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Supporting Information

Extending the Row of Lanthanide Tetrafluorides: A Combined Matrix-Isolation and Quantum-Chemical Study

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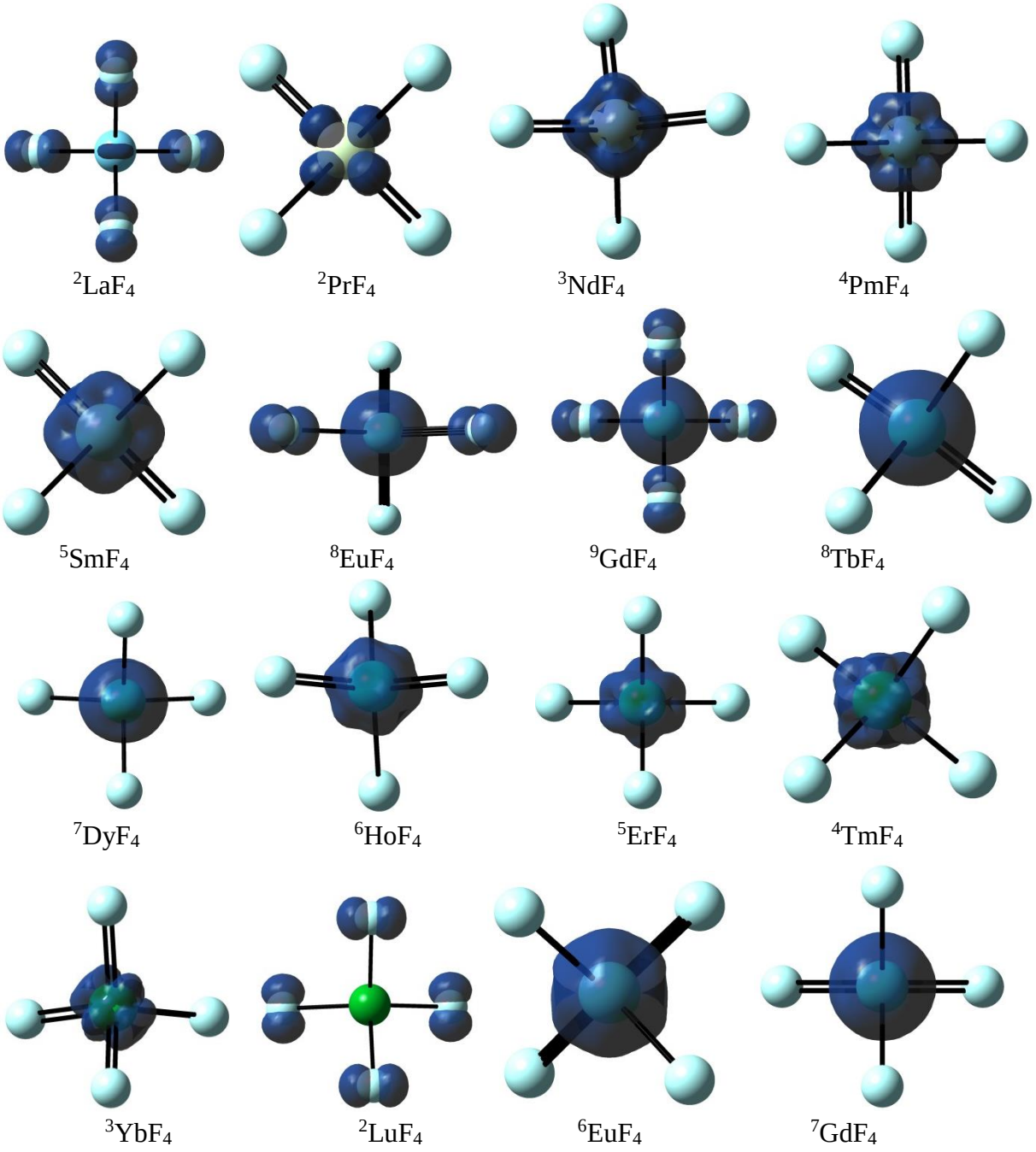
Figures S1 Spin density images at the 0.02 contour level for LnF_4.



Figures S2 Spin density images at the 0.02 contour level for $[LnF_4]^-$.

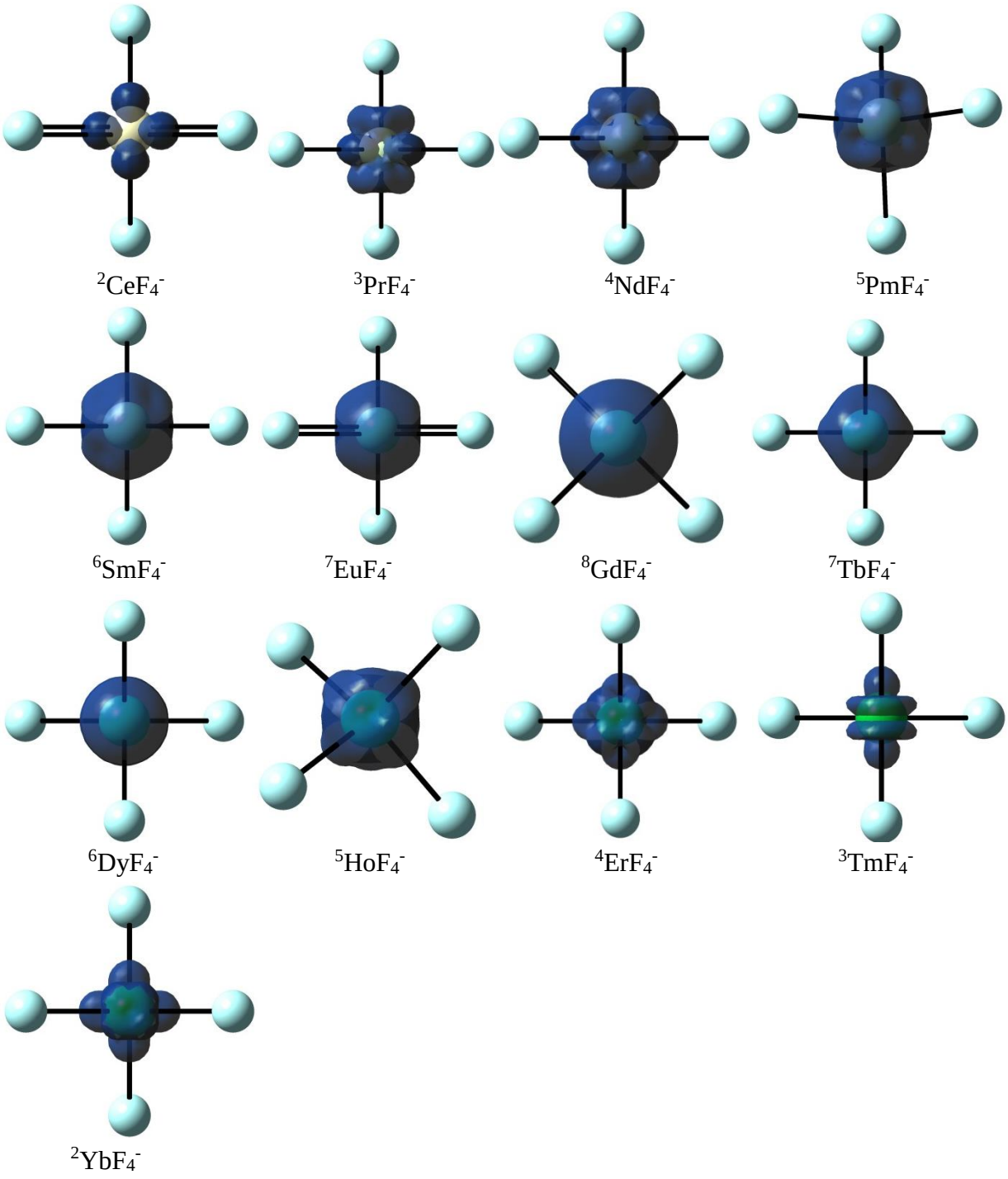


Table S1. Calculated symmetric (sym) and asymmetric (asym) Ln-F vibrational frequencies (cm^{-1}) and intensities (km/mol) at the MP2/Stuttgart/aug-cc-pVDZ level as well as experimental matrix infrared vibrational frequencies (cm^{-1}) for LnF_3.

LnF_3	Spin	$S^2/<S^2>$	Sym ν(I)	Asym ν(I)	*ν*(Ln-F) expt.	*ν*(LnF_3) calc. – expt.
LaF_3	1	0.00/0.00	527.7 (16)	497.2e (265)	479	18
CeF_3	2	0.75/0.75	536.6	504.2, 507.1	488	18
PrF_3	3	2.00/2.00	542.0 (12)	485.0 (240), 513.1 (266)	458	41
NdF_3	4	3.75/3.75	554.1 (24)	519.5 e (246)	504	16
PmF_3	5	6.00/6.00	547.5 (3)	525.9 (256), 526.7 (256)		
SmF_3	6	8.75/8.75	558.3 (10)	525.0 (234), 526.3 (250)	508	18
EuF_3	7	12.01/12.00	559.1 (0)	537.9 e (241)	512	26
GdF_3	8	15.76/15.75	567.3 (11)	541.8 e (224)	519	23
TbF_3	7	12.01/12.00	568.4 (1)	532.9 (219), 550.1 (230)	523	19
DyF_3	6	8.76/8.75	571.1 (0)	552.5 e (215)	532	21
HoF_3	5	6.00/6.00	576.6 (0)	558.2 e (209)	536	22
ErF_3	4	3.75/3.75	577.5 (0)	563.2e (201)	539	24
TmF_3	3	2.00/2.00	583.2 (0)	568.0 (187), 570.7 (202)	545	25
YbF_3	2	0.75/0.75	588.9 (0)	575.1e (185)	546	29
LuF_3	1	0.00/0.00	593.9 (0)	581.4e (186)	552	29

Table S2: Calculated symmetric (sym) and asymmetric (asym) Ln-F vibrational frequencies (cm^{-1}) and intensities (km/mol) at the MP2/Stuttgart/aug-cc-pVDZ level for LnF_2.

LnF_2	Spin	$S^2/<S^2>$	Sym ν(I)	Asym ν(I)
LaF_2	2	0.75/0.75	543.7 (111)	519.6 (214)
CeF_2	3	2.00/2.00	563.3 (0)	479.4 (225)
PrF_2	4	3.76/3.75	498.3 (44)	470.0 (277)
NdF_2	5	6.00/6.00	561.1 (106)	538.5 (206)
PmF_2	6	8.75/8.75	478.7 (82)	456.3 (225)
SmF_2	7	12.01/12.00	577.2 (98)	546.9 (176)
EuF_2	8	15.76/15.75	482.0 (62)	460.2 (217)
GdF_2	9	20.01/20.00	577.1 (78)	550.2 (181)
TbF_2	6	9.19/8.75	554.4 (32)	497.1 (180)
DyF_2	5	7.01/6.00	585.2 (42)	564.3 (159)
HoF_2	4	3.75/3.75	495.7 (55)	481.8 (200)
ErF_2	3	2.00/2.00	500.5 (53)	490.2 (188)
TmF_2	2	0.75/0.75	502.4 (39)	492.1 (191)
YbF_2	1	0.00/0.00	504.9 (43)	493.4 (176)
LuF_2	2	0.75/0.75	603.3 (39)	580.0 (142)

Table S3. B3LYP/Stuttgart/DZVP2 Population Analysis for LnF_4.

LnF_4	$S^2/\langle S^2\rangle$	Pop Ln	Ln Excess Spin	Ln Oxidation State	Ln 4f α	Ln 5d α	Pop 2p F	F 2p α -β
$^2LaF_4$	0.76/0.75	$4f^{0.24}5d^{0.57}$		+III	0.11	0.27	$2p^{5.59}$	0.26
$^1CeF_4$	0.00/0.00	$4f^{0.73}5d^{0.89}$		+IV			$2p^{5.63}$	0
$^2PrF_4$	0.75/0.75	$4f^{1.71}5d^{0.89}$	$4f^1$	+IV	1.33	0.45	$2p^{5.62}$	0
$^3NdF_4$	2.04/2.00	$4f^{2.79}5d^{0.89}$	$4f^2$	+IV	2.47	0.46	$2p^{5.60}$	-0.06
$^4PmF_4$	3.84/3.75	$4f^{3.74}5d^{0.88}$	$4f^3$	+IV	3.45	0.46	$2p^{5.62}$	-0.06
$^5SmF_4$	6.19/6.00	$4f^{4.99}5d^{0.71}$	$4f^4$	+IV	4.85	0.39	$2p^{5.68}$	-0.06
$^6EuF_4$	9.39/8.75	$4f^{6.08}5d^{0.64}$	$4f^5$	+IV	5.96	0.35	$2p^{5.60}$	-0.22
$^8EuF_4$	15.76/15.75	$4f^{6.10}5d^{0.61}$	$4f^6$	+III	6.03	0.30	$2p^{5.64/5.54}$	0.17/0.34
$^7GdF_4$	12.82/12.00	$4f^{6.75}5d^{0.71}$	$4f^6$	+IV	6.67	0.38	$2p^{5.68/5.52}$	0.10/-0.31
$^9GdF_4$	20.23/20.00	$4f^{7.04}5d^{0.56}6s^{0.27}$	$4f^7$	+III	6.99	0.27	$2p^{5.57}$	0.30
$^8TbF_4$	16.30/15.75	$4f^{7.10}5d^{0.83}6s^{0.60}$	$4f^7$	+IV	7.00	0.42	$2p^{5.65}$	0.15
$^7DyF_4$	12.41/12.00	$4f^{8.10}5d^{0.85}6s^{0.57}$	$4f^{5.5}6s^{0.5\ a}$	+IV	6.96	0.47	$2p^{5.64}$	-0.1
$^6HoF_4$	8.76/8.75	$4f^{9.49}5d^{0.95}$	$4f^5$	+IV	7.00	0.48	$2p^{5.65}$	0.13
$^5ErF_4$	6.01/6.00	$4f^{10.76}5d^{0.74}$	$4f^4$	+IV	7.00	0.36	$2p^{5.64}$	0.20
$^4TmF_4$	3.76/3.75	$4f^{11.57}5d^{0.84}$	$4f^3$	+IV	7.00	0.41	$2p^{5.65}$	0.14
$^3YbF_4$	2.01/2.00	$4f^{12.80}5d^{0.67}$	$4f^2$	+IV	7.00	0.32	$2p^{5.61}$	0.23
$^2LuF_4$	0.76/0.75	$6s^{0.10}5d^{0.67}$		+III	7.00	0.31	$2p^{5.59}$	0.25

[a] unpaired 6s α spin = 0.54.

Table S4. B3LYP/Stuttgart/DZVP2 Population Analysis for $[LnF_4]^-$.

$[LnF_4]^-$	$S^2/\langle S^2\rangle$	Pop Ln	Ln Excess Spin	Ln Oxidation state	Ln 4f α	Ln 5d α	Pop 2p F	F 2p α -β
$[^1LaF_4]^-$	0.00/0.00	$4f^{0.19}5d^{0.58}$		+III			$2p^{5.83}$	0
$[^2CeF_4]^-$	0.75/0.75	$4f^{1.13}5d^{0.61}$	$4f^1$	+III	1.04	0.31	$2p^{5.82}$	0
$[^3PrF_4]^-$	2.00/2.00	$4f^{2.15}5d^{0.62}$	$4f^2$	+III	2.06	0.32	$2p^{5.82}$	0
$[^4NdF_4]^-$	3.75/3.75	$4f^{3.13}5d^{0.63}$	$4f^3$	+III	3.05	0.33	$2p^{5.82}$	0
$[^5PmF_4]^-$	6.00/6.00	$4f^{4.11}5d^{0.63}$	$4f^4$	+III	4.04	0.33	$2p^{5.83}$	0
$[^6SmF_4]^-$	8.76/8.75	$4f^{5.09}5d^{0.63}$	$4f^5$	+III	5.03	0.33	$2p^{5.83}$	0
$[^7EuF_4]^-$	12.00/12.00	$4f^{6.08}5d^{0.62}$	$4f^6$	+III	6.03	0.33	$2p^{5.84}$	0
$[^8GdF_4]^-$	15.76/15.75	$4f^{7.03}5d^{0.61}6s^{0.11}$	$4f^7$	+III	6.99	0.33	$2p^{5.84}$	0
$[^7TbF_4]^-$	12.51/12.00	$4f^{8.00}5d^{0.52}6s^{0.85}$	$4f^6$	+III	6.99	0.26	$2p^{5.76}$	0.13
$[^6DyF_4]^-$	8.82/8.75	$4f^{8.63}5d^{0.60}6s^{0.54}$	$4f^{4.5}6s^{0.5\ a}$	+III	6.59	0.31	$2p^{5.83}$	-0.03
$[^5HoF_4]^-$	6.01/6.00	$4f^{10.04}5d^{0.63}$	$4f^4$	+III	7.00	0.32	$2p^{5.84}$	0
$[^4ErF_4]^-$	3.75/3.75	$4f^{11.02}5d^{0.62}$	$4f^3$	+III	7.00	0.31	$2p^{5.84}$	0
$[^3TmF_4]^-$	2.00/2.00	$4f^{12.01}5d^{0.62}$	$4f^2$	+III	7.00	0.31	$2p^{5.84}$	0
$[^2YbF_4]^-$	0.75/0.75	$4f^{13.01}5d^{0.61}$	$4f^1$	+III	7.00	0.30	$2p^{5.85}$	0
$[^1LuF_4]^-$	0.00/0.00	$6s^{0.11}5d^{0.66}$		+III			$2p^{5.84}$	

[a] unpaired 6s α spin = 0.52.

Table S5. Cartesian coordinates for optimized lanthanide species, Zero Point Energies (ZPE, a.u.), enthalpy correction (dH_{298}, a.u.) at 298 K and electronic energies at 0 K ($E_{M,0K}$, a.u.) at the MP2/Stuttgart/aug-cc-pVDZ level.

F ZPE=0 dH_{298}=0.00236 $E_{M,0K}$=-99.535699

F^- ZPE=0 dH_{298}=0.00236 $E_{M,0K}$=-99.665948

$^2F_2$ ZPE=0.002128 dH_{298}=0.00548 $E_{M,0K}$=-199.126917

F	0.000000	0.000000	0.713319
F	0.000000	0.000000	-0.713319

$^2LaF_4$ ZPE=0.006537 dH_{298}=0.014545 $E_{M,0K}$=-833.331065

LA	0.000000	0.000000	0.000000
F	0.000000	1.524770	1.502840
F	1.524770	0.000000	-1.502840
F	0.000000	-1.524770	1.502840
F	-1.524770	0.000000	-1.502840

$^1CeF_4$ ZPE=0.006705 dH_{298}=0.01458 $E_{M,0K}$=-872.904545

CE	0.000000	0.000000	0.000000
F	1.175801	1.175801	1.175801
F	-1.175801	-1.175801	1.175801
F	-1.175801	1.175801	-1.175801
F	1.175801	-1.175801	-1.175801

$^2PrF_4$ ZPE=0.006669 dH_{298}=0.014633 $E_{M,0K}$=-914.656252

PR	0.000000	0.000000	0.000000
F	1.171096	1.171096	1.171096
F	-1.171096	-1.171096	1.171096
F	1.171096	-1.171096	-1.171096
F	-1.171096	1.171096	-1.171096

$^3NdF_4$ ZPE=0.006734 dH_{298}=0.014686 $E_{M,0K}$=-958.956149

ND	0.000000	0.000000	-0.000833
F	0.000000	1.664319	-1.133820
F	1.660878	0.000000	1.136595
F	-1.660878	0.000000	1.136595
F	0.000000	-1.664319	-1.133820

$^{4}PmF_4$ ZPE=0.00689 dH_{298}=0.014754 $E_{M,0K}$=-1005.855557

PM	0.001553	-0.002083	0.000000
F	0.660263	-0.998385	1.607497
F	0.660263	-0.998385	-1.607497
F	-1.991317	0.127590	0.000000
F	0.660263	1.883300	0.000000

$^{5}SmF_4$ ZPE=0.006916 dH_{298}=0.014784 $E_{M,0K}$=-1055.407231

SM	0.000000	0.000000	0.000000
F	1.147132	1.147132	1.147132
F	-1.147132	-1.147132	1.147132
F	1.147132	-1.147132	-1.147132
F	-1.147132	1.147132	-1.147132

$^{8}EuF_4$ ZPE=0.006214 dH_{298}=0.014351 $E_{M,0K}$=-1107.690555

EU	-0.000009	0.000033	0.067807
F	1.979891	-0.000736	0.847189
F	0.000306	1.658320	-1.083879
F	-1.980003	-0.000368	0.847045
F	-0.000134	-1.657448	-1.085004

$^{6}EuF_4$ ZPE=0.007252 dH_{298}=0.014851 $E_{M,0K}$=-1107.683160

F	1.139816	-1.150146	1.127465
F	-1.157363	1.120111	1.139987
F	1.158924	1.148113	-1.110207
F	-1.141418	-1.118570	-1.157264
EU	0.000006	0.000070	0.000002

$^{9}GdF_4$ ZPE=0.006411 dH_{298}=0.01457 $E_{M,0K}$=-1162.866218

F	0.000000	1.554489	1.352400
F	1.554489	0.000000	-1.352400
F	-1.554489	0.000000	-1.352400
F	0.000000	-1.554489	1.352400
GD	0.000000	0.000000	0.000000

$^{7}GdF_4$ ZPE=0.007402 dH_{298}=0.014937 $E_{M,0K}$=-1162.782712

F	0.000000	1.595312	1.144488
F	0.000000	-1.595312	1.144488
F	-1.608442	0.000000	-1.117988
F	1.608442	0.000000	-1.117988
GD	0.000000	0.000000	-0.007453

$^{8}TbF_4$ ZPE=0.007395 dH_{298}=0.014989 $E_{M,0K}$=-1220.847078

F	1.128318	1.128318	1.128318
F	-1.128318	-1.128318	1.128318
F	-1.128318	1.128318	-1.128318
F	1.128318	-1.128318	-1.128318
TB	0.000000	0.000000	0.000000

$^{7}DyF_4$ ZPE=0.007441 dH_{298}=0.015019 $E_{M,0K}$=-1281.556076

F	0.000000	1.600377	1.103978
F	0.000000	-1.600377	1.103978
F	-1.611076	0.000000	-1.086870
F	1.611076	0.000000	-1.086870
DY	0.000000	0.000000	-0.004666

$^{6}HoF_4$ ZPE=0.007548 dH_{298}=0.015063 $E_{M,0K}$=-1345.337751

F	-1.135629	1.135629	1.073181
F	1.135629	1.135629	-1.073181
F	1.135629	-1.135629	1.073181
F	-1.135629	-1.135629	-1.073181
HO	0.000000	0.000000	0.000000

$^{5}ErF_4$ ZPE=0.007613 dH_{298}=0.01514 $E_{M,0K}$=-1412.266485

F	0.000000	1.548635	1.135749
F	1.562666	0.000000	-1.127066
F	0.000000	-1.548635	1.135749
F	-1.562666	0.000000	-1.127066
ER	0.000000	0.000000	-0.002298

$^{4}TmF_4$ ZPE=0.007654 dH_{298}=0.015166 $E_{M,0K}$=-1482.393253

F	0.000000	1.561437	1.104165
F	0.000000	-1.561437	1.104165
F	-1.561549	0.000000	-1.104076
F	1.561549	0.000000	-1.104076
TM	0.000000	0.000000	-0.000023

$^{3}YbF_4$ ZPE=0.00803 dH_{298}=0.015308 $E_{M,0K}$=-1555.771293

YB	0.000002	0.000000	0.000000
F	1.111750	1.155640	1.021868
F	1.111739	-1.155737	-1.021771
F	-1.111653	1.021989	-1.155603
F	-1.111854	-1.021890	1.155502

$^{2}LuF_4$ ZPE=0.006838 dH_{298}=0.014958 $E_{M,0K}$=-1632.675277

F	0.000000	1.674660	1.103844
F	0.000000	-1.674660	1.103844
F	-1.674986	0.000000	-1.103995
F	1.674986	0.000000	-1.103995
LU	0.000000	0.000000	0.000038

$^{1}LaF_4^-$ ZPE=0.005294 dH_{298}=0.01369 $E_{M,0K}$=-833.615904

LA	0.000000	0.000000	0.000000
F	1.280586	1.280586	1.280586
F	-1.280586	-1.280586	1.280586
F	-1.280586	1.280586	-1.280586
F	1.280586	-1.280586	-1.280586

$^{2}CeF_4^-$ ZPE=0.005352 dH_{298}=0.013734 $E_{M,0K}$=-873.001216

F	0.000000	1.794340	-1.268754
F	0.000000	-1.794340	-1.268754
F	1.794613	0.000000	1.268698
F	-1.794613	0.000000	1.268698
CE	0.000000	0.000000	0.000017

$^{3}PrF_4^-$ ZPE=0.005458 dH_{298}=0.013787 $E_{M,0K}$=-914.835394

PR	0.000000	0.000000	0.007364
F	0.000000	1.749221	-1.287696
F	0.000000	-1.749221	-1.287696
F	-1.784100	0.000000	1.263557
F	1.784100	0.000000	1.263557

$^{4}NdF_4^-$ ZPE=0.005525 dH_{298}=0.013825 $E_{M,0K}$=-959.189357

ND	0.000000	0.000000	0.002117
F	0.000000	1.744812	-1.274055
F	0.000000	-1.744812	-1.274055
F	1.756994	0.000000	1.266999
F	-1.756994	0.000000	1.266999

$^{5}PmF_4^-$ ZPE=0.005584 dH_{298}=0.013854 $E_{M,0K}$=-1006.113378

PM	0.000000	0.000000	0.000000
F	-1.240538	1.754390	0.006868
F	-1.240555	-1.754385	-0.004906
F	1.239159	0.005885	-1.755368
F	1.241933	-0.005890	1.753406

$^{6}SmF_4^-$ ZPE=0.00573 dH_{298}=0.013911 $E_{M,0K}$=-1055.678980

SM	0.000000	0.000000	0.011210
F	0.000000	1.732175	-1.235099
F	0.000000	-1.732175	-1.235099
F	1.775229	0.000000	1.196488
F	-1.775229	0.000000	1.196488

$^{7}EuF_4^-$ ZPE=0.005764 dH_{298}=0.013937 $E_{M,0K}$=-1108.001603

F	0.000000	1.732057	-1.211245
F	0.000000	-1.732057	-1.211245
F	1.782628	0.000000	1.166765
F	-1.782628	0.000000	1.166765
EU	0.000000	0.000000	0.012709

$^{8}GdF_4^-$ ZPE=0.005821 dH_{298}=0.01396 $E_{M,0K}$=-1163.167141

F	1.217929	1.217929	1.217929
F	-1.217929	-1.217929	1.217929
F	-1.217929	1.217929	-1.217929
F	1.217929	-1.217929	-1.217929
GD	0.000000	0.000000	0.000000

$^{7}TbF_4^-$ ZPE=0.005429 dH_{298}=0.013755 $E_{M,0K}$=-1220.991670

F	0.000000	1.721681	1.195289
F	0.000000	-1.721681	1.195289
F	-1.706383	0.000000	-1.202639
F	1.706383	0.000000	-1.202639
TB	0.000000	0.000000	0.002035

$^{6}DyF_4^-$ ZPE=0.005935 dH_{298}=0.014021 $E_{M,0K}$=-1281.699178

F	0.000000	1.630483	1.286789
F	0.000000	-1.630483	1.286789
F	-1.631545	0.000000	-1.286052
F	1.631545	0.000000	-1.286052
DY	0.000000	0.000000	-0.000201

$^{5}HoF_4^-$ ZPE=0.006019 dH_{298}=0.014057 $E_{M,0K}$=-1345.558202

F	0.000000	1.685926	1.192718
F	0.000000	-1.685926	1.192718
F	-1.686096	0.000000	-1.192653
F	1.686096	0.000000	-1.192653
HO	0.000000	0.000000	-0.000018

$^{4}ErF_4^-$ ZPE=0.006074 dH_{298}=0.014093 $E_{M,0K}$=-1412.562576

F	0.000000	1.677396	1.187557
F	0.000000	-1.677396	1.187557
F	-1.679326	0.000000	-1.186010
F	1.679326	0.000000	-1.186010
ER	0.000000	0.000000	-0.000409

$^{3}TmF_4^-$ ZPE=0.006279 dH_{298}=0.014162 $E_{M,0K}$=-1482.693522

F	0.000000	1.655574	-1.197746
F	0.000000	-1.655574	-1.197746
F	1.655791	0.000000	1.197527
F	-1.655791	0.000000	1.197527
TM	0.000000	0.000000	0.000057

$^{2}YbF_4^-$ ZPE=0.006223 dH_{298}=0.014168 $E_{M,0K}$=-1556.123953

F	0.000000	1.687048	1.137670
F	0.000000	-1.687048	1.137670
F	-1.657363	0.000000	-1.168013
F	1.657363	0.000000	-1.168013
YB	0.000000	0.000000	0.007802

$^{1}LuF_4^-$ ZPE=0.006349 dH_{298}=0.014225 $E_{M,0K}$=-1632.987867

F	1.163780	1.163780	1.163780
F	-1.163780	-1.163780	1.163780
F	-1.163780	1.163780	-1.163780
F	1.163780	-1.163780	-1.163780
LU	0.000000	0.000000	0.000000

$^{1}LaF_3$ ZPE=0.00415 dH_{298}=0.010793 $E_{M,0K}$=-733.794706

LA	0.000000	0.000000	0.136764
F	0.000000	2.088109	-0.288725
F	1.808355	-1.044054	-0.288725
F	-1.808355	-1.044054	-0.288725

$^{2}CeF_3$ ZPE=0.004708 dH_{298}=0.011178 $E_{M,0K}$=-773.186411

CE	0.000000	0.000000	0.100887
F	0.000000	1.992250	-0.216721
F	1.725339	-0.996125	-0.216721
F	-1.725339	-0.996125	-0.216721

$^{3}PrF_3$ ZPE=0.004109 dH_{298}=0.010811 $E_{M,0K}$=-815.018792

PR	0.003216	-0.000002	0.118620
F	-1.044481	1.772847	-0.257926
F	-1.045076	-1.772501	-0.257928
F	2.068474	-0.000335	-0.261765

$^{4}NdF_3$ ZPE=0.004388 dH_{298}=0.010915 $E_{M,0K}$=-859.371905

ND	0.000000	0.000009	0.166879
F	-1.740640	0.999183	-0.370841
F	1.735684	1.007767	-0.370841
F	0.004956	-2.007010	-0.370846

$^{5}PmF_3$ ZPE=0.004243 dH_{298}=0.01091 $E_{M,0K}$=-906.282224

PM	0.000000	0.000000	0.054160
F	0.000000	2.066454	-0.122362
F	1.789602	-1.033227	-0.122362
F	-1.789602	-1.033227	-0.122362

$^{6}SmF_3$ ZPE=0.004345 dH_{298}=0.010932 $E_{M,0K}$=-955.852089

SM	-0.000053	-0.009245	0.106543
F	0.004562	2.021968	-0.237201
F	1.778074	-0.982887	-0.248358
F	-1.782270	-0.975396	-0.248402

$^{7}EuF_3$ ZPE=0.004308 dH_{298}=0.010964 $E_{M,0K}$=-1008.174382

EU	0.000000	0.000000	0.000292
F	0.000000	2.053881	-0.000682
F	1.778713	-1.026941	-0.000682
F	-1.778713	-1.026941	-0.000682

$^{8}GdF_3$ ZPE=0.004494 dH_{298}=0.011009 $E_{M,0K}$=-1063.331750

GD	0.000000	0.000000	0.117972
F	0.000000	1.998901	-0.279636
F	1.731099	-0.999451	-0.279636
F	-1.731099	-0.999451	-0.279636

$^{7}TbF_3$ ZPE=0.004303 dH_{298}=0.010987 $E_{M,0K}$=-1121.159112

TB	0.011139	0.000017	0.034484
F	2.038128	0.000914	-0.086070
F	-1.058427	-1.718732	-0.081489
F	-1.060153	1.717693	-0.081495

$^{6}DyF_3$ ZPE=0.004487 dH_{298}=0.011047 $E_{M,0K}$=-1181.897622

DY	0.000000	0.000000	0.000000
F	0.000000	2.014458	0.000000
F	-1.744572	-1.007229	0.000000
F	1.744572	-1.007229	0.000000

$^{5}HoF_3$ ZPE=0.004581 dH_{298}=0.011078 $E_{M,0K}$=-1245.752204
HO 0.000000 -0.000035 0.000138
F 1.736136 -1.001762 -0.000373
F -1.735811 -1.002324 -0.000373
F -0.000325 2.004346 -0.000279

$^{4}ErF_3$ ZPE=0.004578 dH_{298}=0.011094 $E_{M,0K}$=-1312.718020
ER 0.000000 0.000000 0.000000
F 0.000000 1.994425 0.000000
F 1.727223 -0.997213 0.000000
F -1.727223 -0.997213 0.000000

$^{3}TmF_3$ ZPE=0.004626 dH_{298}=0.011123 $E_{M,0K}$=-1382.854328
TM 0.000000 0.000000 0.010800
F 0.000000 0.000000 1.995334
F 0.000000 -1.682535 -1.039066
F 0.000000 1.682535 -1.039066

$^{2}YbF_3$ ZPE=0.004697 dH_{298}=0.011155 $E_{M,0K}$=-1456.285878
YB -0.000061 0.000000 -0.000102
F 0.986652 -1.707437 0.000287
F 0.985964 1.707834 0.000287
F -1.972140 -0.000397 0.000218

$^{1}LuF_3$ ZPE=0.004691 dH_{298}=0.011188 $E_{M,0K}$=-1533.141778
LU 0.000000 0.000004 0.001752
F -1.697031 0.979882 -0.004607
F 1.697143 0.979689 -0.004607
F -0.000112 -1.959605 -0.004608

$^{2}LaF_2$ ZPE=0.002671 dH_{298}=0.007569 $E_{M,0K}$=-634.004426
LA 0.000000 0.000000 0.275772
F 0.000000 1.744532 -0.873279
F 0.000000 -1.744532 -0.873279

$^{3}CeF_2$ ZPE=0.002619 dH_{298}=0.007538 $E_{M,0K}$=-673.348447
CE 0.000000 0.000000 0.271680
F 0.000000 1.778340 -0.875413
F 0.000000 -1.778340 -0.875413

$^{4}PrF_2$ ZPE=0.002392 dH_{298}=0.007412 $E_{M,0K}$=-715.200795
PR 0.000000 0.000000 0.182532
F 0.000000 1.977017 -0.598301
F 0.000000 -1.977017 -0.598301

$^{5}NdF_2$ ZPE=0.002745 dH_{298}=0.007626 $E_{M,0K}$=-759.583573
F 0.000000 1.714067 -0.857997
F 0.000000 -1.714067 -0.857997
ND 0.000000 0.000000 0.257399

$^{6}PmF_2$ ZPE=0.00236 dH_{298}=0.007369 $E_{M,0K}$=-806.494166
PM 0.000000 0.000000 0.267467
F 0.000000 1.781747 -0.906416
F 0.000000 -1.781747 -0.906416

$^{7}SmF_2$ ZPE=0.002816 dH_{298}=0.007669 $E_{M,0K}$=-856.066294
SM 0.000000 0.000000 0.267601
F 0.000000 1.633914 -0.921737
F 0.000000 -1.633914 -0.921737

$^{8}EuF_2$ ZPE=0.002371 dH_{298}=0.007378 $E_{M,0K}$=-908.472758
EU 0.000000 0.000000 0.242518
F 0.000000 1.823799 -0.848812
F 0.000000 -1.823799 -0.848812

$^{9}GdF_2$ ZPE=0.002826 dH_{298}=0.007675 $E_{M,0K}$=-963.557372
GD 0.000000 0.000000 0.237419
F 0.000000 1.693930 -0.844156
F 0.000000 -1.693930 -0.844156

$^{6}TbF_2$ ZPE=0.002679 dH_{298}=0.007558 $E_{M,0K}$=-1021.272949
TB 0.000000 0.000000 0.274742
F 0.000000 1.663424 -0.992123
F 0.000000 -1.663424 -0.992123

$^{5}DyF_2$ ZPE=0.002852 dH_{298}=0.007708 $E_{M,0K}$=-1082.149944
DY 0.000000 0.000000 0.202720
F 0.000000 1.748363 -0.743307
F 0.000000 -1.748363 -0.743307

$^{4}HoF_2$ ZPE=0.002467 dH_{298}=0.007433 $E_{M,0K}$=-1145.994052
F 0.000000 1.771355 -0.837163
F 0.000000 -1.771355 -0.837163
HO 0.000000 0.000000 0.224909

$^{3}ErF_2$ ZPE=0.002496 dH_{298}=0.007453 $E_{M,0K}$=-1212.948195
ER 0.000000 0.000000 0.218708
F 0.000000 1.767353 -0.826228
F 0.000000 -1.767353 -0.826228

$^{2}TmF_2$ ZPE=0.002466 dH_{298}=0.007453 $E_{M,0K}$=-1283.135028

TM	0.000000	0.000000	0.186835
F	0.000000	1.841683	-0.716201
F	0.000000	-1.841683	-0.716201

$^{1}YbF_2$ ZPE=0.002503 dH_{298}=0.007463 $E_{M,0K}$=-1356.608693

YB	0.000000	0.000000	0.201455
F	0.000000	1.782813	-0.783434
F	0.000000	-1.782813	-0.783434

$^{2}LuF_2$ ZPE=0.002947 dH_{298}=0.007768 $E_{M,0K}$=-1433.360228

LU	0.000000	0.000000	0.194286
F	0.000000	1.683702	-0.766351
F	0.000000	-1.683702	-0.766351