

## **An insight into the intermolecular vibrational modes of dicationic ionic liquids through far-infrared spectroscopy, and DFT calculations**

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Method	B3LYP/aug-cc-pvtz-pp	m062x/lanl08(d)	mPW2PLYPD/crenbl
<b>Number of basis functions</b>	1858	748	544
<b>Progressive number</b>	19	19	19
<b>Frequency/cm<sup>-1</sup></b>	138.6	149.6	159.9
<b>Intensity/ (Kg/mole)</b>	24.4	17.5	20.9
<b>Red. Mass (a.u.)</b>	4.4608	4.1478	4.7148
<b>Progressive number</b>	41	41	41
<b>Frequency/cm<sup>-1</sup></b>	639.8	640.3	654.8
<b>Intensity/ (Kg/mole)</b>	116.4	102.2	67.8
<b>Red. Mass (a.u.)</b>	2.0376	2.7505	2.7024

In the table some data about test calculations on BIC4IB+2Br Syn system with different functionals and basis sets are reported. All geometries have been re-optimized and frequencies calculations have been performed.

Data about two of the normal modes analyzed in the paper are reported. For all the different calculation schemes, they share the same progressive number, e.g. they are the 19<sup>th</sup> and 41<sup>th</sup> normal modes (ordered with respect to increasing frequency values), they present a large IR intensity with respect to normal modes with similar frequency. A visual analysis shows that all the corresponding normal modes are related to the same molecular motion (the one reported in the main paper body). Reduced masses are similar (this is a synthetic index of similarity between normal modes, especially in the case of normal modes extendedly delocalized in the molecule like these ones). Differences in frequencies are observable. Frequencies (especially lower ones) are the normal-mode related quantity most sensitive to the level of calculation. As reported in the table, the method used in the paper presents a considerable larger basis set.

Conclusion: the calculated infrared quantities reported in the paper are reliable and are not the consequence of level of calculation numerical artifact.

## BIC4IB+2Br Syn

Charge = 0 Multiplicity = 1

C,0,1.2397196542,2.3904481814,1.5446644865  
C,0,2.3270026977,1.7996162075,0.9887474312  
C,0,1.0971351718,2.6615591695,-0.6328437797  
N,0,0.4838899854,2.9267548265,0.5183454685  
H,0,0.9430072686,2.4612657842,2.5731912249  
H,0,3.1121498695,1.1889472506,1.4220825896  
H,0,0.7084643328,2.9010440245,-1.6055986496  
C,0,-0.7938156751,3.6468080231,0.638481437  
H,0,-1.1700601383,3.7663790134,-0.3754443143  
H,0,-0.5848402238,4.6323625436,1.0588235677  
C,0,3.1691173146,0.0399429235,-1.6214191221  
H,0,3.1878867131,-0.4592979328,-0.6482969256  
C,0,1.9956739606,-0.4155739695,-2.4947225367  
H,0,1.0946395002,0.1754711024,-2.3110772456  
H,0,2.2406631756,-0.2692915719,-3.5494881234  
C,0,1.6317114618,-1.8911180791,-2.3030905392  
H,0,1.0827709459,-2.2636667186,-3.1658832864  
H,0,2.5153069303,-2.5135203276,-2.1735267672  
N,0,0.7721442299,-2.109589399,-1.1276844824  
C,0,-0.5469239849,-1.8975732389,-1.1292730203  
C,0,1.170290904,-2.4478350695,0.1529068532  
H,0,-1.1253231022,-1.5161323953,-1.9537437373  
C,0,0.0491047009,-2.451589377,0.9169604416  
H,0,2.2063384958,-2.5581650088,0.4458280025  
H,0,-0.0722226727,-2.6409200108,1.9667278011  
C,0,-2.4136963095,-1.9327973305,0.4974290179  
H,0,-2.4088427555,-1.6462341016,1.5484763804

H,0,-2.7964941336,-1.0887815102,-0.0779255094  
N,0,-1.0116833303,-2.1062505216,0.1001400414  
N,0,2.2246335245,1.9943797855,-0.3770808294  
Br,0,4.0309822712,-1.2008325788,1.7612548177  
Br,0,-1.6688059381,1.1231838034,-1.9603432951  
C,0,3.2150836406,1.5441165548,-1.3721063752  
H,0,3.0341478995,2.1169347828,-2.2815653196  
H,0,4.1919970582,1.8258583179,-0.9844078438  
H,0,4.1116407941,-0.2377159254,-2.0984672089  
C,0,-1.8239703437,2.8991265086,1.4765002249  
H,0,-1.9734792991,1.9156152658,1.0285650536  
H,0,-1.4519972751,2.7560494693,2.4947920452  
C,0,-3.1536639125,3.6535355968,1.5210248853  
H,0,-2.9929113853,4.6608122408,1.9176800416  
H,0,-3.5241412873,3.7751007822,0.5003884621  
C,0,-4.2080101341,2.9377557724,2.3627034473  
H,0,-3.8773857523,2.8184976226,3.3965892248  
H,0,-5.1452442071,3.4946194517,2.3766978432  
H,0,-4.4185354163,1.9447543343,1.9623809715  
C,0,-3.2540812392,-3.1891972677,0.2817740267  
H,0,-3.2257205102,-3.4602658264,-0.7768908844  
H,0,-2.8114902189,-4.0237671039,0.8325341409  
C,0,-4.7049006401,-2.9879073354,0.7215893338  
H,0,-5.1328730983,-2.1436769606,0.1746470004  
H,0,-4.7268473771,-2.7103870082,1.7795152696  
C,0,-5.5671671994,-4.2295310884,0.5029365698  
H,0,-6.5937498362,-4.0572552774,0.8266182423  
H,0,-5.594697013,-4.5095435031,-0.5516003356  
H,0,-5.1810571358,-5.0832600832,1.0629558645

## BIC4IB+2Br anti

Charge = 0 Multiplicity = 1

C,0,0.0198797854,-2.6058224486,-0.5471669788  
C,0,0.5515196613,-2.2939046319,0.6609204965  
C,0,2.1491337456,-2.1378394107,-0.8614148725  
N,0,1.0311052112,-2.5045788394,-1.4839951497  
H,0,-0.9873128814,-2.8642525557,-0.8139111978  
H,0,0.0651405021,-2.1785549042,1.6163879289  
H,0,3.0701546781,-1.8662107539,-1.3518945805  
C,0,0.9113501027,-2.654643842,-2.9404528252  
H,0,1.43965828,-1.805766745,-3.3798604841  
H,0,-0.1475580266,-2.5587600884,-3.1768326844  
C,0,2.9627397035,0.0160838168,1.420505217  
H,0,2.9149723823,0.3506004726,0.3809943627  
C,0,1.9089924194,0.7039878291,2.298573332  
H,0,0.9587832388,0.1637296362,2.3018339107  
H,0,2.2494568553,0.7078677584,3.3362940052  
C,0,1.615970234,2.1542945295,1.8984097911  
H,0,1.2110109747,2.7052190771,2.7448460044  
H,0,2.5103488066,2.6745656047,1.5590295157  
N,0,0.61991232,2.2469660276,0.8193594111  
C,0,-0.697459677,2.1522408577,1.0265891395  
C,0,0.8550223177,2.2981486809,-0.5427133026  
H,0,-1.1780338486,1.9721499518,1.9748504064  
C,0,-0.3579597735,2.2499744766,-1.1474923985  
H,0,1.8410938132,2.285633191,-0.9789453815  
H,0,-0.6113243816,2.2479282633,-2.1906500286  
C,0,-2.7624173665,1.9871034615,-0.3262854888

H,0,-2.9142678239,1.6423383406,-1.3482581558  
H,0,-3.0578717541,1.1855838096,0.3541992526  
N,0,-1.3139573655,2.1607107333,-0.1532231955  
N,0,1.8887437161,-2.0147021316,0.4441318713  
Br,0,3.19521819,0.4452825816,-2.5233041897  
Br,0,-1.8821942151,-0.4599074134,2.5433683448  
C,0,2.8698836389,-1.5138742633,1.4196408746  
H,0,2.5872222687,-1.9079291229,2.3946252191  
H,0,3.8292296517,-1.9503422364,1.1492476275  
H,0,3.9602384264,0.288298321,1.7721978455  
C,0,1.4642187268,-3.9820696668,-3.4519489998  
H,0,2.5207796547,-4.0560361132,-3.1819129487  
H,0,0.9511716195,-4.8101377173,-2.9546037266  
C,0,1.3157521134,-4.1120673886,-4.9685021796  
H,0,0.2581981427,-4.0311853661,-5.2368826979  
H,0,1.8198816901,-3.2710298018,-5.4510738899  
C,0,1.8790331387,-5.4253458974,-5.5077715099  
H,0,1.373675559,-6.2854371688,-5.0641942372  
H,0,1.7577410435,-5.4906062934,-6.5891999747  
H,0,2.9441908869,-5.5164201895,-5.2879113966  
C,0,-3.5534349027,3.2650541933,-0.0607997661  
H,0,-3.3642476638,3.5951405847,0.9638758722  
H,0,-3.1980612217,4.0612909428,-0.7210896974  
C,0,-5.0551809095,3.0544950934,-0.2590302811  
H,0,-5.3930383556,2.2470598892,0.3953903784  
H,0,-5.2413698286,2.7179294381,-1.2832607436  
C,0,-5.8712318308,4.3152649654,0.0190323478  
H,0,-6.9358732194,4.1358063083,-0.1319350809  
H,0,-5.7349928378,4.6532601423,1.0478141502

H, 0, -5.5751704251, 5.1328831419, -0.6410832612

### **BIC5IB+2Br Syn**

Charge = 0 Multiplicity = 1

C, 0, 2.4933531917, -0.8433885016, 1.1622250494

C, 0, 2.1880871681, 0.4087509299, 1.5812486511

C, 0, 0.5430087885, -0.9358337644, 2.1851031356

N, 0, 1.4599141314, -1.6708174263, 1.5556281474

H, 0, 3.3234156632, -1.1906191384, 0.5770806049

H, 0, 2.7016414782, 1.331552692, 1.3883025484

H, 0, -0.429464668, -1.2780338292, 2.5082785307

C, 0, 1.3298119017, -3.1004454145, 1.2522147083

H, 0, 0.7171073792, -3.5421569817, 2.0364737729

H, 0, 2.3269240749, -3.5344121292, 1.3255865986

C, 0, 0.3937744272, 2.7809142401, 2.2834772496

H, 0, 1.4460366564, 3.070326381, 2.3034218453

C, 0, -1.6516315826, 2.8118859453, 0.7279747072

H, 0, -2.0276142456, 1.8788368194, 1.1548704246

H, 0, -2.131098564, 3.6271818452, 1.2782489168

C, 0, -2.1379456626, 2.9039141851, -0.7195078081

H, 0, -3.2126464257, 3.0757193405, -0.7514936598

H, 0, -1.6531898674, 3.7229638999, -1.2486635549

N, 0, -1.8805615931, 1.6822151694, -1.4987243552

C, 0, -2.679941492, 0.6124629582, -1.499758729

C, 0, -0.7703007178, 1.4103853366, -2.276572865

H, 0, -3.576175085, 0.4962659568, -0.919467548

C, 0, -0.9395989887, 0.1565576623, -2.7655576253

H, 0, 0.0872122574, 2.0654816492, -2.3500786792

H, 0, -0.2953296246, -0.4341665532, -3.3885151517  
C, 0, -2.7017344052, -1.6631628101, -2.4811166626  
H, 0, -1.8865732018, -2.2887066184, -2.8413726074  
H, 0, -2.9980003648, -2.0283390754, -1.4959697032  
N, 0, -2.1395318362, -0.3232338855, -2.2767223261  
N, 0, 0.9677840069, 0.3294051997, 2.2240110651  
Br, 0, 2.6125351962, 1.9373910432, -1.53922973  
Br, 0, -2.7279647283, -1.1602698338, 1.3108706342  
C, 0, 0.2326258174, 1.4038288954, 2.920037666  
H, 0, -0.8094131204, 1.0872250826, 2.9339650882  
H, 0, 0.5899305403, 1.4326595557, 3.9503629965  
H, 0, -0.119525295, 3.4818906665, 2.9481601553  
C, 0, -0.1328177083, 2.9233645628, 0.8547807917  
H, 0, 0.1856847902, 3.8981253039, 0.4780868254  
H, 0, 0.3736082752, 2.204500119, 0.2079748237  
C, 0, 0.713087381, -3.3631375702, -0.1192411514  
H, 0, -0.2835337386, -2.9161729356, -0.1391205776  
H, 0, 1.3114345853, -2.8626248881, -0.8848943627  
C, 0, 0.6273616604, -4.8606242005, -0.4178326737  
H, 0, 1.627924156, -5.3009957611, -0.3708660542  
H, 0, 0.0383562588, -5.3512443929, 0.3620962801  
C, 0, 0.0067853826, -5.1578779306, -1.781388069  
H, 0, 0.5848833948, -4.7000324326, -2.5864242899  
H, 0, -0.0332421298, -6.2307217239, -1.971183875  
H, 0, -1.0130378602, -4.773788688, -1.8381602137  
C, 0, -3.8681316637, -1.676992167, -3.4662229596  
H, 0, -4.6641529515, -1.0287415557, -3.0902587076  
H, 0, -3.5440959764, -1.2559776183, -4.4220392513  
C, 0, -4.4179251753, -3.0881440685, -3.6789571789



H,0,-4.7261917111,-3.5029942838,-2.7157868043  
H,0,-3.617772357,-3.7354833136,-4.0496137572  
C,0,-5.5940463257,-3.1247563342,-4.6528146833  
H,0,-5.9631968025,-4.1418296865,-4.7858455135  
H,0,-6.4243676943,-2.5156013139,-4.2911396987  
H,0,-5.3067623798,-2.744493413,-5.63491228

## BIC5IB+2Br Anti

Charge = 0 Multiplicity = 1

Redundant internal coordinates found in file. (old form).

C,0,1.1246296833,-1.9299956778,1.5377619845  
C,0,0.2840319223,-1.1539601356,2.2659237555  
C,0,1.7463976241,0.1681077664,1.2717776862  
N,0,2.0260506365,-1.0885287132,0.9188075522  
H,0,1.1441550209,-2.9929785122,1.3881210087  
H,0,-0.5996091157,-1.3935388391,2.8290260141  
H,0,2.2441192802,1.0277230357,0.8447499662  
C,0,3.0999085034,-1.4784273701,-0.008628865  
H,0,3.1101100685,-0.7274244958,-0.8028014078  
H,0,2.8090954743,-2.4383933322,-0.4344027208  
C,0,0.446226263,2.6642267308,2.248657277  
H,0,1.5312699535,2.784362879,2.2929110084  
C,0,-1.5571823971,3.1755691957,0.7223939277  
H,0,-2.0984393303,2.3650124107,1.2163179872  
H,0,-1.8587091813,4.1035935227,1.2160708032  
C,0,-2.0391363981,3.2552909804,-0.7263226993  
H,0,-3.0731947006,3.5933560271,-0.7690708515  
H,0,-1.4362623794,3.9475537283,-1.3121569832  
N,0,-1.9825765706,1.9559191518,-1.419551625  
C,0,-2.8927599448,0.9878282843,-1.2821972716  
C,0,-0.9731585394,1.5012273642,-2.2480047024  
H,0,-3.7433359138,1.0088641593,-0.623591514  
C,0,-1.3125309986,0.2430909707,-2.6226320816  
H,0,-0.0724803567,2.0614622842,-2.4449248244  
H,0,-0.7925205678,-0.4548646081,-3.2503487322

C, 0, -3.2284530527, -1.3427826902, -2.0671666532  
H, 0, -4.1747200649, -1.1940259423, -1.5512221983  
H, 0, -3.4396037552, -1.5645232887, -3.1144270695  
N, 0, -2.5176988336, -0.0579462968, -2.0153291718  
N, 0, 0.695536172, 0.1529005493, 2.0972486618  
Br, 0, 2.5847355596, 1.7542329071, -1.6463833538  
Br, 0, -3.2107964254, -0.2840773054, 1.744823214  
C, 0, 0.0532325145, 1.2929968582, 2.786817046  
H, 0, -1.0203378457, 1.1113940408, 2.706839096  
H, 0, 0.3305782815, 1.217290578, 3.8389515576  
H, 0, 0.0411514499, 3.3911672889, 2.9577490322  
C, 0, -0.0433549585, 2.9920282845, 0.8349278525  
H, 0, 0.4567751928, 3.9044182673, 0.5030014637  
H, 0, 0.302555903, 2.2255147328, 0.1412116154  
C, 0, 4.4627831694, -1.5718712627, 0.6714705635  
H, 0, 4.7129786925, -0.5953411026, 1.0935914334  
H, 0, 4.4170081755, -2.2789563058, 1.5053820976  
C, 0, 5.5547270088, -1.9938784894, -0.3125891265  
H, 0, 5.2988808075, -2.9671017255, -0.7425919181  
H, 0, 5.5762385232, -1.2854386583, -1.1438609195  
C, 0, 6.9363178797, -2.0702175257, 0.3340060363  
H, 0, 6.9520730178, -2.7904728082, 1.1546358847  
H, 0, 7.6928571407, -2.3749386685, -0.3895162045  
H, 0, 7.2352594164, -1.1009739148, 0.7368739158  
C, 0, -2.4462927116, -2.4717361386, -1.4024965388  
H, 0, -1.4910321318, -2.6108095345, -1.9169019776  
H, 0, -2.2354746628, -2.1726439159, -0.3737802826  
C, 0, -3.234057209, -3.7820632909, -1.4149724599  
H, 0, -3.4850096347, -4.0549371963, -2.4449256997

H,0,-4.1825742031,-3.6306657877,-0.8934699801  
C,0,-2.4732344933,-4.9300005752,-0.7543608144  
H,0,-3.0556450017,-5.851553142,-0.7728409487  
H,0,-1.5282008432,-5.1249356636,-1.2659402984  
H,0,-2.249884033,-4.6986188307,0.2881585168

## MIC6IM+2Tf2N Syn

Charge = 0 Multiplicity = 1

6	1.50404	-1.56859	3.14941
6	1.46977	-0.23655	3.39955
6	-0.49104	-0.82275	2.57744
7	0.27222	-1.91443	2.63653
1	2.304	-2.27881	3.2331
1	2.24033	0.43109	3.73552
1	-1.49896	-0.78678	2.19222
6	0.11773	0.23685	-2.6995
6	0.91378	1.27706	-2.34438
6	-1.01739	2.09215	-3.03053
7	-1.08056	0.76571	-3.13137
1	0.30189	-0.81977	-2.64932
1	1.91001	1.28547	-1.93325
1	-1.82141	2.76983	-3.24847
7	0.21505	0.21115	3.04193
7	0.18552	2.43114	-2.56211
6	-0.21763	1.61718	2.9894
1	0.21147	2.12248	3.85392
1	-1.30099	1.62632	3.08284
6	0.21258	2.25772	1.6728
1	1.29735	2.20282	1.58993
1	-0.20849	1.64806	0.87239
6	-0.2825	3.70013	1.50932
1	0.38954	4.39286	2.02323
1	-1.26289	3.8069	1.97875
6	0.65438	3.79868	-2.27335

1	1.58228	3.93915	-2.82588
1	-0.08916	4.48205	-2.68199
6	0.87186	4.03776	-0.77874
1	1.54463	3.26392	-0.40912
1	1.41774	4.97777	-0.67522
6	-0.43139	4.08617	0.03217
1	-1.16838	3.40713	-0.40203
1	-0.86322	5.08704	-0.04407
6	-5.34567	1.56247	0.7674
6	-5.21182	-2.63818	-0.35429
8	-3.56926	2.1244	-1.11287
8	-2.73714	1.11527	1.01254
8	-2.69883	-2.39551	-1.17813
8	-3.20523	-1.82075	1.19768
9	-5.03463	-3.90154	0.03827
9	-5.64748	-2.63374	-1.61377
9	-6.1296	-2.06755	0.42552
9	-6.34049	1.57593	-0.11879
9	-5.23868	2.77647	1.31652
9	-5.62891	0.68013	1.72662
7	-3.98706	-0.28618	-0.76263
6	4.46145	-2.48145	-1.45325
7	4.0259	-0.79099	0.70818
8	2.93779	-3.00617	0.64246
8	2.13343	-1.28479	-0.97936
9	3.88446	-3.44215	-2.1813
9	5.53635	-2.98567	-0.84799
9	4.84542	-1.49778	-2.26968
16	3.22064	-1.84145	-0.18329

16	-3.56551	-1.73232	-0.21516
16	-3.71621	1.1179	-0.06902
16	4.14568	0.7825	0.44868
8	3.75051	1.26744	-0.87139
8	3.66603	1.52649	1.60751
6	6.01666	1.00033	0.50707
9	6.30065	2.29469	0.33204
9	6.60329	0.29676	-0.46135
9	6.5028	0.60909	1.68451
6	-0.11932	-3.25083	2.18419
1	0.66692	-3.63395	1.53853
1	-0.25564	-3.90561	3.0425
1	-1.0495	-3.16745	1.63158
6	-2.22291	0.00028	-3.63656
1	-3.12003	0.60127	-3.52974
1	-2.05571	-0.25646	-4.6811
1	-2.33514	-0.90001	-3.03936

## MIC6IM+2Tf2N anti

Charge = 0 Multiplicity = 1

C	0.19735	3.2754	-1.84108
C	-0.49082	2.16466	-2.20793
C	1.65312	1.79883	-2.57639
N	1.53384	3.03075	-2.08393
H	-0.1464	4.20207	-1.42155
H	-1.54403	1.94283	-2.14848
H	2.57429	1.29167	-2.80298
C	0.14274	-0.77806	2.63634
C	0.79259	-1.77894	1.9921
C	-1.32125	-2.37028	2.2225
N	-1.17305	-1.16612	2.77469
H	0.50991	0.17009	2.98047
H	1.81667	-1.84472	1.669
H	-2.25809	-2.8922	2.13022
N	0.43873	1.25542	-2.67001
N	-0.13891	-2.76862	1.74497
C	0.15777	-0.11522	-3.13408
H	1.0568	-0.46549	-3.636
H	-0.64708	-0.05078	-3.86579
C	-0.21443	-1.04227	-1.98343
H	0.59791	-1.01839	-1.25627
H	-1.11597	-0.67195	-1.49443
C	-0.46579	-2.47597	-2.45722
H	0.40074	-2.84516	-3.01465
H	-1.31244	-2.47923	-3.14687
C	0.13841	-4.02857	1.03256



H	0.98078	-4.49859	1.53812
H	-0.73344	-4.66789	1.16432
C	0.44943	-3.80246	-0.44693
H	1.23509	-3.04951	-0.51882
H	0.89358	-4.72407	-0.82797
C	-0.77854	-3.41986	-1.28979
H	-1.53891	-2.93899	-0.67317
H	-1.24371	-4.32992	-1.67327
C	-6.13763	-1.36636	-0.50705
C	-5.01206	2.78489	0.53265
O	-4.33171	-2.20687	1.23817
O	-3.51874	-1.45468	-0.99974
O	-2.51134	1.98039	0.91283
O	-3.53908	1.54839	-1.31721
F	-4.62431	3.98104	0.07663
F	-5.20977	2.87176	1.84836
F	-6.15774	2.45031	-0.05857
F	-7.02191	-1.16306	0.46982
F	-6.32313	-2.58973	-1.01039
F	-6.34002	-0.46754	-1.47018
N	-4.30657	0.22507	0.79918
C	5.38786	1.08566	2.15829
N	4.13144	0.72071	-0.30701
O	3.63933	2.72457	1.04004
O	2.80105	0.5338	1.90663
F	5.23408	1.69091	3.33778
F	6.41811	1.63995	1.51851
F	5.65012	-0.2052	2.36855
S	3.79853	1.28473	1.15926

S	-3.66209	1.53166	0.13641
S	-4.37736	-1.22937	0.15391
S	3.97086	-0.78589	-0.81899
O	3.55257	-1.7861	0.15492
O	3.28767	-0.77368	-2.1115
C	5.74286	-1.24338	-1.27622
F	5.74796	-2.47745	-1.78586
F	6.53195	-1.21572	-0.20361
F	6.22208	-0.39771	-2.18989
C	2.64226	3.94156	-1.79203
H	2.39746	4.92984	-2.17324
H	2.8219	3.96825	-0.72028
H	3.53602	3.57188	-2.2849
C	-2.2301	-0.38097	3.41791
H	-3.18015	-0.88037	3.26083
H	-2.01593	-0.29587	4.48137
H	-2.26981	0.60128	2.95476

BIC4IB+Br2				BIC5IB+Br2				MIC6IM+2Tf2N			
syn		anti		Syn		anti		syn		anti	
v (cm-1)	I (Km/mole)	v (cm-1)	I (Km/mole)	v (cm-1)	I (Km/mole)	v (cm-1)	I (Km/mole)	v (cm-1)	I (Km/mole)	v (cm-1)	I (Km/mole)
12.153	0.492	10.205	0.007	-13.786	4.003	11.024	0.047	5.287	0.341	4.268	0.417
15.088	1.569	12.073	0.866	11.540	1.000	16.314	1.158	11.212	0.495	10.397	0.191
20.537	0.279	15.471	2.445	16.619	1.091	17.985	2.458	15.133	0.093	13.364	0.790
25.751	5.773	18.488	5.240	18.988	3.561	22.167	2.095	16.901	0.261	14.957	0.085
31.070	1.303	20.484	4.322	23.076	1.359	33.185	0.463	21.018	2.656	16.927	1.943
39.858	2.107	42.591	3.990	26.644	3.142	37.893	1.534	23.897	0.228	22.843	2.775
43.021	4.920	42.815	10.014	40.485	5.121	48.786	6.330	26.743	2.013	26.025	0.260
48.551	6.081	45.710	0.224	42.117	8.561	50.595	4.764	29.474	0.745	30.345	1.111
55.956	4.970	48.293	4.300	49.102	0.602	56.376	9.877	30.570	0.176	31.970	4.975
56.509	6.009	50.141	6.584	53.703	6.435	58.157	12.871	32.151	0.978	34.128	1.185
71.950	9.962	66.744	0.066	68.953	22.441	61.700	3.161	35.464	2.309	35.853	0.380
74.703	19.163	68.626	22.946	70.799	4.364	67.278	6.059	35.940	0.433	38.350	0.942
79.454	2.692	73.039	9.378	73.455	2.282	80.287	3.850	40.657	4.097	39.457	0.323
85.040	8.038	75.468	1.022	74.773	2.115	82.798	13.054	43.581	1.929	42.979	0.173
92.037	0.910	81.410	0.535	78.335	3.643	84.600	3.572	45.011	0.190	45.294	2.805
105.630	3.636	111.854	0.219	103.599	7.445	104.465	2.799	47.326	4.387	46.931	1.219
114.112	3.624	113.168	0.442	109.788	4.827	114.064	11.292	51.264	1.128	50.217	3.367
119.297	0.277	125.702	0.073	110.726	0.532	117.130	0.931	54.811	0.260	51.798	0.486

126.934	16.075	138.637	24.479	119.729	6.864	122.742	0.979	59.644	3.828	53.987	2.473
154.699	1.206	154.577	0.041	127.890	6.702	131.789	4.338	60.599	1.815	59.655	4.975
174.138	0.725	160.019	1.335	157.440	0.230	157.521	1.381	62.180	2.675	62.937	5.273
206.885	0.175	207.545	0.641	175.490	0.805	181.001	0.594	64.119	9.803	66.734	0.721
225.582	0.592	216.244	0.018	204.577	0.639	203.311	2.542	74.112	14.367	68.532	3.599
238.991	0.606	239.035	0.924	213.995	0.071	228.143	1.091	83.126	5.000	78.078	7.264
240.133	0.029	239.225	0.042	234.280	0.495	239.100	0.042	86.254	8.029	83.582	5.455
244.779	0.021	245.066	1.834	239.829	0.212	239.930	0.227	94.820	9.546	106.252	6.396
256.916	1.171	265.600	0.550	244.177	0.128	245.909	0.083	116.081	0.079	110.572	5.427
274.033	0.853	293.633	0.410	254.257	1.242	252.987	0.232	119.130	0.319	113.977	5.672
292.188	0.431	315.234	0.061	274.578	0.292	267.943	1.221	120.996	0.342	117.720	10.011
318.549	0.227	316.317	0.249	298.332	0.577	296.090	0.861	127.762	0.648	123.628	0.363
322.943	0.676	317.557	0.006	314.332	0.384	309.727	0.477	141.045	0.041	133.239	1.317
382.767	1.657	396.386	0.085	318.246	0.258	316.007	0.166	149.805	1.841	147.368	1.330
401.156	0.146	407.893	0.252	351.113	0.211	358.407	0.377	156.799	1.167	158.049	1.331
412.227	0.270	413.888	2.503	388.633	1.249	383.821	3.078	161.970	0.410	159.033	1.320
431.980	2.243	432.569	0.105	410.785	1.471	402.005	2.554	180.258	0.088	174.369	0.096
463.652	0.503	436.370	3.899	427.471	0.803	429.573	1.221	182.644	0.584	189.247	1.946
526.992	0.707	519.685	0.043	434.529	2.040	444.738	0.770	185.828	2.647	192.837	0.126
612.935	11.730	614.665	0.102	477.130	0.733	471.583	0.861	194.849	1.640	195.805	0.452
621.189	1.827	621.117	14.750	521.599	0.583	518.050	0.277	195.618	0.818	197.021	1.731
641.768	71.054	637.362	0.917	619.836	0.811	618.338	19.992	205.287	0.266	199.708	0.776
649.037	5.822	639.831	116.456	624.356	31.865	623.236	2.409	205.682	1.201	205.693	1.520
661.803	19.335	659.343	2.809	641.406	33.559	636.982	36.570	209.312	0.914	206.899	0.367

662.895	6.504	659.741	2.554	644.925	10.969	651.099	50.158	225.481	1.052	224.973	0.066
				651.831	29.951	652.333	0.755	249.907	2.696	250.832	1.840
				662.113	12.473	656.046	2.248	255.596	0.626	260.572	2.364
								262.793	0.999	261.215	0.477
								263.078	1.054	263.741	0.974
								268.214	3.122	267.820	2.600
								268.744	3.105	268.683	2.029
								278.476	0.238	269.331	1.040
								290.408	0.410	289.679	0.336
								291.013	1.019	290.867	0.527
								294.464	1.405	294.378	0.854
								294.814	0.192	295.428	0.255
								307.509	1.886	306.672	2.244
								307.649	2.337	308.756	2.669
								318.113	0.441	315.658	0.338
								319.038	0.905	320.170	1.170
								334.740	0.333	334.497	0.700
								335.406	1.013	337.111	1.103
								355.222	0.625	354.157	1.070
								390.106	4.591	389.193	3.907
								392.658	4.347	392.947	6.821

								409.906	0.373	399.150	0.322
								413.925	5.391	409.287	6.497
								416.028	5.634	418.652	6.194
								420.001	1.883	421.476	0.120
								439.927	0.196	438.196	0.408
								497.900	6.928	498.244	64.460
								499.673	33.834	500.937	78.607
								520.356	14.984	517.585	1.132
								521.996	15.353	521.635	24.536
								525.542	0.934	522.033	5.563
								539.479	6.235	538.974	5.256
								539.608	3.981	540.973	3.604
								549.939	2.059	549.841	1.755
								550.024	2.336	550.061	1.400
								560.239	6.566	560.533	10.259
								561.468	46.271	561.023	52.901
								563.204	4.209	562.136	51.740
								563.862	20.792	567.647	69.587
								581.923	31.416	582.353	34.773
								582.701	44.039	582.979	63.561
								601.038	1.158	599.045	0.543

								631.742	5.689	629.368	53.984
								633.796	1.473	633.399	3.050
								636.830	68.284	639.143	16.818
								640.422	22.570	643.352	24.356
								644.440	11.940	644.312	14.676
								664.181	13.961	667.685	28.309
								674.158	23.622	672.947	6.183
								697.069	2.924	696.726	2.919