Superalkali-hydroxides as strong bases and superbases

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(A) FLi_2OH

Cartesian coordinates (Å)

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

Vibrational frequency (cm^{-1})	*IR intensity (a.u.)*
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

(B) OLi_3OH

Cartesian coordinates (Å)

O	-1.168445000	0.000043000	-0.000772000
Li	0.258455000	-1.090450000	-0.000116000

Li	0.258728000	1.090943000	-0.000116000
Li	-2.827788000	-0.000180000	0.001452000
O	1.702764000	-0.000133000	0.000183000
H	2.657261000	-0.000220000	0.001053000

Vibrational frequency (cm^{-1})	***IR intensity (a.u.)***
91.3321	52.627
120.9083	61.5722
296.1939	232.3801
344.0627	93.8225
353.4148	2.2148
497.4816	178.8685
539.7261	78.5454
624.1181	139.4422
631.8002	0.5611
676.6609	201.495
909.4555	302.7691
4008.4059	10.9983

(C) NLi_4OH

Cartesian coordinates (Å)

N	1.119137000	-0.000117000	0.000025000
Li	2.114062000	-1.489845000	-0.000057000
Li	2.112673000	1.490523000	0.000072000
Li	-0.444084000	-0.000087000	1.109650000
Li	-0.444128000	0.000086000	-1.109550000
O	-1.877133000	-0.000078000	-0.000234000

H	-2.832464000	-0.000587000	0.001350000

Vibrational frequency (cm^{-1})	***IR intensity (a.u.)***
102.6198	0.471
150.0318	0.0019
160.9118	44.5817
207.963	38.0233
281.4795	82.5169
296.9494	67.8076
350.3434	3.1624
479.5213	6.067
493.7895	164.5163
559.8287	69.6572
595.7089	69.9995
655.1751	109.7337
730.985	126.9237
790.837	43.2817
3995.0702	5.5193