Supporting information for:

Structures of the (Imidazole)$_n$H$^+$ ... X (n=1,2,3) complexes determined from IR spectroscopy and quantum chemical calculations

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1.1 ImH^+ and $ImH^+ \cdot X$

Table S1 Structure of ImH^+ at B3LYP-D3/def-TZVPP

```
################################################################################
10
 ImH+
  N   0.00701163470661     -0.00406658004790     -0.11710526137501
  C   1.21404676191123      0.54827314363036     -0.21268086716380
  N   2.09961472323941     -0.44486816014170     -0.20130077820056
  C   1.44803459078702     -1.65759032673618     -0.09622595143088
  C   0.12101831244689     -1.37796432647204     -0.04302781407143
  H   1.43278453405042      1.59921528425576     -0.28600957573791
  H   3.10011080884571     -0.31895372867882     -0.26223770173535
  H   1.97350067824314     -2.59459883864073     -0.06896749887742
  H  -0.73367658322022     -2.02396982014295      0.03954172808795
  H  -0.85940331560565      0.51501030412125     -0.10166371821554
################################################################################
```

Table S2 Structure of $ImH^+ \cdot He(\sigma)$ at B3LYP-D3/def-TZVPP

```
################################################################################
11
 ImH+ * He(sigma)
  N   6.71783015352535      0.81997230253018     -0.52920432842485
  C   7.17418017045641      2.06808679993092     -0.60269781481884
  N   6.11682702625796      2.87390966727804     -0.54915083209857
  C   4.96024953988534      2.12862285913831     -0.43932936850400
  C   5.34125240419639      0.82592820267226     -0.42672664523301
  H   8.20356176725025      2.36862327508083     -0.68948971019550
  H   6.16377448067181      3.88256496249599     -0.58543588250483
  H   3.98685929694574      2.58004734956267     -0.38051377641743
  H   4.76466960273509     -0.07798747153991     -0.35520284981698
  H   7.30111708962799     -0.00444185653184     -0.54681374366454
  He  6.19945846844767      5.98349390938254     -0.76403504832145
################################################################################
```

Table S3 Structure of $ImH^+ \cdot He(\pi)$ at B3LYP-D3/def-TZVPP

```
################################################################################
11
 ImH+ * He(pi)
  N   0.01244774599605      0.05184094951105     -0.16719239653697
  C   1.21565104186435      0.59334837745225     -0.34021712806664
  N   2.10525471518858     -0.38989996179629     -0.22931749856712
  C   1.46049605650141     -1.58457843876668      0.02061047794768
  C   0.13299956970203     -1.30416843875997      0.06005685016515
  H   1.42895804536327      1.62981322284268     -0.53400007339786
  H   3.10425303268125     -0.26950086635699     -0.31838438452322
  H   1.99056587685472     -2.51085677472166      0.14645990226070
  H  -0.71798407762663     -1.93848137040971      0.22753110307576
```

```
  H  -0.85584499330151      0.56701481564137     -0.19724172333893
  He  1.13280298674208      0.29282848536596      2.70795487108166
################################################################################
```

Table S4 Structure of $ImH^+ \cdot Ar(\sigma)$ at B3LYP-D3/def-TZVPP

```
################################################################################
11
 ImH+ * Ar(sigma)
  N   6.71725249420075      0.79171339730907     -0.52063269502455
  C   7.17230268400405      2.03972858179974     -0.61227957662288
  N   6.11545159682804      2.84561849582676     -0.56789674745471
  C   4.96018715317108      2.10143302681696     -0.44579295491071
  C   5.34099812750722      0.79873660482106     -0.41568120996473
  H   8.20125254815201      2.33966270099588     -0.70537696251373
  H   6.16146753417528      3.85665997555728     -0.61863082564503
  H   3.98685627426305      2.55352580721340     -0.39143782844982
  H   4.76475714592957     -0.10414582079672     -0.33041897594468
  H   7.30087388531936     -0.03243343480597     -0.52778226535854
  Ar  6.20838055644962      6.25832066526255     -0.73266995811062
################################################################################
```

Table S5 Structure of $ImH^+ \cdot Ar(\pi)$ at B3LYP-D3/def-TZVPP

```
################################################################################
11
 ImH+ * Ar(pi)
  N  -0.00639613523758      0.01850352033689     -0.22797924705222
  C   1.19127106725474      0.56477542070235     -0.42178713352924
  N   2.09023020580787     -0.40490852150807     -0.27542345277299
  C   1.45751546581177     -1.59487579548041      0.02274447992990
  C   0.12757522778235     -1.32617196036953      0.05255295638943
  H   1.39439203660824      1.59521549972033     -0.65377879992710
  H   3.08808271448768     -0.27712407714684     -0.36497651185171
  H   1.99699575968770     -2.50979650780979      0.18552114279969
  H  -0.71702097531360     -1.96138647835436      0.24637645603583
  H  -0.87939551694346      0.52409000747632     -0.27424873116470
  Ar  1.26635015005429      0.50903889243311      3.08725884114311
################################################################################
```

1.2 Im_2H^+ and $Im_2H^+ \cdot X$

Table S6 Structure of Im_2H^+ at B3LYP-D3/def-TZVPP

```
################################################################################
19
 Im2H+
  C   1.79886619763377      0.92618574593186     -1.33564567010294
  C   3.13883272417431      0.70965439092448     -1.42282561955004
  H   1.17040481291461      1.62110132362233     -1.86185889782803
  H   3.89694516663274      1.17108389464056     -2.02796823647276
  N   3.42116670268346     -0.29803121885585     -0.52508312517637
```

```
  N   1.29738911824424      0.05504809479100     -0.39499621794585
  C   2.29071796673934     -0.67677830761060      0.08352129868162
  H   0.23950330713089     -0.02734543786162     -0.08610485901073
  H   4.33201788466581     -0.69336318147529     -0.35082534213116
  H   2.20971447997270     -1.44527106857846      0.83153658472387
  N  -1.25402659543165     -0.15824220601362      0.32073923184397
  N  -3.21206705405850      0.12946403060922      1.25610395792042
  C  -1.92429083138355      0.53054342109612      1.22555782172276
  C  -2.15176669630468     -1.03624023782802     -0.25137323571683
  C  -3.37704838171767     -0.86765935709587      0.32279088584931
  H  -4.32205612915600     -1.35070634433638      0.15614223529112
  H  -1.86324415897837     -1.72056969516596     -1.02961381874390
  H  -1.52736587312441      1.30578316702119      1.85814642115478
  H  -3.92894327611034      0.49985833307651      1.85826349734006
################################################################################
```

Table S7 Structure of $ImH^+ \cdot Ar(\pi) \cdots Im$ at B3LYP-D3/def-TZVPP

```
################################################################################
20
 ImH+Ar(pi)...Im
  C   1.80211849393738      0.89902820573589     -1.44214481331873
  C   3.15266551181064      0.74222155309759     -1.47347005185380
  H   1.16053868286784      1.53609920496182     -2.02279590964614
  H   3.91055582999723      1.20375412470058     -2.07879701836404
  N   3.44881454365082     -0.20230334735965     -0.51303771326916
  N   1.30799515522858      0.05527218543731     -0.47353759432028
  C   2.31605997926292     -0.59969820213137      0.07854537851392
  H   0.25240661202375     -0.03449648124918     -0.16558394093101
  H   4.37029285608701     -0.54249587966643     -0.28658728506244
  H   2.24384313774151     -1.32519848901992      0.86900773502051
  N  -1.23316742111340     -0.15227826006667      0.28035234882130
  N  -3.16023665118583      0.20870678784408      1.25370870082713
  C  -1.87291357299199      0.60087087905256      1.15507911167143
  C  -2.14990053945024     -1.06441731627750     -0.20078588396112
  C  -3.35629259296500     -0.85077037939312      0.39789318174099
  H  -4.30732280180509     -1.34003261155049      0.29596191188571
  H  -1.88642001905813     -1.80243130306726     -0.93767773164814
  H  -1.45409361962595      1.41563281707837      1.72007348406357
  H  -3.85716521486637      0.62296443183128      1.85058240050870
 Ar   1.86711163045430      2.44549208004212      1.95289368932161
################################################################################
```

Table S8 Structure of $ImH^+ \cdot Ar(\sigma) \cdots Im$ at B3LYP-D3/def-TZVPP

```
################################################################################
20
 ImH+Ar(sigma)...Im
  C   2.35844053616316      0.22587523293492      0.33938771662137
  C   3.39577159430261     -0.65376042731572      0.33277591155841
  H   2.35088971719573      1.29329348074362      0.46265269207715
  H   4.45380933590231     -0.50750779680110      0.44837326378696
```

```
  N   2.83948384549553     -1.89969693991891      0.13654710284679
  N   1.20196811067964     -0.49567622525787      0.14914191653185
  C   1.51187260706304     -1.77739387232055      0.02802862711118
  H   0.18525887120322     -0.08002824990000      0.09453303842270
  H   3.34831582962695     -2.77042249071200      0.07923251387103
  H   0.81998091044827     -2.58495603689645     -0.13122945069333
  N  -1.25179706651566      0.53001715795703     -0.03647252160732
  N  -3.23384402929831      1.35777048394954      0.38859254356992
  C  -2.11096990187048      0.83025367312246      0.91967210330374
  C  -1.85081247569356      0.88096857059934     -1.22871993484891
  C  -3.08746444111111      1.39827680928270     -0.97879577238601
  H  -3.85283487732942      1.77965111625484     -1.62923644461641
  H  -1.36013261613791      0.74163273577800     -2.17573836358562
  H  -1.96369591571487      0.68612151527876      1.97623087365899
  H  -4.03919481191053      1.66945956698077      0.90629071632737
  Ar  4.60330477750140     -4.90008830375935     -0.10925653194987
################################################################################
```

Table S9 Structure of $\mathrm{Im} \cdot \mathrm{Ar}(\sigma) \cdots \mathrm{ImH}^+$ at B3LYP-D3/def-TZVPP

```
################################################################################
20
 ImAr(sigma)...ImH+
  C  -1.38935590475813      1.08363039981936     -1.70164863583455
  C  -2.33118112821566      2.06439962132256     -1.68335315977093
  H  -0.97906493296423      0.52798275995732     -2.52454078205869
  H  -2.89564116120856      2.52508920212218     -2.47257307781270
  N  -2.47709488921157      2.42778609726102     -0.36103688658565
  N  -0.98451828088330      0.87072446204506     -0.40321868483451
  C  -1.65130591024674      1.69141887824543      0.39254241146859
  H  -0.21800415808257      0.13980603898629     -0.07316630540616
  H  -3.10294554697175      3.13634251460432     -0.01071184553266
  H  -1.55033047086136      1.76032395394659      1.46121738125989
  N   0.87984974202400     -0.84840388225139      0.37303328089729
  N   1.95446864977135     -2.63560437057182      1.03903385304519
  C   0.75240403454411     -2.11772095895697      0.71543691391598
  C   2.22103802920143     -0.54362161194238      0.48158641291686
  C   2.90241008231377     -1.64972551577387      0.89642216889404
  H   3.94414259754948     -1.81915024968244      1.09762887925567
  H   2.60288833344219      0.43604004379132      0.25545618596051
  H  -0.16447582998267     -2.68099337778839      0.74003986217888
  H   2.12828782455746     -3.58316745467457      1.33497397128164
  Ar  2.87858891998272     -5.86110655045962      2.23852805676134
################################################################################
```

Table S10 Structure of $\mathrm{Im} \cdot \mathrm{Ar}(\pi) \cdots \mathrm{ImH}^+$ at B3LYP-D3/def-TZVPP

```
################################################################################
20
 ImAr(pi)...ImH+
  C   1.83976628510816      0.86468896391353     -1.38177793988185
  C   3.19374817507200      0.72538775511059     -1.46554783928512
```

```
 H   1.19732143825483     1.52837455960672    -1.93313133740073
 H   3.93133211826975     1.21615286240556    -2.07332532830879
 N   3.52025725683657    -0.25178159394224    -0.55366721238160
 N   1.34779103974461    -0.01129233782999    -0.43657778420690
 C   2.38516481198026    -0.67016705960315     0.04418776030224
 H  -0.14116719435544    -0.11395995198378    -0.00582864208436
 H   4.44593929947144    -0.60089884581941    -0.36722699931741
 H   2.35912080413878    -1.43311018817053     0.80319212159624
 N  -1.20642114119084    -0.16941401200017     0.28253074371814
 N  -3.08624406727251     0.24783605401530     1.25374269203190
 C  -1.79716166387993     0.60161236296292     1.18167991344959
 C  -2.13661396092874    -1.04058128598941    -0.23794101585395
 C  -3.32550541432698    -0.78372363874413     0.37055281310599
 H  -4.29537914915080    -1.23097926201448     0.25634541172366
 H  -1.88196607779443    -1.76320864625549    -0.99142037654627
 H  -1.32695229837712     1.38027790607945     1.75503883519380
 H  -3.76985579512553     0.67446709928038     1.85948049116367
 Ar  1.30171553352592     2.64623925897832     1.89937369298177
################################################################################
```

1.3 Im_3H^+ and Im_3H^+·Ar

Table S11 Structure of Im_3H^+ at B3LYP-D3/def-TZVP

```
################################################################################
28
 Im3H+
 N          -5.708503   -0.642541   -0.699540
 N          -3.662686   -0.160294   -0.077148
 C          -4.509693   -0.154309   -1.087080
 C          -5.624277   -0.979009    0.631418
 C          -4.348154   -0.673530    1.003300
 H          -4.304344    0.186015   -2.088001
 H          -6.454514   -1.391422    1.175401
 H          -3.886058   -0.787696    1.968484
 H          -2.096430    0.360504   -0.026240
 N           3.662462   -0.160844   -0.077148
 N           5.708404   -0.642290   -0.699698
 C           4.509379   -0.154689   -1.087167
 C           4.348257   -0.673632    1.003305
 C           5.624470   -0.978622    0.631355
 H           4.303716    0.185340   -2.088127
 H           3.886370   -0.787792    1.968591
 H           6.454935   -1.390743    1.175205
 H           6.522259   -0.740304   -1.284365
 N           1.082852    0.699986    0.047450
 N          -1.082768    0.700258    0.046983
 C          -0.000028   -0.052388   -0.131636
 C          -0.680870    1.979010    0.352723
 C           0.681126    1.978845    0.353011
 H          -1.384983    2.768340    0.543000
 H           1.385388    2.767991    0.543492
```

```
 H           2.096498    0.359976   -0.026011
 H          -0.000093   -1.099292   -0.378914
 H          -6.522331   -0.740896   -1.284185
################################################################################
```

Table S12 Structure of $Im_3H^+ \ldots Ar$ conformers at B3LYP-D3/def-TZVPP level of theory.

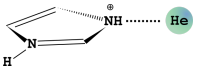
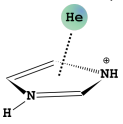
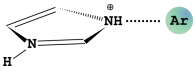
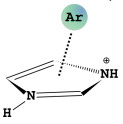
```
################################################################################
29
 Im3H+...Ar(mid) #1
  N    0.96173052993243      0.78375613861156      5.72396619411939
  N    0.53962588841385      0.19726333296925      3.65373526080139
  C    1.48367594101335      0.32345750434272      4.56518320225043
  C   -0.39074465061287      0.96141369228299      5.54431151192227
  C   -0.63722333052824      0.59286267900652      4.25405595704959
  H    2.52818401585136      0.09882574356626      4.43442659328087
  H   -1.03315066934536      1.32163501565166      6.32645373152315
  H   -1.57469338104358      0.58569524214239      3.72650184147592
  H    0.62677092465562     -0.34907538590648      2.09316509002721
  N    0.53962584516261      0.19726327942600     -3.65373529257701
  N    0.96173055086077      0.78375580533598     -5.72396629201653
  C    1.48367584245956      0.32345687610855     -4.56518336516909
  C   -0.63722322084083      0.59286330994364     -4.25405585684199
  C   -0.39074450094845      0.96141414677962     -5.54431145245042
  H    2.52818380064053      0.09882449414478     -4.43442688822384
  H   -1.57469319577851      0.58569646291233     -3.72650162630381
  H   -1.03315042256428      1.32163585006387     -6.32645358428967
  H    1.47430350240245      0.96324568169086     -6.57117066013179
  N    0.61173075872339     -0.69863169244986     -1.08272069206679
  N    0.61173080379404     -0.69863167469327      1.08272071901862
  C    0.71049994290213      0.06870754100095      0.00000000976288
  C    0.43863058105173     -2.00228487247075      0.68118595164697
  C    0.43863055434859     -2.00228489080872     -0.68118591813504
  H    0.32974689758997     -2.80626859303654      1.38514539954665
  H    0.32974685423224     -2.80626863062676     -1.38514537067890
  H    0.62677084814168     -0.34907543918025     -2.09316503392046
  H    0.84179182990287      1.13564284905686      0.00000000956253
  H    1.47430347868617      0.96324633027142      6.57117050447486
  Ar  -2.78749901910321     -0.19779379613555      0.00000005634261
29
 Im3H+...Ar(front) #2
  N    0.10212621174241     -0.88959592168821      5.68456092276284
  N    0.52062087112979     -0.14566222122321      3.66460531901958
  C   -0.41336841780762     -0.62170271287628      4.46415185060916
  C    1.43945837510032     -0.56674670363952      5.66504109399072
  C    1.68381139967960     -0.10623044752583      4.40425466703861
  H   -1.44658242307403     -0.78338693232306      4.20932968969533
  H    2.07418852484250     -0.68982149056092      6.52304041430167
  H    2.61058075704359      0.24768481186393      3.98844084981678
  H    0.37552469875672      0.35793634249872      2.09421842246370
  N    0.52062117098594     -0.14566213623734     -3.66460552867717
  N    0.10212588693186     -0.88959539186992     -5.68456117456928
```

```
  C   -0.41336854375461     -0.62170162709050     -4.46415214638114
  C    1.68381183007304     -0.10623165820174     -4.40425478713223
  C    1.43945839820334     -0.56674762760779     -5.66504124796992
  H   -1.44658274024283     -0.78338475417846     -4.20933008964987
  H    2.61058155278320      0.24768257711293     -3.98844090174879
  H    2.07418847478579     -0.68982311164825     -6.52304052909532
  H   -0.40542043944296     -1.25933897006010     -6.47090975025012
  N    0.29596038354832      0.69664909495311     -1.08278392989541
  N    0.29596017165266      0.69664891837317      1.08278429359231
  C    0.49176502499315     -0.05182219249579      0.00000014577374
  C   -0.03844417474243      1.96847945117102      0.68119390601714
  C   -0.03844404814039      1.96847958228734     -0.68119336345149
  H   -0.24408069769269      2.75329216573318      1.38518191206122
  H   -0.24408045793929      2.75329244122846     -1.38518125208397
  H    0.37552507811356      0.35793660483680     -2.09421815087535
  H    0.76250485547923     -1.09216441763147      0.00000010310047
  H   -0.40541977237163     -1.25934005877524      6.47090945501838
  Ar  -3.03273395063654     -0.17657761442502     -0.00000019348161
29
 Im3H+...Ar(side) #3
  N   -4.95235418015041     -1.69600640817706     -0.61236501150259
  N   -2.92415627703336     -1.05062127815188     -0.08588563504169
  C   -3.75797989363176     -1.27204286668625     -1.08237588913154
  C   -4.87838531570268     -1.74820116785701      0.76058754136438
  C   -3.61300970103624     -1.34409808307602      1.07176535387708
  H   -3.54732578518460     -1.13968700081016     -2.12958812618065
  H   -5.70635090545694     -2.05932104948724      1.37043025977640
  H   -3.16142780474411     -1.24500811733217      2.04301064988811
  H   -1.41973788212530     -0.36570060336575     -0.12514161144592
  N    4.35972247412344     -0.10290728406429     -0.04326208992918
  N    6.46950021924402     -0.41751194650230     -0.55214153300184
  C    5.22861459094412     -0.17889627895243     -1.03190141364884
  C    5.07452361798731     -0.30070170864093      1.11944232300035
  C    6.39057635173926     -0.49823988006977      0.81904540179470
  H    5.01045761662169     -0.06952914491433     -2.08028436740086
  H    4.60303588622489     -0.28706033169158      2.08622540603231
  H    7.25093730105202     -0.68238106523876      1.43558345986924
  H    7.30562004687871     -0.51699285042764     -1.10325945592698
  N    1.68225963691589      0.40942820014367     -0.09929525034622
  N   -0.46336408903592      0.11390882664575     -0.11178687325321
  C    0.71502463959444     -0.50422511892876     -0.13690396435808
  C   -0.24517954962597      1.47071165741745     -0.05461366751280
  C    1.10443600942029      1.65644856713091     -0.04677918142077
  H   -1.05437951302503      2.17630193009423     -0.02327770125122
  H    1.69116913444443      2.55541956079315     -0.00725887224401
  H    2.73155332407459      0.20325559769802     -0.10074052487333
  H    0.86194246508170     -1.56846330261667     -0.17873785814636
  H   -5.75476793054192     -1.93459971048870     -1.17083556382199
  Ar  -4.12429348705257      2.25344185755653      0.11350319483553
29
 Im3H+...Ar(NH) #4
  N    4.45558970139311     -0.18775402701099      0.33304093874567
```

```
  N    2.35455132012443     0.26124467796816    -0.10581722682043
  C    3.24039035218265     0.08686317825590     0.85562592097394
  C    4.34268039184796    -0.18879552495313    -1.03757997883698
  C    3.03235799607386     0.09160683043037    -1.29484743369321
  H    3.05117961123651     0.14945178241586     1.91337072407311
  H    5.17949748588752    -0.38228947966178    -1.68263513970331
  H    2.54106218203944     0.18226918391155    -2.24748365415982
  H    0.75486475355119     0.64747605442130     0.01062919481082
  N   -4.94684342772505    -0.33930213927256     0.08530341609805
  N   -6.92130079505893    -1.12428172563950     0.62778579216641
  C   -5.74294391876914    -0.64963420102321     1.08937917749828
  C   -5.64515402584407    -0.62676203716770    -1.06864106322800
  C   -6.87716625721111    -1.11685433630000    -0.74732835139549
  H   -5.51486956136945    -0.54906819119097     2.13649570280102
  H   -5.22306434611786    -0.46355026311870    -2.04449788350557
  H   -7.70052662434727    -1.44983314276680    -1.35180200476874
  H   -7.69645453084002    -1.42836435540672     1.19289083990161
  N   -2.44145376118461     0.73469472742159     0.10661496882088
  N   -0.28305085043870     0.91113281118563     0.04967388734875
  C   -1.29941878006960     0.05203653912907     0.06560951744554
  C   -0.79027500293061     2.18905229595164     0.07996740921393
  C   -2.14772316058686     2.07820653791662     0.11578003680748
  H   -0.15473764941830     3.05506039366897     0.07205067495377
  H   -2.91494541110952     2.82950082720292     0.14485258019263
  H   -3.42154613262279     0.30630683120473     0.12072695899880
  H   -1.21234949976540    -1.01937479342657     0.04637271480518
  H    5.30053495779186    -0.35959494220602     0.85230041967813
  Ar   7.93213798328076    -0.82481751193965     0.26677386077756
################################################################################
```

2 Motions in ImH^+ and $ImH^+ \ldots X$ (X=He,Ar)

Table S13 Theoretical frequencies for N–H stretching vibrations in ImH^+ and $ImH^+ \cdot X$ (He, Ar). ν_i and I_i denote frequency and relative intensity of the i-th N–H stretching vibration to the intensity of the second one (I_2). If the particle is symmetric enough (ImH^+, $ImH^+ \cdot He$ and $ImH^+ \cdot Ar(\pi)$) ν_1 and ν_2 correspond to symmetric and antisymmetric N–H stretching. In case of the non-symmetric ion $ImH^+ \cdot Ar(\sigma)$ they describe the stretching vibrations of two unequal N–H bonds ($\nu(N-H)$ and $\nu(N-H \cdots Ar)$, respectively). $\Delta E = E(ImH^+ \cdot X(\pi)) - E(ImH^+ \cdot X(\sigma))$ is the energy difference between optimized structures with different locations of He/Ar atom. D_e is the dissociation energy of the tag He/Ar computed as difference between optimized geometries $D_e = E(ImH^+) - E(ImH^+ \cdot X)$ at the same level of theory. "d2DZ" denotes def2-SVPD, "d2TZ" – def2-TZVPP, "accTZ" – aug-cc-pVTZ. All the values (except I) are given in cm^{-1}.

		ImH^+	$ImH^+ \cdot He$		$ImH^+ \cdot Ar$	
			$ImH^+ \cdot He(\sigma)$	$ImH^+ \cdot He(\pi)$	$ImH^+ \cdot Ar(\sigma)$	$ImH^+ \cdot Ar(\pi)$
						
B3LYP-D3/d2DZ[a]	ν_1	3498	3497	3497	3497	3498
	I_1	0.1	0.1	0.1	0.3	0.1
	ν_2	3491	3489	3489	3442	3491
	I_2	1.0	1.0	1.0	1.0	1.0
	ΔE	—	0	109	0	216
	D_e	—	500	391	925	710
B3LYP-D3/d2TZ[b]	ν_1	3490	3490	3490	3490	3492
	I_1	0.1	0.1	0.1	0.3	0.1
	ν_2	3483	3481	3484	3423	3486
	I_2	1.0	1.0	1.0	1.0	1.0
	ΔE	—	0	36	0	171
	D_e	—	211	175	826	655
MP2/d2DZ[c]	ν_1	3472	3475	3472	3471	3473
	I_1	0.1	0.2	0.1	0.3	0.1
	ν_2	3466	3468	3466	3439	3467
	I_2	1.0	1.0	1.0	1.0	1.0
	ΔE	—	0	-64	0	38
	D_e	—	284	348	1132	1094
MP2/d2TZ	ΔE	—	0	39	0	128
	D_e	—	125	86	882	754

[a] – scale factor for harmonic frequency to fundamental transition was 0.9671.[S1]
[b] – scale factor for harmonic frequency to fundamental transition was 0.9657.[S1]
[c] – scale factor for harmonic frequency to fundamental transition was 0.9557.[S1]
[e] – energies computed as single point energy calculations on geometries from ri-B3LYP-D3/def2-TZVPP optimizations.

3 SAPT results

3.1 $ImH^+ \ldots Ar$

Table S14 SAPT+δMP2/aug-cc-pVTZ//B3LYP-D3/def2-TZVPP results for $ImH^+ \ldots Ar(\sigma)$. Calculations were done using Psi4.

```
-------------------------------------------------------
  Electrostatics                    -1.87531238 [kJ/mol]
    Elst10,r                        -1.52048854 [kJ/mol]
    Elst12,r                        -0.35482384 [kJ/mol]

  Exchange                          11.20673279 [kJ/mol]
    Exch10                          10.36850271 [kJ/mol]
    Exch10(S^2)                     10.33814198 [kJ/mol]
    Exch11(S^2)                      0.13113292 [kJ/mol]
    Exch12(S^2)                      0.70709716 [kJ/mol]

  Induction                        -11.11896456 [kJ/mol]
    Ind20,r                        -11.14775371 [kJ/mol]
    Ind22                           -0.70777687 [kJ/mol]
    Exch-Ind20,r                     3.14523132 [kJ/mol]
    Exch-Ind22                       0.19969243 [kJ/mol]
    delta HF,r (2)                  -1.83692259 [kJ/mol]
    delta MP2,r (2)                 -0.77143514 [kJ/mol]

  Dispersion                        -6.63517890 [kJ/mol]
    Disp20                          -7.02420941 [kJ/mol]
    Disp21                           0.69707915 [kJ/mol]
    Disp22 (SDQ)                     0.25944992 [kJ/mol]
    Disp22 (T)                      -1.02790407 [kJ/mol]
    Est. Disp22 (T)                 -1.13383599 [kJ/mol]
    Exch-Disp20                      0.56633743 [kJ/mol]

Total HF                            -0.99143082 [kJ/mol]
Total SAPT0                         -7.44930279 [kJ/mol]
Total SAPT2                         -7.47398100 [kJ/mol]
Total SAPT2+                        -7.65128792 [kJ/mol]
Total SAPT2+dMP2                    -8.42272306 [kJ/mol]

Special recipe for scaled SAPT0
  Electrostatics sSAPT0             -1.52048854 [kJ/mol]
  Exchange sSAPT0                   10.36850271 [kJ/mol]
  Induction sSAPT0                  -9.81165307 [kJ/mol]
  Dispersion sSAPT0                 -6.45286770 [kJ/mol]
Total sSAPT0                        -7.41650661 [kJ/mol]
-------------------------------------------------------
```

Table S15 SAPT+δMP2/aug-cc-pVTZ//B3LYP-D3/def2-TZVPP results for $ImH^+ \ldots Ar(\pi)$. Calculations were done using Psi4.

```
-------------------------------------------------------
  Electrostatics                    -2.09688913 [kJ/mol]
```

```
    Elst10,r                          -1.82969178 [kJ/mol]
    Elst12,r                          -0.26719735 [kJ/mol]

  Exchange                             6.80562330 [kJ/mol]
    Exch10                             6.29648855 [kJ/mol]
    Exch10(S^2)                        6.29125135 [kJ/mol]
    Exch11(S^2)                        0.15386672 [kJ/mol]
    Exch12(S^2)                        0.35526804 [kJ/mol]

  Induction                           -3.04836621 [kJ/mol]
    Ind20,r                           -4.52968134 [kJ/mol]
    Ind22                             -0.29802820 [kJ/mol]
    Exch-Ind20,r                       1.94579024 [kJ/mol]
    Exch-Ind22                         0.12802233 [kJ/mol]
    delta HF,r (2)                    -0.26635659 [kJ/mol]
    delta MP2,r (2)                   -0.02811266 [kJ/mol]

  Dispersion                          -8.45887266 [kJ/mol]
    Disp20                            -9.94583211 [kJ/mol]
    Disp21                             2.26385170 [kJ/mol]
    Disp22 (SDQ)                       0.21317896 [kJ/mol]
    Disp22 (T)                        -1.53833402 [kJ/mol]
    Est. Disp22 (T)                   -1.67519820 [kJ/mol]
    Exch-Disp20                        0.68512700 [kJ/mol]

Total HF                               1.61654908 [kJ/mol]
Total SAPT0                           -7.64415604 [kJ/mol]
Total SAPT2                           -7.57222450 [kJ/mol]
Total SAPT2+                          -6.77039204 [kJ/mol]
Total SAPT2+dMP2                      -6.79850470 [kJ/mol]

Special recipe for scaled SAPT0
  Electrostatics sSAPT0               -1.82969178 [kJ/mol]
  Exchange sSAPT0                      6.29648855 [kJ/mol]
  Induction sSAPT0                    -2.84538428 [kJ/mol]
  Dispersion sSAPT0                   -9.25899268 [kJ/mol]
Total sSAPT0                          -7.63758019 [kJ/mol]
-----------------------------------------------------------
```

3.2 $Im_2H^+ \ldots Ar$

Table S16 SAPT+δMP2/aug-cc-pVTZ//B3LYP-D3/def2-TZVPP results for Im$\cdots$Im$H^+ \ldots$Ar(π). Calculations were done using Psi4.

```
-----------------------------------------------------------
  Electrostatics                      -2.19994238 [kJ/mol]
    Elst10,r                          -1.92944209 [kJ/mol]
    Elst12,r                          -0.27050029 [kJ/mol]

  Exchange                             6.76730570 [kJ/mol]
    Exch10                             6.28945093 [kJ/mol]
    Exch10(S^2)                        6.28265545 [kJ/mol]
```

```
    Exch11(S^2)                        0.16118335 [kJ/mol]
    Exch12(S^2)                        0.31667142 [kJ/mol]

  Induction                           -1.38437156 [kJ/mol]
    Ind20,r                           -3.28119291 [kJ/mol]
    Ind22                             -0.27779214 [kJ/mol]
    Exch-Ind20,r                       2.14219513 [kJ/mol]
    Exch-Ind22                         0.18136239 [kJ/mol]
    delta HF,r (2)                    -0.26894950 [kJ/mol]
    delta MP2,r (2)                    0.12000547 [kJ/mol]

  Dispersion                          -9.40679794 [kJ/mol]
    Disp20                           -10.85287047 [kJ/mol]
    Disp21                             2.51512171 [kJ/mol]
    Disp22 (SDQ)                       0.11662166 [kJ/mol]
    Disp22 (T)                        -1.75277428 [kJ/mol]
    Est. Disp22 (T)                   -1.89787623 [kJ/mol]
    Exch-Disp20                        0.71220538 [kJ/mol]

Total HF                               2.95206156 [kJ/mol]
Total SAPT0                           -7.18860352 [kJ/mol]
Total SAPT2                           -7.07767880 [kJ/mol]
Total SAPT2+                          -6.34381166 [kJ/mol]
Total SAPT2+dMP2                      -6.22380619 [kJ/mol]

Special recipe for scaled SAPT0
  Electrostatics sSAPT0               -1.92944209 [kJ/mol]
  Exchange sSAPT0                      6.28945093 [kJ/mol]
  Induction sSAPT0                    -1.40098860 [kJ/mol]
  Dispersion sSAPT0                  -10.13835156 [kJ/mol]
Total sSAPT0                          -7.17933133 [kJ/mol]
-----------------------------------------------------------
```

Table S17 SAPT+δMP2/aug-cc-pVTZ//B3LYP-D3/def2-TZVPP results for Im$\cdots$ImH$^+\ldots$Ar(σ). Calculations were done using Psi4.

```
-----------------------------------------------------------
  Electrostatics                      -1.59173086 [kJ/mol]
    Elst10,r                          -1.26982904 [kJ/mol]
    Elst12,r                          -0.32190181 [kJ/mol]

  Exchange                             8.84335386 [kJ/mol]
    Exch10                             8.11014618 [kJ/mol]
    Exch10(S^2)                        8.09085580 [kJ/mol]
    Exch11(S^2)                        0.10759856 [kJ/mol]
    Exch12(S^2)                        0.62560912 [kJ/mol]

  Induction                           -7.76446385 [kJ/mol]
    Ind20,r                           -7.93797240 [kJ/mol]
    Ind22                             -0.54861972 [kJ/mol]
    Exch-Ind20,r                       2.32765678 [kJ/mol]
    Exch-Ind22                         0.16087211 [kJ/mol]
    delta HF,r (2)                    -1.26053373 [kJ/mol]
```

delta MP2,r (2)	-0.50586690 [kJ/mol]
Dispersion	-6.00635056 [kJ/mol]
Disp20	-6.28386835 [kJ/mol]
Disp21	0.62737010 [kJ/mol]
Disp22 (SDQ)	0.21168466 [kJ/mol]
Disp22 (T)	-0.94811382 [kJ/mol]
Est. Disp22 (T)	-1.04082501 [kJ/mol]
Exch-Disp20	0.47928803 [kJ/mol]
Total HF	-0.03053221 [kJ/mol]
Total SAPT0	-5.83511253 [kJ/mol]
Total SAPT2	-5.81155426 [kJ/mol]
Total SAPT2+	-6.01332451 [kJ/mol]
Total SAPT2+dMP2	-6.51919140 [kJ/mol]
Special recipe for scaled SAPT0	
Electrostatics sSAPT0	-1.26982904 [kJ/mol]
Exchange sSAPT0	8.11014618 [kJ/mol]
Induction sSAPT0	-6.85416069 [kJ/mol]
Dispersion sSAPT0	-5.80114395 [kJ/mol]
Total sSAPT0	-5.81498750 [kJ/mol]

Table S18 SAPT+δMP2/aug-cc-pVTZ//B3LYP-D3/def2-TZVPP results for $ImH^+ \cdots Im \ldots Ar(\sigma)$. Calculations were done using Psi4.

Electrostatics	-1.34446928 [kJ/mol]
Elst10,r	-1.05189520 [kJ/mol]
Elst12,r	-0.29257409 [kJ/mol]
Exchange	6.86922380 [kJ/mol]
Exch10	6.22060955 [kJ/mol]
Exch10(S^2)	6.20881221 [kJ/mol]
Exch11(S^2)	0.08750581 [kJ/mol]
Exch12(S^2)	0.56110844 [kJ/mol]
Induction	-5.15329727 [kJ/mol]
Ind20,r	-5.37013971 [kJ/mol]
Ind22	-0.44908652 [kJ/mol]
Exch-Ind20,r	1.70406748 [kJ/mol]
Exch-Ind22	0.14250537 [kJ/mol]
delta HF,r (2)	-0.82763467 [kJ/mol]
delta MP2,r (2)	-0.35300921 [kJ/mol]
Dispersion	-5.39449584 [kJ/mol]
Disp20	-5.59810556 [kJ/mol]
Disp21	0.59599138 [kJ/mol]
Disp22 (SDQ)	0.15947025 [kJ/mol]
Disp22 (T)	-0.87336711 [kJ/mol]
Est. Disp22 (T)	-0.95415060 [kJ/mol]
Exch-Disp20	0.40229869 [kJ/mol]

```
Total HF                                0.67500745 [kJ/mol]
Total SAPT0                            -4.52079942 [kJ/mol]
Total SAPT2                            -4.47134041 [kJ/mol]
Total SAPT2+                           -4.67002939 [kJ/mol]
Total SAPT2+dMP2                       -5.02303860 [kJ/mol]

Special recipe for scaled SAPT0
  Electrostatics sSAPT0                -1.05189520 [kJ/mol]
  Exchange sSAPT0                       6.22060955 [kJ/mol]
  Induction sSAPT0                     -4.48397476 [kJ/mol]
  Dispersion sSAPT0                    -5.19350929 [kJ/mol]
Total sSAPT0                           -4.50876969 [kJ/mol]
-----------------------------------------------------------
```

Table S19 SAPT+δMP2/aug-cc-pVTZ//B3LYP-D3/def2-TZVPP results for $ImH^+ \cdots Im...Ar(\pi)$. Calculations were done using Psi4.

```
-----------------------------------------------------------
  Electrostatics                       -2.53397426 [kJ/mol]
    Elst10,r                           -2.19612086 [kJ/mol]
    Elst12,r                           -0.33785340 [kJ/mol]

  Exchange                              8.07477462 [kJ/mol]
    Exch10                              7.51204948 [kJ/mol]
    Exch10(S^2)                         7.50482294 [kJ/mol]
    Exch11(S^2)                         0.17504818 [kJ/mol]
    Exch12(S^2)                         0.38767695 [kJ/mol]

  Induction                            -1.94223020 [kJ/mol]
    Ind20,r                            -4.59784943 [kJ/mol]
    Ind22                              -0.33530002 [kJ/mol]
    Exch-Ind20,r                        2.89873030 [kJ/mol]
    Exch-Ind22                          0.21139107 [kJ/mol]
    delta HF,r (2)                     -0.47257516 [kJ/mol]
    delta MP2,r (2)                     0.35337303 [kJ/mol]

  Dispersion                           -9.77925119 [kJ/mol]
    Disp20                            -11.05227257 [kJ/mol]
    Disp21                              2.29924429 [kJ/mol]
    Disp22 (SDQ)                        0.13268021 [kJ/mol]
    Disp22 (T)                         -1.78058966 [kJ/mol]
    Est. Disp22 (T)                    -1.93815713 [kJ/mol]
    Exch-Disp20                         0.77925401 [kJ/mol]

Total HF                                3.14423434 [kJ/mol]
Total SAPT0                            -7.12878423 [kJ/mol]
Total SAPT2                            -7.02782144 [kJ/mol]
Total SAPT2+                           -6.53405407 [kJ/mol]
Total SAPT2+dMP2                       -6.18068104 [kJ/mol]

Special recipe for scaled SAPT0
  Electrostatics sSAPT0                -2.19612086 [kJ/mol]
```

```
  Exchange sSAPT0                    7.51204948 [kJ/mol]
  Induction sSAPT0                  -2.16331249 [kJ/mol]
  Dispersion sSAPT0                -10.27076532 [kJ/mol]
Total sSAPT0                        -7.11814919 [kJ/mol]
-------------------------------------------------------------
```

3.3 $Im_3H^+ \ldots Ar$

The ordering and naming of the conformers is in accordance with the results given in Table S12.

Table S20 SAPT+δMP2/aug-cc-pVTZ//B3LYP-D3/def2-TZVPP results for Im_3H^+Ar(mid) #1. Calculations were done using Psi4.

```
-------------------------------------------------------------
  Electrostatics                   -2.33200877 [kJ/mol]
    Elst10,r                       -2.01260500 [kJ/mol]
    Elst12,r                       -0.31940377 [kJ/mol]

  Exchange                          6.91098312 [kJ/mol]
    Exch10                          6.32270110 [kJ/mol]
    Exch10(S^2)                     6.31846024 [kJ/mol]
    Exch11(S^2)                     0.17883685 [kJ/mol]
    Exch12(S^2)                     0.40944516 [kJ/mol]

  Induction                        -0.82542438 [kJ/mol]
    Ind20,r                        -2.45992219 [kJ/mol]
    Ind22                          -0.29011149 [kJ/mol]
    Exch-Ind20,r                    1.79004542 [kJ/mol]
    Exch-Ind22                      0.21110942 [kJ/mol]
    delta HF,r (2)                 -0.29485520 [kJ/mol]
    delta MP2,r (2)                 0.21830966 [kJ/mol]

  Dispersion                      -10.35042943 [kJ/mol]
    Disp20                        -11.98470733 [kJ/mol]
    Disp21                          2.90864336 [kJ/mol]
    Disp22 (SDQ)                    0.05897934 [kJ/mol]
    Disp22 (T)                     -1.94970435 [kJ/mol]
    Est. Disp22 (T)                -2.10918323 [kJ/mol]
    Exch-Disp20                     0.77583843 [kJ/mol]

Total HF                            3.34536413 [kJ/mol]
Total SAPT0                        -7.86350476 [kJ/mol]
Total SAPT2                        -7.67362859 [kJ/mol]
Total SAPT2+                       -6.81518912 [kJ/mol]
Total SAPT2+dMP2                   -6.59687946 [kJ/mol]

Special recipe for scaled SAPT0
  Electrostatics sSAPT0            -2.01260500 [kJ/mol]
  Exchange sSAPT0                   6.32270110 [kJ/mol]
  Induction sSAPT0                 -0.96112519 [kJ/mol]
  Dispersion sSAPT0               -11.20730565 [kJ/mol]
```

```
Total sSAPT0                              -7.85833475 [kJ/mol]
-----------------------------------------------------------
```

Table S21 SAPT+δMP2/aug-cc-pVTZ//B3LYP-D3/def2-TZVPP results for Im_3H^+Ar(front) #2. Calculations were done using Psi4.

```
-----------------------------------------------------------
  Electrostatics                          -2.27194847 [kJ/mol]
    Elst10,r                              -1.98417889 [kJ/mol]
    Elst12,r                              -0.28776958 [kJ/mol]

  Exchange                                 6.73911472 [kJ/mol]
    Exch10                                 6.17137935 [kJ/mol]
    Exch10(S^2)                            6.16733260 [kJ/mol]
    Exch11(S^2)                            0.17506821 [kJ/mol]
    Exch12(S^2)                            0.39266716 [kJ/mol]

  Induction                               -0.78376884 [kJ/mol]
    Ind20,r                               -2.32853370 [kJ/mol]
    Ind22                                 -0.28631597 [kJ/mol]
    Exch-Ind20,r                           1.73846007 [kJ/mol]
    Exch-Ind22                             0.21376065 [kJ/mol]
    delta HF,r (2)                        -0.28948703 [kJ/mol]
    delta MP2,r (2)                        0.16834714 [kJ/mol]

  Dispersion                              -9.71745128 [kJ/mol]
    Disp20                               -11.31707374 [kJ/mol]
    Disp21                                 2.71321561 [kJ/mol]
    Disp22 (SDQ)                           0.12060116 [kJ/mol]
    Disp22 (T)                            -1.84383094 [kJ/mol]
    Est. Disp22 (T)                       -1.99565641 [kJ/mol]
    Exch-Disp20                            0.76146209 [kJ/mol]

Total HF                                   3.30763981 [kJ/mol]
Total SAPT0                               -7.24797184 [kJ/mol]
Total SAPT2                               -7.04056138 [kJ/mol]
Total SAPT2+                              -6.20240101 [kJ/mol]
Total SAPT2+dMP2                          -6.03405387 [kJ/mol]

Special recipe for scaled SAPT0
  Electrostatics sSAPT0                   -1.98417889 [kJ/mol]
  Exchange sSAPT0                          6.17137935 [kJ/mol]
  Induction sSAPT0                        -0.87613629 [kJ/mol]
  Dispersion sSAPT0                      -10.55411174 [kJ/mol]
Total sSAPT0                              -7.24304757 [kJ/mol]
-----------------------------------------------------------
```

Table S22 SAPT+δMP2/aug-cc-pVTZ//B3LYP-D3/def2-TZVPP results for Im_3H^+Ar(side) #3. Calculations were done using Psi4.

```
-----------------------------------------------------------
  Electrostatics                          -2.52510680 [kJ/mol]
```

```
    Elst10,r                          -2.23934767 [kJ/mol]
    Elst12,r                          -0.28575913 [kJ/mol]

  Exchange                             7.62046310 [kJ/mol]
    Exch10                             7.07890399 [kJ/mol]
    Exch10(S^2)                        7.07248368 [kJ/mol]
    Exch11(S^2)                        0.18835137 [kJ/mol]
    Exch12(S^2)                        0.35320773 [kJ/mol]

  Induction                           -0.97695538 [kJ/mol]
    Ind20,r                           -3.35524673 [kJ/mol]
    Ind22                             -0.39716080 [kJ/mol]
    Exch-Ind20,r                       2.70200928 [kJ/mol]
    Exch-Ind22                         0.31983703 [kJ/mol]
    delta HF,r (2)                    -0.37630436 [kJ/mol]
    delta MP2,r (2)                    0.12991019 [kJ/mol]

  Dispersion                          -9.99454430 [kJ/mol]
    Disp20                           -11.43386512 [kJ/mol]
    Disp21                             2.52439389 [kJ/mol]
    Disp22 (SDQ)                       0.12287232 [kJ/mol]
    Disp22 (T)                        -1.85539817 [kJ/mol]
    Est. Disp22 (T)                   -2.01198231 [kJ/mol]
    Exch-Disp20                        0.80403692 [kJ/mol]

Total HF                               3.81001451 [kJ/mol]
Total SAPT0                           -6.81981370 [kJ/mol]
Total SAPT2                           -6.64133748 [kJ/mol]
Total SAPT2+                          -6.00605358 [kJ/mol]
Total SAPT2+dMP2                      -5.87614339 [kJ/mol]

Special recipe for scaled SAPT0
  Electrostatics sSAPT0               -2.23934767 [kJ/mol]
  Exchange sSAPT0                      7.07890399 [kJ/mol]
  Induction sSAPT0                    -1.02217658 [kJ/mol]
  Dispersion sSAPT0                  -10.62763653 [kJ/mol]
Total sSAPT0                          -6.81025679 [kJ/mol]
-------------------------------------------------------------
```

Table S23 SAPT+δMP2/aug-cc-pVTZ//B3LYP-D3/def2-TZVPP results for $Im_3H^+Ar(NH)$ #4. Calculations were done using Psi4.

```
-------------------------------------------------------------
  Electrostatics                      -1.23429163 [kJ/mol]
    Elst10,r                          -0.95194602 [kJ/mol]
    Elst12,r                          -0.28234561 [kJ/mol]

  Exchange                             5.32040340 [kJ/mol]
    Exch10                             4.75183773 [kJ/mol]
    Exch10(S^2)                        4.74587148 [kJ/mol]
    Exch11(S^2)                        0.06033984 [kJ/mol]
    Exch12(S^2)                        0.50822582 [kJ/mol]
```

```
  Induction                          -3.11953511 [kJ/mol]
    Ind20,r                          -3.62317511 [kJ/mol]
    Ind22                            -0.36917519 [kJ/mol]
    Exch-Ind20,r                      1.27068861 [kJ/mol]
    Exch-Ind22                        0.12947393 [kJ/mol]
    delta HF,r (2)                   -0.41683386 [kJ/mol]
    delta MP2,r (2)                  -0.11051348 [kJ/mol]

  Dispersion                         -5.66634438 [kJ/mol]
    Disp20                           -5.96168694 [kJ/mol]
    Disp21                            0.83942254 [kJ/mol]
    Disp22 (SDQ)                      0.09807780 [kJ/mol]
    Disp22 (T)                       -0.93607683 [kJ/mol]
    Est. Disp22 (T)                  -1.01974985 [kJ/mol]
    Exch-Disp20                       0.37759206 [kJ/mol]

Total HF                              1.03057134 [kJ/mol]
Total SAPT0                          -4.55352353 [kJ/mol]
Total SAPT2                          -4.50700473 [kJ/mol]
Total SAPT2+                         -4.58925424 [kJ/mol]
Total SAPT2+dMP2                     -4.69976772 [kJ/mol]

Special recipe for scaled SAPT0
  Electrostatics sSAPT0              -0.95194602 [kJ/mol]
  Exchange sSAPT0                     4.75183773 [kJ/mol]
  Induction sSAPT0                   -2.76452201 [kJ/mol]
  Dispersion sSAPT0                  -5.58266902 [kJ/mol]
Total sSAPT0                         -4.54729932 [kJ/mol]
-----------------------------------------------------------
```

4 Experimental spectra of imidazole ionic species

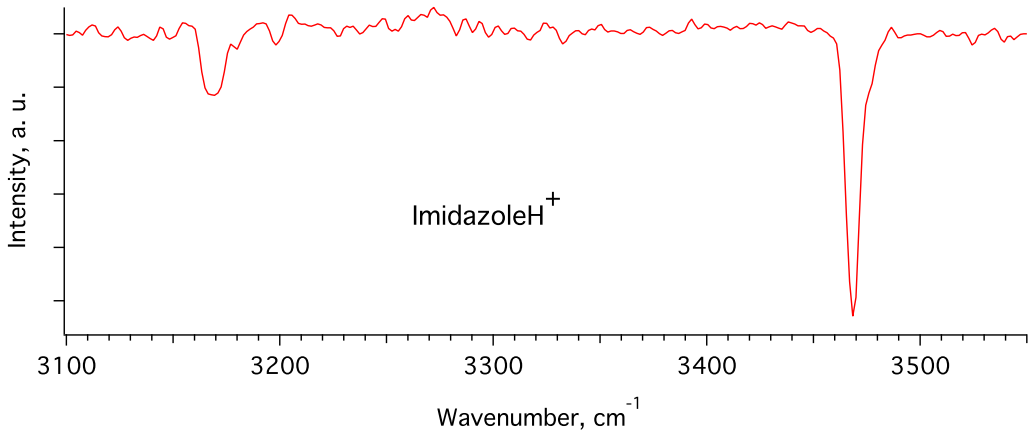


Figure S1 Vibrational spectrum of ImH^+ with He tag.

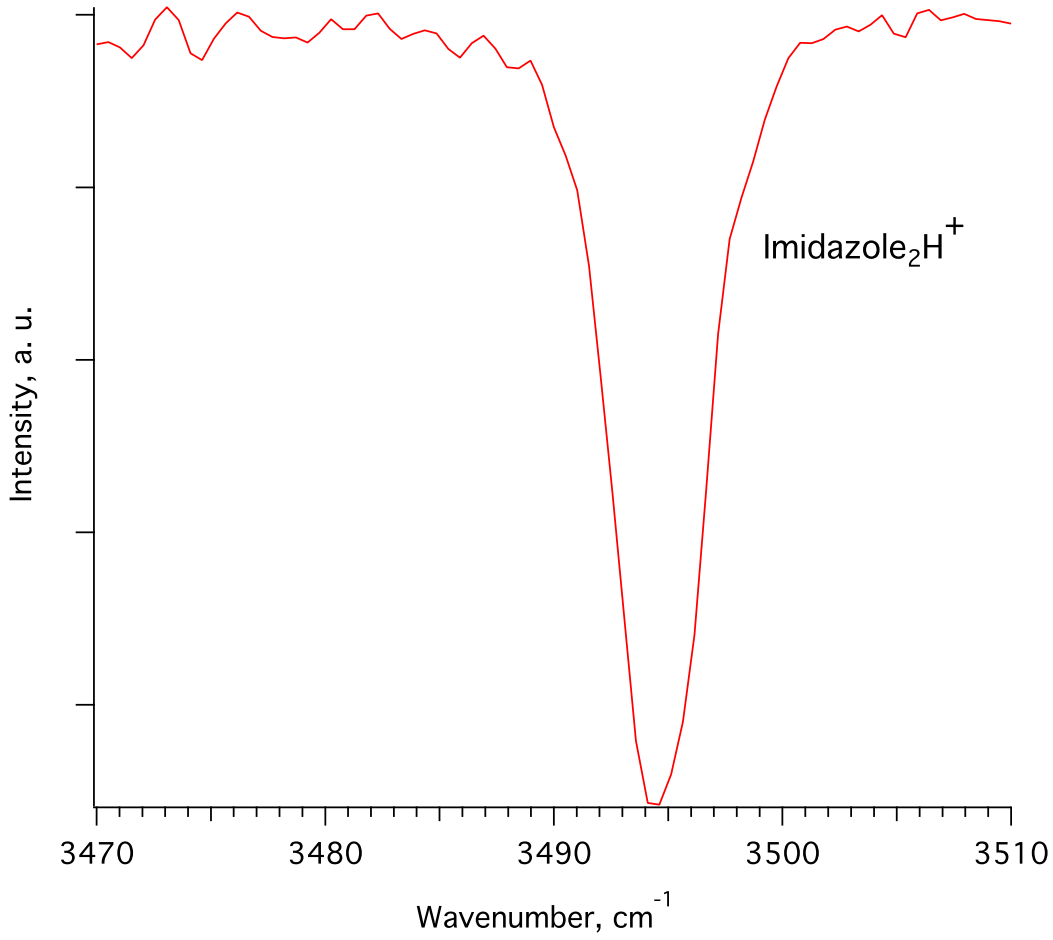


Figure S2 Vibrational spectrum of N-H stretching vibrations of Im_2H^+ with He tag.

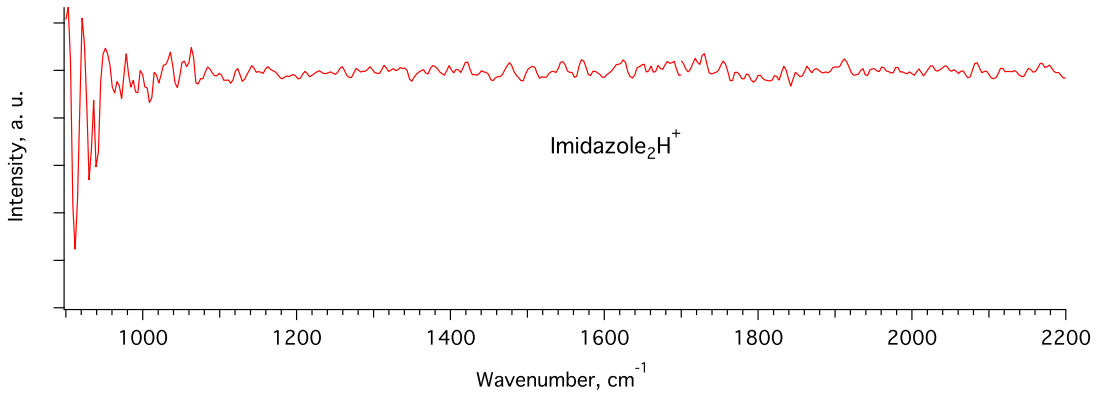


Figure S3 Vibrational spectrum of region with proton transfer motion in Im_2H^+ taken with He tag. The large backgroud noise oscillations appear due to low laser power.

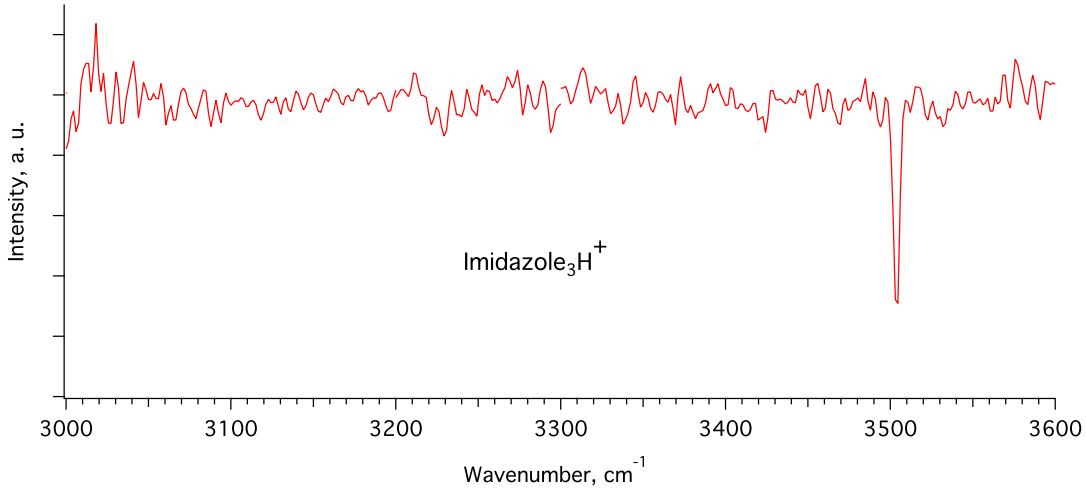


Figure S4 Vibrational spectrum of Im_3H^+ with He tag.

Table S24 Vibrational spectrum of ImH^+ with He tag.

```
################################################################################
      Frequency      Intensity      Absolute noise level
      [cm^{-1}]      [arb.units]    [arb.units]
      3100.00000      0.0179881758   0.0511790929
      3101.51007     -0.0332213369   0.0487982581
      3103.02013     -0.0196744408   0.0463688962
      3104.53020      0.0343441353   0.0456307606
      3106.04027      0.0422039523   0.0440661976
      3107.55034     -0.0114482052   0.0450196689
      3109.06040     -0.0120014328   0.0449100240
      3110.57047      0.0239162639   0.0442357547
      3112.08054     -0.1137070126   0.0441851957
      3113.59060      0.0440720899   0.0433806491
      3115.10067      0.0610418945   0.0423779197
      3116.61074      0.0133306181   0.0424771413
      3118.12081      0.0200291835   0.0401095842
      3119.63087      0.0269715723   0.0415559963
```

3121.14094	0.0039228227	0.0422994916
3122.65101	0.0178942006	0.0411534346
3124.16107	-0.0229525426	0.0416098394
3125.67114	-0.0261083264	0.0408122078
3127.18121	-0.0384892649	0.0417350346
3128.69128	0.0250544442	0.0409247022
3130.20134	-0.0014678141	0.0413568580
3131.71141	0.0141650309	0.0411861675
3133.22148	0.0183953551	0.0432223995
3134.73154	0.0174663863	0.0424916283
3136.24161	0.0194980316	0.0429840749
3137.75168	0.0367871870	0.0426419787
3139.26174	0.0255925858	0.0408923020
3140.77181	0.0189745475	0.0413347609
3142.28188	0.0087157385	0.0418587358
3143.79195	0.0233371512	0.0412247320
3145.30201	-0.0651678516	0.0419549184
3146.81208	0.0015922397	0.0409498395
3148.32215	-0.0336312461	0.0419604825
3149.83222	-0.0777121898	0.0404952711
3151.34228	-0.0455749883	0.0453747720
3152.85235	0.0264062345	0.0442610235
3154.36242	0.0388461452	0.0437157966
3155.87248	-0.0206141799	0.0414153841
3157.38255	-0.0953665722	0.0418405290
3158.89262	0.0156914542	0.0417299113
3160.40269	-0.0567503253	0.0450670132
3161.91275	-0.1035850837	0.0456555176
3163.42282	-0.0314843330	0.0430069280
3164.93289	0.0014467861	0.0457563758
3166.44295	-0.0471474816	0.0465048271
3167.95302	-0.0935188264	0.0512669428
3169.46309	-0.0443175914	0.0493561608
3170.97315	-0.0600584217	0.0491167872
3172.48322	-0.1060367993	0.0529741559
3173.99329	-0.0538745916	0.0535834910
3175.50336	0.0074487937	0.0523568377
3177.01342	-0.0423030923	0.0503167525
3178.52349	0.0373452323	0.0510981753
3180.03356	0.0113539259	0.0483075393
3181.54362	0.0618562192	0.0495952399
3183.05369	0.0564998670	0.0518728413
3184.56376	0.0470949405	0.0558214620
3186.07383	-0.0478569132	0.0518699536
3187.58389	0.0316545239	0.0554630436
3189.09396	0.0427112951	0.0523244208
3190.60403	0.0311143288	0.0489390846
3192.11410	0.0151971011	0.0518106553
3193.62416	0.0434240213	0.0527775051
3195.13423	0.0114811457	0.0492598809
3196.64430	0.0217603912	0.0492948056
3198.15436	-0.0588065502	0.0471748459

3199.66443	-0.0978732916	0.0514745346
3201.17450	-0.0015139294	0.0485603899
3202.68456	-0.0215875859	0.0498425343
3204.19463	0.0198087041	0.0454970629
3205.70470	0.0318681418	0.0493375323
3207.21477	-0.0549537116	0.0502738382
3208.72483	-0.0339337532	0.0497663597
3210.23490	-0.0083192111	0.0560308259
3211.74497	0.0463198417	0.0490096777
3213.25503	0.0333387928	0.0516399454
3214.76510	0.0410727157	0.0532605238
3216.27517	0.0139398980	0.0542719191
3217.78524	-0.0294370605	0.0531954602
3219.29530	0.0592085693	0.0576457301
3220.80537	-0.0842394849	0.0564918175
3222.31544	-0.1357455837	0.0560935812
3223.82550	-0.0339306312	0.0591073619
3225.33557	0.0269027498	0.0581720613
3226.84564	-0.0765224069	0.0564759058
3228.35571	0.0511526779	0.0509574408
3229.86577	0.0583770462	0.0567365477
3231.37584	0.0612719065	0.0570449139
3232.88591	0.0946482484	0.0581785068
3234.39598	0.0394678198	0.0568133563
3235.90604	0.0680489373	0.0579299857
3237.41611	-0.0799053198	0.0592717356
3238.92618	0.0235853380	0.0583716611
3240.43624	0.0163575291	0.0571675400
3241.94631	0.0280751185	0.0632040093
3243.45638	0.0788387313	0.0687746757
3244.96644	0.1043445635	0.0685598629
3246.47651	-0.1278280950	0.0664172511
3247.98658	0.0245490855	0.0731764944
3249.49664	0.0544186275	0.0777345688
3251.00671	-0.0120054479	0.0798868380
3252.51678	0.0524675617	0.0722993280
3254.02685	0.0373039195	0.0769684458
3255.53691	0.0587868264	0.0811004678
3257.04698	0.0325952819	0.0785392723
3258.55705	-0.0039180477	0.0697331771
3260.06712	0.1029063049	0.0786291804
3261.57718	0.0166500614	0.0797022965
3263.08725	-0.0668169809	0.0919916856
3264.59732	-0.0740218061	0.0777477198
3266.10738	0.0230590804	0.0786644078
3267.61745	0.0533759600	0.0788247695
3269.12752	-0.0775847676	0.0728865713
3270.63758	-0.0018124928	0.0654945164
3272.14765	-0.0921244515	0.0759538591
3273.65772	0.0636511067	0.0691714679
3275.16779	0.1314002622	0.0661821874
3276.67785	0.1100036316	0.0748871435

3278.18792	0.0982577240	0.0723983326
3279.69799	-0.0598575246	0.0568817938
3281.20805	0.0066896127	0.0666693434
3282.71812	-0.0897481102	0.0640962537
3284.22819	-0.1161348366	0.0691057681
3285.73826	0.0570486272	0.0667253341
3287.24832	-0.0341321608	0.0612426580
3288.75839	-0.0250403213	0.0623870521
3290.26846	0.0479375734	0.0594237970
3291.77852	0.0019185699	0.0608169686
3293.28859	0.0302099632	0.0588859181
3294.79866	0.0210076283	0.0549062791
3296.30873	0.0396246726	0.0612788090
3297.81879	0.0485669951	0.0559786571
3299.32886	0.0936519132	0.0571328925
3300.83893	0.0935843918	0.0517174469
3302.34899	0.0435553796	0.0524573222
3303.85906	0.0612048851	0.0503649561
3305.36913	0.0323591192	0.0509202375
3306.87920	0.0036857263	0.0525256799
3308.38926	0.0738341873	0.0519795485
3309.89933	-0.1076005902	0.0479355853
3311.40940	-0.0536372219	0.0458236254
3312.91946	-0.0660490635	0.0474864083
3314.42953	-0.0087646567	0.0453240717
3315.93960	0.0220422687	0.0449073230
3317.44967	-0.0856697026	0.0464919753
3318.95973	-0.0157288020	0.0503433776
3320.46980	0.0457056381	0.0461964548
3321.97987	0.0564167229	0.0529073273
3323.48993	0.0450575969	0.0537904555
3325.00000	-0.0145837480	0.0513891024
3326.51007	-0.0796356359	0.0508540947
3328.02013	0.0580187722	0.0511822350
3329.53020	-0.0074525362	0.0505556683
3331.04027	0.0591529349	0.0502125057
3332.55034	-0.0485098670	0.0491215287
3334.06040	-0.0704149133	0.0514270977
3335.57047	-0.0003814520	0.0447568973
3337.08054	0.0434653984	0.0458793345
3338.59060	-0.0161487473	0.0514947878
3340.10067	-0.0449893748	0.0468196388
3341.61074	0.0620388559	0.0477467808
3343.12081	-0.0871185606	0.0500419727
3344.63087	-0.0402964212	0.0507040004
3346.14094	-0.0240870212	0.0478797777
3347.65101	-0.0321966844	0.0467168446
3349.16107	-0.0144894542	0.0483406038
3350.67114	0.0494492734	0.0463024914
3352.18121	0.0454531074	0.0482362994
3353.69128	0.0456916790	0.0483285678
3355.20134	0.0357422510	0.0475075600

3356.71141	-0.0295971030	0.0465761177
3358.22148	-0.0691683384	0.0438156610
3359.73154	0.0315240542	0.0430442662
3361.24161	-0.0337510267	0.0435698882
3362.75168	0.0333636107	0.0420066556
3364.26175	0.0201805362	0.0424626214
3365.77181	0.0176905589	0.0431466152
3367.28188	-0.0845777146	0.0412954053
3368.79195	-0.0145040398	0.0424743790
3370.30201	0.0186473568	0.0393229032
3371.81208	0.0583351665	0.0427432806
3373.32215	0.0823258600	0.0388870968
3374.83222	0.0549638517	0.0395680435
3376.34228	-0.0574969038	0.0400237985
3377.85235	0.0522827881	0.0408324436
3379.36242	-0.0999405970	0.0372403789
3380.87248	-0.0104146905	0.0393835383
3382.38255	0.0180168408	0.0367603943
3383.89262	0.0230230738	0.0385412724
3385.40268	0.0210385668	0.0408293397
3386.91275	-0.0100029726	0.0385449120
3388.42282	-0.0163744612	0.0388317950
3389.93289	-0.0090287901	0.0378297205
3391.44295	-0.0593575668	0.0364409090
3392.95302	0.0031092376	0.0371939597
3394.46309	0.0023579211	0.0344556038
3395.97316	0.0354618018	0.0338112212
3397.48322	0.0292842107	0.0349069483
3398.99329	0.0184778085	0.0336429594
3400.50336	-0.0216115875	0.0330361011
3402.01342	0.0131352301	0.0331703329
3403.52349	0.0236402799	0.0322696895
3405.03356	0.0074350282	0.0321736550
3406.54362	0.0198931463	0.0317976878
3408.05369	-0.0721850263	0.0320185876
3409.56376	-0.0466437118	0.0317579363
3411.07383	0.0261833042	0.0309957700
3412.58389	0.0253173165	0.0318488125
3414.09396	0.0506231134	0.0338891008
3415.60403	0.0355250391	0.0335981104
3417.11409	0.0423736037	0.0345534038
3418.62416	0.0107264813	0.0330714084
3420.13423	0.0025167314	0.0354035438
3421.64430	0.0465361907	0.0350790793
3423.15436	0.0388733217	0.0373783280
3424.66443	0.0601016495	0.0338107686
3426.17450	0.0581897083	0.0338396132
3427.68456	0.0548127566	0.0336123894
3429.19463	0.0453277166	0.0331450096
3430.70470	0.0295118142	0.0339797304
3432.21477	-0.0163603447	0.0332337598
3433.72483	0.0262042117	0.0339944852

3435.23490	-0.0284599188	0.0346131979
3436.74497	-0.0169415237	0.0339281384
3438.25503	-0.0791516256	0.0339302328
3439.76510	-0.0064906113	0.0349232947
3441.27517	0.0033502622	0.0351479303
3442.78524	0.0448259042	0.0352260973
3444.29530	0.0234427068	0.0321126115
3445.80537	-0.0228644623	0.0337078495
3447.31544	0.0083993542	0.0330643327
3448.82550	-0.0228422610	0.0339905181
3450.33557	-0.0340412844	0.0322949339
3451.84564	0.0169056279	0.0329637272
3453.35571	0.0486809241	0.0315119339
3454.86577	0.0199423281	0.0313418425
3456.37584	0.0380797967	0.0313782447
3457.88591	-0.0441295808	0.0314292003
3459.39597	-0.0046054722	0.0311322424
3460.90604	-0.0115020814	0.0324511860
3462.41611	-0.0224459796	0.0319623864
3463.92617	-0.1269210871	0.0332127100
3465.43624	-0.2175994401	0.0324487605
3466.94631	-0.3036003456	0.0331514372
3468.45638	-0.3282287701	0.0339483454
3469.96644	-0.3353764169	0.0329944111
3471.47651	-0.1688255143	0.0327889571
3472.98658	-0.0827510885	0.0331285721
3474.49664	-0.1219053002	0.0343100667
3476.00671	-0.0757995449	0.0335630154
3477.51678	-0.1126181446	0.0336377039
3479.02685	-0.0938941164	0.0340261340
3480.53691	-0.0930820846	0.0327251581
3482.04698	-0.0288280109	0.0329639840
3483.55705	-0.0531290122	0.0351787052
3485.06711	0.0069226321	0.0343097457
3486.57718	0.0279390553	0.0333422527
3488.08725	0.0354156367	0.0336185779
3489.59732	0.0251446175	0.0328326548
3491.10738	0.0189731900	0.0317474686
3492.61745	0.0142860003	0.0321209162
3494.12752	0.0306351458	0.0316669337
3495.63758	0.0153949266	0.0316816348
3497.14765	0.0266443127	0.0312223068
3498.65772	0.0188954068	0.0319043298
3500.16779	-0.0047669549	0.0328468966
3501.67785	-0.0550386231	0.0319308143
3503.18792	0.0103667046	0.0308660022
3504.69799	0.0015831825	0.0319537025
3506.20805	-0.0145157247	0.0336315234
3507.71812	-0.0538906187	0.0314813802
3509.22819	0.0242109762	0.0305599904
3510.73826	0.0005382269	0.0322408022
3512.24832	0.0151525456	0.0316386891

3513.75839	0.0407465215	0.0319418895
3515.26846	0.0310052085	0.0313138418
3516.77852	-0.0436649437	0.0315642580
3518.28859	-0.0454121559	0.0305274900
3519.79866	0.0083735242	0.0325736186
3521.30872	0.0348621978	0.0336146417
3522.81879	0.0742900724	0.0324703358
3524.32886	-0.0234451233	0.0318950511
3525.83893	-0.0154243069	0.0349366999
3527.34899	-0.0476530282	0.0347286079
3528.85906	0.0207586596	0.0344186728
3530.36913	0.0098005240	0.0340520287
3531.87919	0.0178727498	0.0338970981
3533.38926	0.0025789020	0.0332875041
3534.89933	-0.0286294118	0.0321472531
3536.40940	0.0065893254	0.0314830563
3537.91946	-0.0127076670	0.0314158710
3539.42953	-0.0068793046	0.0315137551
3540.93960	-0.0274426809	0.0322684678
3542.44966	-0.0608411639	0.0313796527
3543.95973	-0.0469329261	0.0305576574
3545.46980	0.0388217512	0.0302907875
3546.97987	0.0439573799	0.0308547625
3548.48993	-0.0180847777	0.0319626303
3550.00000	-0.0618566501	0.0330136204

Table S25 Vibrational spectrum of Im_2H^+ with He tag.

Frequency [cm^{-1}]	Intensity [arb.units]	Absolute noise level [arb.units]
3470.00000	0.0052461307	0.0223297337
3470.51282	-0.0158077751	0.0234489974
3471.02564	0.0135503328	0.0254189418
3471.53846	-0.0062339950	0.0247749617
3472.05128	-0.0174832200	0.0231634069
3472.56410	0.0051685600	0.0237214556
3473.07692	0.0095608169	0.0226815061
3473.58974	-0.0074386883	0.0219944647
3474.10256	-0.0506891838	0.0239623178
3474.61538	-0.0444395349	0.0241792649
3475.12820	-0.0436658676	0.0218442526
3475.64102	-0.0112973626	0.0237251900
3476.15385	-0.0328586291	0.0245526692
3476.66667	-0.0162241002	0.0230486862
3477.17949	-0.0154776916	0.0241219596
3477.69231	-0.0278891303	0.0220157648
3478.20513	-0.0119674142	0.0226279729
3478.71795	-0.0080352760	0.0221066251
3479.23077	-0.0070625615	0.0217542912
3479.74359	0.0186282453	0.0240477880

3480.25641	0.0172441885	0.0235357707
3480.76923	0.0006872209	0.0218625913
3481.28205	-0.0152358603	0.0222323241
3481.79487	-0.0618596900	0.0245285739
3482.30769	0.0110954176	0.0231794787
3482.82051	-0.0272886826	0.0274667452
3483.33333	-0.0443970930	0.0223256629
3483.84615	-0.0356933113	0.0243915830
3484.35897	0.0020915404	0.0201485845
3484.87179	-0.0038879996	0.0196912100
3485.38462	0.0170896586	0.0225151735
3485.89744	-0.0434950467	0.0229645740
3486.41026	0.0113419195	0.0212090629
3486.92308	-0.0419668514	0.0201995126
3487.43590	-0.0983495112	0.0230118359
3487.94872	-0.0437324367	0.0190886472
3488.46154	-0.0258098701	0.0197142201
3488.97436	-0.0102345160	0.0208819394
3489.48718	-0.0807528798	0.0197646869
3490.00000	-0.0832515083	0.0215596550
3490.51282	-0.0970748705	0.0210787844
3491.02564	-0.0997045799	0.0189569438
3491.53846	-0.1311074299	0.0174052209
3492.05128	-0.1927013294	0.0176859861
3492.56410	-0.2806779834	0.0183687724
3493.07692	-0.3507407594	0.0169085157
3493.58974	-0.4295301309	0.0181770051
3494.10256	-0.4365650439	0.0175570966
3494.61539	-0.4710109862	0.0186507892
3495.12821	-0.4437956314	0.0177099188
3495.64103	-0.4015043852	0.0176280227
3496.15385	-0.3511990106	0.0174691028
3496.66667	-0.2747348291	0.0177184746
3497.17949	-0.1864949991	0.0185975763
3497.69231	-0.1067157711	0.0182724593
3498.20513	-0.1032229728	0.0179566188
3498.71795	-0.0616126315	0.0163579510
3499.23077	-0.0250774565	0.0168116932
3499.74359	-0.0563287012	0.0181255106
3500.25641	-0.0159519960	0.0168153336
3500.76923	-0.0166487056	0.0168802539
3501.28205	-0.0163671357	0.0170860619
3501.79487	-0.0012990873	0.0163491705
3502.30769	0.0052544594	0.0186331872
3502.82051	-0.0036700578	0.0159648340
3503.33333	-0.0085812022	0.0179329832
3503.84615	-0.0083716253	0.0174987088
3504.35898	0.0103067133	0.0160845717
3504.87180	-0.0265528751	0.0163765354
3505.38462	-0.0114123593	0.0167350616
3505.89744	0.0116799181	0.0167764224
3506.41026	0.0080577460	0.0161693400

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      3506.92308    -0.0391331924    0.0179919038
      3507.43590    -0.0144058607    0.0152870844
      3507.94872     0.0123038156    0.0170588799
      3508.46154     0.0076998541    0.0153221051
      3508.97436    -0.0125087405    0.0159219749
      3509.48718    -0.0272442166    0.0169516605
      3510.00000    -0.0058660013    0.0156116610
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Table S26 Vibrational spectrum of Im_3H^+ with He tag.

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      Frequency      Intensity       Absolute noise level
      [cm^{-1}]      [arb.units]     [arb.units]
      3300.00000     0.0294088259    0.0138934548
      3301.51515     0.0078870462    0.0144895596
      3303.03030     0.0106509554    0.0149166143
      3304.54546    -0.0145299251    0.0143392845
      3306.06061     0.0035025362    0.0151214157
      3307.57576     0.0017597298    0.0139365737
      3309.09091    -0.0008958292    0.0137729007
      3310.60606    -0.0153444405    0.0136003739
      3312.12121     0.0251379072    0.0139187405
      3313.63636     0.0284750181    0.0130793034
      3315.15152    -0.0056251732    0.0137874176
      3316.66667     0.0214084454    0.0132188140
      3318.18182    -0.0300148778    0.0133539184
      3319.69697    -0.0089374975    0.0134421703
      3321.21212    -0.0079241767    0.0131440893
      3322.72727    -0.0158928641    0.0128017092
      3324.24242    -0.0063747780    0.0128476142
      3325.75758    -0.0127177700    0.0127422373
      3327.27273     0.0171688258    0.0128477312
      3328.78788     0.0013551862    0.0135293877
      3330.30303    -0.0169002084    0.0132823598
      3331.81818    -0.0064523983    0.0141000877
      3333.33333    -0.0067963169    0.0128050683
      3334.84849     0.0322564968    0.0144462727
      3336.36364     0.0039187501    0.0131192667
      3337.87879    -0.0065118031    0.0128420190
      3339.39394     0.0039780067    0.0135317149
      3340.90909    -0.0040003835    0.0124178966
      3342.42424     0.0028155557    0.0125446891
      3343.93940    -0.0171333238    0.0127236738
      3345.45455     0.0109794771    0.0130373277
      3346.96970    -0.0073125006    0.0131522774
      3348.48485     0.0032072208    0.0137156692
      3350.00000     0.0024003894    0.0140842144
      3351.51515     0.0002980615    0.0131847837
      3353.03030     0.0090486830    0.0118403870
      3354.54546    -0.0182230675    0.0133643774
      3356.06061     0.0059155069    0.0124964268
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3357.57576	-0.0091061843	0.0116558695
3359.09091	-0.0071726447	0.0130717404
3360.60606	-0.0169802431	0.0128300400
3362.12121	0.0204969555	0.0119695078
3363.63636	-0.0148602636	0.0120722909
3365.15152	-0.0115157014	0.0136729510
3366.66667	0.0063869594	0.0131273035
3368.18182	0.0108359622	0.0119068484
3369.69697	-0.0193092592	0.0110870397
3371.21212	-0.0118212419	0.0106227165
3372.72727	0.0077093926	0.0113761340
3374.24243	-0.0212908239	0.0112727016
3375.75758	0.0162368835	0.0111508597
3377.27273	-0.0098155546	0.0112596193
3378.78788	0.0070104825	0.0121764155
3380.30303	-0.0189905480	0.0118731447
3381.81818	0.0020704815	0.0120831550
3383.33334	-0.0176224577	0.0129950817
3384.84849	-0.0172689587	0.0128226785
3386.36364	-0.0008442796	0.0113975458
3387.87879	0.0012874913	0.0106254283
3389.39394	0.0095624877	0.0108769415
3390.90909	0.0063034106	0.0116187603
3392.42424	-0.0249866638	0.0131732210
3393.93940	-0.0223611717	0.0119133215
3395.45455	-0.0076728549	0.0112908307
3396.96970	-0.0173162570	0.0118180816
3398.48485	-0.0080170738	0.0109599666
3400.00000	-0.0100570540	0.0109136644
3401.51515	0.0003653207	0.0114037562
3403.03031	0.0044132385	0.0104898567
3404.54546	0.0092788681	0.0103808985
3406.06061	-0.0267960780	0.0103152740
3407.57576	-0.0027658557	0.0112006201
3409.09091	-0.0012735733	0.0107957335
3410.60606	-0.0002652560	0.0111468947
3412.12121	-0.0005426688	0.0109086960
3413.63637	-0.0136351185	0.0108646281
3415.15152	-0.0048320787	0.0100949127
3416.66667	-0.0098041394	0.0109116663
3418.18182	-0.0018699958	0.0107623441
3419.69697	-0.0379458618	0.0117667097
3421.21212	-0.0034319794	0.0115923298
3422.72727	0.0212574614	0.0110006190
3424.24243	-0.0280131527	0.0109705765
3425.75758	-0.0084820392	0.0105633074
3427.27273	-0.0033185743	0.0104862515
3428.78788	-0.0047223072	0.0110431243
3430.30303	-0.0096993483	0.0112386655
3431.81818	-0.0174529987	0.0108698916
3433.33334	0.0019146987	0.0105918821
3434.84849	0.0016457804	0.0105171801

3436.36364	0.0115464595	0.0107687157
3437.87879	0.0019727221	0.0111305435
3439.39394	-0.0069210055	0.0119169220
3440.90909	0.0009252469	0.0116313802
3442.42424	-0.0172279456	0.0113702894
3443.93940	0.0125754250	0.0111541632
3445.45455	0.0062031533	0.0111145455
3446.96970	-0.0178781946	0.0126608163
3448.48485	-0.0104266636	0.0115229344
3450.00000	0.0048544133	0.0106309516
3451.51515	-0.0053180294	0.0105202134
3453.03031	-0.0044059074	0.0107888273
3454.54546	-0.0037639112	0.0108954069
3456.06061	0.0040956934	0.0102188690
3457.57576	0.0012787714	0.0104913463
3459.09091	-0.0139607139	0.0105852564
3460.60606	-0.0155452976	0.0114414762
3462.12121	-0.0016899789	0.0111726103
3463.63636	0.0057170575	0.0108584315
3465.15152	-0.0059512422	0.0110546375
3466.66667	-0.0018796856	0.0111929604
3468.18182	-0.0147624371	0.0118135800
3469.69697	-0.0376029529	0.0107656220
3471.21212	-0.0077147154	0.0105695724
3472.72727	-0.0122975774	0.0109083485
3474.24243	-0.0189142103	0.0111569300
3475.75758	-0.0069561526	0.0111726676
3477.27273	0.0022835032	0.0108026801
3478.78788	0.0107451009	0.0108027982
3480.30303	0.0218470493	0.0111098790
3481.81818	-0.0005932087	0.0116161622
3483.33334	-0.0006240073	0.0120272205
3484.84849	0.0127458577	0.0113110470
3486.36364	-0.0050157971	0.0112843244
3487.87879	-0.0222293871	0.0117270638
3489.39394	-0.0068480921	0.0111835892
3490.90909	0.0010945779	0.0101641219
3492.42424	-0.0082774796	0.0104146983
3493.93940	-0.0020474629	0.0105979151
3495.45455	-0.0180377669	0.0112232695
3496.96970	0.0118259952	0.0109523284
3498.48485	0.0008479660	0.0110585576
3500.00000	-0.0135163250	0.0105196006
3501.51515	-0.0573123035	0.0111861827
3503.03030	-0.1622411093	0.0118619842
3504.54546	-0.1834956219	0.0126772257
3506.06061	-0.0579865818	0.0109542125
3507.57576	-0.0148074447	0.0100231068
3509.09091	-0.0037932416	0.0105213018
3510.60606	-0.0044306930	0.0109264378
3512.12121	-0.0264066203	0.0103478108
3513.63636	-0.0131746058	0.0104218449

3515.15152	-0.0082195295	0.0098962183
3516.66667	0.0063768403	0.0101515588
3518.18182	-0.0018146156	0.0097897997
3519.69697	0.0024172281	0.0104476603
3521.21212	-0.0214906352	0.0109325453
3522.72727	-0.0123414493	0.0117191772
3524.24242	-0.0134525836	0.0126580605
3525.75758	0.0073486247	0.0115462749
3527.27273	-0.0236313630	0.0115003142
3528.78788	-0.0059381456	0.0120828413
3530.30303	0.0028877536	0.0122741408
3531.81818	-0.0069165928	0.0104706900
3533.33334	-0.0155430354	0.0096715506
3534.84849	0.0007234642	0.0092604821
3536.36364	-0.0029800920	0.0098228147
3537.87879	-0.0185838759	0.0098835870
3539.39394	-0.0045776836	0.0094626628
3540.90909	0.0073141352	0.0092154680
3542.42424	0.0000437542	0.0100845939
3543.93939	-0.0026296463	0.0110558891
3545.45455	0.0014120271	0.0119380684
3546.96970	0.0052000469	0.0122804329
3548.48485	0.0099380868	0.0114829958
3550.00000	-0.0032351169	0.0102529455
3551.51515	-0.0045026524	0.0102968677
3553.03030	-0.0208366398	0.0115350653
3554.54546	0.0000223099	0.0104218166
3556.06061	-0.0213806152	0.0095496539
3557.57576	-0.0137534177	0.0105591329
3559.09091	0.0221933963	0.0111464425
3560.60606	-0.0151235307	0.0115366820
3562.12121	-0.0235184689	0.0122867062
3563.63636	-0.0099765599	0.0123222481
3565.15151	-0.0016549099	0.0142619843
3566.66667	-0.0269086163	0.0191492739
3568.18182	0.0228839082	0.0242447050
3569.69697	0.0302854353	0.0211827417
3571.21212	-0.0080505056	0.0174941618
3572.72727	0.0015233213	0.0165248421
3574.24243	-0.0052537672	0.0151271429
3575.75758	0.0080167252	0.0142621454
3577.27273	0.0145150139	0.0139092216
3578.78788	-0.0106649082	0.0127956452
3580.30303	-0.0026518642	0.0132824462
3581.81818	0.0043650088	0.0125378923
3583.33333	0.0017599549	0.0122472333
3584.84849	0.0000960963	0.0133751291
3586.36364	0.0230695764	0.0144553600
3587.87879	-0.0046809169	0.0201193543
3589.39394	0.0085253746	0.0196881616
3590.90909	0.0129716989	0.0137291378
3592.42424	0.0118797332	0.0115394946

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      3593.93939    -0.0008442547    0.0130408683
      3595.45455     0.0064927357    0.0139857086
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      3598.48485     0.0043820054    0.0134157054
      3600.00000    -0.0027105984    0.0145635541
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