Supplementary Information

Planar Tetracoordinate Fluorine Atoms

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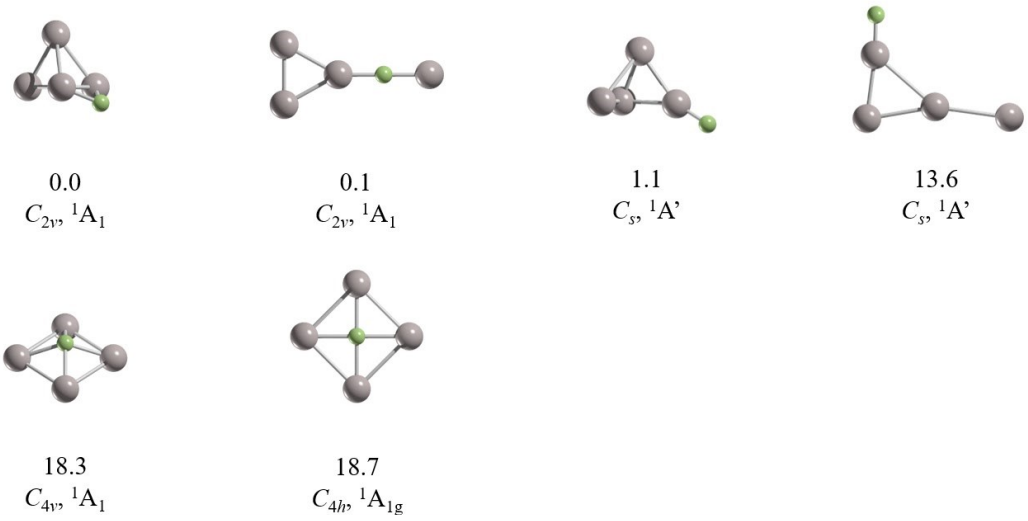


Figure S1. TPSS-D3(BJ)/def2-TZVP structures of the lowest-energy isomers of FAl_4^+. Relative energies in kcal/mol were computed at the CCSD(T)/def2-TZVP//TPSS-D3(BJ)/def2-TZVP level, including the ZPE correction at the TPSS-D3(BJ)/def2-TZVP level.

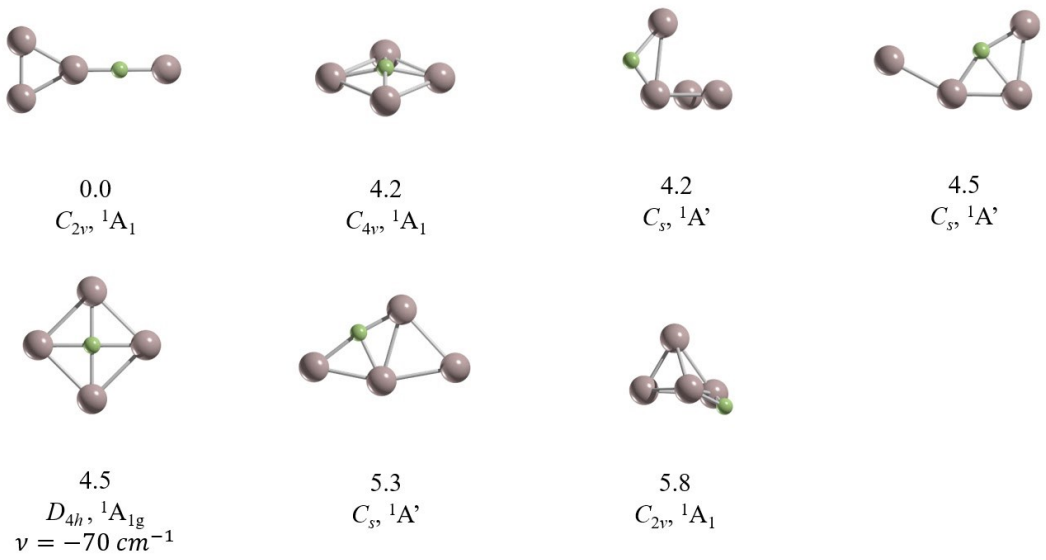
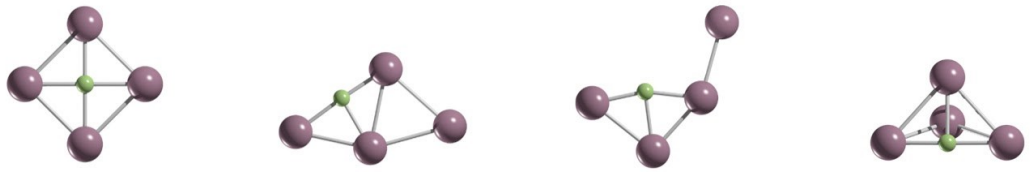


Figure S2. TPSS-D3(BJ)/def2-TZVP structures of the lowest-energy isomers of FGa_4^+. Relative energies in kcal/mol were computed at the CCSD(T)/def2-TZVP//TPSS-D3(BJ)/def2-TZVP level, including the ZPE correction at the TPSS-D3(BJ)/def2-TZVP level.



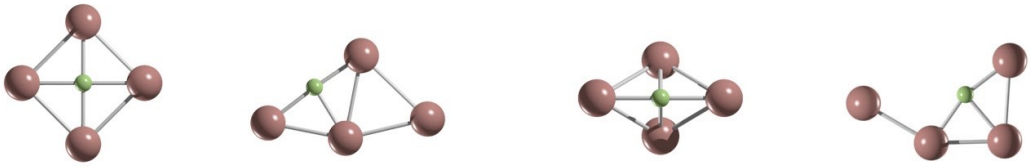
0.0
D_{4h}, $^1A_{1g}$

5.7
C_s, $^1A'$

7.9
C_s, $^1A'$

9.8
C_{2v}, $^1A_1$

Figure S3. TPSS-D3(BJ)/def2-TZVP structures of the lowest-energy isomers of FIn_4^+. Relative energies in kcal/mol were computed at the CCSD(T)/def2-TZVP//TPSS-D3(BJ)/def2-TZVP level, including the ZPE correction at the TPSS-D3(BJ)/def2-TZVP level.



0.0
D_{4h}, $^1A_{1g}$

5.1
C_s, $^1A'$
$\nu = -6cm^{-1}$

6.3
C_{2v}, $^1A_1$

8.7
C_s, $^1A'$

Figure S4. TPSS-D3(BJ)/def2-TZVP structures of the lowest-energy isomers of FTl_4^+. Relative energies in kcal/mol were computed at the CCSD(T)/def2-TZVP//TPSS-D3(BJ)/def2-TZVP level, including the ZPE correction at the TPSS-D3(BJ)/def2-TZVP level.

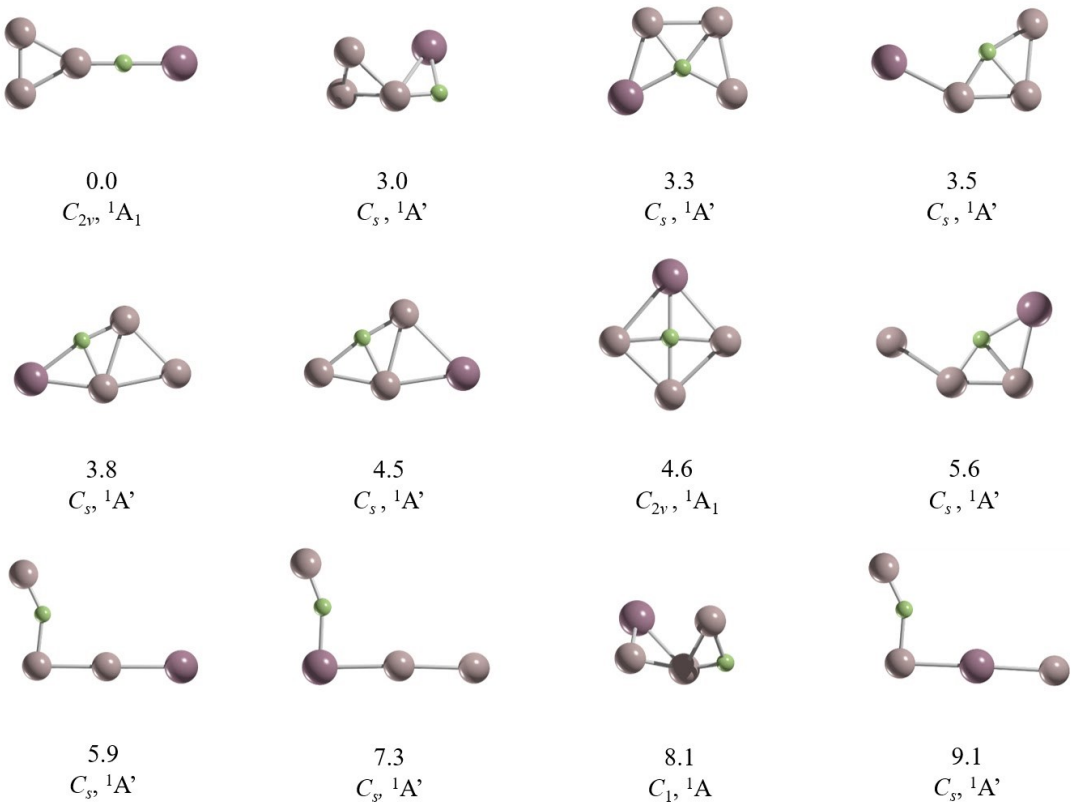


Figure S5. TPSS-D3(BJ)/def2-TZVP structures of the lowest-energy isomers of FGa_3In^+. Relative energies in kcal/mol were computed at the CCSD(T)/def2-TZVP//TPSS-D3(BJ)/def2-TZVP level, including the ZPE correction at the TPSS-D3(BJ)/def2-TZVP level.

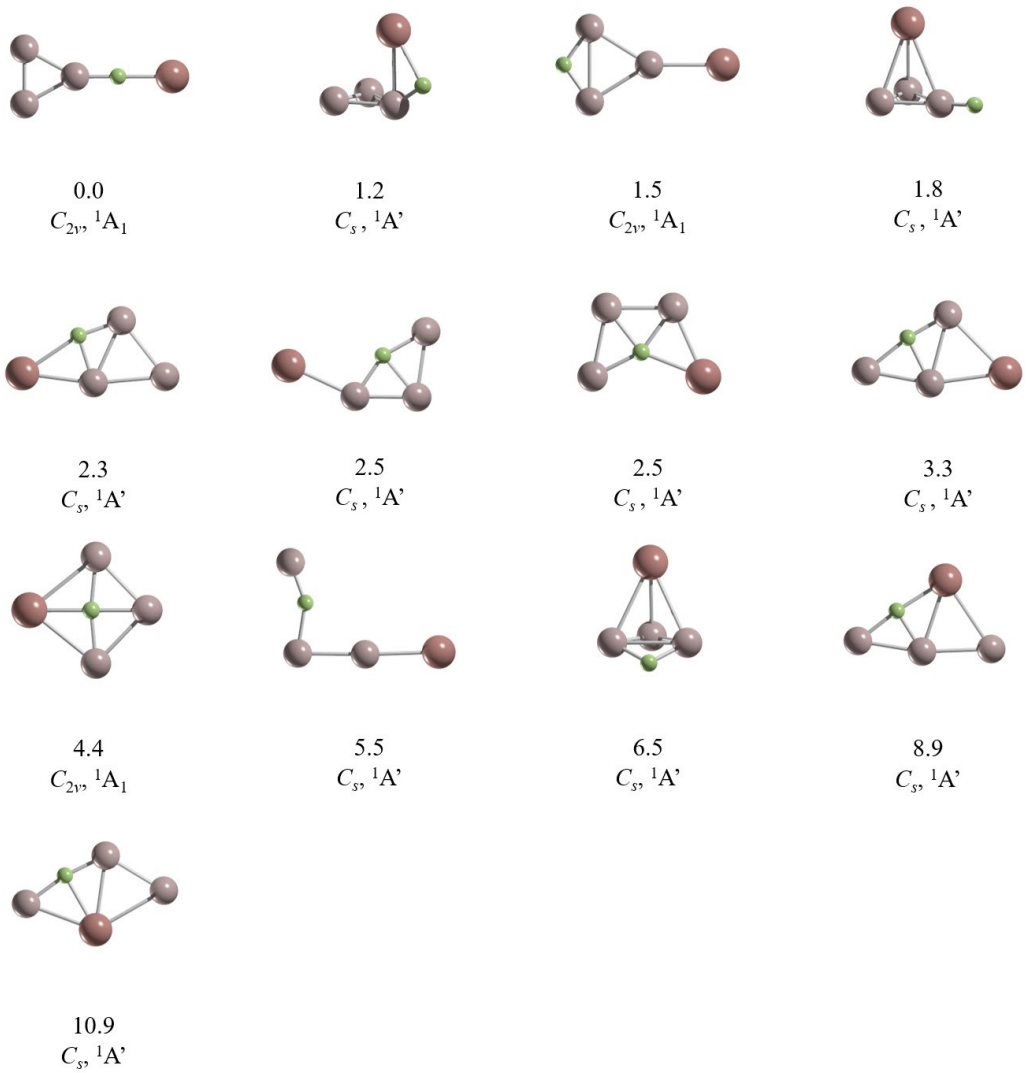


Figure S6. TPSS-D3(BJ)/def2-TZVP structures of the lowest-energy isomers of FGa_3Tl^+. Relative energies in kcal/mol were computed at the CCSD(T)/def2-TZVP//TPSS-D3(BJ)/def2-TZVP level, including the ZPE correction at the TPSS-D3(BJ)/def2-TZVP level.

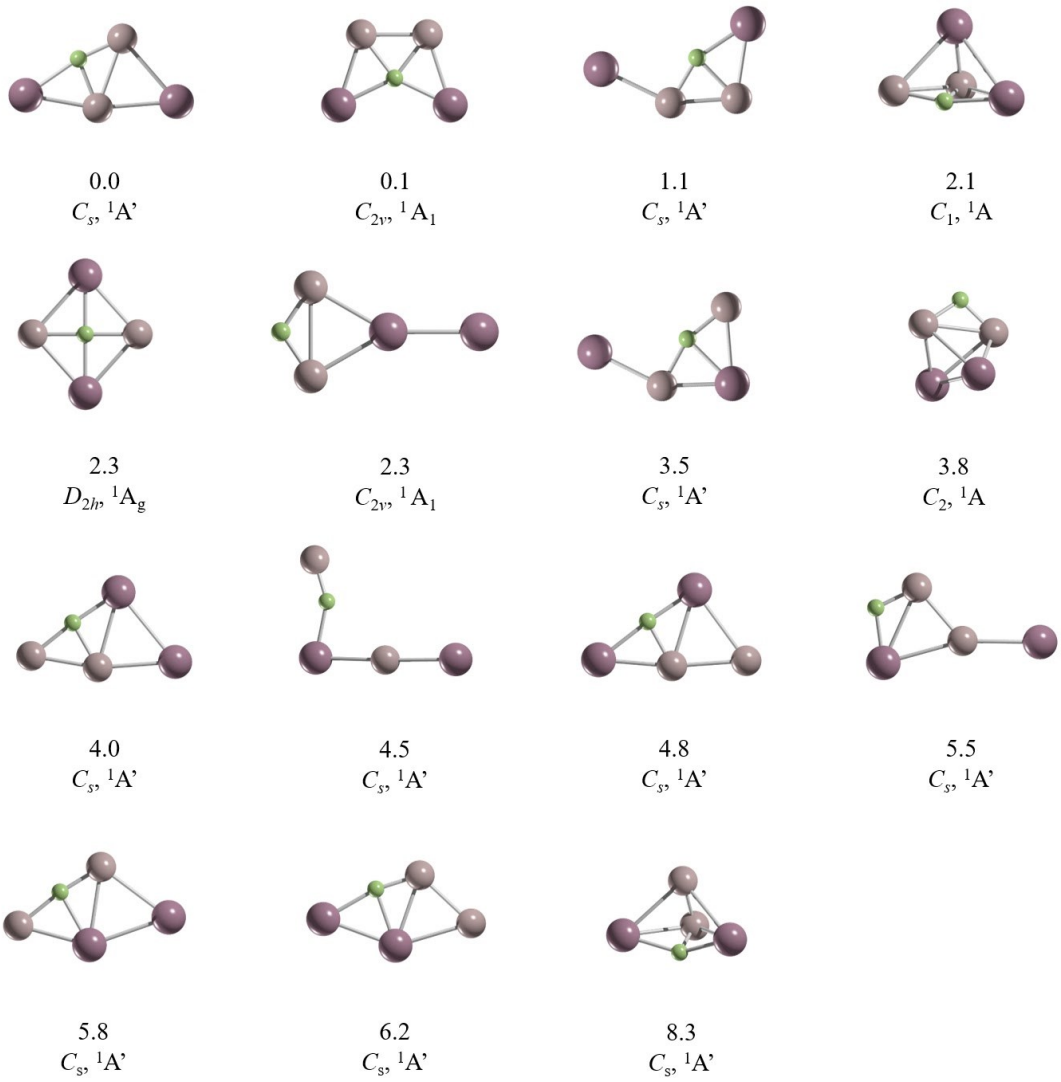


Figure S7. TPSS-D3(BJ)/def2-TZVP structures of the lowest-energy isomers of $FGa_2In_2^+$. Relative energies in kcal/mol were computed at the CCSD(T)/def2-TZVP//TPSS-D3(BJ)/def2-TZVP level, including the ZPE correction at the TPSS-D3(BJ)/def2-TZVP level.

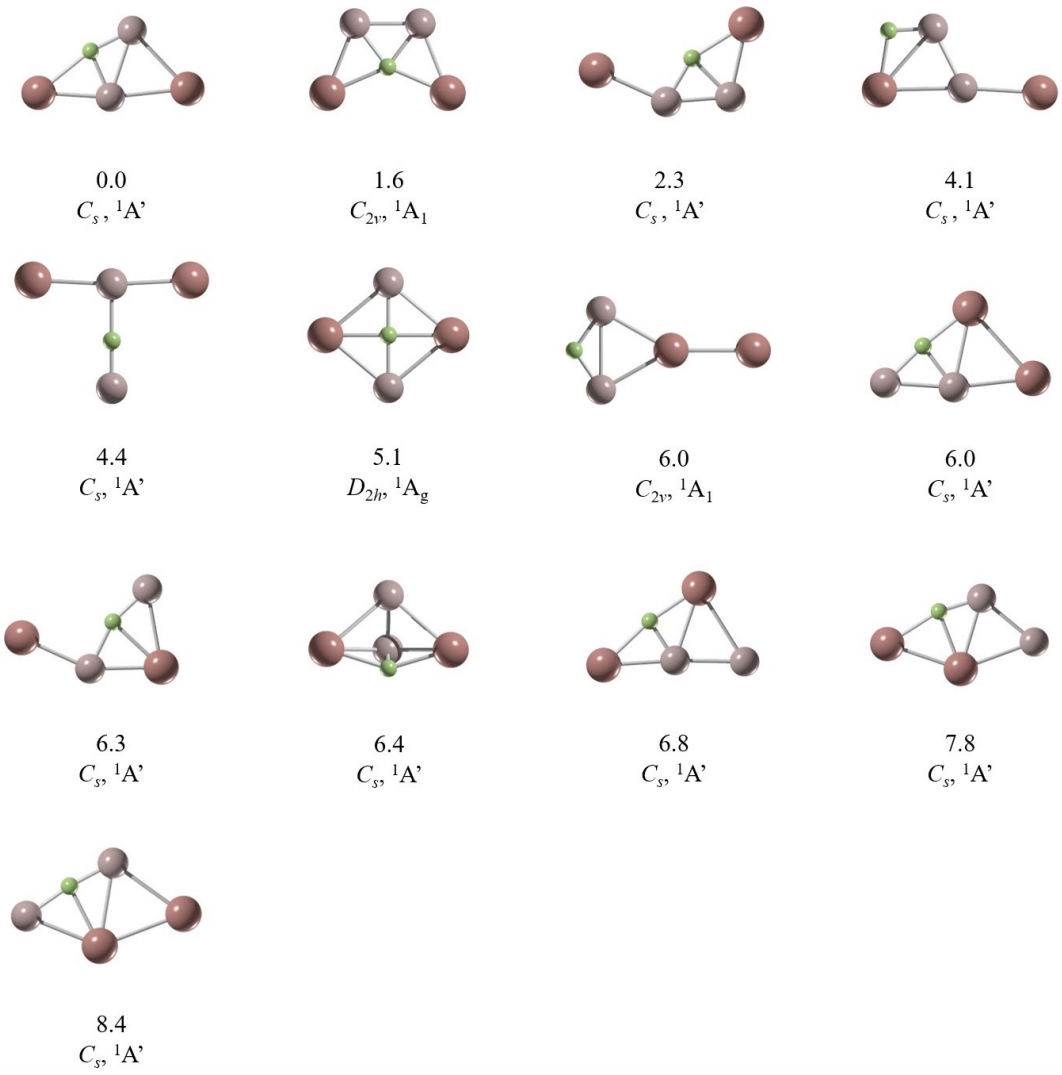


Figure S8. TPSS-D3(BJ)/def2-TZVP structures of the lowest-energy isomers of $FGa_2Tl_2^+$. Relative energies in kcal/mol were computed at the CCSD(T)/def2-TZVP//TPSS-D3(BJ)/def2-TZVP level, including the ZPE correction at the TPSS-D3(BJ)/def2-TZVP level.

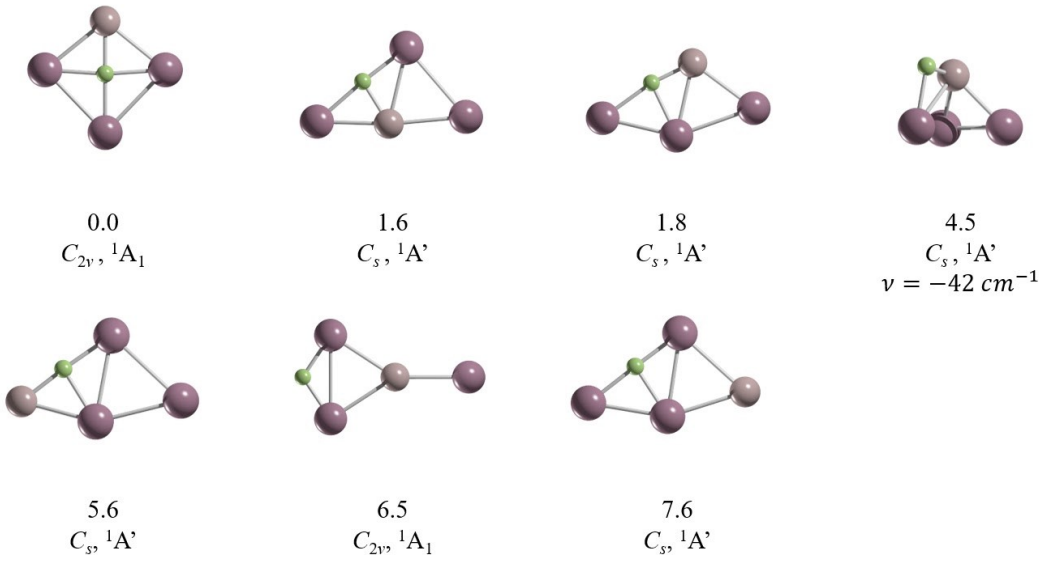


Figure S9. TPSS-D3(BJ)/def2-TZVP structures of the lowest-energy isomers of $FGaIn_3^+$. Relative energies in kcal/mol were computed at the CCSD(T)/def2-TZVP//TPSS-D3(BJ)/def2-TZVP level, including the ZPE correction at the TPSS-D3(BJ)/def2-TZVP level.

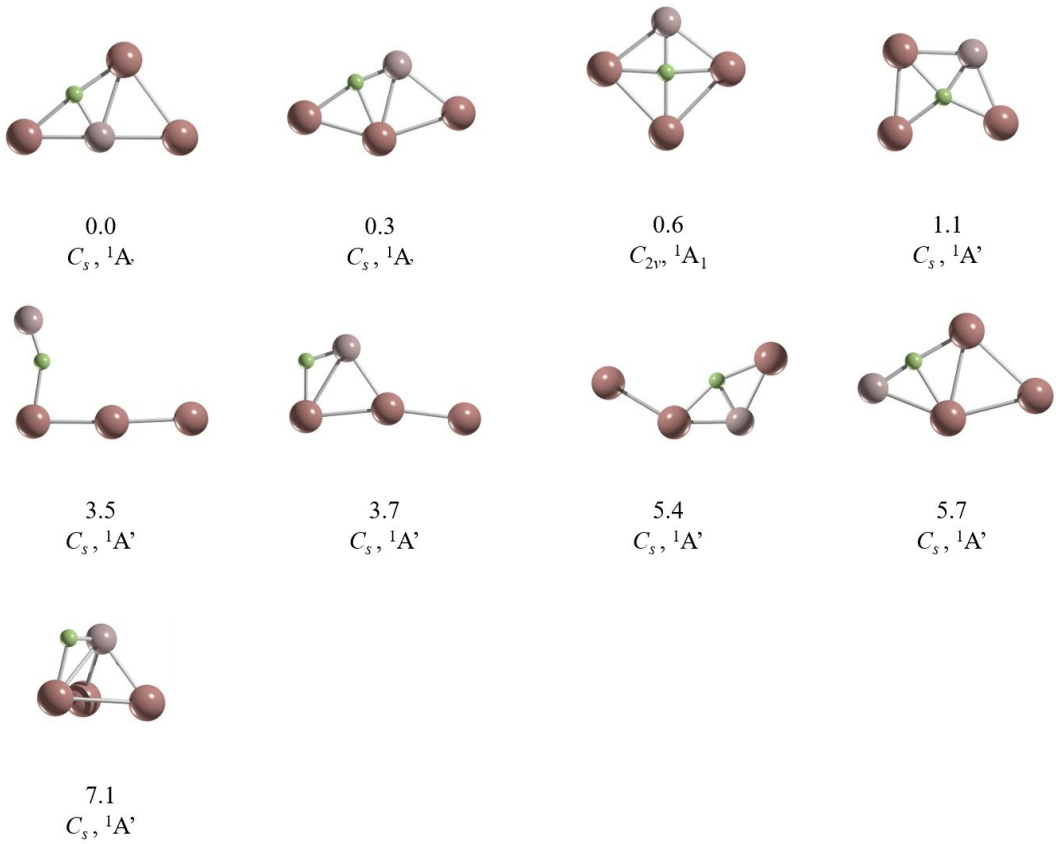


Figure S10. TPSS-D3(BJ)/def2-TZVP structures of the lowest-energy isomers of $FGaTl_3^+$. Relative energies in kcal/mol were computed at the CCSD(T)/def2-TZVP//TPSS-D3(BJ)/def2-TZVP level, including the ZPE correction at the TPSS-D3(BJ)/def2-TZVP level.

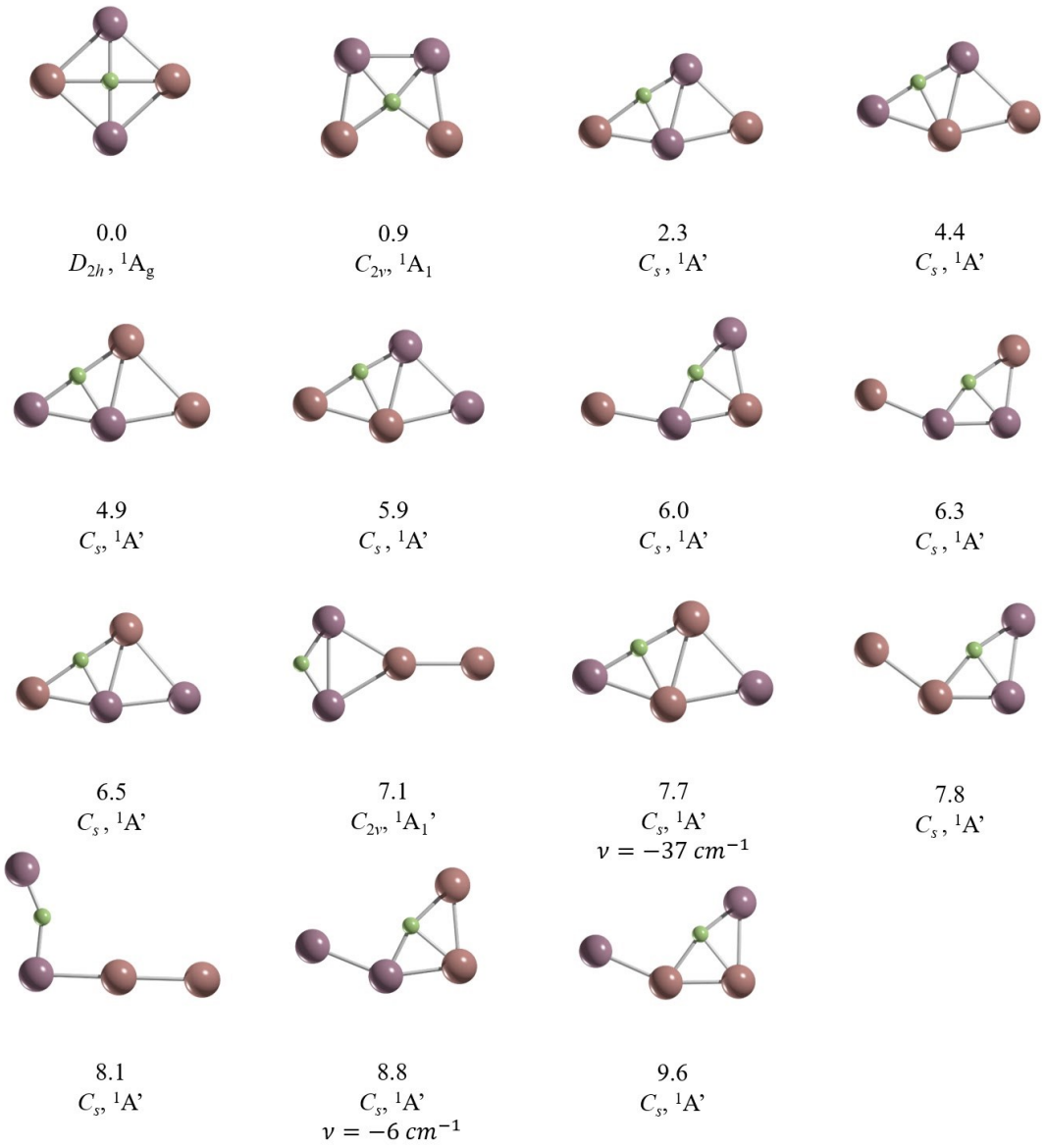


Figure S11. TPSS-D3(BJ)/def2-TZVP structures of the lowest-energy isomers of $FIn_2Tl_2^+$. Relative energies in kcal/mol were computed at the CCSD(T)/def2-TZVP//TPSS-D3(BJ)/def2-TZVP level, including the ZPE correction at the TPSS-D3(BJ)/def2-TZVP level.

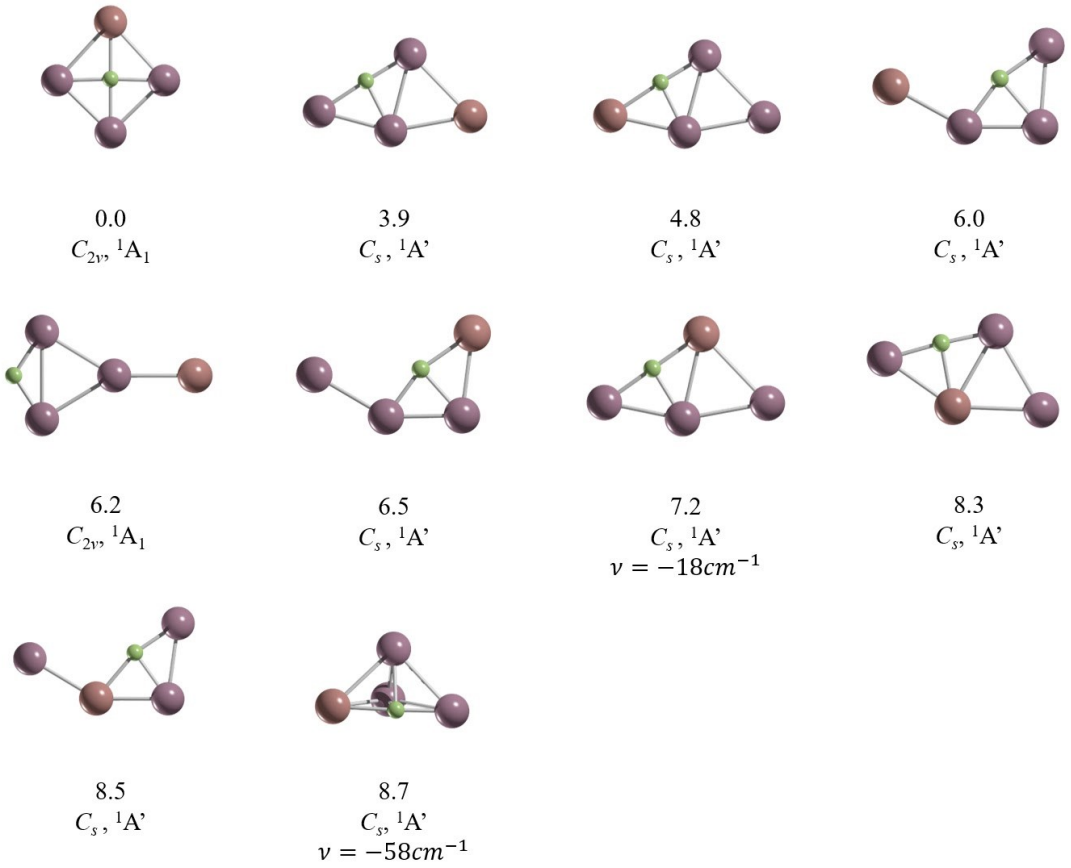


Figure S12. TPSS-D3(BJ)/def2-TZVP structures of the lowest-energy isomers of FIn_3Tl^+. Relative energies in kcal/mol were computed at the CCSD(T)/def2-TZVP//TPSS-D3(BJ)/def2-TZVP level, including the ZPE correction at the TPSS-D3(BJ)/def2-TZVP level.

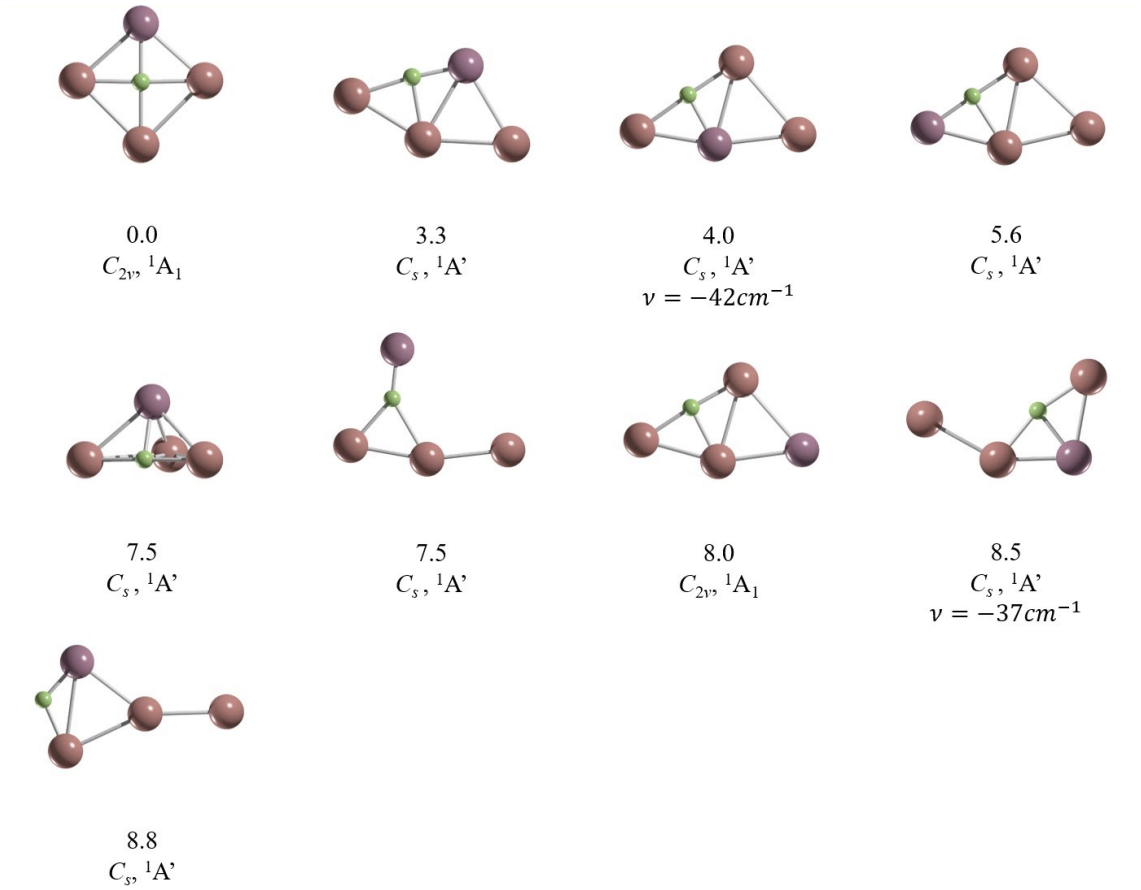


Figure S13. TPSS-D3(BJ)/def2-TZVP structures of the lowest-energy isomers of $FInTl_3^+$. Relative energies in kcal/mol were computed at the CCSD(T)/def2-TZVP//TPSS-D3(BJ)/def2-TZVP level, including the ZPE correction at the TPSS-D3(BJ)/def2-TZVP level.

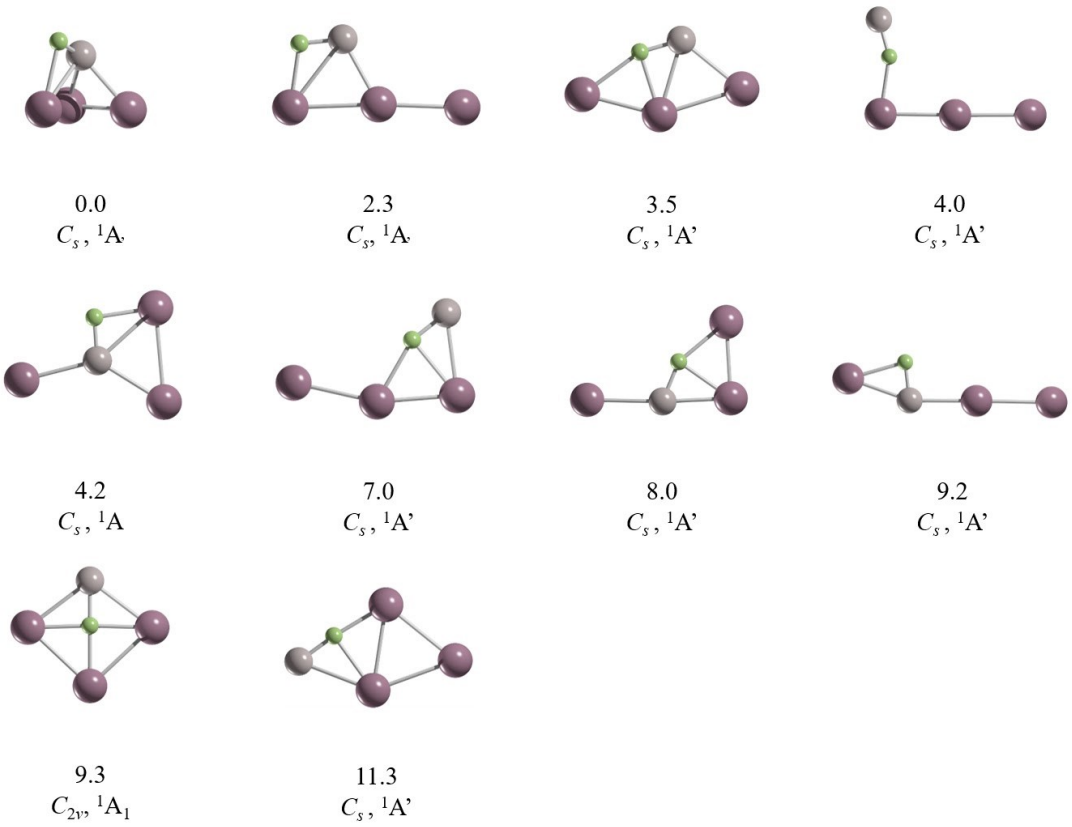


Figure S14. TPSS-D3(BJ)/def2-TZVP structures of the lowest-energy isomers of FIn_3Al^+. Relative energies in kcal/mol were computed at the CCSD(T)/def2-TZVP//TPSS-D3(BJ)/def2-TZVP level, including the ZPE correction at the TPSS-D3(BJ)/def2-TZVP level.

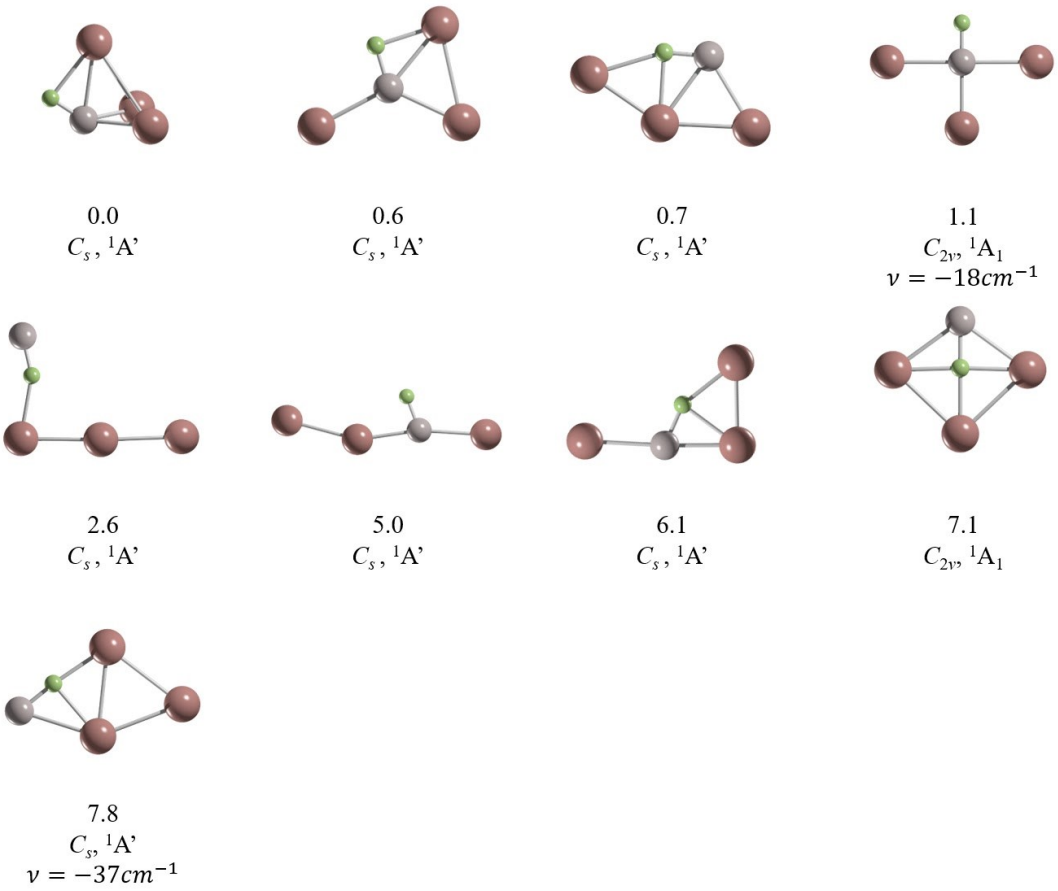


Figure S15. TPSS-D3(BJ)/def2-TZVP structures of the lowest-energy isomers of FTl_3Al^+. Relative energies in kcal/mol were computed at the CCSD(T)/def2-TZVP//TPSS-D3(BJ)/def2-TZVP level, including the ZPE correction at the TPSS-D3(BJ)/def2-TZVP level.

Table S1. First AdNDP solution for CAl_4^{2-}, NAl_4^-, OAl_4, and FAl_4^+. The values indicate occupation number.

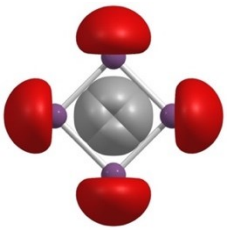
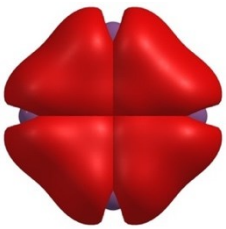
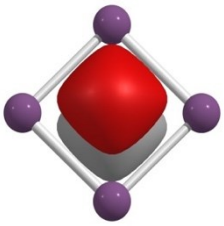
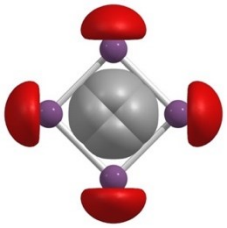
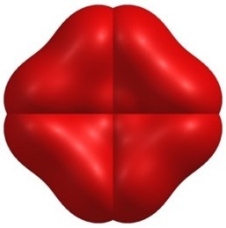
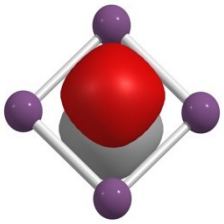
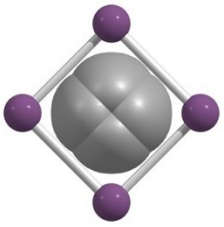
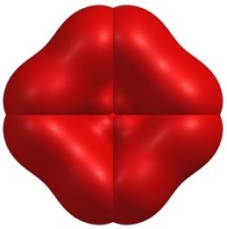
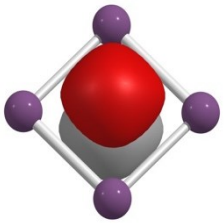
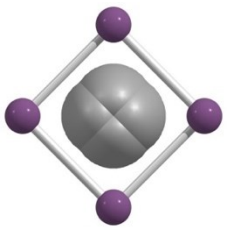
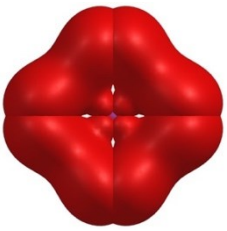
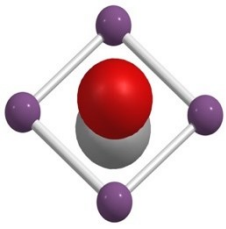
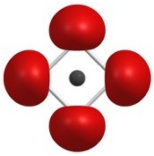
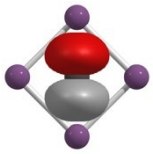
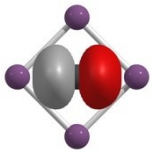
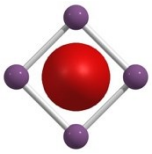
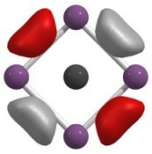
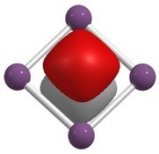
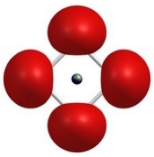
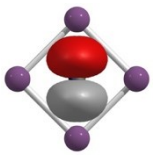
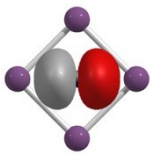
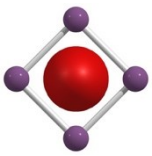
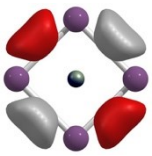
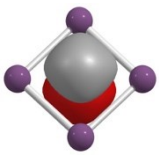
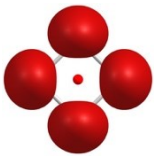
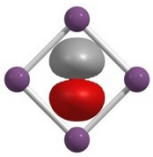
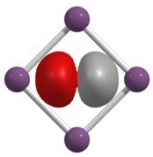
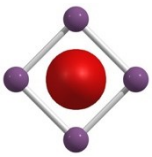
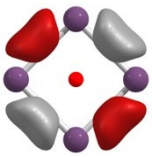
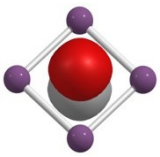
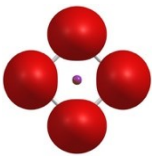
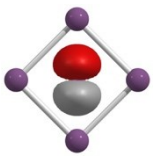
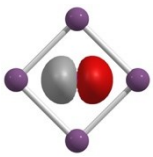
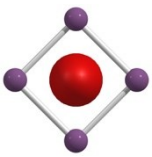
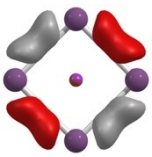
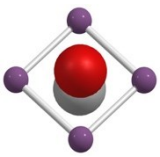
	4 x 2c-2e Center-Al σ-bonds	4 x 3c-2e Center-Al-Al σ-bonds	π-bond
CAl_4^{2-}			
	1.96	1.95	2.00
NAl_4^-			
	1.98	1.97	2.00
OAl_4			
	1.98	1.97	2.00
FAl_4^+			
	1.99	1.98	2.00

Table S2. Second AdNDP solution for CAl_4^{2-}, NAl_4^-, OAl_4, and FAl_4^+. The values indicate occupation number.

	4 x 1c-2e LP Al	1c-2e Central atom			4c-2e Al_4 σ-bond	π-bond
CAl_4^{2-}						
	1.88	1.72	1.72	1.57	2.00	2.00
NAl_4^-						
	1.84	1.82	1.82	1.77	2.00	2.00
OAl_4						
	1.83	1.90	1.90	1.89	2.00	2.00
FAl_4^+						
	1.87	1.94	1.94	1.95	2.00	2.00

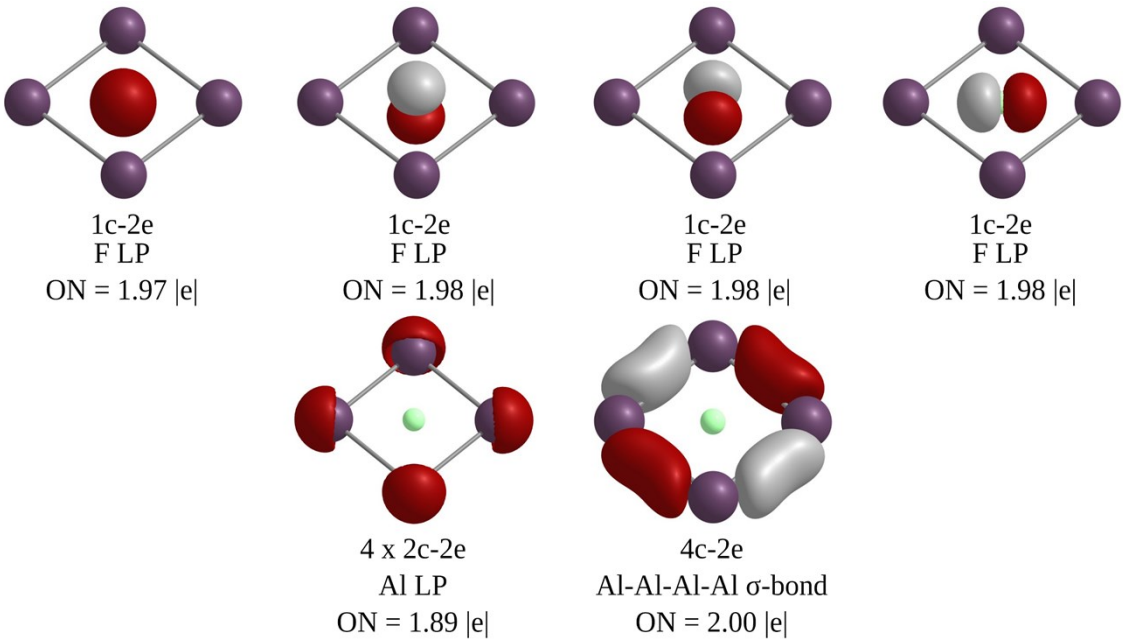


Figure S16. Second AdNDP solution for FAl_4^+. ON stands for occupation number.

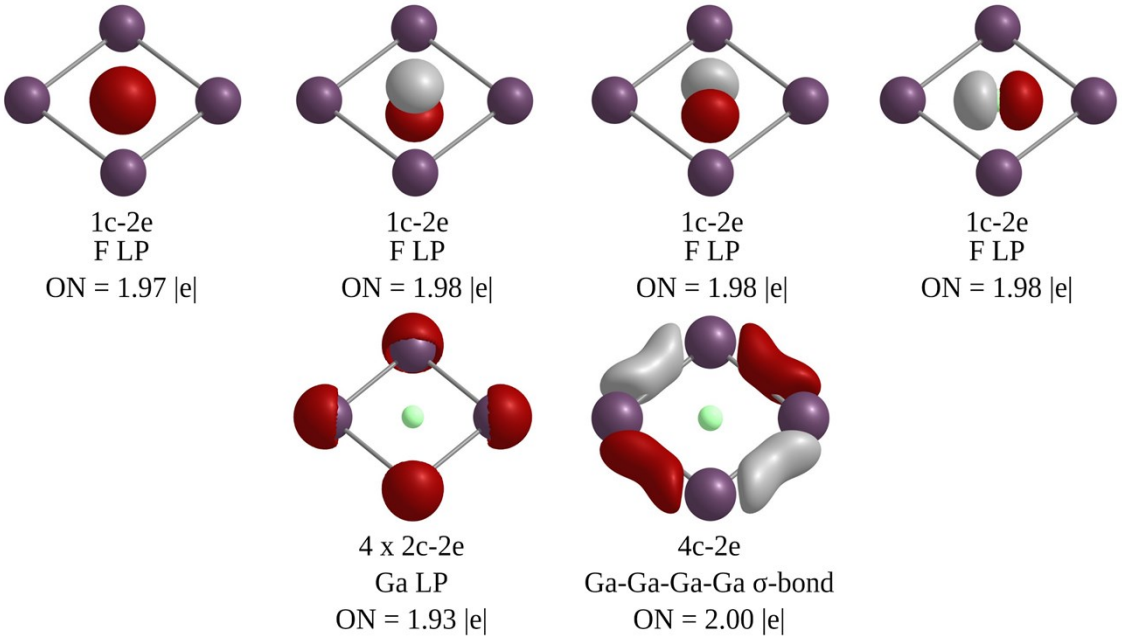


Figure S17. Second AdNDP solution for FGa_4^+. ON stands for occupation number.

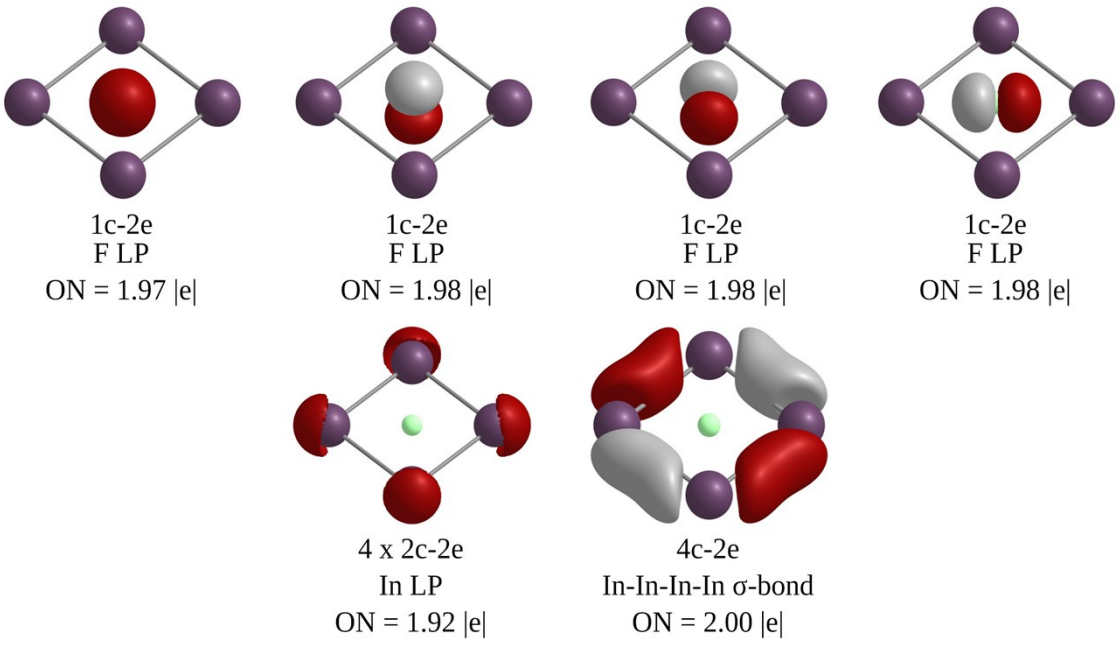


Figure S18. Second AdNDP solution for FIn_4^+. ON stands for occupation number.

Molecular coordinates Figure S1

1 FAl_4^+

Al	0.000000000	-1.386158000	-0.687485241
F	0.000000000	0.000000000	-1.934328241
Al	-1.267410000	0.000000000	1.368490759
Al	0.000000000	1.386158000	-0.687485241
Al	1.267410000	0.000000000	1.368490759

2 FAl_4^+

Al	0.000000000	0.000000000	0.134401931
Al	1.228210000	0.000000000	2.341816931
Al	0.000000000	0.000000000	-3.599763069
Al	-1.228210000	0.000000000	2.341816931
F	0.000000000	0.000000000	-1.730191069

3 FAl_4^+

Al	0.660149000	1.132280000	0.000000000
Al	0.660149000	-1.175465000	1.214310000
F	0.556969000	2.773065000	0.000000000
Al	-2.366040000	-0.701163000	0.000000000
Al	0.660149000	-1.175465000	-1.214310000

4 FAl_4^+

Al	-1.150666096	-2.064627668	0.000000000
Al	1.116419695	-0.361641339	0.000000000
Al	-2.050366393	0.428084971	0.000000000
F	-2.774410313	1.910230486	0.000000000
Al	4.038147560	0.653140857	0.000000000

5 FAl_4^+

Al	0.000000000	2.051350000	-0.121974000
F	0.000000000	0.000000000	0.704741000
Al	-2.051350000	0.000000000	-0.121974000
Al	2.051350000	0.000000000	-0.121974000
Al	0.000000000	-2.051350000	-0.121974000

6 FAl_4^+

Al	0.000000000	2.214294000	0.000000000
F	0.000000000	0.000000000	0.000000000
Al	2.214294000	0.000000000	0.000000000
Al	-2.214294000	0.000000000	0.000000000
Al	0.000000000	-2.214294000	0.000000000

Molecular coordinates Figure S2

1 FGa_4^+

Ga	0.000000000	0.000000000	-0.025910000
Ga	0.000000000	1.224216000	-2.238755000
Ga	0.000000000	0.000000000	3.938604000
Ga	0.000000000	-1.224216000	-2.238755000
F	0.000000000	0.000000000	1.945480000

2 FGa_4^+

Ga	0.000000000	2.204034000	-0.034393000
F	0.000000000	0.000000000	0.473860000
Ga	2.204034000	0.000000000	-0.034393000
Ga	-2.204034000	0.000000000	-0.034393000
Ga	0.000000000	-2.204034000	-0.034393000

3 FGa_4^+

Ga	-0.802199000	1.085260000	0.000000000

Ga	2.219180000	0.713562000	0.000000000
Ga	-0.802199000	-1.227805000	1.236205000
F	0.645547000	2.262273000	0.000000000
Ga	-0.802199000	-1.227805000	-1.236205000

4 FGa_4^+

F	0.000000000	0.802971000	0.000000000
Ga	-1.048708000	2.634300000	0.000000000
Ga	0.153266000	-1.359941000	0.000000000
Ga	-2.207853000	-0.048634000	0.000000000
Ga	3.103295000	-1.458846000	0.000000000

5 FGa_4^+

Ga	0.000000000	2.238115000	0.000000000
Ga	2.238115000	0.000000000	0.000000000
Ga	0.000000000	-2.238115000	0.000000000
Ga	-2.238115000	0.000000000	0.000000000
F	0.000000000	0.000000000	0.000000000

6 FGa_4^+

F	-1.284963000	-0.707265000	0.000000000
Ga	0.313512000	-1.961346000	0.000000000
Ga	0.000000000	1.105242000	0.000000000
Ga	-2.864095000	1.027025000	0.000000000
Ga	2.923637000	0.034414000	0.000000000

7 FGa_4^+

Ga	0.000000000	1.543673000	0.967465000
F	0.000000000	0.000000000	2.214239000
Ga	-1.298455000	0.000000000	-1.288887000

Ga	0.000000000	-1.543673000	0.967465000
Ga	1.298455000	0.000000000	-1.288887000

Molecular coordinates Figure S3

1 FIn_4^+

1.96

2 FIn_4^+

In	3.237975708	-0.355377906	0.000000000
In	-0.157611184	-1.283640087	0.000000000
In	-3.333789452	-0.598254567	0.000000000
F	-1.376796862	0.841135022	0.000000000
In	0.506305782	2.082778562	0.000000000

3 FIn_4^+

F	-0.887180116	0.077618203	0.000000000
In	1.482749421	-0.182419288	0.000000000
In	-3.124374552	-0.402513501	0.000000000
In	2.359770467	3.007223847	0.000000000
In	-0.555193872	-2.436548468	0.000000000

4 FIn_4^+

F	-0.000000001	0.000000000	-1.105734105
In	-0.000000001	-2.390112000	-1.086976105
In	-1.424213999	0.000000000	1.178387896
In	1.424214000	0.000000000	1.178387894
In	-0.000000001	2.390112000	-1.086976105

Molecular coordinates Figure S4

1 FTl_4^+

F	0.000000000	0.000000000	0.000000000
Tl	0.000000000	2.532739000	0.000000000
Tl	2.532739000	0.000000000	0.000000000
Tl	0.000000000	-2.532739000	0.000000000
Tl	-2.532739000	0.000000000	0.000000000

2 FTl_4^+

Tl	-0.176775864	-1.257825627	0.000000000
F	-1.485611485	0.889707732	0.000000000
Tl	0.496795793	2.223935577	0.000000000
Tl	3.288604342	-0.448068839	0.000000000
Tl	-3.443556091	-0.616898232	0.000000000

3 FTl_4^+

Tl	0.000000000	1.481668000	-1.142513000
Tl	0.000000000	-1.481668000	-1.142513000
F	0.000000000	0.000000000	1.111440000
Tl	2.497594000	0.000000000	1.080766000
Tl	-2.497594000	0.000000000	1.080766000

4 FTl_4^+

F	-0.881493542	0.155431094	0.000000000
Tl	1.573792322	-0.352489273	0.000000000
Tl	-0.752105706	-2.427641545	0.000000000
Tl	2.519534866	2.846263500	0.000000000
Tl	-3.243277427	-0.083402863	0.000000000

Molecular coordinates Figure S5

1 FGa_3In^+

Ga	-0.556805000	0.000000000	0.000000000

Ga	-2.772372000	1.218446000	0.000000000
F	1.359833000	0.000000000	0.000000000
In	3.610398000	0.000000000	0.000000000
Ga	-2.772372000	-1.218446000	0.000000000

2 FGa_3In^+

Ga	-0.306554575	1.406442170	-0.000000001
In	2.064693909	-0.727231147	0.000000001
Ga	-1.773487232	-0.337377157	1.227903000
Ga	-1.773487232	-0.337377159	-1.227903000
F	1.493041049	1.743817530	-0.000000001

3 FGa_3In^+

F	0.328648049	-0.153251102	0.000000000
Ga	1.713743960	1.674003609	0.000000000
In	-1.938069158	-1.324947880	0.000000000
Ga	-1.057722667	1.650571623	0.000000000
Ga	2.311963478	-1.185811268	0.000000000

4 FGa_3In^+

F	0.676423400	0.806130017	0.000000000
Ga	-0.073465817	-1.230333424	0.000000000
Ga	2.224667363	2.269045092	0.000000000
In	-3.101399676	-0.421580913	0.000000000
Ga	2.554628414	-0.606379298	0.000000000

5 FGa_3In^+

F	-0.679030439	1.051415088	0.000000000
Ga	1.123044797	1.896793814	0.000000000
Ga	0.223241652	-0.966965827	0.000000000

Ga	3.281899755	-0.335712480	0.000000000
In	-2.803315819	-0.568985922	0.000000000

6 FGa_3In^+

Ga	-0.583012000	-1.009806405	0.000000000
F	-1.567414971	0.990957634	0.000000000
Ga	0.192934730	2.001290756	0.000000000
Ga	-3.392017106	-0.470413968	0.000000000
In	2.680645646	-0.511669544	0.000000000

7 FGa_3In^+

F	0.000000000	-0.262878000	0.000000000
Ga	0.000000000	-2.546314000	0.000000000
In	0.000000000	2.181585000	0.000000000
Ga	-2.224254000	-0.412840000	0.000000000
Ga	2.224254000	-0.412840000	0.000000000

8 FGa_3In^+

F	0.000000000	0.342829000	0.000000000
In	-2.138547000	1.567396000	0.000000000
Ga	1.205884000	-1.391028000	0.000000000
Ga	3.636968000	0.234164000	0.000000000
Ga	-1.462567000	-1.420163000	0.000000000

9 FGa_3In^+

Ga	-2.525073065	-0.925570411	0.000000000
Ga	0.466419010	-0.956300687	0.000000000
F	-2.276851079	1.305102305	0.000000000
Ga	-3.096309839	3.022363261	0.000000000
In	3.679501232	-0.961248941	0.000000000

10 FGa_3In^+

In	-1.827133090	-1.014948957	0.000000000
Ga	1.373373115	-0.961646208	0.000000000
F	-1.719227378	1.433839201	0.000000000
Ga	-2.393120364	3.197817144	0.000000000
Ga	4.406927086	-1.048173583	0.000000000

11 FGa_3In^+

Ga	0.743543301	-1.159566343	-0.546723762
Ga	-1.417536288	-0.729152136	0.871277115
In	-1.146467467	0.878976682	-1.260012465
Ga	1.789501552	0.763814985	1.581528397
F	2.399570247	-0.910868945	0.294677456

12 FGa_3In^+

Ga	-2.211502621	-0.841289485	0.000000000
In	0.961254393	-0.961254393	0.000000000
F	-2.037346464	1.390232036	0.000000000
Ga	-2.866016921	3.104299179	0.000000000
Ga	4.149605234	-1.147222770	0.000000000

Molecular coordinates Figure S6

1 FGa_3Tl^+

F	0.654327000	0.000000000	0.000000000
Tl	3.042980000	0.000000000	0.000000000
Ga	-3.452632000	1.215173000	0.000000000
Ga	-3.452632000	-1.215173000	0.000000000
Ga	-1.235714000	0.000000000	0.000000000

2 FGa_3Tl^+

Ga	1.271925943	1.205063687	0.000000000
Tl	-1.732032012	0.035121093	0.000000000
Ga	1.966726379	-0.966985065	-1.224186000
Ga	1.966726380	-0.966985063	1.224186000
F	-0.198024486	2.265530869	-0.000000002

3 FGa_3Tl^+

Ga	-2.989455000	1.632134000	0.000000000
Tl	2.889552000	0.000000000	0.000000000
Ga	-0.368970000	0.000000000	0.000000000
F	-4.141047000	0.000000000	0.000000000
Ga	-2.989455000	-1.632134000	0.000000000

4 FGa_3Tl^+

Ga	1.890725640	1.073200491	0.000000000
Ga	1.392120946	-1.165116120	1.209397000
Ga	1.392120947	-1.165116121	-1.209397000
Tl	-1.765977092	0.162022162	0.000000000
F	2.092528067	2.812415674	0.000000000

5 FGa_3Tl^+

Ga	0.663748914	-0.791025152	0.000000000
Ga	3.768788637	-0.518338543	0.000000000
F	0.012907068	1.270671058	0.000000000
Tl	-2.417728896	-0.376230361	0.000000000
Ga	1.881007197	1.923513881	0.000000000

6 FGa_3Tl^+

F	1.516312076	0.452912775	0.000000000

Ga	0.102697093	-1.173833148	0.000000000
Ga	3.496868520	1.268007324	0.000000000
Ga	2.774581153	-1.521414761	0.000000000
Tl	-2.607966963	0.495903766	0.000000000

7 FGa_3Tl^+

F	-0.781884000	0.000000000	0.000000000
Tl	1.784104000	-1.013166000	0.000000000
Ga	0.536144000	1.827944000	0.000000000
Ga	-2.196832000	1.824761000	0.000000000
Ga	-2.774004000	-1.005401000	0.000000000

8 FGa_3Tl^+

Ga	-3.872558064	-0.363265270	0.000000000
F	-2.051178925	1.106659815	0.000000000
Ga	-0.288592513	2.111295660	0.000000000
Tl	2.229442086	-0.448774551	0.000000000
Ga	-1.068662640	-0.896714427	0.000000000

9 FGa_3Tl^+

F	0.000000000	0.000000000	0.778643670
Tl	0.000000000	0.000000000	-1.764600330
Ga	2.199266000	0.000000000	0.973766670
Ga	0.000000000	0.000000000	3.085493670
Ga	-2.199266000	0.000000000	0.973766670

10 FGa_3Tl^+

Ga	-2.925828637	-1.899031659	0.000000000
Ga	-0.118197988	-0.901767544	0.000000000
F	-3.383830745	0.312441109	0.000000000

Ga	-4.614044726	1.761139475	0.000000000
Tl	2.888776835	0.320641960	0.000000000

11 FGa_3Tl^+

Ga	1.563720777	-0.656148645	-1.568590999
Ga	1.420392366	1.499354123	-0.000000005
Ga	1.563720778	-0.656148639	1.568591002
Tl	-1.748132800	0.084766016	0.000000000
F	2.361242807	-1.593180842	0.000000002

12 FGa_3Tl^+

Ga	-1.085962256	-1.364030117	0.000000000
F	-1.419866321	0.732892661	0.000000000
Tl	1.081752713	1.156803100	0.000000000
Ga	-3.513072584	0.165653002	0.000000000
Ga	1.773435318	-2.443788423	0.000000000

13 FGa_3Tl^+

Ga	3.020480000	0.570294000	0.000000000
Tl	0.000000000	-1.163537000	0.000000000
Ga	0.447103000	2.126657000	0.000000000
F	-1.354584000	1.242261000	0.000000000
Ga	-3.074316000	-0.017398000	0.000000000

Molecular coordinates Figure S7

1 $FGa_2In_2^+$

Ga	0.000000000	0.899578000	0.000000000
In	3.115006000	-0.210764000	0.000000000

In	-3.032247000	1.164592000	0.000000000
F	-1.297186000	-0.867848000	0.000000000
Ga	0.245790000	-2.155286000	0.000000000

2 $FGa_2In_2^+$

In	-2.301171000	-1.127916000	0.000000000
Ga	1.366719000	1.785803000	0.000000000
In	2.301171000	-1.127916000	0.000000000
F	0.000000000	-0.020444000	0.000000000
Ga	-1.366719000	1.785803000	0.000000000

3 $FGa_2In_2^+$

Ga	1.426959000	-0.686826000	0.000000000
In	2.676136999	2.169973001	0.000000000
In	-3.021637000	-0.291165000	0.000000000
F	-0.570458000	0.000000000	0.000000000
Ga	-0.715229000	-2.282903000	0.000000000

4 $FGa_2In_2^+$

Ga	0.074251184	-0.489636643	-1.524026120
In	-0.181303256	1.912720380	-0.350416260
In	1.885086673	-0.975617083	1.152583607
Ga	-2.596090693	-0.672479352	0.098054680
F	-0.589817636	-1.099163476	0.544329306

5 $FGa_2In_2^+$

Ga	-2.216701000	0.000000000	0.000000000
Ga	2.216701000	0.000000000	0.000000000
F	0.000000000	0.000000000	0.000000000
In	0.000000000	-2.485209000	0.000000000

In	0.000000000	2.485209000	0.000000000

6 $FGa_2In_2^+$

Ga	-2.594788000	1.662582000	0.000000000
In	3.678239000	0.000000000	0.000000000
In	0.285598000	0.000000000	0.000000000
Ga	-2.594788000	-1.662582000	0.000000000
F	-3.705691000	0.000000000	0.000000000

7 $FGa_2In_2^+$

F	0.458874643	-0.829767717	0.000000000
Ga	2.014929422	-2.165917071	0.000000000
Ga	-0.525550715	1.123575792	0.000000000
In	2.381403375	0.975168896	0.000000000
In	-3.350684315	-0.212721244	0.000000000

8 $FGa_2In_2^+$

Ga	0.395085427	1.520654973	1.244314874
In	1.834669661	-0.081846402	-0.950941126
F	0.000000000	0.000000000	2.474077874
In	-1.834669661	0.081846402	-0.950941126
Ga	-0.395085427	-1.520654973	1.244314874

9 $FGa_2In_2^+$

In	2.642903583	-0.949954541	0.000000000
In	0.248526625	2.012002559	0.000000000
Ga	-0.630247733	-1.185323592	0.000000000
F	-1.696304021	0.705866923	0.000000000
Ga	-3.447602162	-0.698327772	0.000000000

10 $FGa_2In_2^+$

In	-2.003405173	-1.664637914	0.000000000
Ga	0.993585614	-0.614043844	0.000000000
F	-2.440567232	0.776971032	0.000000000
Ga	-3.626947029	2.243901576	0.000000000
In	3.986564620	0.558495560	0.000000000

11 $FGa_2In_2^+$

Ga	3.162394004	-0.905610322	0.000000000
Ga	0.098019968	-1.120373356	0.000000000
In	-2.930488988	-0.865558656	0.000000000
F	-0.905760788	0.713516893	0.000000000
In	1.034141558	2.016248811	0.000000000

12 $FGa_2In_2^+$

In	-2.734912036	-1.118275243	0.000000000
Ga	0.558461204	-0.203263255	0.000000000
In	3.789296411	-0.249649403	0.000000000
F	-3.050537281	1.183133903	0.000000000
Ga	-1.339429611	2.021977044	0.000000000

13 $FGa_2In_2^+$

In	0.580765985	-1.139817423	0.000000000
Ga	-0.298414266	2.046034130	0.000000000
In	-2.845789228	-0.392070388	0.000000000
F	1.531145591	1.210171332	0.000000000
Ga	3.434086528	0.023997197	0.000000000

14 $FGa_2In_2^+$

F	-0.513453000	1.302072000	0.000000000

In	-2.882792000	0.335015000	0.000000000
In	0.000000000	-1.186076000	0.000000000
Ga	3.295561000	-0.671305000	0.000000000
Ga	1.410178000	1.638510000	0.000000000

15 $FGa_2In_2^+$

Ga	-0.750472738	1.458402152	0.000000000
Ga	-1.720488292	-0.843398285	0.000000000
In	0.655848445	-0.221827349	2.424174000
In	0.655848445	-0.221827349	-2.424174000
F	1.031316745	0.452047105	0.000000000

Molecular coordinates Figure S8

1 $FGa_2Tl_2^+$

Ga	0.174219640	-0.650196549	0.000000000
Tl	-3.147097996	-0.290325500	0.000000000
F	1.018775796	1.337498743	0.000000000
Tl	3.260959716	-0.462698593	0.000000000
Ga	-0.767502338	2.229470130	0.000000000

2 $FGa_2Tl_2^+$

F	0.000000000	0.267989000	0.000000000
Tl	-2.476715000	-0.801570000	0.000000000
Tl	2.476715000	-0.801570000	0.000000000
Ga	1.348381000	2.055523000	0.000000000
Ga	-1.348381000	2.055523000	0.000000000

3 $FGa_2Tl_2^+$

Ga	-2.328602731	-1.060717976	0.0000000000
F	-0.491772575	0.229317317	0.000000000

Ga	0.240497238	-1.730217425	0.000000000
Tl	-2.444894790	2.005928022	0.000000000
Tl	3.298688090	-0.963271903	0.000000000

4 $FGa_2Tl_2^+$

Ga	-0.876048271	2.174493659	0.000000000
Ga	0.366733053	-0.330207925	0.000000000
Tl	3.620025050	-0.525918426	0.000000000
F	-2.734713296	2.085618191	0.000000000
Tl	-3.121245023	-0.411655191	0.000000000

5 $FGa_2Tl_2^+$

Tl	3.143011000	0.686583000	0.000000000
Ga	0.000000000	0.531569000	0.000000000
Ga	-0.000100000	-3.618287000	0.000000000
Tl	-3.142984000	0.686576000	0.000000000
F	0.000102000	-1.726403000	0.000000000

6 $FGa_2Tl_2^+$

Ga	0.000000000	2.168352000	0.000000000
F	0.000000000	0.000000000	0.000000000
Tl	2.587986000	0.000000000	0.000000000
Tl	-2.587986000	0.000000000	0.000000000
Ga	0.000000000	-2.168352000	0.000000000

7 $FGa_2Tl_2^+$

Ga	-3.192904000	1.654700000	0.000000000
Tl	3.184931000	0.000000000	0.000000000
Tl	-0.261346000	0.000000000	0.000000000

Ga	-3.192904000	-1.654700000	0.000000000
F	-4.316707000	0.000000000	0.000000000

8 $FGa_2Tl_2^+$

Ga	0.950307175	-1.357179298	0.000000000
F	2.227033046	0.355008181	0.000000000
Tl	0.266148698	1.917083200	0.000000000
Tl	-2.330512443	-0.989100898	0.000000000
Ga	3.797117879	-1.170616207	0.000000000

9 $FGa_2Tl_2^+$

F	-0.351007061	1.074232265	0.000000000
Ga	0.187452340	-1.063095045	0.000000000
Ga	-1.488757440	2.723592473	0.000000000
Tl	3.274002899	-0.377518721	0.000000000
Tl	-2.736971388	-0.377339732	0.000000000

10 $FGa_2Tl_2^+$

Ga	-1.803281084	-0.984876260	0.000000001
Ga	-0.969867909	1.371402483	-0.000000001
Tl	0.426779353	-0.092206833	2.559249000
F	0.851837636	0.587338402	0.000000000
Tl	0.426779352	-0.092206833	-2.559249000

11 $FGa_2Tl_2^+$

Tl	2.631502543	-1.288476742	0.000000000
Tl	-1.425701246	1.983580241	0.000000000
F	0.668467308	0.583834045	0.000000000
Ga	-3.365215810	-1.139617835	0.000000000
Ga	-0.404904866	-1.088438396	0.000000000

12 $FGa_2Tl_2^+$

F	0.343214356	1.455752703	0.000000000
Tl	-0.596591000	-1.033325923	0.000000000
Ga	-3.764915555	0.134108973	0.000000000
Ga	-1.494604310	2.025363398	0.000000000
Tl	2.571358494	0.045111556	0.000000000

13 $FGa_2Tl_2^+$

Tl	0.814763607	-1.163603021	0.000000000
Tl	-2.604708053	0.146703946	0.000000000
Ga	0.271325200	2.229278134	0.000000000
F	2.048757604	1.283258820	0.000000000
Ga	3.810825350	0.055221279	0.000000000

Molecular coordinates Figure S9

1 FIn_3Ga^+

In	-2.485003000	0.352878000	0.000000000
F	0.000000000	0.188516000	0.000000000
In	0.000000000	-2.238554000	0.000000000
Ga	0.000000000	2.368078000	0.000000000
In	2.485003000	0.352878000	0.000000000

2 FIn_3Ga^+

Ga	-0.200282471	-1.030363992	0.000000000
F	-1.301410853	0.756257478	0.000000000
In	3.049633008	-0.733578310	0.000000000
In	-3.231009959	-0.935937035	0.000000000
In	0.547119768	2.182473817	0.000000000

3 FIn_3Ga^+

In	-0.101080811	-1.131985442	0.081345887
In	3.205631050	0.046583130	0.136698705
F	-1.174388715	1.130826176	-0.137052615
In	-3.259769476	-0.380043656	-0.113801516
Ga	0.586297656	1.988046938	-0.124981959

4 FIn_3Ga^+

Ga	-0.190482905	-1.587357834	-0.000000001
In	-1.344708082	0.567863160	-1.439480000
In	2.540325931	0.163728527	0.000000000
In	-1.344708082	0.567863159	1.439480000
F	1.592778689	-2.100331590	-0.000000001

5 FIn_3Ga^+

In	-0.501710310	-1.350620373	0.125569859
In	2.879483351	-0.515037099	0.395931220
Ga	-3.443079931	-0.550288085	-0.315911649
In	0.127798928	2.076763966	-0.266032614
F	-1.781949531	0.746076233	-0.302743310

6 FIn_3Ga^+

In	-1.984493000	1.831311000	0.000000000
Ga	0.821486000	0.000000000	0.000000000
In	4.036643000	0.000000000	0.000000000
In	-1.984493000	-1.831311000	0.000000000
F	-3.197916000	0.000000000	0.000000000

7 FIn_3Ga^+

In	0.252236975	-1.301935572	0.000000000

In	-2.962797783	-0.755600881	0.000000000
Ga	3.397917102	-0.300180148	0.000000000
F	-1.060401332	0.742501006	0.000000000
In	0.755625445	2.111068467	0.000000000

Molecular coordinates Figure S10

1 $FGaTl_3^+$

Ga	-0.311481714	-0.958642143	0.000000000
F	-1.347355692	0.784279161	0.000000000
Tl	0.687601247	2.195143499	0.000000000
Tl	2.963491857	-0.972903640	0.000000000
Tl	-3.382178367	-0.942494364	0.000000000

2 $FGaTl_3^+$

Tl	-0.105120722	-1.000156856	0.000000000
Tl	-3.307482109	-0.083856352	0.000000000
F	-1.119763344	1.428040095	0.000000000
Tl	3.281927883	0.100433306	0.000000000
Ga	0.666533702	2.155406800	0.000000000

3 $FGaTl_3^+$

Tl	2.571900000	0.548197000	0.000000000
Tl	-2.571900000	0.548197000	0.000000000
Ga	0.000000000	2.517122000	0.000000000
F	0.000000000	0.407580000	0.000000000
Tl	0.000000000	-2.105023000	0.000000000

4 $FGaTl_3^+$

F	0.277874000	0.000000000	0.000000000
Ga	1.486649000	1.793288000	0.000000000

Tl	-1.747449000	-1.515280000	0.000000000
Tl	2.671172000	-1.081211000	0.000000000
Tl	-1.523562000	1.910171000	0.000000000

5 $FGaTl_3^+$

Tl	-2.908609021	-0.587735026	0.000000000
F	-2.524686485	2.001782065	0.000000000
Tl	0.479501783	-0.613734295	0.000000000
Ga	-3.104676088	3.779182614	0.000000000
Tl	3.897837511	-0.467305307	0.000000000

6 $FGaTl_3^+$

Ga	-1.452914023	2.563274212	0.000000000
Tl	0.379820938	-0.138243516	0.000000000
Tl	-3.258856165	-0.481530383	0.000000000
Tl	3.795831420	-0.582785045	0.000000000
F	-3.246692315	1.993976679	0.000000000

7 $FGaTl_3^+$

Ga	-2.131164739	-1.319916557	0.000000000
Tl	0.761423050	-1.360071794	0.000000000
F	-1.116611969	0.473973660	0.000000000
Tl	-3.482179828	1.439658953	0.000000000
Tl	3.660455833	0.372901849	0.000000000

8 $FGaTl_3^+$

Tl	-0.098580213	2.068026063	0.000000000
Tl	2.707634434	-0.573081592	0.000000000
Tl	-0.857474500	-1.485189400	0.000000000

Ga	-3.918971840	-0.268866340	0.000000000
F	-2.265539015	0.838299320	0.000000000

9 $FGaTl_3^+$

Ga	0.284715802	-2.152051591	0.000000000
Tl	1.159152344	0.358998094	-1.824536000
Tl	-2.267295992	0.209985090	0.000000000
Tl	1.159152344	0.358998094	1.824536000
F	-1.583276116	-2.204435279	0.000000000

Molecular coordinates Figure S11

1 $FIn_2Tl_2^+$

F	0.000000000	0.000000000	0.000000000
In	0.000000000	2.377876000	0.000000000
Tl	2.588298000	0.000000000	0.000000000
Tl	-2.588298000	0.000000000	0.000000000
In	0.000000000	-2.377876000	0.000000000

2 $FIn_2Tl_2^+$

F	0.000000000	0.211361000	0.000000000
Tl	-2.079342000	-1.258605000	0.000000000
In	1.575584000	2.061140000	0.000000000
Tl	2.079342000	-1.258605000	0.000000000
In	-1.575584000	2.061140000	0.000000000

3 $FIn_2Tl_2^+$

Tl	3.273663178	-0.326868512	0.000000000
In	0.619812829	2.248007923	0.000000000
In	-0.186305220	-1.056589405	0.000000000

F	-1.265762295	1.088001503	0.000000000
Tl	-3.395268049	-0.514755178	0.000000000

4 $FIn_2Tl_2^+$

Tl	-0.616805341	-1.112746293	0.000000000
Tl	2.892895796	-0.430864648	0.000000000
F	-1.713566679	1.249469457	0.000000000
In	0.287278553	2.272699297	0.000000000
In	-3.735057840	0.049491193	0.000000000

5 $FIn_2Tl_2^+$

Tl	2.790302368	-0.788149177	0.000000000
In	-0.635133968	-1.362049189	0.000000000
Tl	0.094379106	2.008549074	0.000000000
In	-3.785305499	-0.767661693	0.000000000
F	-1.895295197	0.611497959	0.000000000

6 $FIn_2Tl_2^+$

Tl	0.235533591	-1.108098422	0.000000000
In	3.677375407	-0.331048874	0.000000000
F	-0.884575995	1.191957439	0.000000000
Tl	-2.995748170	-0.193866516	0.000000000
In	1.047901296	2.264345308	0.000000000

7 $FIn_2Tl_2^+$

F	0.512081502	1.049922670	0.000000000
Tl	2.650694221	-0.563412572	0.000000000
In	-0.393827244	-1.143098915	0.000000000

In	2.000564796	2.737136640	0.000000000
Tl	-3.679568574	-0.517539370	0.000000000

8 $FIn_2Tl_2^+$

F	0.557163374	0.557163374	0.000000000
Tl	2.253538705	2.386108498	0.000000000
In	-0.366455261	-1.590643775	0.000000000
In	2.560797814	-0.876503403	0.000000000
Tl	-3.642887564	-0.955543799	0.000000000

9 $FIn_2Tl_2^+$

Tl	0.998081289	2.062667246	0.000000000
In	3.558185950	-0.950399407	0.000000000
F	-1.009373894	0.706771209	0.000000000
Tl	-3.105796171	-0.755458654	0.000000000
In	0.111391162	-1.340310817	0.000000000

10 $FIn_2Tl_2^+$

In	-2.861995000	-1.842784000	0.000000000
Tl	0.237060000	0.000000000	0.000000000
In	-2.861995000	1.842784000	0.000000000
Tl	3.677095000	0.000000000	0.000000000
F	-4.063449000	0.000000000	0.000000000

11 $FIn_2Tl_2^+$

Tl	-0.306124184	-1.440201052	0.000000000
F	-1.495181291	0.844368140	0.000000000
In	-3.468710773	-0.324325775	0.000000000

Tl	0.623700428	2.015913946	0.000000000
In	3.218362878	-0.782452737	0.000000000

12 $FIn_2Tl_2^+$

In	2.812327372	-0.816548733	0.000000000
In	2.702574603	2.475358096	0.000000000
Tl	-0.232010288	-1.315795729	0.000000000
F	1.064446549	0.913284642	0.000000000
Tl	-3.222436651	0.210842422	0.000000000

13 $FIn_2Tl_2^+$

In	-2.976011446	-0.761937384	0.000000000
Tl	0.412932274	-0.885536119	0.000000000
F	-2.727431290	1.596500383	0.000000000
In	-3.543859560	3.555292450	0.000000000
Tl	3.834235438	-0.981659980	0.000000000

14 $FIn_2Tl_2^+$

F	-0.195340016	0.536692285	0.000000000
In	-1.235235685	-1.564610016	0.000000000
Tl	1.819245463	-1.149863670	0.000000000
Tl	1.537712127	2.229375304	0.000000000
In	-4.278143182	-0.318464930	0.000000000

15 $FIn_2Tl_2^+$

Tl	2.198963274	-0.723096520	0.000000000
Tl	-0.940836468	-1.055489928	0.000000000
In	1.951387804	2.702273940	0.000000000

In	-4.097411313	0.021100105	0.000000000
F	0.360765341	1.180010258	0.000000000

Molecular coordinates Figure S12

1 FIn_3Tl^+

F	0.000000000	-0.350347000	0.000000000
Tl	0.000000000	2.212917000	0.000000000
In	-2.392751000	-0.416627000	0.000000000
In	0.000000000	-2.760485000	0.000000000
In	2.392751000	-0.416627000	0.000000000

2 FIn_3Tl^+

Tl	2.799033017	-0.534176603	0.000000000
In	0.171149718	2.190362007	0.000000000
In	-0.675320000	-1.169688551	0.000000000
F	-1.768885453	1.014862523	0.000000000
In	-3.797904801	-0.324050078	0.000000000

3 FIn_3Tl^+

F	-0.801775392	1.013808675	0.000000000
In	0.242840231	-1.142473463	0.000000000
In	3.687990440	-0.496513687	0.000000000
In	1.117496525	2.163863194	0.000000000
Tl	-2.964839746	-0.430163959	0.000000000

4 FIn_3Tl^+

F	1.054733220	0.633747656	0.000000000
In	2.928896189	1.958163889	0.000000000
In	-0.360736506	-1.295173106	0.000000000

In	2.677123783	-1.295894418	0.000000000
Tl	-3.290265234	0.312450239	0.000000000

5 FIn_3Tl^+

In	-2.794647000	-1.845819000	0.000000000
In	0.254157000	0.000000000	0.000000000
Tl	3.670793000	0.000000000	0.000000000
In	-2.794647000	1.845819000	0.000000000
F	-3.990278000	0.000000000	0.000000000

6 FIn_3Tl^+

F	0.120149282	0.330107440	0.000000000
Tl	2.163895474	1.759459554	0.000000000
In	-1.258000290	-1.561023816	0.000000000
In	1.756697187	-1.511547278	0.000000000
In	-4.097817155	0.103445540	0.000000000

7 FIn_3Tl^+

Tl	0.494843422	1.924175897	0.000000000
In	-0.268501064	-1.522745201	0.000000000
F	-1.501844665	0.516732923	0.000000000
In	-3.445099956	-0.864524744	0.000000000
In	3.171443577	-0.888421517	0.000000000

8 FIn_3Tl^+

In	1.215649634	1.938682741	0.000000000
Tl	-0.509985712	-1.093667890	0.000000000
F	-0.976245574	1.468254192	0.000000000

In	-3.247867805	0.828786044	0.000000000
In	3.054566638	-1.229247568	0.000000000

9 FIn_3Tl^+

F	0.827336303	0.887209564	0.000000000
In	2.248478924	-1.113462525	0.000000000
Tl	-0.840963585	-1.102502404	0.000000000
In	2.691759190	2.156354228	0.000000000
In	-3.702033205	0.616655899	0.000000000

10 FIn_3Tl^+

In	0.640720678	1.177178729	-1.422213000
In	2.639046945	-1.415199735	0.000000000
Tl	-2.228483220	-0.431620768	0.000000000
In	0.640720678	1.177178729	1.422213000
F	0.331703253	-1.023342232	-0.000000001

Molecular coordinates Figure S13

1 $FInTl_3^+$

Tl	0.000000000	-2.252043000	0.000000000
Tl	2.563609000	0.318154000	0.000000000
In	0.000000000	2.621386000	0.000000000
Tl	-2.563609000	0.318154000	0.000000000
F	0.000000000	0.269631000	0.000000000

2 $FInTl_3^+$

In	1.258291252	1.997008262	0.000000000
F	-0.895793135	1.540628424	0.000000000
Tl	3.100061531	-1.166644081	0.000000000

Tl	-3.301874107	0.773534450	0.000000000
Tl	-0.459843746	-0.986138096	0.000000000

3 $FInTl_3^+$

Tl	3.197183529	-0.826953572	0.000000000
In	-0.285338715	-1.235937760	0.000000000
Tl	0.614787600	2.169576999	0.000000000
Tl	-3.484809520	-0.686656383	0.000000000
F	-1.390943924	0.825294548	0.000000000

4 $FInTl_3^+$

Tl	-0.549618673	-1.360353952	0.000000000
Tl	2.931866619	-0.551340022	0.000000000
Tl	0.116196118	2.137205214	0.000000000
F	-1.911829641	0.801818307	0.000000000
In	-3.778928398	-0.520055978	0.000000000

5 $FInTl_3^+$

In	0.323138449	1.863975548	0.000000000
Tl	1.891459094	-0.599059795	-0.000000001
Tl	-0.988060042	-0.214350841	2.518615000
F	-1.040961170	-0.184944037	0.000000000
Tl	-0.988060043	-0.214350841	-2.518614999

6 $FInTl_3^+$

Tl	-3.031400262	-0.521396313	0.000000000
F	-1.279330642	1.476224736	0.000000000
Tl	0.193990367	-1.100174042	0.000000000

In	-1.057249768	3.578037941	0.000000000
Tl	3.619128756	-0.706947000	0.000000000

7 $FInTl_3^+$

In	3.565484900	-0.825866760	0.000000000
Tl	0.068538907	-1.307800246	0.000000000
Tl	1.023117731	2.112379788	0.000000000
Tl	-3.131016910	-0.410941946	0.000000000
F	-1.057846483	0.953641525	0.000000000

8 $FInTl_3^+$

In	-2.320090917	-1.327167024	0.000000000
Tl	0.737111280	-1.414073203	0.000000000
F	-0.875612329	0.568629295	0.000000000
Tl	-2.906602294	1.927286029	0.000000000
Tl	3.670292268	0.226460267	0.000000000

9 $FInTl_3^+$

In	-2.289038747	2.219668862	0.000000000
Tl	0.572147251	0.019979822	0.000000000
Tl	-2.775473612	-1.545556143	0.000000000
Tl	4.000459083	0.113809338	0.000000000
F	-3.711647938	0.621037674	0.000000000

Molecular coordinates Figure S14

1 FIn_3Al^+

Al	0.298223862	-1.756583913	-0.000000002
In	-1.372548534	0.022260239	1.413874000

In	2.349555317	0.704644380	0.000000000
In	-1.372548535	0.022260240	-1.413873999
F	1.968735942	-2.036318440	-0.000000002

2 FIn_3Al^+

Al	-1.029021704	2.364856788	0.000000000
In	0.318257760	-0.267049969	0.000000000
F	-2.745400869	2.235038290	0.000000000
In	-3.168611142	-0.298174630	0.000000000
In	3.627616917	-0.472703914	0.000000000

3 FIn_3Al^+

In	3.243961779	0.134741835	0.000000000
In	-0.079747156	-0.911514164	0.000000000
Al	0.797513062	2.127768960	0.000000000
F	-0.881918160	1.643939920	0.000000000
In	-3.213815172	-0.089685833	0.000000000

4 FIn_3Al^+

In	-2.931551836	-0.436058508	0.000000000
In	0.409320079	-0.487808675	0.000000000
F	-2.548443743	2.138337994	0.000000000
Al	-3.009801252	3.806973699	0.000000000
In	3.788832006	-0.478902673	0.000000000

5 FIn_3Al^+

In	1.776015000	2.130982000	0.000000000
In	2.118492000	-1.672323000	0.000000000
F	-0.688914000	1.752714000	0.000000000

In	-3.617125000	-0.780586000	0.000000000
Al	-0.568578000	0.000000000	0.000000000

6 FIn_3Al^+

F	1.154091022	1.785663297	0.000000000
Al	2.524994932	2.871746369	0.000000000
In	-0.254912401	-0.700366066	0.000000000
In	2.954059281	-0.447135339	0.000000000
In	-3.581018843	0.057631162	0.000000000

7 FIn_3Al^+

F	-0.048641881	0.555979250	0.000000000
In	1.964117714	2.234922694	0.000000000
Al	-0.728267900	-1.118725819	0.000000000
In	-3.914434315	-1.052498505	0.000000000
In	2.152465811	-0.987737884	0.000000000

8 FIn_3Al^+

Al	-1.941447621	-0.297532193	0.000000000
In	1.097316661	-0.399390602	0.000000000
F	-2.096274440	1.444126573	0.000000000
In	-4.699532871	0.769731389	0.000000000
In	4.502324591	-0.556650856	0.000000000

9 FIn_3Al^+

Al	0.000000000	2.507937000	0.000000000
In	0.000000000	-1.886576000	0.000000000
F	0.000000000	0.630109000	0.000000000

In	2.580496000	0.552735000	0.000000000
In	-2.580496000	0.552735000	0.000000000

10 FIn_3Al^+

In	2.573437791	-0.361776598	0.000000000
In	-0.814412196	-1.598373931	0.000000000
In	-0.282961413	1.947057340	0.000000000
Al	-3.882709921	-0.405854023	0.000000000
F	-2.427990762	0.657519023	0.000000000

Molecular coordinates Figure S15

1 FTl_3Al^+

Tl	-1.343075830	0.020194285	1.506344000
Tl	2.475164537	-0.510162863	0.000000000
Tl	-1.343075831	0.020194285	-1.506344000
Al	0.265357846	1.916858249	0.000000000
F	1.899486190	2.346088909	0.000000000

2 FTl_3Al^+

Tl	2.242115560	-1.283304608	0.000000000
Tl	1.402807395	2.526687087	0.000000000
Al	-0.611293956	0.053481291	0.000000000
Tl	-3.423870538	-1.443286160	0.000000000
F	-1.106489605	1.721882205	0.000000000

3 FTl_3Al^+

Tl	-0.346735040	-0.743575692	0.000000000
Tl	-3.076439182	1.135410502	0.000000000
Al	1.546031988	1.848365062	0.000000000

Tl	3.195741699	-0.910837150	0.000000000
F	-0.186265879	2.001150589	0.000000000

4 FTl_3Al^+

F	0.000000000	2.498150000	0.000000000
Tl	3.208848000	0.815392000	0.000000000
Al	0.000000000	0.808781000	0.000000000
Tl	-3.208848000	0.815392000	0.000000000
Tl	0.000000000	-2.038160000	0.000000000

5 FTl_3Al^+

Tl	-3.136321077	-0.316296429	0.000000000
F	-2.676744971	2.365829607	0.000000000
Tl	0.251259747	-0.358836106	0.000000000
Al	-3.062478766	4.045176187	0.000000000
Tl	3.673986479	-0.236963247	0.000000000

6 FTl_3Al^+

F	1.265364685	1.600917264	0.090134813
Tl	-1.064975371	-0.432326446	-0.087002480
Al	1.856286552	-0.002814131	0.160857790
Tl	5.012068732	-0.203688168	0.436711872
Tl	-4.385612114	0.458586763	-0.385541069

7 FTl_3Al^+

F	-0.448678235	0.259044500	0.000000000
Al	1.341130890	0.375468841	0.000000000
Tl	-2.772183707	-1.172393029	0.000000000

Tl	0.320876307	-2.375709933	0.000000000
Tl	2.285916666	3.459059808	0.000000000

8 FTl_3Al^+

F	0.000000000	0.745194000	0.000000000
Tl	2.646857000	0.670922000	0.000000000
Tl	0.000000000	-1.841137000	0.000000000
Al	0.000000000	2.595073000	0.000000000
Tl	-2.646857000	0.670922000	0.000000000

9 FTl_3Al^+

Tl	-0.940295500	-1.628639580	0.000000000
Tl	2.474889667	-0.325513354	0.000000000
F	-2.756110701	0.509700234	0.000000000
Tl	-0.564177942	1.994633140	0.000000000
Al	-4.138362805	-0.605092639	0.000000000