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A Molecular Orbital Study of N-H…Cl^- and C-H…Cl^- Hydrogen Bonds. Inferences on Selected Metal Complexes and on Protein ClC Cl^- Channels

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Supporting Material

The orthogonal atomic coordinates for the molecules optimized via DFT, and *ab initio* methods listed in the Tables below are x·10, y·10, z·10 Å.

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ISOLATE MOLECULES
Calibration of the methods on small molecules

HF

Table 1S. Computed atomic orthogonal coordinates for HF optimized at the *ab initio*-RHF/6-31G* level.

Atom	x	y	z
H1	0.00000	0.00000	-0.08196
F2	0.00000	0.00000	0.00911

Table 2S. Computed bond lengths (Å) and angles (°) for HF optimized at the *ab initio*-RHF/6-31G* level.

Vector	Length
F2-H1	0.911

Table 3S. Computed atomic orthogonal coordinates for HF optimized at the DFT-B3LYP/6-31G** level.

Atom	x	y	z
H1	0.00000	0.00000	-0.08329
F2	0.00000	0.00000	0.00925

Table 4S. Computed bond lengths (Å) and angles (°) for HF optimized at the DFT-B3LYP/6-31G** level.

Vector	Length
F2-H1	0.925

Table 5S. Computed atomic orthogonal coordinates for HF optimized at the *ab initio*-CCSD(T)/6-31G** level.

Atom	x	y	z
F2	0.00000	0.00000	0.00921
H1	0.00000	0.00000	-0.08290

Table 6S. Computed bond lengths (Å) and angles (°) for HF optimized at the *ab initio*-CCSD(T)/6-31G** level.

Vector	Length
F2-H1	0.921

Table 7S. Computed atomic orthogonal coordinates for HF optimized at the DFT-B3LYP/6-31+G** level.

Atom	x	Y	z
F1	0.00000	0.00000	0.00928
H1	0.00000	0.00000	-0.08349

Table 8S. Computed bond lengths (Å) and angles (°) for HF optimized at the DFT-B3LYP/6-31+G** level.

Vector	Length
F1-H1	0.928

Table 9S. Computed atomic orthogonal coordinates for HF optimized at the *ab initio*-CCSD(T)/6-31+G** level.

Atom	x	y	z
H1	0.00000	0.00000	-0.08328
F2	0.00000	0.00000	0.00925

Table 10S. Computed bond lengths (Å) and angles (°) for HF optimized at the *ab initio*-CCSD(T)/6-31+G** level.

Vector	Length
F2-H1	0.925

Table 11S. Computed atomic orthogonal coordinates for HF optimized at the *ab initio*-MP4(SDTQ)/6-31+G** level.

Atom	x	y	z
F1	0.00000	0.00000	0.00926
H1	0.00000	0.00000	-0.08338

Table 12S. Computed bond lengths (Å) and angles (°) for HCl optimized at the *ab initio*-MP4(SDTQ)/6-31+G** level.

Vector	Length
F1-H1	0.926

HCl

Table 13S. Computed atomic orthogonal coordinates for HCl optimized at the DFT-B3LYP/6-31G** level

Atom	x	y	z
Cl1	0.00000	0.00000	0.00715
H1	0.00000	0.00000	-0.12146

Table 14S. Computed bond lengths (Å) and angles (°) for HCl optimized at the DFT-B3LYP/6-31G** level.

Vector	Length
Cl1-H1	1.286

Table 15S. Computed atomic orthogonal coordinates for HCl optimized at the DFT-B3LYP/6-31+G** level

Atom	X	y	z
Cl1	0.00000	0.00000	0.00715
H1	0.00000	0.00000	-0.12153

Table 16S. Computed bond lengths (Å) and angles (°) for HCl optimized at the DFT-B3LYP/6-31+G** level.

Vector	Length
Cl1-H1	1.287

Table 17S. Computed atomic orthogonal coordinates for HCl optimized at the DFT-B3LYP/6-31++G** level

Atom	X	y	Z
Cl1	0.00000	0.00000	0.00715
H1	0.00000	0.00000	-0.12154

Table 18S. Computed bond lengths (Å) and angles (°) for HCl optimized at the DFT-B3LYP/6-31++G** level.

Vector	Length
Cl1-H1	1.287

Table 19S. Computed atomic orthogonal coordinates for HCl optimized at the *ab initio*-MP2/6-31+G** level

Atom	x	y	z
Cl1	0.00000	0.00000	0.00706
H1	0.00000	0.00000	-0.11995

Table 20S. Computed bond lengths (Å) and angles (°) for HCl optimized at the *ab initio*-MP2/6-31+G** level.

Vector	Length
Cl1-H1	1.270

Table 21S. Computed atomic orthogonal coordinates for HCl optimized at the *ab initio*-CCSD(T)/6-31G** level

Atom	x	y	z
Cl1	0.00000	0.00000	0.00707
H2	0.00000	0.00000	-0.12027

Table 22S. Computed bond lengths (Å) and angles (°) for HCl optimized at the *ab initio*-CCSD(T)/6-31G** level.

Vector	Length
Cl1-H2	1.273

Table 23S. Computed atomic orthogonal coordinates for HCl optimized at the *ab initio*-CCSD(T)/6-31++G** level

Atom	x	y	z
Cl1	0.00000	0.00000	0.00708
H2	0.00000	0.00000	-0.12036

Table 24S. Computed bond lengths (Å) and angles (°) for HCl optimized at the *ab initio*-CCSD(T)/6-31++G** level.

Vector	Length
Cl1-H2	1.274

Table 25S. Computed atomic orthogonal coordinates for HCl optimized at the *ab initio*-CCSD(T)/6-31+G** level

Atom	x	y	z
Cl1	0.00000	0.00000	0.00708
H2	0.00000	0.00000	-0.12035

Table 26S. Computed bond lengths (Å) and angles (°) for HCl optimized at the *ab initio*-CCSD(T)/6-31+G** level.

Vector	Length
Cl1-H2	1.274

H_2O

Table 27S. Computed atomic orthogonal coordinates for H_2O optimized at the DFT-B3LYP/6-31G** level.

Atom	x	y	z
O1	0.00000	0.00000	0.01192
H2	0.00000	0.07593	-0.04768
H3	0.00000	-0.07593	-0.04768

Table 28S. Computed bond lengths (Å) and angles (°) for H_2O optimized at the DFT-B3LYP/6-31G** level.

Vector	Length
O1-H2	0.965
O1-H3	0.965

Vectors	Angle
H2-O1-H3	103.74

Table 29S. Computed atomic orthogonal coordinates for H_2O optimized at the DFT-B3LYP/6-31+G** level.

Atom	x	y	z
O1	0.00000	0.00000	0.01165
H2	0.00000	0.07695	-0.04659
H3	0.00000	-0.07695	-0.04659

Table 30S. Computed bond lengths (Å) and angles (°) for H_2O optimized at the DFT-B3LYP/6-31+G** level.

Vector	Distance
O1-H2	0.965
O1-H3	0.965

Vectors	Angle
H2-O1-H3	105.76

Table 31S. Computed atomic orthogonal coordinates for H_2O optimized at the DFT-B3LYP/6-31++G** level.

Atom	x	y	z
O1	0.00000	0.00000	0.01166
H2	0.00000	0.07694	-0.04664
H3	0.00000	-0.07694	-0.04664

Table 32S. Computed bond lengths (Å) and angles (°) for H_2O optimized at the DFT-B3LYP/6-31++G** level.

Vector	Length
O1-H2	0.965
O1-H3	0.965

Vectors	Angle
H2-O1-H3	105.70

Table 33S. Computed atomic orthogonal coordinates for H_2O optimized at the *ab initio*-CCSD(T)/6-31G** level.

Atom	x	y	z
O1	0.00000	0.00000	0.01186
H2	0.00000	0.07572	-0.04746
H3	0.00000	-0.07572	-0.04746

Table 34S. Computed bond lengths (Å) and angles (°) for H_2O optimized at the *ab initio*-CCSD(T)/6-31G** level.

Vector	Length
O1-H2	0.962
O1-H3	0.962

Vectors	Angle
H2-O1-H3	103.85

Table 35S. Computed atomic orthogonal coordinates for H_2O optimized at the *ab initio*-CCSD(T)/6-31++G** level.

Atom	x	y	z
O1	0.00000	0.00000	0.01170
H2	0.00000	0.07658	-0.04679
H3	0.00000	-0.07658	-0.04679

Table 36S. Computed bond lengths (Å) and angles (°) for H_2O optimized at the *ab initio*-CCSD(T)/6-31++G** level.

Vector	Length
O1-H2	0.964
O1-H3	0.964

Vectors	Angle
H2-O1-H3	105.26

Table 37S. Computed atomic orthogonal coordinates for H_2O optimized at the *ab initio*-CCSD(T)/6-31+G** level.

Atom	x	y	z
O1	0.00000	0.00000	0.01168
H2	0.00000	0.07660	-0.04674
H3	0.00000	-0.07660	-0.04674

Table 38S. Computed bond lengths (Å) and angles (°) for H_2O optimized at the *ab initio*-CCSD(T)/6-31+G** level.

Vector	Length
O1-H2	0.963
O1-H3	0.963

Vectors	Angle
H2-O1-H3	105.34

Table 39S. Computed atomic orthogonal coordinates for H_2O optimized at the *ab initio* MP2/6-31+G** level.

Atom	x	y	z
O1	0.00000	0.00000	0.01167
H2	0.00000	0.07663	-0.04668
H3	0.00000	-0.07663	-0.04668

Table 40S. Computed bond lengths (Å) and angles (°) for H_2O optimized at the *ab initio* MP2/6-31+G** level.

Vector	Length
O1-H2	0.963
O1-H3	0.963

Vectors	Angle
H2-O1-H3	105.42

ISOLATE MOLECULES
Imidazole and pyrimidine

IM

Table 41S. Computed atomic orthogonal coordinates for IM optimized at the DFT-B3LYP/6-31G** level.

Atom	x	y	z
H2	-0.21025	0.06626	0.00000
H1	-0.00098	0.21142	0.00000
N1	0.00000	0.11060	0.00000
C2	-0.10905	0.02815	0.00000
H5	0.21203	0.07052	0.00000
N3	-0.07429	-0.09868	0.00000
C5	0.11205	0.03001	0.00000
C4	0.06355	-0.09834	0.00000
H4	0.11997	-0.19054	0.00000

Table 42S. Computed bond lengths (Å) and angles (°) for IM optimized at the DFT-B3LYP/6-31G** level.

Vector	Length
N1-C2	1.367
N1-C5	1.380
N3-C2	1.315
N3-C4	1.378
C4-C5	1.372
H1-N1	1.008
H2-C2	1.081
H4-C4	1.081
H5-C5	1.079

Vectors	Angle
H1-N1-C2	126.54
H1-N1-C5	126.28
C2-N1-C5	107.18
C2-N3-C4	105.19
H2-C2-N3	125.96
H2-C2-N1	122.27
N3-C2-N1	111.77
H4-C4-C5	127.84
H4-C4-N3	121.32
C5-C4-N3	110.84
H5-C5-C4	132.76
H5-C5-N1	122.22
C4-C5-N1	105.02

Table 43S. Computed atomic orthogonal coordinates for IM optimized at the DFT-B3LYP/6-31+G** level.

Atom	x	y	z
H5	0.21222	0.07036	0.00000
H4	0.11990	-0.19085	0.00000
H2	-0.21052	0.06617	0.00000
H1	-0.00106	0.21156	0.00000
C5	0.11214	0.03002	0.00000
N3	-0.07423	-0.09861	0.00000
N1	0.00000	0.11067	0.00000
C4	0.06365	-0.09859	0.00000
C2	-0.10927	0.02830	0.00000

Table 44S. Computed bond lengths (Å) and angles (°) for IM optimized at the DFT-B3LYP/6-31+G** level.

Vector	Length
N1-C2	1.368
N1-C5	1.381
N3-C2	1.317
N3-C4	1.379
C4-C5	1.374
H1-N1	1.009
H2-C2	1.081
H4-C4	1.081
H5-C5	1.079

Vectors	Angle
H1-N1-C2	126.41
H1-N1-C5	126.33
C2-N1-C5	107.27
C2-N3-C4	105.43
H2-C2-N3	125.94
H2-C2-N1	122.48
N3-C2-N1	111.57
H4-C4-C5	127.97
H4-C4-N3	121.36
C5-C4-N3	110.67
H5-C5-C4	132.61
H5-C5-N1	122.32
C4-C5-N1	105.07

Table 45S. Computed atomic orthogonal coordinates for IM optimized at the *ab initio*-CCSDT/6-31G** level.

Atom	x	y	Z
H5	0.21221	0.07079	0.00000
H4	0.12026	-0.19037	0.00000
H2	-0.21014	0.06644	0.00000
H1	-0.00124	0.21152	0.00000
C5	0.11246	0.03024	0.00000
N3	-0.07483	-0.09932	0.00000
N1	0.00000	0.11092	0.00000
C4	0.06387	-0.09847	0.00000
C2	-0.10922	0.02830	0.00000

Table 46S. Computed bond lengths (Å) and angles (°) for IM optimized at the *ab initio*-CCSDT/6-31G** level.

Vector	Length
N1-C2	1.369
N1-C5	1.384
N3-C2	1.322
N3-C4	1.387
C4-C5	1.376
H1-N1	1.006
H2-C2	1.079
H4-C4	1.078
H5-C5	1.077

Vectors	Angle
H1-N1-C2	126.40
H1-N1-C5	126.36
C2-N1-C5	107.24
C2-N3-C4	104.73
H2-C2-N3	125.78
H2-C2-N1	122.19
N3-C2-N1	112.02
H4-C4-C5	127.78
H4-C4-N3	121.18
C5-C4-N3	111.03
H5-C5-C4	132.80
H5-C5-N1	122.22
C4-C5-N1	104.97

Table 47S. Computed atomic orthogonal coordinates for IM optimized at the *ab initio*-MP2/6-31+G** level.

Atom	x	Y	z
N1	0.00000	0.11045	0.00000
C2	-0.10915	0.02900	0.00000
N3	-0.07449	-0.09885	0.00000
C4	0.06388	-0.09898	0.00000
C5	0.11193	0.02993	0.00000
H1	-0.00106	0.21254	0.00000
H2	-0.21047	0.06742	0.00000
H4	0.12064	-0.19128	0.00000
H5	0.21235	0.07038	0.00000

Table 48S. Computed bond lengths (Å) and angles (°) for IM optimized at the *ab initio*-MP2/6-31+G** level.

Vector	Length
N1-C2	1.362
N1-C5	1.379
N3-C2	1.325
N3-C4	1.384
C4-C5	1.376
H1-N1	1.021
H2-C2	1.084
H4-C4	1.084
H5-C5	1.083

Vectors	Angle
H1-N1-C2	126.14
H1-N1-C5	126.33
C2-N1-C5	107.54
C2-N3-C4	105.22
H2-C2-N3	125.93
H2-C2-N1	122.50
N3-C2-N1	111.56
H4-C4-C5	127.97
H4-C4-N3	121.64
C5-C4-N3	110.39
H5-C5-C4	132.38
H5-C5-N1	122.33
C4-C5-N1	105.29

IMH^+

Table 49S. Computed atomic orthogonal coordinates for IMH^+ optimized at the DFT-B3LYP/6-31+G**level.

Atom	x	y	z
H4	0.21335	0.07700	0.00000
H5	0.12748	-0.18756	0.00000
H2	-0.21145	0.06861	0.00000
H1	-0.12745	-0.17242	0.00000
H3	-0.00202	0.21439	0.00000
C4	0.11412	0.03471	0.00000
C5	0.07203	-0.09505	0.00000
C2	-0.10875	0.03527	0.00000
N1	-0.06633	-0.09148	0.00000
N3	0.00000	0.11298	0.00000

Table 50S. Computed bond lengths (Å) and angles (°) for IMH^+ optimized at the DFT-B3LYP/6-31+G** level.

Vector	Length
N1-C2	1.337
N1-C5	1.384
N3-C2	1.337
N3-C4	1.384
C4-C5	1.364
H1-N1	1.014
H2-C2	1.080
H3-N3	1.014
H4-C4	1.079
H5-C5	1.079

Vectors	Angle
H1-N1-C2	124.44
H1-N1-C5	125.58
C2-N1-C5	109.98
H3-N3-C2	124.41
H3-N3-C4	125.59
C2-N3-C4	110.01
H2-C2-N1	126.49
H2-C2-N3	126.47
N1-C2-N3	107.04
H4-C4-C5	131.05
H4-C4-N3	122.47
C5-C4-N3	106.47
H5-C5-C4	131.09
H5-C5-N1	122.42
C4-C5-N1	106.49

Table 51S. Computed atomic orthogonal coordinates for IMH^+ optimized at the *ab initio*-MP2/6-31+G** level.

Atom	x	Y	z
N1	-0.06567	-0.09176	0.00000
C2	-0.10921	0.03505	0.00000
N3	0.00000	0.11281	0.00000
C4	0.11390	0.03551	0.00000
C5	0.07197	-0.09514	0.00000
H1	-0.12656	-0.17279	0.00000
H2	-0.21167	0.06795	0.00000
H3	-0.00238	0.21415	0.00000
H4	0.21273	0.07795	0.00000
H5	0.12760	-0.18717	0.00000

Table 52S. Computed bond lengths (Å) and angles (°) for IMH^+ optimized at the *ab initio*-MP2/6-31+G** level.

Vector	Length
N1-C2	1.341
N1-C5	1.377
N3-C2	1.341
N3-C4	1.377
C4-C5	1.372
H1-N1	1.014
H2-C2	1.076
H3-N3	1.014
H4-C4	1.076
H5-C5	1.075

Vectors	Angle
H1-N1-C2	124.13
H1-N1-C5	125.52
C2-N1-C5	110.36
H3-N3-C2	124.11
H3-N3-C4	125.51
C2-N3-C4	110.38
H2-C2-N3	126.75
H2-C2-N1	126.75
N3-C2-N1	106.50
H4-C4-C5	131.03
H4-C4-N3	122.60
C5-C4-N3	106.37
H5-C5-C4	131.05
H5-C5-N1	122.56
C4-C5-N1	106.39

PYM

Table 53S. Computed atomic orthogonal coordinates for PYM optimized at the DFT-B3LYP/6-31G**level.

Atom	x	y	z
H2	0.00002	0.23977	0.00000
H6	-0.21537	-0.11186	0.00000
H4	0.21533	-0.11190	0.00000
H5	-0.00001	-0.24407	0.00000
C2	0.00000	0.13095	0.00000
N3	0.11993	0.07163	0.00000
N1	-0.11988	0.07165	0.00000
C6	-0.11846	-0.06224	0.00000
C4	0.11843	-0.06225	0.00000
C5	-0.00003	-0.13560	0.00000

Table 54S. Computed bond lengths (Å) and angles (°) for PYM optimized at the DFT-B3LYP/6-31G** level.

Vector	Distance
N1-C2	1.337
N1-C6	1.339
N3-C2	1.338
N3-C4	1.339
C4-C5	1.393
C5-C6	1.393
H2-C2	1.088
H4-C4	1.089
H5-C5	1.085
H6-C6	1.089

Vectors	Angle
C2-N1-C6	115.71
C2-N3-C4	115.68
H2-C2-N1	116.33
H2-C2-N3	116.31
N1-C2-N3	127.36
H4-C4-N3	116.49
H4-C4-C5	121.10
N3-C4-C5	122.41
H5-C5-C6	121.79
H5-C5-C4	121.76
C6-C5-C4	116.46
H6-C6-N1	116.51
H6-C6-C5	121.11
N1-C6-C5	122.38

Table 55S. Computed atomic orthogonal coordinates for PYM optimized at the DFT-B3LYP/6-31+G** level.

Atom	x	y	z
H5	-0.00001	-0.24421	0.00000
H6	-0.21559	-0.11172	0.00000
H4	0.21556	-0.11175	0.00000
H2	0.00002	0.24000	0.00000
N3	0.11985	0.07161	0.00000
N1	-0.11981	0.07163	0.00000
C5	-0.00002	-0.13572	0.00000
C6	-0.11862	-0.06235	0.00000
C4	0.11859	-0.06236	0.00000
C2	0.00000	0.13127	0.00000

Table 56S. Computed bond lengths (Å) and angles (°) for PYM optimized at the DFT-B3LYP/6-31+G** level.

Vector	Distance
N1-C2	1.338
N1-C6	1.340
N3-C2	1.339
N3-C4	1.340
C4-C5	1.395
C5-C6	1.395
H2-C2	1.087
H4-C4	1.088
H5-C5	1.085
H6-C6	1.088

Vectors	Angle
C2-N1-C6	115.95
C2-N3-C4	115.92
H2-C2-N1	116.47
H2-C2-N3	116.45
N1-C2-N3	127.07
H4-C4-N3	116.45
H4-C4-C5	121.27
N3-C4-C5	122.28
H5-C5-C4	121.73
H5-C5-C6	121.75
C4-C5-C6	116.52
H6-C6-N1	116.47
H6-C6-C5	121.28
N1-C6-C5	122.25

Table 57S. Computed atomic orthogonal coordinates for PYM optimized at the *ab initio*-MP2/6-31+G** level.

Atom	x	y	z
N1	0.12042	0.07181	0.00000
C2	0.00000	0.13153	0.00000
N3	-0.12043	0.07181	0.00000
C4	-0.11881	-0.06273	0.00000
C5	0.00000	-0.13564	0.00000
C6	0.11881	-0.06274	0.00000
H2	0.00000	0.23980	0.00000
H4	-0.21537	-0.11192	0.00000
H5	-0.00001	-0.24380	0.00000
H6	0.21538	-0.11192	0.00000

Table 58S. Computed bond lengths (Å) and angles (°) for PYM optimized at the *ab initio*-MP2/6-31+G** level.

Vector	Length
N1-C2	1.344
N1-C6	1.346
N3-C2	1.344
N3-C4	1.345
C4-C5	1.394
C5-C6	1.394
H2-C2	1.083
H4-C4	1.084
H5-C5	1.082
H6-C6	1.084

Vectors	Angle
C2-N1-C6	115.69
C2-N3-C4	115.69
H2-C2-N1	116.38
H2-C2-N3	116.38
N1-C2-N3	127.25
H4-C4-N3	116.31
H4-C4-C5	121.47
N3-C4-C5	122.23
H5-C5-C4	121.53
H5-C5-C6	121.54
C6-C5-C4	116.93
H6-C6-N1	116.30
H6-C6-C5	121.48
N1-C6C5	122.22

MePYM

Table 59S. Computed atomic orthogonal coordinates for MePYM optimized at the DFT-B3LYP/Lanl2dz level.

Atom	x	y	z
N1	-0.19094	-0.00638	0.00001
C2	-0.11275	-0.11711	0.00000
N3	0.02292	-0.11963	-0.00001
C4	0.08839	0.00008	-0.00001
C5	0.01493	0.12100	-0.00001
C6	-0.12524	0.11287	0.00000
C7	0.23937	-0.00261	0.00000
H2	-0.16355	-0.21304	0.00000
H5	0.06531	0.21716	-0.00002
H6	-0.18742	0.20200	0.00001
H7a	0.27418	-0.10619	-0.00032
H7b	0.27975	0.04870	-0.08828
H7c	0.27970	0.04808	0.08867

Table 60S. Computed bond lengths (Å) and angles (°) for MePYM optimized at the DFT-B3LYP/Lanl2dz level.

Vector	Length
N1-C2	1.356
N1-C6	1.362
N3-C2	1.357
N3-C4	1.364
C4-C5	1.415
C4-C7	1.510
C5-C6	1.404
H2-C2	1.086
H5-C5	1.086
H6-C6	1.087
H7a-C7	1.093
H7b-C7	1.098
H7c-C7	1.098

Vectors	Angle
C2-N1-C6	115.92
C2-N3-C4	117.61
H2-C2-N1	116.87
H2-C2-N3	116.84
N1-C2-N3	126.29
N3-C4-C5	120.05
N3-C4-C7	117.65
C5-C4-C7	122.30
H5-C5-C6	120.97
H5-C5-C4	121.07
C6-C5-C4	117.96
H6-C6-N1	116.25
H6-C6-C5	121.58
N1-C6-C5	122.17
H7a-C7-H7b	108.87
H7a-C7-H7c	108.84
H7a-C7-C4	109.60
H7b-C7-H7c	107.36

H7b-C7-C4	111.06
H7c-C7-C4	111.04

Table 61S. Computed atomic orthogonal coordinates for MePYM optimized at the DFT-B3LYP/6-31G** level.

Atom	x	y	z
N1	0.18916	-0.00697	0.00000
C2	0.11054	-0.11493	0.00000
N3	-0.02320	-0.11840	0.00000
C4	-0.08671	-0.00006	0.00000
C5	-0.01410	0.11978	0.00000
C6	0.12451	0.11053	0.00000
C7	-0.23726	-0.00208	0.00000
H2	0.16093	-0.21142	0.00000
H5	-0.06409	0.21614	0.00000
H6	0.18653	0.20001	0.00000
H7a	-0.27711	0.04859	0.08859
H7b	-0.27717	0.05002	-0.08773
H7c	-0.27272	-0.10521	-0.00081

Table 62S. Computed bond lengths (Å) and angles (°) for MePYM optimized at the DFT-B3LYP/6-31G** level.

Vector	Distance
N1-C2	1.336
N1-C6	1.341
N3-C2	1.338
N3-C4	1.343
C2-N1	1.336
C2-N3	1.338
C4-C5	1.401
C4-C7	1.506
C5-C6	1.389
H2-C2	1.089
H5-C5	1.086
H6-C6	1.089
H7a-C7	1.096
H7b-C7	1.096
H7c-C7	1.091

Vectors	Angle
C2-N1-C6	115.12
C2-N3-C4	116.74
H2-C2-N1	116.36
H2-C2-N3	116.09
N1-C2-N3	127.55
N3-C4-C5	120.57
N3-C4-C7	117.45
C5-C4-C7	121.98
H5-C5-C6	121.24
H5-C5-C4	121.37
C6-C5-C4	117.39
H6-C6-N1	116.45
H6-C6-C5	120.91
N1-C6-C5	122.64
H7c-C7-H7a	108.97
H7c-C7-H7b	108.98

H7c-C7-C4	109.74
H7a-C7-H7b	107.16
H7a-C7-C4	110.95
H7b-C7-C4	110.97

Table 63S. Computed atomic orthogonal coordinates for MePYM optimized at the DFT-B3LYP/6-31+G** level.

Atom	x	y	z
H7b	-0.27723	0.04992	-0.08783
H7c	-0.27311	-0.10532	-0.00079
H6	0.18660	0.20014	0.00000
H2	0.16129	-0.21148	0.00000
C7	-0.23746	-0.00220	0.00000
H5	-0.06425	0.21616	0.00000
N1	0.18916	-0.00684	0.00000
C6	0.12451	0.11078	0.00000
C2	0.11087	-0.11512	0.00000
C5	-0.01423	0.11979	0.00000
N3	-0.02299	-0.11836	0.00000
C4	-0.08692	-0.00017	0.00000
H7a	-0.27717	0.04852	0.08867

Table 64S. Computed bond lengths (Å) and angles (°) for MePYM optimized at the DFT-B3LYP/6-31+G** level.

Vector	Length
N1-C2	1.336
N1-C6	1.342
N3-C2	1.339
N3-C4	1.344
C4-C5	1.403
C4-C7	1.506
C5-C6	1.390
H2-C2	1.088
H5-C5	1.086
H6-C6	1.088
H7a-C7	1.096
H7b-C7	1.096
H7c-C7	1.091

Vectors	Angle
C2-N1-C6	115.34
C2-N3-C4	117.02
H2-C2-N1	116.51
H2-C2-N3	116.23
N1-C2-N3	127.25
N3-C4-C5	120.38
N3-C4-C7	117.64
C5-C4-C7	121.99
H5-C5-C6	121.15
H5-C5-C4	121.35
C6-C5-C4	117.50
H6-C6-N1	116.41
H6-C6-C5	121.08
N1-C6-C5	122.51
H7c-C7-H7a	108.96
H7c-C7-H7b	108.97
H7c-C7-C4	109.84
H7a-C7-H7b	107.27

H7a-C7-C4	110.86
H7b-C7-C4	110.88

ISOLATE MOLECULES

Acetamide, N-methylacetamide, methylammonium, methylamine, N-methylguanidinium, methanol, 1-hydroxy-4-methylbenzene

AA

Table 65S. Computed atomic orthogonal coordinates for AA optimized at the DFT-B3LYP/6-31+G** level.

Atom	x	y	z
N1	-0.10393	-0.08269	-0.00002
C2	-0.00740	0.01432	-0.00001
C3	0.13646	-0.03474	0.00000
O4	-0.03549	0.13359	0.00000
H5	-0.20072	-0.05392	0.00007
H6	-0.08231	-0.18104	0.00006
H7	0.18711	0.00590	-0.08798
H8	0.14598	-0.14368	-0.00033
H9	0.18691	0.00534	0.08836

Table 66S. Computed bond lengths (Å) and angles (°) for AA optimized at the DFT-B3LYP/6-31+G** level.

Vector	Length
N1-C2	1.369
C2-O4	1.225
C2-C3	1.520
H5-N1	1.010
H6-N1	1.007
H7-C3	1.094
H8-C3	1.094
H9-C3	1.094

Vectors	Angle
H6-N1-H5	118.95
H6-N1-C2	122.74
H5-N1-C2	118.30
O4-C2-N1	121.89
O4-C2-C3	122.08
N1-C2-C3	116.03
H7-C3-H8	109.12
H7-C3-H9	107.47
H7-C3-C2	108.57
H8-C3-H9	109.11
H8-C3-C2	113.82
H9-C3-C2	108.57

Table 67S. Computed atomic orthogonal coordinates for AA optimized at the *ab initio*-MP2/6-31+G** level.

Atom	x	y	z
N1	-0.10121	-0.08567	-0.00437
C2	-0.00732	0.01448	-0.00092
C3	0.13674	-0.03174	0.00004
O4	-0.03913	0.13356	0.00069
H5	-0.19704	-0.05891	0.01193
H6	-0.07545	-0.18115	0.01403
H7	0.19766	0.04403	-0.04834
H8	0.14969	-0.12727	-0.05058
H9	0.17011	-0.04195	0.10334

Table 68S. Computed bond lengths (Å) and angles (°) for AA optimized at the *ab initio*-MP2/6-31+G** level.

Vector	Length
N1-C2	1.373
C2-O4	1.233
C2-C3	1.513
H5-N1	1.008
H6-N1	1.006
H7-C3	1.086
H8-C3	1.089
H9-C3	1.090

Vectors	Angle
H6-N1-H5	117.76
H6-N1-C2	120.83
H5-N1-C2	116.89
O4-C2-N1	121.90
O4-C2-C3	122.73
N1-C2-C3	115.36
H7-C3-H8	109.77
H7-C3-H9	108.40
H7-C3-C2	108.55
H8-C3-H9	108.78
H8-C3-C2	112.23
H9-C3-C2	109.03

MAA

Table 69S. Computed atomic orthogonal coordinates for MAA optimized at the DFT-B3LYP/6-31+G** level.

Atom	x	y	z
H4a	0.25280	-0.04168	0.08955
H3a	-0.23852	-0.02616	0.08840
H3b	-0.17253	-0.16576	-0.00041
H4b	0.19081	0.09861	-0.00077
C4	0.19806	-0.01020	0.00000
C3	-0.18187	-0.05675	0.00000
H1	0.04997	-0.16334	0.00000
O5	-0.04262	0.13912	0.00000
N1	0.06266	-0.06327	0.00000
C2	-0.04861	0.01642	0.00000
H4c	0.25322	-0.04296	-0.08881
H3c	-0.23886	-0.02550	-0.08794

Table 70S. Computed bond lengths (Å) and angles (°) for MAA optimized at the DFT-B3LYP/6-31+G** level.

Vector	Length
N1-C2	1.369
N1-C4	1.454
C2-O5	1.228
C2-C3	1.520
C4-H4b	1.091
C4-H4c	1.096
C4-H4a	1.096
H1-N1	1.009
H3a-C3	1.094
H3b-C3	1.094
H3c-C3	1.094
H4a-C4	1.096
H4b-C4	1.091
H4c-C4	1.096

Vectors	Angle
H1-N1-C2	118.38
H1-N1-C4	118.63
C2-N1-C4	122.99
O5-C2-N1	122.81
O5-C2-C3	121.57
N1-C2-C3	115.62
H3a-C3-H3c	107.47
H3a-C3-H3b	109.02
H3a-C3-C2	108.63
H3c-C3-H3b	109.04
H3c-C3-C2	108.62
H3b-C3-C2	113.87
H4b-C4-H4c	109.03
H4b-C4-H4a	109.00
H4b-C4-N1	107.59
H4c-C4-H4a	108.97
H4c-C4-N1	111.08

H4a-C4-N1	111.12

Table 71S. Computed atomic orthogonal coordinates for MAA optimized at the *ab initio*-MP2/6-31+G** level.

Atom	x	y	z
N1	0.06253	-0.06379	0.00000
C2	-0.04854	0.01604	0.00000
C3	-0.18123	-0.05679	0.00000
C4	0.19736	-0.00994	0.00000
O5	-0.04247	0.13958	0.00000
H1	0.04978	-0.16365	0.00001
H3a	-0.23760	-0.02560	-0.08771
H3b	-0.23715	-0.02647	0.08831
H3c	-0.17094	-0.16520	-0.00055
H4a	0.25204	-0.04249	-0.08843
H4b	0.25151	-0.04088	0.08935
H4c	0.18882	0.09833	-0.00099

Table 72S. Computed bond lengths (Å) and angles (°) for MAA optimized at the *ab initio*-MP2/6-31+G** level.

Vector	Length
N1-C2	1.368
N1-C4	1.452
C2-O5	1.237
C2-C3	1.514
H1-N1	1.007
H3a-C3	1.088
H3b-C3	1.088
H3c-C3	1.089
H4a-C4	1.089
H4b-C4	1.090
H4c-C4	1.086

Vectors	Angle
H1-N1-C2	118.43
H1-N1-C4	119.05
C2-N1-C4	122.52
O5-C2-N1	122.89
O5-C2-C3	121.57
N1-C2-C3	115.53
H3a-C3-H3b	107.94
H3a-C3-H3c	109.28
H3a-C3-C2	108.43
H3b-C3-H3c	109.27
H3b-C3-C2	108.44
H3c-C3-C2	113.34
H4c-C4-H4a	109.26
H4c-C4-H4b	109.25
H4c-C4-N1	107.26
H4a-C4-H4b	109.35
H4a-C4-N1	110.81
H4b-C4-N1	110.87

MA

Table 73S. Computed atomic orthogonal coordinates for MA optimized at the DFT-B3LYP/6-31+G** level.

Atom	x	y	z
H6	0.11446	-0.03019	0.09896
H3	-0.10892	0.06510	0.06985
H5	-0.10891	-0.09304	0.02144
C2	0.08034	0.00000	0.00000
N1	-0.07125	0.00000	0.00000
H7	0.11450	0.10079	-0.02333
H8	0.11447	-0.07061	-0.07561
H4	-0.10888	0.02795	-0.09131

Table 74S. Computed bond lengths (Å) and angles (°) for MA optimized at the DFT-B3LYP/6-31+G** level.

Vector	Length
N1-C2	1.516
H3-N1	1.026
H4-N1	1.026
H5-N1	1.026
H6-C2	1.089
H7-C2	1.089
H8-C2	1.089
Vectors	**Angle**
H3-N1-H4	107.35
H3-N1-H5	107.34
H3-N1-C2	111.53
H4-N1-H5	107.35
H4-N1-C2	111.51
H5-N1-C2	111.53
H6-C2-H8	110.65
H6-C2-H7	110.65
H6-C2-N1	108.25
H8-C2-H7	110.66
H8-C2-N1	108.26
H7-C2-N1	108.27

Table 75S. Computed atomic orthogonal coordinates for MA optimized at the *ab initio*-MP2/6-31+G** level.

Atom	x	y	z
N1	0.07076	0.00000	0.00000
C2	-0.07991	0.00000	0.00000
H3	0.10839	0.07144	0.06285
H4	0.10838	-0.09017	0.03040
H5	0.10834	0.01876	-0.09330
H6	-0.11365	0.09765	-0.03278
H7	-0.11366	-0.02044	0.10096
H8	-0.11365	-0.07721	-0.06820

Table 76S. Computed bond lengths (Å) and angles (°) for MA optimized at the *ab initio*-MP2/6-31+G** level.

Vector	Length
N1-C2	1.507
H3-N1	1.023
H4-N1	1.023
H5-N1	1.023
H6-C2	1.084
H7-C2	1.084
H8-C2	1.084
Vectors	**Angle**
H3-N1-H4	107.31
H3-N1-H5	107.28
H3-N1-C2	111.58
H4-N1-H5	107.30
H4-N1-C2	111.57
H5-N1-C2	111.55
H6-C2-H7	110.77
H6-C2-H8	110.76
H6-C2-N1	108.14
H7-C2-H8	110.78
H7-C2-N1	108.14
H8-C2-N1	108.13

MAB

Table 77S. Computed atomic orthogonal coordinates for MAB optimized at the DFT-B3LYP/6-31+G** level.

Atom	x	y	z
N1	-0.07506	0.00000	-0.01183
C2	0.07096	0.00000	0.00176
H3	-0.11603	0.08181	0.03229
H4	-0.11604	-0.08180	0.03231
H5	0.10852	-0.00017	0.10538
H6	0.11163	-0.08802	-0.04902
H7	0.11157	0.08823	-0.04870

Table 78S. Computed bond lengths (Å) and angles (°) for MAB optimized at the DFT-B3LYP/6-31+G** level.

Vector	Length
N1-C2	1.467
H3-N1	1.016
H4-N1	1.016
H5-C2	1.095
H6-C2	1.095
H7-C2	1.102

Vectors	Angle
H3-N1-H4	107.28
H3-N1-C2	111.18
H4-N1-C2	111.19
H5-C2-H6	107.25
H5-C2-H2c	107.96
H5-C2-N1	109.09
H6-C2-H7	107.95
H6-C2-N1	109.07
H7-C2-N1	115.24

Table 79S. Computed atomic orthogonal coordinates for MAB optimized at the *ab initio*-MP2/6-31+G** level.

Atom	x	y	z
N1	-0.07489	0.00000	-0.01191
C2	0.07092	0.00000	0.00175
H3	-0.11529	-0.08154	0.03259
H4	-0.11530	0.08154	0.03258
H5	0.11084	-0.08776	-0.04874
H6	0.10772	-0.00015	0.10487
H7	0.11077	0.08795	-0.04845

Table 80S. Computed bond lengths (Å) and angles (°) for MAB optimized at the *ab initio*-MP2/6-31+G** level.

Vector	Length
N1-C2	1.464
H3-N1	1.013
H4-N1	1.013
H5-C2	1.088
H6-C2	1.095
H7-C2	1.088

Vectors	Angle
H3-N1-H4	107.21
H3-N1-C2	110.86
H4-N1-C2	110.87
H5-C2-H7	107.66
H5-C2-H6	108.21
H5-C2-N1	108.78
H7-C2-H6	108.21
H7-C2-N1	108.76
H6-C2-N1	114.99

MGU

Table 81S. Computed atomic orthogonal coordinates for MGU optimized at the DFT-B3LYP/6-31+G** level.

Atom	x	y	z
H5b	-0.22280	0.05058	-0.08612
H4	-0.06056	-0.16609	-0.02405
H3b	-0.02994	0.18709	-0.02041
H2a	0.25592	-0.02216	-0.01296
N4	-0.06439	-0.06674	-0.00564
C5	-0.19701	-0.00466	0.00484
N3	0.05320	0.13329	-0.00111
H5a	-0.27024	-0.08415	0.01856
N2	0.16751	-0.06820	0.00305
C1	0.05150	-0.00065	-0.00166
H3a	0.13793	0.18461	0.01839
H2b	0.16996	-0.16747	0.02135
H5c	-0.20149	0.06110	0.09206

Table 82S. Computed bond lengths (Å) and angles (°) for MGU optimized at the DFT-B3LYP/6-31+G** level.

Vector	Length
C1-N2	1.343
C1-N3	1.340
C1-N4	1.335
C5-N4	1.468
N2-H2a	1.010
N2-H2b	1.010
N3-H3a	1.010
N3-H3b	1.009
N4-H4	1.011
C5-H5a	1.089
C5-H5b	1.095
C5-H5c	1.093

Vectors	Angle
N4-C1-N3	120.42
N4-C1-N2	120.13
N3-C1-N2	119.45
H5a-C5-H5c	108.11
H5a-C5-H5b	108.32
H5a-C5-C1	134.50
H5a-C5-N4	107.92
H5c-C5-H5b	110.46
H5c-C5-N4	110.39
H5b-C5-N4	111.52
H2a-N2-H2b	117.12
H2a-N2-C1	121.43
H2b-N2-C1	121.45
H3b-N3-H3a	117.22
H3b-N3-C1	121.46
H3a-N3-C1	121.31
H4-N4-C1	117.33
H4-N4-C5	117.56
C1-N4-C5	124.95

Table 83S. Computed atomic orthogonal coordinates for MGU optimized at the MP2/6-31+G** level.

Atom	x	y	z
C1	0.05115	-0.00076	-0.00259
N2	0.16736	-0.06750	0.00454
N3	0.05206	0.13307	-0.00119
N4	-0.06421	-0.06714	-0.00801
C5	-0.19599	-0.00480	0.00679
H2a	0.25469	-0.02245	-0.01770
H2b	0.16993	-0.16546	0.02791
H3a	0.13520	0.18405	0.02420
H3b	-0.02879	0.18634	-0.02893
H4	-0.06018	-0.16520	-0.03183
H5a	-0.26837	-0.08410	0.02212
H5b	-0.22367	0.05110	-0.08251
H5c	-0.19625	0.06001	0.09415

Table 84S. Computed bond lengths (Å) and angles (°) for MGU optimized at the MP2/6-31+G** level.

Vector	Length
C1-N2	1.342
C1-N3	1.338
C1-N4	1.332
N4-C5	1.465
H2a-N2	1.008
H2b-N2	1.007
H3a-N3	1.008
H3b-N3	1.007
H4-N4	1.010
H5a-C5	1.085
H5b-C5	1.089
H5c-C5	1.088

Vectors	Angle
N4-C1-N3	120.31
N4-C1-N2	120.28
N3-C1-N2	119.40
H5a-C5-H5c	108.70
H5a-C5-H5b	108.75
H5a-C5-N4	107.66
H5c-C5-H5b	110.61
H5c-C5-N4	109.68
H5b-C5-N4	111.35
H2a-N2-H2b	117.64
H2a-N2-C1	121.10
H2b-N2-C1	121.20
H3b-N3-H3a	117.65
H3b-N3-C1	121.37
H3a-N3-C1	120.94
H4-N4-C1	117.32
H4-N4-C5	118.22
C1-N4-C5	124.25

MeOH

Table 85S. Computed atomic orthogonal coordinates for MeOH optimized at the DFT-B3LYP/6-31+G** level.

Atom	x	Y	z
O1	0.07497	0.01224	0.00000
C2	-0.06682	-0.00207	0.00000
H1	0.11543	-0.07538	0.00005
H2a	-0.10824	0.09899	-0.00056
H2b	-0.10306	-0.05404	0.08976
H2c	-0.10299	-0.05506	-0.08919

Table 86S. Computed bond lengths (Å) and angles (°) for MeOH optimized at the DFT-B3LYP/6-31+G** level.

Vector	Length
O1-C2	1.425
H1-O1	0.965
H2a-C2	1.092
H2b-C2	1.099
H2c-C2	1.099
H1-O1-C2	109.02

Vectors	Angle
H2a-C2-H2b	108.47
H2a-C2-H2c	108.50
H2a-C2-O1	106.52
H2b-C2-H2c	109.06
H2b-C2-O1	112.07
H2c-C2-O1	112.08

Table 87S. Computed atomic orthogonal coordinates for MeOH optimized at the *ab initio*-MP2/6-31+G** level.

Atom	x	Y	z
O1	0.07508	0.01223	0.00000
C2	-0.06713	-0.00203	0.00000
H1	0.11460	-0.07573	0.00003
H2a	-0.10751	0.09875	-0.00034
H2b	-0.10246	-0.05464	-0.08888
H2c	-0.10248	-0.05402	0.08923

Table 88S. Computed bond lengths (Å) and angles (°) for MeOH optimized at the *ab initio*-MP2/6-31+G** level.

Vector	Length
O1-C2	1.429
H1-O1	0.964
H2a-C2	1.086
H2b-C2	1.092
H2c-C2	1.092
H1-O1-C2	108.47

Vectors	Angle
H2a-C2-H2b	108.93
H2a-C2-H2c	108.92
H2a-C2-O1	106.11
H2b-C2-H2c	109.34
H2b-C2-O1	111.72
H2c-C2-O1	111.70

HMB

Table 89S. Computed atomic orthogonal coordinates for HMB optimized at the DFT-B3LYP/6-31+G** level.

Atom	x	y	z
O1	-0.28134	-0.00949	0.00011
C2	-0.14418	-0.00175	0.00004
C3	-0.07283	-0.12210	-0.00003
C4	0.06647	-0.11970	-0.00011
C5	0.13831	0.00105	-0.00012
C6	0.06472	0.12007	-0.00011
C7	-0.07517	0.11965	-0.00002
C8	0.28954	0.00157	0.00015
H1	-0.31926	0.07935	0.00000
H3	-0.12747	-0.21587	-0.00005
H4	0.12059	-0.21404	-0.00018
H6	0.11698	0.21541	-0.00018
H7	-0.12988	0.21371	-0.00004
H8a	0.33007	-0.05228	-0.08633
H8b	0.32970	-0.04671	0.09005
H8c	0.32881	0.10363	-0.00295

Table 90S. Computed bond lengths (Å) and angles (°) for HMB optimized at the DFT-B3LYP/6-31+G** level.

Vector	Length
O1-C2	1.374
C2-C7	1.396
C2-C3	1.399
C3-C4	1.393
C4-C5	1.405
C5-C6	1.399
C5-C8	1.512
C6-C7	1.399
H1-O1	0.966
H3-C3	1.085
H4-C4	1.088
H6-C6	1.087
H7-C7	1.088
H8a-C8	1.096
H8b-C8	1.097
H8c-C8	1.094

Vectors	Angle
H1-O1-C2	109.88
O1-C2-C7	122.85
O1-C2-C3	117.43
C7-C2-C3	119.72
H3-C3-C4	121.22
H3-C3-C2	119.11
C4-C3-C2	119.67
H4-C4-C3	118.85
H4-C4-C5	119.41
C3-C4-C5	121.74
C6-C5-C4	117.52
C6-C5-C8	121.53
C4-C5-C8	120.95
H6-C6-C7	118.90
H6-C6-C5	119.54

C7-C6-C5	121.56
H7-C7-C2	120.20
H7-C7-C6	120.01
C2-C7-C6	119.79
H8c-C8-H8a	107.65
H8c-C8-H8b	107.61
H8c-C8-C5	111.23
H8a-C8-H8b	107.16
H8a-C8-C5	111.50
H8b-C8-C5	111.48

Table 91S. Computed atomic orthogonal coordinates for HMB optimized at the *ab initio* MP2/6-31+G** level.

Atom	x	y	z
O1	-0.28141	-0.00951	0.00106
C2	-0.14366	-0.00151	0.00065
C3	-0.07300	-0.12205	-0.00061
C4	0.06651	-0.12000	-0.00087
C5	0.13821	0.00065	-0.00181
C6	0.06518	0.12014	-0.00086
C7	-0.07469	0.12000	-0.00071
C8	0.28887	0.00142	0.00184
H1	-0.31825	0.07987	0.00222
H3	-0.12800	-0.21530	-0.00034
H4	0.12045	-0.21412	-0.00188
H6	0.11765	0.21508	-0.00190
H7	-0.12923	0.21383	-0.00058
H8a	0.32952	-0.08419	-0.05204
H8b	0.32614	-0.00305	0.10436
H8c	0.32847	0.09202	-0.04406

Table 92S. Computed bond lengths (Å) and angles (°) for HMB optimized at the *ab initio* MP2/6-31+G** level.

Vector	Length
O1-C2	1.380
C2-C3	1.397
C2-C7	1.397
C3-C4	1.395
C4-C5	1.404
C5-C6	1.400
C5-C8	1.507
C6-C7	1.399
H1-O1	0.967
H3-C3	1.083
H4-C4	1.085
H6-C6	1.085
H7-C7	1.085
H8a-C8	1.090
H8b-C8	1.092
H8c-C8	1.090

Vectors	Angle
H1-O1-C2	109.08
O1-C2-C3	117.06
O1-C2-C7	122.90
C3-C2-C7	120.03
H3-C3-C4	121.37
H3-C3-C2	119.09
C4-C3-C2	119.54
H4-C4-C3	118.97
H4-C4-C5	119.45
C3-C4-C5	121.56
C6-C5-C4	117.84
C6-C5-C8	121.12
C4-C5-C8	120.99
H6-C6-C7	118.98
H6-C6-C5	119.63
C7-C6-C5	121.37

H7-C7-C2	120.25
H7-C7-C6	120.11
C2-C7-C6	119.64
H8a-C8-H8c	108.01
H8a-C8-H8b	107.74
H8a-C8-C5	110.90
H8c-C8-H8b	107.78
H8c-C8-C5	110.93
H8b-C8-C5	111.33

ISOLATE MOLECULES
Solvent effect on the structure of selected molecules

HF

Table 93S. Computed atomic orthogonal coordinates for HF optimized at the DFT-B3LYP/6-31G** level with solvent treatment via PCM method (water).

Atom	x	y	z
F1	0.00000	0.00000	0.00939
H1	0.00000	0.00000	-0.08450

Table 94S. Computed bond lengths (Å) and angles (°) for HCl optimized at the DFT-B3LYP/6-31G** level, with solvent treatment via PCM method (water).

Vector	Length
F1-H1	0.939

HCl

Table 95S. Computed atomic orthogonal coordinates for HCl optimized at the DFT-B3LYP/6-31G** level with solvent treatment via PCM method (water).

Atom	x	y	z
Cl1	0.00000	0.00000	0.00718
H2	0.00000	0.00000	-0.12214

Table 96S. Computed bond lengths (Å) and angles (°) for HCl optimized at the DFT-B3LYP/6-31G** level, with solvent treatment via PCM method (water).

Vector	Length
Cl1-H2	1.293

Table 97S. Computed atomic orthogonal coordinates for HCl optimized at the DFT-B3LYP/6-31G** level with solvent treatment via PCM method (water).

Atom	x	y	z
Cl1	0.00000	0.00000	0.00719
H2	0.00000	0.00000	-0.12225

Table 98S. Computed bond lengths (Å) and angles (°) for HCl optimized at the DFT-B3LYP/6-31+G** level, with solvent treatment via PCM method (water).

Vector	Length
Cl1-H2	1.274

IM

Table 99S. Computed atomic orthogonal coordinates for IM optimized at the DFT-B3LYP/6-31G** level, with solvent treatment via PCM method (water).

Atom	x	y	z
H5	0.21329	0.07034	0.00000
H4	0.12152	-0.19149	0.00000
H2	-0.21038	0.06774	0.00000
H1	-0.00038	0.21231	0.00000
C5	0.11195	0.02986	0.00000
N3	-0.07473	-0.09877	0.00000
N1	0.00000	0.11039	0.00000
C4	0.06378	-0.09882	0.00000
C2	-0.10922	0.02893	0.00000

Table 100S. Computed bond lengths (Å) and angles (°) for IM optimized at the DFT-B3LYP/6-31G** level, with solvent treatment via PCM method (water).

Vector	Length
N1-C2	1.363
N1-C5	1.379
N3-C2	1.323
N3-C4	1.385
C4-C5	1.374
H1-N1	1.019
H2-C2	1.083
H4-C4	1.092
H5-C5	1.091

Vectors	Angle
H1-N1-C2	126.50
H1-N1-C5	125.94
C2-N1-C5	107.55
C2-N3-C4	105.13
H2-C2-N3	126.10
H2-C2-N1	122.29
N3-C2-N1	111.60
H4-C4-C5	127.55
H4-C4-N3	121.95
C5-C4-N3	110.50
H5-C5-C4	132.30
H5-C5-N1	122.50
C4-C5-N1	105.21

Table 101. Computed atomic orthogonal coordinates for IM optimized at the DFT-B3LYP/6-31+G** level, with solvent treatment via PCM method (water).

Atom	x	y	z
N1	0.00000	0.11044	0.00000
C2	-0.10912	0.02900	0.00000
N3	-0.07447	-0.09886	0.00000
C4	0.06387	-0.09897	0.00000
C5	0.11189	0.02993	0.00000
H1	-0.00103	0.21256	0.00000
H2	-0.21043	0.06745	0.00000
H4	0.12065	-0.19126	0.00000
H5	0.21230	0.07040	0.00000

Table 102S. Computed bond lengths (Å) and angles (°) for IM optimized at the DFT-B3LYP/6-31+G** level, with solvent treatment via PCM method (water).

Vector	Length
N1-C2	1.362
N1-C5	1.378
N3-C2	1.325
N3-C4	1.383
C4-C5	1.376
H1-N1	1.021
H2-C2	1.084
H4-C4	1.084
H5-C5	1.083

Vectors	Angle
H1-N1-C2	126.16
H1-N1-C5	126.31
C2-N1-C5	107.53
C2-N3-C4	105.21
H2-C2-N3	125.95
H2-C2-N1	122.48
N3-C2-N1	111.57
H4-C4-C5	127.97
H4-C4-N3	121.65
C5-C4-N3	110.39
H5-C5-C4	132.38
H5-C5-N1	122.31
C4-C5-N1	105.30

Table 103S. Computed atomic orthogonal coordinates for IM optimized at the DFT-B3LYP/6-31+G** level, with solvent treatment via PCM method (Methanol).

Atom	x	Y	z
N1	0.00000	0.11045	0.00000
C2	-0.10915	0.02900	0.00000
N3	-0.07449	-0.09885	0.00000
C4	0.06388	-0.09898	0.00000
C5	0.11193	0.02993	0.00000
H1	-0.00106	0.21254	0.00000
H2	-0.21047	0.06742	0.00000
H4	0.12064	-0.19128	0.00000
H5	0.21235	0.07038	0.00000

Table 104S. Computed bond lengths (Å) and angles (°) for IM optimized at the DFT-B3LYP/6-31+G** level, with solvent treatment via PCM method (Methanol).

Vector	Length
N1-C2	1.362
N1-C5	1.379
N3-C2	1.325
N3-C4	1.384
C4-C5	1.376
H1-N1	1.021
H2-C2	1.084
H4-C4	1.084
H5-C5	1.083

Vectors	Angle
H1-N1-C2	126.14
H1-N1-C5	126.33
C2-N1-C5	107.54
C2-N3-C4	105.22
H2-C2-N3	125.93
H2-C2-N1	122.50
N3-C2-N1	111.56
H4-C4-C5	127.97
H4-C4-N3	121.64
C5-C4-N3	110.39
H5-C5-C4	132.38
H5-C5-N1	122.33
C4-C5-N1	105.29

PYM

Table 105S. Computed atomic orthogonal coordinates for PYM optimized at the DFT-B3LYP/6-31+G** level, with solvent treatment via PCM method (water).

Atom	x	y	z
N1	-0.11926	0.07184	0.00000
C2	0.00000	0.13247	0.00000
N3	0.11938	0.07168	0.00000
C4	0.11874	-0.06291	0.00000
C5	-0.00008	-0.13623	0.00000
C6	-0.11878	-0.06280	0.00000
H2	0.00012	0.24199	0.00000
H4	0.21692	-0.11203	0.00000
H5	-0.00015	-0.24596	0.00000
H6	-0.21703	-0.11178	0.00000

Table 106S. Computed bond lengths (Å) and angles (°) for PYM optimized at the DFT-B3LYP/6-31+G** level, with solvent treatment via PCM method (water).

Vector	Length
N1-C2	1.338
N1-C6	1.346
N3-C2	1.340
N3-C4	1.346
C4-C5	1.396
C5-C6	1.396
H2-C2	1.095
H4-C4	1.098
H5-C5	1.097
H6-C6	1.098

Vectors	Angle
C2-N1-C6	116.74
C2-N3-C4	116.71
H2-C2-N1	117.01
H2-C2-N3	116.92
N1-C2-N3	126.07
H4-C4-N3	116.31
H4-C4-C5	121.74
N3-C4-C5	121.95
H5-C5-C4	121.71
H5-C5-C6	121.71
C6-C5-C4	116.58
H6-C6-N1	116.29
H6-C6-C5	121.76
N1-C6-C5	121.95

MAA

Table 107S. Computed atomic orthogonal coordinates for MAA optimized at the DFT-B3LYP/6-31+G** level, with solvent treatment via PCM method (water).

Atom	x	y	z
N1	-0.06073	-0.06419	-0.00004
C2	0.04786	0.01535	-0.00003
C3	0.18226	-0.05460	-0.00007
C4	-0.19622	-0.01052	0.00000
O5	0.03923	0.13950	0.00002
H1	-0.04921	-0.16617	-0.00008
H3a	0.23657	-0.02782	0.09120
H3b	0.24114	-0.01878	-0.08516
H3c	0.17381	-0.16350	-0.00556
H4a	-0.26638	-0.09409	0.00506
H4b	-0.21587	0.04732	-0.09104
H4c	-0.21220	0.05496	0.08631

Table 108S. Computed bond lengths (Å) and angles (°) for MAA optimized at the DFT-B3LYP/6-31+G** level, with solvent treatment via PCM method (water).

Vector	Length
N1-C2	1.346
N1-C4	1.457
C2-O5	1.244
C2-C3	1.515
H1-N1	1.026
H3a-C3	1.095
H3b-C3	1.095
H3c-C3	1.094
H4a-C4	1.092
H4b-C4	1.096
H4c-C4	1.095

Vectors	Angle
H1-N1-C2	119.78
H1-N1-C4	118.05
C2-N1-C4	122.17
O5-C2-N1	122.25
O5-C2-C3	121.47
N1-C2-C3	116.28
H3c-C3-H3b	109.16
H3c-C3-H3a	108.88
H3c-C3-C2	113.03
H3b-C3-H3a	107.51
H3b-C3-C2	109.04
H3a-C3-C2	109.07
H4a-C4-H4c	109.10
H4a-C4-H4b	109.08
H4a-C4-N1	108.39
H4c-C4-H4b	108.23
H4c-C4-N1	110.86
H4b-C4-N1	111.14

MA

Table 109S. Computed atomic orthogonal coordinates for MA optimized at the DFT-B3LYP/6-31+G** level, with solvent treatment via PCM method (water).

Atom	x	y	z
N1	0.07030	-0.00005	-0.00002
C2	-0.07935	-0.00002	-0.00003
H3	0.10881	-0.09300	0.02314
H4	0.10855	0.02684	-0.09213
H5	0.10802	0.06673	0.06921
H6	-0.11370	-0.03016	0.09901
H7	-0.11392	-0.07069	-0.07557
H8	-0.11378	0.10080	-0.02331

Table 110S. Computed bond lengths (Å) and angles (°) for MA optimized at the DFT-B3LYP/6-31+G** level, with solvent treatment via PCM method (water).

Vector	Length
N1-C2	1.497
H3-N1	1.032
H4-N1	1.033
H5-N1	1.033
H6-C2	1.091
H7-C2	1.091
H8-C2	1.091

Vectors	Angle
H3-N1-H4	107.23
H3-N1-H5	107.18
H3-N1-C2	111.91
H4-N1-H5	107.10
H4-N1-C2	111.73
H5-N1-C2	111.41
H8-C2-H6	110.48
H8-C2-H7	110.56
H8-C2-N1	108.42
H6-C2-H7	110.49
H6-C2-N1	108.35
H7-C2-N1	108.47

MGU

Table 111S. Computed atomic orthogonal coordinates for MGU optimized at the DFT-B3LYP/6-31+G** level, with solvent treatment via PCM method (water).

Atom	x	y	z
C1	-0.05083	-0.00041	0.00077
N2	-0.16658	-0.06881	-0.00424
N3	-0.05367	0.13335	0.00005
N4	0.06459	-0.06730	0.00097
C5	0.19602	-0.00384	0.00049
H2a	-0.25517	-0.02025	0.00930
H2b	-0.16539	-0.16942	0.01271
H3a	-0.14298	0.18218	0.00615
H3b	0.03070	0.18974	-0.00799
H4	0.05947	-0.17008	-0.00635
H5a	0.27104	-0.08311	-0.00003
H5b	0.21064	0.05768	0.09007
H5c	0.21024	0.05807	-0.08890

Table 112S. Computed bond lengths (Å) and angles (°) for MGU optimized at the DFT-B3LYP/6-31+G** level, with solvent treatment via PCM method (water).

Vector	Length
C1-N4	1.334
C1-N3	1.338
C1-N2	1.345
C5-N4	1.459
H2a-N2	1.019
H2b-N2	1.020
H3a-N3	1.020
H3b-N3	1.018
H4-N4	1.032
H5a-C5	1.091
H5b-C5	1.096
H5c-C5	1.097

Vectors	Angle
N4-C1-N3	121.31
N4-C1-N2	119.31
N3-C1-N2	119.33
H5a-C5-H5b	108.65
H5a-C5-H5c	108.48
H5a-C5-N4	107.65
H5b-C5-H5c	109.38
H5b-C5-N4	111.18
H5c-C5-N4	111.40
H2a-N2-H2b	117.25
H2a-N2-C1	120.04
H2b-N2-C1	119.02
H3b-N3-H3a	117.73
H3b-N3-C1	122.46
H3a-N3-C1	119.80
H4-N4-C1	117.16
H4-N4-C5	118.53
C1-N4-C5	124.13

TWO-PARTICLE SYSTEMS
Small particle systems

$F\text{-}H\ldots F^-$

Table 113S. Computed atomic orthogonal coordinates for $FH\ldots F^-$ optimized at the DFT-B3LYP/6-31G** level.

Atom	x	Y	z
F1	0.00000	-0.11506	0.00000
F3	0.00000	0.11506	0.00000
H2	-0.00003	-0.00001	0.00000

Table 114S. Computed bond lengths (Å) and angles (°) for $FH\ldots F^-$ optimized at the DFT-B3LYP/6-31G** level.

Vector	Length
F1-H2	1.151
F3-H2	1.151

Vectors	Angle
F1-H2-F3	179.97

Table 115S. Computed atomic orthogonal coordinates for FH…F$^-$ optimized at the DFT-B3LYP/6-31++G** level.

Atom	x	y	z
F1	0.00000	-0.11471	0.00000
F3	0.00000	0.11471	0.00000
H2	-0.00002	-0.00001	0.00000

Table 116S. Computed bond lengths (Å) and angles (°) for FH…F$^-$ optimized at the DFT-B3LYP/6-31++G** level.

Vector	Length
F1-H2	1.147
F3-H2	1.147

Vectors	Angle
F1-H2-F3	180.00

Table 117S. Computed atomic orthogonal coordinates for FH…F^- optimized at the *ab initio*-CCSD(T)/6-311++G** level.

Atom	x	y	z
F1	0.00000	0.00000	-0.11346
F3	0.00000	0.00000	0.11347
H2	0.00000	0.00000	-0.00004

Table 118S. Computed bond lengths (Å) and angles (°) for FH…F^- optimized at the *ab initio*-CCSD(T)/6-311++G** level.

Vector	Length
F1-H2	1.1342
H2...F3	1.1351

Vectors	Angle
F1-H2...F3	180.00

$Cl\text{-}H\ldots Cl^-$

Table 119S. Computed atomic orthogonal coordinates for $ClH\ldots Cl^-$ optimized at the DFT-B3LYP/6-31G** level.

Atom	x	Y	z
Cl1	0.00000	0.00000	-0.15778
Cl3	0.00000	0.00000	0.15778
H2	0.00000	0.00000	-0.00005

Table 120S. Computed bond lengths (Å) and angles (°) for $ClH\ldots Cl^-$ optimized at the DFT-B3LYP/6-31G** level.

Vector	Length
Cl1-H2	1.577
Cl3-H2	1.578

Vectors	Angle
Cl1-H2-Cl3	180.00

Table 121S. Computed atomic orthogonal coordinates for ClH…Cl^- optimized at the DFT-B3LYP/6-311++G** level.

Atom	x	y	z
Cl1	0.00000	0.00000	-0.15775
Cl3	0.00000	0.00000	0.15775
H2	0.00000	0.00000	-0.00002

Table 122S. Computed bond lengths (Å) and angles (°) for ClH…Cl^- optimized at the DFT-B3LYP/6-311++G** level.

Vector	Length
Cl1-H2	1.5773
H2…Cl3	1.5777

Vectors	Angle
Cl1-H2…Cl3	180.00

Table 123S. Computed atomic orthogonal coordinates for ClH…Cl^- optimized at the *ab initio*-CCSD(T)/6-311++G** level.

Atom	x	y	z
Cl1	0.00000	0.00000	-0.15552
Cl3	0.00000	0.00000	0.15552
H2	0.00000	0.00000	-0.00005

Table 124S. Computed bond lengths (Å) and angles (°) for ClH…Cl^- optimized at the the *ab initio*-CCSD(T)/6-311++G** level.

Vector	Length
Cl1-H2	1.5547
H2...Cl3	1.5557

Vectors	Angle
Cl1-H2...Cl3	180.00

$FH…OH_2$

Table 125S. Computed atomic orthogonal coordinates for $FH…OH_2$ optimized at the *ab initio*-RHF/6-31G* level.

Atom	x	y	z
F2	0.00000	0.00000	0.14668
O3	0.00000	0.00000	-0.12622
H1	0.00000	0.00000	0.05465
H5	0.00000	-0.07625	-0.18249
H4	0.00000	0.07625	-0.18249

Table 126S. Computed bond lengths (Å) and angles (°) for $FH…OH_2$ optimized at the *ab initio*-RHF/6-31G* level.

Vector	Length
F2-H1	0.920
O3-H4	0.948
O3-H5	0.948
H1...O3	1.809
F2...O3	2.729

Vectors	Angle
H4-O3-H5	107.15
F2-H1...O3	180.00 (fixed)

Table 127S. Computed atomic orthogonal coordinates for FH…OH_2 optimized at the *ab initio*-CCSD(T)/6-31G** level.

Atom	x	y	z
H5	0.00000	-0.07682	-0.18213
H4	0.00000	0.07682	-0.18213
F2	0.00000	0.00000	0.14527
O3	0.00000	0.00000	-0.12442
H1	0.00000	0.00000	0.05221

Table 128S. Computed bond lengths (Å) and angles (°) for FH…OH_2 optimized at the *ab initio*-CCSD(T)/6-31G** level.

Vector	Length
F2-H1	0.931
O3-H4	0.961
O3-H5	0.961
H1...O3	1.766
F2...O3	2.697

Vectors	Angle
H4-O3-H5	106.17
F2-H1...O3	180.00(fixed)

Table 129S. Computed atomic orthogonal coordinates for FH…OH_2 optimized at the *ab initio*-CCSD(T)/6-31+G** level.

Atom	x	y	z
H1	0.00000	0.00000	0.05055
F2	0.00000	0.00000	0.14438
O3	0.00000	0.00000	-0.12356
H4	0.00000	0.07749	-0.18074
H5	0.00000	-0.07749	-0.18074

Table 130S. Computed bond lengths (Å) and angles (°) for FH…OH_2 optimized at the *ab initio*-CCSD(T)/6-31+G** level.

Vector	Length
F2-H1	0.938
O3-H4	0.963
O3-H5	0.963
H1…O3	1.741
F2…O3	2.679

Vectors	Angle
H4-O3-H5	107.15
O3…H1-F2	180.0(fixed)

Table 131S. Computed atomic orthogonal coordinates for FH…OH_2 optimized at the DFT-B3LYP/6-31G** level.

Atom	x	y	z
H1	0.00000	0.00000	0.04953
H4	0.00000	0.07730	-0.18006
H5	0.00000	-0.07730	-0.18006
F2	0.00000	0.00000	0.14342
O3	0.00000	0.00000	-0.12253

Table 132S. Computed bond lengths (Å) and angles (°) for FH…OH_2 optimized at the DFT-B3LYP/6-31G** level.

Vector	Length
F2-H1	0.939
O3-H4	0.964
O3-H5	0.964
H1…O3	1.721
F2…O3	2.659

Vectors	Angle
H4-O3-H5	106.68
F2-H1…O3	180.0(fixed)

Table 133S. Computed atomic orthogonal coordinates for FH…OH_2 optimized at the DFT-B3LYP/6-31+G** level.

Atom	x	y	z
H1	0.00000	0.00000	0.04714
H4	0.00000	0.07803	-0.17768
H5	0.00000	-0.07803	-0.17768
F2	0.00000	0.00000	0.14180
O3	0.00000	0.00000	-0.12100

Table 134S. Computed bond lengths (Å) and angles (°) for FH…OH_2 optimized at the DFT-B3LYP/6-31+G** level.

Vector	Length
F2-H1	0.947
O3-H4	0.964
O3-H5	0.964
H1…O3	1.681
F2…O3	2.628

Vectors	Angle
H4-O3-H5	108.01
F2-H1…O3	180.00(fixed)

HO-H…FH

Table 135S. Computed atomic orthogonal coordinates for HO-H…FH optimized at the DFT-B3LYP/6-31G** level.

Atom	x	y	z
H1	-0.00130	0.23187	0.00000
H5	-0.09150	-0.16732	0.00000
O4	0.00446	-0.15732	0.00000
F2	0.00446	0.13950	0.00000
H3	0.01698	-0.06150	0.00000

Table 136S. Computed bond lengths (Å) and angles (°) for HO-H…FH optimized at the DFT-B3LYP/6-31G** level.

Vector	Lengt
F2-H1	0.925
O4-H5	0.965
O4-H3	0.966
H3…F2	2.014
O4…F2	2.968

Vectors	Angle
H5-O4-H3	103.39
O4-H3…F2	168.99

Table 137S. Computed atomic orthogonal coordinates for HO-H…FH optimized at the DFT-B3LYP/6-31+G** level.

Atom	x	y	z
H1	-0.00144	0.23886	0.00000
H5	-0.09129	-0.17605	0.00000
O4	0.00440	-0.16379	0.00000
F2	0.00440	0.14618	0.00000
H3	0.01790	-0.06808	0.00000

Table 138S. Computed bond lengths (Å) and angles (°) for HO-H…FH optimized at the DFT-B3LYP/6-31+G** level.

Vector	Length
F2-H1	0.929
O4-H5	0.965
O4-H3	0.967
H3…F2	2.147
O4…F2	3.100

Vectors	Angle
H5-O4-H3	105.33
F2…H3-O4	168.37

Table 139S. Computed atomic orthogonal coordinates for HO-H…FH optimized at the *ab initio*-CCSD(T)/6-31G** level.

Atom	x	y	z
H1	-0.00101	0.23450	0.00000
H5	-0.09116	-0.17061	0.00000
O4	0.00444	-0.16022	0.00000
F2	0.00444	0.14251	0.00000
H3	0.01672	-0.06478	0.00000

Table 140S. Computed bond lengths (Å) and angles (°) for HO-H…FH optimized at the *ab initio*-CCSD(T)/6-31G** level.

Vector	Length
F2-H1	0.922
O4-H5	0.962
O4-H3	0.962
H3…F2	2.077
O4…F2	3.027

Vectors	Angle
H5-O4-H3	103.53
O4-H3…F2	169.28

Table 141S. Computed atomic orthogonal coordinates for HO-H…FH optimized at the *ab initio*-CCSD(T)/6-31+G** level.

Atom	x	y	z
H1	-0.00957	0.23751	0.00000
F2	0.00386	0.14587	0.00000
H3	0.03609	-0.07411	0.00000
O4	0.00386	-0.16497	0.00000
H5	-0.09209	-0.15645	0.00000

Table 142S. Computed bond lengths (Å) and angles (°) for HO-H…FH optimized at the *ab initio*-CCSD(T)/6-31+G** level.

Vector	Length
F2-H1	0.926
O4-H5	0.963
O4-H3	0.964
H3…F2	2.223
O4…F2	3.108

Vectors	Angle
H5-O4-H3	104.46
F2…H3-O4	152.13

Table 143S. Computed atomic orthogonal coordinates for HO-H…FH optimized at the *ab initio* MP2/6-31+G** level.

Atom	x	y	z
H1	-0.00796	0.23833	0.00000
H3	0.03247	-0.07307	0.00000
H5	-0.09222	-0.16084	0.00000
F2	0.00398	0.14635	0.00000
O4	0.00398	-0.16520	0.00000

Table 144S. Computed bond lengths (Å) and angles (°) for HO-H…FH optimized at the *ab initio* MP2/6-31+G** level.

Vector	Length
F2-H1	0.928
O4-H5	0.963
O4-H3	0.964
H3…F2	2.213
O4…F2	3.115

Vectors	Angle
H5-O4-H3	104.59
F2…H3-O4	155.42

$ClH\ldots OH_2$

Table 145S. Computed atomic orthogonal coordinates for $ClH\ldots OH_2$ optimized at the *ab initio*-CCSD(T)/6-31G** level.

Atom	x	y	z
Cl2	0.00000	0.00000	0.12306
H1	0.00000	0.00000	-0.00541
O3	0.00000	0.00000	-0.19703
H4	0.00000	0.07654	-0.25523
H5	0.00000	-0.07654	-0.25523

Table 146S. Computed bond lengths (Å) and angles (°) for $ClH\ldots OH_2$ optimized at the *ab initio*-CCSD(T)/6-31G** level.

Vector	Length
O3…H1	1.916
O3…Cl2	3.201
Cl2-H1	1.285
O3-H4	0.962
O3-H5	0.962

Vectors	Angle
H1…O3-H4	127.25
H1…O3-H5	127.25
H4-O3-H5	105.50

Table 147S. Computed atomic orthogonal coordinates for ClH…OH_2 optimized at the *ab initio*-CCSD(T)/6-31+G** level.

Atom	x	y	z
H5	0.00000	-0.07711	-0.25633
H4	0.00000	0.07711	-0.25633
Cl2	0.00000	0.00000	0.12384
O3	0.00000	0.00000	-0.19852
H1	0.00000	0.00000	-0.00457

Table 148S. Computed bond lengths (Å) and angles (°) for ClH…OH_2 optimized at the *ab initio*-CCSD(T)/6-31+G** level.

Vector	Length
O3...H1	1.940
O3...Cl2	3.224
Cl2-H1	1.284
O3-H4	0.964
O3-H5	0.964

Vectors	Angle
H1...O3-H4	126.86
H1...O3-H5	126.86
H4-O3-H5	106.28

Table 149S. Computed atomic orthogonal coordinates for ClH…OH_2 optimized at the DFT-B3LYP/6-31G** level.

Atom	x	y	z
H5	0.00000	-0.07725	-0.24870
H4	0.00000	0.07725	-0.24870
Cl2	0.00000	0.00000	0.11980
O3	0.00000	0.00000	-0.19102
H1	0.00000	0.00000	-0.01113

Table 150S. Computed bond lengths (Å) and angles (°) for ClH…OH_2 optimized at the DFT-B3LYP/6-31G** level.

Vector	Length
O3…H1	1.799
O3…Cl2	3.108
Cl2-H1	1.309
O3-H4	0.964
O3-H5	0.964

Vectors	Angle
H4-O3-H5	106.51
H1…O3-H4	126.75
H1…O3-H5	126.75

Table 151S. Computed atomic orthogonal coordinates for ClH…OH_2 optimized at the DFT-B3LYP/6-31+G** level.

Atom	x	y	z
H5	0.00000	-0.07772	-0.25161
H4	0.00000	0.07772	-0.25161
Cl2	0.00000	0.00000	0.12162
O3	0.00000	0.00000	-0.19442
H1	0.00000	0.00000	-0.00888

Table 152S. Computed bond lengths (Å) and angles (°) for ClH…OH_2 optimized at the DFT-B3LYP/6-31+G** level.

Vector	Length
O3...H1	1.855
O3...Cl2	3.224
Cl2-H1	1.305
O3-H4	0.965
O3-H5	0.965

Vectors	Angle
H1...O3-H4	126.35
H1...O3-H5	126.35
H4-O3-H5	107.31

Table 153S. Computed atomic orthogonal coordinates for ClH…OH_2 optimized at the DFT-B3LYP/6-31++G** level.

Atom	x	y	z
H5	0.00000	-0.07773	-0.25160
H4	0.00000	0.07773	-0.25160
Cl2	0.00000	0.00000	0.12161
O3	0.00000	0.00000	-0.19441
H1	0.00000	0.00000	-0.00892

Table 154S. Computed bond lengths (Å) and angles (°) for ClH…OH_2 optimized at the DFT-B3LYP/6-31++G** level.

Vector	Length
O3…H1	1.855
O3…Cl2	3.160
Cl2-H1	1.305
O3-H4	0.965
O3-H5	0.965

Vectors	Angle
H4-O3-H5	107.31
H1…O3-H4	126.34
H1…O3-H5	126.34

Table 155S. Computed atomic orthogonal coordinates for ClH…OH_2 optimized at the DFT-B3LYP/6-311++G** level.

Atom	x	y	z
H5	0.00000	-0.07728	-0.25225
H4	0.00000	0.07728	-0.25225
Cl2	0.00000	0.00000	0.12191
O3	0.00000	0.00000	-0.19493
H1	0.00000	0.00000	-0.00856

Table 156S. Computed bond lengths (Å) and angles (°) for ClH…OH_2 optimized at the DFT-B3LYP/6-311++G** level.

Vector	Length
O3…H1	1.864
O3…Cl2	3.168
Cl2-H1	1.305
O3-H4	0.962
O3-H5	0.962

Vectors	Angle
H1…O3-H4	126.56
H1...O3-H5	126.56
H4-O3-H5	106.87

Table 157S. Computed atomic orthogonal coordinates for ClH…OH_2 optimized at the *ab initio*-CCSD(T)/6-311++G** level.

Atom	x	y	z
Cl2	0.00000	0.00000	0.12421
H5	0.00000	-0.07609	-0.25759
H4	0.00000	0.07609	-0.25759
H1	0.00000	0.00000	-0.00449
O3	0.00000	0.00000	-0.19900

Table 158S. Computed bond lengths (Å) and angles (°) for ClH…OH_2 optimized at the *ab initio*-CCSD(T)/6-311++G** level.

Vector	Length
O3…H1	1.945
O3…Cl2	3.232
Cl2-H1	1.287
O3-H4	0.960
O3-H5	0.960

Vectors	Angle
H1…O3-H4	127.60
H1…O3-H5	127.60
H4-O3-H5	104.81

Table 159S. Computed atomic orthogonal coordinates for ClH…OH_2 optimized at the *ab initio*-CCSD(T)/6-31++G** level.

Atom	x	y	z
H5	0.00000	-0.07712	-0.25635
H4	0.00000	0.07712	-0.25635
Cl2	0.00000	0.00000	0.12386
O3	0.00000	0.00000	-0.19853
H1	0.00000	0.00000	-0.00461

Table 160S. Computed bond lengths (Å) and angles (°) for ClH…OH_2 optimized at the *ab initio*-CCSD(T)/6-31++G** level.

Vector	Length
O3...H1	1.939
O3...Cl2	3.224
Cl2-H1	1.285
O3-H4	0.964
O3-H5	0.964

Vectors	Angle
H1...O3-H4	126.86
H1...O3-H5	126.86
H4-O3-H5	106.28

HO-H…ClH

Table 161S. Computed atomic orthogonal coordinates for HO-H…ClH optimized at the DFT-B3LYP/6-31G** level.

Atom	x	y	z
H1	0.03361	-0.24040	0.00000
O4	-0.00065	0.23377	0.00000
Cl2	-0.00065	-0.11645	0.00000
H3	-0.08401	0.18513	0.00000
H5	0.06676	0.16468	0.00000

Table 162S. Computed bond lengths (Å) and angles (°) for HO-H…ClH optimized at the DFT-B3LYP/6-31G** level.

Vector	Length
O4...Cl2	3.502
H3...Cl2	3.129
H5...Cl2	2.891
Cl2-H1	1.286
O4-H3	0.965
O4-H5	0.965

Vectors	Angle
Cl2...H5-O4	122.22
Cl2...H3-O4	104.81
H5...Cl2-H1	151.07
H3...Cl2-H1	180.
H3-O4-H5	104.03

Table 163S. Computed atomic orthogonal coordinates for HO-H…ClH optimized at the DFT-B3LYP/6-31+G** level.

Atom	x	y	z
H1	0.03162	-0.24722	0.00000
O4	-0.00073	0.24488	0.00000
Cl2	-0.00073	-0.12268	0.00000
H3	-0.08317	0.19464	0.00000
H5	0.06983	0.17898	0.00000

Table 164S. Computed bond lengths (Å) and angles (°) for HO-H…ClH optimized at the DFT-B3LYP/6-31+G** level.

Vector	Length
O4...Cl2	3.676
H3...Cl2	3.279
H5...Cl2	3.098
Cl2-H1	1.287
O4-H3	0.965
O4-H5	0.965

Vectors	Angle
Cl2...H5-O4	119.88
Cl2...H3-O4	106.80
H5...Cl2-H1	152.27
H3...Cl2-H1	179.98
H3-O4-H5	105.60

TWO-PARTICLE SYSTEMS
Imidazole…X^- (X: Cl^-, F^-) systems

(IM)N1-H…Cl^-

Table 165S. Computed atomic orthogonal coordinates for (IM)N1-H…Cl^- optimized at the DFT-B3LYP/6-31+G** level.

Atom	x	y	z
Cl1	-0.00820	-0.28544	0.00000
N1	0.00000	0.02391	0.00000
C2	0.11071	0.10227	0.00000
N3	0.08166	0.23197	0.00000
C4	-0.05610	0.23626	0.00000
C5	-0.10808	0.10833	0.00000
H1	-0.00279	-0.08134	0.00000
H2	0.21039	0.06045	0.00000
H4	-0.10965	0.33033	0.00000
H5	-0.20927	0.07067	0.00000

Table 166S. Computed bond lengths (Å) and angles (°) for (IM)N1-H…Cl^- optimized at the DFT-B3LYP/6-31+G** level.

Vector	Length
N1-C2	1.356
N1-C5	1.371
N3-C2	1.329
N3-C4	1.378
C4-C5	1.381
H1-N1	1.053
H2-C2	1.081
H4-C4	1.082
H5-C5	1.080
H1…Cl1	2.042
N1…Cl1	3.095

Vectors	Angle
H1-N1-C2	126.81
H1-N1-C5	126.47
C2-N1-C5	106.72
C2-N3-C4	104.41
H2-C2-N3	125.38
H2-C2-N1	121.95
N3-C2-N1	112.67
H4-C4-N3	121.43
H4-C4-C5	128.24
N3-C4-C5	110.33
H5-C5-N1	121.59
H5-C5-C4	132.53
N1-C5-C4	105.88
N1-H1…Cl1	180.00

Table 167S. Computed atomic orthogonal coordinates for (IM)N1-H…Cl^- optimized at the DFT-B3LYP/6-31G** level.

Atom	x	y	z
Cl1	-0.00893	-0.28338	0.00000
H4	-0.10884	0.32940	0.00000
H5	-0.20891	0.07033	0.00000
H2	0.21012	0.05886	0.00000
N3	0.08238	0.23096	0.00000
C4	-0.05531	0.23522	0.00000
H1	-0.00309	-0.08305	0.00000
C5	-0.10763	0.10774	0.00000
C2	0.11059	0.10123	0.00000
N1	0.00000	0.02287	0.00000

Table 168S. Computed bond lengths (Å) and angles (°) for (IM)N1-H…Cl^- optimized at the DFT-B3LYP/6-31G** level.

Vector	Distance
N1-C2	1.355
N1-C5	1.371
N3-C2	1.328
N3-C4	1.378
C4-C5	1.378
H1-N1	1.060
H2-C2	1.082
H4-C4	1.083
H5-C5	1.080
Cl1…H1	2.004
Cl1…N1	3.064

Vectors	Angle
H1-N1-C2	126.99
H1-N1-C5	126.59
C2-N1-C5	106.42
C2-N3-C4	104.04
H2-C2-N3	125.33
H2-C2-N1	121.62
N3-C2-N1	113.05
H4-C4-N3	121.39
H4-C4-C5	128.07
N3-C4-C5	110.54
H5-C5-N1	121.47
H5-C5-C4	132.59
N1-C5-C4	105.94
N1-H1…Cl1	180.00(fixed)

Table 169S. Computed atomic orthogonal coordinates for (IM)N1-H…Cl^- optimized at the *ab initio* MP2/6-31+G** level.

Atom	x	y	z
Cl1	-0.00783	-0.28244	0.00000
N1	0.00000	0.02244	0.00000
C2	0.11078	0.10081	0.00000
N3	0.08125	0.23146	0.00000
C4	-0.05652	0.23480	0.00000
C5	-0.10823	0.10620	0.00000
H1	-0.00269	-0.08247	0.00000
H2	0.21018	0.05928	0.00000
H4	-0.11039	0.32826	0.00000
H5	-0.20896	0.06816	0.00000

Table 170S. Computed bond lengths (Å) and angles (°) for (IM)N1-H…Cl^- optimized at the *ab initio* MP2/6-31+G** level.

Vector	Length
N1-C2	1.357
N1-C5	1.369
N3-C2	1.339
N3-C4	1.378
C4-C5	1.386
H1-N1	1.049
H2-C2	1.077
H4-C4	1.079
H5-C5	1.077
H1…Cl1	2.000
N1…Cl1	3.050

Vectors	Angle
H1-N1-C2	126.75
H1-N1-C5	126.27
C2-N1-C5	106.99
C2-N3-C4	104.12
H2-C2-N3	125.41
H2-C2-N1	122.05
N3-C2-N1	112.54
H4-C4-N3	121.35
H4-C4-C5	128.14
N3-C4-C5	110.52
H5-C5-N1	121.57
H5-C5-C4	132.59
N1-C5-C4	105.83
N1-H1…Cl1	180.00(fixed)

(IM)C2-H…Cl$^-$

Table 171S. Computed atomic orthogonal coordinates for (IM)C2-H…Cl$^-$ optimized at the DFT-B3LYP/6-31+G** level.

Atom	x	y	z
Cl1	-0.12409	-0.28764	0.00000
N1	0.13565	0.05757	0.00000
C2	0.00000	0.03826	0.00000
N3	-0.06353	0.15434	0.00000
C4	0.03497	0.25094	0.00000
C5	0.16003	0.19351	0.00000
H1	0.20360	-0.01702	0.00000
H2	-0.03897	-0.06408	0.00000
H4	0.01045	0.35635	0.00000
H5	0.25971	0.23502	0.00000

Table 172S. Computed bond lengths (Å) and angles (°) for (IM)C2-H…Cl^- optimized at the DFT-B3LYP/6-31+G** level.

Vector	Length
N1-C2	1.370
N1-C5	1.381
N3-C2	1.323
N3-C4	1.380
C4-C5	1.376
H1-N1	1.009
H2-C2	1.095
H4-C4	1.082
H5-C5	1.080
H2…Cl1	2.392
C2…Cl1	3.487

Vectors	Angle
H1-N1-C2	124.23
H1-N1-C5	127.50
C2-N1-C5	108.27
C2-N3-C4	105.75
H2-C2-N3	130.46
H2-C2-N1	118.95
N3-C2-N1	110.59
H4-C4-C5	127.76
H4-C4-N3	121.35
C5-C4-N3	110.89
H5-C5-C4	132.73
H5-C5-N1	122.78
C4-C5-N1	104.50
C2-H2…Cl1	180.00 (fixed)

Table 173S. Computed atomic orthogonal coordinates for (IM)C2-H…Cl^- optimized at the DFT-B3LYP/6-31G** level.

Atom	x	y	z
Cl1	-0.13011	-0.27969	0.00000
N1	0.13609	0.05174	0.00000
C2	0.00000	0.03635	0.00000
N3	-0.06016	0.15419	0.00000
C4	0.04135	0.24758	0.00000
C5	0.16447	0.18681	0.00000
H1	0.20178	-0.02472	0.00000
H2	-0.04189	-0.06540	0.00000
H4	0.02017	0.35380	0.00000
H5	0.26541	0.22515	0.00000

Table 174S. Computed bond lengths (Å) and angles (°) for (IM)C2-H…Cl^- optimized at the DFT-B3LYP/6-31G** level.

Vector	Distance
N1-C2	1.370
N1-C5	1.380
N3-C2	1.323
N3-C4	1.379
C4-C5	1.373
H1-N1	1.008
H2-C2	1.100
H4-C4	1.083
H5-C5	1.080
Cl1…H2	2.317
Cl1…C2	3.418

Vectors	Angle
H1-N1-C2	124.22
H1-N1-C5	127.47
C2-N1-C5	108.32
C2-N3-C4	105.57
H2-C2-N3	130.58
H2-C2-N1	118.83
N3-C2-N1	110.59
H4-C4-C5	127.55
H4-C4-N3	121.34
C5-C4-N3	111.12
H5-C5-C4	132.93
H5-C5-N1	122.66
C4-C5-N1	104.40
C2-H2…Cl1	180.00(fixed)

(IM)C4-H…Cl$^-$

Table 175S. Computed atomic orthogonal coordinates for (IM)C4-H…Cl$^-$ optimized at the DFT-B3LYP/6-31G** level.

Atom	x	y	z
Cl1	-0.01046	-0.32238	0.00000
N1	0.06896	0.24332	0.00000
C2	-0.06786	0.23852	0.00000
N3	-0.11265	0.11498	0.00000
C4	0.00000	0.03399	0.00000
C5	0.11301	0.11194	0.00000
H1	0.12641	0.32605	0.00000
H2	-0.12840	0.32832	0.00000
H4	-0.00321	-0.07549	0.00000
H5	0.21794	0.08674	0.00000

Table 176S. Computed bond lengths (Å) and angles (°) for (IM)C4-H…Cl^- optimized at the DFT-B3LYP/6-31G** level.

Vector	Distance
N1-C2	1.369
N1-C5	1.386
N3-C2	1.314
N3-C4	1.387
C4-C5	1.373
H1-N1	1.007
H2-C2	1.083
H4-C4	1.095
H5-C5	1.079
Cl1…H4	2.470
Cl1…C4	3.565

Vectors	Angle
H1-N1-C2	126.79
H1-N1-C5	126.69
C2-N1-C5	106.53
C2-N3-C4	105.79
H2-C2-N3	126.09
H2-C2-N1	121.98
N3-C2-N1	111.94
H4-C4-C5	126.28
H4-C4-N3	124.03
C5-C4-N3	109.69
H5-C5-C4	131.90
H5-C5-N1	122.04
C4-C5-N1	106.06
C4-H4…Cl1	180.00(fixed)

Table 177S. Computed atomic orthogonal coordinates for (IM)C4-H…Cl^- optimized at the DFT-B3LYP/6-31+G** level.

Atom	x	y	z
Cl1	-0.01159	-0.32833	0.00000
N1	0.06984	0.24589	0.00000
C2	-0.06713	0.24180	0.00000
N3	-0.11217	0.11813	0.00000
C4	0.00000	0.03676	0.00000
C5	0.11355	0.11433	0.00000
H1	0.12759	0.32850	0.00000
H2	-0.12760	0.33156	0.00000
H4	-0.00346	-0.07227	0.00000
H5	0.21830	0.08832	0.00000

Table 178S. Computed bond lengths (Å) and angles (°) for (IM)C4-H…Cl^- optimized at the DFT-B3LYP/6-31+G** level.

Vector	Length
N1-C2	1.370
N1-C5	1.386
N3-C2	1.316
N3-C4	1.386
C4-C5	1.375
H1-N1	1.008
H2-C2	1.082
H4-C4	1.091
H5-C5	1.079
H4…Cl1	2.562
C4…Cl1	3.653

Vectors	Angle
H1-N1-C2	126.67
H1-N1-C5	126.67
C2-N1-C5	106.67
C2-N3-C4	105.95
H2-C2-N3	126.02
H2-C2-N1	122.26
N3-C2-N1	111.72
H4-C4-C5	126.16
H4-C4-N3	124.14
C5-C4-N3	109.70
H5-C5-C4	131.72
H5-C5-N1	122.32
C4-C5-N1	105.96
C4-H4…Cl1	180.00(fixed)

(IM)C5-H…Cl$^-$

Table 179S. Computed atomic orthogonal coordinates for (IM)C5-H…Cl$^-$ optimized at the DFT-B3LYP/6-31G** level.

Atom	x	y	z
Cl1	0.13821	-0.27766	0.00000
N1	0.13723	0.04839	0.00000
C2	0.16630	0.18196	0.00000
N3	0.05676	0.25513	0.00000
C4	-0.04691	0.16325	0.00000
C5	0.00000	0.03403	0.00000
H1	0.20219	-0.02871	0.00000
H2	0.26781	0.21958	0.00000
H4	-0.15008	0.19561	0.00000
H5	-0.04453	-0.06640	0.00000

Table 180S. Computed bond lengths (Å) and angles (°) for (IM)C5-H…Cl^- optimized at the DFT-B3LYP/6-31G** level.

Vector	Length
N1-C2	1.367
N1-C5	1.380
N3-C2	1.317
N3-C4	1.385
C4-C5	1.375
H1-N1	1.008
H2-C2	1.083
H4-C4	1.081
H5-C5	1.099
H5…Cl1	2.311
C5…Cl1	3.410

Vectors	Angle
H1-N1-C2	127.61
H1-N1-C5	124.14
H1-N1-C5	99.13
C2-N1-C5	108.25
C2-N3-C4	104.71
H2-C2-N3	125.92
H2-C2-N1	122.61
N3-C2-N1	111.46
H4-C4-C5	127.37
H4-C4-N3	121.04
C5-C4-N3	111.60
H5-C5-C4	136.14
H5-C5-N1	119.89
C4-C5-N1	103.98
C5-H5…Cl1	180.00 (fixed)

Table 181S. Computed atomic orthogonal coordinates for (IM)C5-H…Cl^- optimized at the DFT-B3LYP/6-31+G** level.

Atom	x	y	z
Cl1	-0.12926	-0.28795	0.00000
H2	0.25975	0.23312	0.00000
H4	-0.15716	0.19147	0.00000
H1	0.20488	-0.01800	0.00000
N3	0.04725	0.25931	0.00000
C2	0.16010	0.19101	0.00000
H5	-0.04047	-0.06521	0.00000
C4	-0.05279	0.16347	0.00000
N1	0.13654	0.05624	0.00000
C5	0.00000	0.03633	0.00000

Table 182S. Computed bond lengths (Å) and angles (°) for (IM)C5-H…Cl^- optimized at the DFT-B3LYP/6-31+G** level.

Vector	Length
N1-C2	1.368
N1-C5	1.380
N3-C2	1.319
N3-C4	1.385
C4-C5	1.377
H1-N1	1.009
H2-C2	1.082
H4-C4	1.081
H5-C5	1.093
H5…Cl1	2.398
C5…Cl1	3.491

Vectors	Angle
H1-N1-C2	127.45
H1-N1-C5	124.33
C2-N1-C5	108.21
C2-N3-C4	105.04
H2-C2-N3	125.91
H2-C2-N1	122.82
N3-C2-N1	111.27
H4-C4-C5	127.57
H4-C4-N3	121.21
C5-C4-N3	111.22
H5-C5-C4	135.72
H5-C5-N1	120.03
C4-C5-N1	104.25
C5-H5…Cl1	180.00 (fixed)

$(IMH^+)N1\ldots H^+\ldots Cl^-$

Table 183S. Computed atomic orthogonal coordinates for $(IMH^+)N1\ldots H^+\ldots Cl^-$ optimized at the DFT- B3LYP/6-31+G** level.

Atom	x	y	z
Cl1	-0.03045	-0.28187	0.00000
H4	-0.08912	0.33454	0.00000
H3	0.16233	0.28814	0.00000
H5	-0.20444	0.08210	0.00000
H1	-0.01733	-0.14566	0.00000
H2	0.21277	0.03792	0.00000
C4	-0.04518	0.23605	0.00000
N3	0.09159	0.21614	0.00000
C5	-0.10025	0.11043	0.00000
C2	0.11415	0.08198	0.00000
N1	0.00000	0.01588	0.00000

Table 184S. Computed bond lengths (Å) and angles (°) for $(IMH^+)N1\ldots H^+\ldots Cl^-$ optimized at the DFT- B3LYP/6-31+G** level.

Vector	Distance
N1-C2	1.319
N1-C5	1.378
N3-C2	1.360
N3-C4	1.382
C4-C5	1.372
H1-Cl1	1.368
H2-C2	1.080
H3-N3	1.009
H4-C4	1.078
H5-C5	1.080
Cl1-H1	1.368
N1…H1	1.625
N1…Cl1	2.993

Vectors	Angle
C2-N1-C5	106.60
H3-N3-C2	125.96
H3-N3-C4	126.21
C2-N3-C4	107.83
H2-C2-N1	125.85
H2-C2-N3	123.62
N1-C2-N3	110.53
H4-C4-C5	132.28
H4-C4-N3	122.33
C5-C4-N3	105.39
H5-C5-C4	128.88
H5-C5-N1	121.46
C4-C5-N1	109.65
N1…H1-Cl1	179.38

Table 185S. Computed atomic orthogonal coordinates for $(IMH^+)N1\ldots H^+\ldots Cl^-$ optimized at the *ab initio*- MP2/6-31+G** level.

Atom	x	y	z
Cl1	-0.05807	-0.28301	0.00000
N1	0.00000	0.01822	0.00000
C2	0.12130	0.07243	0.00000
N3	0.11298	0.20845	0.00000
C4	-0.02026	0.24311	0.00000
C5	-0.08876	0.12348	0.00000
H1	-0.03466	-0.15339	0.00000
H2	0.21463	0.01870	0.00000
H3	0.19100	0.27240	0.00000
H4	-0.05311	0.34554	0.00000
H5	-0.19519	0.10726	0.00000

Table 186S. Computed bond lengths (Å) and angles (°) for $(IMH^+)N1\ldots H^+\ldots Cl^-$ optimized at the *ab initio*- MP2/6-31+G** level.

Atom	Length
N1-C2	1.329
N1-C5	1.377
N3-C2	1.363
N3-C4	1.377
C4-C5	1.379
H1-Cl1	1.317
H2-C2	1.077
H3-N3	1.009
H4-C4	1.076
H5-C5	1.077
N1…H1	1.751

Vectors	Angle
C2-N1-C5	106.06
H3-N3-C2	125.84
H3-N3-C4	126.08
C2-N3-C4	108.08
H2-C2-N1	125.99
H2-C2-N3	123.43
N1-C2-N3	110.58
H4-C4-N3	122.36
H4-C4-C5	132.42
N3-C4-C5	105.21
H5-C5-N1	121.47
H5-C5-C4	128.46
N1-C5-C4	110.07
N1…H1-Cl1	178.82
H1…N1-C2	125.50
H1…N1-C5	128.44

(IM)N1-H…F$^-$

Table 187S. Computed atomic orthogonal coordinates for (IM)N1-H…F$^-$ optimized at the DFT-B3LYP/6-31G** level.

Atom	x	y	z
F1	-0.00012	0.29280	0.00000
H4	0.12050	-0.26714	0.00000
H5	0.21005	-0.00553	0.00000
H1	-0.00007	0.19264	0.00000
H2	-0.20748	-0.00932	0.00000
N3	-0.07448	-0.17627	0.00000
C4	0.06291	-0.17499	0.00000
C5	0.10869	-0.04423	0.00000
C2	-0.10503	-0.04562	0.00000
N1	0.00000	0.03959	0.00000

Table 188S. Computed bond lengths (Å) and angles (°) for (IM)N1-H…F^- optimized at the DFT-B3LYP/6-31G** level.

Vector	Distance
N1-C2	1.352
N1-C5	1.373
N3-C3	1.342
C4-C5	1.385
H1-F1	1.002
H2-C2	1.087
H4-C4	1.087
H5-C5	1.085
H1…N1	1.531
F1…N1	2.532

Vectors	Angle
C2-N1-C5	103.31
C2-N3-C4	102.63
H2-C2-N3	122.67
H2-C2-N1	121.44
N3-C2-N1	115.89
H4-C4-N3	121.47
H4-C4-C5	128.70
N3-C4-C5	109.83
H5-C5-N1	121.46
H5-C5-C4	130.19
N1-C5-C4	108.34

(IM)C2-H…F$^-$

Table 189S. Computed atomic orthogonal coordinates for (IM)C2-H…F$^-$ optimized at the DFT-B3LYP/6-31G** level.

Atom	x	y	z
F1	-0.09117	0.28335	0.00000
H5	-0.05930	-0.28198	0.00000
H4	0.20649	-0.20505	0.00000
H2	-0.05240	0.18167	0.00000
H1	-0.18574	-0.05869	0.00000
C5	-0.01304	-0.18415	0.00000
C4	0.11766	-0.14239	0.00000
N3	0.12572	-0.00457	0.00000
N1	-0.08518	-0.06575	0.00000
C2	0.00000	0.04422	0.00000

Table 190S. Computed bond lengths (Å) and angles (°) for (IM)C2-H…F^- optimized at the DFT-B3LYP/6-31G** level.

Vector	Distance
N1-C5	1.386
N1-C2	1.391
N3-C2	1.349
N3-C4	1.381
C4-C5	1.372
H1-N1	1.008
H2-F1	1.088
H4-C4	1.087
H5-C5	1.082
H2…C2	1.471
F1…C2	2.559

Vectors	Angle
H1-N1-C2	124.22
H1-N1-C5	127.47
C2-N1-C5	108.32
C2-N1-C2	26.46
C2-N3-C4	105.57
H2-C2-N3	130.58
H2-C2-N1	118.83
N3-C2-N1	110.59
H4-C4-C5	127.55
H4-C4-N3	121.34
C5-C4-N3	111.12
H5-C5-C4	132.93
H5-C5-N1	122.66
C4-C5-N1	104.40
C2-H2…F1	180.00(fixed)

TWO-PARTICLE SYSTEMS
Imidazole…Imidazole systems

(IM)N1-H…N3’(IM) (coplanar)

Table 191S. Computed atomic orthogonal coordinates for (IM)N1-H…N3’(IM)(coplanar) optimized at the DFT- B3LYP/6-31+G** level.

Atom	x	y	z
N1	-0.00511	0.15664	0.00000
N3	-0.09213	0.36186	0.00000
N1'	0.08120	-0.35339	0.00000
N3'	0.00808	-0.14450	0.00000
C2	-0.11850	0.23241	0.00000
C4	0.04536	0.37019	0.00000
C5	0.10120	0.24430	0.00000
C2'	0.11528	-0.22139	0.00000
C4'	-0.09981	-0.23057	0.00000
C5'	-0.05668	-0.36087	0.00000
H1	0.00000	0.05414	0.00000
H2	-0.21738	0.18865	0.00000
H4	0.09606	0.46567	0.00000
H5	0.20372	0.21050	0.00000
H1'	0.14523	-0.43142	0.00000
H2'	0.21785	-0.18738	0.00000
H4'	-0.20141	-0.19391	0.00000
H5'	-0.10945	-0.45495	0.00000

Table 192S. Computed bond lengths (Å) and angles (°) for (IM)N1-H…N3’(IM) (coplanar) optimized at the DFT- B3LYP/6-31+G** level.

Vector	Distance
N1'-C2'	1.363
N1'-C5'	1.381
N1-C2	1.364
N1-C5	1.378
N3-C2	1.321
N3-C4	1.377
N3'-C2'	1.319
N3'-C4'	1.380
C4-C5	1.377
C4'-C5'	1.373
H1-N1	1.026
H1'-N1'	1.009
H2-C2	1.081
H2'-C2'	1.081
H4-C4	1.081
H4'-C4'	1.080
H5'-C5'	1.079
H5-C5	1.079
N3'…H1	1.988
N3'…N1	3.014

Vectors	Angle
H1'-N1'-C2'	126.15
H1'-N1'-C5'	126.27
C2'-N1'-C5'	107.58
H1-N1-C2	126.61
H1-N1-C5	126.65
C2-N1-C5	106.74
C2-N3-C4	104.98
C2'-N3'-C4'	105.77
H2'-C2'-N3'	126.01
H2'-C2'-N1'	122.82
N3'-C2'-N1'	111.17

H2-C2-N3	125.39
H2-C2-N1	122.38
N3-C2-N1	112.24
H4-C4-C5	128.11
H4-C4-N3	121.44
C5-C4-N3	110.45
H4'-C4'-C5'	128.16
H4'-C4'-N3'	121.58
C5'-C4'-N3'	110.27
H5'-C5'-C4'	132.40
H5'-C5'-N1'	122.39
C4'-C5'-N1'	105.21
H5-C5-C4	132.17
H5-C5-N1	122.25
C4-C5-N1	105.59
N3'…H1-N1	179.48
H1…N3'-C2'	127.98
H1…N3'-C4'	126.25

(IM)N1-H…N3’(IM) (free)

Table 193S. Computed atomic orthogonal coordinates for (IM)N1-H…N3’(IM) (free) optimized at the DFT- B3LYP/6-31+G** level.

Atom	x	y	z
N1	0.15542	0.00028	0.00070
C2	0.23693	-0.02005	-0.10677
N3	0.36485	-0.01417	-0.07424
C4	0.36603	0.01126	0.06116
C5	0.23744	0.02059	0.10956
N1'	-0.35412	-0.06581	0.01225
C2'	-0.22309	-0.10279	0.01905
N3'	-0.14348	0.00075	0.00031
C4'	-0.22659	0.10914	-0.01942
C5'	-0.35796	0.07004	-0.01240
H1	0.05274	0.00043	0.00049
H2	0.19819	-0.03863	-0.20600
H5	0.19815	0.03922	0.20836
H4	0.45877	0.02136	0.11580
H1'	-0.43382	-0.12675	0.02326
H2'	-0.19160	-0.20449	0.03753
H4'	-0.18703	0.20804	-0.03734
H5'	-0.45065	0.12432	-0.02231

Table 194S. Computed bond lengths (Å) and angles (°) for (IM)N1-H…N3’(IM) (free) optimized at the DFT- B3LYP/6-31+G** level.

Vector	Length
N1-C2	1.364
N1-C5	1.378
N1'-C2'	1.363
N1'-C5'	1.381
N3-C2	1.321
N3-C4	1.378
N3'-C2'	1.319
N3'-C4'	1.380
C4'-C5'	1.372
C4-C5	1.377
H1'-N1'	1.009
H1-N1	1.027
H2-C2	1.081
H2'-C2'	1.081
H4'-C4'	1.080
H4-C4	1.081
H5'-C5'	1.079
H5-C5	1.079
H1…N3'	1.962
N1…N3'	2.989

Vectors	Angle
H1-N1-C2	126.59
H1-N1-C5	126.63
C2-N1-C5	106.78
H1'-N1'-C2'	126.14
H1'-N1'-C5'	126.25
C2'-N1'-C5'	107.60
C2-N3-C4	104.98
C2'-N3'-C4'	105.86
H2'-C2'-N3'	125.95
H2'-C2'-N1'	122.95
N3'-C2'-N1'	111.10

H2-C2-N3	125.48
H2-C2-N1	122.31
N3-C2-N1	112.21
H4'-C4'-C5'	128.31
H4'-C4'-N3'	121.49
C5'-C4'-N3'	110.21
H4-C4-C5	128.10
H4-C4-N3	121.42
C5-C4-N3	110.48
H5'-C5'-C4'	132.41
H5'-C5'-N1'	122.36
C4'-C5'-N1'	105.23
H5-C5-C4	132.32
H5-C5-N1	122.13
C4-C5-N1	105.55
N1-H1…N3'	179.93

(IM)C2-H…N3’(IM)

Table 195S. Computed atomic orthogonal coordinates for (IM)C2-H…N3’(IM) optimized at the DFT- B3LYP/6-31+G** level.

Atom	x	y	z
H5'	-0.08890	-0.44173	0.00000
H4	-0.25417	0.40190	0.00000
C5'	-0.01981	-0.35887	0.00000
C4	-0.16262	0.34444	0.00000
H4'	-0.13142	-0.16804	0.00000
H1'	0.16582	-0.46524	0.00000
N3	-0.16424	0.20652	0.00000
C4'	-0.03822	-0.22277	0.00000
N1'	0.11717	-0.37685	0.00000
H5	0.00812	0.49098	0.00000
C5	-0.03342	0.39138	0.00000
C2	-0.03757	0.16959	0.00000
H2	0.00000	0.06805	0.00000
N3'	0.08349	-0.15760	0.00000
C2'	0.17456	-0.25282	0.00000
N1	0.04570	0.27813	0.00000
H2'	0.28167	-0.23829	0.00000
H1	0.14653	0.27526	0.00000

Table 196S. Computed bond lengths (Å) and angles (°) for (IM)C2-H…N3'(IM) optimized at the DFT- B3LYP/6-31+G** level.

Vector	Length
N1'-C2'	1.367
N1'-C5'	1.382
N1-C2	1.368
N1-C5	1.382
N3-C2	1.319
N3-C4	1.379
N3'-C2'	1.318
N3'-C4'	1.381
C4-C5	1.375
C4'-C5'	1.373
H1'-N1'	1.009
H1-N1	1.009
H2-C2	1.083
H2'-C2'	1.081
H4-C4	1.081
H4'-C4'	1.081
H5'-C5'	1.079
H5-C5	1.079
H2…N3'	2.406
C2…N3'	3.489

Vectors	Angle
H1'-N1'-C2'	126.34
H1'-N1'-C5'	126.31
C2'-N1'-C5'	107.35
H1-N1-C2	125.86
H1-N1-C5	126.57
C2-N1-C5	107.57
C2-N3-C4	105.58
C2'-N3'-C4'	105.56
H2'-C2'-N3'	126.00
H2'-C2'-N1'	122.56
N3'-C2'-N1'	111.45

H2-C2-N3	126.56
H2-C2-N1	122.20
N3-C2-N1	111.24
H4-C4-C5	127.92
H4-C4-N3	121.44
C5-C4-N3	110.64
H4'-C4'-C5'	128.13
H4'-C4'-N3'	121.41
C5'-C4'-N3'	110.46
H5-C5-C4	132.61
H5-C5-N1	122.42
C4-C5-N1	104.97
H5'-C5'-C4'	132.47
H5'-C5'-N1'	122.34
C4'-C5'-N1'	105.18
C2-H2…N3'	180.00(fixed)
H2…N3'-C2'	156.58
H2…N3'-C4'	97.86

TWO-PARTICLE SYSTEMS
Pyrimidine…Cl^- systems

(PYM)C2-H…Cl^-

Table 197S. Computed atomic orthogonal coordinates for (PYM)C2-H…Cl^- optimized at the DFT-B3LYP/6-31+G** level.

Atom	x	y	z
Cl1	-0.00033	-0.34778	0.00000
H5	0.00038	0.38595	0.00000
H6	0.21558	0.25256	0.00000
H4	-0.21509	0.25298	0.00000
H2	-0.00010	-0.10225	0.00000
C5	0.00027	0.27734	0.00000
C6	0.11838	0.20313	0.00000
C4	-0.11799	0.20336	0.00000
N3	-0.11953	0.06977	0.00000
N1	0.11965	0.06954	0.00000
C2	0.00000	0.00748	0.00000

Table 198S. Computed bond lengths (Å) and angles (°) for (PYM)C2-H…Cl^- optimized at the DFT- B3LYP/6-31+G** level.

Vector	Length
N1-C6	1.336
N1-C2	1.348
N3-C4	1.336
N3-C2	1.348
C2-H2	1.097
C4-H4	1.090
C4-C5	1.395
C5-H5	1.086
C5-C6	1.395
C6-H6	1.090
H2…Cl1	2.455
C2…Cl1	2.553

Vectors	Angle
C6-N1-C2	116.87
C4-N3-C2	116.86
H2-C2-N1	117.47
H2-C2-N3	117.47
N1-C2-N3	125.06
H4-C4-N3	116.41
H4-C4-C5	120.90
N3-C4-C5	122.69
H5-C5-C4	122.09
H5-C5-C6	122.08
C4-C5-C6	115.83
H6-C6-N1	116.41
H6-C6-C5	120.90
N1-C6-C5	122.69
C2-H2…Cl1	180.0 (fixed)

Table 199S. Computed atomic orthogonal coordinates for (PYM)C2-H…Cl^- optimized at the DFT-B3LYP/6-31+G** level. The C2-H…Cl angle was fixed at 140°.

Atom	x	y	z
Cl1	0.32767	-0.09312	0.00000
H5	-0.37702	0.01906	0.00000
H4	-0.26077	0.24408	0.00000
H6	-0.22755	-0.18539	0.00000
C5	-0.26873	0.02746	0.00000
C4	-0.20409	0.15094	0.00000
H2	0.10887	0.05763	0.00000
C6	-0.18565	-0.08473	0.00000
N3	-0.07086	0.16224	0.00000
N1	-0.05243	-0.07625	0.00000
C2	0.00000	0.04728	0.00000

Table 200S. Computed bond lengths (Å) and angles (°) for (PYM)C2-H… Cl^- optimized at the DFT- B3LYP/6-31+G** level. The C2-H…Cl angle was fixed at 140°.

Vector	Distance
N1-C6	1.335
N1-C2	1.342
N3-C4	1.337
N3-C2	1.350
C4-C5	1.394
C5-C6	1.396
H2-C2	1.094
H4-C4	1.090
H5-C5	1.086
H6-C6	1.090
Cl1…H2	2.657
Cl1…C2	3.500

Vectors	Angle
C6-N1-C2	116.64
C4-N3-C2	116.80
H2-C2-N1	118.43
H2-C2-N3	116.22
N1-C2-N3	125.35
H4-C4-N3	116.47
H4-C4-C5	121.05
N3-C4-C5	122.48
H5-C5-C4	122.07
H5-C5-C6	122.09
C4-C5-C6	115.85
H6-C6-N1	116.24
H6-C6-C5	120.88
N1-C6-C5	122.88
Cl1…H2-C2	140.00(fixed)

(PYM)C5-H…Cl$^-$

Table 201S. Computed atomic orthogonal coordinates for (PYM)C5-H…Cl$^-$ optimized at the DFT-B3LYP/6-31+G** level.

Atom	x	y	z
Cl1	-0.00142	-0.34332	0.00000
N1	0.12076	0.21060	0.00000
C2	0.00112	0.27054	0.00000
N3	-0.11901	0.21161	0.00000
C4	-0.11770	0.07707	0.00000
C5	0.00000	0.00224	0.00000
C6	0.11833	0.07609	0.00000
H2	0.00158	0.37945	0.00000
H4	-0.21460	0.02761	0.00000
H5	-0.00045	-0.10756	0.00000
H6	0.21480	0.02580	0.00000

Table 202S. Computed bond lengths (Å) and angles (°) for (PYM)C5-H…Cl^- optimized at the DFT- B3LYP/6-31+G** level.

Vector	Length
N1-C2	1.338
N1-C6	1.345
N3-C2	1.338
N3-C4	1.345
C4-C5	1.395
C5-C6	1.395
H2-C2	1.089
H4-C4	1.088
H5-C5	1.098
H6-C6	1.088
H5…Cl1	2.358
C5…Cl1	3.456

Vectors	Angle
C2-N1-C6	115.58
C2-N3-C4	115.57
H2-C2-N1	116.37
H2-C2-N3	116.37
N1-C2-N3	127.26
H4-C4-N3	116.48
H4-C4-C5	120.51
N3-C4-C5	123.00
H5-C5-C4	122.21
H5-C5-C6	122.20
C6-C5-C4	115.58
H6-C6-N1	116.50
H6-C6-C5	120.50
N1-C6-C5	123.00
C5-H5…Cl1	180.00

(PYM)C6-H…Cl$^-$

Table 203S. Computed atomic orthogonal coordinates for (PYM)C6-H…Cl$^-$ optimized at the DFT-B3LYP/6-31+G** level.

Atom	x	y	z
Cl1	0.20595	-0.27645	0.00000
N1	0.05526	0.12766	0.00000
C2	-0.02945	0.23109	0.00000
N3	-0.16342	0.22752	0.00000
C4	-0.21719	0.10433	0.00000
C5	-0.13925	-0.01076	0.00000
C6	0.00000	0.00493	0.00000
H2	0.01559	0.33027	0.00000
H4	-0.32604	0.09929	0.00000
H5	-0.18316	-0.11001	0.00000
H6	0.06489	-0.08372	0.00000

Table 204S. Computed bond lengths (Å) and angles (°) for (PYM)C6-H…Cl^- optimized at the DFT- B3LYP/6-31+G** level.

Vector	Length
N1-C2	1.337
N1-C6	1.346
N3-C2	1.340
N3-C4	1.344
C4-C5	1.390
C5-C6	1.401
H2-C2	1.089
H4-C4	1.090
H5-C5	1.085
H6-C6	1.099
H6…Cl1	2.388
C6…Cl1	3.456

Vectors	Angle
C2-N1-C6	116.44
C2-N3-C4	115.11
H2-C2-N1	116.26
H2-C2-N3	115.95
N1-C2-N3	127.79
H4-C4-N3	116.23
H4-C4-C5	121.46
N3-C4-C5	122.31
H5-C5-C4	122.03
H5-C5-C6	120.29
C6-C5-C4	117.68
H6-C6-N1	119.56
H6-C6-C5	119.77
N1-C6-C5	120.67
C6-H6…Cl1	180.00

Table 205S. Computed atomic orthogonal coordinates for (PYM)C6-H…Cl^- optimized at the DFT-B3LYP/6-31+G** level. The C6-H…Cl angle was fixed at 140.0°.

Atom	x	y	z
Cl1	0.32767	-0.09312	0.00000
H5	-0.37702	0.01906	0.00000
H4	-0.26077	0.24408	0.00000
H6	-0.22755	-0.18539	0.00000
C5	-0.26873	0.02746	0.00000
C4	-0.20409	0.15094	0.00000
H2	0.10887	0.05763	0.00000
C6	-0.18565	-0.08473	0.00000
N3	-0.07086	0.16224	0.00000
N1	-0.05243	-0.07625	0.00000
C2	0.00000	0.04728	0.00000

Table 206S. Computed bond lengths (Å) and angles (°) for (PYM)C6-H… Cl^- optimized at the DFT- B3LYP/6-31+G** level. The C6-H…Cl angle was fixed at 140.0°.

Vector	Distance
N1-C2	1.335
N1-C6	1.342
N3-C2	1.342
N3-C4	1.342
C4-C5	1.391
C5-C4	1.391
C5-C6	1.403
H2-C2	1.089
H4-C4	1.090
H5-C5	1.086
Cl1…H6	2.560
Cl1…C6	3.472

Vectors	Angle
C2-N1-C6	116.42
C2-N3-C4	115.00
H2-C2-N1	116.15
H2-C2-N3	115.88
N1-C2-N3	127.97
H4-C4-N3	116.37
H4-C4-C5	121.44
N3-C4-C5	122.19
H5-C5-C4	121.41
H5-C5-C6	120.79
C4-C5-C6	117.80
H6-C6-N1	119.54
H6-C6-C5	119.83
N1-C6-C5	120.62
Cl1…H6-C6	140.00(fixed)

(**MePYM)C-H…Cl$^-$**

Table 207S. Computed atomic orthogonal coordinates for (MePYM)C-H…Cl$^-$ optimized at the DFT- B3LYP/6-31G** level.

Atom	x	y	z
Cl1	-0.35265	-0.03693	-0.00003
N1	0.27037	-0.10289	-0.00002
C2	0.27903	0.03052	-0.00004
N3	0.17949	0.11958	-0.00003
C4	0.05416	0.06949	0.00002
C5	0.03248	-0.06934	0.00005
C6	0.14473	-0.15098	0.00003
C7	-0.06392	0.16234	0.00004
H2	0.38005	0.07176	-0.00008
H5	-0.06959	-0.10759	0.00009
H6	0.13474	-0.25951	0.00005
H7a	-0.15447	0.09984	0.00002
H7b	-0.06179	0.22713	0.08841
H7c	-0.06178	0.22719	-0.08828

Table 208S. Computed bond lengths (Å) and angles (°) for (MePYM)C-H…Cl^- optimized at the DFT- B3LYP/6-31G** level.

Vector	Length
N1-C2	1.337
N1-C6	1.345
N3-C2	1.336
N3-C4	1.350
C4-C5	1.405
C4-C7	1.502
C5-C6	1.388
H2-C2	1.091
H5-C5	1.090
H6-C6	1.090
H7a-C7	1.100
H7b-C7	1.096
H7c-C7	1.096
H7a…Cl1	2.408
C7…Cl1	3.508
H5…Cl1	2.917
C5…Cl1	3.865

Vectors	Angle
C2-N1-C6	114.66
C2-N3-C4	116.40
H2-C2-N3	115.97
H2-C2-N1	115.92
N3-C2-N1	128.11
N3-C4-C5	120.66
N3-C4-C7	120.04
C5-C4-C7	119.30
H5-C5-C6	123.43
H5-C5-C4	119.42
C6-C5-C4	117.15
H6-C6-N1	116.20
H6-C6-C5	120.77
N1-C6-C5	123.03

H7b-C7-H7c	107.43
H7b-C7-H7a	110.61
H7b-C7-C4	110.50
H7c-C7-H7a	110.61
H7c-C7-C4	110.51
H7a-C7-C4	107.21
C7-H7a…Cl1	180.00(fixed)
C5-H5…Cl1	145.44

TWO-PARTICLE SYSTEMS
Pyrimidine…Pyrimidine systems

PYM…PYM
(PYM)C2-H…N1'(PYM)/(PYM)C6'-H…N3(PYM)

Table 209S. Computed atomic orthogonal coordinates for (PYM)C2-H…N1'(PYM)/(PYM)C6'-H…N3(PYM) optimized at the DFT- B3LYP/6-31G** level.

Atom	x	y	z
H5	0.48543	-0.18210	0.00000
H4'	-0.36302	0.37181	0.00000
H6	0.33541	-0.38539	0.00000
C5	0.37736	-0.17292	0.00000
N3'	-0.38184	0.16585	0.00000
C4'	-0.30820	0.27774	0.00000
C6	0.29411	-0.28465	0.00000
H5'	-0.11055	0.36696	0.00000
H4	0.37202	0.04356	0.00000
H2'	-0.37161	-0.04040	0.00000
C5'	-0.16894	0.27555	0.00000
C4	0.31432	-0.04876	0.00000
N1	0.16063	-0.27484	0.00000
C2'	-0.31293	0.05126	0.00000
C2	0.11093	-0.15055	0.00000
N3	0.18104	-0.03616	0.00000
C6'	-0.10819	0.15011	0.00000
N1'	-0.17998	0.03673	0.00000
H2	0.00262	-0.14004	0.00000
H6'	0.00000	0.13795	0.00000

Table 210S. Computed bond lengths (Å) and angles (°) for (PYM)C2-H…N1'(PYM)/(PYM)C6'-H…N3(PYM)optimized at the DFT- B3LYP/6-31G** level.

Vector	Length
N1-C6	1.338
N1-C2	1.339
N1'-C2'	1.337
N1'-C6'	1.342
N3-C4	1.339
N3-C2	1.342
N3'-C2'	1.337
N3'-C4'	1.339
C4-C5	1.392
C4'-C5'	1.393
C5-C6	1.393
C5'-C6'	1.394
H2'-C2'	1.088
H2-C2	1.088
H4'-C4'	1.089
H4-C4	1.089
H5-C5	1.085
H5'-C5'	1.085
H6-C6	1.089
H6'-C6'	1.089
H2…N1'	2.541
C2…N1'	3.460
H6'…N3	2.512
C6'…N3	3.440

Vectors	Angle
C6-N1-C2	116.00
C2'-N1'-C6'	116.10
C4-N3-C2	116.10
C2'-N3'-C4'	115.63
H2'-C2'-N3'	116.35
H2'-C2'-N1'	116.39
N3'-C2'-N1'	127.26

H2-C2-N1	117.34
H2-C2-N3	115.96
N1-C2-N3	126.70
H4-C4-N3	116.60
H4-C4-C5	121.08
N3-C4-C5	122.32
H4'-C4'-N3'	116.42
H4'-C4'-C5'	121.13
N3'-C4'-C5'	122.45
H5-C5-C4	121.77
H5-C5-C6	121.83
C4-C5-C6	116.39
H5'-C5'-C4'	121.67
H5'-C5'-C6'	121.59
C4'-C5'-C6'	116.74
H6-C6-N1	116.50
H6-C6-C5	121.02
N1-C6-C5	122.49
H6'-C6'-N1'	115.93
H6'-C6'-C5'	122.25
N1'-C6'-C5'	121.82
C2-H2…N1'	141.47
C6'-H6'…N3	142.53

Table 211S. Computed atomic orthogonal coordinates for (PYM)C2-H…N1’(PYM)/(PYM)C6’-H…N3(PYM) optimized at the DFT- B3LYP/6-31+G** level.

Atom	x	y	z
H5	0.48252	-0.20261	0.00000
H4’	-0.34654	0.39080	0.00000
H6	0.32445	-0.40019	0.00000
C5	0.37485	-0.18929	0.00000
N3’	-0.37907	0.18654	0.00000
C4	-0.29811	0.29335	0.00000
C6	0.28735	-0.29789	0.00000
H2’	-0.38319	-0.02005	0.00000
H5’	-0.09460	0.36867	0.00000
H4	0.37767	0.02747	0.00000
C4	0.31663	-0.06263	0.00000
C2’	-0.31837	0.06726	0.00000
C5’	-0.15921	0.28150	0.00000
N1	0.15429	-0.28269	0.00000
C2	0.10920	-0.15657	0.00000
N3	0.18381	-0.04501	0.00000
N1’	-0.18659	0.04382	0.00000
C6’	-0.10715	0.15207	0.00000
H2	0.00138	-0.14249	0.00000
H6’	0.00000	0.13297	0.00000

Table 212S. Computed bond lengths (Å) and angles (°) for (PYM)C2-H…N1’(PYM)/(PYM)C6’-H…N3(PYM)optimized at the DFT- B3LYP/6-31+G** level.

Vector	Length
N1'-C2'	1.338
N1'-C6'	1.343
N1-C2	1.339
N1-C6	1.342
N3'-C2'	1.338
N3'-C4'	1.340
N3-C4	1.340
N3-C2	1.342
C4'-C5'	1.394
C4-C5	1.394
C5'-C6'	1.395
C5-C6	1.395
H2'-C2'	1.087
H2-C2	1.087
H4'-C4'	1.088
H4-C4	1.088
H5'-C5'	1.085
H5-C5	1.085
H6'-C6'	1.088
H6-C6	1.088
H2…N1'	2.647
C2…N1'	3.573
H6'…N3	2.559
C6'…N3	3.514

Vectors	Angle
C2'-N1'-C6'	116.19
C2-N1-C6	116.19
C2'-N3'-C4'	115.87
C4-N3-C2	116.22
H2-C2-N1	117.11
H2-C2-N3	116.33
N1-C2-N3	126.55

H2'-C2'-N1'	116.50
H2'-C2'-N3'	116.44
N1'-C2'-N3'	127.06
H4'-C4'-N3'	116.41
H4'-C4'-C5'	121.30
N3'-C4'-C5'	122.29
H4-C4-N3	116.56
H4-C4-C5	121.20
N3-C4-C5	122.24
H5'-C5'-C4'	121.67
H5'-C5'-C6'	121.54
C4'-C5'-C6'	116.79
H5-C5-C4	121.74
H5-C5-C6	121.81
C4-C5-C6	116.46
H6'-C6'-N1'	116.17
H6'-C6'-C5'	122.02
N1'-C6'-C5'	121.82
H6-C6-N1	116.45
H6-C6-C5	121.21
N1-C6-C5	122.34
C2-H2…N1'	142.69
H2…N1'-C2'	145.34
H2…N1'-C6'	98.47
C6'-H6'…N3	146.03
H6'…N3-C2	100.03
H6'…N3-C4	143.48

(PYM)C2-H…N1’(PYM)

Table 213S. Computed atomic orthogonal coordinates for (PYM)C2-H…N1’(PYM) optimized at the DFT- B3LYP/6-31+G** level.

Atom	x	y	z
H5	0.00230	0.55754	0.00000
H4'	-0.01593	-0.55542	0.00000
H5'	0.20845	-0.43855	0.00000
H4	0.21714	0.42400	0.00000
H6	-0.21383	0.42607	0.00000
C5	0.00178	0.44904	0.00000
C4'	-0.00851	-0.44686	0.00000
C5'	0.11538	-0.38282	0.00000
N3'	-0.12414	-0.37917	0.00000
C4	0.11995	0.37501	0.00000
C6	-0.11711	0.37615	0.00000
H2'	-0.20714	-0.18977	0.00000
H6'	0.20550	-0.18541	0.00000
N3	0.12056	0.24107	0.00000
N1	-0.11902	0.24224	0.00000
C2'	-0.11392	-0.24573	0.00000
C6'	0.11345	-0.24341	0.00000
C2	0.00045	0.18132	0.00000
N1'	-0.00103	-0.17374	0.00000
H2	0.00000	0.07251	0.00000

Table 214S. Computed bond lengths (Å) and angles (°) for (PYM)C2-H…N1’(PYM) optimized at the DFT- B3LYP/6-31+G** level.

Vector	Length
N1-C6	1.339
N1-C2	1.341
N1'-C2'	1.339
N1'-C6'	1.340
N3-C4	1.339
N3-C2	1.342
N3'-C2'	1.338
N3'-C4'	1.340
C2'-H2'	1.087
C2-H2	1.088
C4'-H4'	1.088
C4'-C5'	1.395
C4-H4	1.088
C4-C5	1.394
C5-H5	1.085
C5-C6	1.395
C5'-H5'	1.085
C5'-C6'	1.394
C6'-H6'	1.088
C6-H6	1.088
H2…N1'	2.462
C2…N1'	3.551

Vectors	Angle
C6-N1-C2	116.20
C2'-N1'-C6'	116.15
C4-N3-C2	116.19
C2'-N3'-C4'	115.97
H2'-C2'-N3'	116.60
H2'-C2'-N1'	116.50
N3'-C2'-N1'	126.91
H2-C2-N1	116.78
H2-C2-N3	116.69

N1-C2-N3	126.53
H4'-C4'-N3'	116.43
H4'-C4'-C5'	121.24
N3'-C4'-C5'	122.32
H4-C4-N3	116.49
H4-C4-C5	121.18
N3-C4-C5	122.33
H5-C5-C4	121.79
H5-C5-C6	121.79
C4-C5-C6	116.42
H5'-C5'-C6'	121.71
H5'-C5'-C4'	121.75
C6'-C5'-C4'	116.54
H6'-C6'-N1'	116.46
H6'-C6'-C5'	121.42
N1'-C6'-C5'	122.12
H6-C6-N1	116.48
H6-C6-C5	121.19
N1-C6-C5	122.33
C2-H2…N1'	180.00(fixed)
H2…N1'-C2'	122.76
H2…N1'-C4'	121.09

(PYM)C5-H…N1’(PYM)

Table 215S. Computed atomic orthogonal coordinates for (PYM)C5-H…N1’(PYM) optimized at the DFT- B3LYP/6-31G** level.

Atom	x	y	z
N1	0.38600	0.07462	-0.09384
C2	0.44528	-0.00014	-0.00008
H2	0.55411	-0.00042	-0.00026
N3	0.38596	-0.07454	0.09393
C4	0.25199	-0.07317	0.09281
H4	0.20241	-0.13342	0.16875
C5	0.17816	0.00055	0.00039
H5	0.06950	0.00089	0.00063
C6	0.25203	0.07386	-0.09232
H6	0.20247	0.13425	-0.16816
N1'	-0.17477	0.00180	0.00129
N3'	-0.37810	-0.10029	-0.07357
C2'	-0.24508	-0.09005	-0.06610
H2'	-0.18754	-0.16449	-0.12074
C4'	-0.44759	-0.00801	-0.00586
C5'	-0.38577	0.09268	0.06799
C6'	-0.24654	0.09300	0.06822
H4'	-0.55606	-0.01534	-0.01122
H5'	-0.44304	0.16696	0.12253
H6'	-0.19037	0.16814	0.12338

Table 216S. Computed bond lengths (Å) and angles (°) for (PYM)C5-H…N1’(PYM) optimized at the DFT- B3LYP/6-31G** level.

Vector	Distance
N1-C2	1.338
N1-C6	1.340
N1'-C2'	1.339
N1'-C6'	1.340
N3'-C2'	1.336
N3'-C4'	1.339
N3-C2	1.338
N3-C4	1.340
C4-C5	1.394
C4'-C5'	1.393
C5'-C6'	1.392
C5-C6	1.394
H2-C2	1.088
H2'-C2'	1.088
H4'-C4'	1.088
H4-C4	1.089
H5'-C5'	1.085
H5-C5	1.087
H6-C6	1.089
H6'-C6'	1.088
H5…N1'	2.443
C5…N1'	3.529

Vectors	Angle
C2-N1-C6	115.59
C2'-N1'-C6'	115.93
C2'-N3'-C4'	115.82
C2-N3-C4	115.59
H2'-C2'-N3'	116.48
H2'-C2'-N1'	116.39
N3'-C2'-N1'	127.13
H2-C2-N1	116.32
H2-C2-N3	116.31

N1-C2-N3	127.37
H4-C4-N3	116.35
H4-C4-C5	120.93
N3-C4-C5	122.72
H4'-C4'-N3'	116.48
H4'-C4'-C5'	121.12
N3'-C4'-C5'	122.40
H5'-C5'-C6'	121.70
H5'-C5'-C4'	121.80
C6'-C5'-C4'	116.50
H5-C5-C4	122.00
H5-C5-C6	121.99
C4-C5-C6	116.01
H6-C6-N1	116.37
H6-C6-C5	120.92
N1-C6-C5	122.72
H6'-C6'-N1'	116.53
H6'-C6'-C5'	121.24
N1'-C6'-C5'	122.23
C5-H5…N1'	179.97

Table 217S. Computed atomic orthogonal coordinates for (PYM)C5-H…N1’(PYM) optimized at the DFT- B3LYP/6-31+G** level.

Atom	x	y	z
H5'	0.44600	0.18194	0.09933
H6'	0.19306	0.18303	0.09993
H6	-0.20548	-0.10587	0.18756
C5'	0.38872	0.10099	0.05513
C6'	0.24935	0.10129	0.05530
N1	-0.38887	-0.05922	0.10415
C6	-0.25481	-0.05808	0.10316
H2	-0.55732	-0.00054	-0.00029
H4'	0.55917	-0.01676	-0.00915
C2	-0.44858	-0.00019	-0.00010
C4'	0.45075	-0.00866	-0.00473
N1'	0.17767	0.00184	0.00100
C5	-0.18103	0.00068	0.00037
H5	-0.07246	0.00103	0.00056
N3	-0.38890	0.05923	-0.10415
C4	-0.25484	0.05896	-0.10268
N3'	0.38110	-0.10911	-0.05957
C2'	0.24793	-0.09826	-0.05365
H4	-0.20552	0.10706	-0.18690
H2'	0.19059	-0.17936	-0.09793

Table 218S. Computed bond lengths (Å) and angles (°) for (PYM)C5-H…N1’(PYM) optimized at the DFT- B3LYP/6-31+G** level.

Vector	Length
N1-C2	1.339
N1-C6	1.341
N1'-C2'	1.340
N1'-C6'	1.341
N3-C2	1.339
N3-C4	1.341
N3'-C2'	1.337
N3'-C4'	1.340
C2-H2	1.087
C2'-H2'	1.087
C4'-H4'	1.088
C4'-N3'	1.340
C4'-C5'	1.395
C4-H4	1.088
C4-N3	1.341
C4-C5	1.395
C5'-H5'	1.086
C5'-C6'	1.394
C5-H5	1.086
C5-C6	1.395
C6'-H6'	1.088
C6-H6	1.088
N1’…H5	2.501
N1’…C5	3.587

Vectors	Angle
C2-N1-C6	115.88
C2'-N1'-C6'	116.05
C2-N3-C4	115.87
C2'-N3'-C4'	116.02
H2-C2-N1	116.49
H2-C2-N3	116.48
N1-C2-N3	127.03

H2'-C2'-N3'	116.52
H2'-C2'-N1'	116.54
N3'-C2'-N1'	126.94
H4'-C4'-N3'	116.46
H4'-C4'-C5'	121.27
N3'-C4'-C5'	122.27
H4-C4-N3	116.35
H4-C4-C5	121.10
N3-C4-C5	122.55
H5'-C5'-C6'	121.70
H5'-C5'-C4'	121.75
C6'-C5'-C4'	116.55
H5-C5-C4	121.94
H5-C5-C6	121.93
C4-C5-C6	116.13
H6'-C6'-N1'	116.53
H6'-C6'-C5'	121.29
N1'-C6'-C5'	122.18
H6-C6-N1	116.35
H6-C6-C5	121.11
N1-C6-C5	122.54
C2'-N1'…H5	121.42
C6'-N1'…H5	122.53
C5-H5…N1'	180.00

TWO-PARTICLE SYSTEMS
Other molecule…Cl^- systems

(AA)N1-H…Cl^-

Table 219S. Computed atomic orthogonal coordinates for (AA)N1-H…Cl^- optimized at the DFT-B3LYP/6-31+G** level.

Atom	x	y	z
N1	0.04717	-0.09745	-0.00003
C2	0.14929	-0.00944	-0.00001
C3	0.10804	0.13710	-0.00002
O4	0.26884	-0.04314	0.00003
H5	-0.05260	-0.06863	-0.00013
H6	0.07035	-0.19574	0.00005
H7	0.15181	0.18558	-0.08793
H8	0.15067	0.18520	0.08865
H9	-0.00057	0.14980	-0.00063
Cl10	-0.25556	0.00030	0.00001

Table 220S. Computed bond lengths (Å) and angles (°) for (AA)N1-H…Cl^- optimized at the DFT-B3LYP/6-31+G** level.

Vector	Length
N1-C2	1.348
C2-O4	1.242
C2-C3	1.522
H5-N1	1.038
H6-N1	1.010
H7-C3	1.095
H8-C3	1.095
H9-C3	1.094
H5…Cl10	2.143
N1…Cl10	3.181

Vectors	Angle
H6-N1-H5	119.38
H6-N1-C2	117.49
H5-N1-C2	123.13
O4-C2-N1	123.50
O4-C2-C3	121.46
N1-C2-C3	115.03
H9-C3-H7	109.94
H9-C3-H8	109.88
H9-C3-C2	112.39
H7-C3-H8	107.45
H7-C3-C2	108.53
H8-C3-C2	108.50
N1-H5…Cl10	177.35

Table 221S. Computed atomic orthogonal coordinates for (AA)N1-H…Cl^- optimized at the *ab initio*- MP2/6-31+G** level.

Atom	x	y	z
N1	0.04787	-0.09897	0.01216
C2	0.14731	-0.00859	-0.00007
C3	0.10231	0.13598	0.00456
O4	0.26787	-0.03951	-0.01074
H5	-0.05157	-0.07175	0.00865
H6	0.07304	-0.19622	0.00400
H7	0.14983	0.18937	-0.07758
H8	0.13747	0.17990	0.09795
H9	-0.00600	0.14471	-0.00152
Cl10	-0.25168	-0.00008	-0.00339

Table 222S. Computed bond lengths (Å) and angles (°) for (AA)N1-H…Cl^- optimized at the *ab initio*- MP2/6-31+G** level.

Vector	Length
N1-C2	1.349
C2-O4	1.249
C2-C3	1.515
H5-N1	1.032
H6-N1	1.008
H7-C3	1.089
H8-C3	1.090
H9-C3	1.088
H5…Cl10	2.129
N1…Cl10	3.158

Vectors	Angle
H6-N1-H5	119.51
H6-N1-C2	117.06
H5-N1-C2	122.04
O4-C2-N1	123.59
O4-C2-C3	121.70
N1-C2-C3114.68	55501
H9-C3-H7110.66	55501
H9-C3-H8	109.66
H9-C3-C2	111.75
H7-C3-H8	107.93
H7-C3-C2	108.38
H8-C3-C2	108.35
N1-H5…Cl10	175.42

(MAA)N1-H…Cl$^-$

Table 223S. Computed atomic orthogonal coordinates for (MAA)N1-H…Cl$^-$ optimized at the DFT-B3LYP/6-31+G** level.

Atom	x	y	z
N1	-0.04184	0.05579	0.00000
C2	-0.13665	-0.03987	0.00000
C3	-0.08453	-0.18286	0.00000
C4	-0.07612	0.19644	0.00000
O5	-0.25862	-0.01517	0.00000
H1	0.05882	0.03033	0.00000
H3a	0.02473	-0.18750	0.00002
H3b	-0.12381	-0.23445	0.08827
H3c	-0.12377	-0.23444	-0.08829
H4a	0.01691	0.25368	-0.00014
H4b	-0.13522	0.22327	0.08850
H4c	-0.13547	0.22319	-0.08835
Cl1	0.26844	-0.01092	0.00000

Table 224S. Computed bond lengths (Å) and angles (°) for (MAA)N1-H…Cl^- optimized at the DFT- B3LYP/6-31+G** level.

Atom	Length
N1-C2	1.347
N1-C4	1.448
C2-O5	1.244
C2-C3	1.522
H1-N1	1.038
H3a-C3	1.094
H3b-C3	1.095
H3c-C3	1.095
H4a-C4	1.092
H4b-C4	1.097
H4c-C4	1.097
Cl1…H1	2.136
Cl1…N1	3.174

Vectors	Angle
H1-N1-C2	120.55
H1-N1-C4	117.89
C2-N1-C4	121.56
O5-C2-N1	123.30
O5-C2-C3	121.47
N1-C2-C3	115.23
H3a-C3-H3b	109.77
H3a-C3-H3c	109.76
H3a-C3-C2	112.46
H3b-C3-H3c	107.42
H3b-C3-C2	108.65
H3c-C3-C2	108.65
H4a-C4-H4b	109.36
H4a-C4-H4c	109.38
H4a-C4-N1	107.91
H4b-C4-H4c	107.36
H4b-C4-N1	111.41
H4c-C4-N1	111.40

N1-H1…Cl1	176.94

Table 225S. Computed atomic orthogonal coordinates for (MAA)N1-H…Cl^- optimized at the *ab initio*- MP2/6-31+G** level.

Atom	x	y	z
N1	-0.04075	0.05606	0.00000
C2	-0.13394	-0.04097	0.00000
C3	-0.07942	-0.18227	0.00000
C4	-0.07906	0.19539	0.00000
O5	-0.25711	-0.01788	0.00000
H1	0.05983	0.03225	0.00000
H3a	-0.11751	-0.23403	-0.08804
H3b	-0.11743	-0.23399	0.08809
H3c	0.02942	-0.18384	-0.00005
H4a	0.01207	0.25473	-0.00015
H4b	-0.13860	0.21969	0.08821
H4c	-0.13885	0.21960	-0.08806
Cl1	0.26516	-0.00921	0.00000

Table 226S. Computed bond lengths (Å) and angles (°) for (MAA)N1-H…Cl^- optimized at the *ab initio*- MP2/6-31+G** level.

Vector	Length
N1-C2	1.345
N1-C4	1.445
C2-O5	1.253
C2-C3	1.515
H1-N1	1.034
H3a-C3	1.090
H3b-C3	1.090
H3c-C3	1.089
H4a-C4	1.087
H4b-C4	1.092
H4c-C4	1.092
H1…Cl1	2.095
N1…Cl1	3.128

Vectors	Angle
H1-N1-C2	120.53
H1-N1-C4	118.69
C2-N1-C4	120.78
O5-C2-N1	123.23
O5-C2-C3	121.72
N1-C2-C3	115.06
H3c-C3-H3a	110.01
H3c-C3-H3b	110.01
H3c-C3-C2	111.93
H3a-C3-H3b	107.79
H3a-C3-C2	108.50
H3b-C3-C2	108.49
H4a-C4-H4b	109.68
H4a-C4-H4c	109.69
H4a-C4-N1	107.70
H4b-C4-H4c	107.68
H4b-C4-N1	111.05
H4c-C4-N1	111.04

N1-H1…Cl1	178.10

(MAA)N1-H…F$^-$

Table 227S. Computed atomic orthogonal coordinates for (MAA)N1-H…F$^-$ optimized at the DFT-B3LYP/6-31+G** level.

Atom	x	y	z
N1	0.02618	0.04754	0.00000
C2	-0.08598	-0.02532	0.00000
C3	-0.06436	-0.17645	0.00000
C4	0.01628	0.19190	0.00000
O5	-0.20222	0.02178	0.00000
H1	0.12944	-0.00058	0.00000
H3a	0.04188	-0.20227	0.00004
H3b	-0.11334	-0.21929	0.08824
H3c	-0.11328	-0.21928	-0.08828
H4a	0.11764	0.23313	-0.00008
H4b	-0.03760	0.22946	0.08826
H4c	-0.03774	0.22945	-0.08818
F1	0.25021	-0.05538	0.00000

Table 228S. Computed bond lengths (Å) and angles (°) for (MAA)N1-H…F^- optimized at the DFT- B3LYP/6-31+G** level.

Vector	Length
N1-C2	1.337
N1-C4	1.447
C2-O5	1.254
C2-C3	1.527
H1-N1	1.139
H3a-C3	1.093
H3b-C3	1.096
H3c-C3	1.096
H4a-C4	1.094
H4b-C4	1.100
H4c-C4	1.100
H1…F1	1.326
N1…F1	2.465

Vectors	Angle
H1-N1-C2	122.01
H1-N1-C4	118.91
C2-N1-C4	119.08
O5-C2-N1	124.93
O5-C2-C3	120.20
N1-C2-C3	114.87
H3a-C3-H3b	109.97
H3a-C3-H3c	109.97
H3a-C3-C2	111.80
H3b-C3-H3c	107.22
H3b-C3-C2	108.88
H3c-C3-C2	108.88
H4a-C4-H4b	109.00
H4a-C4-H4c	109.00
H4a-C4-N1	108.21
H4b-C4-H4c	106.62
H4b-C4-N1	111.97
H4c-C4-N1	111.97

N1-H1…F1	179.42

Table 229S. Computed atomic orthogonal coordinates for (MAA)N1-H…F^- optimized at the *ab initio* MP2/6-31+G** level.

Atom	x	y	z
N1	0.02647	0.04698	0.00000
C2	-0.08547	-0.02619	0.00000
C3	-0.06347	-0.17644	0.00000
C4	0.01409	0.19104	0.00000
O5	-0.20250	0.02126	0.00000
H1	0.12939	0.00000	0.00000
H3a	0.04257	-0.20103	-0.00003
H3b	-0.11186	-0.21891	0.08805
H3c	-0.11192	-0.21892	-0.08801
H4a	0.11447	0.23327	-0.00007
H4b	-0.04027	0.22666	0.08798
H4c	-0.04040	0.22664	-0.08791
F1	0.25132	-0.05301	0.00000

Table 230S. Computed bond lengths (Å) and angles (°) for (MAA)N1-H…F^- optimized at the *ab initio* MP2/6-31+G** level.

Vector	Length
N1-C2	1.337
N1-C4	1.446
C2-O5	1.263
C2-C3	1.519
H1-N1	1.131
H3a-C3	1.089
H3b-C3	1.091
H3c-C3	1.091
H4a-C4	1.089
H4b-C4	1.094
H4c-C4	1.094
H1…F1	1.330
N1…F1	2.461

Vectors	Angle
H1-N1-C2	122.29
H1-N1-C4	119.45
C2-N1-C4	118.26
O5-C2-N1	124.76
O5-C2-C3	120.40
N1-C2-C3	114.84
H3a-C3-H3b	110.15
H3a-C3-H3c	110.15
H3a-C3-C2	111.39
H3b-C3-H3c	107.62
H3b-C3-C2	108.72
H3c-C3-C2	108.72
H4a-C4-H4b	109.41
H4a-C4-H4c	109.42
H4a-C4-N1	107.90
H4b-C4-H4c	107.03
H4b-C4-N1	111.53
H4c-C4-N1	111.53

N1-H1…F1	178.96

(MA)N1…H^+…Cl^-

Table 231S. Computed atomic orthogonal coordinates for (MA)N1…H^+…Cl^- optimized at the DFT- B3LYP/6-31+G** level.

Atom	x	y	z
N1	-0.11415	0.06761	0.00000
C2	-0.19707	-0.05457	0.00000
H3	0.03265	0.03036	0.00004
H4	-0.13261	0.12496	-0.08205
H5	-0.13268	0.12504	0.08199
H6	-0.17230	-0.11379	0.08838
H7	-0.17214	-0.11388	-0.08827
H8	-0.30463	-0.03360	-0.00010
Cl9	0.16842	-0.00970	0.00000

Table 232S. Computed bond lengths (Å) and angles (°) for (MA)N1…H^+…Cl^- optimized at the DFT- B3LYP/6-31+G** level.

Vector	Length
N1-C2	1.477
H3-Cl9	1.416
H4-N1	1.018
H5-N1	1.018
H6-C2	1.092
H7-C2	1.092
H8-C2	1.096
H3…N1	1.515
Cl9…N1	2.930

Vectors	Angle
H4-N1-H5	107.36
H4-N1-C2	111.37
H5-N1-C2	111.38
H6-C2-H7	107.92
H6-C2-H8	109.09
H6-C2-N1	108.74
H7-C2-H8	109.10
H7-C2-N1	108.73
H8-C2-N1	113.13
Cl9-H3…N1	177.80
H3…N1-C2	109.93
H3…N1-H4	108.33
H3…N1-H5	108.36

Table 233S. Computed atomic orthogonal coordinates for (MA)N1…H^{+}…Cl^{-} optimized at the *ab initio*- MP2/6-31+G** level.

Atom	x	y	z
N1	0.12053	0.06928	0.00000
C2	0.19574	-0.05723	0.00000
H3	-0.04332	0.03149	-0.00004
H4	0.14414	0.12504	0.08151
H5	0.14416	0.12506	-0.08150
H6	0.16735	-0.11449	-0.08798
H7	0.16734	-0.11449	0.08797
H8	0.30401	-0.04371	0.00001
Cl9	-0.17070	-0.00885	0.00000

Table 234S. Computed bond lengths (Å) and angles (°) for (MA)N1…H^+…Cl^- optimized at the *ab initio*- MP2/6-31+G** level.

Vector	Length
N1-C2	1.472
H4-N1	1.015
H5-N1	1.015
H6-C2	1.087
H7-C2	1.087
H8-C2	1.091
Cl9-H3	1.336
H3…N1	1.683
Cl9…N1	3.015

Vectors	Angle
H4-N1-H5	106.77
H4-N1-C2	110.68
H5-N1-C2	110.69
H6-C2-H7	108.00
H6-C2-H8	108.93
H6-C2-N1	108.61
H7-C2-H8	108.93
H7-C2-N1	108.61
H8-C2-N1	113.61
Cl9-H3…N1	175.41
H3…N1-C2	107.74
H3…N1-H4	110.50
H3…N1-H5	110.49

(MAB)N1-H…Cl$^-$

Table 235S. Computed atomic orthogonal coordinates for (MAB)N1-H…Cl$^-$ optimized at the DFT-B3LYP/6-31+G** level.

Atom	x	y	z
N1	0.14429	0.07610	-0.01256
C2	0.21000	-0.05389	0.00221
H3	0.04340	0.06026	-0.02626
H4	0.15035	0.12688	0.07547
H5	0.20051	-0.10946	-0.09175
H6	0.16852	-0.11792	0.08197
H7	0.31735	-0.04015	0.02149
Cl8	-0.18530	-0.00759	0.00081

Table 236S. Computed bond lengths (Å) and angles (°) for (MAB)N1-H…Cl^- optimized at the DFT- B3LYP/6-31+G** level.

Vector	Length
N1-C2	1.464
H3-N1	1.030
H4-N1	1.018
H5-C2	1.096
H6-C2	1.104
H7-C2	1.099
H3…Cl8	2.401
N1…Cl8	3.403

Vectors	Angle
H4-N1-H3	104.47
H4-N1-C2	109.20
H3-N1-C2	108.44
H5-C2-H7	107.36
H5-C2-H6	107.03
H5-C2-N1	108.96
H7-C2-H6	108.23
H7-C2-N1	110.18
H6-C2-N1	114.79
N1-H3…Cl8	163.98

Table 237S. Computed atomic orthogonal coordinates for (MAB)N1-H…Cl^- optimized at the *ab initio*- MP2/6-31+G** level.

Atom	x	y	z
N1	0.14392	0.07705	-0.01248
C2	0.20321	-0.05586	0.00205
H3	0.04289	0.06491	-0.02473
H4	0.15360	0.12723	0.07522
H5	0.18841	-0.11081	-0.09082
H6	0.16022	-0.11611	0.08289
H7	0.31081	-0.04692	0.01889
Cl8	-0.18133	-0.00721	0.00080

Table 238S. Computed bond lengths (Å) and angles (°) for (MAB)N1-H…Cl^- optimized at the *ab initio*- MP2/6-31+G** level.

Vector	Length
N1-C2	1.463
H3-N1	1.025
H4-N1	1.015
H5-C2	1.089
H6-C2	1.096
H7-C2	1.093
H3…Cl8	2.369
N1…Cl8	3.362

Vectors	Angle
H4-N1-H3	104.82
H4-N1-C2	108.95
H3-N1-C2	107.69
H5-C2-H7	107.85
H5-C2-H6	107.35
H5-C2-N1	108.58
H7-C2-H6	108.51
H7-C2-N1	109.88
H6-C2-N1	114.44
N1-H3…Cl8	162.96

(MGU) $NH_2NH\ldots Cl^-$

Table 239S. Computed atomic orthogonal coordinates for (MGU)$NH_2NH\ldots Cl^-$ optimized at the DFT-B3LYP/6-31+G** level.

Atom	x	y	z
Cl1	0.24744	0.01163	0.00285
C1	-0.09371	-0.05531	-0.00051
N2	-0.00666	-0.15646	-0.01090
N3	-0.22742	-0.08018	0.00347
N4	-0.04802	0.06906	0.00017
C5	-0.13057	0.18838	-0.00392
H2a	-0.03426	-0.25030	0.01345
H2b	0.09451	-0.12960	-0.00913
H3a	-0.26094	-0.17513	0.00661
H3b	-0.29146	-0.00796	0.03218
H4	0.05734	0.07615	0.00142
H5a	-0.06408	0.27415	-0.01465
H5b	-0.18817	0.20217	0.08857
H5c	-0.19907	0.18731	-0.08954

Table 240S. Computed bond lengths (Å) and angles (°) for (MGU)$NH_2NH\ldots Cl^-$ optimized at the DFT-B3LYP/6-31+G** level.

Vector	Length
C1-N4	1.325
C1-N2	1.339
C1-N3	1.361
C5-N4	1.451
H2a-N2	1.008
H2b-N2	1.047
H3a-N3	1.007
H3b-N3	1.007
H4-N4	1.056
H5a-C5	1.091
H5b-C5	1.098
H5c-C5	1.097
H2b…Cl1	2.085
N2…Cl1	3.050
H4…Cl1	2.008
N4…Cl1	3.010

Vectors	Angle
N4-C1-N2	119.04
N4-C1-N3	120.68
N2-C1-N3	120.21
H5a-C5-H5c	108.16
H5a-C5-H5b	107.69
H5a-C5-N4	107.61
H5c-C5-H5b	109.34
H5c-C5-N4	111.67
H5b-C5-N4	112.19
H2a-N2-H2b	119.96
H2a-N2-C1	120.44
H2b-N2-C1	115.68
H3b-N3-H3a	117.09
H3b-N3-C1	120.15
H3a-N3-C1	120.01

H4-N4-C1	114.02
H4-N4-C5	120.83
C1-N4-C5	125.12
N2-H2b…Cl1	152.07
N4-H4…Cl1	157.04

Table 241S. Computed atomic orthogonal coordinates for (MGU)$NH_2NH\ldots Cl^-$ optimized at the *ab initio*-MP2/6-31+G** level.

Atom	x	y	z
Cl1	0.24519	0.01008	0.00451
C1	-0.09386	-0.05422	-0.00024
N2	-0.01051	-0.15836	-0.01661
N3	-0.22868	-0.07494	0.00480
N4	-0.04477	0.06813	-0.00115
C5	-0.12521	0.18869	-0.00565
H2a	-0.03746	-0.24809	0.02043
H2b	0.08998	-0.13284	-0.01392
H3a	-0.26129	-0.16983	0.01358
H3b	-0.28548	-0.00536	0.05037
H4	0.06084	0.07198	0.00057
H5a	-0.05784	0.27191	-0.02353
H5b	-0.17715	0.20648	0.08877
H5c	-0.19776	0.18384	-0.08692

Table 242S. Computed bond lengths (Å) and angles (°) for (MGU)NH_2NH…Cl^- optimized at the *ab initio*-MP2/6-31+G** level.

Vector	Length
C1-N4	1.318
C1-N2	1.344
C1-N3	1.365
C5-N4	1.450
H2a-N2	1.007
H2b-N2	1.037
H3a-N3	1.007
H3b-N3	1.007
H4-N4	1.057
H5a-C5	1.086
H5b-C5	1.092
H5c-C5	1.090
H2b…Cl1	2.118
N2…Cl1	3.069
H4…Cl1	1.945
N4…Cl1	2.954

Vectors	Angle
N4-C1-N2	119.17
N4-C1-N3	120.59
N2-C1-N3	119.96
H5a-C5-H5c	108.92
H5a-C5-H5b	108.22
H5a-C5-N4	107.35
H5c-C5-H5b	109.58
H5c-C5-N4	110.81
H5b-C5-N4	111.86
H2a-N2-H2b	117.96
H2a-N2-C1	118.65
H2b-N2-C1	114.02
H3a-N3-H3b	115.39
H3a-N3-C1	117.78
H3b-N3-C1	117.96

H4-N4-C1	113.94
H4-N4-C1	7.83
H4-N4-C5	121.64
C1-N4-C5	124.42
N2-H2b…Cl1	151.44
N4-H4…Cl1	159.35

(MGU)NH_2NH_2…Cl^-

Table 243S. Computed atomic orthogonal coordinates for (MGU)NH_2NH_2…Cl^- optimized at the DFT-B3LYP/6-31+G** level.

Atom	x	y	z
Cl1	-0.27654	-0.02273	-0.00230
C1	0.06733	0.02890	0.00247
N2	-0.01599	0.13357	0.00554
N3	0.01580	-0.09362	0.00334
N4	0.20140	0.04895	-0.00143
C5	0.29957	-0.05869	-0.00496
H2a	-0.11821	0.11001	0.00323
H2b	0.01532	0.22398	-0.02636
H3a	-0.08957	-0.09960	0.00198
H3b	0.07262	-0.17459	0.02216
H4	0.23381	0.14222	0.01926
H5a	0.40006	-0.01818	-0.02010
H5b	0.27836	-0.12695	-0.08778
H5c	0.29885	-0.11407	0.08939

Table 244S. Computed bond lengths (Å) and angles (°) for (MGU)NH_2NH_2…Cl^- optimized at the DFT-B3LYP/6-31+G** level.

Vector	Length
C1-N3	1.329
C1-N2	1.338
C1-N4	1.356
C5-N4	1.457
H2a-N2	1.049
H2b-N2	1.009
H3a-N3	1.055
H3b-N3	1.007
H4-N4	1.009
H5a-C5	1.094
H5b-C5	1.094
H5c-C5	1.094
H2a…Cl1	2.067
N2…Cl1	3.039
H3a…Cl1	2.022
N3a…Cl1	3.009

Vectors	Angle
N3-C1-N2	118.65
N3-C1-N4	121.31
N2-C1-N4	120.04
H5a-C5-H5b	107.72
H5a-C5-H5c	108.23
H5a-C5-N4	110.40
H5b-C5-H5c	109.62
H5b-C5-N4	110.40
H5c-C5-N4	110.40
H2b-N2-H2a	119.79
H2b-N2-C1	120.04
H2a-N2-C1	115.50
H3b-N3-H3a	121.35
H3b-N3-C1	121.58
H3a-N3-C1	116.05

H4-N4-C1	116.64
H4-N4-C5	118.13
C1-N4-C5	123.88
N2-H2a…Cl1	153.01
N3-H3a…Cl1	154.40

Table 245S. Computed atomic orthogonal coordinates for (MGU)NH_2NH_2…Cl^- optimized at the *ab initio*-MP2/6-31+G** level.

Atom	x	y	z
Cl1	0.27479	-0.02314	0.00200
C1	-0.06718	0.02948	-0.00217
N2	0.01561	0.13470	-0.00600
N3	-0.01548	-0.09283	-0.00171
N4	-0.20117	0.04922	0.00114
C5	-0.29691	-0.06022	0.00538
H2a	0.11676	0.11007	-0.00303
H2b	-0.01461	0.22162	0.03504
H3a	0.08952	-0.09707	-0.00120
H3b	-0.07035	-0.17202	-0.03068
H4	-0.23341	0.13929	-0.03060
H5a	-0.39545	-0.01811	0.02290
H5b	-0.27288	-0.12655	0.08824
H5c	-0.29915	-0.11709	-0.08782

Table 246S. Computed bond lengths (Å) and angles (°) for (MGU)NH_2NH_2…Cl^- optimized at the *ab initio*-MP2/6-31+G** level.

Vector	Length
C1-N3	1.328
C1-N2	1.339
C1-N4	1.355
C5-N4	1.455
H2a-N2	1.041
H2b-N2	1.008
H3a-N3	1.051
H3b-N3	1.006
H4-N4	1.008
H5a-C5	1.086
H5b-C5	1.088
H5c-C5	1.092
H2a…Cl1	2.067
N2…Cl1	3.036
H3a…Cl1	1.995
N3…Cl1	2.985

Vectors	Angle
N3-C1-N2	118.88
N3-C1-N4	121.28
N2-C1-N4	119.84
H5a-C5-H5b	108.30
H5a-C5-H5c	108.73
H5a-C5-N4	108.07
H5b-C5-H5c	109.69
H5b-C5-N4	109.60
H5c-C5-N4	112.36
H2b-N2-H2a	118.93
H2b-N2-C1	118.73
H2a-N2-C1	114.44
H3b-N3-H3a	120.97
H3b-N3-C1	120.78
H3a-N3-C1	115.23

H4-N4-C1	116.03
H4-N4-C5	118.10
C1-N4-C5	122.82
N2-H2a…Cl1	153.56
N3-H3a…Cl1	155.93

(MeOH)O-H…Cl$^-$

Table 247S. Computed atomic orthogonal coordinates for (MeOH)O-H…Cl$^-$ optimized at the DFT-B3LYP/6-31+G** level.

Atom	x	Y	z
O1	0.13101	0.07691	0.00002
C2	0.19295	-0.04958	0.00000
Cl1	-0.16902	-0.00746	0.00000
H1	0.03283	0.06143	-0.00016
H2a	0.30169	-0.03402	-0.00017
H2b	0.16671	-0.10918	0.08892
H2c	0.16644	-0.10928	-0.08877

Table 248S. Computed bond lengths (Å) and angles (°) for (MeOH)O-H…Cl^- optimized at the DFT-B3LYP/6-31+G** level.

Vector	Length
O1-C2	1.408
H1-O1	0.994
H2a-C2	1.098
H2b-C2	1.102
H2c-C2	1.102
H1…Cl1	2.133
O1…Cl1	3.117

Vectors	Angle
H1-O1-C2	107.13
H2a-C2-H2b	108.27
H2a-C2-H2c	108.28
H2a-C2-O1	107.95
H2b-C2-H2c	107.44
H2b-C2-O1	112.39
H2c-C2-O1	112.38
O1-H1…Cl1	170.11

Table 249S. Computed atomic orthogonal coordinates for (MeOH)O-H…Cl^- optimized at the *ab initio*-MP2/6-31+G** level.

Atom	x	y	z
O1	-0.13152	0.07799	-0.00002
C2	-0.18865	-0.05143	0.00000
Cl1	0.16671	-0.00722	0.00000
H1	-0.03359	0.06453	0.00017
H2a	-0.29711	-0.03930	-0.00015
H2b	-0.15979	-0.10889	0.08853
H2c	-0.15955	-0.10901	-0.08838

Table 250S. Computed bond lengths (Å) and angles (°) for (MeOH)O-H…Cl^- optimized at the *ab initio*-MP2/6-31+G** level.

Vector	Length
O1-C2	1.415
H1-O1	0.989
H2a-C2	1.091
H2b-C2	1.094
H2c-C2	1.094
H1…Cl1	2.128
O1…Cl1	3.102

Vectors	Angles
H1-O1-C2	105.99
H2a-C2-H2b	108.76
H2a-C2-H2c	108.76
H2a-C2-O1	107.44
H2b-C2-H2c	107.88
H2b-C2-O1	111.96
H2c-C2-O1	111.96
C1-H1…Cl1	168.12

(HMB)O1-H…Cl$^-$

Table 251S. Computed atomic orthogonal coordinates for (HMB)O1-H…Cl$^-$ optimized at the DFT-B3LYP/6-31+G** level.

Atom	x	y	z
Cl1	-0.35706	-0.07076	0.00003
O1	-0.14402	0.15029	-0.00004
C2	-0.02677	0.08400	-0.00002
C3	0.09074	0.16125	0.00002
C4	0.21631	0.10009	0.00003
C5	0.22997	-0.03935	0.00000
C6	0.11161	-0.11510	-0.00003
C7	-0.01490	-0.05641	-0.00004
C8	0.36665	-0.10533	0.00002
H1	-0.22617	0.09256	0.00001
H3	0.08150	0.26951	0.00004
H4	0.30548	0.16273	0.00006
H6	0.11816	-0.22387	-0.00004
H7	-0.10566	-0.11607	-0.00006
H8a	0.38361	-0.16761	0.08873
H8b	0.43996	-0.02380	0.00001
H8c	0.38361	-0.16763	-0.08869

Table 252S. Computed bond lengths (Å) and angles (°) for (HMB)O1-H…Cl^- optimized at the DFT- B3LYP/6-31+G** level.

Vector	Length
O1-C2	1.347
C2-C3	1.406
C2-C7	1.409
C3-C4	1.397
C4-C5	1.401
C5-C6	1.405
C5-C8	1.518
C6-C7	1.395
H1-O1	1.004
H3-C3	1.087
H4-C4	1.090
H6-C6	1.090
H7-C7	1.086
H8a-C8	1.097
H8b-C8	1.096
H8c-C8	1.097
H1…Cl1	2.093
O1…Cl1	3.070
H7…Cl1	2.554
C7…Cl1	3.425

Vectors	Angle
H1-O1-C2	115.42
O1-C2-C3	117.20
O1-C2-C7	124.31
C3-C2-C7	118.49
H3-C3-C4	120.85
H3-C3-C2	118.44
C4-C3-C2	120.71
H4-C4-C3	118.94
H4-C4-C5	119.49
C3-C4-C5	121.56
C4-C5-C6	117.02

C4-C5-C8	121.36
C6-C5-C8	121.61
H6-C6-C7	118.33
H6-C6-C5	119.17
C7-C6-C5	122.49
H7-C7-C6	121.79
H7-C7-C2	118.49
C6-C7-C2	119.72
H8b-C8-H8a	108.59
H8b-C8-H8c	108.59
H8b-C8-C5	106.19
H8a-C8-H8c	107.91
H8a-C8-C5	112.71
H8c-C8-C5	112.70
O1-H1…Cl1	163.81
C7-H7…Cl1	136.46

Table 253S. Computed atomic orthogonal coordinates for (HMB)O1-H…Cl^- optimized at the *ab initio*-MP2/6-31+G** level.

Atom	x	y	z
Cl1	-0.35287	-0.07199	0.00003
O1	-0.14450	0.15238	-0.00004
C2	-0.02709	0.08478	-0.00002
C3	0.09044	0.16169	0.00002
C4	0.21583	0.09995	0.00003
C5	0.22830	-0.03964	0.00001
C6	0.10979	-0.11493	-0.00003
C7	-0.01656	-0.05552	-0.00005
C8	0.36401	-0.10636	0.00002
H1	-0.22517	0.09341	-0.00002
H3	0.08139	0.26970	0.00004
H4	0.30520	0.16179	0.00006
H6	0.11586	-0.22345	-0.00005
H7	-0.10752	-0.11418	-0.00008
H8a	0.37960	-0.16828	0.08854
H8b	0.43757	-0.02565	0.00003
H8c	0.37962	-0.16827	-0.08850

Table 254S. Computed bond lengths (Å) and angles (°) for (HMB)O1-H…Cl^- optimized at the *ab initio*-MP2/6-31+G** level.

Vector	Length
O1-C2	1.355
C2-C3	1.405
C2-C7	1.407
C3-C4	1.398
C4-C5	1.401
C5-C6	1.404
C5-C8	1.512
C6-C7	1.396
H1-O1	0.999
H3-C3	1.084
H4-C4	1.087
H6-C6	1.087
H7-C7	1.082
H8a-C8	1.091
H8b-C8	1.092
H8c-C8	1.091
H1…Cl1	2.090
O1…Cl1	3.062
H7…Cl1	2.490
C7…Cl1	3.367

Vectors	Angle
H1-O1-C2	113.90
O1-C2-C3	116.87
O1-C2-C7	124.22
C3-C2-C7	118.91
H3-C3-C4	121.00
H3-C3-C2	118.41
C4-C3-C2	120.58
H4-C4-C3	119.10
H4-C4-C5	119.58
C3-C4-C5	121.32
C4-C5-C6	117.32

C4-C5-C8	121.29
C6-C5-C8	121.39
H6-C6-C7	118.38
H6-C6-C5	119.23
C7-C6-C5	122.39
H7-C7-C6	122.00
H7-C7-C2	118.53
C6-C7-C2	119.48
H8a-C8-H8c	108.39
H8a-C8-H8b	108.84
H8a-C8-C5	112.24
H8c-C8-H8b	108.84
H8c-C8-C5	112.24
H8b-C8-C5	106.17
O1-H1…Cl1	163.84
C7-H7…Cl1	137.43

TWO-PARTICLE SYSTEMS

Solvent effects on the structure of selected two-particle systems

(IM)N1-H…Cl$^-$

Table 255S. Computed atomic orthogonal coordinates for (IM)N1-H…Cl$^-$ optimized at the DFT-B3LYP/6-31G** level with solvent treatment via PCM method (water).

Atom	x	y	z
Cl1	-0.01878	-0.28717	0.00000
H1	-0.00620	-0.07769	0.00000
H5	-0.20884	0.08186	0.00000
N1	0.00000	0.02550	0.00000
H2	0.21248	0.05132	0.00000
C5	-0.10477	0.11469	0.00000
C2	0.11467	0.09800	0.00000
N3	0.09141	0.22841	0.00000
C4	-0.04670	0.23948	0.00000
H4	-0.09720	0.33610	0.00000

Table 256S. Computed bond lengths (Å) and angles (°)for (IM)N1-H…Cl^- optimized at the DFT-B3LYP/6-31G** level with solvent treatment via PCM method (water).

Vector	Length
N1-C2	1.357
N1-C5	1.376
N3-C2	1.325
N3-C4	1.386
C4-C5	1.376
H1-N1	1.034
H2-C2	1.084
H4-C4	1.090
H5-C5	1.091
Cl1…H1	2.099
Cl1…N1	3.132

Vectors	Angle
H1-N1-C2	125.74
H1-N1-C5	126.97
C2-N1-C5	107.29
C2-N3-C4	104.70
H2-C2-N3	125.63
H2-C2-N1	122.18
N3-C2-N1	112.19
H4-C4-C5	127.45
H4-C4-N3	122.18
C5-C4-N3	110.37
H5-C5-N1	122.08
H5-C5-C4	132.46
N1-C5-C4	105.45
N1-H1…Cl1	180.00(fixed)

(IM)C2-H…Cl$^-$

Table 257S. Computed atomic orthogonal coordinates for (IM)C2-H…Cl$^-$ optimized at the DFT-B3LYP/6-31G** level with solvent treatment via PCM method (water).

Atom	x	y	z
Cl1	-0.06622	-0.32715	0.00000
H5	0.20075	0.30126	0.00000
H4	-0.07195	0.35626	0.00000
H1	0.21318	0.04553	0.00000
C5	0.11428	0.23546	0.00000
C4	-0.02092	0.25998	0.00000
H2	-0.01896	-0.06115	0.00000
N3	-0.09133	0.14109	0.00000
N1	0.12597	0.09801	0.00000
C2	0.00000	0.04556	0.00000

Table 258S. Computed bond lengths (Å) and angles (°)for (IM)C2-H…Cl^- optimized at the DFT-B3LYP/6-31G** level with solvent treatment via PCM method (water).

Vector	Length
N1-H1	1.018
N1-C2	1.365
N1-C5	1.379
N3-C2	1.322
N3-C4	1.382
C2-H2	1.084
C4-H4	1.090
C4-C5	1.374
C5-H5	1.087
C5C4	1.374
Cl1…H2	2.7.02
Cl1…C2	3.785

Vectors	Angle
H1-N1-C2	126.36
H1-N1-C5	125.90
C2-N1-C5	107.74
C2-N3-C4	105.65
H2-C2-N3	126.21
H2-C2-N1	122.68
N3-C2-N1	111.11
H4-C4-C5	128.20
H4-C4-N3	121.44
C5-C4-N3	110.36
H5-C5-C4	132.45
H5-C5-N1	122.41
C4-C5-N1	105.14
Cl1…H2-C2	180.00

IM…F$^-$
(IM)N1-H…F$^-$

Table 259S. Computed atomic orthogonal coordinates for (IM)N1…H…F$^-$ optimized at the DFT-B3LYP/6-31G** level with solvent treatment via PCM method (water).

Atom	x	y	z
F1	-0.01510	0.28127	0.00000
N1	0.00000	0.04163	0.00000
C2	-0.10372	-0.04520	0.00000
N3	-0.06737	-0.17366	0.00000
C4	0.07060	-0.16893	0.00000
C5	0.11270	-0.03736	0.00000
H1	-0.00796	0.16796	0.00000
H2	-0.20693	-0.01141	0.00000
H4	0.13153	-0.25963	0.00000
H5	0.21338	0.00474	0.00000

Table 260S. Computed bond lengths (Å) and angles (°)for (IM)N1…H…F^- optimized at the DFT-B3LYP/6-31G** level with solvent treatment via PCM method (water).

Vector	Length
N1-C2	1.353
N1-C5	1.376
N3-C2	1.335
N3-C4	1.381
C4-C5	1.381
H1-F1	1.135
H2-C2	1.086
H4-C4	1.093
H5-C5	1.091
H1…N1	1.266
F1…N1	2.401

Vectors	Angle
C2-N1-C5	105.04
C2-N3-C4	103.84
H2-C2-N3	123.93
H2-C2-N1	121.94
N3-C2-N1	114.13
H4-C4-N3	121.93
H4-C4-C5	128.36
N3-C4-C5	109.71
H5-C5-N1	122.28
H5-C5-C4	130.44
N1-C5-C4	107.28
H1…N1-C2	126.33
H1…N1-C5	128.63
F1-H1…N1	180.00(fixed)

ENERGY

Table 261S. Total electronic energy (Eel, hartrees) for the selected isolate molecules and adduct systems as computed through Gaussian98 via *ab initio* and DFT methods. IM = 1,3-imidazole, PYM = 1,3-pyrimidine, MePym = 4-methyl-1,3-pyrimidine, AA = acetamide, MA = methylammonium, MAA = N-methylacetamide, , MAB = methylamine, HMB = hydroxyl-4-methylbenzene, MeOH = methanol, MGU = methylguanidinium. In the case of aggregates, particle number 1 is the first typed, number 2 is the second one (i.e. Cl-H…Cl^-, Cl-H is 1; Cl^- is 2); so BSSE correction 1 means that the massage test was performed by removing the nuclei of particle 1.

Theory	Molecule/Eel						
Isolate Monoatomic Ions							
	Cl^-	**F^-**					
MP2/6-31+G**	-459.67115	-99.62385					
MP4(SDTQ)/6-31+G**	-459.68584	---					
B3LYP/6-31G**	-460.25223	-99.75409					
B3LYP/6-31+G**	-460.27473	-99.85969					
Isolate Molecules							
	H-F	**H-Cl**	**H_2O**	**IM**	**IMH^+**	**PYM**	**MePYM**
RHF/6-31G*	-100.00291	---	---	---	---	---	---
MP2/6-31+G**	-100.21581	-460.20762	-76.23311	-225.56846	-225.93974	-263.55699 (-263.55675§)	---
MP3/6-31+G**	-100.21481	---	---	---	---	-263.57221§ (-263.57221$)	---
MP4(SDTQ)/6-31+G**	-100.22298	---	---	-225.62499§	---	---	---
CCSD(T)/6-31G**	-100.20115	-460.22457	-76.23158	-225.60592	---	-263.60579§	---
CCSD(T)/6-31+G**	-100.22158	-460.22691	-76.24439	---	---	---	---
CCSD(T)/6-31++G**	---	-460.22706	-76.24468	---	---	---	---

B3LYP/LANL2DZ	---	---	---	---	---	---	-303.58179
B3LYP/6-31G**	-100.42746	-460.80078	-76.41974	-226.22309	---	-264.32949	-303.65460
B3LYP/6-31+G**	-100.45137	-460.80321	-76.43405	-226.23538	-226.60810	-264.34081	-303.66670
B3LYP/6-31++G**	---	-460.80327	-76.43412	---	---	---	---
RHF/6-31G* †	-100.00291	-460.05998	-76.01075	---	---	---	---
RHF/6-31+G* †	-100.01487	-460.06102	-76.01774	---	---	---	---
MP2/6-311+G(3df,2p) #	---	-460.29699	---	---	---	---	---

Isolate Molecules

	AA	**MAA**	**MA**	**MAB**	**HMB**	**MeOH**	**MGU**
B3LYP/6-31+G**	-209.23796	-248.54874	-96.22822	-95.87185	-346.81408	-115.73487	-245.10152
MP2/6-31+G**	-208.62882	-247.80372	-95.91782	-95.55901	-345.75024	-115.39352	-244.36477

Isolate Molecules in reaction field&

	HF	**HCl**	**H_2O**	**IM**	**PYM**
B3LYP/6-31G**	-100.43778	-460.80467	---	-226.24360	---
B3LYP/6-31+G**	---	-460.80722	---	-226.25228	-264.35997
B3LYP/6-31+G**~	---	---	---	-226.25172	---

Isolate Molecules in reaction field&

	MAA	**MA**	**MGU**
B3LYP/6-31+G**	-284.56778	-96.34109	-245.21067

Molecular Aggregates

	Cl-H…Cl^-	**F-H…F^-**	**ClH…OH_2**	**HO-H…ClH**	**FH…OH_2**	**HO-H…FH**
RHF/6-31G*	---	---	---	---	-176.02806	---
CCSD(T)/6-31G**	---	---	-536.46694	---	-176.44793	-176.43802
(BSSE correction 1)			-76.23317		-76.23337	-76.23185

(BSSE correction 2)			-460.22535		-100.20180	-100.20285	
CCSD(T)/6-31+G**	---	---	-536.48157	---	-176.48140	-176.46989	
(BSSE correction 1)			-76.24598		-76.24642	-76.24504	
(BSSE correction 2)			-460.22820		-100.22209	-100.22181	
CCSD(T)/6-311++G**	-921.01781	-200.03573	-536.56057	---	---	---	
B3LYP/6-31G**	-921.10225	-200.28999	-537.23341	-537.22185	-176.86369	-176.85312	
B3LYP/6-31+G**	---	---	-537.24779	-537.23774	-176.90146	-176.88893	
B3LYP/6-31++G**	---	---	-537.24795	---	---	---	
B3LYP/6-311++G**	-921.17766	-200.44523	-537.30278	---	---	---	
MP2/6-31+G**	---	---	---	---	---	-176.45284	
(BSSE correction 1)						-76.23371	
(BSSE correction 2)						-100.21603	

Molecular Aggregates

	(IM)N1-H…Cl^-	**(IM)C2-H…Cl^-**	**(IM)C4-H…Cl^-**	**(IM)C5-H…Cl^-**	**(IM)N1-H…F^-**	**(IM)C2-H…F^-**	**(IMH^+)N1…H^+ …Cl^-**
B3LYP/6-31G**	-686.51920	-686.49297	-686.48135	-686.49686	-326.10935	-326.05063	---
B3LYP/6-31+G**	-686.54793	-686.52402	-686.51315	-686.52803	---	---	-687.05590
MP2/6-31+G**	-685.28240	---	---	---	---	---	-685.79360
(BSSE correction 1)	-459.67590						-460.20957
(BSSE correction 2)	-225.56709						-225.56954
MP4(STDQ)/6-31+G**	-685.35262§	---	---	---	---	---	---
(BSSE correction 1)	-459.69091§						
(BSSE correction 2)	-225.62296§						

Molecular Aggregates

	(IM)N-H…N(IM) (coplanar)	**(IM)N-H…N(IM) (free)**	**(IM)C2-H…N(IM) (C2-H2…N1' 180.0)**
B3LYP/6-31+G**	-452.48378	-452.48484	-452.47518

MP2/6-31+G**	-451.15334$		---		---	
(BSSE correction 1)	-225.56992$					
(BSSE correction 2)	-225.56915$					
Molecular Aggregates						
	(PYM)C2-H…Cl$^-$		**(PYM)C5-H…Cl$^-$**		**(PYM)C6-H…Cl$^-$**	**(MePYM)C7-H…Cl$^-$**
B3LYP/6-31G**	---		---		---	-763.93089
B3LYP/6-31+G**	-724.62089		724.63635		-724.63042	---
MP2/6-31+G**	-723.23546$		-723.25304$		-723.24565$	---
(BSSE correction 1)	-459.67410$		-459.67499$		-459.67453$	
(BSSE correction 2)	-263.55648$		-263.55686$		-263.55651$	
Molecular Aggregates						
	(PYM)C2-H…N1(PYM)		**(PYM)C2-H…N1(PYM)/ (PYM)C6'-H…N3(PYM)**		**(PYM)C5-H…N1(PYM)**	
B3LYP/6-31G**	---		-528.66489		-528.66342	
B3LYP/6-31+G**	-528.68391		-528.68541		-528.68480	
MP2/6-31+G**	-527.11836$		-527.12085$		-527.11969 § (-527.11972$)	
(BSSE correction 1)	-263.55776$		-263.55780$		-263.55791 § (-263.55789$)	
(BSSE correction 2)	-263.55752$		-263.55793$		-263.55751 § (-263.55756$)	
MP3/6-31+G**	---		---		-527.14999 § (-527.14995$)	
(BSSE correction 1)					-263.57332 § (-263.57323$)	
(BSSE correction 2)					-263.57292§ (-263.57292$)	
Molecular Aggregates						
	(AA)NH…Cl$^-$	**(MAA)NH…Cl$^-$**	**(MA)N…H-Cl**	**(MAB)NH…Cl$^-$**	**(HMB)OH…Cl$^-$**	**MeOH…Cl$^-$**
B3LYP/6-31+G**	-669.54618	-708.85704	-556.69493	-556.15988	-807.12115	-576.03341
MP2/6-31+G**	-668.33620	-707.51306	-555.78458	-555.24522	-805.45789	-575.09019

(BSSE correction 1)	-459.67545	-459.67592	-460.20782	-459.67332	-459.67729	-459.67449
(BSSE correction 2)	-208.62761	-247.80311	-95.56121	-95.55875	-345.74767	-115.39310

Molecular Aggregates

	(MGU)NH_2..Cl^-	**(MGU)(CH_3)NH..Cl^-**	**(MAA)NH…F^-**
B3LYP/6-31+G**	-705.54452	-705.54606	-348.46996
MP2/6-31+G**	-704.20801	-704.21068	-347.48901
(BSSE correction 1)	-459.67859	-459.67814	
(BSSE correction 2)	-244.35907	-244.35919	

Molecular Aggregates in reaction field[&]

	(IM)N1-H…Cl^-	**(IM)N1…H…F^-**
B3LYP/6-31G** (water)	-686.62412	-326.21230

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§ Single point calculation with the coordinates optimized at B3LYP/6-31G** level.

$ Single point calculation with the coordinates optimized at B3LYP/6-31+G** level.

† Ref. 35-37.

Ref. 38.

&Dielectric constant for water unless otherwise specified.

~Dielectric constant for methanol.

VIBRATION FREQUENCIES

Table 262S. Selected vibration (cm^{-1}) for isolate molecules and aggregates obtained from the analysis of the hessian. Force constants (mdyne/Å) and IR intensities (km/mol) are given in parenthesis in the order.

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	H-F	**H-Cl**	**H_2O**
B3LYP/6-31G**	4084.8 (10.4043; 61.0551)		
B3LYP/6-31G**&	3887.4 (9.4228; 59.3220)		
B3LYP/6-31+G**	4069.9 (10.3281; 114.8018)	2943.0 (5.2869; 22.0887)	1603.1 (1.6411; 91.2244)
			3809.3 (8.9293; 6.4134)
			3931.9 (9.8654; 57.2947)
B3LYP/6-31+G**&		2880.9 (5.0660; 21.8644)	
MP2/6-31+G**			1623.0 (1.6815; 92.8970)
			3867.3 (9.2030; 10.0857)
			4014.2 (10.2798; 66.7177)
	$FH\ldots OH_2$	**HO-H…FH**	
B3LYP/6-31G**		4083.7 (10.3983; 83.6761) ν_{F-H}	
		3807.3 (8.9266; 32.1312) ν_{O-H}	
		3911.4 (9.7382; 67.6479) ν_{O-H}	
B3LYP/6-31+G**	3659.9 (8.3697; 976.5180) ν_{F-H}	4056.9 (10.2616; 138.4978) ν_{F-H}	
	3825.7 (8.9976; 12.0123) ν_{O-H}	3809.7 (8.9319; 138.4978) ν_{O-H}	
	3947.5 (9.9609; 123.8684) ν_{O-H}	3925.3 (9.8258; 99.4225) ν_{O-H}	
CCSD(T)/6-31+G**			
MP2/6-31+G**		4104.7 (10.5047; 150.2562) ν_{F-H}	

		3870.7 (9.2228; 29.1431) ν_{O-H}	
		4007.3 (10.2351; 96.0553) ν_{O-H}	
	$ClH\cdots OH_2$		
B3LYP/6-31+G**	2709.8 (4.4863; 646.1660) ν_{Cl-H}		
	3815.8 (8.9513; 17.6650) ν_{O-H}		
	3939.1 (9.9145; 104.6889) ν_{O-H1}		
	IM	**(IM)N1-H…Cl^-**	**(IM)C2-H…Cl^-**
B3LYP/6-31G**			3670.9 (8.5819; 38.9381) ν_{N-H1}
			2998.9 (5.9220; 609.9454) ν_{C-H2}
B3LYP/6-31+G**	3667.5 (8.5729; 57.7220) ν_{N-H1}	2920.1 (5.5594; 2578.5933) ν_{N-H1}	3667.5 (8.5694; 50.4677) ν_{N-H1}
	3267.1 (6.8958; 0.9525) ν_{C-H2}		3070.2 (6.1854; 484.3194) ν_{C-H2}
	3262.6 (6.8478; 4.5833) ν_{C-H4}		
	3291.8 (7.0481; 1.2684) ν_{C-H5}		
MP2/6-31+G**	3724.1 (8.8461; 77.3160) ν_{N-H1}	2979.6 5.8032; 2652.9469) ν_{N-H1}	
	(IM)C4-H…Cl^-	**(IM)C5-H…Cl^-**	
B3LYP/6-31G**	3671.0 (8.5806; 14.8471) ν_{N-H1}		
	3280.0 (6.9605; 3.8073) ν_{C-H4}		
B3LYP/6-31+G**	3672.0 (8.5878; 24.6168) ν_{N-H1}	3666.2 (8.5630; 50.2180) ν_{N-H1}	
	3136.4 (6.4124; 291.5873) ν_{C-H4}	3262.5 (6.8816; 5.3902) ν_{C-H5}	
	(IM)N1-H…N(IM)	**(IM)N1-H…N(IM)**	**(IM)C2-H…N(IM)**
	(coplanar)	**(free)**	**(C2-H…N 180° fixed)**
B3LYP/6-31+G**	3260.5 (6.8621;3.6616) ν_{N-H1}	3260.8 (6.8638; 3.0271) ν_{N-H1}	3669.9 (8.5829; 51.4803) ν_{N-H1}

	3667.1 (8.5740; 75.0519) ν$_{N'-H1'}$ There is an immaginary frequency.	3666.6 (8.5717; 74.6994) ν$_{N'-H1'}$	3667.6 (8.5740; 64.4861) ν$_{N'-H1'}$ There is an immaginary frequency.
	IMH$^+$	**(IM)N1…H$^+$…Cl$^-$**	
B3LYP/6-31+G**	3617.4(8.3412; 363.6195)ν$_{N-H(1,3)}$ 3624.2 (8.4128;28.5526) ν$_{N-H(1,3)}$	1902.6 (2.2651; 3476.3718) ν$_{Cl-H1}$ 3666.5 (8.5720; 76.2819) ν$_{N-H3}$	
MP2/6-31+G**	3666.0 (8.5740; 393.6321) ν$_{N-H(1,3)}$ 3672.4 (8.6441; 31.2580) ν$_{N-H(1,3)}$	2416.4 (3.5891; 2409.1485) ν$_{Cl-H1}$ 3719.7 (8.8276; 93.8078) ν$_{N-H3}$	
	PYM	**(PYM)C2-H…Cl$^-$**	**(PYM)C2-H…N1'(PYM)/(PYM)C6'-H…N3'(PYM)**
B3LYP/6-31+G**	3192.1 (6.5531; 15.6651) ν$_{C2-H}$	3059.1 (6.0987; 320.5396) ν$_{C2-H}$	3189.9 (6.5623; 5.6287) ν$_{C2-H}$ There is an immaginary frequency. .
	(PYM)C5-H…Cl$^-$	**(PYM)C6-H…Cl$^-$**	
B3LYP/6-31+G**	3020.6 (5.9416; 550.0952) ν$_{C5-H}$ 3159.5 (6.4028; 46.6804) ν$_{C2-H}$	3028.9 (5.9750; 396.9294) ν$_{C6-H}$ 3159.2 (6.4081; 39.4463) ν$_{C2-H}$	
	AA	**(AA)N-H…Cl$^-$**	
B3LYP/6-31+G**	3601.1 (7.9897; 36.2015) ν$_{NH}$ 3744.3 (9.1285; 41.4036) ν$_{NH}$	3125.6 (6.2615; 1067.0896) ν$_{NH}$ + ν$_{CH3}$ 3139.0 (6.3764; 393.5288) ν$_{NH}$ +ν$_{CH3}$ 3656.3 (8.5225; 29.8931) ν$_{NH}$	
MP2/6-31+G**	3659.8 (8.2585; 45.1757) ν$_{NH}$ 3809.2 (9.4383; 49.5114) ν$_{NH}$	3238.5 (6.8312; 60.0307) + ν$_{CH3}$ 3261.9 (6.7525; 1318.9938) ν$_{NH}$ + ν$_{CH3}$ 3733.8 (6.7525; 1318.9938) ν$_{NH}$	

	MAA	**(MAA)N-H…Cl^-**
B3LYP/6-31+G**	3652.5 (8.4719; 22.8543) ν_{NH}	3144.7 (6.3694; 1074.2019) ν_{NH}
MP2/6-31+G**	3727.0 (8.8261; 37.5779) ν_{NH}	3231.6 (6.7778; 566.2145) $\nu_{NH+}\nu_{CH3}$
	There is an immaginary frequency.	3242.1 (6.7848; 920.6167) $\nu_{NH+}\ \nu_{CH3}$
	MA	**(MA)N…H…Cl^-**
B3LYP/6-31+G**	3401.8 (7.0319; 47.0931) ν_{NH}	1517.5 (1.4607; 661.2298) ν_{Cl-H}
	3488.8 (7.8439; 124.5034) ν_{NH}	1491.9 ((1.4479; 359.5643) $\nu_{NH2+}\nu_{Cl-H}$
	3489.3 (7.8462; 124.5674) ν_{NH}	3585.3 (8.2901; 17.7382) ν_{NH}
		3500.4 (7.5807; 5.0138) ν_{NH}
MP2/6-31+G**	3464.0 (7.2991; 53.7963) ν_{NH}	2158.3 (2.8770; 2523.5043) $\nu_{ClH+}\nu_{NH}$
	3575.0 (8.2317; 134.6890) ν_{NH}	3569.7 (7.8889; 3.2435) ν_{NH}
	3575.4 (8.2335; 134.8086) ν_{NH}	3670.4 (8.6793; 15.0143) ν_{NH}
	MAB	**(MAB)NH…Cl^-**
B3LYP/6-31+G**	3513.1 (7.6285; 0.4991)	3326.1 (6.9481; 408.1720)
	3601.2 (8.3606; 1.7444)	3525.7 (7.8923; 17.9341)
MP2/6-31+G**	3590.7 (7.9754; 0.1130)	3445.3 (7.4287; 336.5644)
	3697.8 (8.8132; 3.9856)	3621.8 (8.3564; 30.2328)
	MeOH	**(MeOH)OH…Cl^-**
B3LYP/6-31+G**	3839.7 (9.2669; 28.0942) ν_{O-H}	3309.2 (6.9012; 1257.9276) ν_{O-H}
MP2/6-31+G**	3897.3 (9.5488; 34.0101) ν_{O-H}	3437.8 (7.4439; 1117.5219) ν_{O-H}

	MGU	**(MGU) NH_2NH_2…Cl^-**	**(MGU)NH_2NH…Cl^-**
B3LYP/6-31+G**	3602.3 (8.0060; 192.2091)	2996.9 (5.7176; 2590.7084) ν_{N-H2a}	2818.9 (5.1232; 722.3038) νNH(2b ,4)

	νN-H(2a,2b,3a,3b) 3612.2 (8.0696; 126.3175) νN-H(2a,2b,3a,3b) 3724.3 (9.0408; 96.3697) νN-H(2a,2b,3a,3b) 3729.3 (9.0657; 132.7382) νN-H(2a,2b,3a,3b) 3634.8 (8.3907; 70.8345) ν_{N-H4}	2823.2 (5.0972; 431.8023) ν_{N-H3a} 3656.1 (8.4904; 41.1479) ν_{N-H4}	3015.4 (5.6268; 618.2597)νNH2b+νCH3 3028.5 (5.7889; 1549.2417)νNH2b+νCH3 3627.7 (8.1191; 55.8883) νNH(3a,3b) 3678.9 (8.6291; 69.6928) νNH2a 3750.5 (9.1554; 65.5217) νNH(3a,3b)
MP2/6-31+G**	3662.3 (8.2721; 224.4326) νN-H(2a,2b,3a,3b) 3670.4 (8.3320; 138.2874) νN-H(2a,2b,3a,3b) 3800.3 (9.4146; 87.4460) νN-H(2a,2b,3a,3b) 3802.2 (9.4299; 170.2081) νN-H(2a,2b,3a,3b) 3670.4 (8.3320; 138.2874) ν_{N-H4} 3693.8 (8.6693; 90.4686) ν_{N-H4}	2906.4 (5.4037; 808.7985) νN-H(2a,2b,3a,3b) 3121.5 (6.1283; 1463.5228) νN-H(2a,3a) + νCH3 3715.5 (8.7692; 60.8991) ν_{N-H4} 3735.4 (8.8979; 95.9092) $\nu_{N-H(2a,2b)}$ 3753.7 (8.9819; 90.7784) $\nu_{N-H(3a,3b)}$	3194.6 (6.4644; 1424.4196) νNH(2a,2b,4) 3668.3 (8.3085; 56.8486) νNH(3a,3b) 3736.1 (8.9068; 86.4433) νNH(2a,2b) 3799.0 (9.3770; 66.0391) νNH(3a,3b)
	HMB	**(HMB)OH…Cl^-**	
B3LYP/6-31+G**	3829.7 (9.2149; 56.6372) ν_{O-H}	3114.2 (6.1343; 1899.1950) ν_{O-H}	

&Dielectric constant for water.