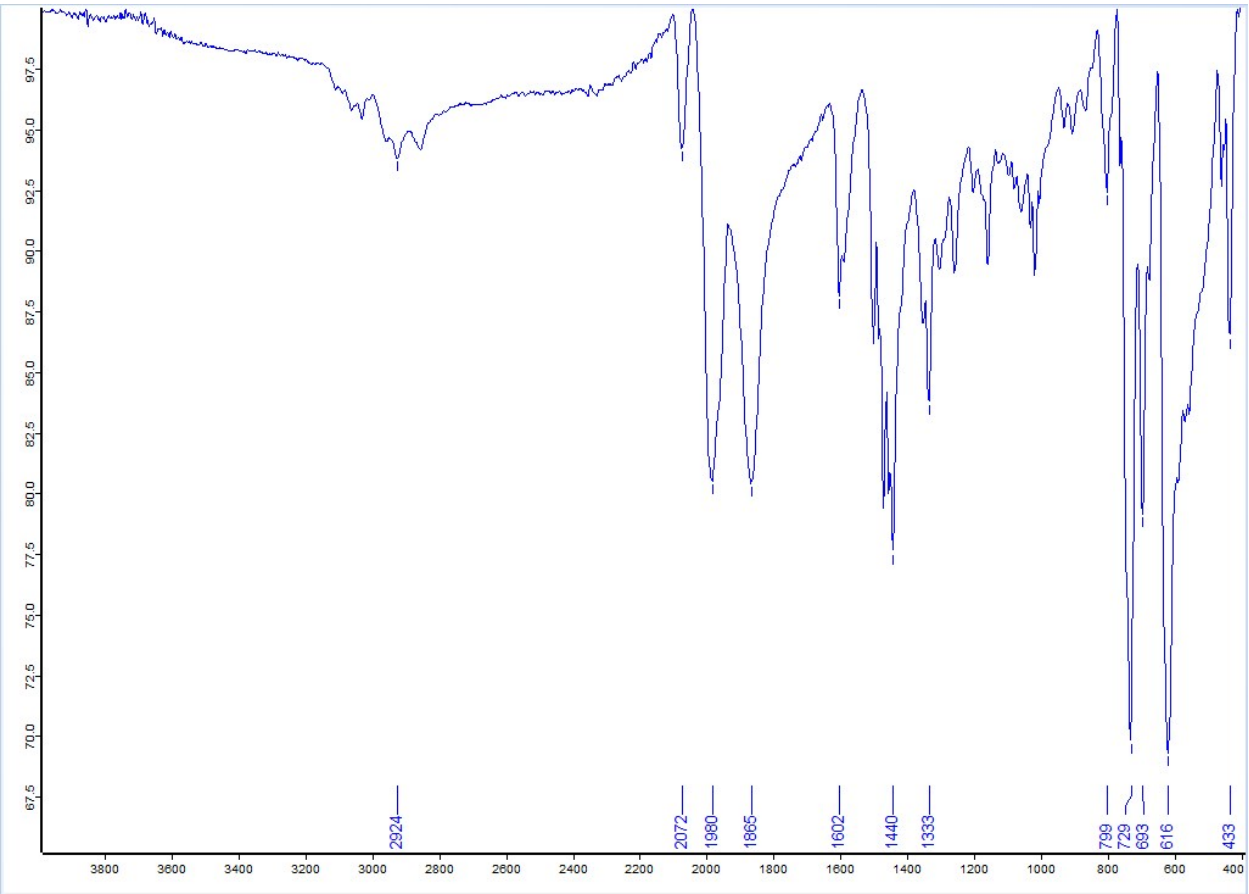
IR-Spectrum of complex 7



Computational Information

General Remarks

Calculations were performed with the Gaussian 09 suite of programs[1] using Compute Canada's Shared Hierarchical Academic Research Computing Network (SHARCNET). Model complexes were fully optimized with no symmetry constraints using the M06-2X density functional method,[2] in conjunction with the cc-pVTZ basis set.[3,4] Geometry optimizations were started using models in which the relevant non-hydrogen atoms were placed in positions found experimentally by X-ray crystallography using Gaussview.[5] Frequency calculations were also performed at the same level of theory in order to confirm that the optimized structures were minima on the potential energy hypersurface and to determine thermochemical and vibrational information. Natural bond orbital (NBO) analyses[6] to determine orbital contributions, Wiberg Bond Indices and orbital energies were obtained using the routine included in the Gaussian distributions.[7] Visualizations of the Kohn-Sham orbitals and optimized geometries were made using VMD.[8] Snapping energies were calculated by subtracting the sum of the single point energies of the $GaCl_2$+ and ligand fragments (separately) from the energy of their optimized complexes.

Parameters for $[Cl_2GaDimpy]^+$

1\1\GINC-ORC51\FOpt\RM062X\CC-pVTZ\C7H7Cl2Ga1N3(1+)\BINDERJ\25-Jul-201
8\0\\# M062X/cc-pVTZ scf=tight opt=tight freq pop=(full,nbo6read)\\Opt
imization, frequency test and nbo analysis for GaCl2 HDimpy complex\\1
,1\Cl,1.8257697142,-0.0000051479,-1.9460922182\N,0.3122616001,-2.09005

73243,0.000005388\N,0.3122637743,2.0900570377,-0.0000038492\N,-1.17957
90856,0.0000006329,0.0000125856\C,-0.9265678122,2.3357519433,0.0000059
658\C,-0.9265702422,-2.3357509406,0.0000165236\C,-3.9096639617,0.00000
20524,0.0000362646\C,-1.8294684952,1.1580308089,0.0000157182\C,-3.2141
113228,-1.2030275409,0.0000326199\C,-1.8294696997,-1.158028867,0.00002
07093\C,-3.2141100708,1.2030309243,0.0000274945\H,-3.731774047,-2.1520
718399,0.0000395083\H,-4.9907309763,0.0000026145,0.0000459477\H,-3.731
7718081,2.1520757614,0.0000301739\Cl,1.8258008089,0.0000032884,1.94606
99198\Ga,0.8973441557,-0.0000004469,-0.0000037039\H,-1.3519162889,3.33
57327599,0.0000065426\H,-1.351919759,-3.335731315,0.000021473\H,0.9386
813037,-2.8906491947,0.0000010745\H,0.9386843126,2.8906482548,-0.00001
14981\\Version=EM64L-G09RevE.01\State=1-A\HF=-3280.4416409\RMSD=4.325e
-09\RMSF=1.174e-06\Dipole=-4.0830462,0.0000021,0.000033\Quadrupole=7.0
72622,15.6854684,-22.7580904,0.0000045,-0.0002506,-0.0000845\PG=C01 [X
(C7H7Cl2Ga1N3)]\\@

Zero-point correction= 0.140660 (Hartree/Particle)
Thermal correction to Energy= 0.153246
Thermal correction to Enthalpy= 0.154190
Thermal correction to Gibbs Free Energy= 0.100470
Sum of electronic and zero-point Energies= -3280.300981
Sum of electronic and thermal Energies= -3280.288395
Sum of electronic and thermal Enthalpies= -3280.287451
Sum of electronic and thermal Free Energies= -3280.341171

Parameters for [$Cl_2GaBzimpy$]$^+$

1\1\GINC-ORC294\FOpt\RM062X\CC-pVTZ\C11H9Cl2Ga1N5(1+)\BINDERJ\12-Jun-2
018\0\\# M062X/cc-pVTZ scf=tight opt=tight freq pop=(full,nbo6read)\\O
ptimization, frequency test and nbo analysis for GaCl2 Bzimpy\\1,1\Cl,
0.0000003043,-2.557176606,1.3490204071\N,3.6137326032,0.7682238868,-0.
0780611417\N,2.0518389908,-0.7347564394,-0.3175744747\N,-2.0518403457,
-0.7347589377,-0.3175747423\N,-0.0000016381,0.8169862268,-0.0702686686
\N,-3.6137358203,0.7682189398,-0.0780581669\C,-2.2883988973,0.54572011
03,-0.1135042758\C,2.2883959559,0.5457230289,-0.1135048087\C,3.2563965
252,-1.3634147348,-0.4177787422\C,-0.0000033056,3.5105372172,0.3590344
122\C,-1.1627478357,1.4627970373,0.0326616984\C,-3.2563971013,-1.36341
82879,-0.4177817464\C,-4.2455759714,-0.4332375373,-0.2695468327\C,1.20
5190169,2.8309611311,0.250721541\C,1.1627437603,1.4627985232,0.0326614
073\C,4.2455742437,-0.4332322533,-0.2695470065\C,-1.2051959394,2.83095
95033,0.250722399\H,2.1452182745,3.355962989,0.334398156\H,-0.00000396
65,4.5781169074,0.5291879738\H,-2.1452246952,3.3559600845,0.3343997256
\H,5.3165201005,-0.5205701166,-0.2834806448\H,3.3347615544,-2.42261958
94,-0.586585499\H,4.0724256449,1.6540209233,0.0630992274\H,-4.07242995
87,1.654015029,0.0631045854\H,-5.3165217199,-0.5205767411,-0.283480378
5\H,-3.3347608187,-2.4226227596,-0.5865915136\Ga,-0.0000003396,-1.2804
653327,-0.4045647801\Cl,0.0000002207,-1.948690502,-2.4681861309\\Versi
on=EM64L-G09RevE.01\State=1-A\HF=-3543.6356997\RMSD=3.223e-09\RMSF=2.6
28e-07\Dipole=-0.0000027,4.4619009,0.7111458\Quadrupole=36.8598487,-1.
2162473,-35.6436014,0.0000242,-0.0000141,5.6300611\PG=C01 [X(C11H9Cl2G
a1N5)]\\@

Zero-point correction= 0.200667 (Hartree/Particle)
Thermal correction to Energy= 0.217079
Thermal correction to Enthalpy= 0.218023
Thermal correction to Gibbs Free Energy= 0.154712
Sum of electronic and zero-point Energies= -3543.435033
Sum of electronic and thermal Energies= -3543.418620
Sum of electronic and thermal Enthalpies= -3543.417676
Sum of electronic and thermal Free Energies= -3543.480987

Parameters for Dimpy from $[Cl_2GaDimpy]^+$ complex

1\1\GINC-ORC343\SP\RM062X\CC-pVTZ\C7H7N3\BINDERJ\25-Jul-2018\0\\# M062
X/cc-pVTZ sp\\Single point calculation on HDimpy ligand fragment from
DimpyGaCl2+ complex\\0,1\N,0,0.477978,2.090057,0.\N,0,0.477978,-2.0900
57,0.000009\N,0,-1.013864,0.,-0.000008\C,0,-0.760854,-2.335751,-0.0000
01\C,0,-0.760854,2.335751,-0.000012\C,0,-3.743949,0.,-0.000031\C,0,-1.
663754,-1.15803,-0.000011\C,0,-3.048396,1.203029,-0.000028\C,0,-1.6637
54,1.15803,-0.000016\C,0,-3.048396,-1.203029,-0.000023\H,0,-3.566058,2
.152074,-0.000035\H,0,-4.825016,0.,-0.000041\H,0,-3.566058,-2.152074,-
0.000025\H,0,-1.186203,-3.335732,-0.000002\H,0,-1.186203,3.335732,-0.0
00017\H,0,1.104398,2.890649,0.000004\H,0,1.104398,-2.890649,0.000016\\
Version=EM64L-G09RevE.01\State=1-A\HF=-435.1240529\RMSD=9.436e-09\Dipo
le=-1.311463,0.,-0.0000112\Quadrupole=-2.5615021,9.3595681,-6.798066,0
.,0.0000385,-0.0000356\PG=C01 [X(C7H7N3)]\\@

Single Point energy = -435.12405293

Parameters for $GaCl_2$ from $[Cl_2GaDimpy]^+$ complex

1\1\GINC-ORC343\SP\RM062X\CC-pVTZ\Cl2Ga1(1+)\BINDERJ\25-Jul-2018\0\\#
M062X/cc-pVTZ sp\\Single point calculation on GaCl2+ fragment from HDi
mpyGaCl2+ complex\\1,1\Cl,0,1.991485,0.000004,1.946097\Cl,0,1.991516,-
0.000004,-1.946065\Ga,0,1.063059,0.,0.000009\\Version=EM64L-G09RevE.01
\State=1-A1\HF=-2845.0545566\RMSD=6.274e-09\Dipole=-1.1008816,0.,-0.00
00088\Quadrupole=0.7393437,-2.0052955,1.2659517,0.,-0.0000042,0.000006
7\PG=C02V [C2(Ga1),SGV(Cl2)]\\@

Single Point energy = -2845.05455665

Parameters for Bzimpy from $[Cl_2GaBzimpy]^+$ complex

1\1\GINC-ORC83\SP\RM062X\CC-pVTZ\C11H9N5\BINDERJ\13-Jun-2018\0\\# M062
X/cc-pVTZ sp\\Single point energy of Bzimpy ligand from BzimpyGaCl2+ c
omplex\\0,1\N,0,-3.613734,1.031464,0.000008\N,0,-2.05184,-0.49048,-0.0
00018\N,0,2.05184,-0.49048,-0.000018\N,0,0.,1.080847,-0.000012\N,0,3.6
13734,1.031464,0.000006\C,0,2.288397,0.806159,-0.000009\C,0,-2.288397,
0.806159,-0.000009\C,0,-3.256397,-1.127075,-0.000008\C,0,0.,3.808395,-
0.000025\C,0,1.162746,1.73481,-0.000014\C,0,3.256397,-1.127075,-0.0000
04\C,0,4.245575,-0.185156,0.00001\C,0,-1.205193,3.120241,-0.000021\C,0
,-1.162746,1.73481,-0.000014\C,0,-4.245575,-0.185156,0.00001\C,0,1.205
193,3.120241,-0.000021\H,0,-2.145221,3.651869,-0.000024\H,0,0.,4.88945
,-0.00003\H,0,2.145221,3.651869,-0.000026\H,0,-5.316521,-0.273599,0.00
0023\H,0,-3.334761,-2.199647,-0.000014\H,0,-4.072428,1.928438,0.000023
\H,0,4.072428,1.928438,0.000018\H,0,5.316521,-0.273599,0.000024\H,0,3.
334761,-2.199647,-0.000007\\Version=EM64L-G09RevE.01\State=1-A\HF=-698
.2937814\RMSD=4.655e-09\Dipole=0.,2.1698342,0.0000341\Quadrupole=17.87
64866,-3.2044118,-14.6720748,0.,-0.0000091,-0.0000284\PG=C01 [X(C11H9N
5)]\\@

Single Point energy = -698.29378142

Parameters for $GaCl_2$ from $[Cl_2GaBzimpy]^+$ complex

1\1\GINC-ORC9\SP\RM062X\CC-pVTZ\Cl2Ga1(1+)\BINDERJ\13-Jun-2018\0\\# M0
62X/cc-pVTZ sp\\Single point calculation on GaCl2+ fragment from Bzimp
yGaCl2+ complex\\1,1\Cl,0,0.,-2.027879,-1.932673\Ga,0,0.,-1.043077,-0.
000001\Cl,0,0.,-2.027769,1.932728\\Version=EM64L-G09RevE.01\State=1-A1
\HF=-2845.0504565\RMSD=6.746e-09\Dipole=0.,1.1673438,-0.0000331\Quadru
pole=-2.0555571,1.0105431,1.045014,0.,0.,0.000001\PG=C02V [C2(Ga1),SGV
(Cl2)]\\@

Single Point energy = -2845.05045646

Parameters for Dimpy ligand

1\1\GINC-ORC335\FOpt\RM062X\CC-pVTZ\C7H7N3\BINDERJ\25-Jul-2018\0\\# M0
62X/cc-pVTZ scf=tight opt=tight freq pop=(full,nbo6read)\\Optimization
, frequency test and nbo analysis for HDimpy Ligand\\0,1\N,0.297406524
3,-2.4781300175,0.1958898525\N,0.3035306174,2.4719252318,0.1779076855\
N,-1.023050993,-0.0017871967,0.0987229093\C,-0.9536416117,2.4210717323
,0.0943224303\C,-0.9596406226,-2.4247798099,0.1119748019\C,-3.80409376
51,0.0009834202,-0.086470198\C,-1.7034228263,1.137277689,0.0491748533\
C,-3.0974382921,-1.186934597,-0.0349827214\C,-1.706246695,-1.139502154
2,0.0574655467\C,-3.0945005727,1.187485528,-0.0436493583\H,-3.60577453
86,-2.1414791217,-0.065262753\H,-4.8830556784,0.0020530165,-0.15831764
96\H,-3.600462219,2.1430438991,-0.0809131924\H,-1.5917136144,3.3102108
843,0.048466438\H,-1.5999115319,-3.3126498385,0.072651924\H,0.60986916
99,-3.4474555791,0.2203105378\H,0.6183895793,3.4406275334,0.1952568936
\\Version=EM64L-G09RevE.01\State=1-A\HF=-435.1376009\RMSD=3.496e-09\RM
SF=1.296e-06\Dipole=-1.8685729,0.0018611,-0.1244693\Quadrupole=-5.2816
914,11.24257,-5.9608786,0.0206377,0.0452481,-0.0629134\PG=C01 [X(C7H7N
3)]\\@

Zero-point correction= 0.133182 (Hartree/Particle)
Thermal correction to Energy= 0.141717
Thermal correction to Enthalpy= 0.142661
Thermal correction to Gibbs Free Energy= 0.098933
Sum of electronic and zero-point Energies= -435.004419
Sum of electronic and thermal Energies= -434.995884
Sum of electronic and thermal Enthalpies= -434.994940
Sum of electronic and thermal Free Energies= -435.038668

Parameters for Bzimpy ligand

1\1\GINC-ORC360\FOpt\RM062X\CC-pVTZ\C11H9N5\ROOT\24-Jul-2018\0\\# M062
X/cc-pVTZ opt=tight scf=tight freq\\Optimization of Bzimpy ligand from
BzimpyGaCl2+ complex\\0,1\N,-3.6094957136,1.14952551,-0.0835176188\N,
-2.4615968266,-0.5792180577,-0.8296499686\N,2.3662707215,-0.6187911953
,1.0718758695\N,-0.0295745172,0.7155917352,0.1025213799\N,3.5610006585
,1.0558993222,0.2775378202\C,2.310211497,0.5830678678,0.5559161784\C,-
2.3722937541,0.6347585293,-0.3478727947\C,-3.7963370673,-0.8645519772,
-0.873025651\C,0.0086629708,3.4930514909,0.0632754616\C,1.1004647072,1
.3832049752,0.3109490725\C,3.6926697376,-0.9394196768,1.1237687166\C,4
.4549078356,0.0811443134,0.6291217384\C,-1.1671084993,2.803521203,-0.1
692213847\C,-1.1408920084,1.4078995331,-0.1251240389\C,-4.5300198464,0
.1901926745,-0.4077759316\C,1.1651018258,2.7782648305,0.3156140063\H,-
2.0784490865,3.3327955561,-0.4107958852\H,0.0235489608,4.5743612298,0.
0479966968\H,2.0907605238,3.2888658734,0.5424930953\H,-5.5860262752,0.
339105334,-0.2750065793\H,-4.1577086229,-1.8099912964,-1.2395909901\H,
-3.8023044109,2.030252916,0.3600609702\H,3.7777860763,1.9180822605,-0.
1907173267\H,5.5145556642,0.1971137035,0.4925573907\H,4.0280370393,-1.
8837008152,1.5170586733\\Version=EM64L-G09RevE.01\State=1-A\HF=-698.31
23027\RMSD=6.267e-09\RMSF=2.204e-07\Dipole=0.0357153,2.5958924,-0.0367
588\Quadrupole=17.4346874,-4.3546082,-13.0800792,-0.340907,-2.8814978,
-0.0835739\PG=C01 [X(C11H9N5)]\\@

Zero-point correction= 0.193524 (Hartree/Particle)
Thermal correction to Energy= 0.205411
Thermal correction to Enthalpy= 0.206355
Thermal correction to Gibbs Free Energy= 0.153626
Sum of electronic and zero-point Energies= -698.118779
Sum of electronic and thermal Energies= -698.106892
Sum of electronic and thermal Enthalpies= -698.105947
Sum of electronic and thermal Free Energies= -698.158677

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