

Gas phase basicity and nonlinear optical properties of FLi_nOH species ($n = 2-5$)

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Cartesian coordinates (x, y, z in Å), Frequency (in cm^{-1}) and Infrared intensity (in a.u.)

(1) FLi_2OH

F	-1.387790000	0.000064000	-0.000002000
Li	-0.061513000	-1.143908000	0.000032000
Li	-0.060942000	1.144023000	0.000032000
O	1.322570000	-0.000127000	-0.000048000
H	2.276914000	0.000091000	0.000214000

Frequency IR Intensity

276.8196	175.0454
357.7405	3.7632
403.6918	157.6727
520.8374	70.7397
556.7032	261.4034
626.9966	87.285
648.9774	0.9282
686.17	297.6193
4012.5763	21.9952

(2) FLi_3OH

Li	0.020520000	-1.007386000	0.000192000
Li	1.285380000	1.536765000	0.000130000
Li	-1.715612000	1.335721000	-0.000068000
F	-1.592082000	-0.368307000	-0.000018000
O	1.633397000	-0.206102000	-0.000056000

H	2.490696000	-0.631721000	-0.000153000
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Frequency	IR Intensity
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137.1795	3.9761
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144.0658	42.9185
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188.1805	16.0306
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189.4583	25.1868
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301.9084	42.4499
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330.2559	160.8483
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469.1565	38.4951
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572.2964	206.6367
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658.8293	20.4826
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670.6426	127.9367
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760.3241	93.2154
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3970.9163	13.0097
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(3) FLi₄OH

Li	1.424172000	1.179124000	0.367417000
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Li	1.423378000	-1.178151000	-0.367871000
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Li	-1.532513000	0.368096000	-1.177792000
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Li	-1.531934000	-0.367693000	1.177875000
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F	-2.725053000	-0.000180000	0.000093000
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O	2.691063000	-0.000035000	-0.000090000
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H	3.647667000	-0.002224000	0.000992000
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Frequency	IR Intensity
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115.3769	0.6835
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120.5839	5.6217
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139.8758	0.1517
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163.387	44.726
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165.3587	11.1533
316.4019	36.8378
344.3568	99.2756
359.6104	125.5429
522.7546	115.5348
628.6461	5.6653
640.6309	10.2734
680.3353	83.7715
694.8908	34.0286
3977.566	3.9639

(4) FLi₅OH

Li	0.000000000	1.265973000	-2.964472000
Li	0.000000000	-1.265973000	-2.964472000
Li	-0.964757000	0.820817000	3.061703000
Li	0.964757000	-0.820817000	3.061703000
F	0.000000000	0.000000000	4.216188000
O	0.000000000	0.000000000	-4.198604000
Li	0.000000000	0.000000000	0.071707000
H	0.000000000	0.000000000	-5.155368000

Frequency IR Intensity

47.5235	6.7435
87.9636	5.0279
101.0938	41.1612
126.0722	0.9874
167.7845	20.3993
174.9533	79.4408
242.997	621.1789

245.2672	198.6446
286.3247	377.3669
318.8724	124.2757
356.7169	440.8468
542.4606	81.0149
644.4414	39.831
661.5801	437.5372
676.7918	138.6199
688.892	218.286
3974.5346	1.8232