Supplementary Material

Pushing the limits in accurate vibrational structure calculations: Anharmonic frequencies of lithium fluoride clusters $(LiF)_n$, n=2-10

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Table 1 Anharmonic frequencies in cm^{-1} and IR intensities in km/mol for Li_4F_4(a) at the VCI level.

Mode	Sym.	Freq.	Int.	Mode	Sym.	Freq.	Int.	Mode	Sym.	Freq.	Int.	Mode	Sym.	Freq.	Int.
ZPVE	A_1	3774.2		6	T_2	470.5	3796.7	4	T_1	375.2	0.0	2	T_2	270.0	67.5
8	A_1	575.6	43.8	5	E	429.3	3.2	3	A_1	388.0	68.2	1	E	253.0	0.1
7	T_2	541.5	3389.7												

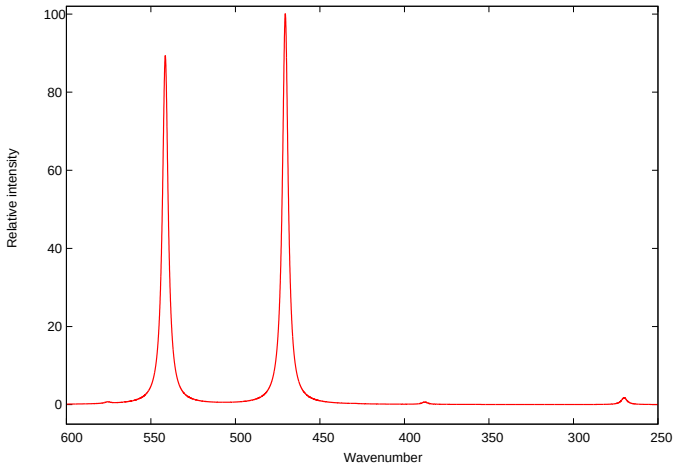

Fig. 1 Simulated IR spectra of Li_4F_4(a) at the VCI level.

Table 2 Anharmonic frequencies in cm^{-1} and IR intensities in km/mol for Li_4F_4(b) at the VCI level.

Mode	Sym.	Freq.	Int.	Mode	Sym.	Freq.	Int.	Mode	Sym.	Freq.	Int.	Mode	Sym.	Freq.	Int.
ZPVE	A_{1g}	3267.5		11	B_{1g}	500.3	0.0	7	A_{1g}	259.9	1.5	3	B_{1g}	102.3	0.0
14	E_u	768.9	3245.3	10	E_u	420.3	985.8	6	E_g	187.5	0.0	2	B_{1u}	55.4	0.0
13	A_{2g}	757.8	0.0	9	A_{1g}	396.6	202.5	5	E_u	184.9	2066.2	1	B_{2g}	53.4	0.5
12	B_{2g}	744.9	9.0	8	A_{2u}	266.3	6859.5	4	B_{2u}	120.6	0.0				

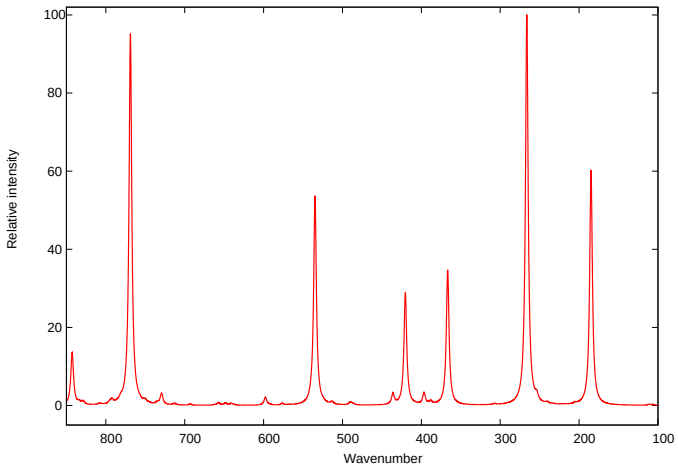

Fig. 2 Simulated IR spectra of Li_4F_4(b) at the VCI level.

Table 3 Anharmonic frequencies in cm^{-1} and IR intensities in km/mol for Li_4F_4(c) at the VCI level.

Mode	Sym.	Freq.	Int.	Mode	Sym.	Freq.	Int.	Mode	Sym.	Freq.	Int.	Mode	Sym.	Freq.	Int.
ZPVE	A_g	3383.6		14	A_g	592.7	10.4	9	A_g	293.9	1.6	4	B_u	175.7	10.8
18	B_u	725.7	196.8	13	B_u	602.0	57.3	8	B_u	257.9	113.6	3	A_u	121.5	38.6
17	A_g	714.4	0.2	12	B_u	367.7	46.6	7	A_g	252.6	4.7	2	B_g	110.3	0.5
16	B_u	654.7	223.6	11	A_g	335.5	0.2	6	B_g	240.8	0.0	1	A_u	38.9	0.1
15	A_g	652.4	21.0	10	A_u	323.4	417.0	5	A_g	147.6	0.3				

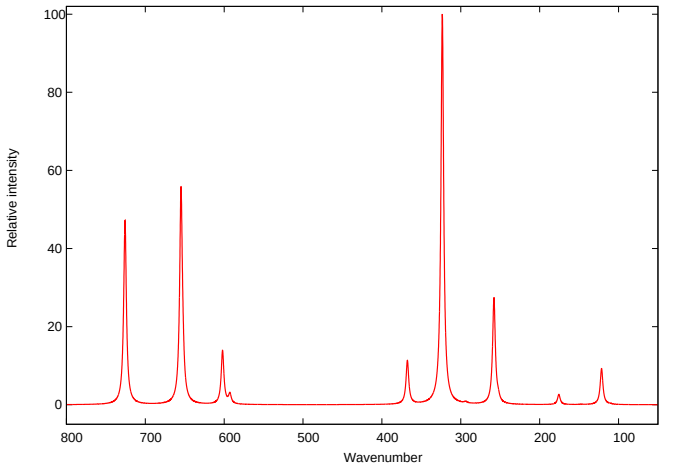

Fig. 3 Simulated IR spectra of Li_4F_4(c) at the VCI level.

Table 4 Anharmonic frequencies in cm^{-1} and IR intensities in km/mol for Li_4F_4(d) at the VCI level.

Mode	Sym.	Freq.	Int.	Mode	Sym.	Freq.	Int.	Mode	Sym.	Freq.	Int.	Mode	Sym.	Freq.	Int.
ZPVE	A1	3344.2		14	A1	543.4	7.8	9	B1	319.6	86.4	4	A2	181.8	0.0
18	A1	742.1	43.0	13	B2	524.7	109.9	8	A1	317.9	7.1	3	A2	136.6	0.0
17	B2	722.0	17.8	12	A1	509.2	28.5	7	B1	268.1	93.4	2	B2	105.0	31.6
16	A1	701.5	36.9	11	B2	335.8	69.0	6	B2	215.3	54.1	1	B1	79.1	11.4
15	B1	566.4	59.4	10	A1	338.7	12.4	5	A1	205.6	13.2				

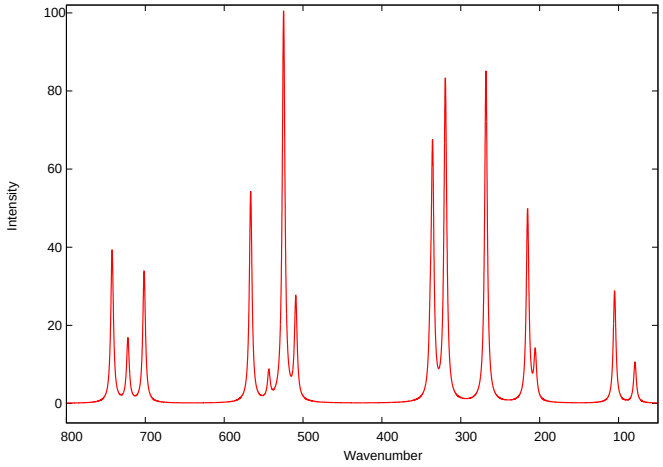

Fig. 4 Simulated IR spectra of Li_4F_4(d) at the VCI level.

Table 5 Anharmonic frequencies in cm^{-1} and IR intensities in km/mol for Li_4F_4(e) at the VCI level.

Mode	Sym.	Freq.	Int.	Mode	Sym.	Freq.	Int.	Mode	Sym.	Freq.	Int.	Mode	Sym.	Freq.	Int.
ZPVE	A1	3373.8		14	B1	586.5	142.2	9	B1	289.7	136.7	4	A2	129.1	0.0
18	B2	710.3	89.5	13	A1	540.1	66.8	8	A1	273.9	7.3	3	A2	96.0	0.0
17	A1	699.9	13.6	12	A1	444.4	2.5	7	B2	225.8	4.7	2	B2	84.3	19.0
16	B2	650.0	1.9	11	A1	379.7	14.1	6	B1	200.0	34.4	1	B1	91.2	15.4
15	A1	615.6	115.3	10	B2	314.2	80.4	5	A1	200.5	15.3				

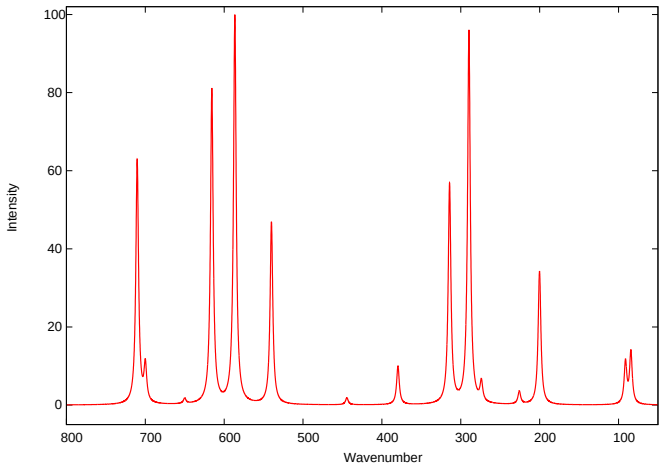

Fig. 5 Simulated IR spectra of Li_4F_4(e) at the VCI level.

Table 6 Anharmonic frequencies in cm^{-1} and IR intensities in km/mol for Li_5F_5 at the VCI level.

Mode	Sym.	Freq.	Int.	Mode	Sym.	Freq.	Int.	Mode	Sym.	Freq.	Int.	Mode	Sym.	Freq.	Int.
ZPVE	A1	4357.6		18	A1	532.3	28.8	12	A1	296.7	14.8	6	A1	138.0	35.8
24	B1	714.2	157.1	17	A1	516.3	18.4	11	A2	254.0	0.0	5	B2	130.8	13.8
23	A1	708.4	151.8	16	A1	446.6	1.8	10	B1	236.5	107.4	4	B1	123.6	15.8
22	B2	684.8	72.5	15	B2	400.7	211.9	9	A1	223.1	4.6	3	A2	112.6	0.0
21	A1	671.1	125.0	14	B1	360.1	246.5	8	B2	209.1	132.8	2	B2	72.9	12.0
20	B1	620.1	2.6	13	A1	319.9	1.1	7	A2	193.0	0.0	1	B1	46.2	7.3
19	B2	509.2	123.5												

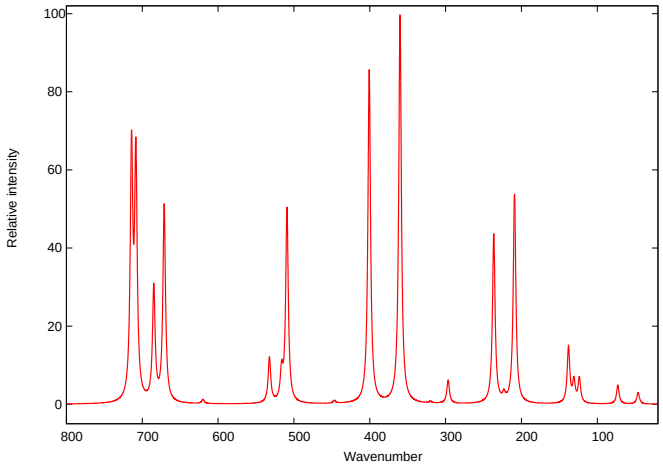

Fig. 6 Simulated IR spectra of Li_5F_5 at the VCI level.

Table 7 Anharmonic frequencies in cm^{-1} and IR intensities in km/mol for Li_6F_6 at the VCI level.

Mode	Sym.	Freq.	Int.	Mode	Sym.	Freq.	Int.	Mode	Sym.	Freq.	Int.
ZPVE	A_{1g}	5785.8		15	E_g	437.4	0.0	7	A_{1u}	264.1	42.2
22	E_u	621.9	48583.8	14	A_{1g}	383.5	0.0	6	A_{1g}	241.8	0.0
21	E_g	602.1	0.0	13	E_g	384.3	0.0	5	E_g	235.1	0.0
20	A_{1u}	579.1	16.0	12	A_{1u}	365.0	178.7	3	A_{2u}	207.7	23.1
19	A_{2g}	543.0	0.0	11	A_{2u}	376.5	96.3	2	E_u	157.6	1627.0
18	A_{1g}	504.5	0.0	10	A_{2u}	366.8	335.0	1	E_g	106.0	0.0
17	A_{2u}	487.9	737.4	9	A_{1g}	339.2	0.0				
16	E_u	455.4	16027.4	8	E_u	300.2	3622.1				

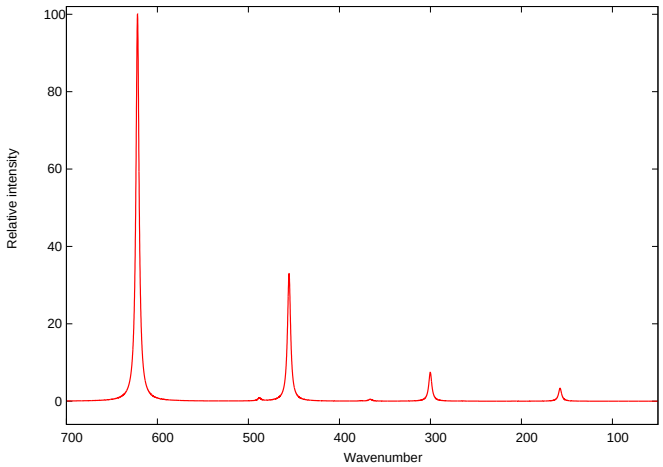

Fig. 7 Simulated IR spectra of Li_6F_6 at the VCI level.

Table 8 Anharmonic frequencies in cm^{-1} and IR intensities in km/mol for Li_7F_7 at the VCI level.

Mode	Sym.	Freq.	Int.	Mode	Sym.	Freq.	Int.	Mode	Sym.	Freq.	Int.	Mode	Sym.	Freq.	Int.
ZPVE	A′	6664.0		27	A″	473.2	109.1	18	A″	367.0	33.7	9	A″	184.4	6.3
36	A′	729.3	52.1	26	A′	483.0	221.7	17	A′	360.2	78.5	8	A′	180.9	4.8
35	A′	622.1	147.1	25	A″	448.6	76.2	16	A′	329.3	36.1	7	A′	160.3	111.4
34	A′	608.2	68.4	24	A′	441.1	12.8	15	A″	298.5	128.7	6	A″	150.1	56.0
33	A″	593.6	140.2	23	A″	405.3	0.0	14	A′	288.6	4.0	5	A″	133.4	1.5
32	A″	585.7	0.3	22	A′	414.7	99.0	13	A′	270.6	14.7	4	A′	129.1	3.8
31	A′	576.9	18.9	21	A′	387.6	34.4	12	A″	261.1	0.2	3	A″	99.4	14.3
30	A″	544.3	14.7	20	A″	377.8	62.2	11	A′	228.8	19.6	2	A′	98.5	17.7
29	A′	496.5	185.3	19	A′	379.5	24.7	10	A′	213.1	8.0	1	A″	72.2	0.5
28	A′	510.1	7.5												

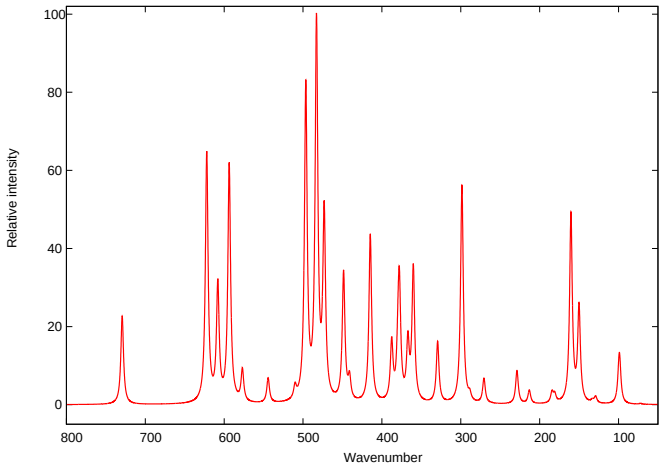

Fig. 8 Simulated IR spectra of Li_7F_7 at the VCI level.

Table 9 Anharmonic frequencies in cm^{-1} and IR intensities in km/mol for Li_8F_8 at the VCI level.

Mode	Sym.	Freq.	Int.	Mode	Sym.	Freq.	Int.	Mode	Sym.	Freq.	Int.	Mode	Sym.	Freq.	Int.
ZPVE	A	7817.6		24	B	480.0	383.3	16	B	389.2	38.1	8	B	214.1	13.3
32	B	657.7	510.1	23	B	457.7	4.8	15	E	361.9	91.5	7	B	187.7	8.1
31	E	639.1	76.3	22	A	436.3	0.0	14	B	340.9	70.2	6	A	174.8	0.0
30	A	609.2	0.0	21	E	441.8	69.6	13	A	310.4	0.0	5	E	149.6	31.8
29	B	604.1	66.9	20	B	409.9	6.9	12	E	267.9	71.8	4	B	126.1	15.0
28	A	595.3	0.0	19	E	400.7	13.0	11	E	266.7	0.1	3	E	116.7	3.7
27	E	570.8	436.8	18	A	404.9	0.0	10	A	248.8	0.0	2	A	94.9	0.0
26	E	505.5	235.4	17	A	386.6	0.0	9	B	213.5	6.5	1	B	89.2	1.5
25	A	509.2	0.0												

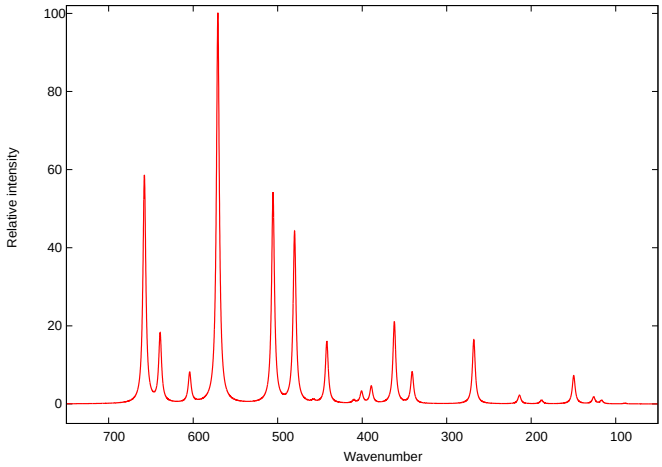

Fig. 9 Simulated IR spectra of Li_8F_8 at the VCI level.

Table 10 Anharmonic frequencies in cm^{-1} and IR intensities in km/mol for $Li_{10}F_{10}$ at the VCI level.

Mode	Sym.	Freq.	Int.	Mode	Sym.	Freq.	Int.	Mode	Sym.	Freq.	Int.	Mode	Sym.	Freq.	Int.
ZPVE	A_g	9808.9		41	A_g	493.7	0.0	27	B_g	370.7	0.0	13	A_g	199.3	0.0
54	A_u	665.6	635.8	40	B_g	495.7	0.0	26	B_u	357.2	136.3	12	A_u	188.2	14.6
53	A_g	654.3	0.0	39	A_u	499.0	298.9	25	A_u	344.5	52.7	11	B_u	162.8	46.3
52	B_u	656.3	143.5	38	B_u	457.5	242.4	24	B_u	340.2	98.2	10	B_g	154.3	0.0
51	B_g	642.2	0.0	37	A_g	428.0	0.0	23	A_g	316.4	0.0	9	A_g	140.0	0.0
50	A_g	610.5	0.0	36	B_g	444.6	0.0	22	A_g	276.6	0.0	8	B_g	133.8	0.0
49	B_g	610.0	0.0	35	A_u	437.5	2.4	21	A_u	274.8	1.4	7	B_g	111.5	0.0
48	A_u	608.1	99.2	34	A_g	416.1	0.0	20	B_g	268.6	0.0	6	B_u	109.5	35.3
47	B_u	604.7	576.9	33	A_u	417.3	7.2	19	B_u	255.4	147.0	5	A_u	95.8	17.1
46	A_u	603.4	1.5	32	B_u	415.2	35.4	18	A_g	246.5	0.0	4	B_u	95.2	7.5
45	B_g	564.6	0.0	31	B_g	405.3	0.0	17	A_g	237.8	0.0	3	A_g	87.4	0.0
44	B_u	546.6	774.1	30	A_g	398.3	0.0	16	B_u	237.0	89.5	2	A_g	69.9	0.0
43	A_g	523.0	0.0	29	A_g	379.0	0.0	15	B_g	225.3	0.0	1	A_g	62.1	0.0
42	B_u	510.6	248.4	28	A_u	384.8	2.2	14	B_u	204.0	60.1				

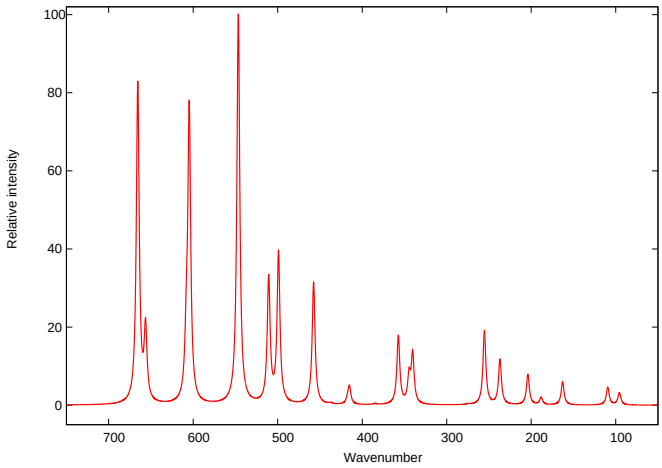

Fig. 10 Simulated IR spectra of $Li_{10}F_{10}$ at the VCI level.

Table 11 Equilibrium and vibrationally averaged geometry of Li_2F_2 at the DF-LCCSD(T)-F12a/cc-pVTZ-F12 level or VCI level in Å

Equilibrium structure				Vibrationally averaged structure			
Atom	X	Y	Z	Atom	X	Y	Z
Li	0.0000000000	1.1155555473	0.0000000000	Li	0.0000000000	1.1246487746	0.0000000000
F	0.0000000000	0.0000000000	-1.3274795329	F	0.0000000000	0.0000000000	-1.3347292166
Li	0.0000000000	-1.1155555473	0.0000000000	Li	0.0000000000	-1.1246487751	0.0000000000
F	0.0000000000	0.0000000000	1.3274795329	F	0.0000000000	0.0000000000	1.3347292166

Table 12 Equilibrium and vibrationally averaged geometry of Li_3F_3 at the DF-LCCSD(T)-F12a/cc-pVTZ-F12 level or VCI level in Å

Equilibrium structure				Vibrationally averaged structure			
Atom	X	Y	Z	Atom	X	Y	Z
Li	0.0000000000	0.0000000000	-1.6334717677	Li	0.0000000000	0.0000000005	-1.6392427313
F	0.0000000000	1.5497718716	-0.8947627753	F	0.0000000000	1.5558844486	-0.8982783096
Li	0.0000000000	1.4146324067	0.8167459238	Li	0.0000000000	1.4199002688	0.8197164463
F	0.0000000000	0.0000000000	1.7895181352	F	0.0000000000	0.0000000016	1.7964863964
Li	0.0000000000	-1.4146324067	0.8167459238	Li	0.0000000000	-1.4199002683	0.8197164463
F	0.0000000000	-1.5497718716	-0.8947627753	F	0.0000000000	-1.5558844502	-0.8982783123

Table 13 Equilibrium and vibrationally averaged geometry of Li_4F_4(a) at the DF-LCCSD(T)-F12a/cc-pVTZ-F12 level or VCI level in Å

Equilibrium structure				Vibrationally averaged structure			
Atom	X	Y	Z	Atom	X	Y	Z
Li	0.8618462130	0.8618462130	0.8618462130	Li	0.8697077940	0.8697418148	0.8697135483
F	0.9641675198	-0.9641675198	0.9641675198	F	0.9712904566	-0.9713238281	0.9712898449
Li	-0.8618462130	-0.8618462130	0.8618462130	Li	-0.8697060773	-0.8697436648	0.8697131852
F	-0.9641675198	0.9641675198	0.9641675198	F	-0.9712910149	0.9713244779	0.9712902650
Li	-0.8618462130	0.8618462130	-0.8618462130	Li	-0.8697069833	0.8697422545	-0.8697141002
F	-0.9641675198	-0.9641675198	-0.9641675198	F	-0.9712907677	-0.9713240011	-0.9712900004
Li	0.8618462130	-0.8618462130	-0.8618462130	Li	0.8697067997	-0.8697431361	-0.8697126672
F	0.9641675198	0.9641675198	-0.9641675198	F	0.9712907598	0.9713243604	-0.9712900967

Table 14 Equilibrium and vibrationally averaged geometry of Li_4F_4(b) at the DF-LCCSD(T)-F12a/cc-pVTZ-F12 level or VCI level in Å

Equilibrium structure				Vibrationally averaged structure			
Atom	X	Y	Z	Atom	X	Y	Z
Li	0.0000000000	2.1662763410	0.0000000000	Li	0.0000000016	2.1705109036	0.0000000000
F	1.6222250758	1.6222250758	0.0000000000	F	1.6256864563	1.6256935843	0.0000000000
Li	2.1662763410	0.0000000000	0.0000000000	Li	2.1704623770	-0.0000000026	0.0000000000
F	1.6222250758	-1.6222250758	0.0000000000	F	1.6256864584	-1.6256935886	0.0000000000
Li	0.0000000000	-2.1662763410	0.0000000000	Li	0.0000000048	-2.1705108999	0.0000000000
F	-1.6222250758	-1.6222250758	0.0000000000	F	-1.6256864537	-1.6256935954	0.0000000000
Li	-2.1662763410	0.0000000000	0.0000000000	Li	-2.1704623860	0.0000000000	0.0000000000
F	-1.6222250758	1.6222250758	0.0000000000	F	-1.6256864600	1.6256935992	0.0000000000

Table 15 Equilibrium and vibrationally averaged geometry of Li_4F_4(c) at the DF-LCCSD(T)-F12a/cc-pVTZ-F12 level or VCI level in Å

Equilibrium structure				Vibrationally averaged structure			
Atom	X	Y	Z	Atom	X	Y	Z
Li	1.1102112638	2.4435637681	0.0000000000	Li	1.1115679236	2.4398671227	0.0000000000
F	-0.5584592313	2.7685660175	0.0000000000	F	-0.5624843914	2.7705294592	0.0000000000
Li	-0.7903974432	1.0242634311	0.0000000000	Li	-0.8191120969	1.0298844153	0.0000000000
F	1.1970384815	0.7044507578	0.0000000000	F	1.2188171575	0.7035745217	0.0000000000
Li	0.7903974432	-1.0242634311	0.0000000000	Li	0.8175660760	-1.0282101161	0.0000000000
F	-1.1970384815	-0.7044507578	0.0000000000	F	-1.2181014199	-0.7017486481	0.0000000000
Li	-1.1102112638	-2.4435637681	0.0000000000	Li	-1.1129803933	-2.4448961012	0.0000000000
F	0.5584592313	-2.7685660175	0.0000000000	F	0.5628612079	-2.7711164697	0.0000000000

Table 16 Equilibrium and vibrationally averaged geometry of Li_4F_4(d) at the DF-LCCSD(T)-F12a/cc-pVTZ-F12 level or VCI level in Å

Equilibrium structure				Vibrationally averaged structure			
Atom	X	Y	Z	Atom	X	Y	Z
Li	1.0153577444	0.0000000000	-1.1671249056	Li	1.0271001309	-0.0000000111	-1.1976531299
Li	-1.0153577444	0.0000000000	-1.1671249056	Li	-1.0271001315	0.0000000085	-1.1976531357
F	0.0000000000	0.0000000000	-2.5744387008	F	0.0000000053	0.0000000000	-2.5963323809
F	0.0000000000	-1.3017798939	-0.1613199738	F	-0.0000000048	-1.3215035938	-0.1526258494
F	0.0000000000	1.3017798939	-0.1613199738	F	-0.0000000058	1.3215035949	-0.1526258494
Li	0.0000000000	-1.3510584341	1.5557003104	Li	0.0000000053	-1.3540043896	1.5681634416
Li	0.0000000000	1.3510584341	1.5557003104	Li	-0.0000000064	1.3540043901	1.5681634416
F	0.0000000000	0.0000000000	2.6100813181	F	0.0000000053	0.0000000000	2.6279294224

Table 17 Equilibrium and vibrationally averaged geometry of Li_4F_4(e) at the DF-LCCSD(T)-F12a/cc-pVTZ-F12 level or VCI level in Å

Equilibrium structure				Vibrationally averaged structure			
Atom	X	Y	Z	Atom	X	Y	Z
F	-1.2201750000	0.0000000000	1.2506941814	F	-1.2292193770	-0.0000000011	1.2658076137
F	1.2201750000	0.0000000000	1.2506941814	F	1.2292193754	0.0000000011	1.2658076105
Li	0.0000000000	0.0000000000	2.4781371814	Li	0.0000000011	0.0000000005	2.4927012527
Li	0.0000000000	1.1627590000	0.2839061815	Li	0.0000000000	1.1741983630	0.2775922015
Li	0.0000000000	-1.1627590000	0.2839061815	Li	-0.0000000016	-1.1741983635	0.2775922015
F	0.0000000000	1.4973030000	-1.4009208186	F	0.0000000011	1.5009027651	-1.4132586646
F	0.0000000000	-1.4973030000	-1.4009208186	F	0.0000000000	-1.5009027651	-1.4132586652
Li	0.0000000000	0.0000000000	-2.2323618185	Li	0.0000000011	0.0000000000	-2.2493297591

Table 18 Equilibrium and vibrationally averaged geometry of Li_5F_5 at the DF-LCCSD(T)-F12a/cc-pVTZ-F12 level or VCI level in Å

Equilibrium structure				Vibrationally averaged structure			
Atom	X	Y	Z	Atom	X	Y	Z
Li	0.0000000000	0.0000000000	-2.8660542289	Li	0.0000000000	0.0000000011	-2.8831880395
F	1.5176870000	0.0000000000	-2.0685602290	F	1.5218087268	0.0000000037	-2.0831838157
F	-1.5176870000	0.0000000000	-2.0685602290	F	-1.5218087268	-0.0000000026	-2.0831838146
Li	1.1546110000	0.0000000000	-0.3791552289	Li	1.1637341467	-0.0000000016	-0.3873374056
Li	-1.1546110000	0.0000000000	-0.3791552289	Li	-1.1637341467	0.0000000005	-0.3873374051
F	0.0000000000	-1.2934230000	0.3913017710	F	-0.0000000016	-1.3017409148	0.3986003614
F	0.0000000000	1.2934230000	0.3913017710	F	0.0000000021	1.3017409137	0.3986003604
Li	0.0000000000	1.3821660000	2.1164087710	Li	0.0000000037	1.3849422133	2.1291343074
Li	0.0000000000	-1.3821660000	2.1164087710	Li	-0.0000000037	-1.3849422128	2.1291343079
F	0.0000000000	0.0000000000	3.1298187711	F	-0.0000000005	0.0000000005	3.1474405080

Table 19 Equilibrium and vibrationally averaged geometry of Li_6F_6 at the DF-LCCSD(T)-F12a/cc-pVTZ-F12 level or VCI level in Å

Equilibrium structure				Vibrationally averaged structure			
Atom	X	Y	Z	Atom	X	Y	Z
Li	0.8673616608	1.7491637713	0.0000000000	Li	0.8771785241	1.7598497775	0.0000000360
F	1.0020896191	0.9166428663	1.5876580904	F	1.0098957252	0.9222412984	1.5973196056
Li	0.8673722012	-0.8745782656	1.5148191808	Li	0.8776181598	-0.8798084650	1.5241170353
F	1.0021025489	-1.8332575984	0.0000000000	F	1.0096826774	-1.8443892769	-0.0000000064
Li	0.8673722012	-0.8745782656	-1.5148191808	Li	0.8776183953	-0.8798084550	-1.5241169914
F	1.0020896191	0.9166428663	-1.5876580904	F	1.0098956686	0.9222413042	-1.5973196421
F	-1.0021025489	1.8332575984	0.0000000000	F	-1.0096826669	1.8443892139	-0.0000000085
Li	-0.8673722012	0.8745782656	1.5148191808	Li	-0.8776181244	0.8798082698	1.5241167951
F	-1.0020896191	-0.9166428663	1.5876580904	F	-1.0098957332	-0.9222412952	1.5973195014
Li	-0.8673616608	-1.7491637713	0.0000000000	Li	-0.8771786554	-1.7598493055	-0.0000000471
F	-1.0020896191	-0.9166428663	-1.5876580904	F	-1.0098958020	-0.9222412634	-1.5973194575
Li	-0.8673722012	0.8745782656	-1.5148191808	Li	-0.8776179465	0.8798082280	-1.5241168078

Table 20 Equilibrium and vibrationally averaged geometry of Li_7F_7 at the DF-LCCSD(T)-F12a/cc-pVTZ-F12 level or VCI level in Å

Equilibrium structure				Vibrationally averaged structure			
Atom	X	Y	Z	Atom	X	Y	Z
Li	0.9219672655	-1.3202210397	1.4646291862	Li	0.9336897832	-1.3279647581	1.4721586037
F	1.1467215016	-2.3396317845	0.0000000000	F	1.1578469555	-2.3553379810	0.0000000042
Li	0.9219672655	-1.3202210397	-1.4646291862	Li	0.9336897880	-1.3279647533	-1.4721585958
F	0.8889663402	0.4715496744	-1.4498002925	F	0.8954182576	0.4730356294	-1.4585660230
Li	1.3086106944	1.5294788858	0.0000000000	Li	1.3197542610	1.5411232864	-0.0000000016
F	0.8889663402	0.4715496744	1.4498002925	F	0.8954182560	0.4730356252	1.4585660187
Li	-0.9269744863	0.2688185995	1.3811618221	Li	-0.9344238658	0.2678435381	1.3890880834
F	-0.9360613999	-1.5182449929	1.5413561238	F	-0.9408005607	-1.5286394049	1.5485263623
Li	-0.7221670274	-2.4136783125	0.0000000000	Li	-0.7277844266	-2.4329264334	-0.0000000032
F	-0.9360613999	-1.5182449929	-1.5413561238	F	-0.9408005565	-1.5286394002	-1.5485263665
Li	-0.9269744863	0.2688185995	-1.3811618221	Li	-0.9344238653	0.2678435428	-1.3890880754
F	-1.6122132082	1.2762074763	0.0000000000	F	-1.6201420725	1.2871112578	0.0000000058
Li	-0.9652771683	2.9207519186	0.0000000000	Li	-0.9638723208	2.9363458788	0.0000000026
F	0.6861257673	3.1891953224	0.0000000000	F	0.6909433554	3.2073897366	-0.0000000069

Table 21 Equilibrium and vibrationally averaged geometry of Li_8F_8 at the DF-LCCSD(T)-F12a/cc-pVTZ-F12 level or VCI level in Å

Equilibrium structure				Vibrationally averaged structure			
Atom	X	Y	Z	Atom	X	Y	Z
Li	0.9581349529	1.5820410299	-0.7478321358	Li	0.9589107188	1.5946626339	-0.7541983239
F	-0.0003277843	1.9357855642	0.7148909752	F	0.0017261734	1.9459475052	0.7210962765
F	1.9357859795	0.0003278490	-0.7148911139	F	1.9459843635	-0.0017041289	-0.7210642978
Li	0.3038702236	1.1739699821	2.3214154579	Li	0.3088145601	1.1836685104	2.3391099522
Li	1.5820410427	-0.9581346202	0.7478320834	Li	1.5946832173	-0.9589149914	0.7541788592
F	1.3237027452	-0.3005157561	2.4144220435	F	1.3325613242	-0.3017519267	2.4325351259
F	-1.9357859795	-0.0003278490	-0.7148911139	F	-1.9459843794	0.0017041745	-0.7210643386
Li	-1.5820410427	0.9581346202	0.7478320834	Li	-1.5946832596	0.9589150591	0.7541788624
Li	-0.9581349529	-1.5820410299	-0.7478321358	Li	-0.9589108458	-1.5946628053	-0.7541983451
F	-1.3237027452	0.3005157561	2.4144220435	F	-1.3325613427	0.3017519140	2.4325351296
F	0.0003277843	-1.9357855642	0.7148909752	F	-0.0017260872	-1.9459474745	0.7210962765
Li	-0.3038702236	-1.1739699821	2.3214154579	Li	-0.3088145305	-1.1836685554	2.3391100581
Li	1.1739699781	-0.3038704338	-2.3214153485	Li	1.1836665021	-0.3088484259	-2.3391158340
F	0.3005157839	1.3237027280	-2.4144219260	F	0.3017750924	1.3325292513	-2.4325577265
Li	-1.1739699781	0.3038704338	-2.3214153485	Li	-1.1836664736	0.3088484137	-2.3391158409
F	-0.3005157839	-1.3237027280	-2.4144219260	F	-0.3017751030	-1.3325292555	-2.4325577546

Table 22 Equilibrium and vibrationally averaged geometry of $Li_{10}F_{10}$ at the DF-LCCSD(T)-F12a/cc-pVTZ-F12 level or VCI level in Å

Equilibrium structure				Vibrationally averaged structure			
Atom	X	Y	Z	Atom	X	Y	Z
Li	-1.6096229893	0.6989944790	-1.5708503267	Li	-1.6156126495	0.6895523866	-1.5841430048
F	-1.3527934375	0.1364724801	-3.2703281041	F	-1.3607340134	0.1364859752	-3.2965537976
Li	-0.1627728357	-1.2059717098	-3.1942541120	Li	-0.1638589041	-1.2133409883	-3.2203179936
F	1.3527934566	-0.1364723122	-3.2703281062	F	1.3607340832	-0.1364857784	-3.2965537643
Li	0.1627728423	1.2059718750	-3.1942540074	Li	0.1638589862	1.2133411937	-3.2203179645
F	-0.1810489144	1.8694112149	-1.5624003017	F	-0.1764586008	1.8684380680	-1.5752032644
Li	1.6096230309	-0.6989945609	-1.5708504065	Li	1.6156126966	-0.6895523581	-1.5841430630
F	1.7850406329	0.1594686448	-0.0000000523	F	1.7935613366	0.1589772846	0.0000000582
Li	1.6096228787	-0.6989943560	1.5708504073	Li	1.6156130083	-0.6895528729	1.5841429286
F	0.1810488305	-1.8694110876	1.5624003101	F	0.1764589040	-1.8684385823	1.5752035591
Li	-0.6701130691	-1.6334514130	-0.0000000755	Li	-0.6682907126	-1.6398321151	0.0000002963
F	0.1810488626	-1.8694111634	-1.5624004398	F	0.1764585061	-1.8684378489	-1.5752031935
F	-1.7850406426	-0.1594687861	-0.0000000214	F	-1.7935613620	-0.1589773984	0.0000000751
Li	-1.6096229079	0.6989943548	1.5708503592	Li	-1.6156129368	0.6895525438	1.5841430090
F	-0.1810488143	1.8694110582	1.5624003276	F	-0.1764589331	1.8684382765	1.5752034173
Li	0.6701131450	1.6334513541	-0.0000000267	Li	0.6682908174	1.6398320696	0.0000002413
Li	-0.1627728150	-1.2059718212	3.1942540774	Li	-0.1638587946	-1.2133410227	3.2203178354
F	-1.3527934459	0.1364723397	3.2703281740	F	-1.3607341991	0.1364858070	3.2965535256
Li	0.1627728071	1.2059717708	3.1942540746	Li	0.1638587808	1.2133410159	3.2203178502
F	1.3527934398	-0.1364723784	3.2703282273	F	1.3607341705	-0.1364857498	3.2965533341