
4	9	0.00	0.53	0.00	-0.02	0.00	-0.32	0.00	-0.41	0.00
5	9	0.00	0.53	0.00	-0.02	0.00	-0.32	0.00	0.41	0.00
6	9	0.00	-0.32	0.00	0.03	0.00	-0.32	0.41	0.00	0.00
7	9	0.00	-0.32	0.00	0.03	0.00	-0.32	-0.41	0.00	0.00

	13	14	15
	T1U	T1U	T1U
Frequencies --	475.8792	475.8792	475.8792
Red. masses --	24.6754	24.6754	24.6754
Frc consts --	3.2924	3.2924	3.2924
IR Inten --	390.3657	390.3657	390.3657
Raman Activ --	0.0000	0.0000	0.0000
Depolar (P) --	0.0000	0.0000	0.0000
Depolar (U) --	0.0000	0.0000	0.0000

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	13	-0.01	0.84	0.00	-0.04	0.00	0.84	0.84	0.01	0.04
2	9	0.00	-0.14	0.00	0.01	0.00	-0.33	-0.14	0.00	-0.01
3	9	0.00	-0.14	0.00	0.01	0.00	-0.33	-0.14	0.00	-0.01

4	9	0.00	-0.33	0.00	0.01	0.00	-0.14	-0.14	-0.01	-0.01
5	9	0.00	-0.33	0.00	0.01	0.00	-0.14	-0.14	-0.01	-0.01
6	9	0.01	-0.14	0.00	0.01	0.00	-0.14	-0.33	0.00	-0.01
7	9	0.01	-0.14	0.00	0.01	0.00	-0.14	-0.33	0.00	-0.01

$Al_2F_9^{3-}$ (D_{3h})

	1	2	3
	A1"	E'	E'
Frequencies --	90.4832	124.1860	124.1895
Red. masses --	18.9984	19.0196	19.0196
Frc consts --	0.0916	0.1728	0.1728
IR Inten --	0.0000	0.9675	0.9653
Raman Activ --	0.0000	0.0031	0.0031
Depolar (P) --	0.7500	0.7498	0.7500
Depolar (U) --	0.8571	0.8570	0.8571

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	13	0.00	0.00	0.00	0.00	-0.04	0.00	0.04	0.00	0.00
2	9	-0.41	0.00	0.00	0.00	0.23	0.44	-0.09	0.00	0.00
3	9	0.20	0.35	0.00	-0.06	0.12	-0.22	-0.19	0.06	-0.38
4	9	0.20	-0.35	0.00	0.06	0.12	-0.22	-0.19	-0.06	0.38
5	13	0.00	0.00	0.00	0.00	-0.04	0.00	0.04	0.00	0.00
6	9	0.00	0.00	0.00	0.00	-0.22	0.00	0.34	0.00	0.00
7	9	0.00	0.00	0.00	-0.05	-0.31	0.00	0.25	0.05	0.00
8	9	0.00	0.00	0.00	0.05	-0.31	0.00	0.25	-0.05	0.00
9	9	0.41	0.00	0.00	0.00	0.23	-0.44	-0.09	0.00	0.00
10	9	-0.20	-0.35	0.00	-0.06	0.12	0.22	-0.19	0.06	0.38
11	9	-0.20	0.35	0.00	0.06	0.12	0.22	-0.19	-0.06	-0.38

	4	5	6
	A2'	E"	E"
Frequencies --	168.3523	173.0467	173.0775
Red. masses --	18.9984	20.5601	20.5595
Frc consts --	0.3173	0.3627	0.3629
IR Inten --	0.0000	0.0000	0.0000
Raman Activ --	0.0000	0.2802	0.2792
Depolar (P) --	0.7500	0.7500	0.7500
Depolar (U) --	0.8571	0.8571	0.8571

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	13	0.00	0.00	0.00	0.00	0.31	0.00	0.31	0.00	0.00
2	9	-0.22	0.00	0.00	0.00	0.12	-0.42	0.09	0.00	0.00
3	9	0.11	0.19	0.00	-0.01	0.10	0.21	0.12	-0.01	-0.36
4	9	0.11	-0.19	0.00	0.01	0.10	0.21	0.12	0.01	0.36
5	13	0.00	0.00	0.00	0.00	-0.31	0.00	-0.31	0.00	0.00
6	9	-0.49	0.00	0.00	0.00	0.00	0.37	0.00	0.00	0.00
7	9	0.24	0.42	0.00	0.00	0.00	-0.19	0.00	0.00	0.32
8	9	0.24	-0.42	0.00	0.00	0.00	-0.19	0.00	0.00	-0.32
9	9	-0.22	0.00	0.00	0.00	-0.12	-0.42	-0.09	0.00	0.00
10	9	0.11	0.19	0.00	0.01	-0.10	0.21	-0.12	0.01	-0.36
11	9	0.11	-0.19	0.00	-0.01	-0.10	0.21	-0.12	-0.01	0.36

	7	8	9
	A1'	E"	E"
Frequencies --	210.7721	214.5706	214.5723
Red. masses --	19.5191	19.1470	19.1471
Frc consts --	0.5109	0.5194	0.5194
IR Inten --	0.0000	0.0000	0.0000
Raman Activ --	0.4409	0.0002	0.0002
Depolar (P) --	0.1579	0.7500	0.7500
Depolar (U) --	0.2727	0.8571	0.8571

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	13	0.00	0.00	0.18	0.00	0.10	0.00	0.10	0.00	0.00
2	9	0.00	0.10	0.38	0.00	0.26	0.23	-0.37	0.00	0.00
3	9	0.09	-0.05	0.38	-0.27	-0.21	-0.12	0.11	-0.27	0.20
4	9	-0.09	-0.05	0.38	0.27	-0.21	-0.12	0.11	0.27	-0.20
5	13	0.00	0.00	-0.18	0.00	-0.10	0.00	-0.10	0.00	0.00
6	9	0.00	-0.03	0.00	0.00	0.00	0.37	0.00	0.00	0.00
7	9	-0.03	0.02	0.00	0.00	0.00	-0.19	0.00	0.00	0.32
8	9	0.03	0.02	0.00	0.00	0.00	-0.19	0.00	0.00	-0.32

9	9	0.00	0.10	-0.38	0.00	-0.26	0.23	0.37	0.00	0.00
10	9	0.09	-0.05	-0.38	0.27	0.21	-0.12	-0.11	0.27	0.20
11	9	-0.09	-0.05	-0.38	-0.27	0.21	-0.12	-0.11	-0.27	-0.20

	10	11	12
	E'	E'	A2"
Frequencies --	235.7206	235.7216	310.2313
Red. masses --	19.0396	19.0396	19.5441
Frc consts --	0.6233	0.6233	1.1082
IR Inten --	2.2745	2.2737	40.4308
Raman Activ --	0.0191	0.0196	0.0000
Depolar (P) --	0.7500	0.7500	0.7500
Depolar (U) --	0.8571	0.8571	0.8571

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	13	0.00	-0.05	0.00	-0.05	0.00	0.00	0.00	0.00	0.18
2	9	0.00	-0.13	-0.19	0.45	0.00	0.00	0.00	-0.26	-0.22
3	9	0.25	0.30	0.10	0.01	0.25	-0.17	-0.23	0.13	-0.22
4	9	-0.25	0.30	0.10	0.01	-0.25	0.17	0.23	0.13	-0.22
5	13	0.00	-0.05	0.00	-0.05	0.00	0.00	0.00	0.00	0.18
6	9	0.00	-0.33	0.00	-0.21	0.00	0.00	0.00	0.00	0.27
7	9	0.06	-0.24	0.00	-0.30	0.06	0.00	0.00	0.00	0.27
8	9	-0.06	-0.24	0.00	-0.30	-0.06	0.00	0.00	0.00	0.27
9	9	0.00	-0.13	0.19	0.45	0.00	0.00	0.00	0.26	-0.22
10	9	0.25	0.30	-0.10	0.01	0.25	0.17	0.23	-0.13	-0.22
11	9	-0.25	0.30	-0.10	0.01	-0.25	-0.17	-0.23	-0.13	-0.22

	13	14	15
	E"	E"	E'
Frequencies --	341.4081	341.4108	364.9204
Red. masses --	19.4845	19.4845	19.4724
Frc consts --	1.3381	1.3381	1.5278
IR Inten --	0.0000	0.0000	15.3364
Raman Activ --	0.0006	0.0005	0.2736
Depolar (P) --	0.7500	0.7500	0.7500
Depolar (U) --	0.8571	0.8571	0.8571

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	13	0.00	-0.17	0.00	-0.17	0.00	0.00	-0.17	0.00	0.00
2	9	0.00	-0.12	0.17	0.29	0.00	0.00	0.19	0.00	0.00
3	9	0.18	0.18	-0.09	-0.02	0.18	0.15	-0.19	0.22	0.26
4	9	-0.18	0.18	-0.09	-0.02	-0.18	-0.15	-0.19	-0.22	-0.26
5	13	0.00	0.17	0.00	0.17	0.00	0.00	-0.17	0.00	0.00
6	9	0.00	0.00	0.61	0.00	0.00	0.00	0.28	0.00	0.00
7	9	0.00	0.00	-0.30	0.00	0.00	0.53	0.29	-0.01	0.00
8	9	0.00	0.00	-0.30	0.00	0.00	-0.53	0.29	0.01	0.00
9	9	0.00	0.12	0.17	-0.29	0.00	0.00	0.19	0.00	0.00
10	9	-0.18	-0.18	-0.09	0.02	-0.18	0.15	-0.19	0.22	-0.26
11	9	0.18	-0.18	-0.09	0.02	0.18	-0.15	-0.19	-0.22	0.26

	16	17	18
	E'	E'	E'
Frequencies --	364.9220	385.8193	385.8199
Red. masses --	19.4724	19.0336	19.0336
Frc consts --	1.5278	1.6693	1.6693
IR Inten --	15.3410	0.0786	0.0785
Raman Activ --	0.2739	0.1702	0.1702
Depolar (P) --	0.7500	0.7500	0.7500
Depolar (U) --	0.8571	0.8571	0.8571

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	13	0.00	-0.17	0.00	0.00	0.05	0.00	-0.05	0.00	0.00
2	9	0.00	-0.32	0.30	0.00	-0.06	-0.06	-0.03	0.00	0.00
3	9	0.22	0.07	-0.15	0.04	0.01	0.03	0.04	-0.04	0.05
4	9	-0.22	0.07	-0.15	-0.04	0.01	0.03	0.04	0.04	-0.05
5	13	0.00	-0.17	0.00	0.00	0.05	0.00	-0.05	0.00	0.00
6	9	0.00	0.30	0.00	0.00	0.55	0.00	0.59	0.00	0.00
7	9	-0.01	0.28	0.00	-0.49	-0.30	0.00	-0.27	0.49	0.00
8	9	0.01	0.28	0.00	0.49	-0.30	0.00	-0.27	-0.49	0.00
9	9	0.00	-0.32	-0.30	0.00	-0.06	0.06	-0.03	0.00	0.00
10	9	0.22	0.07	0.15	0.04	0.01	-0.03	0.04	-0.04	-0.05
11	9	-0.22	0.07	0.15	-0.04	0.01	-0.03	0.04	0.04	0.05

	19	20	21

		A1'			A2"			A1'		
Frequencies --		401.6701			455.5800			519.5091		
Red. masses --		20.5953			20.4801			19.0877		
Frc consts --		1.9577			2.5044			3.0352		
IR Inten --		0.0000			237.4286			0.0000		
Raman Activ --		2.3705			0.0000			2.4820		
Depolar (P) --		0.0053			0.7500			0.0039		
Depolar (U) --		0.0106			0.8571			0.0078		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	13	0.00	0.00	-0.32	0.00	0.00	0.30	0.00	0.00	0.07
2	9	0.00	0.36	-0.02	0.00	-0.19	0.07	0.00	-0.04	0.02
3	9	0.31	-0.18	-0.02	-0.16	0.09	0.07	-0.04	0.02	0.02
4	9	-0.31	-0.18	-0.02	0.16	0.09	0.07	0.04	0.02	0.02
5	13	0.00	0.00	0.32	0.00	0.00	0.30	0.00	0.00	-0.07
6	9	0.00	0.09	0.00	0.00	0.00	-0.44	0.00	0.57	0.00
7	9	0.08	-0.05	0.00	0.00	0.00	-0.44	0.49	-0.29	0.00
8	9	-0.08	-0.05	0.00	0.00	0.00	-0.44	-0.49	-0.29	0.00
9	9	0.00	0.36	0.02	0.00	0.19	0.07	0.00	-0.04	-0.02
10	9	0.31	-0.18	0.02	0.16	-0.09	0.07	-0.04	0.02	-0.02
11	9	-0.31	-0.18	0.02	-0.16	-0.09	0.07	0.04	0.02	-0.02

		22			23			24		
		?A			?A			?A		
Frequencies --		550.3452			559.4693			559.4987		
Red. masses --		21.7032			22.4357			22.4363		
Frc consts --		3.8730			4.1375			4.1381		
IR Inten --		554.2148			0.0001			0.0000		
Raman Activ --		0.0000			0.6685			0.6644		
Depolar (P) --		0.7500			0.7500			0.7500		
Depolar (U) --		0.8571			0.8571			0.8571		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	13	0.00	0.00	0.41	0.00	0.46	0.00	0.46	0.00	0.00
2	9	0.00	0.28	-0.18	0.00	-0.38	0.21	-0.02	0.00	0.00
3	9	0.24	-0.14	-0.18	0.15	-0.11	-0.11	-0.29	0.15	0.18
4	9	-0.24	-0.14	-0.18	-0.15	-0.11	-0.11	-0.29	-0.15	-0.18
5	13	0.00	0.00	0.41	0.00	-0.46	0.00	-0.46	0.00	0.00
6	9	0.00	0.00	-0.03	0.00	0.00	0.00	0.00	0.00	0.00
7	9	0.00	0.00	-0.03	0.00	0.00	0.00	0.00	0.00	0.00
8	9	0.00	0.00	-0.03	0.00	0.00	0.00	0.00	0.00	0.00
9	9	0.00	-0.28	-0.18	0.00	0.38	0.21	0.02	0.00	0.00
10	9	-0.24	0.14	-0.18	-0.15	0.11	-0.11	0.29	-0.15	0.18
11	9	0.24	0.14	-0.18	0.15	0.11	-0.11	0.29	0.15	-0.18

		25			26			27		
		E'			E'			A1'		
Frequencies --		617.5854			617.6063			634.4568		
Red. masses --		23.6131			23.6132			23.3679		
Frc consts --		5.3064			5.3067			5.5421		
IR Inten --		547.9183			547.8443			0.0000		
Raman Activ --		0.2489			0.2483			3.7079		
Depolar (P) --		0.7500			0.7500			0.0028		
Depolar (U) --		0.8571			0.8571			0.0055		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	13	0.00	0.54	0.00	0.54	0.00	0.00	0.00	0.00	0.52
2	9	0.00	-0.31	0.14	-0.06	0.00	0.00	0.00	0.21	-0.18
3	9	0.11	-0.13	-0.07	-0.25	0.11	0.12	0.18	-0.11	-0.18
4	9	-0.11	-0.13	-0.07	-0.25	-0.11	-0.12	-0.18	-0.11	-0.18
5	13	0.00	0.54	0.00	0.54	0.00	0.00	0.00	0.00	-0.52
6	9	0.00	-0.20	0.00	-0.08	0.00	0.00	0.00	-0.02	0.00
7	9	0.05	-0.11	0.00	-0.17	0.05	0.00	-0.02	0.01	0.00
8	9	-0.05	-0.11	0.00	-0.17	-0.05	0.00	0.02	0.01	0.00
9	9	0.00	-0.31	-0.14	-0.06	0.00	0.00	0.00	0.21	0.18
10	9	0.11	-0.13	0.07	-0.25	0.11	-0.12	0.18	-0.11	0.18
11	9	-0.11	-0.13	0.07	-0.25	-0.11	0.12	-0.18	-0.11	0.18

Calculated frequencies and vibrational modes of AlF_4^-, AlF_6^{3-} and $Al_2F_9^{3-}$ from Gaussian result files at MP2/aug-cc-pVTZ level.

AlF_4^- (T_d)

	1			2			3		
	E			E			T2		
Frequencies --	194.3336			194.3337			301.1063		
Red. masses --	18.9984			18.9984			20.2529		
Frc consts --	0.4227			0.4227			1.0819		
IR Inten --	0.0000			0.0000			40.3189		
Raman Activ --	0.1456			0.1456			0.1816		
Depolar (P) --	0.7500			0.7500			0.7500		
Depolar (U) --	0.8571			0.8571			0.8571		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 13	0.00	0.00	0.00	0.00	0.00	0.00	-0.28	0.28	0.00
2 9	-0.35	0.35	0.00	-0.20	-0.20	0.41	0.32	-0.32	0.00
3 9	0.35	-0.35	0.00	0.20	0.20	0.41	0.32	-0.32	0.00
4 9	-0.35	-0.35	0.00	-0.20	0.20	-0.41	-0.12	0.12	0.44
5 9	0.35	0.35	0.00	0.20	-0.20	-0.41	-0.12	0.12	-0.44

	4			5			6		
	T2			T2			A1		
Frequencies --	301.1063			301.1063			603.4054		
Red. masses --	20.2529			20.2529			18.9984		
Frc consts --	1.0819			1.0819			4.0755		
IR Inten --	40.3189			40.3189			0.0000		
Raman Activ --	0.1816			0.1816			6.6823		
Depolar (P) --	0.7500			0.7500			0.0000		
Depolar (U) --	0.8571			0.8571			0.0000		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 13	0.16	0.16	0.32	0.23	0.23	-0.23	0.00	0.00	0.00
2 9	0.32	0.32	0.14	-0.08	-0.08	0.44	0.29	0.29	0.29
3 9	-0.18	-0.19	-0.37	0.28	0.27	-0.28	-0.29	-0.29	0.29
4 9	-0.44	0.07	-0.11	-0.08	-0.44	0.08	0.29	-0.29	-0.29
5 9	0.07	-0.43	-0.12	-0.44	-0.08	0.08	-0.29	0.29	-0.29

	7			8			9		
	T2			T2			T2		
Frequencies --	774.1558			774.1558			774.1558		
Red. masses --	22.5208			22.5208			22.5208		
Frc consts --	7.9523			7.9523			7.9523		
IR Inten --	212.6385			212.6385			212.6385		
Raman Activ --	0.4151			0.4151			0.4151		
Depolar (P) --	0.7500			0.7500			0.7500		
Depolar (U) --	0.8571			0.8571			0.8571		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 13	-0.38	-0.38	0.39	0.28	0.28	0.54	-0.47	0.47	0.00
2 9	0.13	0.13	0.09	-0.35	-0.35	-0.36	0.02	-0.02	0.00
3 9	0.37	0.37	-0.37	-0.02	-0.02	-0.02	0.02	-0.02	0.00
4 9	0.14	-0.10	-0.14	0.15	-0.18	-0.19	0.31	-0.31	-0.29
5 9	-0.10	0.14	-0.14	-0.18	0.15	-0.19	0.31	-0.31	0.29

AlF_6^{3-} (O_h)

	1			2			3		
	T2U			T2U			T2U		
Frequencies --	163.6900			163.6900			163.6900		
Red. masses --	18.9984			18.9984			18.9984		
Frc consts --	0.2999			0.2999			0.2999		
IR Inten --	0.0000			0.0000			0.0000		
Raman Activ --	0.0000			0.0000			0.0000		
Depolar (P) --	0.0000			0.0000			0.0000		
Depolar (U) --	0.0000			0.0000			0.0000		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 13	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2 9	0.00	0.00	0.00	0.00	0.50	0.00	0.50	0.00	0.00
3 9	0.00	0.00	0.00	0.00	0.50	0.00	0.50	0.00	0.00
4 9	0.00	0.00	0.50	0.00	0.00	0.00	-0.50	0.00	0.00

5	9	0.00	0.00	0.50	0.00	0.00	0.00	-0.50	0.00	0.00
6	9	0.00	0.00	-0.50	0.00	-0.50	0.00	0.00	0.00	0.00
7	9	0.00	0.00	-0.50	0.00	-0.50	0.00	0.00	0.00	0.00

	4	5	6
	EG	EG	T2G
Frequencies --	251.5220	251.5220	261.0503
Red. masses --	18.9984	18.9984	18.9984
Frc consts --	0.7081	0.7081	0.7628
IR Inten --	0.0000	0.0000	0.0000
Raman Activ --	1.3336	1.3336	0.0508
Depolar (P) --	0.7500	0.7500	0.7500
Depolar (U) --	0.8571	0.8571	0.8571

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	13	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2	9	0.00	0.00	0.39	0.00	0.00	-0.43	-0.50	0.00	0.00
3	9	0.00	0.00	-0.39	0.00	0.00	0.43	0.50	0.00	0.00
4	9	0.00	0.17	0.00	0.00	0.55	0.00	0.00	0.00	0.00
5	9	0.00	-0.17	0.00	0.00	-0.55	0.00	0.00	0.00	0.00
6	9	0.56	0.00	0.00	0.13	0.00	0.00	0.00	0.00	0.50
7	9	-0.56	0.00	0.00	-0.13	0.00	0.00	0.00	0.00	-0.50

	7	8	9
	T2G	T2G	T1U
Frequencies --	261.0503	261.0503	322.4501
Red. masses --	18.9984	18.9984	19.1548
Frc consts --	0.7628	0.7628	1.1734
IR Inten --	0.0000	0.0000	0.3975
Raman Activ --	0.0508	0.0508	0.0000
Depolar (P) --	0.7500	0.7500	0.0000
Depolar (U) --	0.8571	0.8571	0.0000

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	13	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.14	0.00
2	9	0.00	-0.50	0.00	0.00	0.00	0.00	0.00	-0.32	0.00
3	9	0.00	0.50	0.00	0.00	0.00	0.00	0.00	-0.32	0.00
4	9	0.00	0.00	-0.50	0.50	0.00	0.00	0.00	0.54	0.00
5	9	0.00	0.00	0.50	-0.50	0.00	0.00	0.00	0.54	0.00
6	9	0.00	0.00	0.00	0.00	-0.50	0.00	0.00	-0.32	0.00
7	9	0.00	0.00	0.00	0.00	0.50	0.00	0.00	-0.32	0.00

	10	11	12
	T1U	T1U	A1G
Frequencies --	322.4501	322.4501	425.6951
Red. masses --	19.1548	19.1548	18.9984
Frc consts --	1.1734	1.1734	2.0285
IR Inten --	0.3975	0.3975	0.0000
Raman Activ --	0.0000	0.0000	2.5384
Depolar (P) --	0.0000	0.0000	0.0000
Depolar (U) --	0.0000	0.0000	0.0000

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	13	-0.14	0.00	0.00	0.00	0.00	0.14	0.00	0.00	0.00
2	9	0.32	0.00	0.00	0.00	0.00	0.54	0.00	0.00	-0.41
3	9	0.32	0.00	0.00	0.00	0.00	0.54	0.00	0.00	0.41
4	9	0.32	0.00	0.00	0.00	0.00	-0.32	0.00	-0.41	0.00
5	9	0.32	0.00	0.00	0.00	0.00	-0.32	0.00	0.41	0.00
6	9	-0.54	0.00	0.00	0.00	0.00	-0.32	0.41	0.00	0.00
7	9	-0.54	0.00	0.00	0.00	0.00	-0.32	-0.41	0.00	0.00

	13	14	15
	T1U	T1U	T1U
Frequencies --	473.5908	473.5908	473.5908
Red. masses --	24.7080	24.7080	24.7080
Frc consts --	3.2651	3.2651	3.2651
IR Inten --	410.8442	410.8442	410.8442
Raman Activ --	0.0000	0.0000	0.0000
Depolar (P) --	0.0000	0.0000	0.0000
Depolar (U) --	0.0000	0.0000	0.0000

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	13	0.00	0.00	0.85	0.00	0.85	0.00	0.85	0.00	0.00
2	9	0.00	0.00	-0.32	0.00	-0.14	0.00	-0.14	0.00	0.00
3	9	0.00	0.00	-0.32	0.00	-0.14	0.00	-0.14	0.00	0.00

4	9	0.00	0.00	-0.14	0.00	-0.32	0.00	-0.14	0.00	0.00
5	9	0.00	0.00	-0.14	0.00	-0.32	0.00	-0.14	0.00	0.00
6	9	0.00	0.00	-0.14	0.00	-0.14	0.00	-0.32	0.00	0.00
7	9	0.00	0.00	-0.14	0.00	-0.14	0.00	-0.32	0.00	0.00

$Al_2F_9^{3-}$ (D_{3h})

	1	2	3
	A1"	E'	E'
Frequencies --	90.4608	123.4839	123.4839
Red. masses --	18.9984	19.0196	19.0196
Frc consts --	0.0916	0.1709	0.1709
IR Inten --	0.0000	1.0132	1.0132
Raman Activ --	0.0000	0.0039	0.0039
Depolar (P) --	0.7498	0.7500	0.7500
Depolar (U) --	0.8570	0.8571	0.8571

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	13	0.00	0.00	0.00	0.04	0.01	0.00	0.01	-0.04	0.00
2	9	-0.41	0.00	0.00	-0.09	-0.04	-0.07	-0.01	0.22	0.43
3	9	0.20	0.35	0.00	-0.18	0.04	-0.34	-0.09	0.13	-0.28
4	9	0.20	-0.35	0.00	-0.20	-0.08	0.41	0.03	0.11	-0.15
5	13	0.00	0.00	0.00	0.04	0.01	0.00	0.01	-0.04	0.00
6	9	0.00	0.00	0.00	0.34	0.04	0.00	0.06	-0.22	0.00
7	9	0.00	0.00	0.00	0.26	0.10	0.00	-0.01	-0.30	0.00
8	9	0.00	0.00	0.00	0.24	0.00	0.00	0.09	-0.32	0.00
9	9	0.41	0.00	0.00	-0.09	-0.04	0.07	-0.01	0.22	-0.43
10	9	-0.20	-0.35	0.00	-0.18	0.04	0.34	-0.09	0.13	0.28
11	9	-0.20	0.35	0.00	-0.20	-0.08	-0.41	0.03	0.11	0.15

	4	5	6
	A2'	E"	E"
Frequencies --	168.3925	174.4539	174.4539
Red. masses --	18.9984	20.5263	20.5263
Frc consts --	0.3174	0.3681	0.3681
IR Inten --	0.0000	0.0000	0.0000
Raman Activ --	0.0000	0.2416	0.2416
Depolar (P) --	0.7499	0.7500	0.7500
Depolar (U) --	0.8571	0.8571	0.8571

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	13	0.00	0.00	0.00	0.09	0.29	0.00	0.29	-0.09	0.00
2	9	-0.22	0.00	0.00	0.03	0.11	-0.41	0.10	-0.03	0.13
3	9	0.11	0.19	0.00	0.03	0.10	0.09	0.11	-0.04	-0.42
4	9	0.11	-0.19	0.00	0.04	0.10	0.32	0.10	-0.03	0.29
5	13	0.00	0.00	0.00	-0.09	-0.29	0.00	-0.29	0.09	0.00
6	9	-0.49	0.00	0.00	0.00	0.00	0.33	0.00	0.00	-0.11
7	9	0.24	0.42	0.00	0.00	0.00	-0.07	0.00	0.00	0.34
8	9	0.24	-0.42	0.00	0.00	0.00	-0.26	0.00	0.00	-0.23
9	9	-0.22	0.00	0.00	-0.03	-0.11	-0.41	-0.10	0.03	0.13
10	9	0.11	0.19	0.00	-0.03	-0.10	0.09	-0.11	0.04	-0.42
11	9	0.11	-0.19	0.00	-0.04	-0.10	0.32	-0.10	0.03	0.29

	7	8	9
	A1'	E"	E"
Frequencies --	209.9844	215.2461	215.2461
Red. masses --	19.5039	19.2017	19.2017
Frc consts --	0.5067	0.5242	0.5242
IR Inten --	0.0000	0.0000	0.0000
Raman Activ --	0.5497	0.0000	0.0000
Depolar (P) --	0.1732	0.7500	0.7500
Depolar (U) --	0.2953	0.8571	0.8571

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	13	0.00	0.00	0.18	0.10	0.05	0.00	-0.05	0.10	0.00
2	9	0.00	0.10	0.38	-0.32	0.13	0.10	0.18	0.24	0.19
3	9	0.09	-0.05	0.38	-0.04	-0.34	0.11	-0.30	-0.05	-0.18
4	9	-0.09	-0.05	0.38	0.23	0.14	-0.21	0.19	-0.32	0.00
5	13	0.00	0.00	-0.18	-0.10	-0.05	0.00	0.05	-0.10	0.00
6	9	0.00	-0.03	0.00	0.00	0.00	0.18	0.00	0.00	0.33
7	9	-0.03	0.02	0.00	0.00	0.00	0.19	0.00	0.00	-0.32
8	9	0.03	0.02	0.00	0.00	0.00	-0.38	0.00	0.00	-0.01

9	9	0.00	0.10	-0.38	0.32	-0.13	0.10	-0.18	-0.24	0.19
10	9	0.09	-0.05	-0.38	0.04	0.34	0.11	0.30	0.05	-0.18
11	9	-0.09	-0.05	-0.38	-0.23	-0.14	-0.21	-0.19	0.32	0.00

	10	11	12
	E'	E'	A2"
Frequencies --	233.8578	233.8578	307.6274
Red. masses --	19.0377	19.0377	19.5539
Frc consts --	0.6134	0.6134	1.0903
IR Inten --	2.2047	2.2047	42.5979
Raman Activ --	0.0402	0.0402	0.0000
Depolar (P) --	0.7500	0.7500	0.7495
Depolar (U) --	0.8571	0.8571	0.8568

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	13	-0.05	-0.02	0.00	0.02	-0.05	0.00	0.00	0.00	0.19
2	9	0.41	-0.05	-0.08	-0.18	-0.12	-0.18	0.00	-0.26	-0.22
3	9	0.11	0.35	-0.12	0.22	0.18	0.16	-0.23	0.13	-0.22
4	9	-0.09	-0.11	0.19	-0.23	0.38	0.02	0.23	0.13	-0.22
5	13	-0.05	-0.02	0.00	0.02	-0.05	0.00	0.00	0.00	0.19
6	9	-0.19	-0.13	0.00	0.08	-0.30	0.00	0.00	0.00	0.27
7	9	-0.25	-0.05	0.00	0.17	-0.24	0.00	0.00	0.00	0.27
8	9	-0.30	-0.15	0.00	0.07	-0.19	0.00	0.00	0.00	0.27
9	9	0.41	-0.05	0.08	-0.18	-0.12	0.18	0.00	0.26	-0.22
10	9	0.11	0.35	0.12	0.22	0.18	-0.16	0.23	-0.13	-0.22
11	9	-0.09	-0.11	-0.19	-0.23	0.38	-0.02	-0.23	-0.13	-0.22

	13	14	15
	E"	E"	E'
Frequencies --	340.3645	340.3645	362.8052
Red. masses --	19.4577	19.4577	19.4660
Frc consts --	1.3281	1.3281	1.5096
IR Inten --	0.0000	0.0000	16.1706
Raman Activ --	0.0081	0.0081	0.2943
Depolar (P) --	0.7500	0.7500	0.7500
Depolar (U) --	0.8571	0.8571	0.8571

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	13	0.14	0.09	0.00	0.09	-0.14	0.00	0.13	0.11	0.00
2	9	-0.24	0.06	-0.09	-0.15	-0.10	0.14	-0.15	0.21	-0.20
3	9	-0.08	-0.24	-0.08	0.15	0.06	-0.15	-0.01	-0.21	-0.09
4	9	0.11	0.04	0.17	-0.14	0.25	0.01	0.29	0.12	0.29
5	13	-0.14	-0.09	0.00	-0.09	0.14	0.00	0.13	0.11	0.00
6	9	0.00	0.00	-0.34	0.00	0.00	0.52	-0.21	-0.20	0.00
7	9	0.00	0.00	-0.28	0.00	0.00	-0.55	-0.21	-0.18	0.00
8	9	0.00	0.00	0.62	0.00	0.00	0.03	-0.23	-0.20	0.00
9	9	0.24	-0.06	-0.09	0.15	0.10	0.14	-0.15	0.21	0.20
10	9	0.08	0.24	-0.08	-0.15	-0.06	-0.15	-0.01	-0.21	0.09
11	9	-0.11	-0.04	0.17	0.14	-0.25	0.01	0.29	0.12	-0.29

	16	17	18
	E'	E'	E'
Frequencies --	362.8052	384.8789	384.8789
Red. masses --	19.4660	19.0338	19.0338
Frc consts --	1.5096	1.6612	1.6612
IR Inten --	16.1706	0.0918	0.0918
Raman Activ --	0.2943	0.1940	0.1940
Depolar (P) --	0.7500	0.7500	0.7500
Depolar (U) --	0.8571	0.8571	0.8571

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	13	0.11	-0.13	0.00	-0.05	-0.01	0.00	-0.01	0.05	0.00
2	9	-0.13	-0.24	0.22	-0.03	0.01	0.01	-0.01	-0.06	-0.06
3	9	0.29	-0.10	-0.28	0.03	-0.04	0.05	0.04	0.00	0.04
4	9	-0.04	0.20	0.06	0.04	0.04	-0.06	-0.03	0.02	0.02
5	13	0.11	-0.13	0.00	-0.05	-0.01	0.00	-0.01	0.05	0.00
6	9	-0.18	0.22	0.00	0.58	-0.09	0.00	0.10	0.54	0.00
7	9	-0.20	0.22	0.00	-0.18	0.54	0.00	-0.53	-0.22	0.00
8	9	-0.19	0.20	0.00	-0.34	-0.44	0.00	0.44	-0.38	0.00
9	9	-0.13	-0.24	-0.22	-0.03	0.01	-0.01	-0.01	-0.06	0.06
10	9	0.29	-0.10	0.28	0.03	-0.04	-0.05	0.04	0.00	-0.04
11	9	-0.04	0.20	-0.06	0.04	0.04	0.06	-0.03	0.02	-0.02

	19	20	21

		A1'			A2"			A1'		
Frequencies --		399.8295			456.8616			518.3633		
Red. masses --		20.5560			20.3186			19.0782		
Frc consts --		1.9361			2.4987			3.0203		
IR Inten --		0.0000			213.2370			0.0000		
Raman Activ --		2.9717			0.0000			2.8459		
Depolar (P) --		0.0001			0.7499			0.0002		
Depolar (U) --		0.0002			0.8571			0.0004		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	13	0.00	0.00	-0.31	0.00	0.00	0.29	0.00	0.00	0.07
2	9	0.00	0.36	-0.03	0.00	-0.20	0.08	0.00	-0.04	0.02
3	9	0.31	-0.18	-0.03	-0.17	0.10	0.08	-0.04	0.02	0.02
4	9	-0.31	-0.18	-0.03	0.17	0.10	0.08	0.04	0.02	0.02
5	13	0.00	0.00	0.31	0.00	0.00	0.29	0.00	0.00	-0.07
6	9	0.00	0.09	0.00	0.00	0.00	-0.43	0.00	0.57	0.00
7	9	0.08	-0.04	0.00	0.00	0.00	-0.43	0.49	-0.29	0.00
8	9	-0.08	-0.04	0.00	0.00	0.00	-0.43	-0.49	-0.29	0.00
9	9	0.00	0.36	0.03	0.00	0.20	0.08	0.00	-0.04	-0.02
10	9	0.31	-0.18	0.03	0.17	-0.10	0.08	-0.04	0.02	-0.02
11	9	-0.31	-0.18	0.03	-0.17	-0.10	0.08	0.04	0.02	-0.02

		22			23			24		
		A2"			E"			E"		
Frequencies --		546.8924			555.6838			555.6838		
Red. masses --		21.8752			22.4353			22.4353		
Frc consts --		3.8548			4.0817			4.0817		
IR Inten --		584.0190			0.0000			0.0000		
Raman Activ --		0.0000			0.6876			0.6876		
Depolar (P) --		0.7412			0.7500			0.7500		
Depolar (U) --		0.8514			0.8571			0.8571		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	13	0.00	0.00	0.42	-0.20	0.42	0.00	0.42	0.20	0.00
2	9	0.00	0.27	-0.18	0.01	-0.34	0.19	-0.02	-0.16	0.09
3	9	0.24	-0.14	-0.18	0.26	-0.17	-0.17	-0.20	0.09	0.12
4	9	-0.24	-0.14	-0.18	-0.02	-0.04	-0.02	-0.33	-0.19	-0.21
5	13	0.00	0.00	0.42	0.20	-0.42	0.00	-0.42	-0.20	0.00
6	9	0.00	0.00	-0.05	0.00	0.00	0.00	0.00	0.00	0.00
7	9	0.00	0.00	-0.05	0.00	0.00	0.00	0.00	0.00	0.00
8	9	0.00	0.00	-0.05	0.00	0.00	0.00	0.00	0.00	0.00
9	9	0.00	-0.27	-0.18	-0.01	0.34	0.19	0.02	0.16	0.09
10	9	-0.24	0.14	-0.18	-0.26	0.17	-0.17	0.20	-0.09	0.12
11	9	0.24	0.14	-0.18	0.02	0.04	-0.02	0.33	0.19	-0.21

		25			26			27		
		E'			E'			A1'		
Frequencies --		613.7478			613.7478			631.8033		
Red. masses --		23.6250			23.6250			23.4548		
Frc consts --		5.2433			5.2433			5.5163		
IR Inten --		559.1713			559.1713			0.0000		
Raman Activ --		0.1970			0.1972			4.2546		
Depolar (P) --		0.7500			0.7500			0.0001		
Depolar (U) --		0.8571			0.8571			0.0003		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	13	0.54	-0.03	0.00	0.03	0.54	0.00	0.00	0.00	0.53
2	9	-0.06	0.02	-0.01	0.00	-0.31	0.14	0.00	0.21	-0.17
3	9	-0.25	0.11	0.12	0.09	-0.12	-0.06	0.18	-0.10	-0.17
4	9	-0.24	-0.10	-0.11	-0.12	-0.13	-0.08	-0.18	-0.10	-0.17
5	13	0.54	-0.03	0.00	0.03	0.54	0.00	0.00	0.00	-0.53
6	9	-0.08	0.01	0.00	0.00	-0.20	0.00	0.00	-0.02	0.00
7	9	-0.17	0.06	0.00	0.04	-0.10	0.00	-0.02	0.01	0.00
8	9	-0.16	-0.04	0.00	-0.06	-0.11	0.00	0.02	0.01	0.00
9	9	-0.06	0.02	0.01	0.00	-0.31	-0.14	0.00	0.21	0.17
10	9	-0.25	0.11	-0.12	0.09	-0.12	0.06	0.18	-0.10	0.17
11	9	-0.24	-0.10	0.11	-0.12	-0.13	0.08	-0.18	-0.10	0.17

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