

Distinguishing lactose and lactulose in the gas phase by complexation with sodiated L-Arginine by IRMPD and DFT methods

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Mode #	Frequency	Scaled Freq
197	3456.32	3290.42
198	3531.84	3362.31
199	3569.16	3397.84
200	3613.56	3440.11
201	3625.61	3451.58
202	3719.96	3541.41
203	3813.58	3630.53
204	3847.93	3663.23
205	3871.15	3685.34
206	3882.26	3695.91
207	3886.16	3699.62
208	3900.23	3713.02
209	3902.66	3715.33
210	3907.32	3719.77

OH stretch

Table S1. Calculated harmonic frequencies for lactose/ArgNa⁺ in Figure 4 (a)

Mode #	Frequency	Scaled Freq
197	3501.42	3333.35
198	3522.33	3353.26
199	3540.51	3370.57
200	3620.77	3446.97
201	3621.86	3448.02
202	3630.53	3456.27
203	3658.28	3482.68
204	3709.30	3531.26
205	3810.66	3627.75
206	3826.29	3642.63
207	3860.79	3675.48
208	3863.56	3678.11
209	3869.07	3683.36
210	3883.10	3696.71

OH stretch

Table S2. Calculated harmonic frequencies for lactulose/ArgNa⁺ in Figure 4 (b).

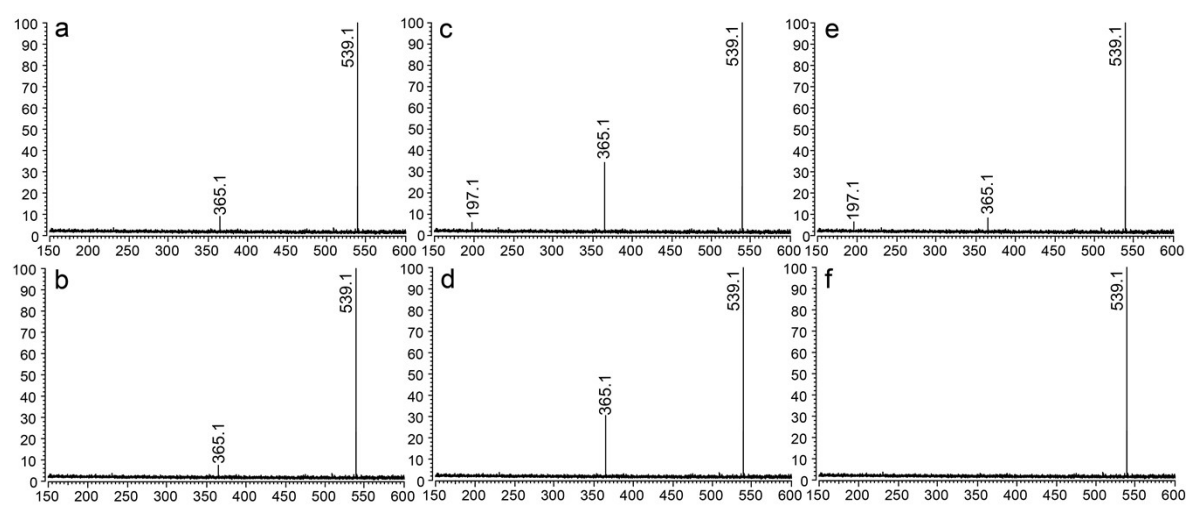
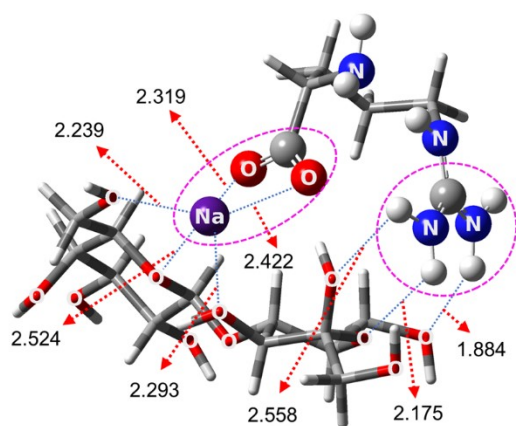
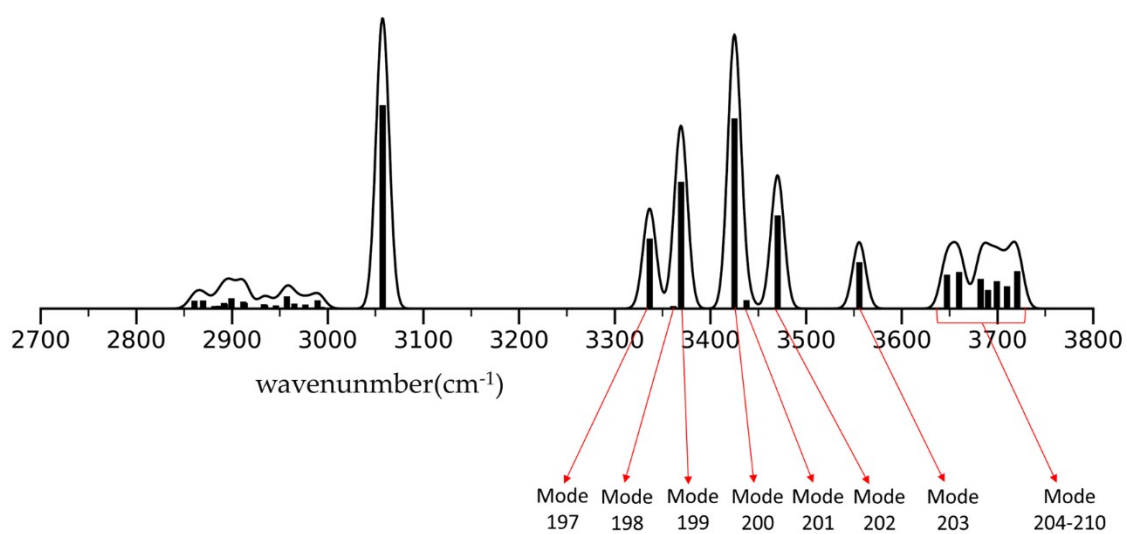


Figure S1 Tandem mass spectra of [lactose/ArgNa]⁺ and [lactulose/ArgNa]⁺, obtained with the method of (a, b) CID, (c, d) IRMPD at 3490 cm⁻¹ and (e, f) IRMPD at 3700 cm⁻¹, respectively.



197 – 199 : NH₂ symmetric stretching vibration
 200 - 203 : NH₂ asymmetric stretching vibration
 200, 204 - 210 : OH stretching vibration

Mode #	Frequency	Scaled Freq
197	3504.67	3336.45
198	3530.64	3361.17
199	3539.15	3369.27
200	3597.74	3425.05
201	3611.01	3437.69
202	3645.11	3470.14
203	3734.75	3555.48
204	3831.21	3647.31
205	3844.29	3659.76
206	3867.99	3682.33
207	3875.95	3689.90
208	3885.74	3699.23
209	3896.91	3709.86
210	3908.07	3720.48

↓
OH stretch

Figure S2. Calculated IR spectrum, structure and harmonic frequencies for the most stable lactulose/ArgNa⁺ in the gas phase.

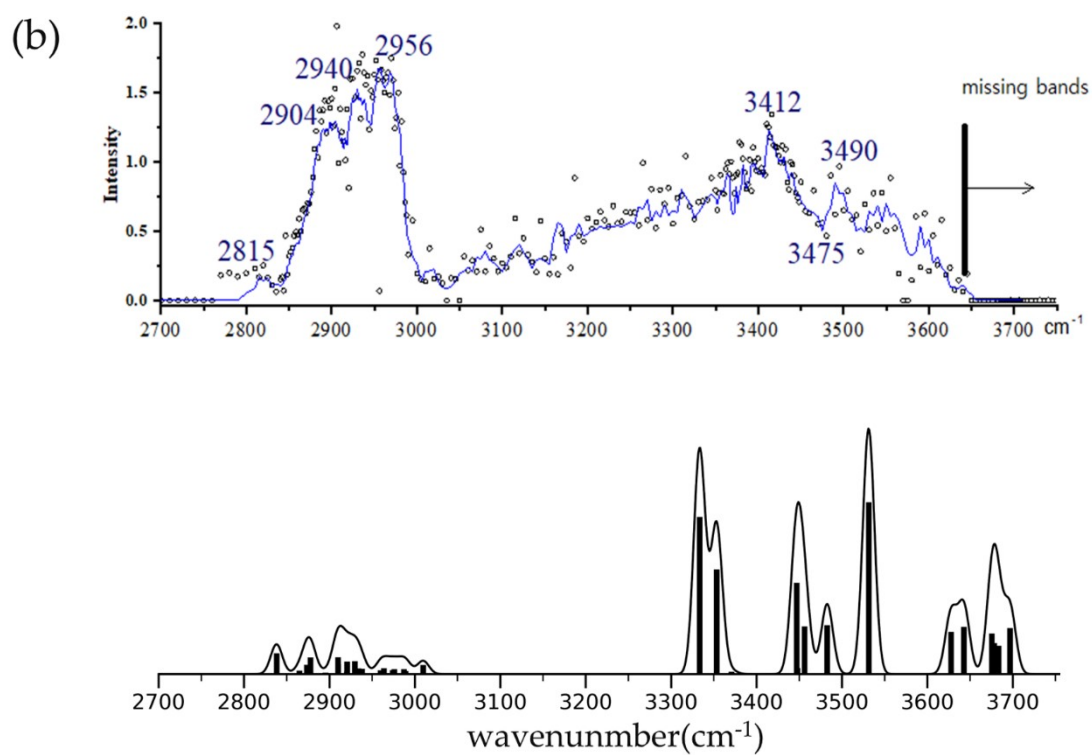
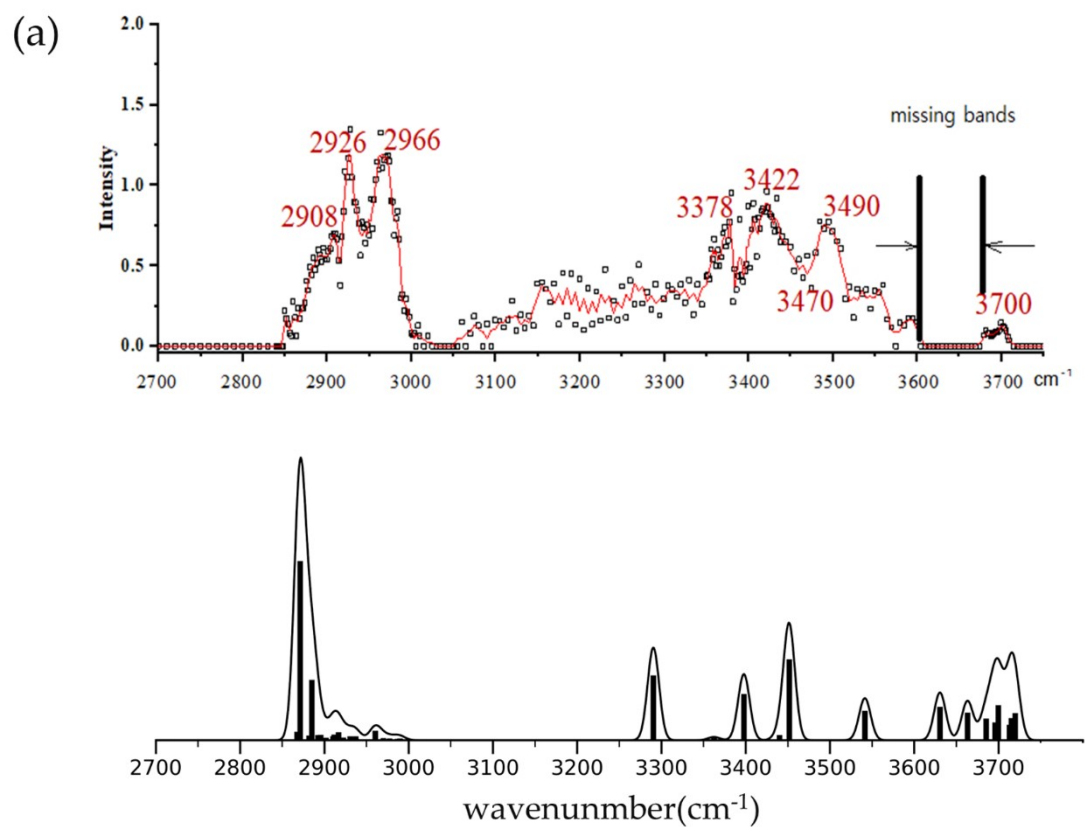


Figure S3. Comparison of experimental IRMPD and calculated IR spectra for (a) lactose/ ArgNa^+ and (b) lactulose/ ArgNa^+ complexes.

Cartesian Coordinates

Figure 5 (a)

O 1.2627460000 -1.6830590000 0.8372550000
O 2.5128390000 -0.4258080000 -0.5927420000
O -2.3530560000 -2.1109990000 0.8036190000
O 0.7137570000 -2.1369150000 -1.9414350000
O 2.7048640000 -0.6777390000 3.0481150000
O 5.1867930000 0.5161210000 2.4058680000
O 5.4276230000 -0.2857970000 -0.1696640000
O -1.5896910000 -3.6952420000 -2.3901520000
O -3.7759380000 -2.9436740000 -0.7421300000
O -2.1573800000 -1.1613760000 3.3823910000
O 2.7318940000 0.6573610000 -3.1229820000
C -0.0492260000 -1.6452220000 0.2938860000
C -0.1152580000 -2.6024700000 -0.8933030000
C 2.0151810000 -0.5125670000 0.7340430000
C -1.0564810000 -2.0285730000 1.3785730000
C 3.1704510000 -0.6237290000 1.7137820000
C 4.0432020000 0.6134620000 1.5903810000
C 4.5361200000 0.7562230000 0.1537940000
C -1.5375570000 -2.6972560000 -1.4097800000
C 3.3600140000 0.7113480000 -0.8186830000
C -2.4734360000 -3.0414470000 -0.2535740000
C -1.1156930000 -0.9505030000 2.4517460000
C 3.8597310000 0.6040720000 -2.2431180000
H -0.2900540000 -0.6274610000 -0.0490140000
H 0.2117600000 -3.6004650000 -0.5734040000
H 1.3954550000 0.3714830000 0.9440030000
H -0.7789600000 -3.0007120000 1.8142990000
H 3.7591330000 -1.5109370000 1.4569110000
H 3.4449190000 1.4951860000 1.8610810000
H 5.0285010000 1.7320000000 0.0485750000
H 2.7528190000 1.6179080000 -0.6976600000
H -1.8372750000 -1.7143030000 -1.8060020000
H -2.2574470000 -4.0553220000 0.1119280000
H -1.3377940000 0.0009430000 1.9593670000
H -0.1381730000 -0.8591210000 2.9350160000
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H 4.5371560000 1.4392310000 -2.4421950000
H 1.6309040000 -2.1806260000 -1.6367020000
H 2.4238280000 -1.5768220000 3.2382920000
H 4.9054460000 0.2899480000 3.2991160000
H 6.0798980000 -0.3381200000 0.5394560000
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H -4.3744470000 -3.4867520000 -0.2196640000
H -1.8890720000 -1.8110490000 4.0375210000
H 3.0432120000 0.6131980000 -4.0307970000
C -1.2086690000 3.5047470000 -1.0824540000
C -1.0916320000 4.0436680000 0.3543830000
C -1.5644460000 3.1487780000 1.5077670000
C -3.0689850000 2.8864140000 1.5997140000
N -3.5502250000 2.0943970000 0.4739160000
C -3.7705700000 0.7889320000 0.4549520000
N -4.0636250000 0.0867050000 1.5604520000
N -3.7580390000 0.1626140000 -0.7290110000
H -3.4243210000 2.5742280000 -0.4417650000
H -4.1075700000 0.5499740000 2.4532090000
H -3.7735930000 -0.8849290000 1.5882870000

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 H -3.1238360000 0.5410520000 -1.4326780000
 H -0.5073910000 4.0913130000 -1.6909400000
 H -0.0345720000 4.2530810000 0.5261410000
 H -1.6114440000 5.0077850000 0.3997850000
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 H -1.2617500000 3.6286190000 2.4431930000
 H -3.2957350000 2.3831990000 2.5403640000
 H -3.6231060000 3.8285040000 1.6051390000
 N -2.5744800000 3.6126730000 -1.6130350000
 H -2.8318640000 4.5865940000 -1.7382420000
 H -2.6177890000 3.1595690000 -2.5216260000
 C -0.6977660000 2.0623620000 -1.2155510000
 O 0.3977050000 1.7913350000 -0.6766360000
 O -1.3603850000 1.2468620000 -1.9189500000
 Na 0.6895200000 0.1483470000 -2.2923630000

Figure 5 (b)

O 0.4532920000 -2.0927040000 -0.2641550000
 O 3.1252880000 -0.8102360000 0.4655330000
 O -1.4333460000 -0.9769130000 -0.9273950000
 O 1.3621100000 0.6762730000 -2.2022790000
 O 3.8995320000 0.5281520000 -1.2054970000
 O -1.0606930000 -4.4962590000 0.1639940000
 O -3.5323870000 -3.6313390000 1.4907740000
 O -2.9568270000 -0.9367570000 1.4034780000
 O 5.1815670000 -2.1648350000 -0.8174750000
 O 3.8061840000 1.5456060000 1.6473800000
 O -3.0257710000 0.8353290000 -2.5168200000
 C 1.4942700000 -1.5204740000 -1.0546580000
 C 1.5090200000 0.0255790000 -0.9647000000
 C 2.8019300000 -1.9353210000 -0.3728200000
 C 2.8567450000 0.3557260000 -0.2726360000
 C -0.8238560000 -2.2611420000 -0.7704070000
 C -1.5100240000 -3.1665360000 0.2725810000
 C -3.0282520000 -3.0836640000 0.2966280000
 C -3.4492700000 -1.6253710000 0.2591960000
 C -2.8703260000 -0.9883340000 -0.9908210000
 C 3.9095420000 -2.2885460000 -1.3798930000
 C 2.8108580000 1.5787850000 0.6458900000
 C -3.3608340000 0.4272020000 -1.2017270000
 H 1.4189100000 -1.8698300000 -2.0910790000
 H 0.7038300000 0.3222850000 -0.2845170000
 H 2.6400000000 -2.7732760000 0.3045970000
 H -0.7912120000 -2.7553610000 -1.7569930000
 H -1.1634270000 -2.8304760000 1.2517540000
 H -3.4558140000 -3.5952400000 -0.5789970000
 H -4.5422960000 -1.5648410000 0.2218360000
 H -3.1887650000 -1.5883210000 -1.8566410000
 H 3.8124230000 -1.6850580000 -2.2884290000
 H 3.7765340000 -3.3368610000 -1.6590410000
 H 1.8456290000 1.6424520000 1.1487270000
 H 2.8908150000 2.4701800000 0.0213330000
 H -2.9118280000 1.0990560000 -0.4663670000
 H -4.4471810000 0.4406250000 -1.0691270000
 H 1.1886470000 1.6475640000 -1.9207950000
 H 3.5185650000 0.8514910000 -2.0337670000
 H -1.3574220000 -4.8801840000 -0.6682960000

H -3.1464880000 -4.5030090000 1.6340450000
 H -3.3054880000 -1.4085120000 2.1718430000
 H 5.3352830000 -1.2244800000 -0.6732800000
 H 4.6729010000 1.6195910000 1.2354290000
 H -2.7942990000 1.7778770000 -2.4633020000
 O 0.7696890000 2.8292570000 -1.0291590000
 O -1.1316170000 2.6177260000 -2.1544520000
 N -2.5615600000 4.0493110000 -0.4320380000
 N 0.1460680000 1.3618590000 3.3026400000
 N 2.0159290000 -0.0052740000 3.1499720000
 N 0.0306260000 -0.6430170000 2.1642250000
 C -0.8266910000 3.5552640000 1.2420530000
 C -1.4576420000 2.2008480000 1.5580780000
 C -1.1207980000 4.0130800000 -0.1957060000
 C -1.2424720000 1.7283940000 2.9955800000
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 H 0.2583870000 3.5246890000 1.3725030000
 H -1.2214330000 4.3087950000 1.9333680000
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 H 2.6042830000 0.7791690000 3.4058970000
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 Na -0.7911980000 0.5552570000 -2.9383950000

Figure S2

O -1.5639800000 1.4524520000 1.1447130000
 O 1.8080610000 2.4970240000 0.5305800000
 O -2.6441810000 0.2632530000 -0.4794110000
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 O 1.8386370000 2.0124030000 -1.7283340000
 O -3.0412210000 0.1421380000 3.1588570000
 O -5.3998220000 -1.1324560000 2.2716220000
 O -5.5646570000 -0.1157830000 -0.2290270000
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 O 2.9899970000 4.4155450000 -1.3297690000
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 C 0.7845750000 2.1199480000 1.4412670000
 C 1.2619440000 2.8210020000 -0.7650880000
 C -2.2303910000 0.2569010000 0.8838970000
 C -3.4358320000 0.1963460000 1.8052060000
 C -4.2106690000 -1.0777140000 1.5206950000
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N 4.1497830000 -1.9263440000 0.3408590000
C 4.0151990000 -0.7361790000 0.9229770000
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C 0.9875320000 -1.7508530000 -1.2128560000
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O 1.5335950000 -0.6931900000 -1.6575120000
Na -0.7623380000 -0.0797240000 -2.1263620000