

Supporting Information

Part I - Benchmarking

SI.1. 1 Reference Spectra

1. Pyridine

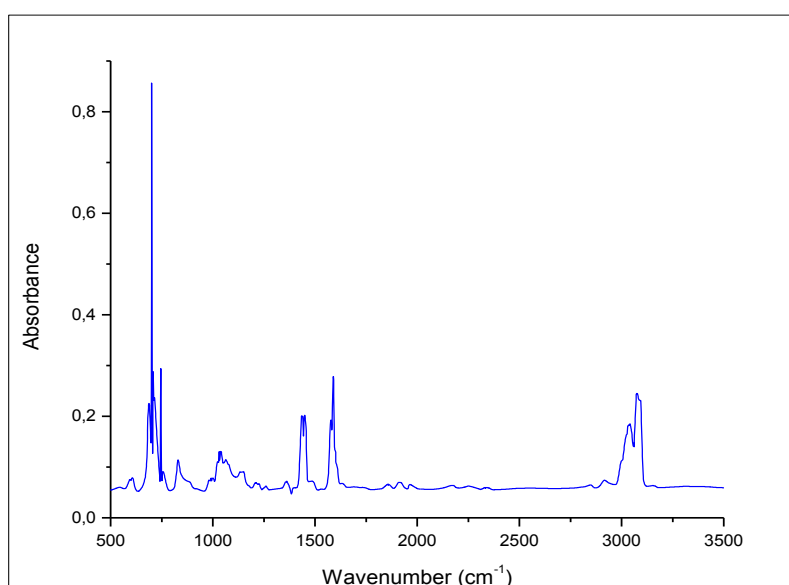


Figure SI.1.1 Infrared Spectrum of Pyridine in the Gas Phase. Adapted from: *Webbook.nist.gov*, 2018.

Table SI.1.1 Infrared Wavenumbers of Pyridine in the Gas Phase. Data from: J. K. Wilmschurst, H. J. Bernstein, *Can. J. Chem.*, 1957, **35**, 1183-1194.

Wavenumber (cm^{-1})	749	1148	3036
374	886	1217	3054
405	942	1218	3054
605	981	1375	3054
652	992	1439	3083
675	1029	1482	
703	1068	1572	
	1068	1580	

2. CHF₃

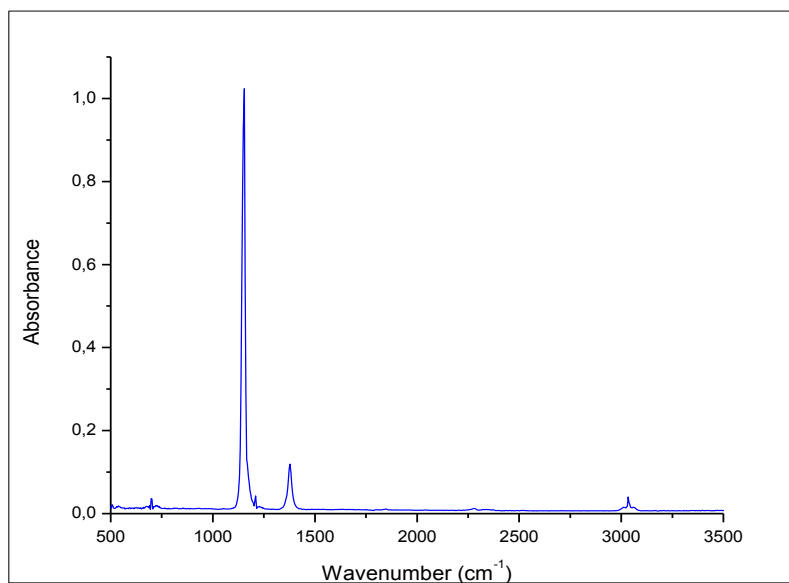


Figure SI.1.2 Infrared Spectrum of Fluoroform in the Gas Phase. Adapted from: *Webbook.nist.gov*, 2018.

Table SI.1.2 Infrared Wavenumbers of Fluoroform in the Gas Phase. Data from: T. Shimanouchi, *Tables of molecular vibrational frequencies*, National Bureau of Standards; for sale by the Supt. of Docs., U.S. Govt. Print. Off., Washington, 1972.

Wavenumber (cm ⁻¹)
507
507
700
1117
1152
1152
1372
1372
3036

3. CHCl₃

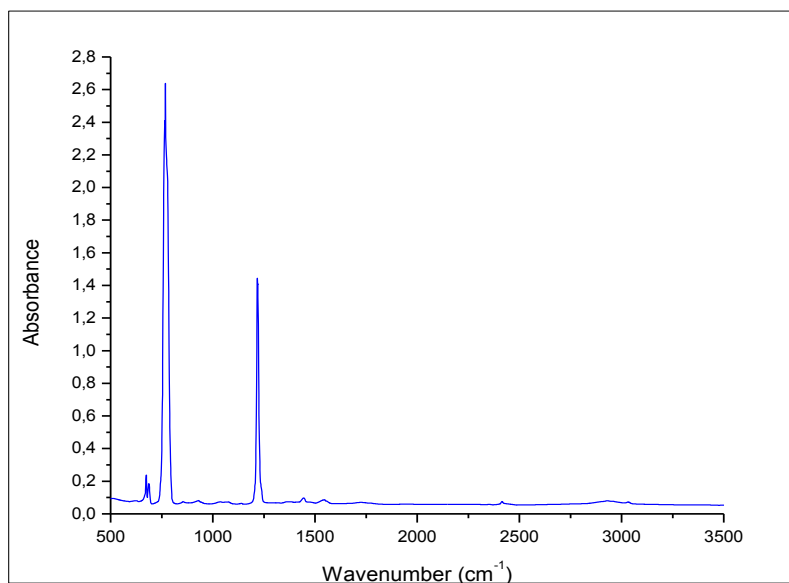


Figure SI.1.3 Infrared Spectrum of Chloroform in the Gas Phase. Adapted from: *Webbook.nist.gov*, 2018.

Table SI.1.3 Infrared Wavenumbers of Chloroform in the Gas Phase. Data from: T. Shimanouchi, *Tables of molecular vibrational frequencies*, National Bureau of Standards; for sale by the Supt. of Docs., U.S. Govt. Print. Off., Washington, 1972.

Wavenumber (cm ⁻¹)
261
261
363
680
774
774
1220
1220
3034

4. CHBr_3

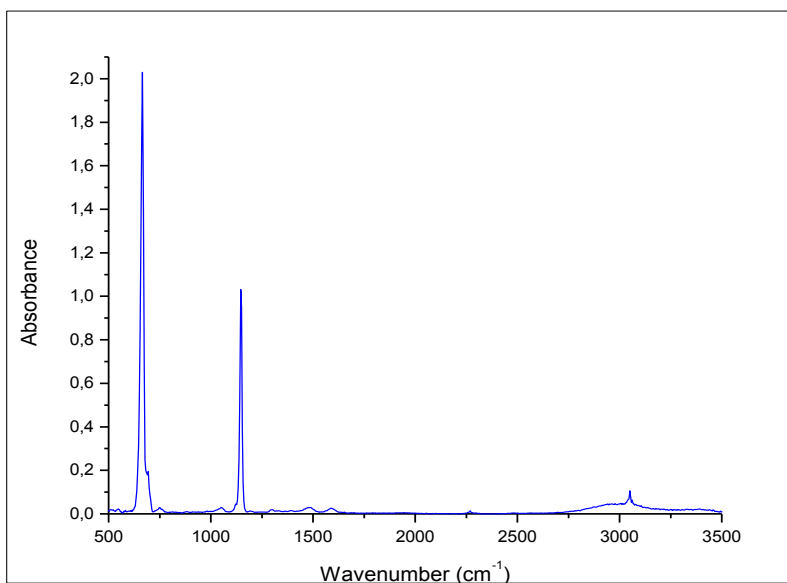


Figure SI.1.4 Infrared Spectrum of Bromoform in the Gas Phase. Adapted from: *Webbook.nist.gov*, 2018.

Table SI.1.4 Infrared Wavenumbers of Bromoform in the Gas Phase. Data from: T. Shimanouchi, *Tables of molecular vibrational frequencies*, National Bureau of Standards; for sale by the Supt. of Docs., U.S. Govt. Print. Off., Washington, 1972.

Wavenumber (cm^{-1})
155
155
222
541
669
669
1149
1149
3042

5. CH_3

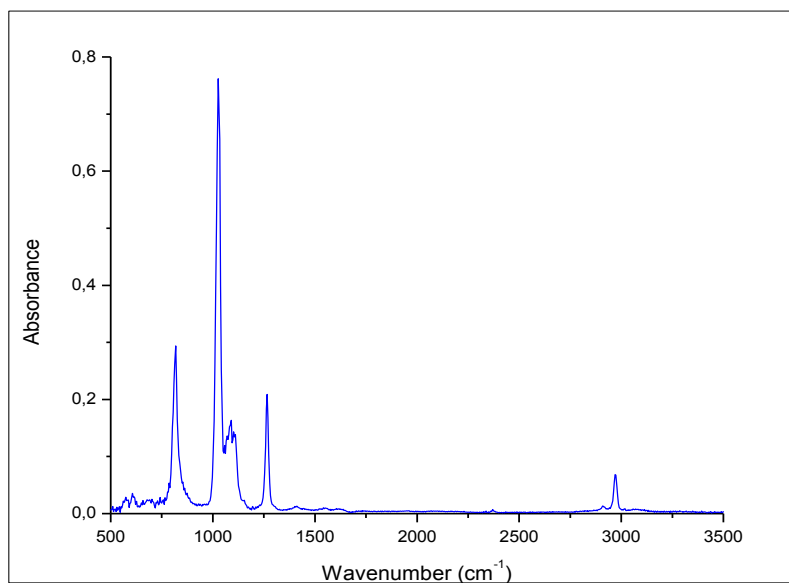


Figure SI.1.5 Infrared Spectrum of Bromoform in the Gas Phase. Adapted from: *Webbook.nist.gov*, 2018.

Table SI.1.5 Infrared Wavenumbers of Bromoform in the Gas Phase. Data from: N. Neto, O. Oehler and R. Hexter, *The Journal of Chemical Physics*, 1973, **58**, 5661-5672.

Wavenumber (cm^{-1})
110
110
154
425
578
578
1068
1068
2982

SI.1.2 Optimised Geometries

1. Pyridine

B3LYP / 6-311++G**

C	0.721166000	1.141491000	0.000000000
C	-0.671490000	1.196239000	0.000000000
C	-1.382631000	0.000000000	0.000000000
C	-0.671490000	-1.196240000	0.000000000
C	0.721166000	-1.141491000	0.000000000
N	1.416184000	0.000000000	0.000000000
H	-2.466582000	0.000000000	0.000000000
H	1.306252000	2.056533000	0.000000000
H	-1.179769000	2.152923000	0.000000000
H	-1.179768000	-2.152923000	0.000000000
H	1.306252000	-2.056533000	0.000000000

B3LYP / aug-cc-PVTZ

C	0.719454000	1.139658000	0.000000000
C	-0.669549000	1.193136000	0.000000000
C	-1.378525000	0.000000000	0.000000000
C	-0.669549000	-1.193135000	0.000000000
C	0.719453000	-1.139658000	0.000000000
N	1.411743000	0.000000000	0.000000000
H	-2.459969000	0.000000000	0.000000000
H	1.302383000	2.053254000	0.000000000
H	-1.177354000	2.147260000	0.000000000
H	-1.177354000	-2.147260000	0.000000000
H	1.302383000	-2.053253000	0.000000000

B3LYP / DGDZVP

C	0.000000000	1.144436000	0.723784000
C	0.000000000	1.200386000	-0.674122000
C	0.000000000	0.000000000	-1.388955000

C	0.000000000	-1.200386000	-0.674122000
C	0.000000000	-1.144436000	0.723784000
N	0.000000000	0.000000000	1.422699000
H	0.000000000	0.000000000	-2.476123000
H	0.000000000	2.062578000	1.309958000
H	0.000000000	2.160669000	-1.182452000
H	0.000000000	-2.160669000	-1.182452000
H	0.000000000	-2.062578000	1.309958000

PBE0/6-311++G**

C	0.000000000	1.345196000	0.000000000
C	-1.204203000	0.649911000	0.000000000
C	-1.165630000	-0.737881000	0.000000000
C	0.072241000	-1.366478000	0.000000000
C	1.215872000	-0.575507000	0.000000000
N	1.193848000	0.755741000	0.000000000
H	-2.082540000	-1.318329000	0.000000000
H	0.005078000	2.432656000	0.000000000
H	-2.145770000	1.187848000	0.000000000
H	0.155656000	-2.447665000	0.000000000
H	2.200963000	-1.036147000	0.000000000

PBE0/ aug-cc-PVTZ

C	1.213620000	0.575407000	0.000000000
C	0.071732000	1.363346000	0.000000000
C	-1.162961000	0.735662000	0.000000000
C	-1.201169000	-0.648891000	0.000000000
C	0.000000000	-1.343118000	0.000000000
N	1.191110000	-0.753466000	0.000000000
H	-2.078513000	1.314832000	0.000000000
H	2.196509000	1.036790000	0.000000000
H	0.154032000	2.442807000	0.000000000

H	-2.141302000	-1.185697000	0.000000000
H	0.004170000	-2.428903000	0.000000000

PBE0/DGDZVP

C	0.000000000	1.347907000	0.000000000
C	-1.207252000	0.651065000	0.000000000
C	-1.169164000	-0.740334000	0.000000000
C	0.072342000	-1.369708000	0.000000000
C	1.218475000	-0.576345000	0.000000000
N	1.197826000	0.758481000	0.000000000
H	-2.087340000	-1.321752000	0.000000000
H	0.004393000	2.436951000	0.000000000
H	-2.149921000	1.190413000	0.000000000
H	0.156846000	-2.452474000	0.000000000
H	2.204827000	-1.038022000	0.000000000

B2PLYP-D3 / 6-311++G**

C	0.721533000	1.142502000	0.000000000
C	-0.672813000	1.197586000	0.000000000
C	-1.385544000	0.000000000	0.000000000
C	-0.672813000	-1.197586000	0.000000000
C	0.721533000	-1.142502000	0.000000000
N	1.420890000	0.000000000	0.000000000
H	-2.469239000	0.000000000	0.000000000
H	1.306174000	2.057087000	0.000000000
H	-1.180356000	2.154412000	0.000000000
H	-1.180356000	-2.154412000	0.000000000
H	1.306175000	-2.057087000	0.000000000

B2PLYP-D3 / aug-cc-PVTZ

C	0.719442000	1.140622000	0.000000000
C	-0.670551000	1.193979000	0.000000000
C	-1.380711000	0.000000000	0.000000000

C	-0.670551000	-1.193979000	0.000000000
C	0.719441000	-1.140622000	0.000000000
N	1.415751000	0.000000000	0.000000000
H	-2.461346000	0.000000000	0.000000000
H	1.301814000	2.053181000	0.000000000
H	-1.177481000	2.147719000	0.000000000
H	-1.177481000	-2.147719000	0.000000000
H	1.301814000	-2.053181000	0.000000000

B2PLYP-D3 / DGDZVP

C	0.724006000	1.146573000	0.000000000
C	-0.675330000	1.201683000	0.000000000
C	-1.391205000	0.000000000	0.000000000
C	-0.675330000	-1.201683000	0.000000000
C	0.724006000	-1.146573000	0.000000000
N	1.426748000	0.000000000	0.000000000
H	-2.477926000	0.000000000	0.000000000
H	1.310531000	2.063487000	0.000000000
H	-1.183629000	2.161592000	0.000000000
H	-1.183629000	-2.161592000	0.000000000
H	1.310531000	-2.063487000	0.000000000

M06-2X / 6-311++G**

C	0.000000000	1.346416000	0.000000000
C	-1.204979000	0.650265000	0.000000000
C	-1.166434000	-0.738180000	0.000000000
C	0.071868000	-1.367363000	0.000000000
C	1.216878000	-0.576288000	0.000000000
N	1.194492000	0.755940000	0.000000000
H	-2.082151000	-1.317842000	0.000000000
H	0.005247000	2.432104000	0.000000000
H	-2.144742000	1.188021000	0.000000000

H	0.155821000	-2.446850000	0.000000000
H	2.200386000	-1.036120000	0.000000000

M06-2X / aug-cc-PVTZ

C	0.718342000	1.136524000	0.000000000
C	-0.668704000	1.191120000	0.000000000
C	-1.376229000	0.000000000	0.000000000
C	-0.668704000	-1.191120000	0.000000000
C	0.718342000	-1.136524000	0.000000000
N	1.409594000	0.000000000	0.000000000
H	-2.457906000	0.000000000	0.000000000
H	1.301434000	2.049988000	0.000000000
H	-1.175200000	2.145749000	0.000000000
H	-1.175200000	-2.145749000	0.000000000
H	1.301434000	-2.049988000	0.000000000

M06-2X / DGDZVP

C	0.721663000	1.140306000	0.000000000
C	-0.672343000	1.196774000	0.000000000
C	-1.384581000	0.000000000	0.000000000
C	-0.672343000	-1.196774000	0.000000000
C	0.721663000	-1.140306000	0.000000000
N	1.418393000	0.000000000	0.000000000
H	-2.470258000	0.000000000	0.000000000
H	1.307829000	2.056398000	0.000000000
H	-1.179251000	2.155848000	0.000000000
H	-1.179251000	-2.155848000	0.000000000
H	1.307829000	-2.056398000	0.000000000

ω B97X-D / 6-311++G**

C	0.719373000	1.137541000	0.000000000
C	-0.669818000	1.193236000	0.000000000
C	-1.379342000	0.000000000	0.000000000

C	-0.669818000	-1.193236000	0.000000000
C	0.719373000	-1.137541000	0.000000000
N	1.412825000	0.000000000	0.000000000
H	-2.463676000	0.000000000	0.000000000
H	1.305003000	2.052621000	0.000000000
H	-1.177357000	2.150451000	0.000000000
H	-1.177357000	-2.150451000	0.000000000
H	1.305003000	-2.052621000	0.000000000

ωB97X-D / aug-cc-PVTZ

C	0.717541000	1.135604000	0.000000000
C	-0.667983000	1.190083000	0.000000000
C	-1.375422000	0.000000000	0.000000000
C	-0.667983000	-1.190083000	0.000000000
C	0.717541000	-1.135604000	0.000000000
N	1.409026000	0.000000000	0.000000000
H	-2.457020000	0.000000000	0.000000000
H	1.300703000	2.049228000	0.000000000
H	-1.174866000	2.144582000	0.000000000
H	-1.174866000	-2.144582000	0.000000000
H	1.300703000	-2.049228000	0.000000000

ωB97X-D / DGDZVP

C	0.721075000	1.139763000	0.000000000
C	-0.671703000	1.196102000	0.000000000
C	-1.383838000	0.000000000	0.000000000
C	-0.671703000	-1.196102000	0.000000000
C	0.721075000	-1.139763000	0.000000000
N	1.417737000	0.000000000	0.000000000
H	-2.469242000	0.000000000	0.000000000
H	1.306828000	2.056122000	0.000000000
H	-1.179006000	2.154793000	0.000000000

H	-1.179006000	-2.154793000	0.000000000
H	1.306828000	-2.056122000	0.000000000

MP2 / 6-311++G**

C	0.723134000	1.144879000	0.000000000
C	-0.674919000	1.199434000	0.000000000
C	-1.391747000	0.000000000	0.000000000
C	-0.674919000	-1.199434000	0.000000000
C	0.723134000	-1.144879000	0.000000000
N	1.428308000	0.000000000	0.000000000
H	-2.478190000	0.000000000	0.000000000
H	1.308550000	2.061927000	0.000000000
H	-1.182585000	2.159423000	0.000000000
H	-1.182585000	-2.159423000	0.000000000
H	1.308550000	-2.061927000	0.000000000

MP2 / aug-cc-PVTZ

C	0.720134000	1.142639000	0.000000000
C	-0.671832000	1.194475000	0.000000000
C	-1.385142000	0.000000000	0.000000000
C	-0.671832000	-1.194476000	0.000000000
C	0.720134000	-1.142638000	0.000000000
N	1.421310000	0.000000000	0.000000000
H	-2.467043000	0.000000000	0.000000000
H	1.302938000	2.056149000	0.000000000
H	-1.178386000	2.150020000	0.000000000
H	-1.178386000	-2.150020000	0.000000000
H	1.302938000	-2.056148000	0.000000000

MP2 / DGDZVP

C	0.000000000	1.152483000	0.726021000
C	0.000000000	1.204577000	-0.677838000
C	0.000000000	0.000000000	-1.397544000

C	0.000000000	-1.204577000	-0.677838000
C	0.000000000	-1.152483000	0.726021000
N	0.000000000	0.000000000	1.434181000
H	0.000000000	0.000000000	-2.488122000
H	0.000000000	2.071279000	1.316000000
H	0.000000000	2.167950000	-1.188038000
H	0.000000000	-2.167950000	-1.188038000
H	0.000000000	-2.071279000	1.316000000

2. CHF₃

B3LYP / 6-311++G** (C,H), DGDZVP (F)

C	0.000000000	0.000000000	0.340955000
H	-0.000005000	0.000001000	1.430912000
F	-0.084438000	1.258854000	-0.128765000
F	-1.047981000	-0.702553000	-0.128765000
F	1.132420000	-0.556301000	-0.128764000

B3LYP / aug-cc-PVTZ (C,H), DGDZVP (F)

C	0.000002000	0.000001000	0.341030000
H	0.000009000	0.000001000	1.428906000
F	1.255723000	-0.077126000	-0.128708000
F	-0.561070000	1.126049000	-0.128707000
F	-0.694656000	-1.048924000	-0.128706000

B3LYP / DGDZVP

C	0.000001000	0.000000000	0.339698000
H	0.000003000	-0.000002000	1.432059000
F	0.094556000	-1.259953000	-0.128528000
F	1.043875000	0.711865000	-0.128528000
F	-1.138431000	0.548089000	-0.128527000

B3LYP / 6-311++G**

C	0.000000000	0.000000000	0.341396000
H	0.000002000	0.000000000	1.430982000
F	0.370124000	-1.203008000	-0.128865000
F	0.856776000	0.922041000	-0.128865000
F	-1.226900000	0.280968000	-0.128865000

B3LYP / aug-cc-PVTZ

C	0.000000000	0.000001000	0.340216000
H	-0.000003000	0.000004000	1.429082000
F	0.553341000	-1.128242000	-0.128532000
F	0.700417000	1.043327000	-0.128533000

F	-1.253758000	0.084914000	-0.128533000
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PBE0/ 6-311++G (C,H), DGDZVP (F)**

C	0.000000000	-0.000001000	0.337669000
H	0.000002000	0.000007000	1.429284000
F	-1.245708000	-0.139684000	-0.127974000
F	0.743825000	-1.008972000	-0.127974000
F	0.501884000	1.148656000	-0.127975000

PBE0/ aug-cc-PVTZ (C,H), DGDZVP (F)

C	0.000000000	0.000001000	0.337880000
H	0.000000000	0.000002000	1.428307000
F	-0.436668000	1.171148000	-0.127985000
F	-0.795911000	-0.963740000	-0.127984000
F	1.232579000	-0.207409000	-0.127985000

PBE0/ DGDZVP

C	-0.000001000	0.000000000	0.336352000
H	0.000001000	0.000001000	1.428763000
F	1.250793000	0.101202000	-0.127662000
F	-0.713040000	1.032616000	-0.127662000
F	-0.537752000	-1.133819000	-0.127662000

PBE0/ 6-311++G**

C	-0.000001000	0.000001000	0.338299000
H	-0.000004000	0.000003000	1.429692000
F	0.456468000	-1.163922000	-0.128128000
F	0.779755000	0.977272000	-0.128129000
F	-1.236221000	0.186649000	-0.128130000

PBE0/ aug-cc-PVTZ

C	0.000001000	0.000000000	0.337173000
H	-0.000003000	0.000003000	1.428667000
F	1.241681000	0.131155000	-0.127841000
F	-0.734425000	1.009748000	-0.127841000

F	-0.507257000	-1.140903000	-0.127841000
B2PLYP-D3 / 6-311++G** (C,H), DGDZVP (F)			
C	0.000000000	0.000000000	0.340322000
H	0.000000000	0.000002000	1.427909000
F	0.208257000	-1.242052000	-0.128512000
F	0.971521000	0.801382000	-0.128513000
F	-1.179778000	0.440670000	-0.128513000
B2PLYP-D3 / aug-cc-PVTZ (C,H), DGDZVP (F)			
C	0.000002000	0.000000000	0.339145000
H	0.000003000	0.000007000	1.423740000
F	-0.680905000	-1.052883000	-0.128096000
F	1.252277000	-0.063238000	-0.128097000
F	-0.571374000	1.116120000	-0.128097000
B2PLYP-D3 / DGDZVP			
C	0.000000000	0.000000000	0.340052000
H	0.000000000	0.000002000	1.429958000
F	-1.239051000	0.236048000	-0.128528000
F	0.415102000	-1.191073000	-0.128529000
F	0.823949000	0.955025000	-0.128529000
B2PLYP-D3 / 6-311++G**			
C	0.000000000	-0.000001000	0.340584000
H	-0.000001000	-0.000004000	1.427730000
F	1.027227000	-0.722662000	-0.128565000
F	0.112231000	1.250935000	-0.128564000
F	-1.139459000	-0.528272000	-0.128565000
B2PLYP-D3 / aug-cc-PVTZ			
C	0.000002000	0.000000000	0.340141000
H	0.000000000	-0.000010000	1.426271000
F	1.251693000	-0.072279000	-0.128412000
F	-0.563251000	1.120136000	-0.128411000

F	-0.688444000	-1.047855000	-0.128412000
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M06-2X / 6-311++G** (C,H), DGDZVP (F)

C	0.000001000	0.000000000	0.339079000
H	-0.000007000	0.000000000	1.426730000
F	-0.623231000	-1.079365000	-0.128193000
F	1.246392000	-0.000040000	-0.128192000
F	-0.623161000	1.079405000	-0.128193000

M06-2X / aug-cc-PVTZ (C,H), DGDZVP (F)

C	-0.000001000	0.000001000	0.339079000
H	-0.000008000	0.000001000	1.426730000
F	-0.618396000	-1.082142000	-0.128193000
F	1.246379000	0.005535000	-0.128192000
F	-0.627982000	1.076607000	-0.128193000

M06-2X / DGDZVP

C	-0.000009000	-0.000012000	0.339395000
H	0.000026000	-0.000041000	1.429019000
F	-0.605244000	-1.096545000	-0.128750000
F	1.252231000	0.024134000	-0.128730000
F	-0.646991000	1.072415000	-0.128726000

M06-2X / 6-311++G**

C	0.000020000	0.000009000	0.340507000
H	-0.000022000	0.000037000	1.429020000
F	0.634373000	1.075047000	-0.129135000
F	-1.248218000	0.011852000	-0.129091000
F	0.613845000	-1.086885000	-0.129081000

M06-2X / aug-cc-PVTZ

C	-0.000004000	-0.000004000	0.339787000
H	-0.000034000	0.000001000	1.427566000
F	-1.136555000	-0.513297000	-0.128379000
F	1.012772000	-0.727638000	-0.128405000

F	0.123807000	1.240921000	-0.128367000
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ω B97X-D / 6-311++G** (C,H), DGDZVP (F)

C	0.000010000	-0.000006000	0.337391000
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H	-0.000009000	-0.000003000	1.427356000
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F	1.222688000	-0.256278000	-0.127842000
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F	-0.389401000	1.187011000	-0.127839000
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F	-0.833293000	-0.930729000	-0.127841000
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ω B97X-D / aug-cc-PVTZ (C,H), DGDZVP (F)

C	-0.000001000	-0.000006000	0.337392000
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H	0.000005000	-0.000006000	1.427357000
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F	-0.143490000	1.240981000	-0.127840000
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F	-1.002982000	-0.744754000	-0.127842000
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F	1.146472000	-0.496223000	-0.127842000
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ω B97X-D / DGDZVP

C	0.000001000	0.000000000	0.337388000
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H	-0.000003000	0.000009000	1.427353000
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F	-1.091840000	0.607064000	-0.127841000
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F	0.020185000	-1.249091000	-0.127839000
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F	1.071655000	0.642026000	-0.127840000
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ω B97X-D / 6-311++G**

C	0.000000000	0.000005000	0.337389000
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H	0.000002000	0.000005000	1.427354000
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F	-0.143735000	-1.240955000	-0.127839000
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F	1.146571000	0.495998000	-0.127841000
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F	-1.002836000	0.744953000	-0.127841000
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ω B97X-D / aug-cc-PVTZ

C	-0.000001000	0.000006000	0.337392000
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H	0.000000000	0.000013000	1.427357000
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F	0.146167000	-1.240671000	-0.127839000
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F	1.001373000	0.746916000	-0.127842000
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F	-1.147540000	0.493749000	-0.127842000
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MP2 / 6-311++G** (C,H), DGDZVP (F)

C	0.000000000	0.000000000	0.339067000
H	0.000000000	-0.000001000	1.427251000
F	0.980723000	-0.789420000	-0.128209000
F	0.193297000	1.244041000	-0.128209000
F	-1.174020000	-0.454620000	-0.128209000

MP2 / aug-cc-PVTZ (C,H), DGDZVP (F)

C	0.000000000	0.000000000	0.334582000
H	0.000000000	0.000000000	1.417073000
F	0.735074000	-1.009797000	-0.126836000
F	0.506975000	1.141490000	-0.126836000
F	-1.242049000	-0.131692000	-0.126836000

MP2 / DGDZVP

C	0.000000000	0.000000000	0.341237000
H	0.000000000	0.000000000	1.432456000
F	1.064088000	0.678281000	-0.128884000
F	-1.119453000	0.582387000	-0.128884000
F	0.055365000	-1.260668000	-0.128884000

MP2 / 6-311++G**

C	0.000000000	0.000000000	0.338737000
H	-0.000002000	-0.000001000	1.426343000
F	0.767305000	-0.991905000	-0.128102000
F	0.475364000	1.160457000	-0.128102000
F	-1.242668000	-0.168552000	-0.128103000

MP2 / aug-cc-PVTZ

C	0.000000000	0.000000000	0.339471000
H	-0.000001000	-0.000001000	1.425000000
F	0.688740000	-1.044722000	-0.128216000
F	0.560388000	1.118827000	-0.128216000

F -1.249127000 -0.074104000 -0.128216000

3. CHCl₃

B3LYP / 6-311++G** (C,H), DGDZVP (Cl)

C	-0.000002000	0.000028000	0.455654000
H	0.000007000	-0.000001000	1.537986000
Cl	1.348081000	1.041948000	-0.083451000
Cl	-1.576403000	0.646459000	-0.083441000
Cl	0.228332000	-1.688428000	-0.083447000

B3LYP / aug-cc-PVTZ (C,H), DGDZVP (Cl)

C	-0.000002000	-0.000031000	0.458460000
H	-0.000009000	-0.000018000	1.537210000
Cl	-1.357956000	-1.022563000	-0.084155000
Cl	1.564548000	-0.664722000	-0.084134000
Cl	-0.206603000	1.687284000	-0.084121000

B3LYP / DGDZVP

C	0.000000000	0.000009000	0.457679000
H	-0.000002000	0.000001000	1.537596000
Cl	0.168642000	-1.686252000	-0.083993000
Cl	1.376021000	0.989172000	-0.083994000
Cl	-1.544663000	0.697077000	-0.083994000

B3LYP / 6-311++G**

C	-0.000014000	0.000024000	0.454776000
H	-0.000017000	0.000004000	1.537292000
Cl	0.242442000	-1.685046000	-0.082933000
Cl	1.338088000	1.052486000	-0.082919000
Cl	-1.580541000	0.632543000	-0.082944000

B3LYP / aug-cc-PVTZ

C	0.000001000	0.000001000	0.457675000
H	0.000000000	0.000000000	1.537593000
Cl	-0.706355000	1.540439000	-0.083993000
Cl	-0.980888000	-1.381939000	-0.083993000

C1	1.687243000	-0.158501000	-0.083993000
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PBE0/ 6-311++G (C,H), DGDZVP (Cl)**

C	-0.000004000	0.000020000	0.451161000
H	0.000000000	0.000001000	1.536152000
Cl	0.647283000	-1.557037000	-0.082074000
Cl	1.024796000	1.339091000	-0.082074000
Cl	-1.672070000	0.217931000	-0.082067000

PBE0/ aug-cc-PVTZ (C,H), DGDZVP (Cl)

C	0.000010000	0.000003000	0.455228000
H	-0.000011000	-0.000008000	1.537363000
Cl	-0.419472000	1.629089000	-0.083827000
Cl	-1.201104000	-1.177832000	-0.083830000
Cl	1.620567000	-0.451262000	-0.083830000

PBE0/ DGDZVP

C	-0.000004000	-0.000006000	0.451605000
H	-0.000020000	0.000031000	1.538367000
Cl	1.170444000	1.215147000	-0.082942000
Cl	-1.637563000	0.406068000	-0.082965000
Cl	0.467102000	-1.621188000	-0.082927000

PBE0/ 6-311++G**

C	-0.000011000	-0.000003000	0.450160000
H	-0.000006000	0.000014000	1.535319000
Cl	0.438203000	-1.627864000	-0.081453000
Cl	1.190675000	1.193453000	-0.081456000
Cl	-1.628884000	0.434420000	-0.081471000

PBE0/ aug-cc-PVTZ

C	0.000006000	0.000004000	0.454292000
H	-0.000004000	-0.000003000	1.537580000
Cl	1.677620000	-0.041442000	-0.083592000
Cl	-0.802941000	1.473585000	-0.083582000

C1	-0.874679000	-1.432152000	-0.083593000
B2PLYP-D3 / 6-311++G** (C,H), DGDZVP (CI)			
C	-0.000001000	-0.000001000	0.459011000
H	-0.000005000	0.000002000	1.538740000
C1	0.941159000	-1.400350000	-0.084173000
C1	0.742166000	1.515238000	-0.084173000
C1	-1.683324000	-0.114888000	-0.084173000
B2PLYP-D3 / aug-cc-PVTZ (C,H), DGDZVP (CI)			
C	-0.000003000	0.000000000	0.459016000
H	0.000004000	0.000001000	1.538745000
C1	1.681987000	-0.132996000	-0.084173000
C1	-0.725815000	1.523137000	-0.084173000
C1	-0.956171000	-1.390142000	-0.084173000
B2PLYP-D3 / DGDZVP			
C	-0.000002000	0.000002000	0.459011000
H	-0.000002000	-0.000002000	1.538740000
C1	0.735657000	1.518410000	-0.084173000
C1	-1.682815000	-0.122110000	-0.084173000
C1	0.947159000	-1.396300000	-0.084172000
B2PLYP-D3 / 6-311++G**			
C	-0.000006000	-0.000002000	0.459014000
H	-0.000002000	0.000004000	1.538743000
C1	0.742819000	1.514918000	-0.084173000
C1	-1.683372000	-0.114162000	-0.084174000
C1	0.940555000	-1.400756000	-0.084173000
B2PLYP-D3 / aug-cc-PVTZ			
C	-0.000008000	0.000008000	0.459021000
H	0.000002000	-0.000002000	1.538749000
C1	-1.659981000	0.302029000	-0.084175000
C1	0.568426000	-1.588600000	-0.084173000

C1	1.091558000	1.286568000	-0.084174000
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M06-2X / 6-311++G** (C,H), DGDZVP (CI)

C	-0.000020000	0.000080000	0.456494000
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H	-0.000036000	0.000081000	1.539413000
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C1	1.416730000	-0.913779000	-0.083469000
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C1	0.083210000	1.683931000	-0.083505000
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C1	-1.499776000	-0.770143000	-0.083298000
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M06-2X / aug-cc-PVTZ (C,H), DGDZVP (CI)

C	0.000010000	0.000033000	0.459855000
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H	-0.000065000	-0.000119000	1.539347000
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C1	0.979106000	1.368437000	-0.084609000
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C1	-1.674618000	0.163951000	-0.084495000
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C1	0.695548000	-1.532280000	-0.084467000
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M06-2X / DGDZVP

C	-0.000024000	0.000007000	0.457032000
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H	0.000033000	0.000071000	1.541912000
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C1	0.421246000	-1.633506000	-0.084508000
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C1	1.203968000	1.181575000	-0.084433000
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C1	-1.625299000	0.451884000	-0.084547000
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M06-2X / 6-311++G**

C	0.000020000	0.000028000	0.455675000
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H	0.000120000	0.000140000	1.538734000
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C1	-1.632495000	0.419045000	-0.082978000
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C1	0.453236000	-1.623290000	-0.082978000
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C1	1.179204000	1.204182000	-0.082934000
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M06-2X / aug-cc-PVTZ

C	-0.000015000	-0.000187000	0.458616000
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H	0.000043000	-0.000450000	1.539208000
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C1	0.435734000	1.621330000	-0.083793000
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C1	-1.622128000	-0.433253000	-0.084177000
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C1	1.186253000	-1.188245000	-0.084112000
ω B97X-D / 6-311++G** (C,H), DGDZVP (Cl)			
C	0.000048000	0.000013000	0.453862000
H	-0.000016000	0.000007000	1.537605000
Cl	-0.861258000	1.455963000	-0.082984000
Cl	-0.830274000	-1.473847000	-0.082976000
Cl	1.691481000	0.017889000	-0.082964000
ω B97X-D / aug-cc-PVTZ (C,H), DGDZVP (Cl)			
C	0.000015000	0.000042000	0.457631000
H	0.000021000	-0.000010000	1.537634000
Cl	-1.472160000	-0.826211000	-0.084223000
Cl	1.451601000	-0.861838000	-0.084252000
Cl	0.020567000	1.688000000	-0.084217000
ω B97X-D / DGDZVP			
C	0.000012000	-0.000028000	0.454383000
H	0.000026000	-0.000018000	1.539376000
Cl	1.069364000	-1.311137000	-0.083671000
Cl	0.600769000	1.581705000	-0.083692000
Cl	-1.670124000	-0.270527000	-0.083669000
ω B97X-D / 6-311++G**			
C	0.000023000	0.000041000	0.453229000
H	0.000023000	0.000035000	1.537148000
Cl	1.566092000	0.638837000	-0.082624000
Cl	-1.336293000	1.036797000	-0.082560000
Cl	-0.229760000	-1.675652000	-0.082571000
ω B97X-D / aug-cc-PVTZ			
C	-0.000002000	-0.000018000	0.456568000
H	0.000020000	0.000020000	1.537627000
Cl	-1.515608000	-0.734528000	-0.083861000
Cl	1.393980000	-0.945255000	-0.083892000

C1	0.121668000	1.679877000	-0.083970000
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MP2 / 6-311++G** (C,H), DGDZVP (Cl)

C	0.000001000	0.000000000	0.449496000
H	-0.000002000	0.000000000	1.534638000
C1	1.676923000	-0.159101000	-0.082973000
C1	-0.700676000	1.531806000	-0.082973000
C1	-0.976247000	-1.372705000	-0.082973000

MP2 / aug-cc-PVTZ (C,H), DGDZVP (Cl)

C	0.000000000	0.000000000	0.451162000
H	-0.000001000	0.000000000	1.529138000
C1	1.668911000	0.025837000	-0.083061000
C1	-0.856831000	1.432400000	-0.083061000
C1	-0.812080000	-1.458237000	-0.083061000

MP2 / DGDZVP

C	0.000000000	0.000000000	0.456450000
H	0.000000000	0.000000000	1.548449000
C1	0.452184000	1.627506000	-0.084062000
C1	-1.635554000	-0.422151000	-0.084062000
C1	1.183371000	-1.205355000	-0.084062000

MP2 / 6-311++G**

C	0.000001000	0.000000000	0.451146000
H	-0.000002000	0.000000000	1.536853000
C1	1.675439000	-0.155748000	-0.083210000
C1	-0.702838000	1.528844000	-0.083210000
C1	-0.972601000	-1.373096000	-0.083210000

MP2 / aug-cc-PVTZ

C	0.000001000	0.000000000	0.459846000
H	0.000000000	0.000000000	1.542171000
C1	1.652687000	0.275683000	-0.084338000
C1	-1.065093000	1.293426000	-0.084338000

C1	-0.587595000	-1.569109000	-0.084338000
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4. CHBr₃

B3LYP / 6-311++G** (C,H), DGDZVP (Br)

C	0.000023000	-0.000009000	0.522387000
H	0.000000000	-0.000006000	1.602850000
Br	-1.846333000	-0.279805000	-0.046896000
Br	1.165474000	-1.459089000	-0.046874000
Br	0.680821000	1.738906000	-0.046884000

B3LYP / aug-cc-PVTZ (C,H), DGDZVP (Br)

C	0.000027000	-0.000007000	0.522230000
H	0.000000000	-0.000015000	1.599007000
Br	0.306197000	1.837624000	-0.045548000
Br	-1.744565000	-0.653621000	-0.045568000
Br	1.438332000	-1.184011000	-0.045548000

B3LYP / DGDZVP

C	0.000036000	0.000010000	0.522512000
H	0.000005000	-0.000002000	1.605872000
Br	1.868258000	0.044584000	-0.047934000
Br	-0.972733000	1.595667000	-0.047936000
Br	-0.895540000	-1.640249000	-0.047930000

B3LYP / 6-311++G**

C	0.000010000	0.000015000	0.519196000
H	-0.000002000	0.000004000	1.600132000
Br	0.331020000	1.837591000	-0.044916000
Br	-1.756912000	-0.632126000	-0.044913000
Br	1.425881000	-1.205474000	-0.044914000

B3LYP / aug-cc-PVTZ

C	-0.000055000	0.000024000	0.521421000
H	-0.000017000	0.000003000	1.599775000
Br	1.258347000	1.368242000	-0.045539000
Br	-1.814135000	0.405563000	-0.045520000

Br	0.555848000	-1.773828000	-0.045549000
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PBE0/ 6-311++G (C,H), DGDZVP (Br)**

C	-0.000052000	0.000325000	0.518357000
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H	-0.000008000	0.000604000	1.601480000
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Br	0.429994000	-1.794502000	-0.046438000
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Br	1.339261000	1.269925000	-0.047229000
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Br	-1.769278000	0.525156000	-0.047010000
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PBE0/ aug-cc-PVTZ (C,H), DGDZVP (Br)

C	0.000029000	0.000016000	0.519075000
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H	0.000042000	0.000001000	1.599257000
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Br	-0.545681000	1.758324000	-0.046434000
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Br	-1.249873000	-1.351772000	-0.046425000
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Br	1.795606000	-0.406573000	-0.046460000
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PBE0/ DGDZVP

C	0.000049000	0.000004000	0.518989000
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H	0.000021000	-0.000003000	1.603173000
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Br	1.770711000	-0.524950000	-0.047722000
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Br	-0.430744000	1.795930000	-0.047702000
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Br	-1.339975000	-1.270999000	-0.047712000
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PBE0/ 6-311++G**

C	-0.000035000	0.000012000	0.514674000
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H	-0.000031000	0.000011000	1.598314000
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Br	-1.845920000	0.049627000	-0.044639000
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Br	0.879966000	-1.623434000	-0.044641000
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Br	0.965976000	1.573782000	-0.044619000
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PBE0/ aug-cc-PVTZ

C	-0.000019000	-0.000007000	0.518183000
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H	-0.000007000	0.000001000	1.599985000
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Br	-1.753240000	-0.552449000	-0.046356000
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Br	1.355075000	-1.242105000	-0.046362000
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Br	0.398178000	1.794555000	-0.046354000
B2PLYP-D3 / 6-311++G** (C,H), DGDZVP (Br)			
C	-0.000056000	-0.000028000	0.524231000
H	-0.000027000	-0.000010000	1.605151000
Br	-1.810988000	-0.425086000	-0.045246000
Br	1.273645000	-1.355783000	-0.045242000
Br	0.537353000	1.780874000	-0.045241000
B2PLYP-D3 / aug-cc-PVTZ (C,H), DGDZVP (Br)			
C	0.000006000	-0.000001000	0.520374000
H	-0.000001000	-0.000005000	1.601749000
Br	1.427041000	-1.189531000	-0.044991000
Br	0.316650000	1.830612000	-0.044990000
Br	-1.743693000	-0.641080000	-0.044990000
B2PLYP-D3 / DGDZVP			
C	0.000024000	0.000009000	0.524004000
H	0.000007000	0.000002000	1.608144000
Br	1.862588000	0.044441000	-0.049190000
Br	-0.969782000	1.590824000	-0.049188000
Br	-0.892811000	-1.635265000	-0.049186000
B2PLYP-D3 / 6-311++G**			
C	0.000006000	-0.000001000	0.520363000
H	-0.000002000	0.000005000	1.601739000
Br	0.796620000	-1.678343000	-0.044990000
Br	1.055189000	1.529059000	-0.044990000
Br	-1.851811000	0.149284000	-0.044989000
B2PLYP-D3 / aug-cc-PVTZ			
C	-0.000050000	0.000067000	-0.524011000
H	-0.000120000	0.000211000	-1.602484000
Br	1.727866000	0.653356000	0.045160000
Br	-0.298087000	-1.823038000	0.044999000

Br	-1.429749000	1.169663000	0.045471000
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M06-2X / 6-311++G** (C,H), DGDZVP (Br)

C	0.000120000	-0.000081000	0.522522000
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H	0.000284000	-0.000136000	1.603407000
---	-------------	--------------	-------------

Br	-1.295688000	1.309646000	-0.046374000
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Br	-0.486340000	-1.777003000	-0.046249000
----	--------------	--------------	--------------

Br	1.782082000	0.467537000	-0.046405000
----	-------------	-------------	--------------

M06-2X / aug-cc-PVTZ (C,H), DGDZVP (Br)

C	0.000036000	-0.000032000	0.523052000
---	-------------	--------------	-------------

H	0.000117000	0.000084000	1.600552000
---	-------------	-------------	-------------

Br	-1.305837000	-1.293045000	-0.045800000
----	--------------	--------------	--------------

Br	1.772762000	-0.484519000	-0.045605000
----	-------------	--------------	--------------

Br	-0.467109000	1.777363000	-0.045621000
----	--------------	-------------	--------------

M06-2X / DGDZVP

C	-0.000085000	0.000002000	0.523431000
---	--------------	-------------	-------------

H	-0.000248000	0.000075000	1.605809000
---	--------------	-------------	-------------

Br	0.492031000	-1.776365000	-0.047353000
----	-------------	--------------	--------------

Br	1.292373000	1.314328000	-0.047749000
----	-------------	-------------	--------------

Br	-1.784348000	0.462411000	-0.047739000
----	--------------	-------------	--------------

M06-2X / 6-311++G**

C	-0.000097000	-0.000105000	0.519701000
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H	-0.000076000	-0.000064000	1.601205000
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Br	-1.744539000	-0.606394000	-0.044830000
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Br	1.397307000	-1.207419000	-0.045085000
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Br	0.347550000	1.813706000	-0.044830000
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M06-2X / aug-cc-PVTZ

C	-0.000172000	-0.000071000	0.521868000
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H	-0.000021000	-0.000288000	1.601138000
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Br	0.722128000	1.693332000	-0.045716000
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Br	-1.827813000	-0.221038000	-0.045527000
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Br	1.105774000	-1.471947000	-0.045404000
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ω B97X-D / 6-311++G** (C,H), DGDZVP (Br)

C	0.000043000	0.000003000	0.518856000
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H	0.000003000	0.000003000	1.601001000
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Br	-0.548963000	1.767119000	-0.046566000
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Br	-1.255920000	-1.358941000	-0.046538000
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Br	1.804857000	-0.408150000	-0.046543000
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ω B97X-D / aug-cc-PVTZ (C,H), DGDZVP (Br)

C	-0.000039000	0.000029000	0.519920000
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H	-0.000002000	0.000000000	1.598310000
---	--------------	-------------	-------------

Br	-1.787639000	-0.461247000	-0.045999000
----	--------------	--------------	--------------

Br	1.293247000	-1.317532000	-0.046015000
----	-------------	--------------	--------------

Br	0.494432000	1.778743000	-0.046001000
----	-------------	-------------	--------------

ω B97X-D / DGDZVP

C	-0.000030000	0.000010000	0.519913000
---	--------------	-------------	-------------

H	0.000006000	0.000027000	1.602796000
---	-------------	-------------	-------------

Br	1.831331000	0.269054000	-0.047520000
----	-------------	-------------	--------------

Br	-1.148676000	1.451474000	-0.047499000
----	--------------	-------------	--------------

Br	-0.682614000	-1.720534000	-0.047502000
----	--------------	--------------	--------------

ω B97X-D / 6-311++G**

C	-0.000014000	0.000030000	0.515805000
---	--------------	-------------	-------------

H	0.000007000	-0.000002000	1.598499000
---	-------------	--------------	-------------

Br	-0.409608000	1.803918000	-0.044697000
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Br	-1.357430000	-1.256715000	-0.044703000
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Br	1.767050000	-0.547236000	-0.044703000
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ω B97X-D / aug-cc-PVTZ

C	0.000017000	0.000001000	0.518879000
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H	-0.000007000	0.000002000	1.598818000
---	--------------	-------------	-------------

Br	-0.127823000	-1.838293000	-0.045828000
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Br	1.655891000	0.808474000	-0.045840000
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Br	-1.528070000	1.029843000	-0.045841000
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MP2 / 6-311++G** (C,H), DGDZVP (Br)

C	0.000000000	0.000000000	0.521004000
H	-0.000001000	0.000000000	1.606025000
Br	0.777557000	-1.680345000	-0.045067000
Br	1.066443000	1.513556000	-0.045067000
Br	-1.844000000	0.166789000	-0.045067000

MP2 / aug-cc-PVTZ (C,H), DGDZVP (Br)

C	0.000000000	0.000000000	0.512574000
H	-0.000001000	0.000000000	1.589680000
Br	-1.779070000	0.424677000	-0.044430000
Br	0.521754000	-1.753058000	-0.044430000
Br	1.257316000	1.328381000	-0.044430000

MP2 / DGDZVP

C	0.000000000	0.000000000	0.529950000
H	-0.000001000	0.000000000	1.620298000
Br	0.898177000	-1.626564000	-0.045714000
Br	0.959558000	1.591126000	-0.045714000
Br	-1.857735000	0.035438000	-0.045714000

MP2 / 6-311++G**

C	0.000000000	0.000000000	0.519297000
H	-0.000001000	0.000000000	1.604733000
Br	0.638839000	-1.730619000	-0.044957000
Br	1.179341000	1.418560000	-0.044957000
Br	-1.818180000	0.312059000	-0.044957000

MP2 / aug-cc-PVTZ

C	0.000003000	0.000004000	0.521279000
H	0.000012000	-0.000007000	1.602447000
Br	-0.126729000	-1.822617000	-0.047863000
Br	1.641802000	0.801575000	-0.047852000

Br -1.515080000 1.021071000 -0.047822000

5. CHI₃

B3LYP / 6-311++G** (C,H), DGDZVP (I)

C	0.000028000	0.000053000	0.555225000
H	0.000107000	0.000050000	1.635764000
I	2.098030000	-0.064520000	-0.030938000
I	-1.104714000	-1.784746000	-0.030946000
I	-0.993322000	1.849213000	-0.030924000

B3LYP / aug-cc-PVTZ (C,H), DGDZVP (I)

C	-0.000022000	-0.000150000	0.553624000
H	-0.000038000	-0.000266000	1.630786000
I	-1.027161000	-1.816779000	-0.029170000
I	-1.059765000	1.797746000	-0.028801000
I	2.086706000	0.018787000	-0.028772000

B3LYP / DGDZVP

C	-0.000012000	0.000062000	0.554171000
H	0.000018000	0.000017000	1.637686000
I	-1.873766000	0.943568000	-0.031147000
I	1.753907000	1.150964000	-0.031287000
I	0.120010000	-2.094435000	-0.031126000

PBE0 / 6-311++G** (C,H), DGDZVP (I)

C	0.000032000	-0.000018000	0.555035000
H	0.000066000	-0.000006000	1.638477000
I	-0.997106000	-1.818065000	-0.030990000
I	-1.075901000	1.772484000	-0.031026000
I	2.072928000	0.045624000	-0.030957000

PBE0 / aug-cc-PVTZ (C,H), DGDZVP (I)

C	-0.000009000	-0.000007000	0.554739000
H	-0.000009000	0.000019000	1.635532000
I	-1.752000000	-1.085888000	-0.029961000
I	-0.064441000	2.060177000	-0.029860000

I	1.816422000	-0.974409000	-0.029938000
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PBE0 / DGDZVP

C	-0.000001000	0.000008000	0.554790000
H	-0.000030000	-0.000034000	1.639470000
I	1.830448000	0.973475000	-0.031244000
I	-0.072358000	-2.071858000	-0.031228000
I	-1.758200000	1.098464000	-0.031342000

B2PLYP-D3 / 6-311++G (C,H), DGDZVP (I)**

C	-0.000028000	0.000043000	0.559916000
H	0.000025000	0.000066000	1.641436000
I	2.085689000	-0.176960000	-0.029941000
I	-1.196019000	-1.717729000	-0.029901000
I	-0.889610000	1.894721000	-0.029943000

B2PLYP-D3 / aug-cc-PVTZ (C,H), DGDZVP (I)

C	-0.000067000	0.000200000	0.557304000
H	-0.000125000	0.000230000	1.634546000
I	-0.240847000	-2.057143000	-0.026591000
I	-1.661293000	1.237217000	-0.026849000
I	1.901964000	0.820225000	-0.026620000

B2PLYP-D3 / DGDZVP

C	0.000004000	-0.000004000	0.560568000
H	0.000006000	0.000009000	1.645523000
I	1.812041000	-1.049932000	-0.031520000
I	-1.815279000	-1.044322000	-0.031509000
I	0.003249000	2.094162000	-0.031456000

M06-2X / 6-311++G (C,H), DGDZVP (I)**

C	0.000336000	0.000027000	0.558812000
H	-0.000260000	0.000055000	1.639965000
I	-1.493908000	-1.433760000	-0.031056000
I	-0.494837000	2.010992000	-0.030840000

I	1.988472000	-0.577358000	-0.031006000
M06-2X / aug-cc-PVTZ (C,H), DGDZVP (I)			
C	0.000399000	0.000439000	0.557961000
H	-0.000168000	-0.000056000	1.636088000
I	1.987046000	-0.535077000	-0.029070000
I	-1.456468000	-1.453537000	-0.029383000
I	-0.531144000	1.988157000	-0.029165000
M06-2X / DGDZVP			
C	-0.000277000	-0.000154000	0.557939000
H	-0.000529000	0.000107000	1.640889000
I	0.047555000	-2.069460000	-0.031017000
I	-1.815913000	0.994534000	-0.030903000
I	1.768738000	1.075017000	-0.031022000
ωB97X-D / 6-311++G** (C,H), DGDZVP (I)			
C	0.000057000	-0.000018000	0.551580000
H	0.000072000	-0.000090000	1.635190000
I	2.034921000	-0.419865000	-0.031101000
I	-1.381113000	-1.552200000	-0.031098000
I	-0.653816000	1.972069000	-0.031097000
ωB97X-D / aug-cc-PVTZ (C,H), DGDZVP (I)			
C	-0.000019000	-0.000015000	0.552095000
H	0.000021000	-0.000091000	1.631130000
I	0.572961000	1.985842000	-0.029770000
I	1.433551000	-1.489077000	-0.029905000
I	-2.006300000	-0.497008000	-0.029754000
ωB97X-D / DGDZVP			
C	0.000032000	0.000010000	0.551602000
H	0.000032000	0.000078000	1.635212000
I	2.035669000	0.416107000	-0.031054000
I	-0.657467000	-1.970860000	-0.031101000

I	-1.378268000	1.554728000	-0.031086000
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MP2 / 6-311++G** (C,H), DGDZVP (I)

C	0.000000000	0.000000000	0.555117000
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H	0.000000000	0.000001000	1.641458000
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I	-0.033913000	-2.087064000	-0.031271000
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I	-1.790495000	1.072902000	-0.031271000
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I	1.824408000	1.014163000	-0.031271000
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MP2 / aug-cc-PVTZ (C,H), DGDZVP (I)

C	0.000000000	0.000000000	0.543966000
---	-------------	-------------	-------------

H	0.000001000	0.000000000	1.623141000
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I	-1.870264000	-0.827983000	-0.030735000
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I	0.218077000	2.033687000	-0.030735000
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I	1.652187000	-1.205704000	-0.030735000
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MP2 / DGDZVP

C	0.000000000	0.000001000	0.564438000
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H	0.000001000	0.000001000	1.656622000
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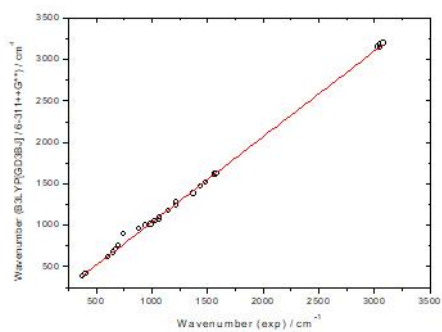
I	-0.334652000	-2.066216000	-0.031719000
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I	-1.622071000	1.322925000	-0.031719000
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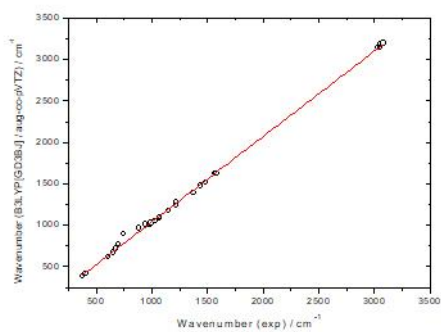
I	1.956723000	0.743291000	-0.031719000
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SI.1.3 Regressions

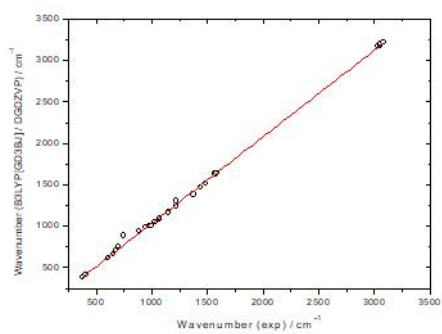
1. Pyridine



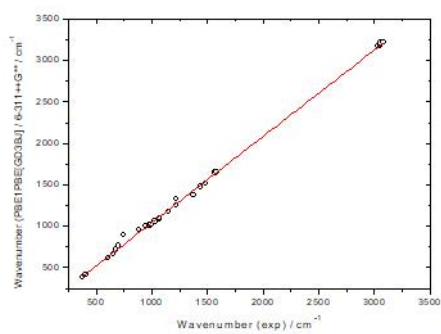
B3LYP / 6-311++G**



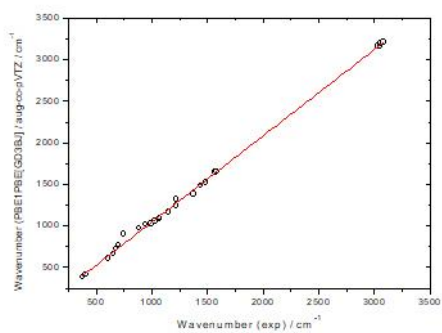
B3LYP / aug-cc-PVTZ



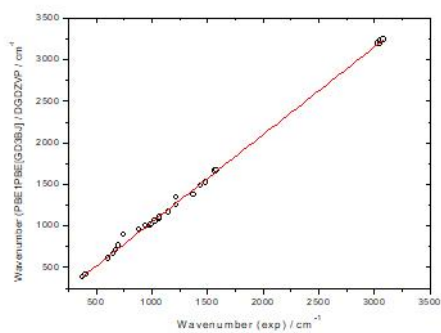
B3LYP / DGDZVP



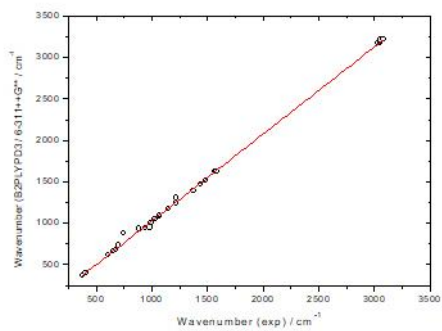
PBE0 / 6-311++G**



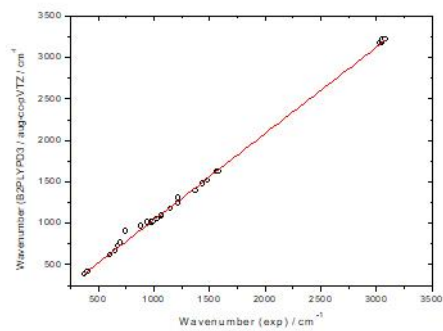
PBE0 / aug-cc-PVTZ



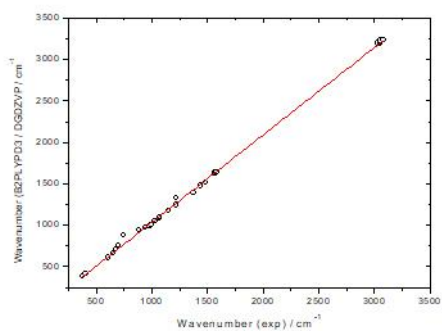
PBE0 / DGDZVP



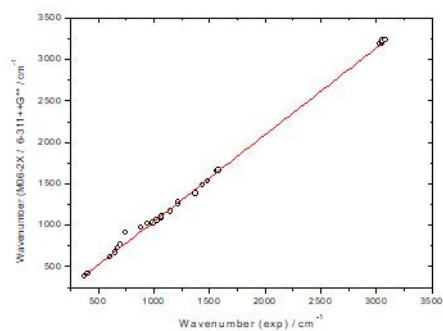
B2PLYP-D3 / 6-311++G**



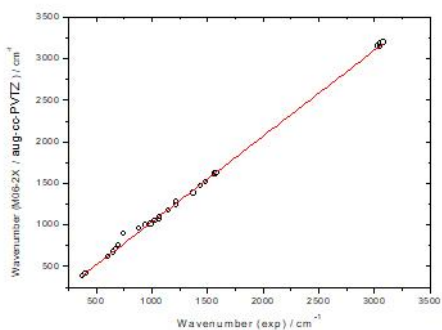
B2PLYP-D3 / aug-cc-pVTZ



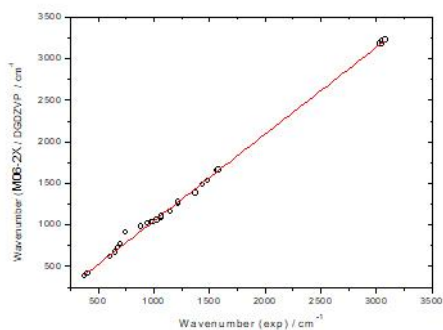
B2PLYP-D3 / DGDZVP



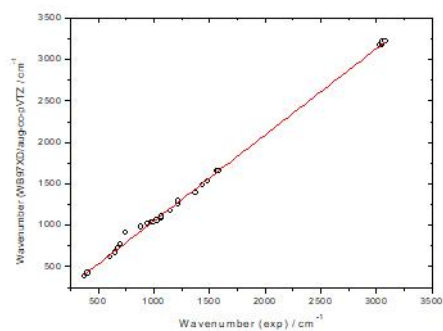
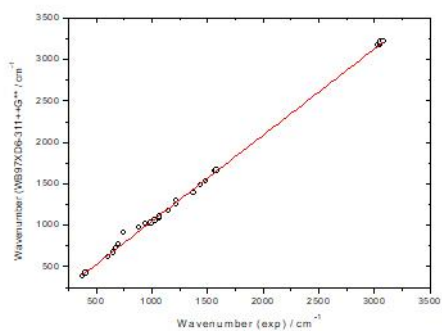
M06-2X / 6-311++G**



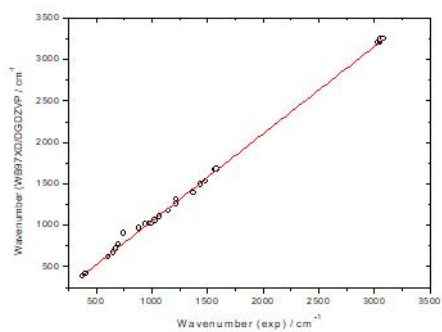
M06-2X / aug-cc-pVTZ



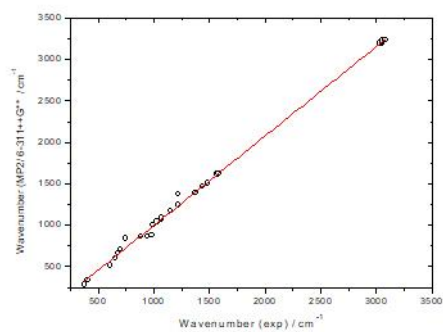
M06-2X / DGDZVP



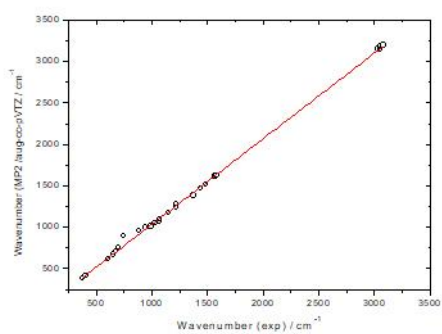
ω B97X-D / 6-311++G**



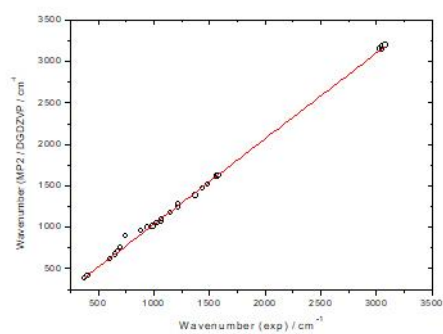
ω B97X-D / aug-cc-PVTZ



ω B97X-D / DGDZVP



MP2 / 6-311++G**



MP2 / aug-cc-PVTZ

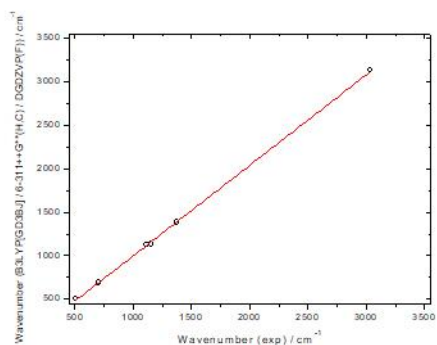
MP2 / DGDZVP

Figure SI.1. 6 Linear Regression of Computed vs. Experimental Infrared Wavenumbers of Pyridine.

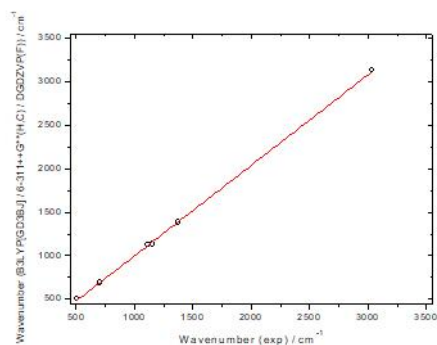
Table SI.1.6 Statistical Parameters of Linear Regression of Computed vs. Experimental Infrared Wavenumbers of Pyridine.

Method	Basis Sets	No.	adj- R^2	Slope	Error	Intercept	Error
B3LYP	6-311++G**	11	0.998921218	1.03369	0.00679	3.36926	11.06941
	aug-cc-PVTZ	12	0.998798219	1.03146	0.00716	10.5898	11.65892
	DGDZVP	13	0.998877266	1.04464	0.007	-7.17633	11.41251
PBE0	6-311++G**	21	0.998689750	1.04271	0.00755	1.78763	12.30718
	aug-cc-PVTZ	22	0.998597874	1.03884	0.00779	8.07573	12.68472
	DGDZVP	23	0.998666430	1.05462	0.00771	-8.33241	12.55823
B2PLYP-D3	6-311++G**	31	0.998720018	1.05142	0.00693	-23.5015	11.29913
	aug-cc-PVTZ	32	0.998630910	1.04197	0.00772	1.00022	12.5719
	DGDZVP	33	0.998845157	1.0553	0.00718	-18.1441	11.69289
M06-2X	6-311++G**	41	0.998656287	1.04769	0.00769	-0.77957	12.52306
	aug-cc-PVTZ	42	0.998562905	1.04769	0.00769	-0.77957	12.52306
	DGDZVP	43	0.998668233	1.04492	0.00793	4.59257	12.91729
ω B97X-D	6-311++G**	51	0.998756153	1.04034	0.00734	9.08554	11.96363
	aug-cc-PVTZ	52	0.998676604	1.03991	0.00757	12.84679	12.33563
	DGDZVP	53	0.998775162	1.0545	0.00739	-2.62665	12.03333
MP2	6-311++G**	61	0.997563863	1.08003	0.01067	-80.7441	17.39199
	aug-cc-PVTZ	62	0.998054366	1.03369	0.00679	3.36926	11.06941
	DGDZVP	63	0.998289840	1.03369	0.00679	3.36926	11.06941

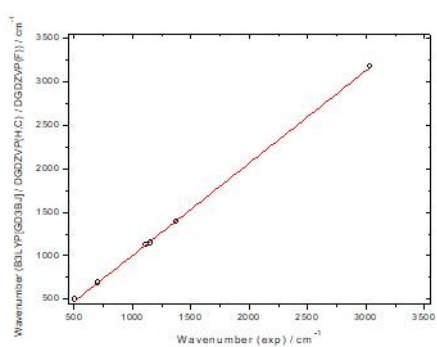
2. CHF₃



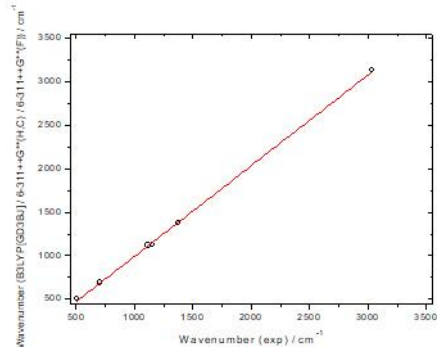
B3LYP / 6-311++G** (C,H), DGDZVP (F)



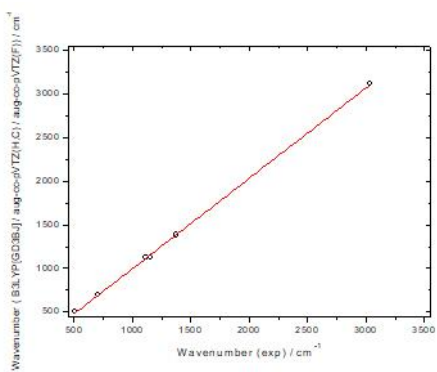
B3LYP / aug-cc-PVTZ (C,H), DGDZVP (F)



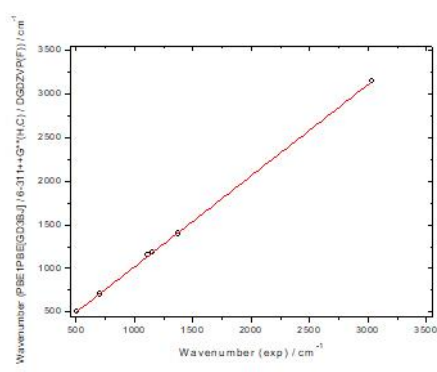
B3LYP / DGDZVP



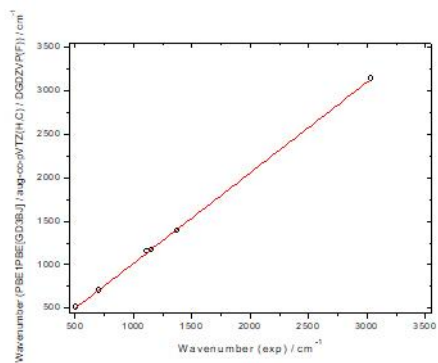
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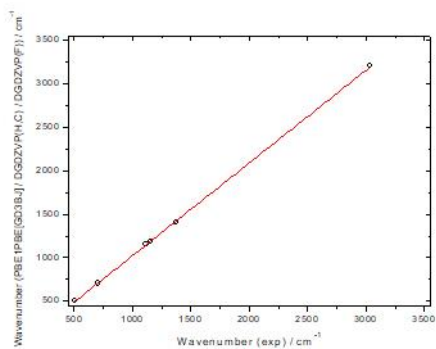
B3LYP / aug-cc-PVTZ



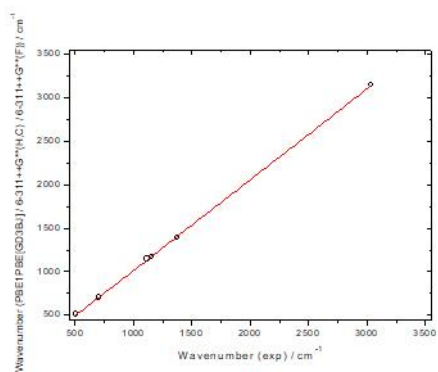
PBE0 / 6-311++G** (C,H), DGDZVP (F)



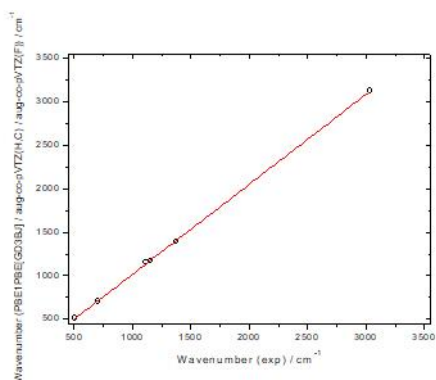
PBE0 / aug-cc-PVTZ (C,H), DGDZVP (F)



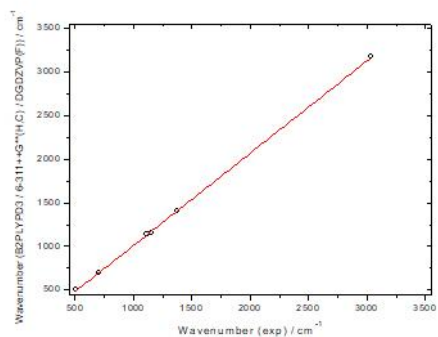
PBE0 / DGDZVP



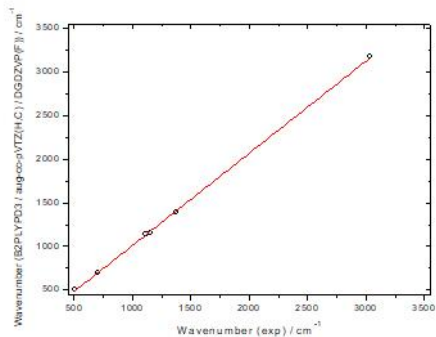
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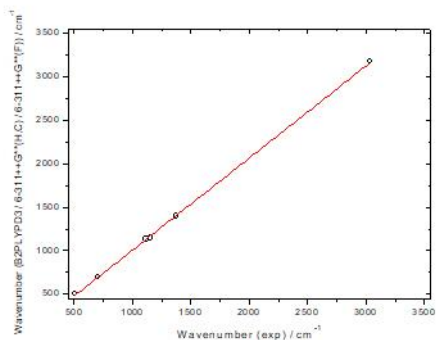
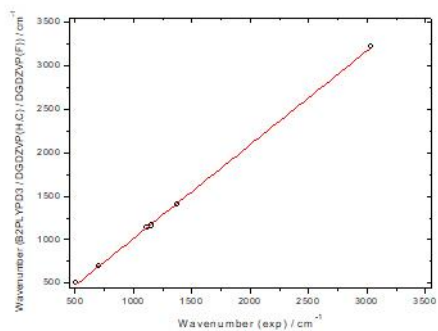
PBE0 / aug-cc-PVTZ



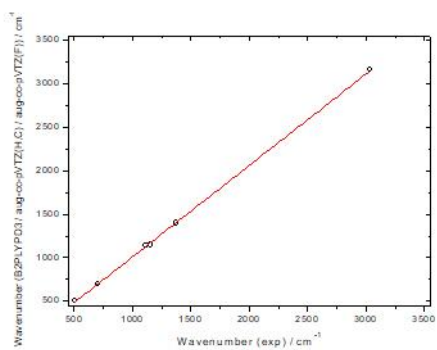
B2PLYP-D3 / 6-311++G** (C,H), DGDZVP (F)



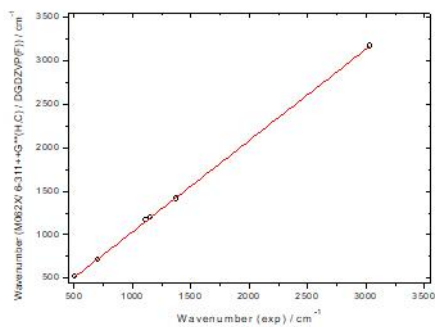
B2PLYP-D3 / aug-cc-PVTZ (C,H), DGDZVP (F)



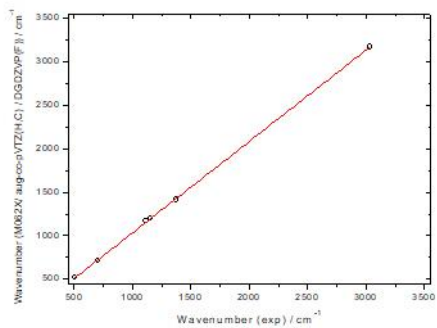
B2PLYP-D3 / DGDZVP



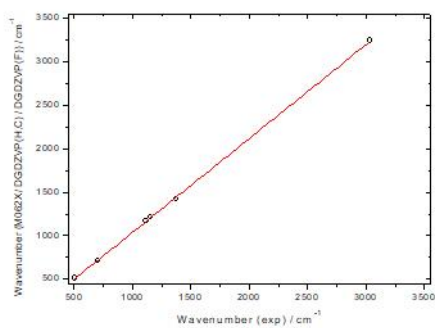
B2PLYP-D3 / 6-311++G**



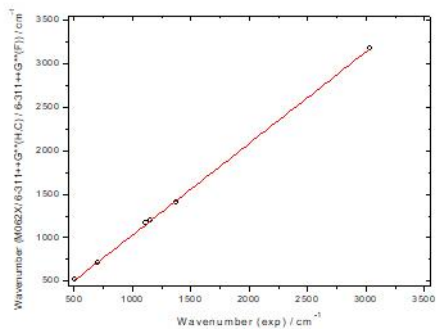
B2PLYP-D3 / aug-cc-PVTZ



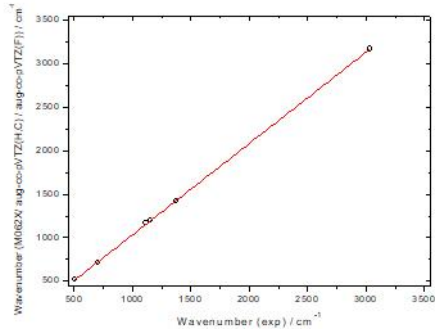
M06-2X / 6-311++G** (C,H), DGDZVP (F)



M06-2X / aug-cc-PVTZ (C,H), DGDZVP (F)

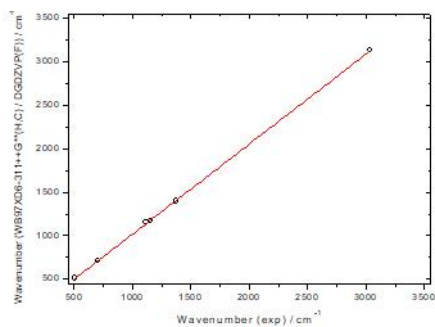


M06-2X / DGDZVP

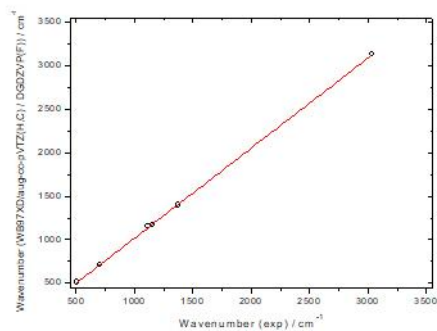


M06-2X / 6-311++G**

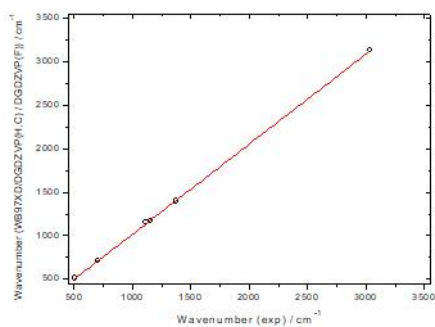
M06-2X / aug-cc-PVTZ



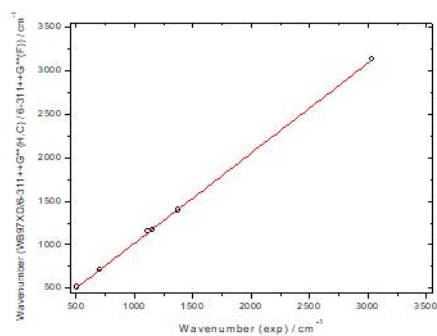
ω B97X-D / 6-311++G** (C,H), DGDZVP (F)



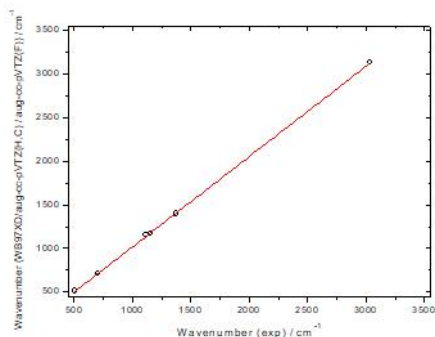
ω B97X-D / aug-cc-PVTZ (C,H), DGDZVP (F)



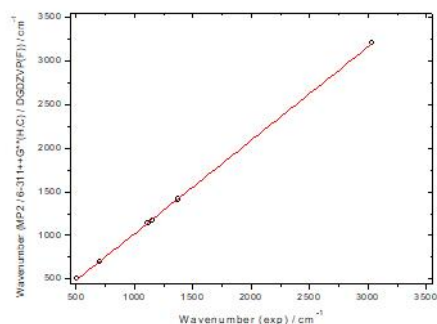
ω B97X-D / DGDZVP



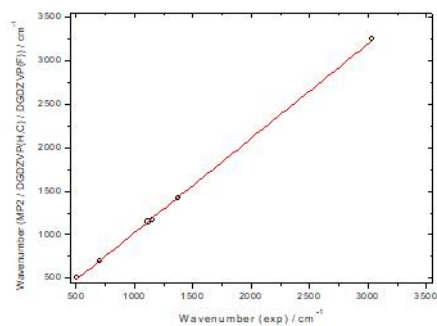
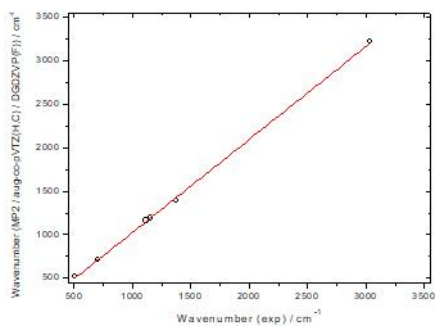
ω B97X-D / 6-311++G**



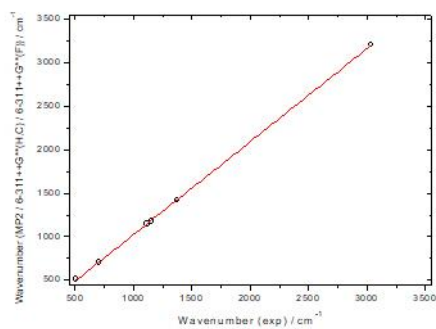
ω B97X-D / aug-cc-PVTZ



MP2 / 6-311++G** (C,H), DGDZVP (F)

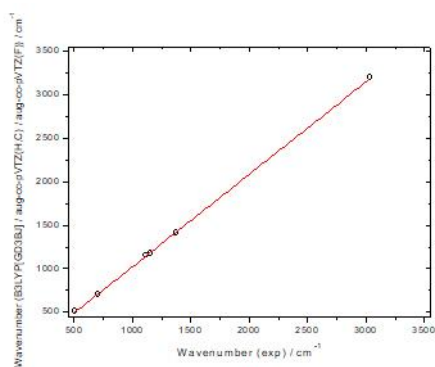


MP2 / aug-cc-PVTZ (C,H), DGDZVP (F)



MP2 / 6-311++G**

MP2 / DGDZVP



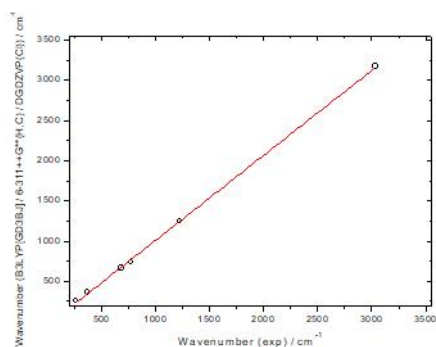
MP2 / aug-cc-PVTZ

Figure SI.1.7 Linear Regression of Computed vs. Experimental Infrared Wavenumbers of Fluoroform.

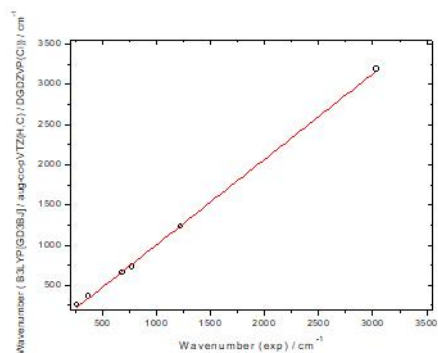
Table SI.1.7 Statistical Parameters of Linear Regression of Computed vs. Experimental Infrared Wavenumbers of Fluoroform.

Method	Basis Sets	No.	adj- R^2	Slope	Error	Intercept	Error
B3LYP	6-311++G** (C,H) DGDZVP (F)	11	0.999755939	1.04377	0.00616	-44.7571	8.68998
	aug-cc-PVTZ (C,H) DGDZVP (F)	12	0.999585455	1.04343	0.00803	-45.007	11.32268
	DGDZVP	13	0.999708804	1.06394	0.00686	-60.9988	9.67577
	6-311++G**	14*	0.999431677	1.04403	0.00941	-50.3839	13.26614
	aug-cc-PVTZ	15*	0.999616151	1.03729	0.00768	-39.6023	10.83115
PBE0	6-311++G** (C,H) DGDZVP (F)	21	0.999901421	1.04512	0.00392	-25.5601	5.52957
	aug-cc-PVTZ (C,H) DGDZVP (F)	22	0.999811326	1.04151	0.00541	-24.3964	7.62384
	DGDZVP	23	0.999869225	1.0673	0.00461	-43.1315	6.50413
	6-311++G**	24*	0.999794353	1.04441	0.00566	-29.6868	7.98157
	aug-cc-PVTZ	25*	0.999877499	1.03531	0.00433	-18.0712	6.10631
B2PLYP-D3	6-311++G** (C,H) DGDZVP (F)	31	0.999817756	1.0597	0.00541	-48.4619	7.62358
	aug-cc-PVTZ (C,H) DGDZVP (F)	32	0.999658830	1.05814	0.00739	-45.8682	10.41636
	DGDZVP	33	0.999730508	1.07968	0.0067	-64.5425	9.44578
	6-311++G**	34*	0.999603083	1.05946	0.00798	-51.3397	11.24951
	aug-cc-PVTZ	35*	0.999733354	1.05249	0.0065	-42.3523	9.15917
M06-2X	6-311++G** (C,H) DGDZVP (F)	41	0.999899738	1.05128	0.00398	-17.0823	5.60945
	aug-cc-PVTZ (C,H) DGDZVP (F)	42	0.999899731	1.05128	0.00398	-17.083	5.60966
	DGDZVP	43	0.999815799	1.08103	0.00555	-42.4298	7.81874
	6-311++G**	44*	0.999847288	1.05451	0.00493	-22.8605	6.94439
	aug-cc-PVTZ	45*	0.999902666	1.05105	0.00392	-17.268	5.52574
ω B97X-D	6-311++G** (C,H) DGDZVP (F)	51	0.999911884	1.03655	0.00368	-18.222	5.18501
	aug-cc-PVTZ (C,H) DGDZVP (F)	52	0.999912035	1.03656	0.00367	-18.206	5.18059
	DGDZVP	53	0.999912440	1.03659	0.00367	-18.2816	5.16881
	6-311++G**	54*	0.999912052	1.03656	0.00367	-18.2067	5.18007
	aug-cc-PVTZ	55*	0.999912010	1.03656	0.00368	-18.2034	5.18131
MP2	6-311++G** (C,H) DGDZVP (F)	61	0.999834618	1.07147	0.00521	-50.4963	7.34298
	aug-cc-PVTZ (C,H) DGDZVP (F)	62	0.999267011	1.0706	0.01096	-43.5638	15.45061
	DGDZVP	63	0.999761481	1.08686	0.00635	-63.1879	8.94534
	6-311++G**	64*	0.999846891	1.07038	0.00501	-45.3578	7.05802
	aug-cc-PVTZ	65*	0.999867941	1.06443	0.00462	-40.993	6.51841

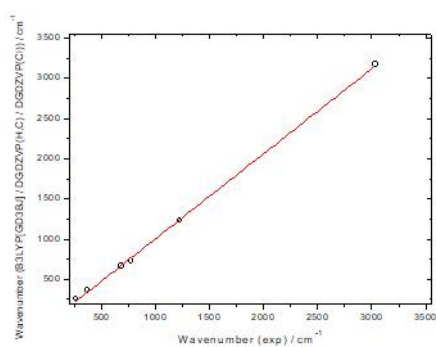
3. CHCl₃



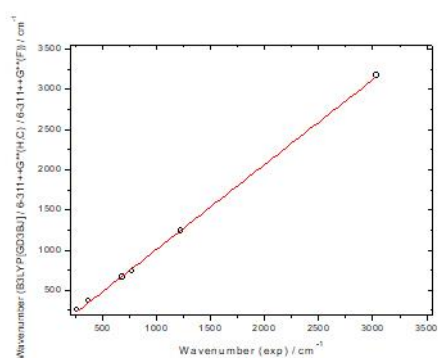
B3LYP / 6-311++G** (C,H), DGDZVP (CI)



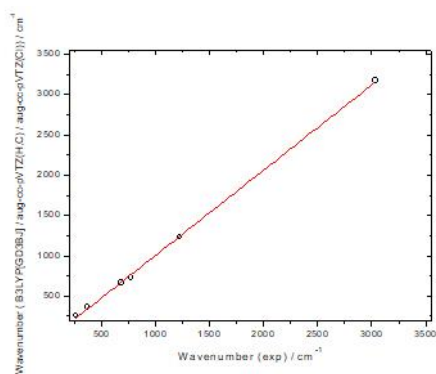
B3LYP / aug-cc-pVTZ (C,H), DGDZVP (CI)



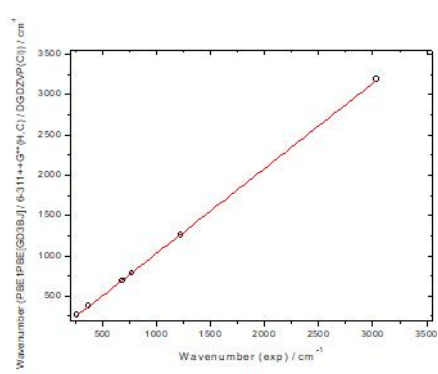
B3LYP / DGDZVP



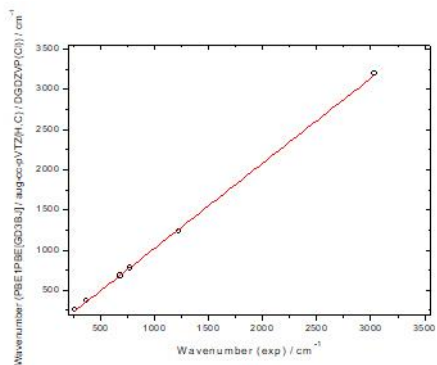
B3LYP / 6-311++G**



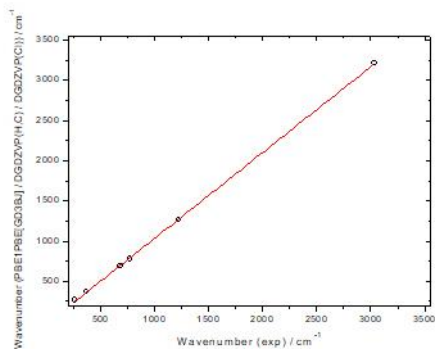
B3LYP / aug-cc-pVTZ



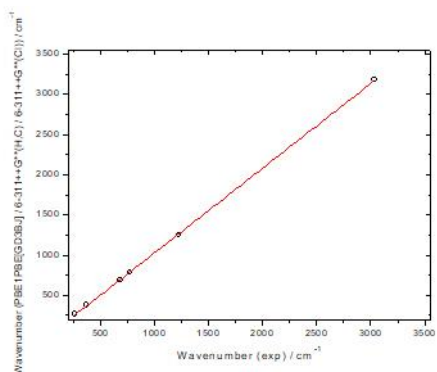
PBE0 / 6-311++G** (C,H), DGDZVP (CI)



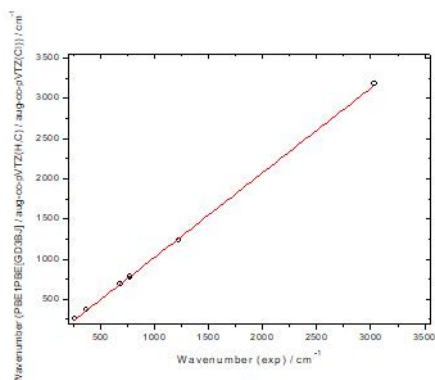
PBE0 / aug-cc-pVTZ (C,H), DGDZVP (CI)



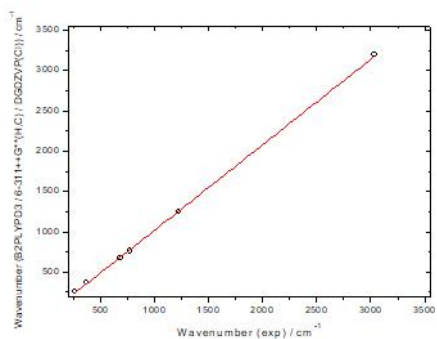
PBE0 / DGDZVP



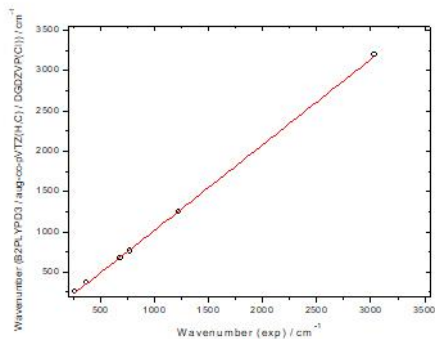
PBE0 / 6-311++G**



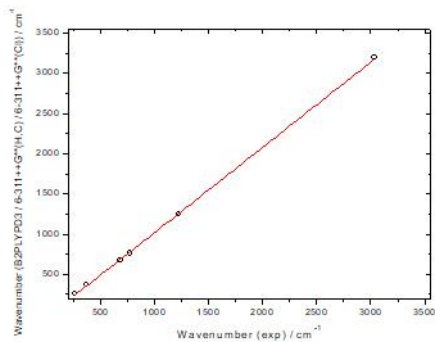
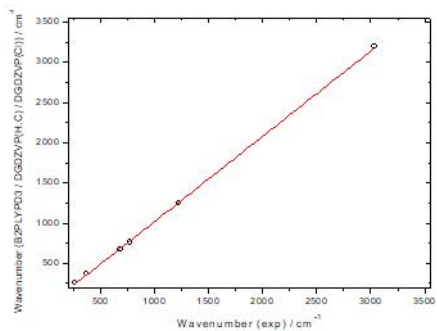
PBE0 / aug-cc-pVTZ



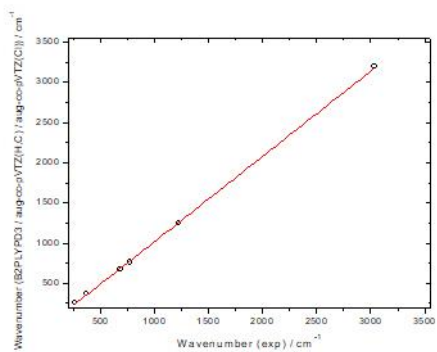
B2PLYP-D3 / 6-311++G** (C,H), DGDZVP (CI)



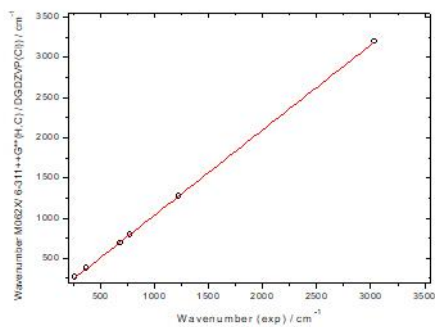
B2PLYP-D3 / aug-cc-pVTZ (C,H), DGDZVP (CI)



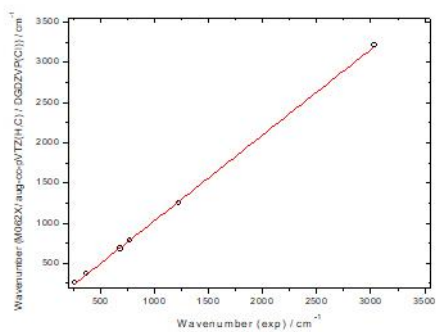
B2PLYP-D3 / DGDZVP



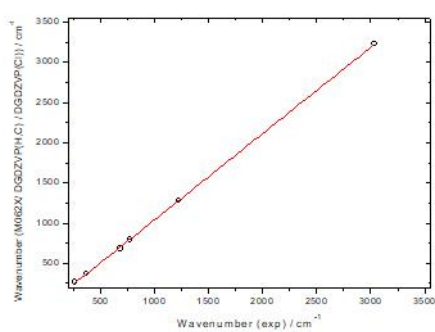
B2PLYP-D3 / 6-311++G**



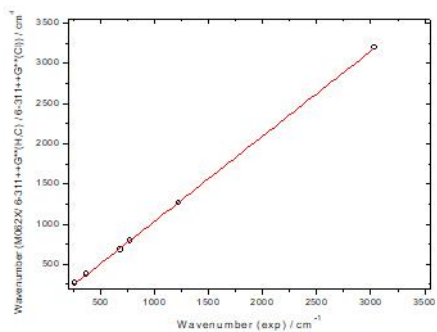
B2PLYP-D3 / aug-cc-PVTZ



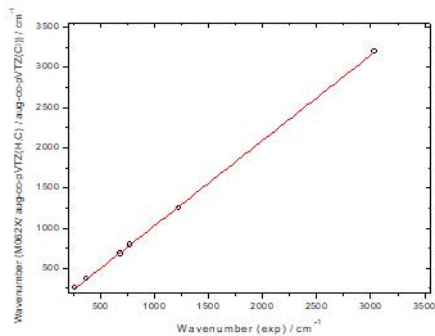
M06-2X / 6-311++G** (C,H), DGDZVP (Cl)



M06-2X / aug-cc-PVTZ (C,H), DGDZVP (Cl)

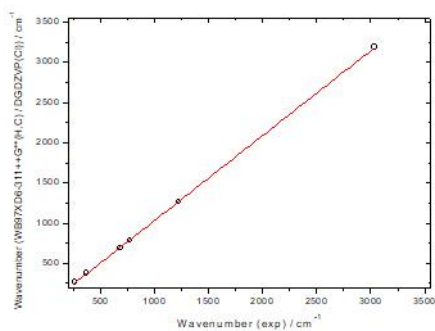


M06-2X / DGDZVP

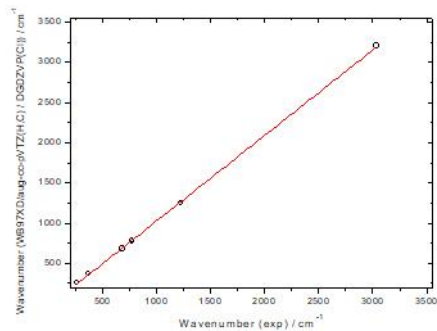


M06-2X / 6-311++G**

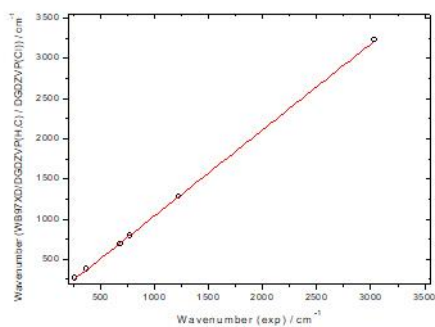
M06-2X / aug-cc-PVTZ



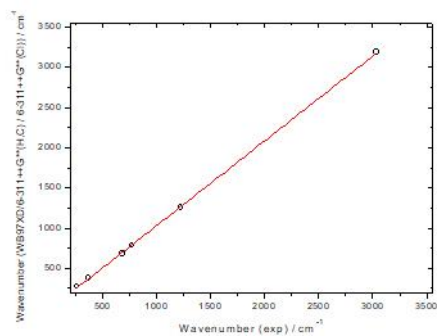
ω B97X-D / 6-311++G** (C,H), DGDZVP (CI)



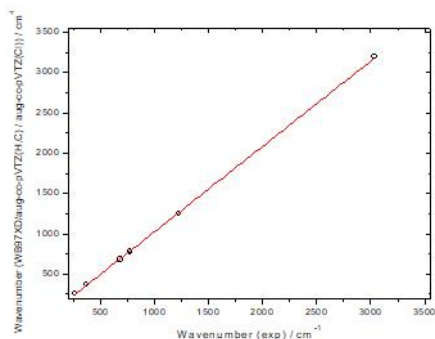
ω B97X-D / aug-cc-PVTZ (C,H), DGDZVP (CI)



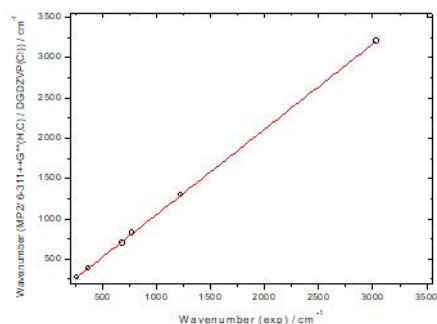
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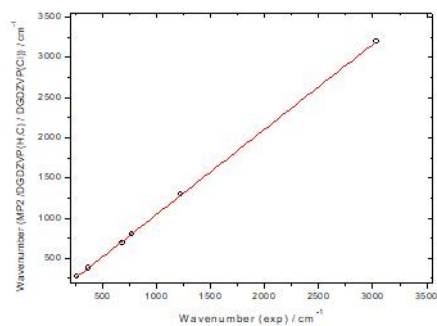
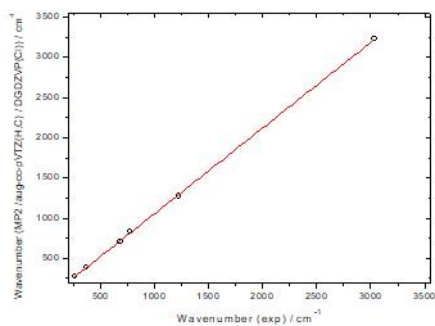
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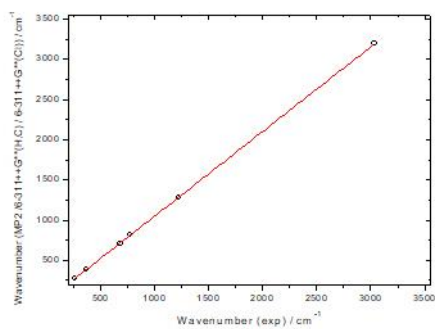
ω B97X-D / aug-cc-PVTZ



MP2 / 6-311++G** (C,H), DGDZVP (CI)

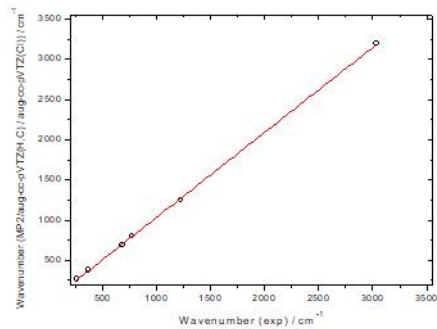


MP2 / aug-cc-PVTZ (C,H), DGDZVP (Cl)



MP2 / 6-311++G**

MP2 / DGDZVP

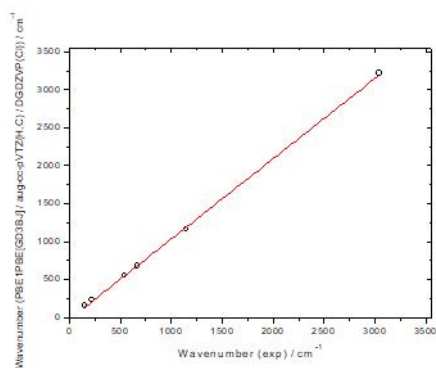


MP2 / aug-cc-PVTZ

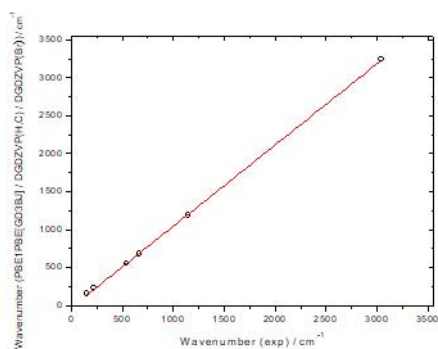
Figure SI.1.8 Linear Regression of Computed vs. Experimental Infrared Wavenumbers of Chloroform.

Table SI.1.8 Statistical Parameters of Linear Regression of Computed vs. Experimental Infrared Wavenumbers of Chloroform.

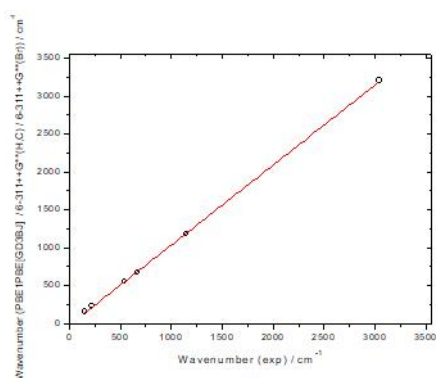
Method	Basis Sets	No.	adj- R^2	Slope	Error	Intercept	Error
B3LYP	6-311++G** (C,H) DGDZVP (Cl)	11	0.999178112	1.05563	0.01144	-41.8739	14.32841
	aug-cc-PVTZ (C,H) DGDZVP (Cl)	12	0.998991650	1.06136	0.01275	-51.9403	15.95843
	DGDZVP	13	0.999126433	1.05564	0.0118	-46.5469	14.77255
	6-311++G**	14*	0.999136224	1.05396	0.01171	-40.6332	14.66609
	aug-cc-PVTZ	15*	0.999126504	1.05564	0.0118	-46.5464	14.77195
PBE0	6-311++G** (C,H) DGDZVP (Cl)	21	0.999810622	1.05349	0.00548	-20.2708	6.86176
	aug-cc-PVTZ (C,H) DGDZVP (Cl)	22	0.999612987	1.0567	0.00786	-30.1628	9.84009
	DGDZVP	23	0.999745728	1.06535	0.00642	-26.812	8.04077
	6-311++G**	24*	0.999770018	1.05193	0.00603	-19.7039	7.55067
	aug-cc-PVTZ	25*	0.999708812	1.05153	0.00678	-25.7965	8.49319
B2PLYP-D3	6-311++G** (C,H) DGDZVP (Cl)	31	0.999593306	1.0588	0.00807	-35.6416	10.10732
	aug-cc-PVTZ (C,H) DGDZVP (Cl)	32	0.999593132	1.0588	0.00807	-35.6441	10.10948
	DGDZVP	33	0.999593265	1.0588	0.00807	-35.6423	10.10782
	6-311++G**	34*	0.999593229	1.0588	0.00807	-35.6438	10.10829
	aug-cc-PVTZ	35*	0.999594491	1.05878	0.00806	-35.5988	10.09247
M06-2X	6-311++G** (C,H) DGDZVP (Cl)	41	0.999887590	1.05879	0.00424	-18.5641	5.31298
	aug-cc-PVTZ (C,H) DGDZVP (Cl)	42	0.999702335	1.06432	0.00694	-30.0277	8.69167
	DGDZVP	43	0.999812444	1.07145	0.00555	-26.1673	6.94511
	6-311++G**	44*	0.999856319	1.05734	0.00479	-18.261	5.99857
	aug-cc-PVTZ	45*	0.999794933	1.05955	0.00574	-25.888	7.18153
ω B97X-D	6-311++G** (C,H) DGDZVP (Cl)	51	0.999871290	1.05481	0.00452	-18.3441	5.66385
	aug-cc-PVTZ (C,H) DGDZVP (Cl)	52	0.999686912	1.06223	0.00711	-31.3691	8.89651
	DGDZVP	53	0.999834770	1.06846	0.00519	-23.8856	6.50041
	6-311++G**	54*	0.999806936	1.0536	0.00553	-19.2503	6.92897
	aug-cc-PVTZ	55*	0.999768933	1.05734	0.00608	-27.5563	7.6074
MP2	6-311++G** (C,H) DGDZVP (Cl)	61	0.999926129	1.05684	0.00343	-0.13663	4.29897
	aug-cc-PVTZ (C,H) DGDZVP (Cl)	62	0.999806910	1.06485	0.00559	-6.24889	7.00341
	DGDZVP	63	0.999890831	1.05746	0.00418	-7.43779	5.22925
	6-311++G**	64*	0.999927687	1.05231	0.00338	0.47084	4.23517
	aug-cc-PVTZ	65*	0.999797902	1.05545	0.00567	-16.8217	7.10174



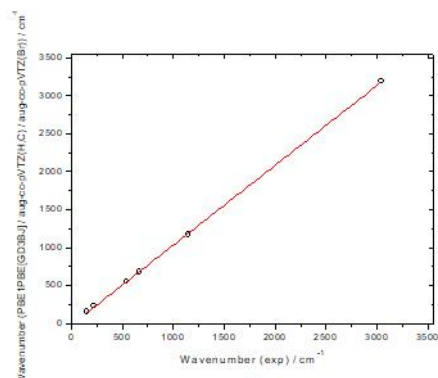
PBE0 / aug-cc-pVTZ (C,H), DGDZVP (Br)



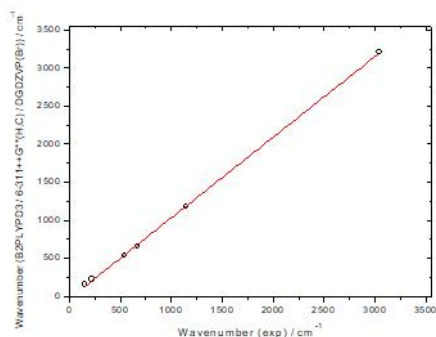
PBE0 / DGDZVP



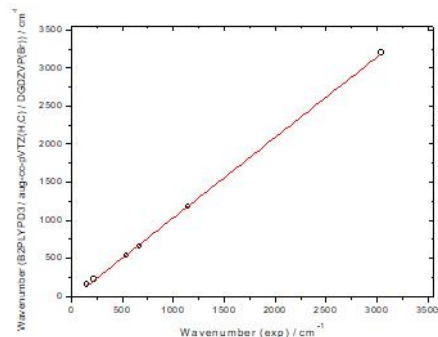
PBE0 / 6-311++G**



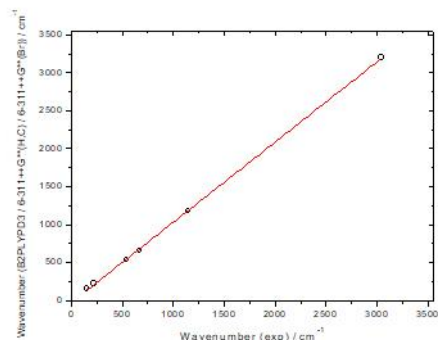
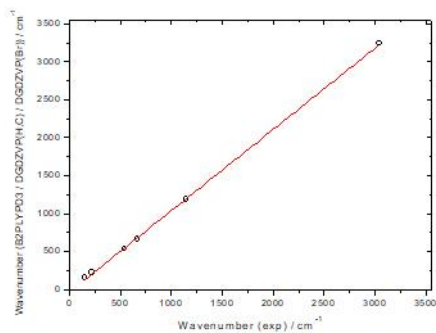
PBE0 / aug-cc-pVTZ



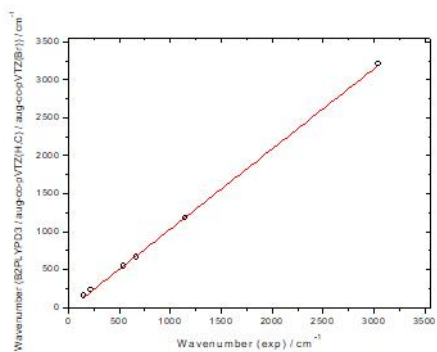
B2PLYP-D3 / 6-311++G** (C,H), DGDZVP (Br)



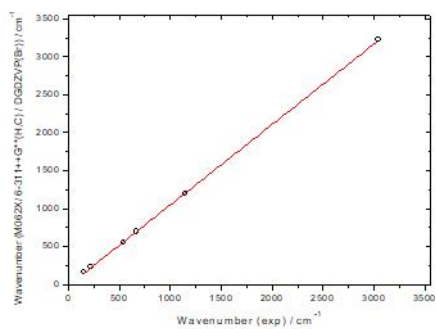
B2PLYP-D3 / aug-cc-pVTZ (C,H), DGDZVP (Br)



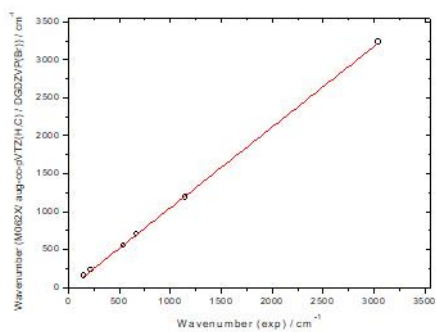
B2PLYP-D3 / DGDZVP



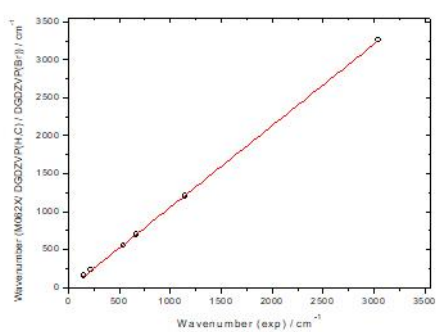
B2PLYP-D3 / 6-311++G**



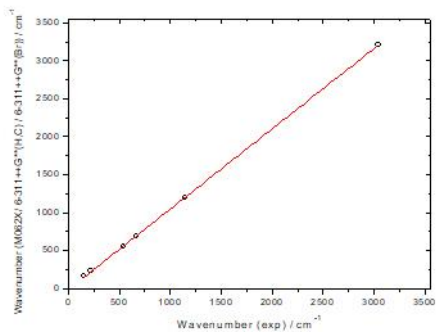
B2PLYP-D3 / aug-cc-PVTZ



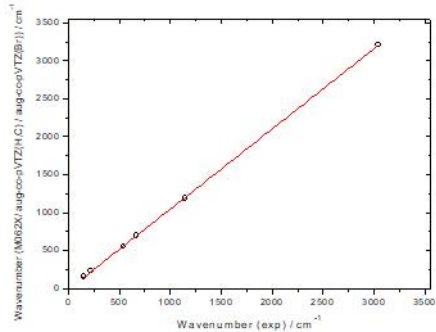
M06-2X / 6-311++G** (C,H), DGDZVP (Br)



M06-2X / aug-cc-PVTZ (C,H), DGDZVP (Br)

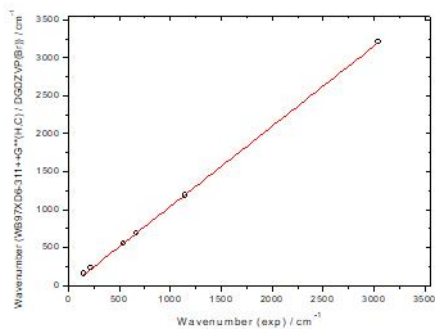


M06-2X / DGDZVP

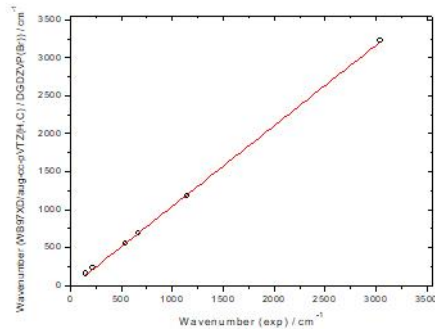


M06-2X / 6-311++G**

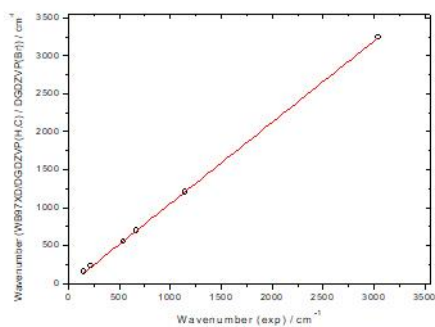
M06-2X / aug-cc-PVTZ



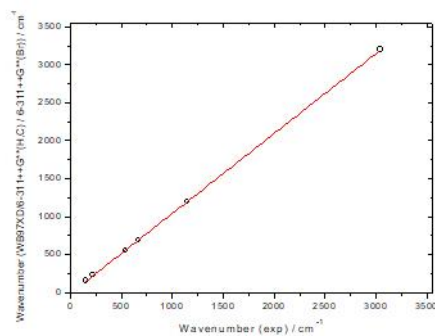
ω B97X-D / 6-311++G** (C,H), DGDZVP (Br)



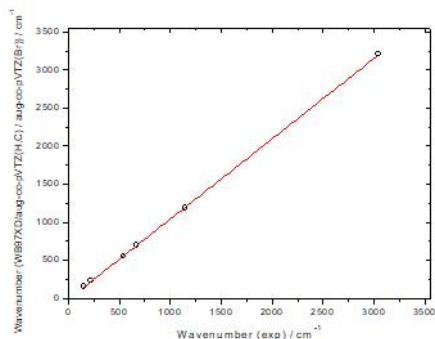
ω B97X-D / aug-cc-PVTZ (C,H), DGDZVP (Br)



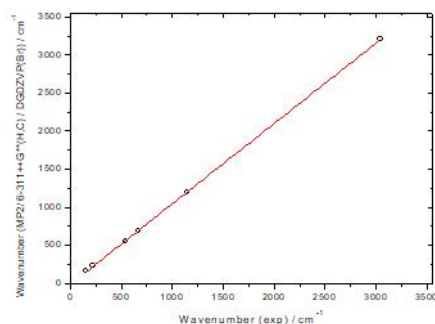
ω B97X-D / DGDZVP



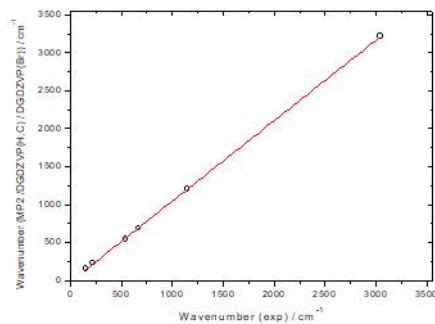
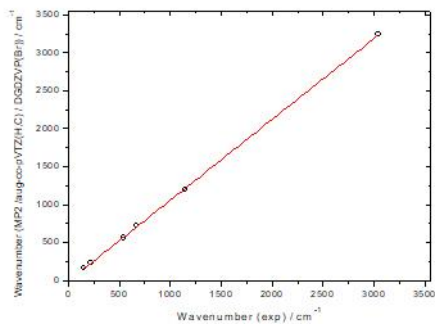
ω B97X-D / 6-311++G**



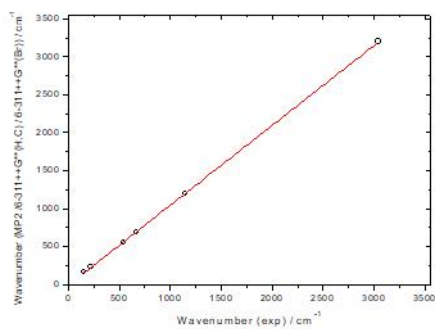
ω B97X-D / aug-cc-PVTZ



MP2 / 6-311++G** (C,H), DGDZVP (Br)

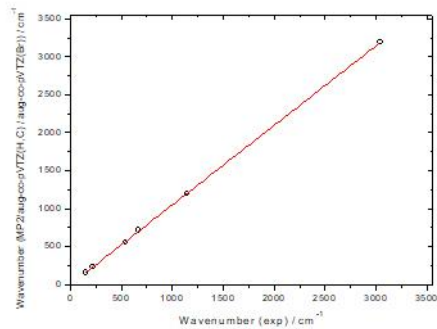


MP2 / aug-cc-PVTZ (C,H), DGDZVP (Br)



MP2 / 6-311++G**

MP2 / DGDZVP



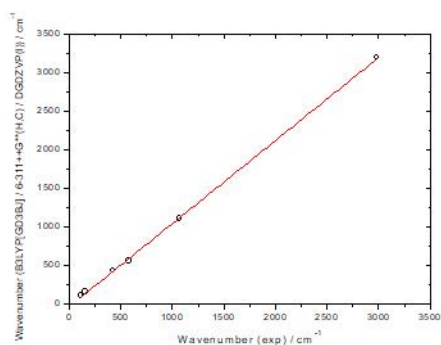
MP2 / aug-cc-PVTZ

Figure SI.1.9 Linear Regression of Computed vs. Experimental Infrared Wavenumbers of Bromoform.

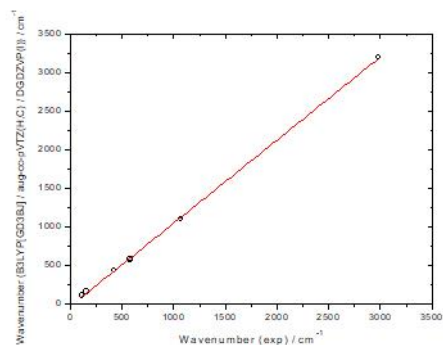
Table SI.1.9 Statistical Parameters of Linear Regression of Computed vs. Experimental Infrared Wavenumbers of Bromoform.

Method	Basis Sets	No.	adj- R^2	Slope	Error	Intercept	Error
B3LYP	6-311++G** (C,H) DGDZVP (Br)	11	0.999323118	1.05767	0.0104	-39.6925	12.59015
	aug-cc-PVTZ (C,H) DGDZVP (Br)	12	0.999252881	1.06255	0.01098	-42.0728	13.28873
	DGDZVP	13	0.999338653	1.06931	0.0104	-42.5699	12.58165
	6-311++G**	14*	0.999302773	1.05587	0.01054	-37.8634	12.75633
	aug-cc-PVTZ	15*	0.999410420	1.05553	0.00969	-36.207	11.72585
PBE0	6-311++G** (C,H) DGDZVP (Br)	21	0.999775671	1.05772	0.00599	-22.6974	7.24665
	aug-cc-PVTZ (C,H) DGDZVP (Br)	22	0.999660476	1.05944	0.00738	-24.3696	8.93016
	DGDZVP	23	0.999762896	1.07139	0.00624	-26.3028	7.54647
	6-311++G**	24*	0.999800623	1.05565	0.00563	-21.3726	6.81832
	aug-cc-PVTZ	25*	0.999792125	1.05286	0.00574	-19.4171	6.94371
B2PLYP-D3	6-311++G** (C,H) DGDZVP (Br)	31	0.999688555	1.06065	0.00708	-29.1162	8.56262
	aug-cc-PVTZ (C,H) DGDZVP (Br)	32	0.999695011	1.05818	0.00699	-26.656	8.45363
	DGDZVP	33	0.999661157	1.07173	0.00746	-32.9831	9.02472
	6-311++G**	34*	0.999694028	1.05818	0.007	-26.6732	8.46724
	aug-cc-PVTZ	35*	0.999772336	1.05784	0.00603	-24.8616	7.30119
M06-2X	6-311++G** (C,H) DGDZVP (Br)	41	0.999951535	1.06122	0.00279	-12.0906	3.37914
	aug-cc-PVTZ (C,H) DGDZVP (Br)	42	0.999807400	1.06455	0.00558	-14.8918	6.7579
	DGDZVP	43	0.999912937	1.07498	0.00379	-16.5827	4.58788
	6-311++G**	44*	0.999948679	1.05901	0.00287	-12.2256	3.47001
	aug-cc-PVTZ	45*	0.999909578	1.05813	0.0038	-12.3444	4.60227
ω B97X-D	6-311++G** (C,H) DGDZVP (Br)	51	0.999934893	1.05702	0.00322	-15.1453	3.90108
	aug-cc-PVTZ (C,H) DGDZVP (Br)	52	0.999842205	1.06267	0.00505	-19.325	6.106
	DGDZVP	53	0.999918102	1.07174	0.00367	-18.7241	4.43631
	6-311++G**	54*	0.999954070	1.05464	0.0027	-12.4868	3.26916
	aug-cc-PVTZ	55*	0.999920750	1.05572	0.00355	-13.576	4.29876
MP2	6-311++G** (C,H) DGDZVP (Br)	61	0.999920750	1.05676	0.0029	-11.6714	3.5135
	aug-cc-PVTZ (C,H) DGDZVP (Br)	62	0.999797202	1.0654	0.00574	-6.27761	6.94009
	DGDZVP	63	0.999934011	1.06139	0.00326	-15.8141	3.94368
	6-311++G**	64*	0.999962363	1.05344	0.00244	-8.49079	2.95598
	aug-cc-PVTZ	65*	0.999962363	1.04951	0.00389	-0.97566	4.71175

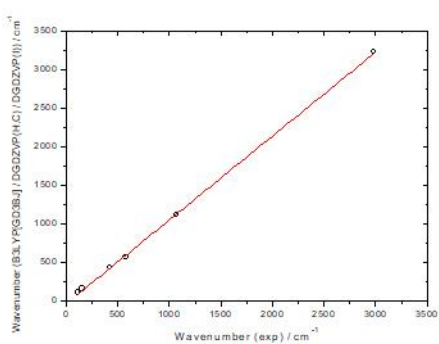
5. CH₃



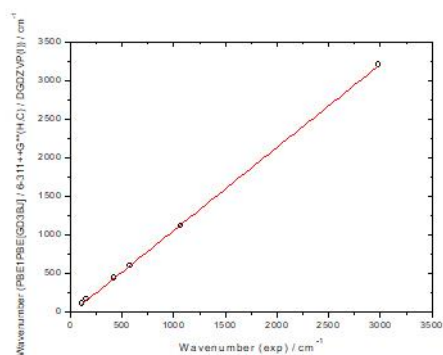
B3LYP / 6-311++G** (C,H), DGDZVP (I)



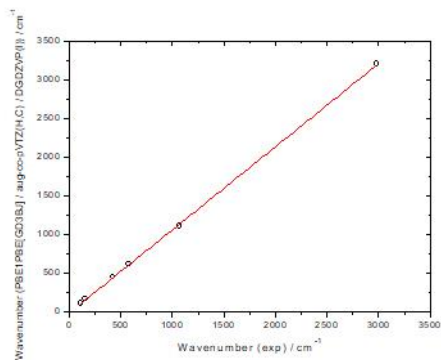
B3LYP / aug-cc-PVTZ (C,H), DGDZVP (I)



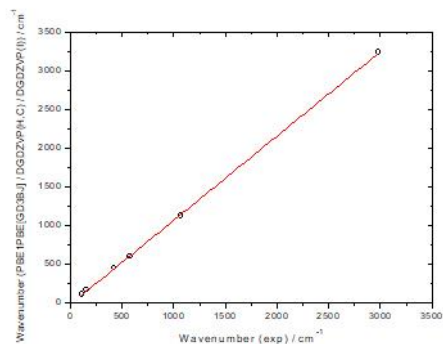
B3LYP / DGDZVP



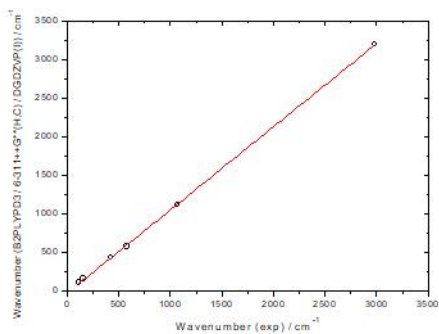
PBE0 / 6-311++G** (C,H), DGDZVP (I)



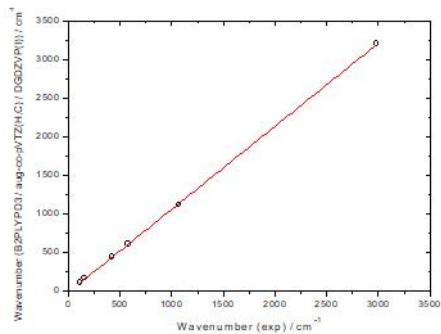
PBE0 / aug-cc-PVTZ (C,H), DGDZVP (I)



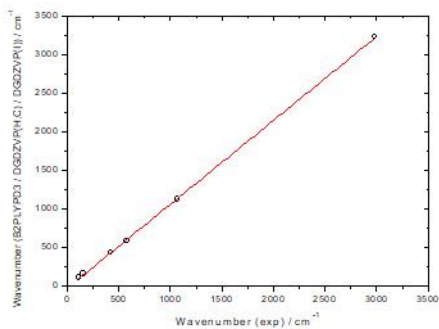
PBE0 / DGDZVP



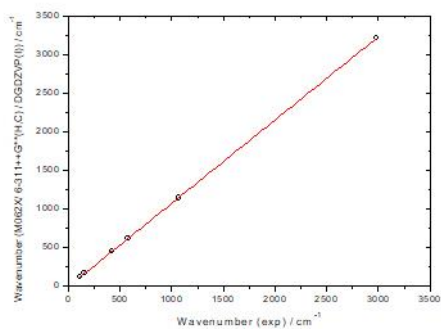
B2PLYP-D3 / 6-311++G** (C,H), DGDZVP (I)



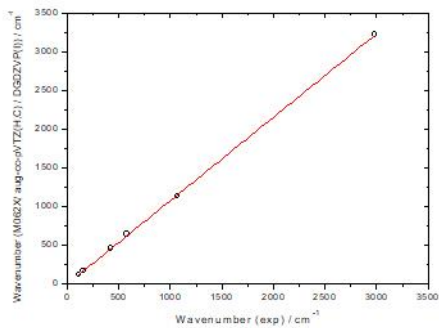
B2PLYP-D3 / aug-cc-pVTZ (C,H), DGDZVP (I)



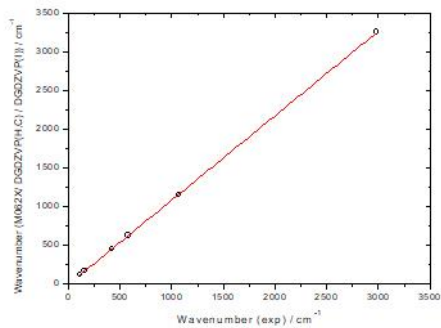
B2PLYP-D3 / DGDZVP



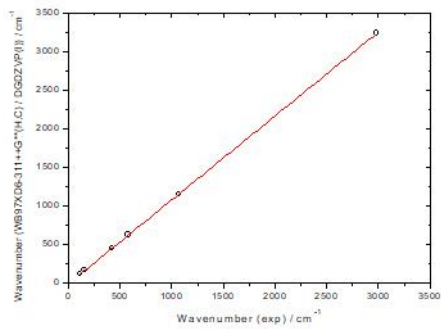
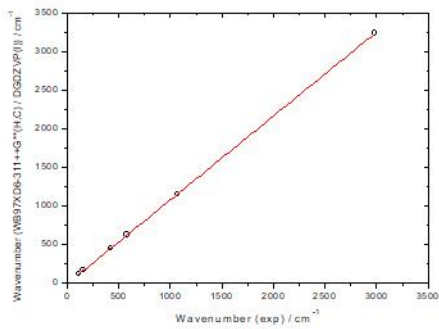
M06-2X / 6-311++G** (C,H), DGDZVP (I)



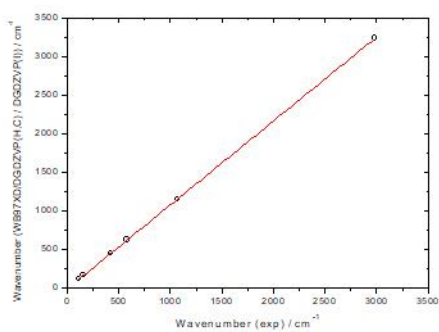
M06-2X / aug-cc-pVTZ (C,H), DGDZVP (I)



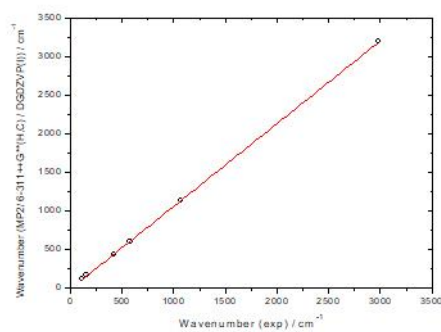
M06-2X / DGDZVP



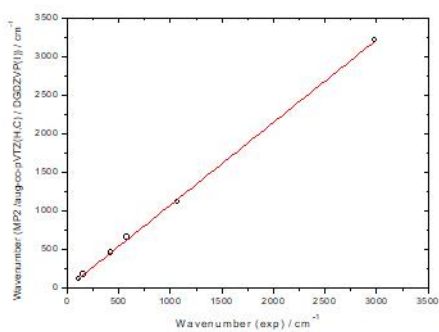
ω B97X-D / 6-311++G** (C,H), DGDZVP (I)



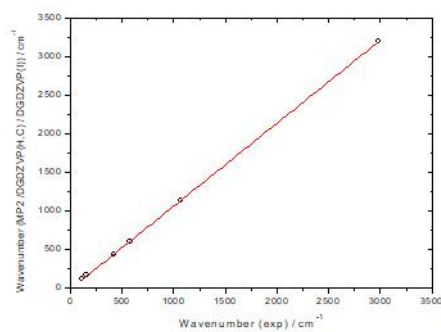
ω B97X-D / aug-cc-PVTZ (C,H), DGDZVP (I)



ω B97X-D / DGDZVP



MP2 / 6-311++G** (C,H), DGDZVP (I)



MP2 / aug-cc-PVTZ (C,H), DGDZVP (I)

MP2 / DGDZVP

Figure SI.1.10 Linear Regression of Computed vs. Experimental Infrared Wavenumbers of Iodoform.

Table SI.1.10 Statistical Parameters of Linear Regression of Computed vs. Experimental Infrared Wavenumbers of Iodoform.

Method	Basis Sets	No.	adj- R^2	Slope	Error	Intercept	Error
B3LYP	6-311++G** (C,H) DGDZVP (I)	11	0.999453219	1.07881	0.00954	-37.9981	11.04483
	aug-cc-PVTZ (C,H) DGDZVP (I)	12	0.999647663	1.07939	0.00766	-32.7338	8.86999
	DGDZVP	13	0.999483457	1.08907	0.00936	-39.2867	10.83701
	6-311++G**	14*	0.999815823	1.07947	0.00554	-23.9418	6.41294
	aug-cc-PVTZ	15*	0.999714997	1.07686	0.00687	-18.6596	7.95855
PBE0	6-311++G** (C,H) DGDZVP (I)	21	0.999812334	1.09161	0.00565	-25.6354	6.54621
	aug-cc-PVTZ (C,H) DGDZVP (I)	22	0.999697328	1.08029	0.0071	-30.9269	8.2277
	DGDZVP	23	0.999804081	1.07889	0.00571	-21.2621	6.61071
	6-311++G**	24*	0.999714617	1.08979	0.00696	-32.1508	8.05946
	aug-cc-PVTZ	25*	0.999984079	1.0822	0.00163	-11.6092	1.89012
B2PLYP-D3	6-311++G** (C,H) DGDZVP (I)	31	0.999810651	1.08117	0.00562	-7.53247	6.5126
	aug-cc-PVTZ (C,H) DGDZVP (I)	32	0.999964545	1.0943	0.00246	-13.6277	2.85215
	DGDZVP	33	0.999965809	1.09044	0.00241	-14.8925	2.79096
	6-311++G**	34*	0.999836260	1.07895	0.00522	-9.98625	6.04367
	aug-cc-PVTZ	35*	0.999965764	1.09044	0.00241	-14.9156	2.79282
M06-2X	6-311++G** (C,H) DGDZVP (I)	41	0.999933878	1.07495	0.0033	-17.9394	3.82619
	aug-cc-PVTZ (C,H) DGDZVP (I)	42	0.999423705	1.07371	0.00975	-0.23083	11.28552
	DGDZVP	43	0.999929053	1.07804	0.00343	-19.0846	3.97473
	6-311++G**	44*	0.999453219	1.07881	0.00954	-37.9981	11.04483
	aug-cc-PVTZ	45*	0.999647663	1.07939	0.00766	-32.7338	8.86999
ω B97X-D	6-311++G** (C,H) DGDZVP (I)	51	0.999483457	1.08907	0.00936	-39.2867	10.83701
	aug-cc-PVTZ (C,H) DGDZVP (I)	52	0.999815823	1.07947	0.00554	-23.9418	6.41294
	DGDZVP	53	0.999714997	1.07686	0.00687	-18.6596	7.95855
	6-311++G**	54*	0.999812334	1.09161	0.00565	-25.6354	6.54621
	aug-cc-PVTZ	55*	0.999697328	1.08029	0.0071	-30.9269	8.2277
MP2	6-311++G** (C,H) DGDZVP (I)	61	0.999804081	1.07889	0.00571	-21.2621	6.61071
	aug-cc-PVTZ (C,H) DGDZVP (I)	62	0.999714617	1.08979	0.00696	-32.1508	8.05946
	DGDZVP	63	0.999984079	1.0822	0.00163	-11.6092	1.89012
	6-311++G**	64*	0.999810651	1.08117	0.00562	-7.53247	6.5126
	aug-cc-PVTZ	65*	0.999964545	1.0943	0.00246	-13.6277	2.85215

SI.1. 4 Electronic Polarizability

Calculated isotropic static electronic polarizability (α_e), discrepancies with respect to the experimental values (Δ), their quadratic averages ($\langle\Delta^2\rangle$), and differences of quadratic averages with respect to the minimum value ($\langle\Delta^2\rangle-\langle\Delta^2\rangle_{min}$). Calculated values are obtained with the same levels of theory as reported above.

Table SI.1.11 Pyridine

No.	$\alpha_e / \text{\AA}^3$	$\Delta / \text{\AA}^3$	$\langle\Delta^2\rangle / \text{\AA}^6$	$(\langle\Delta^2\rangle-\langle\Delta^2\rangle_{min})/\text{\AA}^6$
		exp ^a : 9.17 \AA^3		
11	9.05	-0.12	0.01	0.01
12	9.46	0.29	0.09	0.08
13	8.02	-1.15	1.32	1.31
21	8.91	-0.26	0.07	0.06
22	9.33	0.16	0.03	0.02
23	7.98	-1.19	1.41	1.41
31	9.02	-0.15	0.02	0.02
32	9.45	0.28	0.08	0.07
33	8.01	-1.16	1.34	1.33
41	8.79	-0.38	0.14	0.14
42	9.26	0.09	0.01	0.00
43	7.98	-1.19	1.42	1.41
51	8.89	-0.28	0.08	0.07
52	9.32	0.15	0.02	0.01
53	7.97	-1.20	1.44	1.44
61	8.99	-0.18	0.03	0.02
62	9.44	0.27	0.07	0.07

^a From: CRC Handbook of Chemistry and Physics, 99th Edition, Editor-in-Chief: John R. Rumble.**Table SI.1.12** CHF₃

No.	$\alpha_e / \text{\AA}^3$	$\Delta_1 / \text{\AA}^3$	$\Delta_2 / \text{\AA}^3$	$\Delta_3 / \text{\AA}^3$	$\Delta_4 / \text{\AA}^3$	$\Delta_5 / \text{\AA}^3$	$\Delta_6 / \text{\AA}^3$	$\Delta_7 / \text{\AA}^3$	$\langle \Delta \rangle / \text{\AA}^6$	$(\langle \Delta \rangle - \langle \Delta \rangle_{min}) / \text{\AA}^6$
		exp ^a : 2.62 \AA^3	exp ^b : 2.75 \AA^3	exp ^c : 2.77 \AA^3	exp ^d : 2.76 \AA^3	exp ^e : 2.79 \AA^3	exp ^f : 2.85 \AA^3	exp ^g : 2.55 \AA^3		
11	2.29	-0.33	-0.47	-0.48	-0.48	-0.50	-0.56	-0.26	0.20	0.19
12	2.63	0.01	-0.12	-0.14	-0.13	-0.16	-0.22	0.08	0.02	0.01
13	2.12	-0.50	-0.64	-0.65	-0.65	-0.67	-0.73	-0.43	0.38	0.37
14	2.39	-0.23	-0.36	-0.37	-0.37	-0.39	-0.45	-0.15	0.12	0.11
15	2.81	0.19	0.06	0.04	0.05	0.02	-0.04	0.26	0.02	0.01
21	2.25	-0.37	-0.50	-0.52	-0.51	-0.54	-0.60	-0.30	0.24	0.23
22	2.58	-0.04	-0.17	-0.19	-0.18	-0.20	-0.26	0.04	0.03	0.02
23	2.09	-0.53	-0.66	-0.68	-0.67	-0.70	-0.76	-0.46	0.41	0.41
24	2.34	-0.28	-0.41	-0.43	-0.42	-0.45	-0.51	-0.21	0.16	0.15
25	2.75	0.13	0.00	-0.02	-0.01	-0.04	-0.09	0.20	0.01	0.00
31	2.26	-0.36	-0.49	-0.51	-0.50	-0.53	-0.59	-0.29	0.23	0.22
32	2.60	-0.02	-0.15	-0.17	-0.16	-0.19	-0.25	0.05	0.03	0.02
33	2.10	-0.52	-0.65	-0.67	-0.66	-0.68	-0.74	-0.45	0.40	0.39
34	2.36	-0.26	-0.40	-0.41	-0.40	-0.43	-0.49	-0.19	0.15	0.14
35	2.77	0.15	0.02	0.00	0.01	-0.01	-0.07	0.22	0.01	0.00
41	2.57	-0.05	-0.19	-0.20	-0.19	-0.22	-0.28	0.02	0.03	0.03
42	2.57	-0.05	-0.19	-0.20	-0.19	-0.22	-0.28	0.02	0.03	0.03
43	2.05	-0.57	-0.70	-0.72	-0.71	-0.74	-0.80	-0.50	0.47	0.46
44	2.25	-0.37	-0.50	-0.52	-0.51	-0.54	-0.60	-0.30	0.24	0.23
45	2.67	0.05	-0.08	-0.10	-0.09	-0.12	-0.18	0.12	0.01	0.00

51	2.75	0.13	0.00	-0.02	-0.01	-0.03	-0.09	0.21	0.01	0.00
52	2.75	0.13	0.00	-0.02	-0.01	-0.03	-0.09	0.21	0.01	0.00
53	2.75	0.13	0.00	-0.02	-0.01	-0.03	-0.09	0.21	0.01	0.00
54	2.75	0.13	0.00	-0.02	-0.01	-0.03	-0.09	0.21	0.01	0.00
55	2.75	0.13	0.00	-0.02	-0.01	-0.03	-0.09	0.21	0.01	0.00
61	2.23	-0.39	-0.52	-0.54	-0.53	-0.55	-0.61	-0.32	0.25	0.24
62	2.57	-0.05	-0.19	-0.20	-0.19	-0.22	-0.28	0.02	0.03	0.03
63	2.10	-0.52	-0.66	-0.67	-0.66	-0.69	-0.75	-0.45	0.41	0.40
64	2.30	-0.32	-0.45	-0.47	-0.46	-0.48	-0.54	-0.25	0.19	0.18
65	2.73	0.11	-0.03	-0.04	-0.03	-0.06	-0.12	0.18	0.01	0.00

^a From: CRC Handbook of Chemistry and Physics, 99th Edition, Editor-in-Chief: John R. Rumble.

^{b-g} From: M. Gussoni, M. Rui, G. Zerbi, *J. Mol. Struct.* **1998**, *447*, 163-215 and references therein.

Table SI.1.13 CHCl₃

No.	$\alpha_e / \text{\AA}^3$	$\Delta_1 / \text{\AA}^3$ exp ^a : 8.13 \AA^3	$\Delta_2 / \text{\AA}^3$ exp ^b : 8.33 \AA^3	$\Delta_3 / \text{\AA}^3$ exp ^c : 9.13 \AA^3	$\Delta_4 / \text{\AA}^3$ exp ^d : 9.22 \AA^3	$\langle \Delta \rangle / \text{\AA}^6$	$(\langle \Delta \rangle - \langle \Delta \rangle_{min}) / \text{\AA}^6$
11	6.67	-1.46	-1.66	-2.46	-2.55	4.36	4.12
12	7.72	-0.41	-0.61	-1.41	-1.49	1.19	0.94
13	8.59	0.46	0.26	-0.54	-0.63	0.24	0.00
14	7.23	-0.90	-1.10	-1.90	-1.99	2.40	2.16
15	8.59	0.46	0.26	-0.54	-0.63	0.24	0.00
21	6.49	-1.64	-1.84	-2.63	-2.72	5.10	4.86
22	7.56	-0.57	-0.77	-1.57	-1.66	1.54	1.30
23	5.96	-2.17	-2.37	-3.17	-3.26	7.76	7.52
24	6.99	-1.14	-1.35	-2.14	-2.23	3.17	2.93
25	8.37	0.24	0.04	-0.76	-0.85	0.34	0.10
31	8.45	0.32	0.12	-0.68	-0.77	0.29	0.05
32	8.45	0.32	0.12	-0.68	-0.77	0.29	0.05
33	8.45	0.32	0.12	-0.68	-0.77	0.29	0.05
34	8.45	0.32	0.12	-0.68	-0.77	0.29	0.05
35	8.45	0.32	0.12	-0.68	-0.77	0.29	0.05
41	6.48	-1.65	-1.85	-2.65	-2.74	5.16	4.92
42	7.56	-0.57	-0.77	-1.57	-1.66	1.54	1.30
43	5.95	-2.18	-2.38	-3.18	-3.27	7.81	7.57
44	6.98	-1.15	-1.35	-2.15	-2.24	3.20	2.96
45	8.34	0.21	0.01	-0.79	-0.87	0.36	0.12
51	6.45	-1.68	-1.88	-2.68	-2.77	5.29	5.05
52	7.54	-0.59	-0.79	-1.58	-1.67	1.57	1.33
53	5.91	-2.22	-2.42	-3.22	-3.31	8.01	7.77
54	6.97	-1.16	-1.36	-2.16	-2.25	3.24	3.00
55	8.36	0.23	0.03	-0.76	-0.85	0.34	0.10

61	6.35	-1.78	-1.99	-2.78	-2.87	5.78	5.54
62	7.44	-0.69	-0.89	-1.69	-1.78	1.82	1.58
63	5.82	-2.31	-2.51	-3.30	-3.39	8.51	8.27
64	6.84	-1.29	-1.50	-2.29	-2.38	3.71	3.47
65	8.29	0.16	-0.04	-0.84	-0.93	0.40	0.16

^a From: CRC Handbook of Chemistry and Physics, 99th Edition, Editor-in-Chief: John R. Rumble.

^{b-d} From: M. Gussoni, M. Rui, G. Zerbi, *J. Mol. Struct.***1998**, 447, 163-215 and references therein.

Table SI.1.14 CHBr₃

No.	$\alpha_e / \text{\AA}^3$	$\Delta / \text{\AA}^3$ exp ^a : 11.84 \AA^3	$\langle \Delta \rangle / \text{\AA}^6$	$(\langle \Delta \rangle - \langle \Delta \rangle_{min}) / \text{\AA}^6$
11	10.01	-1.83	3.33	3.33
12	10.94	-0.90	0.81	0.80
13	9.43	-2.41	5.80	5.79
14	10.35	-1.49	2.22	2.22
15	12.03	0.19	0.04	0.03
21	9.76	-2.08	4.33	4.32
22	10.68	-1.16	1.35	1.34
23	9.24	-2.60	6.74	6.73
24	9.99	-1.85	3.42	3.42
25	11.69	-0.15	0.02	0.02
31	9.81	-2.03	4.12	4.11
32	10.05	-1.79	3.21	3.20
33	9.27	-2.57	6.60	6.60
34	10.05	-1.79	3.21	3.20
35	11.76	-0.08	0.01	0.00
41	9.59	-2.25	5.05	5.04
42	10.48	-1.36	1.84	1.84
43	9.12	-2.72	7.42	7.42
44	9.87	-1.97	3.87	3.86
45	11.60	-0.24	0.06	0.05
51	9.69	-2.15	4.64	4.63
52	10.63	-1.21	1.46	1.45
53	9.17	-2.67	7.15	7.14
54	9.90	-1.94	3.74	3.74
55	11.66	-0.18	0.03	0.03

61	9.53	-2.31	5.34	5.33
62	10.44	-1.40	1.96	1.95
63	9.04	-2.80	7.85	7.85
64	9.62	-2.22	4.91	4.90
65	11.55	-0.29	0.08	0.08

^a From: CRC Handbook of Chemistry and Physics, 99th Edition, Editor-in-Chief: John R. Rumble.

Table SI.1.15 CH₃

No.	$\alpha_e / \text{Å}^3$	$\Delta / \text{Å}^3$ exp ^a : 18.04 Å ³	$\langle \Delta \rangle / \text{Å}^6$	$(\langle \Delta \rangle - \langle \Delta \rangle_{min}) / \text{Å}^6$
11	15.58	-2.46	6.06	3.21
12	16.35	-1.69	2.85	0.00
13	14.94	-3.10	9.58	6.73
21	15.22	-2.82	7.94	5.08
22	15.98	-2.06	4.23	1.37
23	14.67	-3.37	11.38	8.53
31	15.28	-2.76	7.63	4.78
32	16.00	-2.04	4.16	1.31
33	14.68	-3.36	11.30	8.44
41	14.93	-3.11	9.69	6.84
42	15.65	-2.39	5.72	2.86
43	14.43	-3.61	13.02	10.17
51	14.47	-3.57	12.72	9.87
52	15.84	-2.20	4.84	1.99
53	14.47	-3.57	12.72	9.87
61	14.87	-3.17	10.08	7.23
62	15.54	-2.50	6.24	3.39
63	14.30	-3.74	13.96	11.11

^a From: CRC Handbook of Chemistry and Physics, 99th Edition, Editor-in-Chief: John R. Rumble.

Part II – Pyridine-Haloforms Complexes

SI.2. 1 Optimised Geometries

1. Py-CHF₃

C	1.97789000	0.84663700	-0.00509600
C	3.32758200	1.17561600	-0.00840500
C	4.25952300	0.14691000	-0.00167500
C	3.80374800	-1.16455100	0.00805000
C	2.43298000	-1.38921700	0.01061900
N	1.52913300	-0.40930900	0.00422200
H	5.32193700	0.36305700	-0.00396700
H	1.21978900	1.62448600	-0.01013800
H	3.63428100	2.21437300	-0.01607200
H	4.49248500	-2.00052000	0.01355500
H	2.04090700	-2.40197800	0.01815100
C	-1.68500400	0.02457400	0.00327000
H	-0.68794800	-0.42152600	0.00561400
F	-2.38519200	-0.33159500	1.08834500
F	-2.38466700	-0.34192000	-1.07870700
F	-1.59087500	1.36599100	-0.00310600

2. Py-CHCl₃

C	2.07566100	1.00243900	-0.01115900
C	3.45061500	1.19877700	-0.01534300
C	4.27858300	0.08459000	-0.00200900
C	3.69892000	-1.17690500	0.01493000
C	2.31310600	-1.26857500	0.01777200
N	1.50965200	-0.20496000	0.00504100
H	5.35687700	0.19721800	-0.00476800
H	1.39441400	1.84811300	-0.02121100
H	3.85661400	2.20277900	-0.02876800
H	4.30392700	-2.07521600	0.02576700
H	1.82333500	-2.23771400	0.03085200
C	-1.64415700	-0.07910800	0.00303500
H	-0.56925900	-0.26581800	0.00572300
Cl	-2.33892100	-0.79886000	1.47035800
Cl	-2.33399000	-0.81364400	-1.45927600
Cl	-1.86880900	1.68791400	-0.00628500

3. Py-CHBr₃

C	2.13777100	1.04762400	-0.01598300
C	3.52137300	1.16944800	-0.01716800
C	4.28782400	0.01204800	0.00164000

C	3.64098100	-1.21632900	0.02084000
C	2.25224900	-1.23309100	0.02032800
N	1.50805600	-0.12741900	0.00232800
H	5.37064000	0.06631000	0.00137700
H	1.50285300	1.92853900	-0.03017300
H	3.98123500	2.14993100	-0.03248100
H	4.19671300	-2.14586400	0.03594300
H	1.71001400	-2.17388300	0.03503300
C	-1.63965500	-0.05149400	0.00046900
H	-0.55351300	-0.15465500	0.00031000
Br	-2.30001800	-0.92183900	1.59588700
Br	-2.29877400	-0.89830600	-1.60799000
Br	-2.01117900	1.85000900	0.01430200

4. Py-CHI₃

C	2.19077000	1.11688100	-0.03423400
C	3.57881600	1.16396400	-0.03049400
C	4.28167100	-0.03280800	0.00657500
C	3.56991800	-1.22451300	0.03831100
C	2.18239700	-1.16684800	0.03145400
N	1.50018700	-0.02261900	-0.00415300
H	5.36575600	-0.03672700	0.01073400
H	1.60335200	2.02971700	-0.06225200
H	4.09098400	2.11787800	-0.05600700
H	4.07487600	-2.18213500	0.06790700
H	1.58892100	-2.07601100	0.05578500
C	-1.61743100	-0.07778800	-0.00179000
H	-0.52540700	-0.06517800	-0.01243600
I	-2.16588400	-1.17478000	1.77259200
I	-2.20734300	-1.06621500	-1.82558600
I	-2.20501200	1.99821100	0.06825500

SI.2.2 Geometrical and Topological Parameters of [Pyr-Hal] Dimers

Table SI.2.1 Distances between Atoms and between Atoms and Critical Points (CPs). Data Reported in Units of 10^{-10} m.

Hal	$r(\text{N}\dots\text{H})$	$r(\text{H}'\dots\text{X})$	$r(\text{N}\dots\text{BCP1})$	$r(\text{H}\dots\text{BCP1})$	$r(\text{H}'\dots\text{BCP2})$	$r(\text{X}\dots\text{BCP2})$	$r(\text{N}\dots\text{RCP})$	$r(\text{H}\dots\text{RCP})$	$r(\text{X}\dots\text{RCP})$	$r(\text{H}'\dots\text{RCP})$
CHF₃	2.217	2.823	1.407	0.810	1.220	1.608	1.983	1.513	1.698	1.380
CHCl₃	2.080	3.267	1.341	0.739	1.290	1.979	1.988	1.616	2.033	1.441
CHBr₃	2.062	3.515	1.333	0.729	1.354	2.162	2.053	1.699	2.193	1.467
CHI₃	2.026	3.811	1.314	0.712	1.410	2.403	2.109	1.826	2.414	1.485

SI.2.3 Vibrational Frequencies, Normal Modes Decomposition, and Electric Properties of [Pyr-Hal] Dimers

Table SI.2.2 Computed Ring Breathing (ω_1) and Triangle Mode (ω_2) Vibrational Frequencies (in harmonic and anharmonic approximation), Percentage Contribution of Selected Bond Distances to ω_1 , Modulus of the Electric Dipole Moment (p), and Isotropic Static Electronic Polarizability (α_e).

Hal	$\omega_1 / \text{cm}^{-1}$	$\omega_2 / \text{cm}^{-1}$	$\omega_1 / \text{cm}^{-1}$	$\omega_2 / \text{cm}^{-1}$	% Contribution of Internal Coordinates to ω_1						p / D	$\alpha_e / \text{\AA}^3$	
	(harm.)	(harm.)	(anharm.)	(anharm.)	$r(1,2)$	$r(4,5)$	$r(1,6)$	$r(5,6)$	$r(2,3)$	$r(3,4)$			$r(6,13)$
CHF₃	1028.34	1059.84	1010.62	1093.41	7.9	7.7	4.9	4.8	3.2	3.1	7.5	4.91	66.44
CHCl₃	1031.17	1061.15	1012.96	1039.64	8.5	8.2	4.9	4.8	3.2	3.1	8.4	4.77	121.95
CHBr₃	1031.81	1060.74	1013.40	1012.44	8.7	8.3	4.8	4.8	3.3	3.2	8.5	4.72	135.93
CHI₃	1032.62	1060.56	1014.01	999.15	8.8	8.4	4.8	4.8	3.3	3.2	8.8	4.68	167.73

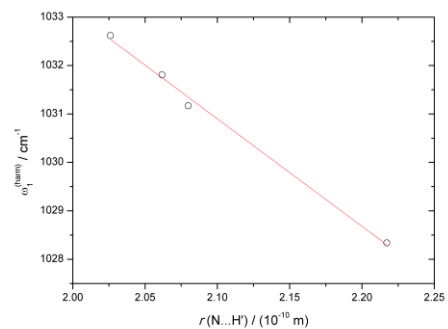
Table SI.2.3 Statistical Parameters of Linear Regression of the Ring Breathing Wavenumber (Computed in Harmonic and Anharmonic Approximation) with Geometrical and Topological Parameters, Contribution of Selected Internal Coordinates to Normal Mode, and Electric Properties.

#	x	<i>Harmonic Approximation</i>					<i>Anharmonic Approximation</i>				
		Intercept		Slope		Adj-R^2	Intercept		Slope		Adj-R^2
		Value	Error	Value	Error		Value	Error	Value	Error	
1	$r(\text{N}\dots\text{H}')$	1077.50	2.13	-22.19	1.02	0.99374	1049.86	0.94	-17.71	0.45	0.99807
2	$r(\text{H}\dots\text{X})$	1016.48	2.48	4.33	0.73	0.91820	1001.28	2.22	3.42	0.66	0.89635
3	$r(\text{N}\dots\text{BCP1})$	1092.97	2.68	-45.97	1.99	0.99443	1062.19	1.32	-36.67	0.98	0.99786
4	$r(\text{H}\dots\text{BCP1})$	1063.05	1.62	-42.89	2.17	0.99237	1038.34	0.74	-34.23	0.98	0.99752
5	$r(\text{X}\dots\text{BCP2})$	1002.64	6.65	21.50	5.04	0.85161	990.40	5.79	16.95	4.39	0.82284
6	$r(\text{H}'\dots\text{BCP2})$	1019.95	1.76	5.41	0.86	0.92848	1004.02	1.59	4.28	0.77	0.90818
7	$r(\text{N}\dots\text{RCP})$	980.41	27.07	24.88	13.31	0.45393	973.41	22.43	19.35	11.03	0.40919
8	$r(\text{H}\dots\text{RCP})$	1009.31	6.24	13.03	3.74	0.78732	995.69	5.33	10.25	3.20	0.75580
9	$r(\text{X}\dots\text{RCP})$	1018.41	2.01	6.03	0.96	0.92829	1002.80	1.81	4.77	0.86	0.90814
10	$r(\text{H}'\dots\text{RCP})$	972.64	4.05	40.43	2.81	0.98568	966.40	4.13	32.11	2.86	0.97659
11	$r(\text{N}\dots\text{BCP1})/r(\text{N}\dots\text{H}')$	839.04	10.32	298.30	16.04	0.99138	859.54	5.02	238.08	7.79	0.99679
12	$r(\text{H}'\dots\text{BCP1})/r(\text{N}\dots\text{H}')$	1137.36	5.72	-298.38	16.03	0.99139	1097.65	2.78	-238.15	7.80	0.99679
13	$r(\text{H}\dots\text{BCP2})/r(\text{H}\dots\text{X})$	1058.74	1.51	-70.17	3.80	0.99125	1034.81	1.62	-55.77	4.09	0.98407
14	$r(\text{X}\dots\text{BCP2})/r(\text{H}\dots\text{X})$	987.69	2.71	71.53	4.48	0.98832	978.35	2.82	56.83	4.65	0.98016

15	% $r(1,2)$	992.00	2.25	4.60	0.27	0.99009	981.70	1.92	3.66	0.23	0.98868
16	% $r(4,5)$	982.31	2.14	5.97	0.26	0.99424	973.92	1.07	4.76	0.13	0.99775
17	% $r(6,13)$	1003.46	1.33	3.32	0.16	0.99303	990.81	0.89	2.64	0.11	0.99506
18	p	1118.28	4.41	-18.30	0.93	0.99237	1082.14	4.80	-14.55	1.01	0.98580
19	α_e	1025.64	0.62	0.04	0.00	0.96349	1008.51	0.57	0.03	0.00	0.95123

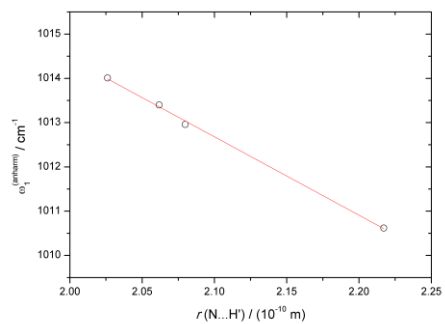
SI.2.4 Regressions

Harmonic Approximation

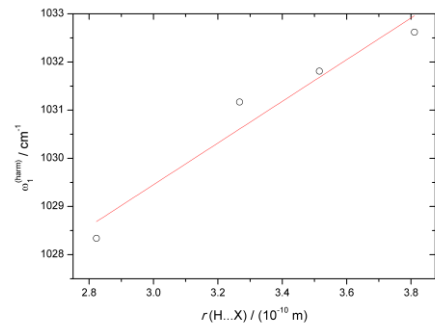


(1.h)

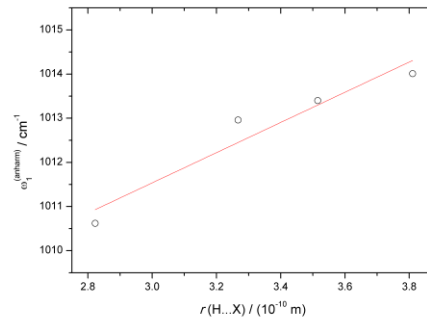
Anharmonic Approximation



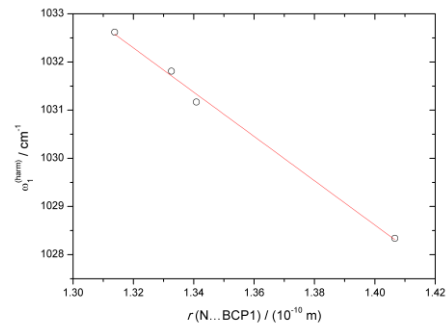
(1.a)



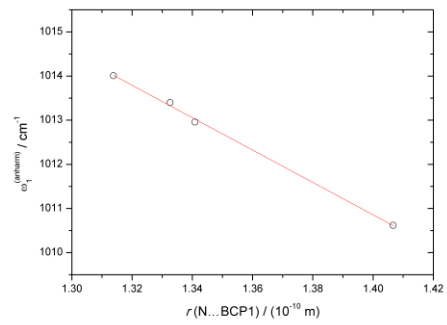
(2.h)



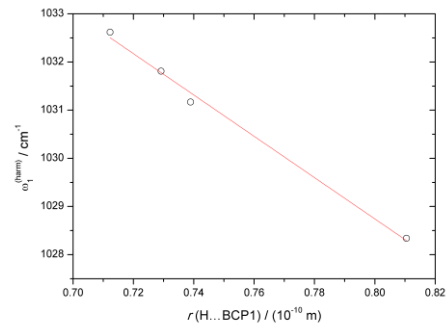
(2.a)



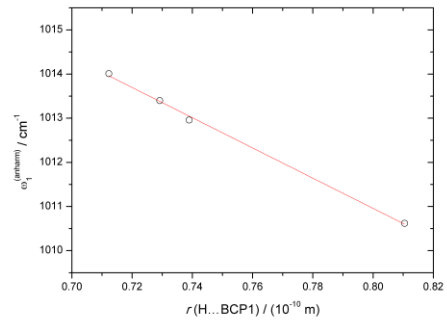
(3.h)



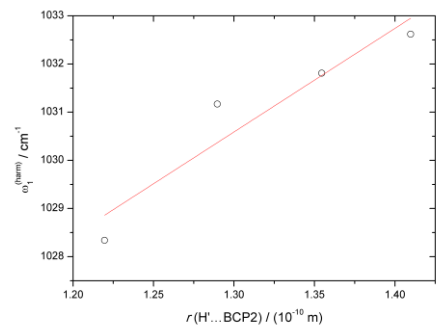
(3.a)



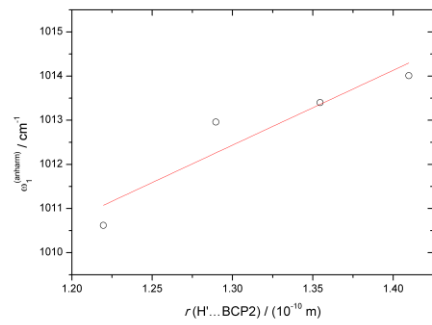
(4.h)



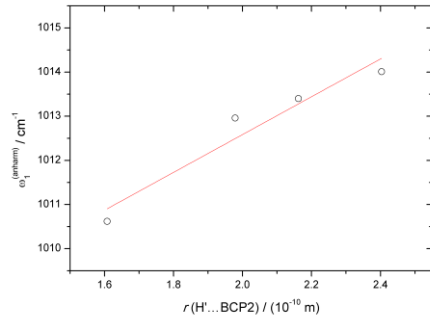
(4.a)



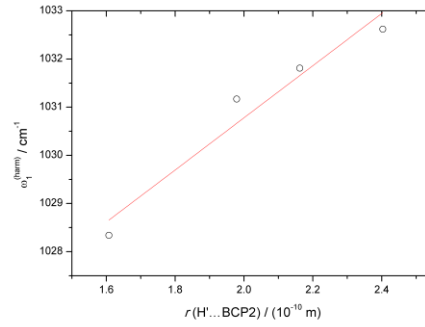
(5.h)



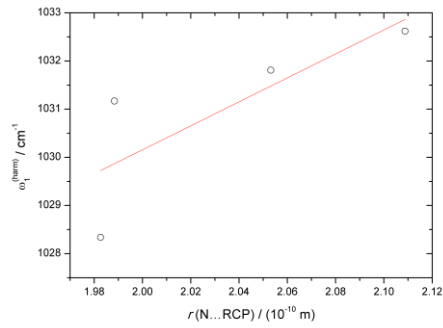
(5.a)



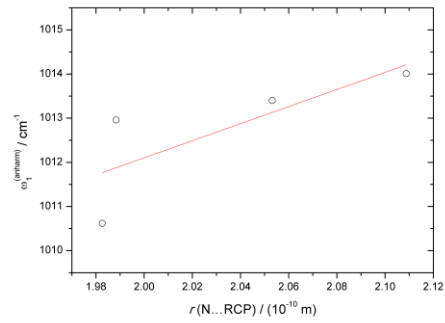
(6.h)



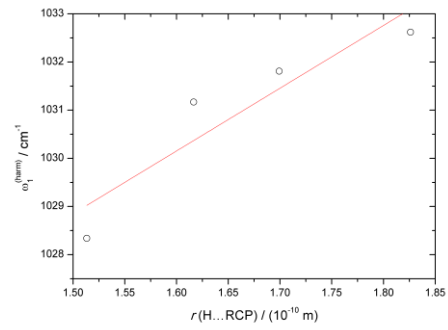
(6.a)



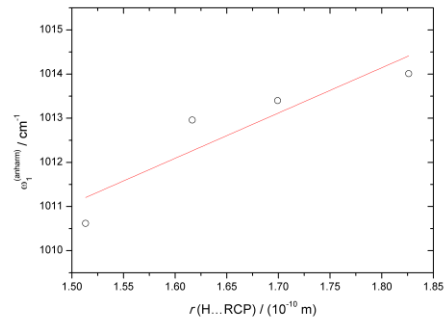
(7.h)



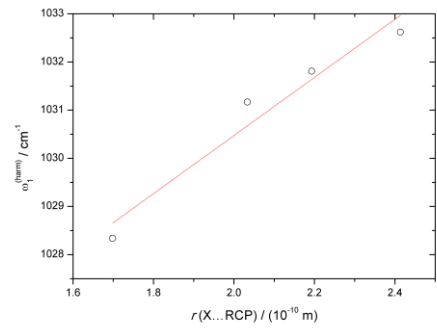
(7.a)



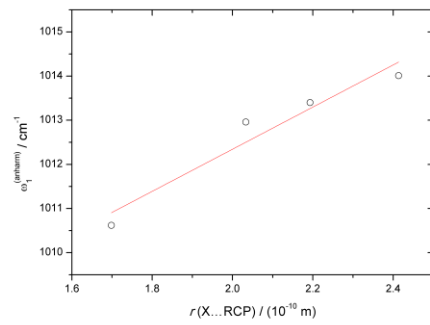
(8.h)



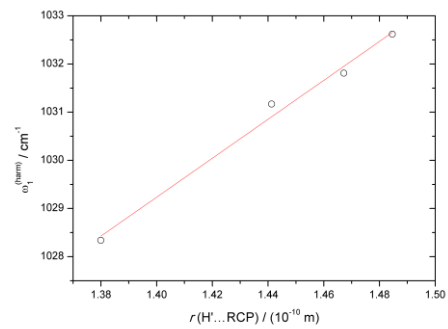
(8.a)



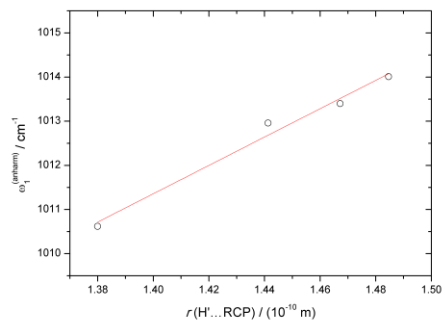
(9.h)



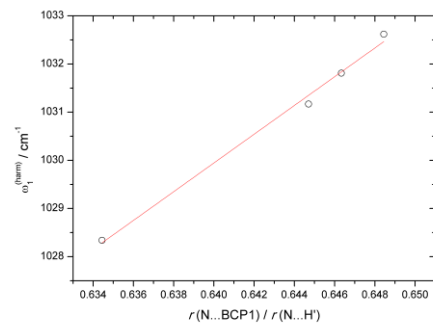
(9.a)



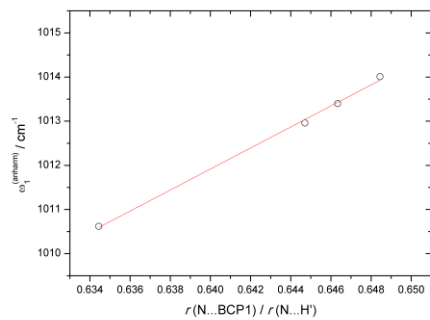
(10.h)



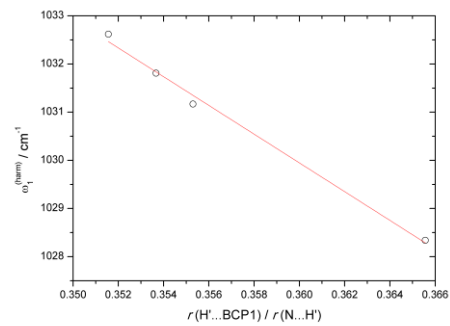
(10.a)



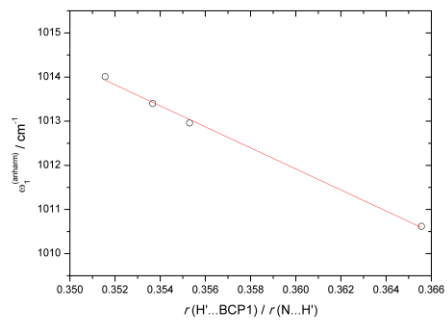
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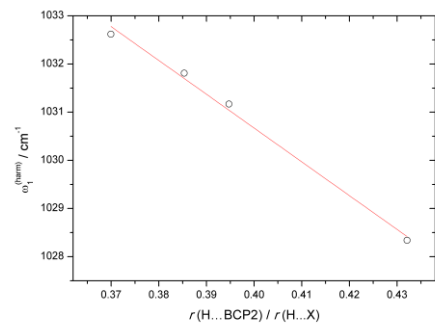
(11.a)



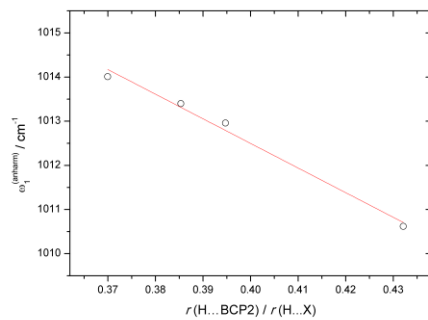
(12.h)



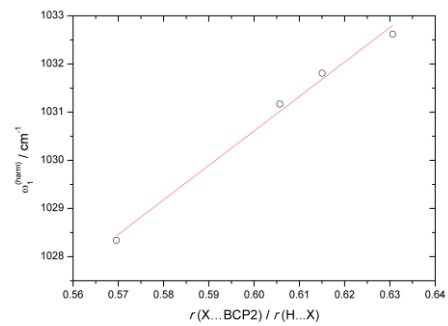
(12.a)



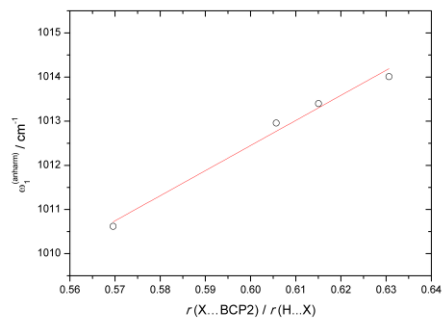
(13.h)



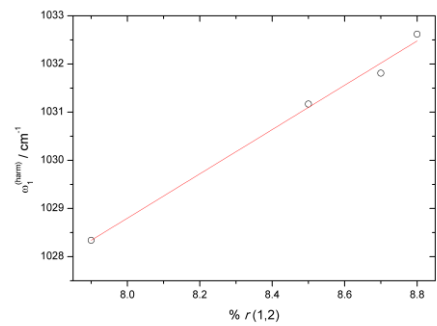
(13.a)



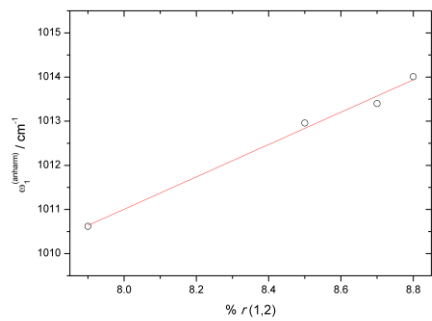
(14.h)



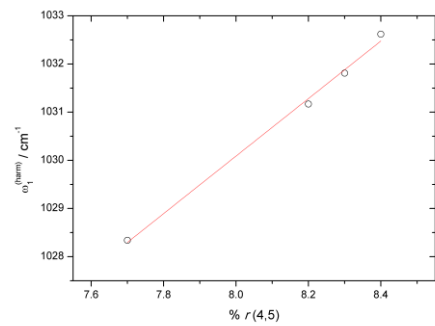
(14.a)



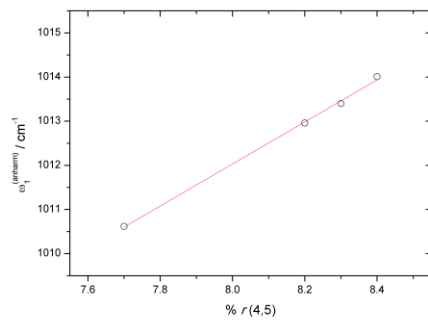
(15.h)



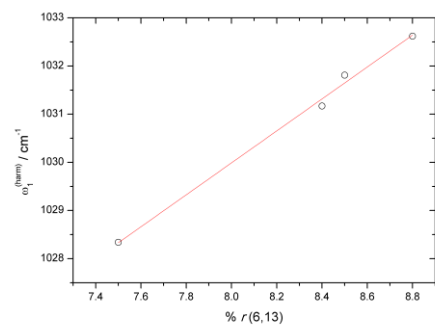
(15.a)



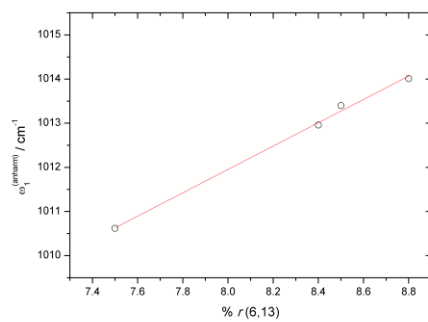
(16.h)



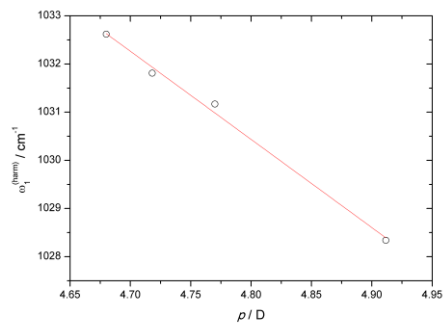
(16.a)



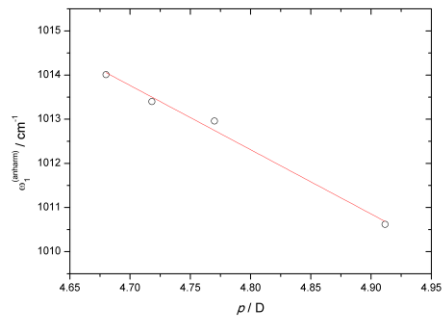
(17.h)



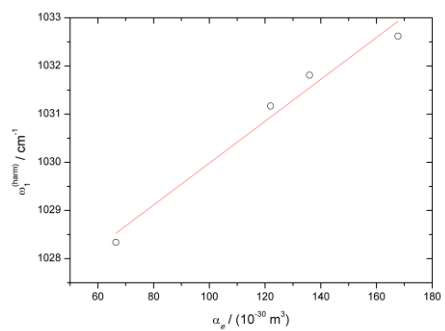
(17.a)



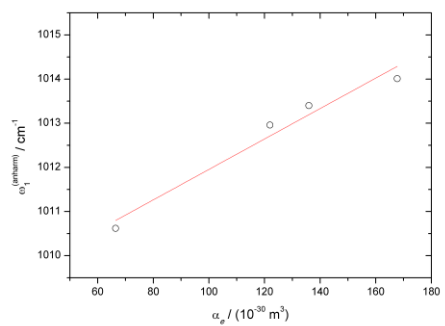
(18.h)



(18.a)



(19.h)



(19.a)

Figure SI.2.1 Regressions of the Ring Breathing Wavenumber (Computed in Harmonic and Anharmonic Approximation) with Geometrical and Topological Parameters, Contribution of Selected Internal Coordinates to Normal Mode, and Electric Properties.

SI.2.5 Geometrical , Charges of [Pyr–Hal] Dimers at MP2 / 6-311++G(d,p) (H, C, N) & DGDZVP (X)

Table SI.2.4 Analysis of geometrical parameters. (Distances B in 10⁻¹⁰ m; bond angles A and dihedral angles D in degrees.)

py-CHF ₃				r		a		b1		b2		c	
				*	**	*	**	*	**	*	**	*	**
B	1	2		1.397426	1.397567	1.397437	1.397448	1.398390	1.397564	1.398319	1.397433	1.398289	1.398355
B	1	6		1.346013	1.345721	1.345227	1.345254	1.344141	1.345727	1.344189	1.345123	1.343788	1.344057
B	1	8		1.087431	1.087737	1.087686	1.087623	1.087788	1.087737	1.087846	1.087484	1.087991	1.087846
B	2	3		1.396218	1.396235	1.396356	1.396294	1.396574	1.396233	1.396506	1.396353	1.396607	1.396513
B	2	9		1.085462	1.085464	1.085456	1.085463	1.085758	1.085464	1.085766	1.085494	1.085795	1.085768
B	3	4		1.396425	1.396353	1.396356	1.396294	1.396419	1.396353	1.396506	1.396234	1.396607	1.396512
B	3	7		1.086080	1.086054	1.086066	1.086036	1.086235	1.086055	1.086238	1.086055	1.086276	1.086254
B	4	5		1.397432	1.397434	1.397437	1.397448	1.398233	1.397434	1.398318	1.397567	1.398289	1.398355
B	4	10		1.085494	1.085494	1.085455	1.085463	1.085771	1.085494	1.085765	1.085464	1.085795	1.085768
B	5	6		1.345177	1.345121	1.345227	1.345254	1.344222	1.345123	1.344189	1.345720	1.343789	1.344057
B	5	11		1.087497	1.087483	1.087687	1.087625	1.087902	1.087484	1.087847	1.087736	1.087990	1.087847
B	12	13		1.088305	1.088475	1.089724	1.089200	1.337935	1.346596	1.337872	1.346591	1.089979	1.089081
B	12	14		1.346494	1.346588	1.346812	1.348037	1.089234	1.088477	1.344132	1.350111	1.342343	1.342219
B	12	15		1.346492	1.346588	1.346812	1.348002	1.344099	1.350129	1.344132	1.346592	1.342336	1.342215
B	12	16		1.351725	1.350124	1.346115	1.347570	1.343968	1.346581	1.089220	1.088476	1.341251	1.341950
A	1	2	3	118.7	118.7	118.7	118.7	118.7	118.7	118.6	118.7	118.6	118.6
A	1	2	9	120.0	120.0	120.0	120.0	120.1	120.0	120.1	120.0	120.1	120.1
A	2	3	4	118.3	118.3	118.4	118.3	118.3	118.3	118.3	118.3	118.3	118.3
A	2	3	7	120.8	120.8	120.8	120.8	120.9	120.8	120.9	120.8	120.9	120.9
A	3	4	5	118.7	118.7	118.7	118.7	118.6	118.7	118.6	118.7	118.6	118.6
A	3	4	10	121.3	121.3	121.3	121.3	121.2	121.3	121.2	121.3	121.2	121.2
A	4	5	6	123.6	123.6	123.6	123.6	123.9	123.6	123.9	123.6	123.8	123.8

A	4	5	11		120.4	120.4	120.4	120.4	120.3	120.4	120.4	120.5	120.5	120.4
D	1	2	3	4	0.0	0.0	0.2	0.1	0.0	0.0	0.0	0.0	0.1	0.0
D	1	2	3	7	180.0	180.0	180.0	180.0	180.0	180.0	180.0	180.0	179.9	180.0
D	2	3	4	5	0.0	0.0	0.2	0.1	0.0	0.0	0.1	0.0	0.2	0.0
D	2	3	4	10	180.0	180.0	180.0	180.0	180.0	180.0	179.9	180.0	180.0	180.0
D	3	4	5	6	0.0	0.0	0.2	0.0	0.0	0.0	0.1	0.0	0.3	0.0
D	3	4	5	11	180.0	180.0	180.0	180.0	179.9	180.0	179.9	180.0	180.0	180.0

py-CHCl ₃				r		a		b1		b2		c	
				*	**	*	**	*	**	*	**	*	**
B	1	2		1.397153	1.397438	1.397113	1.397383	1.397927	1.397388	1.397726	1.397384	1.398106	1.398323
B	1	6		1.345277	1.345510	1.344724	1.345169	1.344130	1.345169	1.344224	1.345169	1.343118	1.343878
B	1	8		1.087446	1.087519	1.087632	1.087602	1.087894	1.087603	1.087879	1.087600	1.088184	1.088036
B	2	3		1.396484	1.396348	1.396561	1.396382	1.396599	1.396379	1.396721	1.396381	1.396772	1.396592
B	2	9		1.085453	1.085477	1.085432	1.085472	1.085652	1.085473	1.085661	1.085471	1.085862	1.085775
B	3	4		1.396531	1.396372	1.396558	1.396382	1.396551	1.396382	1.396453	1.396381	1.396777	1.396591
B	3	7		1.086067	1.086056	1.086060	1.086050	1.086174	1.086049	1.086186	1.086051	1.086247	1.086243
B	4	5		1.397183	1.397374	1.397115	1.397382	1.397784	1.397381	1.398034	1.397384	1.398095	1.398323
B	4	10		1.085466	1.085483	1.085431	1.085471	1.085671	1.085474	1.085660	1.085471	1.085863	1.085774
B	5	6		1.344743	1.345123	1.344722	1.345169	1.344210	1.345166	1.344086	1.345169	1.343135	1.343876
B	5	11		1.087571	1.087548	1.087633	1.087602	1.087933	1.087598	1.087919	1.087600	1.088178	1.088037
B	12	13		1.089398	1.088720	1.090228	1.088983	1.768573	1.088960	1.769071	1.088936	1.084854	1.085177
B	12	14		1.768252	1.768444	1.773217	1.769849	1.084867	1.770270	1.773323	1.769806	1.771530	1.766993
B	12	15		1.768248	1.768441	1.773215	1.769866	1.773488	1.769755	1.773329	1.769823	1.771531	1.766985
B	12	16		1.771649	1.771921	1.772264	1.769038	1.773456	1.769095	1.084837	1.769001	1.770176	1.764927
A	1	2	3	118.7	118.7	118.7	118.7	118.7	118.7	118.7	118.7	118.6	118.6
A	1	2	9	120.0	120.0	120.0	120.0	120.1	120.0	120.1	120.0	120.2	120.1

A	2	3	4	118.4	118.4	118.4	118.4	118.3	118.4	118.3	118.4	118.3	118.3	
A	2	3	7	120.8	120.8	120.8	120.8	120.8	120.8	120.8	120.8	120.9	120.9	
A	3	4	5	118.7	118.7	118.7	118.7	118.6	118.7	118.6	118.7	118.6	118.6	
A	3	4	10	121.3	121.3	121.3	121.3	121.3	121.3	121.3	121.3	121.2	121.2	
A	4	5	6	123.5	123.6	123.4	123.5	123.7	123.5	123.7	123.5	123.8	123.8	
A	4	5	11	120.6	120.5	120.7	120.5	120.5	120.5	120.5	120.5	120.6	120.5	
D	1	2	3	4	0.0	0.0	0.1	0.1	0.0	0.1	0.2	0.0	0.3	0.2
D	1	2	3	7	180.0	180.0	180.0	180.0	180.0	180.0	180.0	180.0	179.8	180.0
D	2	3	4	5	0.0	0.0	0.1	0.1	0.0	0.1	0.2	0.0	0.1	0.2
D	2	3	4	10	180.0	180.0	180.0	180.0	180.0	180.0	179.9	180.0	179.9	180.0
D	3	4	5	6	0.0	0.0	0.1	0.1	0.0	0.0	0.1	0.0	0.1	0.1
D	3	4	5	11	180.0	180.0	179.9	180.0	180.0	180.0	180.0	180.0	180.0	180.0

py-CHBr ₃			r		a		b1		b2		c	
			*	**	*	**	*	**	*	**	*	**
B	1	2	1.397173	1.397423	1.397056	1.397324	1.397518	1.397601	1.397436	1.397685	1.398074	1.398273
B	1	6	1.345497	1.345524	1.344897	1.345191	1.344006	1.344584	1.344072	1.344500	1.343480	1.343954
B	1	8	1.087343	1.087511	1.087680	1.087629	1.087858	1.087968	1.087869	1.087805	1.088153	1.088076
B	2	3	1.396536	1.396414	1.396619	1.396445	1.396708	1.396546	1.396658	1.396564	1.396764	1.396639
B	2	9	1.085523	1.085488	1.085432	1.085471	1.085563	1.085582	1.085565	1.085590	1.085880	1.085794
B	3	4	1.396584	1.396430	1.396613	1.396444	1.396634	1.396503	1.396682	1.396564	1.396767	1.396638
B	3	7	1.086076	1.086070	1.086061	1.086057	1.086107	1.086126	1.086111	1.086122	1.086242	1.086244
B	4	5	1.397181	1.397351	1.397064	1.397323	1.397323	1.397751	1.397392	1.397684	1.398064	1.398273
B	4	10	1.085518	1.085489	1.085432	1.085471	1.085578	1.085606	1.085574	1.085590	1.085880	1.085794
B	5	6	1.344909	1.345140	1.344886	1.345191	1.344127	1.344548	1.344129	1.344501	1.343488	1.343952
B	5	11	1.087693	1.087628	1.087683	1.087628	1.087850	1.087612	1.087854	1.087809	1.088149	1.088074
B	12	13	1.090153	1.089965	1.092994	1.090839	1.948178	1.934244	1.948372	1.934570	1.084916	1.084800
B	12	14	1.936696	1.938887	1.943762	1.938584	1.085357	1.085301	1.944747	1.945059	1.942856	1.936469

B	12	15		1.934986	1.933927	1.943769	1.938597	1.944659	1.942360	1.944739	1.945116	1.942857	1.936462	
B	12	16		1.941688	1.942695	1.942631	1.937585	1.944562	1.945300	1.085335	1.085290	1.941611	1.934312	
A	1	2	3	118.8	118.7	118.7	118.7	118.7	118.7	118.7	118.7	118.6	118.6	
A	1	2	9	120.0	120.0	120.0	120.0	120.1	120.1	120.1	120.1	120.1	120.1	
A	2	3	4	118.4	118.4	118.4	118.4	118.4	118.4	118.4	118.4	118.3	118.3	
A	2	3	7	120.8	120.8	120.8	120.8	120.8	120.8	120.8	120.8	120.9	120.9	
A	3	4	5	118.7	118.7	118.7	118.7	118.7	118.7	118.7	118.7	118.6	118.6	
A	3	4	10	121.3	121.3	121.3	121.3	121.2	121.3	121.2	121.2	121.2	121.2	
A	4	5	6	123.5	123.5	123.4	123.5	123.5	123.6	123.5	123.6	123.8	123.8	
A	4	5	11	120.6	120.5	120.7	120.6	120.7	120.5	120.7	120.6	120.5	120.5	
D	1	2	3	4	0.5	0.5	1.3	0.2	0.1	0.4	0.1	0.4	0.1	0.1
D	1	2	3	7	180.0	180.0	179.9	180.0	180.0	180.0	180.0	180.0	179.8	180.0
D	2	3	4	5	0.3	0.5	1.2	0.2	0.1	0.4	0.1	0.4	0.0	0.1
D	2	3	4	10	180.0	180.0	179.8	180.0	180.0	180.0	180.0	180.0	179.9	180.0
D	3	4	5	6	0.3	0.5	0.8	0.1	0.1	0.3	0.1	0.4	0.2	0.0
D	3	4	5	11	179.9	180.0	179.7	179.9	179.9	179.9	179.9	179.9	179.9	180.0

py-CHI ₃			r		a		b1		b2		c	
			*	**	*	**	*	**	*	**	*	**
B	1	2	1.397178	1.397357	1.396995	1.397293	1.396617	1.397092	1.396561	1.397157	1.397840	1.398127
B	1	6	1.344615	1.345192	1.344820	1.345311	1.343929	1.344435	1.343911	1.344505	1.344146	1.344480
B	1	8	1.087501	1.087571	1.087699	1.087629	1.087682	1.087904	1.087672	1.087714	1.087706	1.087842
B	2	3	1.396663	1.396460	1.396677	1.396483	1.396839	1.396626	1.396789	1.396657	1.396638	1.396535
B	2	9	1.085498	1.085483	1.085453	1.085478	1.085434	1.085470	1.085434	1.085476	1.085903	1.085790
B	3	4	1.396732	1.396526	1.396702	1.396485	1.396723	1.396606	1.396808	1.396657	1.396577	1.396527
B	3	7	1.086061	1.086063	1.086052	1.086065	1.085982	1.086038	1.085985	1.086034	1.086210	1.086229
B	4	5	1.396820	1.397219	1.396959	1.397292	1.396479	1.397238	1.396539	1.397156	1.397815	1.398133

B	4	10		1.085467	1.085471	1.085454	1.085478	1.085440	1.085496	1.085436	1.085475	1.085901	1.085789	
B	5	6		1.345025	1.345292	1.344936	1.345312	1.344000	1.344654	1.343977	1.344507	1.344145	1.344469	
B	5	11		1.087895	1.087750	1.087695	1.087630	1.087638	1.087512	1.087668	1.087718	1.087661	1.087831	
B	12	13		1.095072	1.093483	1.096559	1.093477	2.196962	2.174957	2.197152	2.176082	1.086063	1.086152	
B	12	14		2.165787	2.167671	2.178314	2.167869	1.087126	1.086954	2.178803	2.180847	2.178149	2.167109	
B	12	15		2.165392	2.167121	2.178322	2.167858	2.178816	2.178087	2.178803	2.180888	2.178190	2.167097	
B	12	16		2.167597	2.167533	2.177142	2.166684	2.179013	2.181034	1.087092	1.086940	2.178509	2.166822	
A	1	2	3	118.7	118.7	118.7	118.7	118.7	118.7	118.7	118.7	118.7	118.7	
A	1	2	9	120.0	120.0	120.0	120.0	120.0	120.0	120.0	120.0	120.0	120.1	
A	2	3	4	118.5	118.4	118.5	118.4	118.5	118.4	118.5	118.5	118.2	118.2	
A	2	3	7	120.8	120.8	120.8	120.8	120.8	120.8	120.8	120.8	120.9	120.9	
A	3	4	5	118.7	118.7	118.7	118.7	118.7	118.7	118.7	118.7	118.7	118.7	
A	3	4	10	121.3	121.3	121.3	121.3	121.3	121.3	121.3	121.3	121.2	121.2	
A	4	5	6	123.3	123.5	123.3	123.5	123.1	123.3	123.1	123.3	123.8	123.8	
A	4	5	11	120.7	120.6	120.8	120.6	121.0	120.7	121.1	120.8	120.5	120.5	
D	1	2	3	4	0.1	0.0	1.2	0.3	0.3	0.4	0.2	0.6	0.6	0.1
D	1	2	3	7	180.0	180.0	179.9	180.0	180.0	180.0	180.0	180.0	179.7	179.9
D	2	3	4	5	0.1	0.0	1.1	0.3	0.3	0.4	0.2	0.6	0.9	0.1
D	2	3	4	10	180.0	180.0	179.8	180.0	180.0	180.0	179.9	180.0	179.9	180.0
D	3	4	5	6	0.0	0.0	0.7	0.2	0.2	0.4	0.1	0.6	1.2	0.1
D	3	4	5	11	180.0	180.0	179.6	179.8	180.0	179.9	180.0	179.9	179.6	180.0

Table SI.2.5 Charges (Mul = Mulliken Population; NPA = Natural Population Analysis; ESP)

			*			**			***			****		
			Mul	NPA	ESP	Mul	NPA	ESP	Mul	NPA	ESP	Mul	NPA	ESP
pyr	1	C	-0.384	0.025	0.451	-0.059	0.028	0.432	0.213	0.020	0.425	0.239	0.012	0.427
	2	C	0.063	-0.222	-0.378	-0.312	-0.226	-0.374	-0.718	-0.234	-0.383	-0.237	-0.228	-0.369
	3	C	-0.229	-0.183	0.212	-0.099	-0.185	0.203	0.306	-0.193	0.201	0.234	-0.190	0.206
	4	C	0.063	-0.222	-0.394	-0.312	-0.226	-0.386	-0.718	-0.234	-0.393	-0.234	-0.228	-0.378
	5	C	-0.384	0.025	0.462	-0.059	0.028	0.441	0.213	0.020	0.432	0.241	0.012	0.433
	6	N	-0.055	-0.410	-0.651	-0.245	-0.419	-0.635	-0.717	-0.423	-0.631	-0.693	-0.398	-0.627
	7	H	0.192	0.205	0.044	0.237	0.208	0.048	0.289	0.216	0.053	0.061	0.213	0.045
	8	H	0.187	0.183	-0.005	0.206	0.185	0.002	0.307	0.195	0.009	0.063	0.189	0.002
	9	H	0.180	0.208	0.131	0.218	0.211	0.133	0.259	0.219	0.139	0.134	0.214	0.130
	10	H	0.180	0.208	0.137	0.218	0.211	0.137	0.259	0.219	0.143	0.128	0.214	0.133
	11	H	0.187	0.183	-0.009	0.206	0.185	-0.001	0.307	0.195	0.006	0.065	0.189	-0.001
CHF ₃	1	C	0.614	0.890	0.660	0.362	0.860	0.568	0.223	0.856	0.631	-0.288	0.801	0.504
	2	H	0.075	0.097	0.048	0.049	0.095	0.061	0.252	0.103	0.050	0.491	0.092	0.072
	3	F	-0.230	-0.329	-0.236	-0.137	-0.318	-0.210	-0.158	-0.320	-0.227	-0.068	-0.298	-0.192
	4	F	-0.230	-0.329	-0.236	-0.137	-0.318	-0.210	-0.158	-0.320	-0.227	-0.068	-0.298	-0.192
	5	F	-0.230	-0.329	-0.236	-0.137	-0.318	-0.209	-0.158	-0.320	-0.227	-0.068	-0.298	-0.192
CHCl ₃	1	C	-0.391	-0.350	-0.059	-0.560	-0.398	-0.172	-0.849	-0.414	-0.253	-0.804	-0.459	-0.257
	2	H	0.204	0.189	0.190	0.192	0.192	0.213	0.395	0.208	0.235	0.303	0.190	0.236
	3	Cl	0.062	0.054	-0.044	0.123	0.069	-0.014	0.151	0.069	0.006	0.167	0.090	0.007
	4	Cl	0.062	0.054	-0.044	0.123	0.069	-0.013	0.151	0.069	0.006	0.167	0.090	0.007
	5	Cl	0.062	0.054	-0.044	0.123	0.069	-0.014	0.151	0.069	0.006	0.167	0.090	0.007
CHBr ₃	1	C	-0.244	-0.595		-0.318	-0.645		-0.628	-0.659		-0.684	-0.677	

	2	H	0.208	0.194	0.143	0.198	0.394	0.213	0.156	0.188
	3	Br	0.012	0.134	0.058	0.149	0.078	0.148	0.176	0.163
	4	Br	0.012	0.134	0.058	0.149	0.078	0.148	0.176	0.163
	5	Br	0.012	0.134	0.058	0.149	0.078	0.148	0.176	0.163
CHI ₃	1	C	-0.441	-0.934	-0.484	-0.986	-0.771	-1.012	-1.016	-1.029
	2	H	0.210	0.196	0.140	0.196	0.354	0.212	0.341	0.178
	3	I	0.077	0.246	0.115	0.264	0.139	0.266	0.225	0.284
	4	I	0.077	0.246	0.115	0.264	0.139	0.266	0.225	0.284
	5	I	0.077	0.246	0.115	0.264	0.139	0.266	0.225	0.284

py-CHF ₃							py-CHCl ₃								
Mul		r				ESP		Mul		r				ESP	
#	##	#	##	#	##	#	##	#	##	#	##	#	##		
C	-0.434	-0.375	0.024	0.025	0.214	0.214	C	-0.331	-0.310	0.030	0.029	0.199	0.211		
C	0.059	-0.006	-0.214	-0.215	-0.191	-0.190	C	-0.026	-0.052	-0.213	-0.214	-0.183	-0.188		
C	-0.278	-0.254	-0.178	-0.178	0.027	0.033	C	-0.282	-0.271	-0.178	-0.178	0.030	0.027		
C	-0.002	-0.034	-0.216	-0.216	-0.176	-0.184	C	-0.076	-0.080	-0.214	-0.215	-0.171	-0.176		
C	-0.257	-0.242	0.029	0.029	0.192	0.202	C	-0.236	-0.236	0.033	0.031	0.166	0.174		
N	-0.048	-0.043	-0.440	-0.438	-0.366	-0.371	N	-0.015	-0.012	-0.445	-0.442	-0.331	-0.357		
H	0.195	0.196	0.207	0.207	0.082	0.080	H	0.195	0.195	0.208	0.207	0.079	0.082		
H	0.186	0.173	0.192	0.190	0.034	0.034	H	0.166	0.170	0.191	0.189	0.031	0.028		
H	0.202	0.201	0.212	0.212	0.113	0.111	H	0.205	0.203	0.212	0.212	0.111	0.112		
H	0.199	0.198	0.211	0.211	0.102	0.104	H	0.205	0.203	0.212	0.211	0.106	0.108		
H	0.181	0.180	0.185	0.185	0.047	0.046	H	0.164	0.166	0.187	0.186	0.050	0.050		
C	0.498	0.491	0.865	0.866	0.828	0.818	C	-0.444	-0.433	-0.363	-0.361	-0.033	-0.033		
H	0.230	0.241	0.144	0.142	-0.069	-0.066	H	0.372	0.347	0.242	0.237	0.146	0.156		

F	-0.240	-0.240	-0.337	-0.338	-0.283	-0.281	Cl	0.039	0.040	0.036	0.039	-0.069	-0.068
F	-0.240	-0.240	-0.337	-0.338	-0.283	-0.281	Cl	0.039	0.040	0.036	0.039	-0.070	-0.068
F	-0.251	-0.247	-0.345	-0.343	-0.271	-0.268	Cl	0.028	0.031	0.028	0.031	-0.060	-0.058

a							a						
Mul		NPA		ESP		Mul		NPA		ESP			
#	##	#	##	#	##	#	##	#	##	#	##		
C	-0.255	-0.255	0.029	0.028	0.157	0.181	C	-0.254	-0.255	0.033	0.031	0.199	0.201
C	-0.099	-0.098	-0.215	-0.215	-0.176	-0.198	C	-0.089	-0.092	-0.213	-0.214	-0.179	-0.182
C	-0.228	-0.226	-0.178	-0.178	0.034	0.050	C	-0.280	-0.271	-0.177	-0.178	0.032	0.033
C	-0.099	-0.098	-0.215	-0.215	-0.175	-0.199	C	-0.089	-0.092	-0.213	-0.214	-0.186	-0.182
C	-0.255	-0.256	0.029	0.028	0.161	0.178	C	-0.254	-0.255	0.033	0.031	0.206	0.201
N	-0.035	-0.037	-0.437	-0.438	-0.306	-0.322	N	-0.009	-0.002	-0.446	-0.442	-0.369	-0.367
H	0.196	0.196	0.208	0.208	0.079	0.077	H	0.195	0.195	0.208	0.208	0.081	0.078
H	0.172	0.173	0.186	0.186	0.058	0.051	H	0.163	0.165	0.188	0.187	0.038	0.037
H	0.200	0.200	0.211	0.212	0.108	0.113	H	0.206	0.203	0.212	0.212	0.108	0.108
H	0.200	0.200	0.211	0.212	0.107	0.114	H	0.206	0.203	0.212	0.212	0.110	0.108
H	0.172	0.173	0.186	0.186	0.056	0.053	H	0.163	0.165	0.188	0.187	0.036	0.037
C	0.469	0.468	0.863	0.863	0.918	0.908	C	-0.461	-0.444	-0.357	-0.362	-0.026	-0.001
H	0.281	0.284	0.139	0.144	-0.123	-0.115	H	0.397	0.362	0.245	0.237	0.173	0.147
F	-0.240	-0.241	-0.339	-0.340	-0.298	-0.297	Cl	0.035	0.038	0.029	0.035	-0.073	-0.072
F	-0.240	-0.241	-0.339	-0.340	-0.298	-0.296	Cl	0.035	0.038	0.029	0.035	-0.074	-0.072
F	-0.240	-0.241	-0.338	-0.339	-0.301	-0.299	Cl	0.037	0.040	0.031	0.037	-0.077	-0.075

b1							b1						
Mul		NPA		ESP		Mul		NPA		ESP			
#	##	#	##	#	##	#	##	#	##	#	##		
C	-0.340	-0.375	0.026	0.025	0.288	0.218	C	-0.359	-0.255	0.028	0.030	0.181	0.219
C	-0.016	-0.006	-0.222	-0.215	-0.266	-0.204	C	-0.003	-0.092	-0.219	-0.214	-0.195	-0.193
C	-0.200	-0.254	-0.183	-0.178	0.099	0.046	C	-0.197	-0.271	-0.181	-0.178	0.040	0.033
C	-0.015	-0.034	-0.223	-0.216	-0.263	-0.192	C	0.005	-0.091	-0.220	-0.214	-0.193	-0.185
C	-0.332	-0.242	0.025	0.029	0.296	0.203	C	-0.366	-0.255	0.028	0.031	0.198	0.214

N	-0.018	-0.043	-0.406	-0.438	-0.468	-0.374	N	0.020	-0.002	-0.419	-0.442	-0.321	-0.387
H	0.193	0.196	0.204	0.207	0.064	0.077	H	0.195	0.195	0.205	0.208	0.075	0.081
H	0.186	0.173	0.184	0.190	0.035	0.035	H	0.179	0.165	0.185	0.187	0.053	0.032
H	0.181	0.201	0.208	0.212	0.114	0.115	H	0.184	0.203	0.209	0.212	0.105	0.111
H	0.180	0.198	0.207	0.211	0.113	0.106	H	0.184	0.203	0.209	0.212	0.104	0.108
H	0.180	0.180	0.181	0.185	0.019	0.046	H	0.178	0.165	0.184	0.187	0.033	0.034
C	0.630	0.491	0.890	0.866	0.823	0.822	C	-0.423	-0.444	-0.347	-0.362	0.078	-0.019
F	-0.221	-0.240	-0.316	-0.338	-0.296	-0.281	H	0.100	0.362	0.075	0.237	-0.132	0.162
H	0.060	0.241	0.089	0.142	-0.003	-0.065	Cl	0.207	0.038	0.189	0.035	0.155	-0.069
F	-0.234	-0.247	-0.332	-0.343	-0.278	-0.271	Cl	0.049	0.038	0.037	0.035	-0.092	-0.068
F	-0.234	-0.240	-0.332	-0.338	-0.277	-0.282	Cl	0.048	0.040	0.037	0.037	-0.088	-0.072

	b2						b2						
	Mul		NPA		ESP		Mul		NPA		ESP		
	#	##	#	##	#	##	#	##	#	##	#	##	
C	-0.341	-0.242	0.025	0.029	0.293	0.199	C	-0.255	-0.369	0.028	0.031	0.185	0.198
C	-0.011	-0.034	-0.223	-0.216	-0.264	-0.191	C	-0.092	0.010	-0.219	-0.214	-0.198	-0.181
C	-0.202	-0.254	-0.184	-0.178	0.102	0.047	C	-0.271	-0.205	-0.182	-0.178	0.045	0.038
C	-0.011	-0.006	-0.223	-0.215	-0.271	-0.201	C	-0.092	0.010	-0.219	-0.214	-0.204	-0.181
C	-0.341	-0.375	0.025	0.025	0.301	0.221	C	-0.255	-0.368	0.028	0.031	0.192	0.198
N	-0.019	-0.043	-0.406	-0.438	-0.469	-0.372	N	-0.002	0.021	-0.420	-0.442	-0.316	-0.372
H	0.193	0.196	0.204	0.207	0.062	0.076	H	0.195	0.195	0.205	0.208	0.073	0.076
H	0.184	0.180	0.183	0.185	0.025	0.047	H	0.165	0.178	0.185	0.187	0.044	0.039
H	0.181	0.198	0.208	0.211	0.113	0.106	H	0.203	0.184	0.209	0.212	0.107	0.108
H	0.181	0.201	0.208	0.212	0.115	0.113	H	0.203	0.184	0.209	0.212	0.109	0.108
H	0.184	0.173	0.183	0.190	0.023	0.033	H	0.165	0.178	0.185	0.187	0.041	0.039
C	0.626	0.491	0.890	0.866	0.819	0.831	C	-0.444	-0.423	-0.346	-0.362	0.082	0.015
F	-0.221	-0.240	-0.316	-0.338	-0.294	-0.284	Cl	0.362	0.100	0.074	0.237	-0.134	0.146
F	-0.234	-0.247	-0.332	-0.343	-0.275	-0.273	Cl	0.038	0.049	0.037	0.035	-0.088	-0.076
F	-0.234	-0.240	-0.332	-0.338	-0.275	-0.284	Cl	0.038	0.049	0.037	0.035	-0.088	-0.076
H	0.065	0.241	0.089	0.142	-0.005	-0.070	H	0.040	0.205	0.189	0.037	0.149	-0.080

	c						c						
	Mul		NPA		ESP		Mul		NPA		ESP		
	#	##	#	##	#	##	#	##	#	##	#	##	
C	-0.279	-0.277	0.027	0.026	0.179	0.242	C	-0.321	-0.316	0.026	0.026	0.120	0.166
C	-0.097	-0.087	-0.222	-0.222	-0.200	-0.241	C	0.006	-0.021	-0.220	-0.221	-0.172	-0.184
C	-0.204	-0.184	-0.185	-0.184	0.046	0.082	C	-0.264	-0.239	-0.184	-0.184	0.030	0.034
C	-0.097	-0.087	-0.222	-0.222	-0.200	-0.241	C	0.005	-0.020	-0.220	-0.221	-0.177	-0.183
C	-0.279	-0.277	0.027	0.026	0.180	0.242	C	-0.321	-0.316	0.026	0.026	0.126	0.165
N	0.037	-0.009	-0.414	-0.408	-0.322	-0.404	N	0.023	0.020	-0.421	-0.417	-0.244	-0.317
H	0.191	0.192	0.204	0.204	0.071	0.066	H	0.189	0.191	0.204	0.204	0.073	0.072
H	0.179	0.179	0.184	0.184	0.055	0.043	H	0.159	0.166	0.184	0.184	0.073	0.057
H	0.184	0.182	0.207	0.207	0.102	0.109	H	0.190	0.187	0.207	0.208	0.096	0.098
H	0.184	0.182	0.207	0.207	0.102	0.109	H	0.190	0.187	0.207	0.208	0.099	0.098
H	0.180	0.179	0.184	0.184	0.054	0.043	H	0.159	0.166	0.184	0.184	0.070	0.057
C	0.613	0.626	0.896	0.893	0.616	0.593	C	-0.412	-0.404	-0.333	-0.343	-0.208	-0.185
H	0.095	0.079	0.089	0.091	0.068	0.077	H	0.272	0.255	0.193	0.187	0.262	0.237
F	-0.236	-0.233	-0.328	-0.328	-0.249	-0.239	Cl	0.039	0.045	0.047	0.052	-0.049	-0.038
F	-0.236	-0.233	-0.328	-0.328	-0.249	-0.239	Cl	0.039	0.045	0.047	0.052	-0.048	-0.038
F	-0.233	-0.232	-0.326	-0.328	-0.251	-0.241	Cl	0.047	0.055	0.054	0.057	-0.050	-0.041

py-CHBr ₃					py-CHI ₃				
	r					r			
	Mul		NPA			Mul		NPA	
	#	##	#	##		#	##	#	##
C	-0.340	-0.310	0.031	0.030	C	-0.268	-0.255	0.036	0.033
C	0.004	-0.032	-0.213	-0.214	C	-0.022	-0.048	-0.212	-0.213
C	-0.321	-0.308	-0.178	-0.178	C	-0.364	-0.354	-0.177	-0.178
C	-0.043	-0.058	-0.214	-0.215	C	-0.126	-0.095	-0.211	-0.213

C	-0.235	-0.234	0.033	0.032	C	-0.181	-0.206	0.033	0.032
N	-0.022	-0.020	-0.447	-0.445	N	-0.049	-0.038	-0.450	-0.447
H	0.194	0.194	0.208	0.207	H	0.194	0.193	0.208	0.208
H	0.170	0.173	0.191	0.190	H	0.173	0.173	0.190	0.189
H	0.205	0.204	0.212	0.212	H	0.209	0.207	0.212	0.212
H	0.205	0.204	0.212	0.211	H	0.207	0.206	0.212	0.212
H	0.167	0.166	0.187	0.187	H	0.168	0.167	0.189	0.188
C	-0.301	-0.311	-0.599	-0.598	C	-0.283	-0.266	-0.937	-0.934
H	0.370	0.377	0.244	0.241	H	0.326	0.285	0.244	0.241
Br	-0.011	-0.011	0.114	0.114	I	0.006	0.011	0.221	0.224
Br	-0.013	-0.010	0.116	0.120	I	0.004	0.008	0.222	0.225
Br	-0.028	-0.024	0.104	0.106	I	0.007	0.011	0.219	0.223

a					a				
Mul		NPA			Mul		NPA		
#	##	#	##	#	##	#	##	#	##
C	-0.260	-0.262	0.034	0.032	C	-0.241	-0.241	0.035	0.033
C	-0.059	-0.063	-0.213	-0.214	C	-0.063	-0.066	-0.211	-0.213
C	-0.330	-0.320	-0.177	-0.178	C	-0.360	-0.347	-0.177	-0.178
C	-0.059	-0.063	-0.213	-0.214	C	-0.063	-0.066	-0.211	-0.213
C	-0.260	-0.261	0.034	0.032	C	-0.240	-0.241	0.035	0.033
N	-0.020	-0.012	-0.448	-0.445	N	-0.051	-0.039	-0.451	-0.447
H	0.193	0.194	0.208	0.208	H	0.193	0.193	0.208	0.208
H	0.163	0.165	0.189	0.188	H	0.167	0.171	0.189	0.189
H	0.208	0.206	0.212	0.212	H	0.209	0.206	0.213	0.212
H	0.208	0.206	0.212	0.212	H	0.209	0.206	0.213	0.212
H	0.163	0.165	0.189	0.188	H	0.167	0.171	0.189	0.189
C	-0.373	-0.358	-0.590	-0.600	C	-0.336	-0.273	-0.909	-0.934
H	0.481	0.448	0.248	0.243	H	0.377	0.291	0.245	0.241
Br	-0.019	-0.016	0.104	0.112	I	0.009	0.009	0.210	0.222
Br	-0.019	-0.016	0.104	0.112	I	0.009	0.009	0.210	0.222

Br	-0.019	-0.015	0.107	0.114	I	0.013	0.015	0.213	0.226
b1					b1				
Mul		NPA			Mul		NPA		
	#	##	#	##		#	##	#	##
C	-0.332	-0.381	0.031	0.027	C	-0.276	-0.320	0.033	0.029
C	-0.022	0.018	-0.216	-0.216	C	-0.076	-0.036	-0.209	-0.212
C	-0.164	-0.199	-0.179	-0.180	C	-0.119	-0.147	-0.176	-0.178
C	-0.013	0.041	-0.216	-0.218	C	-0.068	-0.039	-0.210	-0.214
C	-0.344	-0.364	0.030	0.029	C	-0.286	-0.292	0.033	0.031
N	-0.024	-0.018	-0.425	-0.425	N	-0.064	-0.070	-0.433	-0.430
H	0.197	0.195	0.207	0.206	H	0.201	0.199	0.209	0.208
H	0.178	0.165	0.188	0.188	H	0.179	0.167	0.193	0.192
H	0.188	0.190	0.211	0.210	H	0.193	0.193	0.213	0.212
H	0.187	0.186	0.210	0.210	H	0.193	0.190	0.213	0.212
H	0.178	0.188	0.187	0.185	H	0.178	0.188	0.192	0.188
C	-0.299	-0.287	-0.593	-0.597	C	-0.582	-0.566	-0.937	-0.937
Br	0.080	0.072	0.156	0.164	I	0.227	0.213	0.272	0.282
H	0.209	0.209	0.193	0.192	H	0.219	0.226	0.195	0.194
Br	-0.010	-0.006	0.108	0.113	I	0.041	0.047	0.205	0.213
Br	-0.010	-0.010	0.109	0.111	I	0.043	0.047	0.206	0.211
b2					b2				
Mul		NPA			Mul		NPA		
	#	##	#	##		#	##	#	##
C	-0.344	-0.348	0.030	0.029	C	-0.283	-0.291	0.033	0.031
C	-0.006	-0.002	-0.216	-0.217	C	-0.065	-0.056	-0.210	-0.213
C	-0.174	-0.177	-0.179	-0.180	C	-0.126	-0.136	-0.176	-0.177
C	-0.006	-0.003	-0.216	-0.217	C	-0.065	-0.056	-0.210	-0.213
C	-0.344	-0.348	0.030	0.029	C	-0.283	-0.291	0.033	0.031
N	-0.024	-0.025	-0.425	-0.424	N	-0.066	-0.077	-0.433	-0.430
H	0.197	0.196	0.207	0.206	H	0.201	0.199	0.209	0.208

H	0.177	0.179	0.188	0.187	H	0.178	0.180	0.193	0.190
H	0.188	0.188	0.211	0.210	H	0.194	0.191	0.213	0.212
H	0.188	0.188	0.211	0.210	H	0.194	0.191	0.213	0.212
H	0.177	0.179	0.188	0.187	H	0.178	0.180	0.193	0.190
C	-0.301	-0.295	-0.592	-0.595	C	-0.586	-0.580	-0.937	-0.936
Br	0.080	0.076	0.156	0.165	I	0.229	0.223	0.272	0.281
Br	-0.009	-0.007	0.108	0.110	I	0.042	0.048	0.205	0.210
Br	-0.009	-0.007	0.108	0.110	I	0.042	0.048	0.205	0.210
H	0.209	0.209	0.193	0.192	H	0.218	0.227	0.195	0.194

	c					c			
	Mul		NPA			Mul		NPA	
	#	##	#	##		#	##	#	##
C	-0.314	-0.309	0.025	0.026	C	-0.288	-0.290	0.022	0.024
C	0.028	0.003	-0.220	-0.220	C	0.002	-0.011	-0.218	-0.219
C	-0.301	-0.278	-0.184	-0.184	C	-0.334	-0.318	-0.183	-0.183
C	0.027	0.003	-0.220	-0.220	C	0.002	-0.008	-0.218	-0.219
C	-0.313	-0.309	0.025	0.026	C	-0.287	-0.294	0.022	0.024
N	0.008	0.009	-0.422	-0.419	N	0.025	0.022	-0.428	-0.425
H	0.189	0.190	0.205	0.204	H	0.190	0.190	0.205	0.205
H	0.163	0.168	0.184	0.184	H	0.166	0.175	0.185	0.184
H	0.191	0.189	0.208	0.208	H	0.192	0.191	0.208	0.208
H	0.191	0.189	0.208	0.208	H	0.192	0.191	0.208	0.208
H	0.162	0.168	0.184	0.184	H	0.165	0.174	0.184	0.184
C	-0.223	-0.221	-0.572	-0.584	C	-0.399	-0.394	-0.900	-0.920
H	0.230	0.225	0.198	0.193	H	0.252	0.249	0.201	0.195
Br	-0.015	-0.012	0.125	0.130	I	0.037	0.039	0.234	0.242
Br	-0.015	-0.012	0.125	0.130	I	0.038	0.039	0.235	0.242
Br	-0.008	-0.003	0.132	0.137	I	0.045	0.048	0.241	0.248

* 6-311++G(d,p)
** 6-311++G(2df,2p)
*** 6-311++G(3df,3pd)
**** aug-cc-pVTZ

w/o CPC
w/ CPC