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Supplementary Information

Interaction strength of osmolytes with the anion of a salt-bridge determines its stability

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Table S1 Energetics in kcal/mol of the noncovalent complex formed between the guanidinium ion and the salt-bridge model complex

Orientation	Level of theory	ΔE	E_b	ΔH_b	ΔG_b	$I_{ca\cdots an,osm}$	$I_{osm\cdots SB}$
Ort1	L_1	0.1	-15.8	-13.7	-0.8	-24.2	-19.7
	L_2	0.1	-12.7	-10.4	-0.2	-17.8	-15.9
Ort2	L_1	0.9	-14.9	-13.0	-1.6	-26.6	-17.5
	L_2	0.6	-12.1	-9.8	0.0	-19.6	-14.3
	L_3	0.3	-15.4	-13.5	-3.1	-27.9	-17.5
Ort3	L_1	5.6	-10.2	-8.2	5.4	-27.3	-12.6
	L_2	8.7	-4.0	-1.8	8.7	-21.5	-4.4
Ort4	L_1	0.0	-15.8	-13.8	-1.4	-24.2	-19.7
	L_2	0.0	-12.7	-10.4	0.2	-17.9	-15.9
	L_3	0.0	-15.7	-13.9	-2.8	-24.7	-19.8
Ort5	L_1	0.9	-14.9	-12.9	-1.5	-26.7	-17.4
	L_2	0.7	-12.1	-9.8	0.1	-19.7	-14.3
Ort6	L_1	1.1	-14.8	-12.6	0.0	-26.4	-17.5
	L_2	0.7	-12.1	-9.4	1.8	-19.4	-14.4
Ort7	L_1	5.1	-10.7	-8.4	5.6	-26.5	-12.9
	L_2	-	-	-	-	-	-

Ort 1 to Ort7 represent the different orientations in which one Gdm^+ ion was optimized with the salt-bridge model complex. Please see Fig. S1 for the structures.

We could not locate the geometry in Ort7 at the L_2 level of theory. Ort 3 is a π-π stacking complex, whereas all other geometries belong to the hydrogen bonding complex.

L_1, L_2 and L_3 are the CPCM(water)/M06-2X/6-311G**, CPCM(water)/M06-2X/6-311++G** and CPCM(water)/MP2/6-311G** levels of theory, respectively.

ΔE = Relative electronic energy of the given geometry with respect to the lowest energy one.

E_b, ΔH_b and ΔG_b are binding energy, enthalpy of binding and the free energy of binding, respectively.

$I_{ca\cdots an,osm} =$ Energy of interaction between cation and anion of the SB in osmolyte···SB complex

$I_{osm\cdots SB} =$ Energy of interaction between osmolyte and the SB in the osmolyte···SB complex

Table S2 Energetics in kcal/mol of the noncovalent complex formed between the guanidinium chloride and the salt-bridge model complex

Orientation	Level of theory	ΔE	E_b	ΔH_b	ΔG_b	$I_{ca\cdots an,osm}$	$I_{osm\cdots SB}$
Ort1	L_1	6.6	-10.6	-8.4	5.2	-26.9	-12.5
	L_2	5.6	-8.7	-5.6	8.5	-19.8	-10.6
Ort2	L_1	0.0	-17.2	-14.2	3.5	-24.1	-24.2
	L_2	0.0	-14.3	-11.0	4.5	-17.5	-20.8
Ort3	L_1	0.7	-16.4	-13.6	3.3	-25.4	-24.1
	L_2	0.1	-14.3	-10.9	3.9	-18.9	-20.9
Ort4	L_1	3.4	-13.8	-11.3	2.3	-26.9	-16.1
	L_2	3.2	-11.2	-8.2	3.4	-19.8	-13.1
Ort5	L_1	2.7	-14.5	-12.0	2.0	-25.8	-23.2
	L_2	0.4	-14.0	-10.6	4.2	-18.8	-19.4
Ort6	L_1	3.0	-14.2	-11.6	3.8	-25.9	-18.1
	L_2	2.8	-11.6	-8.4	5.5	-19.0	-14.9
Ort7	L_1	1.2	-16.0	-13.2	3.1	-26.6	-20.5
	L_2	0.4	-14.0	-10.6	4.3	-18.8	-19.3
Ort8	L_1	11.1	-6.1	-4.2	11.4	-28.8	-6.2
	L_2	9.1	-5.3	-2.6	11.3	-21.3	-5.4
Ort9	L_1	1.1	-16.1	-13.3	2.1	-24.8	-20.2
	L_2	1.0	-13.4	-10.2	4.1	-18.3	-17.1
Ort10	L_1	0.7	-16.5	-13.5	3.7	-23.6	-23.9
	L_2	0.7	-13.7	-10.3	5.1	-17.5	-20.1
Ort11	L_1	3.4	-13.8	-11.4	2.5	-26.6	-16.2
	L_2	3.2	-11.2	-8.3	3.4	-19.6	-13.1
Ort12	L_1	3.2	-14.0	-11.7	1.3	-26.8	-16.3
	L_2	3.0	-11.3	-8.5	2.7	-19.8	-13.2
Ort13	L_1	2.3	-14.9	-12.4	1.9	-24.7	-18.3
	L_2	2.4	-12.0	-8.9	3.7	-18.3	-14.5
Ort14	L_1	3.4	-13.8	-11.5	2.1	-26.7	-16.1
	L_2	3.1	-11.2	-8.3	3.0	-19.6	-13.2
Ort15	L_1	3.2	-13.9	-11.5	2.2	-26.8	-16.3
	L_2	1.7	-12.7	-9.5	3.8	-19.7	-14.6

Ort 1 to Ort15 represent the different orientations in which one GdmCl molecule was optimized with the salt-bridge model complex. Please see Fig. S2 for the structures.

L_1, L_2 and L_3 are the CPCM(water)/M06-2X/6-311G**, CPCM(water)/M06-2X/6-311++G** and CPCM(water)/MP2/6-311G** levels of theory, respectively.

ΔE = Relative electronic energy of the given geometry with respect to the lowest energy one.

E_b, ΔH_b and ΔG_b are binding energy, enthalpy of binding and the free energy of binding, respectively.

$I_{ca\cdots an,osm} =$ Energy of interaction between cation and anion of the SB in osmolyte···SB complex

$I_{osm\cdots SB} =$ Energy of interaction between osmolyte and the SB in the osmolyte···SB complex

Table S3 Energetics in kcal/mol of the noncovalent complex formed between the urea and the salt-bridge model complex

Orientation	Level of theory	ΔE	E_b	ΔH_b	ΔG_b	$I_{ca\cdots an,osm}$	$I_{osm\cdots SB}$
Ort1	L_1	0.1	-12.5	-10.0	3.8	-26.2	-15.4
	L_2	0.2	-9.1	-6.4	4.4	-19.6	-11.1
Ort2	L_1	0.4	-12.2	-9.8	4.6	-27.0	-16.2
	L_2	0.3	-9.0	-6.5	2.1	-20.1	-10.6
Ort3	L_1	1.8	-10.9	-8.9	2.1	-27.6	-12.7
	L_2	0.7	-8.6	-6.2	1.7	-20.3	-9.9
Ort4	L_1	0.9	-11.7	-9.6	1.6	-27.8	-13.0
	L_2	0.3	-9.0	-6.6	2.6	-20.7	-9.9
Ort5	L_1	1.8	-10.8	-9.0	1.8	-27.5	-12.3
	L_2	0.7	-8.6	-6.1	3.3	-20.3	-9.9
Ort6	L_1	1.0	-11.6	-9.8	0.2	-27.8	-12.9
	L_2	0.3	-9.0	-6.7	1.8	-20.7	-9.9
	L_3	0.1	-10.9	-9.1	0.9	-28.2	-12.4
Ort7	L_1	0.0	-12.6	-10.3	2.7	-27.0	-15.1
	L_2	0.0	-9.3	-6.6	4.1	-19.9	-11.3
	L_3	0.0	-11.0	-9.2	2.1	-27.9	-13.1
Ort8	L_1	3.5	-9.1	-7.5	2.6	-28.3	-10.1
	L_2	2.3	-7.0	-4.9	3.1	-20.8	-7.8
Ort9	L_1	2.4	-10.2	-8.7	0.8	-28.2	-11.0
	L_2	0.9	-8.4	-6.1	2.1	-20.9	-9.0
Ort10	L_1	2.7	-10.0	-8.2	2.0	-26.9	-11.7
	L_2	1.7	-7.6	-5.3	2.7	-20.0	-8.8
Ort11	L_1	1.6	-11.0	-9.1	2.0	-26.6	-13.4
	L_2	1.0	-8.3	-5.8	3.7	-19.7	-10.0
Ort12	L_1	5.8	-6.9	-5.4	3.8	-28.3	-7.7
	L_2	4.3	-5.0	-2.9	4.1	-20.9	-5.7

Ort 1 to Ort12 represent the different orientations in which one urea molecule was optimized with the salt-bridge model complex. Please see Fig. S3 for the structures.

L_1, L_2 and L_3 are the CPCM(water)/M06-2X/6-311G**, CPCM(water)/M06-2X/6-311++G** and CPCM(water)/MP2/6-311G** levels of theory, respectively.

For the definition of the energy terms, please see the "Computational Methods" section in the main manuscript.

Table S4 Energetics in kcal/mol of the noncovalent complex formed between the trimethylamine N-oxide and the salt-bridge model complex

Orientation	Level of theory	ΔE	E_b	ΔH_b	ΔG_b	$I_{ca\cdots an,osm}$	$I_{osm\cdots SB}$
Ort1	L_1	3.0	-14.6	-12.5	-0.2	-26.2	-18.6
	L_2	3.9	-9.3	-6.8	2.1	-19.3	-12.1
Ort2	L_1	2.9	-14.7	-12.8	-0.6	-26.9	-17.2
	L_2	3.3	-9.9	-7.7	1.8	-19.9	-11.7
Ort3	L_1	9.4	-8.2	-6.3	6.5	-28.1	-8.9
	L_2	8.9	-4.4	-2.1	8.0	-21.0	-4.7
Ort4	L_1	0.0	-17.6	-15.5	-4.2	-28.2	-18.8
	L_2	0.0	-13.2	-10.6	-1.1	-20.8	-14.2
	L_3	0.0	-18.2	-16.4	-6.2	-28.4	-19.8

Ort 1 to Ort4 represent different orientations in which one TMAO molecule was optimized with the salt-bridge model complex. Please see Fig. S4 for the structures.

L_1, L_2 and L_3 are the CPCM(water)/M06-2X/6-311G**, CPCM(water)/M06-2X/6-311++G** and CPCM(water)/MP2/6-311G** levels of theory, respectively.

ΔE = Relative electronic energy of the given geometry with respect to the lowest energy one.

E_b, ΔH_b and ΔG_b are binding energy, enthalpy of binding and the free energy of binding, respectively.

$I_{ca\cdots an,osm} =$ Energy of interaction between cation and anion of the SB in osmolyte···SB complex

$I_{osm\cdots SB} =$ Energy of interaction between osmolyte and the SB in the osmolyte···SB complex

Table S5 Energetics in kcal/mol of the noncovalent complex formed between the glycerol and the salt-bridge model complex

Orientation	Level of theory	ΔE	E_b	ΔH_b	ΔG_b	$I_{ca\cdots an,osm}$	$I_{osm\cdots SB}$
Ort1	L_1	1.0	-15.4	-13.2	0.7	-25.9	-23.8
	L_2	0.0	-11.8	-9.2	3.1	-18.9	-18.5
	L_3	0.1	-14.8	-12.9	-0.4	-26.8	-22.9
Ort2	L_1	5.0	-11.4	-9.3	4.8	-27.8	-17.2
	L_2	3.3	-8.6	-6.1	5.4	-20.5	-12.0
Ort3	L_1	4.1	-12.3	-10.4	2.5	-27.4	-15.9
	L_2	2.7	-9.1	-6.8	4.0	-20.1	-11.5
Ort4	L_1	2.5	-13.9	-11.8	1.1	-27.4	-17.9
	L_2	1.7	-10.2	-7.7	1.9	-20.5	-12.5
	L_3	0.6	-14.5	-12.5	-1.1	-27.8	-18.3
Ort5	L_1	4.15	-12.2	-10.3	3.7	-28.1	-17.1
	L_2	1.6	-10.2	-7.9	3.9	-20.9	-13.4
Ort6	L_1	1.1	-15.3	-13.2	1.4	-26.4	-20.7
	L_2	1.0	-10.8	-8.1	4.2	-18.9	-15.3
Ort7	L_1	1.4	-15.0	-12.9	0.9	-26.9	-19.7
	L_2	0.8	-11.0	-8.4	2.6	-19.5	-14.4
Ort8	L_1	3.4	-13.0	-10.8	4.4	-26.7	-19.3
	L_2	3.0	-8.8	-6.2	6.2	-19.6	-13.2
Ort9	L_1	1.8	-14.6	-12.3	2.1	-26.5	-18.7
	L_2	3.9	-7.9	-5.5	6.1	-20.6	-11.5
Ort10	L_1	5.9	-10.5	-8.3	5.9	-27.3	-16.1
	L_2	1.3	-10.5	-7.9	3.7	-19.6	-13.2
Ort11	L_1	7.9	-8.5	-7.0	6.2	-28.3	-16.3
	L_2	5.5	-6.3	-4.3	6.9	-20.9	-12.1
Ort12	**L_1**	**0.0**	**-16.4**	**-14.1**	**0.9**	**-25.9**	**-24.4**
	L_2	0.4	-11.4	-8.8	3.1	-19.0	-17.7
	L_3	**0.0**	**14.9**	**-12.9**	**0.5**	**-26.4**	**-22.2**

Ort 1 - Ort12 represent different orientations in which one glycerol molecule was optimized with the salt-bridge. Please see Fig. S5 for the structures.

L_1, L_2 and L_3 are the CPCM(water)/M06-2X/6-311G**, CPCM(water)/M06-2X/6-311++G** and CPCM (water)/MP2/6-311G** levels of theory, respectively.

For the definition of energy terms, please see the "Computational Methods" section in the main manuscript.

Table S6 Energetics in kcal/mol of the noncovalent complex formed between two guanidinium ions and the salt-bridge model complex

Orientation	Level of theory	ΔE	E_b	ΔH_b	ΔG_b	$I_{ca\cdots an,osm}$	$I_{osm\cdots SB}$
Ort1	L_1	0.0	-27.5	-23.4	0.5	-23.4	-33.9
	L_2	0.0	-22.7	-18.2	4.5	-17.4	-27.9
Ort2	L_1	0.0	-27.5	-23.7	-1.1	-24.0	-33.3
	L_2	0.1	-22.6	-18.7	1.6	-17.9	-27.6
Ort3	L_1	8.4	-19.1	-15.3	8.7	-23.9	-20.9
	L_2	7.6	-15.1	-11.0	11.3	-17.9	-16.5
Ort4	L_1	0.0	-27.5	-23.7	-1.4	-26.3	-30.6
	L_2	0.2	-22.5	-18.7	0.7	-19.8	-25.1

Ort 1 to Ort4 represent different orientations in which two Gdm^+ ions were optimized with the salt-bridge model complex. Please see Fig. S6 for the structures.

L_1 and L_2 are the CPCM(water)/M06-2X/6-311G** and CPCM(water)/M06-2X/6-311++G** levels of theory, respectively.

ΔE = Relative electronic energy of the given geometry with respect to the lowest energy one.
E_b, ΔH_b and ΔG_b are binding energy, enthalpy of binding and the free energy of binding, respectively.

$I_{ca\cdots an,osm} =$ Energy of interaction between cation and anion of the SB in osmolyte···SB complex

$I_{osm\cdots SB} =$ Energy of interaction between osmolyte and the SB in the osmolyte···SB complex

Table S7 Energetics in kcal/mol of the noncovalent complex formed between two trimethylamine N-oxide molecules and the salt-bridge model complex

Orientation	Level of theory	ΔE	E_b	ΔH_b	ΔG_b	$I_{ca\cdots an,osm}$	$I_{osm\cdots SB}$
Ort1	L_1	9.5	-22.6	-18.8	4.0	-26.7	-23.0
	L_2	7.8	-14.5	-10.6	10.6	-19.9	-15.2
Ort2	L_1	0.0	-32.1	-27.5	-3.0	-25.5	-37.2
	L_2	0.5	-21.9	-17.7	3.9	-18.8	-25.9
Ort3	L_1	5.7	-26.4	-22.5	0.3	-27.3	-33.3
	L_2	3.8	-18.5	-14.4	6.7	-20.7	-19.3
Ort4	L_1	0.6	-31.5	-27.6	-5.3	-26.4	-35.0
	L_2	0.0	-22.4	-18.5	-0.4	-19.6	-24.8
Ort5	L_1	10.1	-22.0	-18.6	5.5	-27.2	-33.7
	L_2	7.8	-14.6	-10.8	10.3	-20.1	-15.7

Ort1 to Ort5 represent different orientations in which two TMAO molecules were optimized with the salt-bridge model complex. Please see Fig. S7 for the structures.

L_1 and L_2 are the CPCM(water)/M06-2X/6-311G** and CPCM(water)/M06-2X/6-311++G** levels of theory, respectively.

ΔE = Relative electronic energy of the given geometry with respect to the lowest energy one.
E_b, ΔH_b and ΔG_b are binding energy, enthalpy of binding and the free energy of binding, respectively.

$I_{ca\cdots an,osm} =$ Energy of interaction between cation and anion of the SB in osmolyte···SB complex

$I_{osm\cdots SB} =$ Energy of interaction between osmolyte and the SB in the osmolyte···SB complex

Table S8 Energetics in kcal mol^{-1} for the adsorption of the second molecule of osmolytes on the salt-bridge model complex (the minimum energy geometries)

Level of theory	Osmolyte	E_b	ΔH_b	ΔG_b	K_{A2} (M^{-1})
L_1	Gdm^+	-11.7	-10.0	1.8	4.8×10^{-2}
	TMAO	-14.5	-12.0	1.2	1.3×10^{-1}
L_2	Gdm^+	-10.0	-7.8	4.4	6.0×10^{-4}
	TMAO	-9.1	-7.9	0.7	3.1×10^{-1}

L_1 and L_2 are the CPCM(water)/M06-2X/6-311G** and CPCM(water)/M06-2X/6-311++G** levels of theory, respectively.

E_b, ΔH_b and ΔG_b are binding energy, enthalpy of binding and the free energy of binding, respectively.

$K_{A2} =$ Computed association constant for the adsorption of the second molecule of the osmolyte on the SB

Table S9 Energetics in kcal mol^{-1} of binding of osmolytes with the free acetate ion

Level of theory	Osmolyte	E_b	ΔH_b	ΔG_b	$K_{A,os\cdots an}$ (M^{-1})
L_1	Gdm^+	-26.6	-26.0	-15.7	3.1×10^{11}
	Urea	-17.6	-16.5	-7.3	2.2×10^{5}
	Glycerol	-21.3	-20.4	-9.4	7.6×10^{6}
L_2	Gdm^+	-19.8	-18.6	-10.1	2.5×10^{7}
	Urea	-12.6	-10.8	-2.8	1.1×10^{2}
	Glycerol	-15.9	-14.4	-5.6	1.3×10^{4}
L_3	Gdm^+	-27.2	-26.2	-14.7	5.8×10^{10}
	Urea	-17.2	-15.8	-5.8	1.8×10^{4}
	Glycerol	-21.3	-20.0	-9.4	7.7×10^{6}

L_1 and L_2 are the CPCM(water)/M06-2X/6-311G** and CPCM(water)/M06-2X/6-311++G** levels of theory, respectively.

E_b, ΔH_b and ΔG_b are binding energy, enthalpy of binding and the free energy of binding, respectively.

$K_{A,osm\cdots an} =$ Computed association constant for binding of TMAO with free $MeGdm^+$ ion

Table S10 Energetics in kcal/mol of binding of TMAO with the free $MeGdm^+$ ion

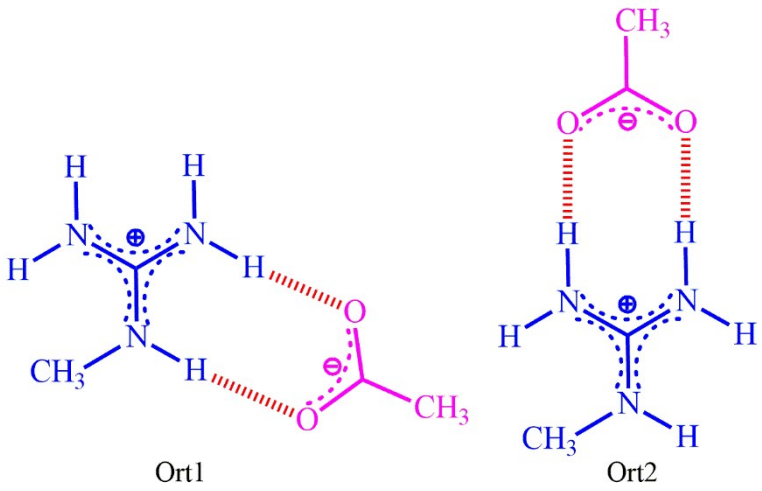
Orientation	Level of theory	ΔE	E_b	ΔH_b	ΔG_b	$K_{a,osm\cdots an}$ (M^{-1})
Ort1	L_1	0.0	-20.3	-18.7	-8.1	8.6×10^5
	L_2	0.0	-15.5	-14.5	-4.8	3.9×10^4
	L_3	0.0	-21.1	-19.7	-8.9	3.3×10^6
Ort2	L_1	0.1	-20.2	-18.5	-7.9	–
	L_2	0.1	-15.4	-14.4	-5.1	–
	L_3	0.6	-20.5	-19.1	-8.0	–

L_1, L_2 and L_3 represent CPCM(water)/M06-2X/6-311G**, CPCM(water)/M06-2X/6-311++G** and CPCM(water)/MP2/6-311G** levels of theory, respectively.

E_b, ΔH_b and ΔG_b are binding energy, enthalpy of binding and the free energy of binding, respectively. For the definition, please see the "Computational Methods" section.

ΔE = Relative electronic energy of the two conformers shown in the below figure.

$K_{A,osm\cdots an}$ = Computed association constant for binding of TMAO with free $MeGdm^+$ ion



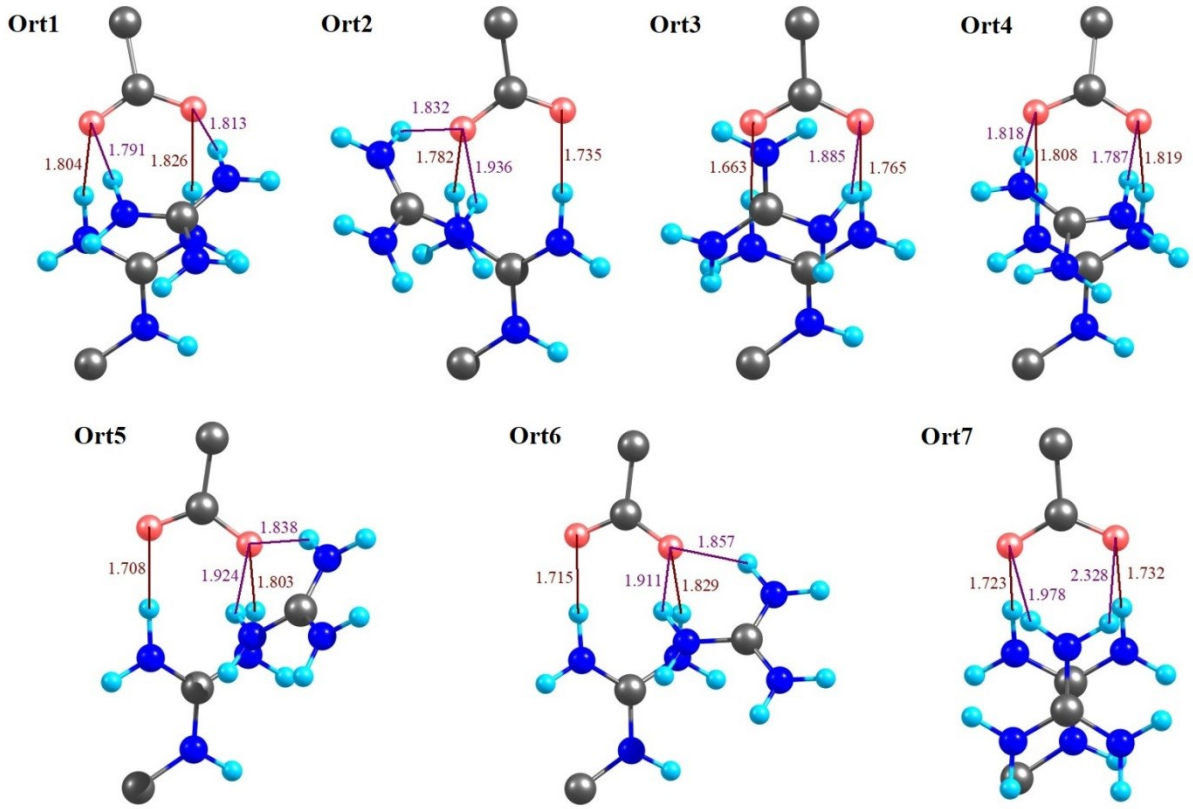


Fig. S1 Optimized geometries at the CPCM(water)/M06-2X/6-311G** level of theory of the salt-bridge model complex in the presence of one guanidinium ion (Gdm^+). Ort1 to Ort7 represent the different orientations in which Gdm^+ is optimized with the salt-bridge model complex. Colour scheme: black – carbon, cyan – hydrogen, blue – nitrogen, red – oxygen, maroon line – salt-bridge hydrogen bond, purple line – hydrogen bond between the Gdm^+ and the salt-bridge model complex.

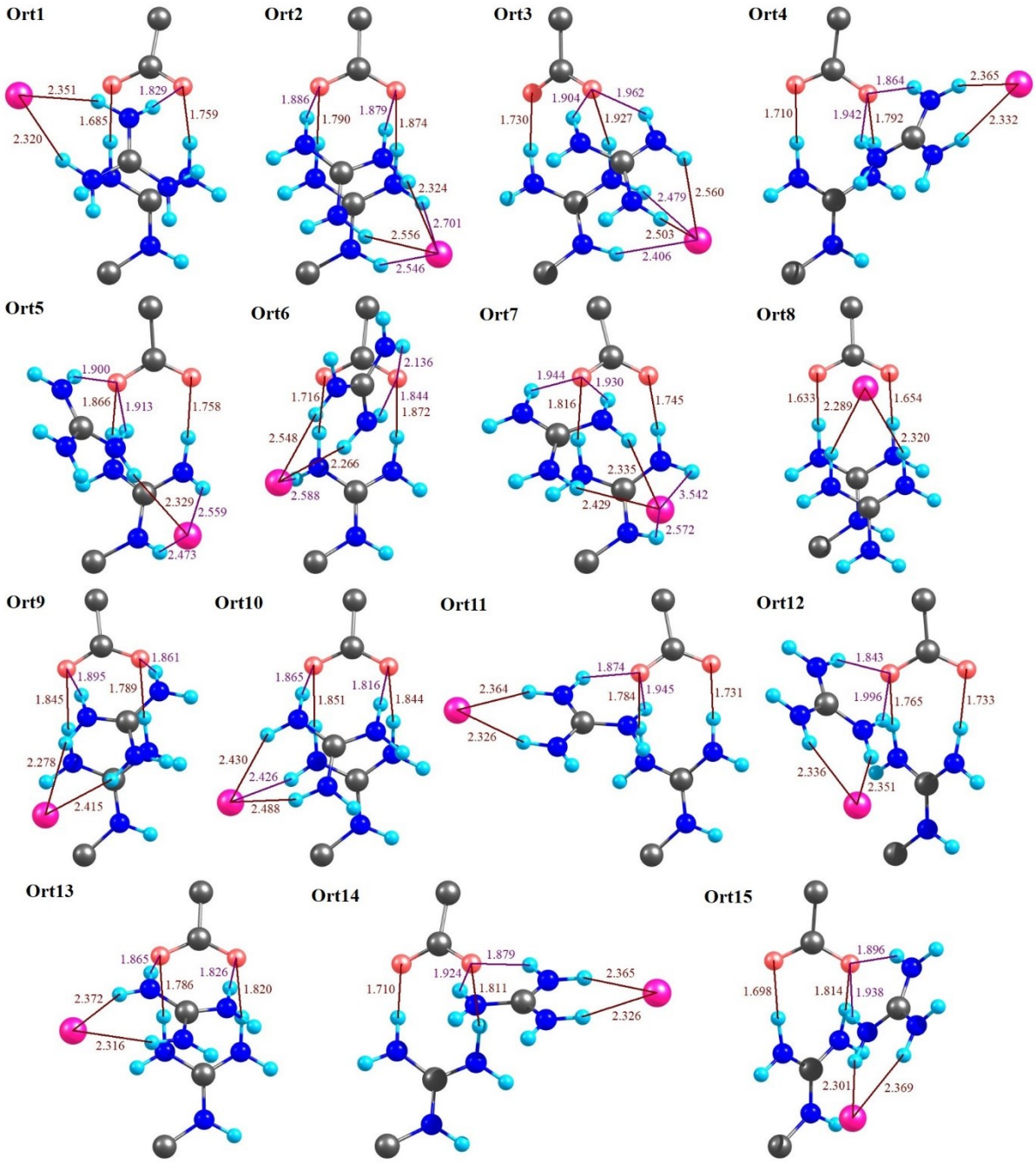


Fig. S2 Optimized geometries at the CPCM(water)/M06-2X/6-311G** level of theory of the salt-bridge model complex in the presence of one molecule of guanidinium chloride (GdmCl). Ort1 to Ort15 represent the different orientations in which the GdmCl is optimized with the salt-bridge model complex. Colour scheme: black – carbon, cyan – hydrogen, blue – nitrogen, red – oxygen, pink – chloride, maroon line – salt-bridge hydrogen bond and the hydrogen bond between the chloride and the Gdm^+ ion, purple line – hydrogen bond between the GdmCl and the salt-bridge model complex.

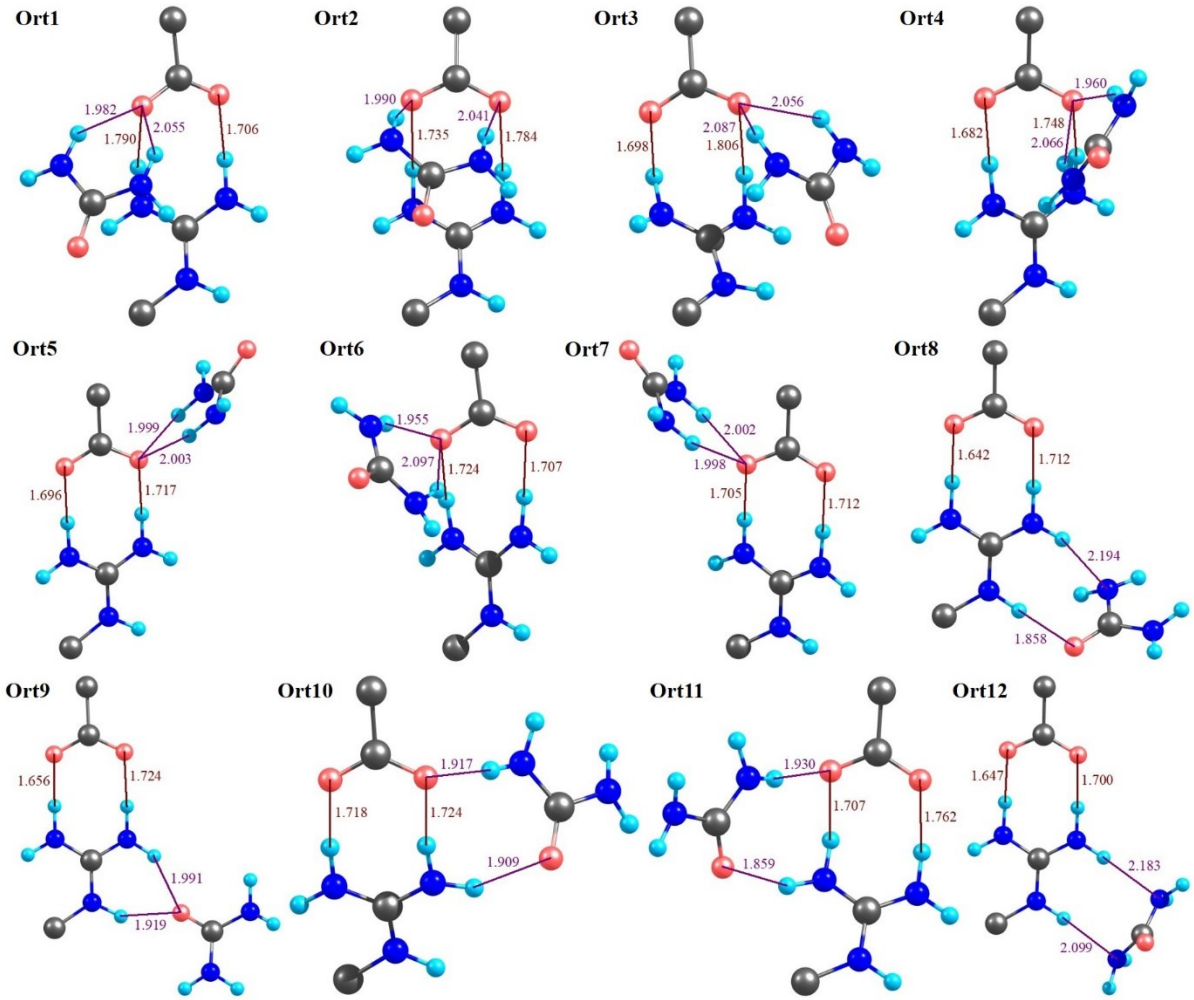


Fig. S3 Optimized geometries at the CPCM(water)/M06-2X/6-311G** level of theory of the salt-bridge model complex in the presence of one molecule of urea. Ort1 to Ort12 represent the different orientations in which the urea molecule is optimized with the salt-bridge model complex. Colour scheme: black – carbon, cyan – hydrogen, blue – nitrogen, red – oxygen, maroon line – salt-bridge hydrogen bond, purple line – hydrogen bond between the urea and the salt-bridge model complex.

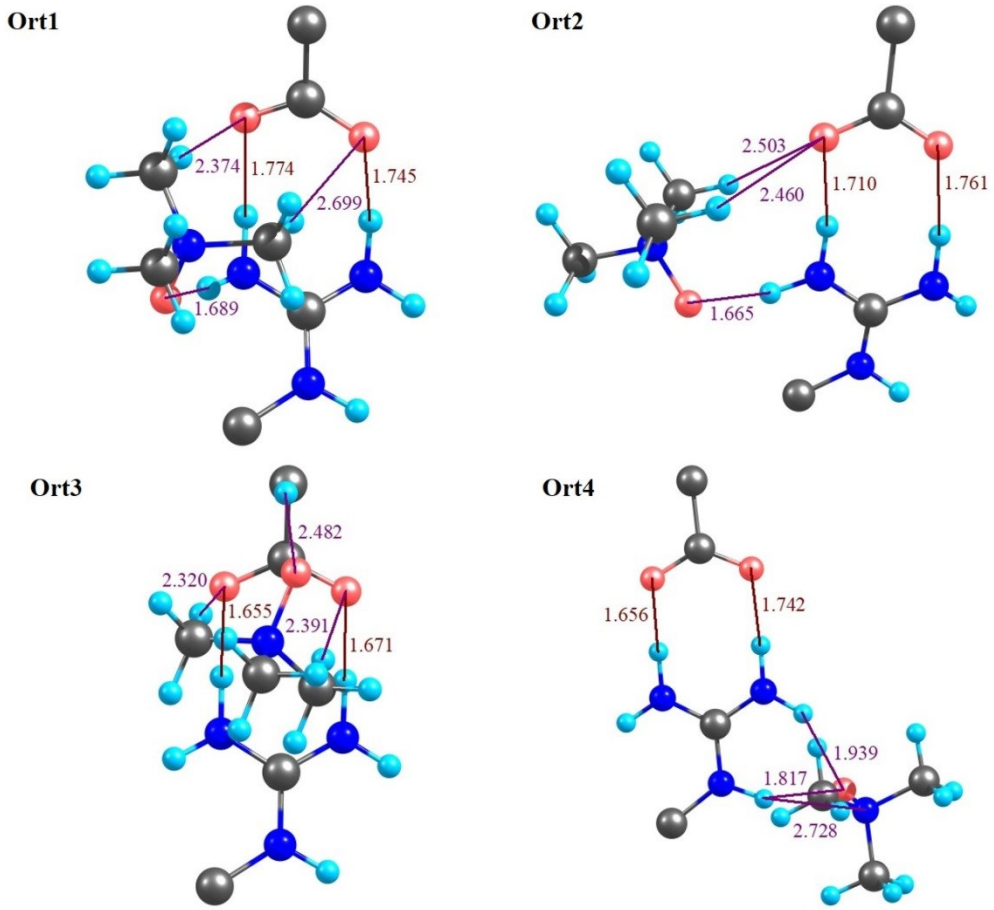


Fig. S4 Optimized geometries at the CPCM(water)/M06-2X/6-311G** level of theory of the salt-bridge model complex in the presence of one molecule of trimethylamine N-oxide (TMAO). Ort1 to Ort4 represent the different orientations in which the TMAO molecule is optimized with the salt-bridge model complex. Colour scheme: black – carbon, cyan – hydrogen, blue – nitrogen, red – oxygen, maroon line – salt-bridge hydrogen bond, purple line – hydrogen bond between the TMAO and the salt-bridge model complex.

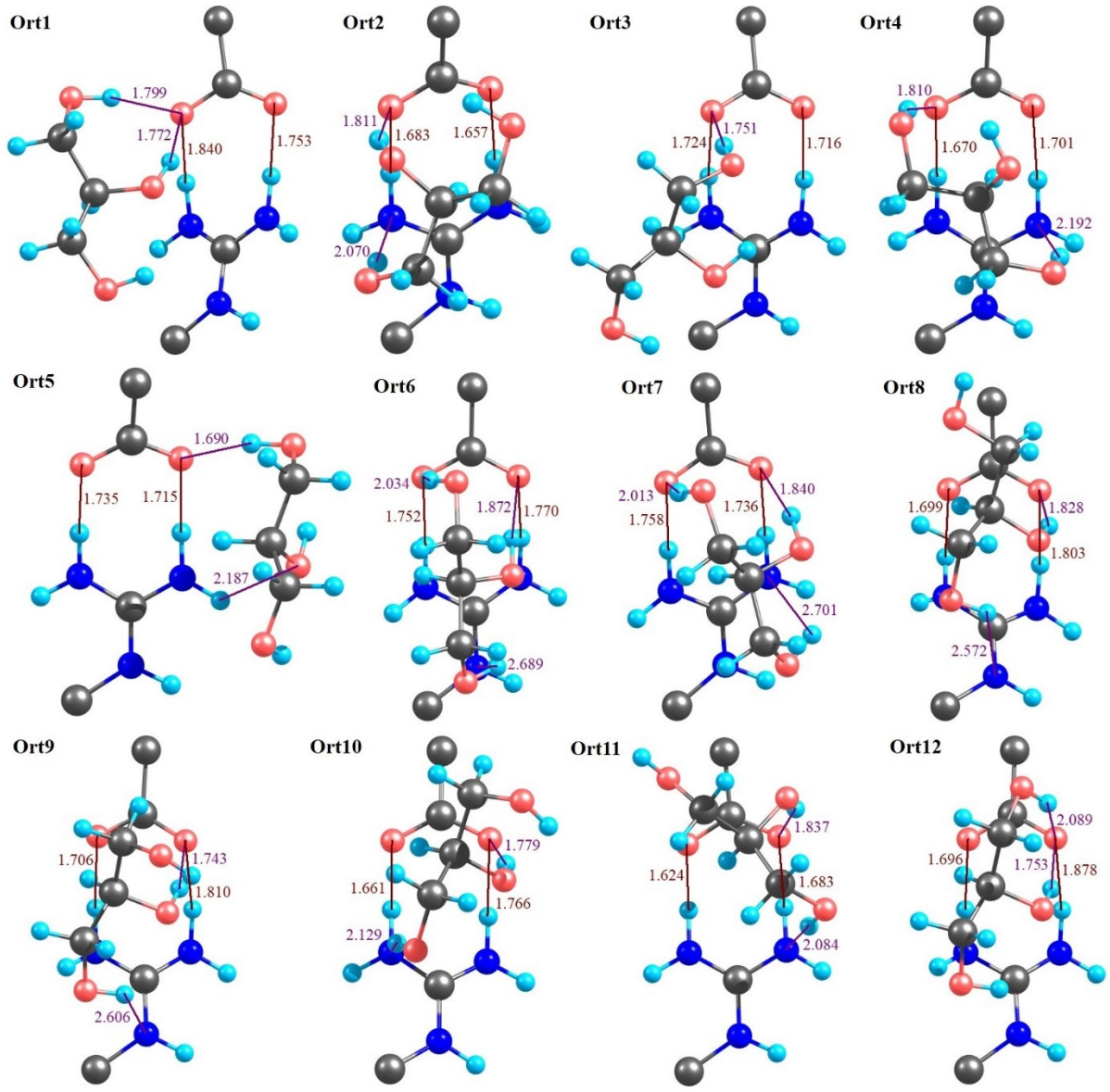


Fig. S5 Optimized geometries at the CPCM(water)/M06-2X/6-311G** level of theory of the salt-bridge model complex in the presence of one molecule of glycerol. Ort1 to Ort12 represent the different orientations in which the glycerol molecule is optimized with the salt-bridge model complex. Colour scheme: black – carbon, cyan – hydrogen, blue – nitrogen, red – oxygen, maroon line – salt-bridge hydrogen bond, purple line – hydrogen bond between the glycerol and the salt-bridge model complex.

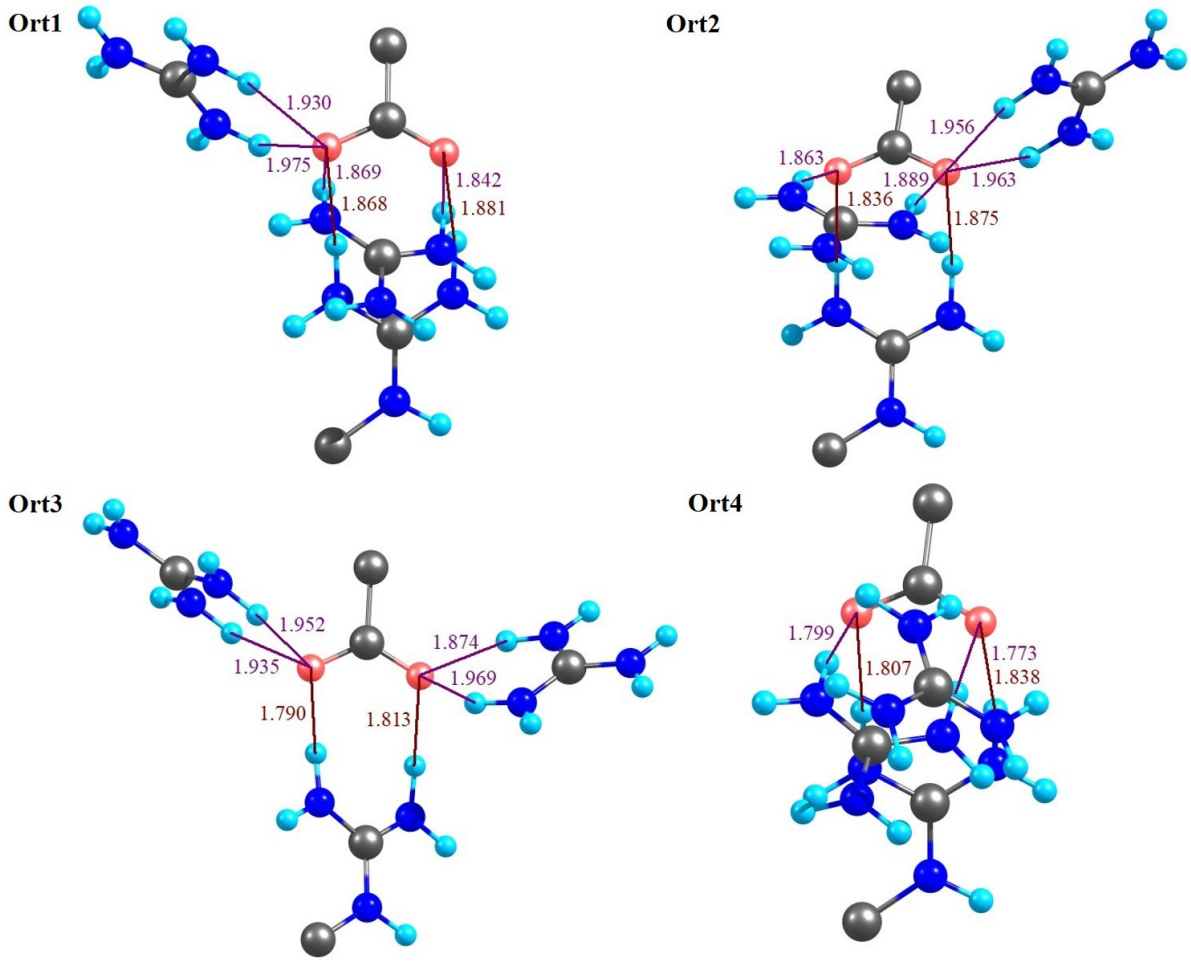


Fig. S6 Optimized geometries at the CPCM(water)/M06-2X/6-311G** level of theory of the salt-bridge model complex in the presence of two guanidinium ions (Gdm^+). Ort1 to Ort4 represent the different orientations in which the two Gdm^+ ions are optimized with the salt-bridge model complex. Colour scheme: black – carbon, cyan – hydrogen, blue – nitrogen, red – oxygen, maroon line – salt-bridge hydrogen bond, purple line – hydrogen bond between the Gdm^+ and the salt-bridge model complex.

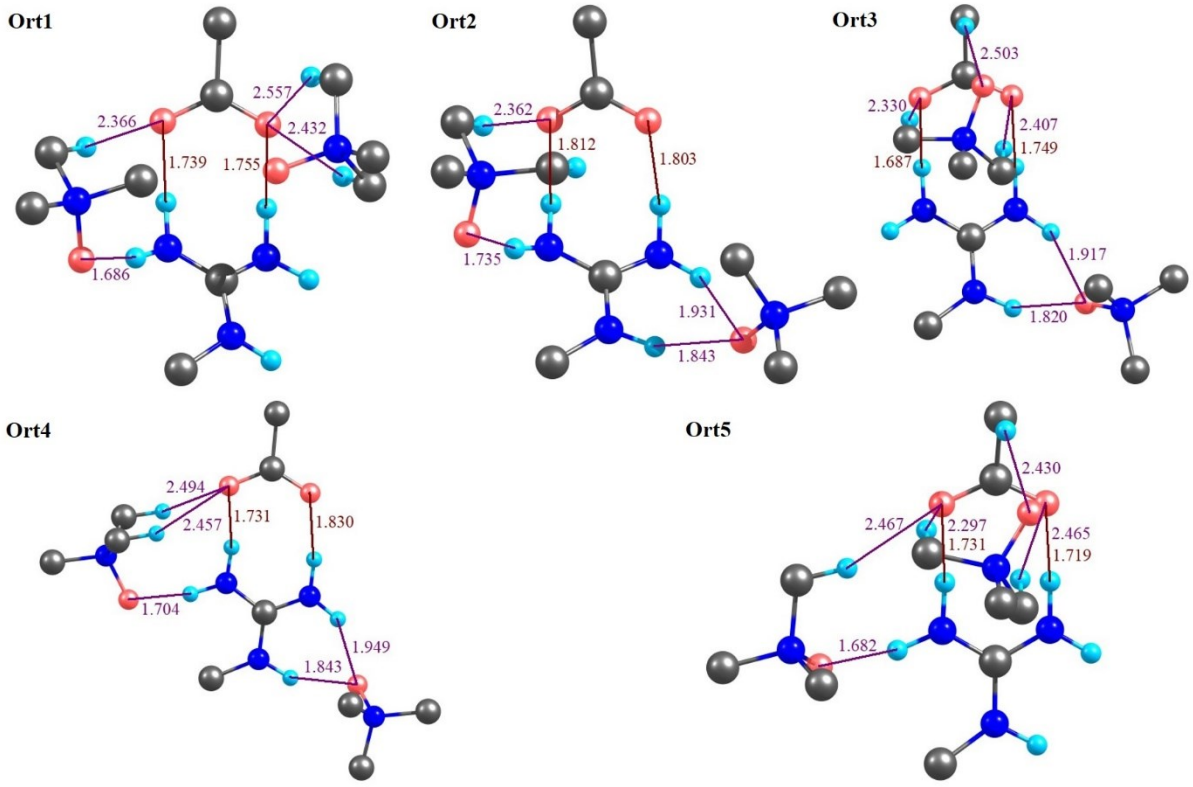


Fig. S7 Optimized geometries at the CPCM(water)/M06-2X/6-311G** level of theory of the salt-bridge model complex in the presence of two molecules of trimethylamine N-oxide (TMAO). Ort1 to Ort5 represent the different orientations in which two TMAO molecules are optimized with the salt-bridge model complex. Colour scheme: black – carbon, cyan – hydrogen, blue – nitrogen, red – oxygen, maroon line – salt-bridge hydrogen bond, purple line – hydrogen bond between the TMAO and the salt-bridge model complex.

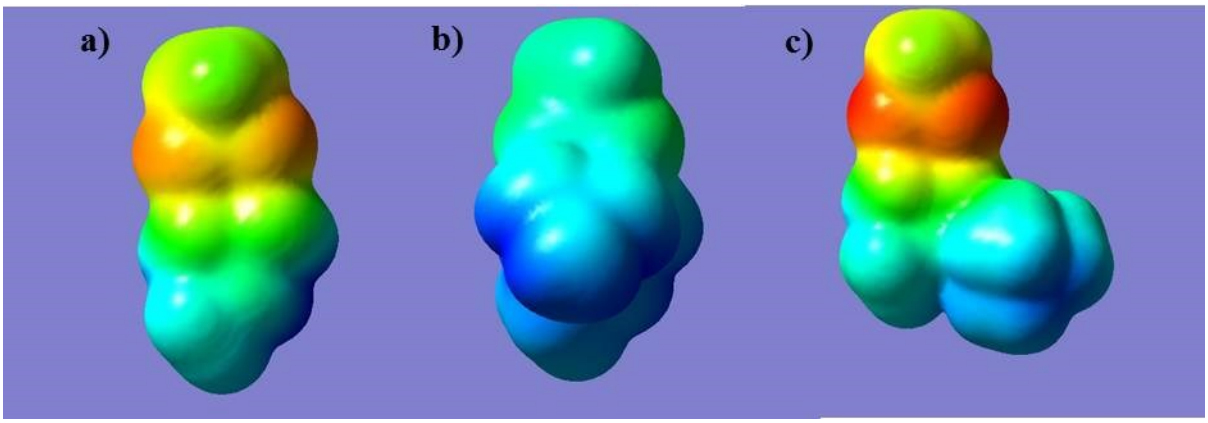


Fig. S8 The molecular surface electrostatic potential computed on the 0.0004 au contour of electron density at the CPCM(water)/M06-2X/6-311++G** level of theory: a) model salt-bridge, b) Gdm^+···SB complex, and d) TMAO···SB complex. The blue colour on potential surfaces indicates a positive electrostatic potential. The transition from negative to positive potential is represented by red to yellow to green to blue.

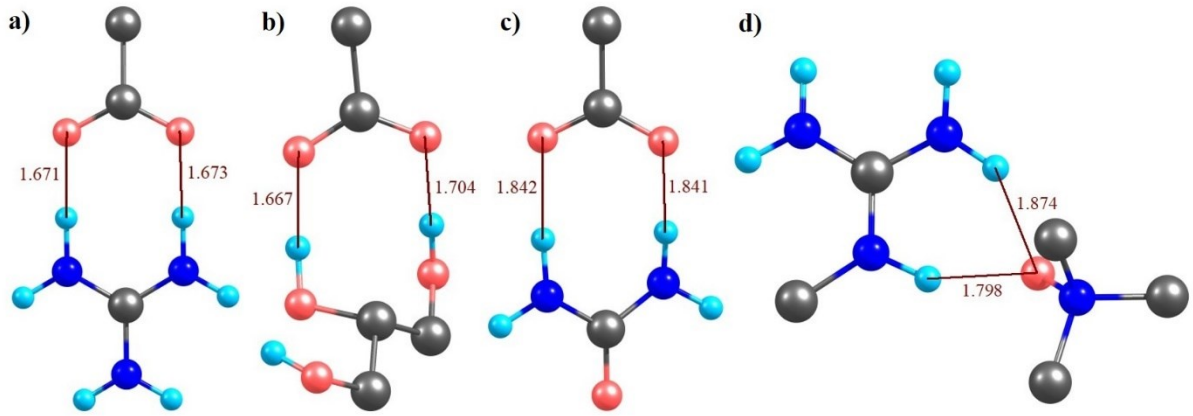


Fig. S9 Optimized geometries at the CPCM(water)/M06-2X/6-311++G** level of theory. a) Gdm^+···acetate, b) glycerol···acetate, c) urea···acetate and d) TMAO···$MeGdm^+$ complexes in their lowest energy conformations. Colour scheme: carbon–black, hydrogen–cyan, nitrogen–blue, oxygen–red, maroon line represents hydrogen bond. Hydrogen atoms from methyl/methylene groups have been removed for the clarity.

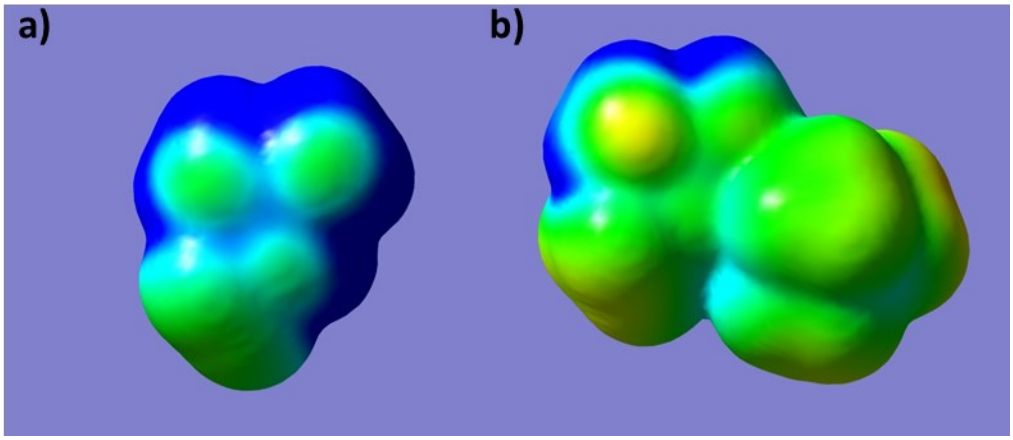


Fig. S10 The molecular surface electrostatic potential computed on the 0.0004 au contour of electron density at the CPCM(water)/M06-2X/6-311++G** level of theory: a) MeGdm+, b) MeGdm+···TMAO complex. The red colour on potential surfaces indicates a negative and blue colour a positive electrostatic potential. The transition from negative to positive potential is represented by red to yellow to green to blue. The TMAO is at the right hand side in Figure b.

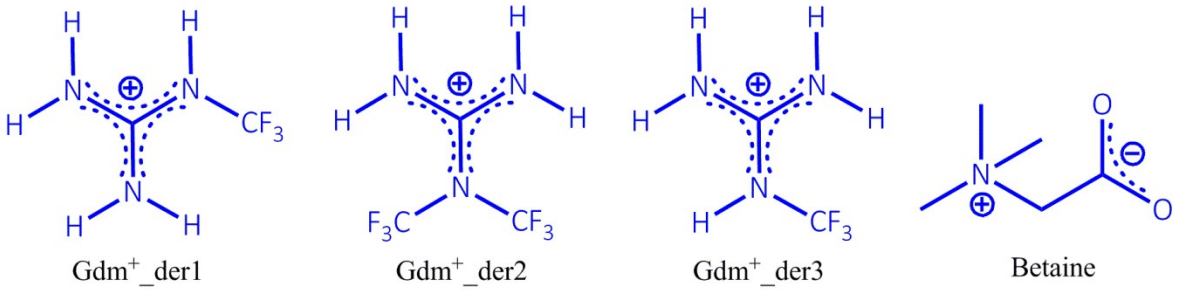


Fig. S11 Schematic representations of designed Gdm^+-based osmolytes (a-c) and the glycine betaine (d). Energy of interactions in kcal mol^{-1} between different interacting units in osmolyte···SB complex is provided in the following table.

	Gdm^+_der1	Gdm^+_der2	Gdm^+_der3	Betaine
$I_{os\cdots an,ca}$	-28.9	-22.6	-26.6	0.2
$I_{ca\cdots an,os}$	-16.1	-17.1	-16.4	-20.5

$I_{os\cdots an,ca} =$ Energy of interaction between osmolyte and anion in the osmolyte···SB complex

$I_{ca\cdots an,os} =$ Energy of interaction between cation and anion of the SB in osmolyte···SB complex

XYZ Coordinates of the optimized geometries obtained at the CPCM(water)/M06-2X/6-311G** level of theory

Guanidinium ion

Gdm$^+$_Orientation1

C	4.289664	-0.380039	-0.230321
C	2.781572	-0.305160	-0.068872
O	2.315890	-0.121528	1.081708
O	2.079442	-0.447780	-1.111274
N	-0.474603	-1.401668	-0.734452
C	-1.057558	-1.217802	0.446481
N	-0.311530	-0.882913	1.498353
N	-2.377030	-1.373443	0.576848
C	-3.258289	-1.696752	-0.534048
C	-0.895326	1.938271	-0.195238
N	-1.637137	1.617060	-1.256876
N	-1.471525	2.495426	0.865435
N	0.410096	1.693605	-0.198441
H	4.591656	0.056013	-1.181610
H	-4.280446	-1.686598	-0.166743
H	4.792921	0.115262	0.597895
H	4.581354	-1.433507	-0.236087
H	-3.166778	-0.947746	-1.323917
H	-3.043747	-2.688717	-0.938520
H	-2.773293	-1.286573	1.499426
H	-1.021740	-1.691901	-1.528354
H	0.520111	-1.143867	-0.875638
H	-0.764045	-0.626470	2.361279
H	0.688493	-0.639186	1.367494
H	-2.583490	1.953569	-1.342951
H	-1.190881	1.279283	-2.095182
H	0.823268	1.064254	-0.887516
H	0.915972	1.694468	0.678128
H	-0.925956	2.751310	1.673058
H	-2.454333	2.717295	0.871681

Gdm$^+$_Orientation2

C	-2.589688	2.806372	-0.326829
C	-1.271724	2.117703	-0.030272
O	-1.087101	0.981312	-0.584323
O	-0.446190	2.662895	0.719958
N	1.579449	0.326595	-1.029229
C	2.189552	0.285224	0.151736
N	3.371377	-0.316756	0.283531
C	4.032845	-1.035799	-0.795713
N	1.583132	0.836336	1.206698
C	-1.846809	-2.065979	0.141319
N	-2.179019	-3.326775	0.416746
N	-2.502572	-1.378087	-0.785000
N	-0.837694	-1.480618	0.782725
H	-2.685357	2.951351	-1.404167
H	4.926926	-1.500588	-0.390348
H	-3.408576	2.156618	-0.011206
H	-2.657485	3.763034	0.185791
H	3.382446	-1.819602	-1.189223
H	4.327406	-0.360512	-1.602638
H	3.845595	-0.234833	1.169277
H	2.003762	-0.084681	-1.844129
H	0.592599	0.616198	-1.053300
H	2.051641	0.824198	2.099128
H	0.833115	1.538436	1.052108
H	-0.382673	-1.932520	1.558700
H	-0.654493	-0.498549	0.585921
H	-2.227533	-0.405475	-0.948781
H	-3.262159	-1.794944	-1.297147
H	-2.935074	-3.781530	-0.068508
H	-1.671580	-3.860242	1.103700

Gdm$^+$_Orientation3

C	3.148191	-1.899110	-0.681398
C	1.774302	-1.353386	-0.332851
O	1.386266	-1.506616	0.863747
O	1.112991	-0.784147	-1.229478
N	-1.417796	0.080849	-0.800942
C	-2.084107	-0.582635	0.148998
N	-1.400568	-1.319921	1.021540
N	-3.408122	-0.468532	0.251187
C	-4.211318	0.368435	-0.627765
H	3.414443	-1.666519	-1.710219
H	-5.238932	0.332812	-0.278050
H	3.888991	-1.479592	0.001693
H	3.148935	-2.980891	-0.534896
H	-3.868297	1.404492	-0.597121
H	-4.183535	0.001122	-1.655804
H	-3.869673	-0.960903	0.999894
H	-1.942167	0.471349	-1.569063
H	-0.430056	-0.213531	-0.986025
H	-1.886936	-1.802477	1.760294
H	-0.376777	-1.445559	0.933204
C	1.308019	1.807558	0.371891
N	0.662821	2.657948	-0.417885
N	0.663899	1.160742	1.346251
N	2.617853	1.624738	0.239762
H	0.983689	0.207130	1.538267
H	-0.326755	1.325943	1.445382
H	-0.344071	2.632908	-0.467185
H	1.156305	3.243946	-1.072322
H	3.118327	1.965269	-0.565420
H	3.125331	1.094675	0.930575

Gdm$^+$_Orientation4

C	3.692301	-1.661174	-0.246143
C	2.351645	-0.963573	-0.144251
O	1.802516	-0.544540	-1.197408
O	1.847895	-0.836692	1.005667
N	-1.010968	-0.713919	-0.896145
C	-1.599719	-1.202567	0.190489
N	-2.929726	-1.260989	0.262889
C	-3.814313	-0.825273	-0.807073
N	-0.853291	-1.655010	1.197524
N	0.318253	1.519801	1.193328
C	0.203473	2.367771	0.178460
N	-0.493586	3.496598	0.322782
N	0.788954	2.091242	-0.981723
H	4.027271	-1.723085	-1.278721
H	-4.836363	-1.031287	-0.502468
H	4.423121	-1.113473	0.351091
H	3.606480	-2.661930	0.180410
H	-3.715359	0.247257	-0.988868
H	-3.611137	-1.376216	-1.727599
H	-3.339580	-1.599428	1.119011
H	-1.563685	-0.358845	-1.658929
H	0.012505	-0.703786	-0.995919
H	-1.294889	-1.986197	2.039851
H	0.153568	-1.467600	1.205467
H	0.703590	2.728410	-1.756836
H	1.233694	1.179909	-1.129965
H	0.908150	0.678029	1.125112
H	-0.127083	1.725996	2.072893
H	-0.896776	3.748942	1.209953
H	-0.624555	4.127985	-0.450037

Gdm$^+$_Orientation5

C	-2.329283	2.981200	-0.141823
C	-1.066211	2.142623	-0.153860
O	-1.079893	1.080574	0.555054
O	-0.090313	2.509354	-0.829987
N	1.818513	0.530410	-0.764051
C	2.194306	0.050314	0.418731
N	1.451028	0.331787	1.491403
N	3.295824	-0.691103	0.534535
C	4.194653	-0.975796	-0.573938
H	-2.246149	3.825109	-0.822673
H	5.041942	-1.532978	-0.184797
H	-3.179351	2.355823	-0.421096
H	-2.507510	3.340506	0.873456
H	3.702473	-1.580010	-1.339277
H	4.565602	-0.049510	-1.016785
H	3.485343	-1.117593	1.427827
H	2.384727	0.351208	-1.577474
H	1.105427	1.289279	-0.810426
H	1.686768	-0.074806	2.382315
H	0.495434	0.673418	1.331664
C	-2.097218	-1.902479	-0.113962
N	-2.546965	-3.124962	-0.395093
N	-0.904256	-1.507655	-0.551619
N	-2.825138	-1.061418	0.610360
H	-0.624656	-0.546520	-0.363814
H	-0.366722	-2.078287	-1.182819
H	-1.983752	-3.779012	-0.913423
H	-3.442936	-3.437489	-0.058821
H	-3.709562	-1.345859	0.997643
H	-2.445963	-0.127289	0.788336

Gdm$^+$_Orientation6

C	3.880349	-1.151273	-0.105373
C	2.364792	-1.197240	-0.097735
O	1.759618	-0.119110	0.215975
O	1.781692	-2.254031	-0.396807
N	-0.914584	-1.704375	-0.534444
C	-1.489747	-1.065776	0.476798
N	-0.717102	-0.594242	1.463736
N	-2.812806	-0.914768	0.525949
C	-3.722822	-1.471106	-0.463859
N	-0.750216	3.618237	-0.340483
C	0.032261	2.544183	-0.243777
N	-0.154332	1.499644	-1.044213
N	1.015283	2.501190	0.649075
H	4.301089	-2.133483	-0.309905
H	-4.739251	-1.269058	-0.138037
H	4.208259	-0.443414	-0.869854
H	4.238052	-0.781700	0.857037
H	-3.572743	-1.010593	-1.443060
H	-3.592795	-2.552256	-0.541533
H	-3.193638	-0.344153	1.264121
H	-1.475612	-2.065564	-1.288442
H	0.099280	-1.941166	-0.496667
H	-1.137950	-0.025009	2.181448
H	0.266434	-0.425131	1.226440
H	-0.904400	1.482575	-1.715531
H	0.438743	0.681504	-0.908985
H	-0.618075	4.412469	0.263748
H	-1.504561	3.653348	-1.006400
H	1.608405	1.671679	0.681024
H	1.195589	3.282554	1.257593

Urea

Urea_Orientation1

C	4.150076	-0.252175	-0.228939
C	2.638460	-0.370096	-0.138291
O	2.134599	-0.803597	0.928195
O	1.970886	0.005748	-1.140379
N	-0.691905	-0.747862	-1.121436
C	-1.215239	-1.346318	-0.055797
N	-0.403032	-1.985636	0.795174
N	-2.535013	-1.359299	0.127012
C	-3.465709	-0.643400	-0.734937

N	0.142988	2.273280	-0.598809
C	-0.698416	1.899249	0.417127
N	-0.113493	1.177858	1.420700
O	-1.876038	2.244548	0.459936
H	4.494633	-0.648258	-1.184365
H	-4.469555	-0.805983	-0.352974
H	4.419604	0.806092	-0.195518
H	4.634781	-0.771529	0.594981
H	-3.251171	0.428365	-0.717987
H	-3.419721	-1.023679	-1.757517
H	-2.895098	-1.820914	0.947424
H	-1.286665	-0.175636	-1.700248
H	0.327336	-0.548747	-1.153208
H	-0.796455	-2.319228	1.661948
H	0.579379	-1.670876	0.828779
H	-0.336470	2.646549	-1.403873
H	0.936436	1.671953	-0.806315
H	0.737088	0.644780	1.259670
H	-0.761548	0.781570	2.083718

Urea_Orientation2

C	4.114612	-0.064160	-0.368281
C	2.684682	-0.432722	-0.006087
O	1.864156	0.524215	0.124022
O	2.394236	-1.639948	0.136602
N	-0.309583	-1.974509	-0.119110
C	-1.057636	-1.085600	0.519155
N	-0.468959	-0.293335	1.431103
N	-2.376561	-1.008028	0.321943
C	-3.094252	-1.906499	-0.569465
N	-0.542125	1.301992	-1.372311
C	-1.008976	1.994398	-0.287740
O	-2.200903	2.034101	0.014991
N	-0.047999	2.682035	0.399473
H	4.755542	-0.943080	-0.386531
H	-4.159771	-1.753046	-0.420365
H	4.119384	0.413938	-1.350024
H	4.495934	0.663117	0.350022
H	-2.855857	-1.722819	-1.620996
H	-2.857254	-2.941147	-0.318945
H	-2.798691	-0.113023	0.542546
H	-0.678931	-2.440891	-0.932813
H	0.725678	-1.932888	0.013062
H	-1.057359	0.408489	1.857619
H	0.481706	0.012650	1.168569
H	-1.212749	0.675517	-1.790663
H	0.412189	0.960454	-1.310606
H	0.900756	2.325534	0.351267
H	-0.344482	3.050672	1.289759

Urea_Orientation3

C	4.282884	-0.926749	-0.633511
N	3.459960	-0.521895	0.495679
C	2.300277	0.126945	0.368955
N	1.628185	0.528360	1.448509
N	1.801005	0.393870	-0.833569
O	-0.314450	2.100151	-1.056403
C	-1.172291	1.895085	-0.174830
O	-0.999620	1.142027	0.833931
C	-2.533998	2.554945	-0.302128
N	-2.864464	-1.069347	0.819082
C	-2.238110	-1.898885	-0.067458
O	-2.797936	-2.845766	-0.607535
N	-0.903693	-1.628268	-0.244220
H	-2.565105	3.234853	-1.150512
H	5.199222	-1.360407	-0.243083
H	-3.287956	1.774141	-0.429814
H	-2.769202	3.088981	0.619395
H	3.776828	-1.676379	-1.246170
H	4.545373	-0.064174	-1.249202
H	3.759381	-0.774879	1.423884
H	2.298616	0.102213	-1.658724
H	0.997516	1.055073	-0.932233
H	1.969522	0.290645	2.365637
H	0.645942	0.827447	1.329985
H	-0.577695	-0.700277	-0.002195
H	-0.479106	-2.068855	-1.044402
H	-3.867037	-1.146174	0.861811
H	-2.429777	-0.180581	1.051139

Urea_Orientation4

C	1.864659	2.272891	-0.076721
C	0.544957	1.516815	-0.049502
O	0.620411	0.247610	-0.042665
O	-0.517810	2.165088	-0.035533
N	-2.883543	0.800370	0.153548
C	-2.895566	-0.514112	-0.031476
N	-1.744166	-1.156120	-0.207136
N	-4.053030	-1.184969	-0.047213
C	-5.351277	-0.548718	0.107002
N	3.109692	-0.869390	-1.110906
C	3.822399	-0.922409	0.057206
O	5.036484	-1.085505	0.092656
N	3.045347	-0.854376	1.182849
H	1.697822	3.347628	-0.068569
H	-6.116293	-1.309896	-0.018475
H	2.466999	1.984276	0.787359
H	2.426820	1.992720	-0.970026
H	-5.463720	-0.103774	1.098573
H	-5.500123	0.217098	-0.657057
H	-4.014293	-2.189306	-0.113898
H	-3.739878	1.292133	0.346608
H	-1.988259	1.328117	0.092741
H	-1.745189	-2.140730	-0.416655
H	-0.844289	-0.642334	-0.148305
H	2.110692	-0.469016	1.085888
H	3.540589	-0.697480	2.045246
H	3.653061	-0.722391	-1.945627
H	2.172251	-0.479998	-1.070514

Urea_Orientation5

C	-2.658979	-2.525342	0.204783
C	-1.254574	-1.967194	0.054604
O	-0.928595	-1.037036	0.857730
O	-0.510344	-2.421724	-0.836089
N	1.579795	-0.686893	-1.252066
C	2.255842	-0.230103	-0.196791
N	3.424651	0.393790	-0.357457
C	4.172447	0.994143	0.736288
N	1.735273	-0.392268	1.015369
N	-2.746986	1.186678	0.678595
C	-2.068663	2.049595	-0.131091
O	-2.528210	3.126099	-0.496190
N	-0.818660	1.618821	-0.497065
H	-2.793497	-2.900707	1.220478
H	5.033639	1.504199	0.314052
H	-3.374914	-1.713285	0.058127
H	-2.846395	-3.319133	-0.514835
H	3.560861	1.728629	1.263904
H	4.526811	0.236931	1.439181
H	3.826046	0.410562	-1.281367
H	2.210904	-0.035398	1.827186
H	0.746141	-0.693761	1.083392
H	1.984301	-0.593983	-2.170274
H	0.805048	-1.368905	-1.111368
H	-0.419680	2.072787	-1.302529
H	-0.581139	0.647249	-0.341890
H	-2.272869	0.369562	1.052142
H	-3.563009	1.549049	1.141806

Urea_Orientation6

C	-1.997496	2.261063	-0.179222
C	-0.607536	1.649188	-0.093953
O	0.381819	2.403730	-0.089136
O	-0.551722	0.379794	-0.029511
N	1.933627	-0.777319	-0.151056
C	3.009432	-0.029384	0.063461
N	4.226728	-0.583443	0.077522
C	4.463242	-2.005759	-0.108813
N	2.860090	1.273358	0.286450
N	-2.881042	-1.054774	-1.085628
C	-3.613460	-1.118671	0.069714
N	-2.876091	-0.907473	1.204023
O	-4.804634	-1.406479	0.090744
H	-2.518577	1.863721	-1.052414
H	5.522643	-2.193992	0.041783
H	-2.575726	1.972657	0.701318
H	-1.940892	3.345372	-0.243806
H	3.902497	-2.588240	0.624928
H	4.192888	-2.328655	-1.117135
H	5.021454	0.030139	0.158412
H	2.031664	-1.746416	-0.403260
H	0.986052	-0.350547	-0.110080
H	3.667440	1.842939	0.479788
H	1.931597	1.719758	0.155862
H	-3.405425	-0.757618	2.047108
H	-1.983176	-0.434359	1.102490
H	-1.989514	-0.569449	-1.049801
H	-3.414911	-1.012728	-1.938251

Urea_Orientation7

C	4.154297	0.366288	-0.140684
C	2.763121	-0.243586	-0.104652
O	1.790746	0.542094	-0.324845
O	2.642502	-1.461115	0.138830
N	0.004218	-1.977164	0.718599
C	-0.936323	-1.466774	-0.067469
N	-2.228144	-1.701023	0.165662
C	-3.306704	-1.096224	-0.606270
N	-0.559725	-0.726780	-1.117218
N	-0.309152	2.480492	-0.590402
C	-1.138843	1.940378	0.351172
O	-2.359371	2.068400	0.315830
N	-0.489797	1.303501	1.378053
H	4.305539	0.863324	-1.100209
H	-4.248830	-1.432145	-0.181648
H	4.229216	1.129015	0.636992
H	4.920523	-0.390775	0.011921
H	-3.258894	-0.006655	-0.537981
H	-3.267343	-1.413971	-1.650617
H	-2.465163	-2.342446	0.906143
H	-1.268638	-0.226006	-1.630638
H	0.360095	-0.268528	-1.020684
H	-0.256698	-2.509607	1.532710
H	1.011112	-1.824698	0.498541
H	-1.086966	0.732505	1.956791
H	0.428438	0.923758	1.168007
H	0.631707	2.109931	-0.673894
H	-0.760218	2.807593	-1.429398

Urea_Orientation8

C	-4.978098	-1.372155	-0.047324
C	-3.600355	-0.718038	-0.034067
O	-3.576571	0.538691	0.025179
O	-2.597563	-1.466502	-0.103066
N	-1.179151	1.760776	-0.077096
C	-0.055199	1.055999	-0.031118
N	1.136174	1.663602	0.039171
C	1.279521	3.108641	0.066617
N	-0.116841	-0.277304	-0.052426
C	3.398156	-1.029195	-0.006124
N	2.656183	-1.239261	1.138606
N	3.973422	-2.119322	-0.553857
O	3.484023	0.090279	-0.508884
H	-5.620099	-0.905208	0.700044
H	2.330863	3.338084	0.223237
H	-5.435766	-1.205052	-1.025485
H	-4.906021	-2.443166	0.132209

H	0.958308	3.573360	-0.870395
H	0.710249	3.536336	0.894325
H	1.967658	1.108132	-0.167729
H	-1.136978	2.757944	-0.206943
H	-2.113377	1.278969	-0.044749
H	0.690537	-0.798680	0.266885
H	-1.049412	-0.737722	-0.067858
H	4.375694	-2.021937	-1.471622
H	3.816521	-3.048100	-0.198829
H	2.795144	-2.099454	1.649500
H	2.584899	-0.424177	1.732886

Urea_Orientation9

C	-5.052230	-1.534227	-0.105305
C	-3.705498	-0.820968	-0.026059
O	-2.668913	-1.524167	-0.060651
O	-3.740689	0.434606	0.048491
N	-1.391544	1.761593	-0.132756
C	-0.248424	1.112129	0.068292
N	-0.267820	-0.203165	0.273930
N	0.919378	1.764309	0.075595
C	1.030700	3.198776	-0.109068
N	4.752641	-0.353790	-0.280738
C	3.638134	-1.061005	0.040382
N	3.719368	-2.409043	-0.091741
O	2.605495	-0.506964	0.432738
H	-5.742420	-1.109777	0.624402
H	2.083638	3.465021	-0.063494
H	-5.479369	-1.367496	-1.097237
H	-4.941411	-2.604645	0.058130
H	0.641575	3.508784	-1.082628
H	0.504590	3.744527	0.678638
H	1.752555	1.197706	0.206689
H	-1.384443	2.760799	-0.249183
H	-2.305068	1.250806	-0.065186
H	0.623071	-0.678257	0.359389
H	-1.156071	-0.725266	0.153233
H	4.470989	-2.831535	-0.612632
H	2.850473	-2.916767	-0.051456
H	4.770723	0.607634	0.019670
H	5.643783	-0.816895	-0.362451

Urea_Orientation10

C	1.270500	3.839302	-0.268976
C	0.345367	2.682870	0.084804
O	0.872273	1.700315	0.680748
O	-0.858689	2.768307	-0.239317
N	-2.530457	0.585358	-0.118422
C	-1.940990	-0.558393	0.217277
N	-0.732266	-0.529938	0.768270
N	-2.568975	-1.725898	0.030058
C	-3.897927	-1.840678	-0.546875
H	0.705816	4.704016	-0.612003
H	-4.132389	-2.896792	-0.647807
H	1.879037	4.104006	0.596379
H	1.949539	3.514991	-1.061200
H	-4.654728	-1.375190	0.089647
H	-3.927903	-1.387728	-1.539986
H	-2.135015	-2.550528	0.413427
H	-3.461851	0.588555	-0.498536
H	-1.959389	1.452527	-0.132476
H	-0.139093	-1.357282	0.785381
H	-0.220137	0.371203	0.803023
O	1.602168	-2.140295	0.741015
C	2.471926	-1.720053	-0.025009
N	3.469349	-2.543668	-0.476502
N	2.520096	-0.437049	-0.463235
H	1.950853	0.269794	-0.000798
H	3.345968	-0.107496	-0.936751
H	3.988250	-2.288158	-1.302204
H	3.287542	-3.528460	-0.364179

Urea_Orientation11

C	3.670083	-1.578182	-0.257240
C	2.707264	-0.458748	0.114690
O	1.739447	-0.775237	0.866805
O	2.914146	0.681469	-0.350163
N	-0.308940	1.008788	0.654447
C	-0.227519	2.158262	0.000706
N	-1.341251	2.812239	-0.342822
C	-2.670246	2.335102	0.009105
N	0.977528	2.679911	-0.256113
O	-2.234833	-1.052365	0.480929
C	-1.812723	-2.097832	-0.023396
N	-0.495082	-2.359730	-0.200844
N	-2.677843	-3.077879	-0.427454
H	3.922835	-2.162365	0.627964
H	-3.397656	3.045074	-0.374571
H	3.168252	-2.247243	-0.961083
H	4.572101	-1.184219	-0.721362
H	-2.864921	1.354298	-0.430091
H	-2.779906	2.264744	1.093897
H	-1.251983	3.677086	-0.851201
H	-1.171035	0.462526	0.653604
H	0.555566	0.454939	0.813834
H	1.039425	3.516047	-0.814596
H	1.776334	2.023050	-0.255062
H	-2.368324	-3.780911	-1.080203
H	-3.637757	-2.786084	-0.520529
H	0.208637	-1.774722	0.246650
H	-0.203666	-3.288087	-0.461516

Urea_Orientation12

C	4.999378	-1.217662	0.119743
C	3.605887	-0.603606	0.034171
O	3.543831	0.651977	0.084150
O	2.628142	-1.381418	-0.068331
N	1.097172	1.786145	0.110913
C	0.010407	1.050893	-0.099990
N	-1.201259	1.619344	-0.110515
C	-1.416159	3.041454	0.088465
N	0.141519	-0.255501	-0.315488
N	-3.793609	-0.081658	-0.352820
C	-3.333131	-1.281824	0.161692
N	-2.515040	-1.987346	-0.696128
O	-3.527685	-1.617800	1.311055
H	5.652121	-0.749145	-0.618224
H	-2.482163	3.234986	-0.004762
H	5.419394	-1.009350	1.106150
H	4.966996	-2.293486	-0.040078
H	-1.094050	3.362727	1.082493
H	-0.892462	3.628971	-0.669438
H	-2.017466	1.026690	-0.222059
H	1.005072	2.765214	0.323361
H	2.049346	1.342766	0.100292
H	-0.677224	-0.827572	-0.483928
H	1.080091	-0.697897	-0.229652
H	-2.326115	-2.933092	-0.395786
H	-2.653680	-1.888421	-1.692207
H	-4.528804	0.334464	0.201860
H	-3.955122	-0.021357	-1.349240

Guanidinium chloride

GdmCl_Orientation1

C	2.866476	-3.151548	-0.094082
C	1.691474	-2.189695	-0.099108
O	1.443461	-1.550095	-1.143260
O	1.011848	-2.105226	0.970551
N	-1.015226	-0.367122	-1.142308
C	-1.980277	-0.918128	-0.419012
N	-3.229756	-0.450750	-0.482396
C	-3.607215	0.697313	-1.291191
N	-1.694450	-1.973007	0.350721
C	-0.153302	1.421198	1.283358
N	-1.178118	0.880016	1.949677
N	0.966677	0.729421	1.120584
N	-0.256321	2.651167	0.788836
Cl	2.548954	2.834008	-0.860776
H	3.535117	-2.956320	-0.929959
H	-4.679787	0.840497	-1.195772
H	3.402813	-3.080912	0.851937
H	2.477653	-4.169408	-0.180048
H	-3.100459	1.605054	-0.952239
H	-3.376578	0.518450	-2.342952
H	-3.902633	-0.818616	0.171670
H	-1.200392	0.459391	-1.686954
H	-0.055741	-0.781274	-1.146195
H	-2.416910	-2.362153	0.935306
H	-0.708881	-2.134904	0.610224
H	-1.047245	3.235723	1.004434
H	0.509798	3.020743	0.229779
H	1.674030	1.139844	0.514467
H	0.950739	-0.293409	1.214747
H	-1.061818	0.001348	2.429088
H	-2.026972	1.397465	2.111750

GdmCl_Orientation2

C	-4.560132	0.233148	-0.610341
C	-3.062870	0.120304	-0.395935
O	-2.667569	-0.634900	0.537035
O	-2.292962	0.780784	-1.137164
N	-0.200264	-1.843678	-0.026311
C	0.671654	-1.245164	-0.834457
N	1.976783	-1.495739	-0.729558
C	2.542864	-2.311026	0.333991
N	0.228269	-0.438975	-1.808201
C	0.270872	0.830306	1.640115
N	1.549367	0.806988	2.018824
N	-0.062492	1.485656	0.533737
N	-0.674011	0.248949	2.384167
Cl	2.812544	1.691866	-1.030294
H	-4.981797	-0.764845	-0.737525
H	3.618414	-2.355247	0.186909
H	-5.012748	0.667077	0.283371
H	-4.789194	0.850819	-1.475721
H	2.339596	-1.884178	1.320382
H	2.150445	-3.328039	0.284769
H	2.589134	-0.838390	-1.198929
H	0.143147	-2.406303	0.736271
H	-1.160311	-1.476560	0.065599
H	0.911810	0.186161	-2.218034
H	-0.718917	-0.060087	-1.707883
H	-0.385813	-0.359306	3.135219
H	-1.550397	0.013336	1.910686
H	-0.964286	1.315679	0.078561
H	0.700540	1.793985	-0.066084
H	2.253705	1.222168	1.419411
H	1.829773	0.387132	2.890186

GdmCl_Orientation3

C	-4.506129	-0.844764	0.338823
C	-3.176182	-0.111655	0.325459
O	-3.166858	1.128306	0.451929
O	-2.132062	-0.822369	0.175525
N	-0.647851	2.074660	-0.184116
C	0.349532	1.444678	0.423780
N	1.621300	1.694898	0.120992
C	2.021773	2.658325	-0.890662
N	0.058687	0.575850	1.410456
C	0.688814	-1.392727	-1.243131
N	0.370570	-2.119918	-0.171350
N	-0.288015	-0.826097	-1.946346
N	1.961208	-1.314061	-1.638402
Cl	3.072538	-1.013699	1.461465
H	-5.326644	-0.168371	0.568139
H	3.104498	2.745948	-0.866178
H	-4.667576	-1.298362	-0.641445
H	-4.468157	-1.653356	1.069887

H	1.718646	2.338397	-1.891571
H	1.590841	3.638181	-0.676315
H	2.314868	1.064755	0.516391
H	-0.467864	2.624883	-1.008228
H	-1.622863	1.790712	0.039487
H	0.838228	0.019525	1.748484
H	-0.818966	0.071052	1.266597
H	2.680353	-1.529231	-0.956510
H	2.211133	-0.680418	-2.381629
H	-0.066958	-0.205191	-2.708546
H	-1.190792	-0.737253	-1.477170
H	-0.577745	-2.020028	0.182440
H	1.109071	-2.336323	0.487374

GdmCl_Orientation4

C	-0.080742	3.810913	-0.149510
C	0.767190	2.554136	-0.100752
O	0.230078	1.526019	0.429561
O	1.920582	2.572355	-0.565068
N	2.880567	-0.007909	-0.580562
C	2.803230	-0.726758	0.535497
N	2.054566	-0.269804	1.542715
N	3.468659	-1.876184	0.652932
C	4.367614	-2.391702	-0.368845
H	0.446022	4.621671	-0.647645
H	4.816852	-3.305529	0.009079
H	-1.013144	3.592526	-0.673713
H	-0.340586	4.105776	0.868798
H	3.828574	-2.625208	-1.289729
H	5.164197	-1.675533	-0.579033
H	3.308431	-2.432599	1.477955
H	3.460717	-0.324697	-1.340244
H	2.532881	0.974544	-0.590558
H	1.920674	-0.843550	2.359783
H	1.353788	0.448414	1.317342
C	-1.752644	-0.831711	-0.563061
N	-2.199399	0.195301	0.147579
N	-2.595868	-1.783908	-0.959881
N	-0.454615	-0.898739	-0.869254
H	-2.256126	-2.614765	-1.415235
H	-3.564220	-1.740059	-0.651758
H	-3.175100	0.210333	0.427477
H	-1.532364	0.917496	0.423188
H	0.127542	-0.101573	-0.622801
H	-0.117917	-1.581244	-1.528106
Cl	-5.345339	-0.730210	0.463799

GdmCl_Orientation5

C	4.204146	-0.607934	0.588372
C	2.737128	-0.966087	0.436226
O	2.223614	-1.794374	1.208438
O	2.102781	-0.377226	-0.501182
N	-0.152373	-1.807790	-1.424213
C	-1.006330	-1.614562	-0.409796
N	-0.536969	-1.624943	0.834916
N	-2.311427	-1.456775	-0.632456
C	-2.864803	-1.232830	-1.959999
H	4.727488	-0.836663	-0.341606
H	-3.936521	-1.086977	-1.855495
H	4.292056	0.467612	0.755598
H	4.659594	-1.149857	1.414224
H	-2.432731	-0.345590	-2.430987
H	-2.701847	-2.103521	-2.597140
H	-2.856055	-1.147861	0.166374
H	-0.494707	-1.701061	-2.366124
H	0.809190	-1.496320	-1.247405
H	-1.137780	-1.284508	1.575598
H	0.477675	-1.748233	1.005891
C	0.423539	2.420666	-0.454308
N	-0.089718	1.322393	0.083941
N	-0.263489	3.563493	-0.443658
N	1.631777	2.356820	-1.007838
H	0.114315	4.405635	-0.845278
H	-1.179484	3.604752	-0.027451
H	-0.961545	1.319407	0.610249
H	0.506643	0.496829	0.089020
H	2.114864	1.456453	-1.000261
H	2.031269	3.151457	-1.478390
Cl	-2.797075	0.641373	1.872783

GdmCl_Orientation6

C	3.654128	-1.668566	-0.880559
C	2.182201	-1.486392	-0.553653
O	1.881243	-1.346829	0.676222
O	1.360578	-1.451327	-1.489288
N	-1.250309	-0.946591	-0.779151
C	-1.661002	-1.569832	0.320385
N	-0.798076	-2.342642	0.991197
N	-2.926217	-1.465125	0.724362
C	-3.956368	-0.776494	-0.042462
H	3.783561	-2.061199	-1.886959
H	-4.916850	-0.986576	0.420341
H	4.143552	-0.692427	-0.818357
H	4.124462	-2.324208	-0.148426
H	-3.790447	0.302966	-0.052291
H	-3.970244	-1.150253	-1.067833
H	-3.167137	-1.845685	1.625912
H	-1.760021	-0.136885	-1.114144
H	-0.270677	-1.094716	-1.093805
H	-1.115977	-2.849670	1.801901
H	0.205126	-2.149033	0.901555
C	1.446305	1.900097	0.675201
N	1.187699	3.161031	0.328279
N	0.444003	1.045572	0.848591
N	2.692192	1.489031	0.906956
H	0.706560	0.058152	0.895148
H	-0.465224	1.310499	0.474719
H	0.253160	3.384024	0.002692
H	1.937312	3.796980	0.109497
H	3.480454	2.104342	0.793435
H	2.841636	0.508352	1.119215
Cl	-1.964144	2.425222	-0.806658

GdmCl_Orientation7

C	-4.615329	0.251168	-0.425062
C	-3.196750	-0.274809	-0.309080
O	-2.936190	-1.425345	-0.705018
O	-2.334529	0.514412	0.198818
N	-0.293178	-0.877990	1.524560
C	0.421301	-1.480843	0.569527
N	-0.190728	-1.841792	-0.552689
N	1.720588	-1.743722	0.748628
C	2.487504	-1.143618	1.832444
H	-4.965049	0.563586	0.560129
H	3.519727	-1.467348	1.728221
H	-4.615118	1.135046	-1.065803
H	-5.282304	-0.503101	-0.836405
H	2.455340	-0.050391	1.794065
H	2.120157	-1.493784	2.797931
H	2.240355	-1.920536	-0.103258
H	0.181375	-0.491231	2.324771
H	-1.167159	-0.426312	1.223964
H	0.334941	-2.297938	-1.281377
H	-1.217679	-1.723804	-0.649740
C	0.523660	1.965348	0.130660
N	0.164119	1.236241	-0.923042
N	1.810433	2.244934	0.332177
N	-0.421830	2.445390	0.938423
H	2.105164	2.815705	1.107810
H	2.508940	1.785405	-0.244683
H	0.895622	0.743130	-1.430127
H	-0.774832	0.841002	-0.890154
H	-1.363789	2.074497	0.834769
H	-0.170372	2.914686	1.793131
Cl	3.065430	-0.079768	-1.698881

GdmCl_Orientation8

C	4.898944	0.162559	-0.094930
C	3.458932	-0.320650	0.023997
O	2.953146	-0.353314	1.172715
O	2.869281	-0.622096	-1.044617
N	0.330817	-1.481863	-0.862029
C	-0.305026	-1.434119	0.300996
N	0.325058	-0.953033	1.367697
N	-1.579223	-1.845904	0.397671
C	-2.322483	-2.413110	-0.713798
C	-2.769633	0.918716	0.070452
N	-2.193979	1.001956	-1.126860
N	-3.994825	0.407512	0.194474
N	-2.092940	1.310352	1.142544
Cl	0.484502	2.628319	-0.331215
H	5.411400	-0.359068	-0.902586
H	-3.344377	-2.582214	-0.384318
H	4.884840	1.228309	-0.338127
H	5.431770	0.029747	0.845103
H	-2.344542	-1.712997	-1.552104
H	-1.897126	-3.364159	-1.044721
H	-1.983753	-1.899205	1.319090
H	-0.113869	-1.907360	-1.658161
H	1.323231	-1.136275	-0.937311
H	-0.165333	-0.881900	2.244117
H	1.341933	-0.703735	1.307978
H	-2.734629	0.854883	-1.964303
H	-1.293194	1.475205	-1.196641
H	-1.168817	1.720968	1.018992
H	-2.490869	1.237709	2.064786
H	-4.459814	0.395194	1.087935
H	-4.541557	0.173234	-0.618652

GdmCl_Orientation9

C	-4.442147	0.787101	-0.801079
C	-2.989429	0.539413	-0.443183
O	-2.118133	0.713277	-1.332676
O	-2.730005	0.132866	0.723782
N	0.445020	1.711293	-0.537111
C	0.774538	1.405221	0.720458
N	2.009039	1.644569	1.158630
C	3.034691	2.296739	0.355972
N	-0.144481	0.901317	1.541335
N	-1.191766	-2.202198	1.156928
C	-0.106895	-2.039590	0.396078
N	1.047190	-2.626001	0.718749
N	-0.184362	-1.352904	-0.738192
H	-4.865077	-0.149283	-1.174375
H	3.876109	2.521377	1.006004
H	-5.006871	1.088525	0.079390
H	-4.522679	1.535529	-1.587398
H	3.372342	1.642867	-0.451373
H	2.651217	3.233441	-0.052647
H	2.250791	1.322593	2.082508
H	1.185488	1.766388	-1.221199
H	-0.485679	1.440703	-0.874087
H	0.048640	0.839288	2.528386
H	-1.092506	0.661742	1.213677
H	0.692967	-1.135468	-1.208432
H	-0.991931	-0.762124	-0.946896
H	-1.950160	-1.527907	1.035110
H	-1.090862	-2.630886	2.063600
H	1.160169	-3.076115	1.612247
H	1.876066	-2.387453	0.181987
Cl	2.952239	-0.918718	-1.405129

GdmCl_Orientation10

C	4.391903	0.356331	-1.022813
C	2.986371	0.241300	-0.464553
O	2.046550	0.742991	-1.135771
O	2.825287	-0.372460	0.625469
N	-0.396326	-0.747575	-0.890149

C	-0.402889	-1.841049	-0.134278
N	-1.546022	-2.482387	0.104678
C	-2.828522	-2.050614	-0.432907
N	0.751503	-2.322503	0.338099
N	-0.001549	2.036342	0.361146
C	-0.356565	1.279348	1.402069
N	0.558052	0.553837	2.038080
N	-1.618386	1.324849	1.841484
H	4.529822	1.328004	-1.495639
H	-3.561653	-2.823475	-0.219372
H	5.134993	0.198075	-0.244079
H	4.518699	-0.410159	-1.791478
H	-3.152494	-1.108538	0.015113
H	-2.758756	-1.923279	-1.514934
H	-1.532655	-3.239315	0.770035
H	-1.255314	-0.234701	-1.077792
H	0.491196	-0.256930	-1.052890
H	0.742219	-3.156964	0.902829
H	1.558367	-1.695571	0.422758
H	-1.918597	0.684415	2.559680
H	-2.326074	1.661243	1.196547
H	-0.763420	2.360505	-0.227761
H	0.853788	1.769806	-0.135279
H	1.456658	0.340147	1.583311
H	0.265209	-0.056909	2.784994
Cl	-2.837022	1.597033	-1.237182

GdmCl_Orientation11

C	1.327553	3.967285	-0.425566
C	1.658712	2.508185	-0.176289
O	2.821178	2.186000	0.123896
O	0.697946	1.676858	-0.288626
N	-1.883037	0.673266	-0.063775
C	-1.646098	-0.181784	0.923077
N	-0.461914	-0.158688	1.537848
N	-2.589643	-1.045509	1.294670
N	2.798926	-0.507297	0.772556
C	2.278841	-1.351775	-0.120446
N	2.512182	-2.661481	-0.037491
C	1.905343	-3.642167	-0.925178
N	1.506353	-0.863582	-1.088480
H	0.871983	4.071075	-1.411628
H	2.233310	-4.628764	-0.611263
H	0.590934	4.295298	0.310659
H	2.218197	4.588135	-0.357861
H	0.816103	-3.602150	-0.859509
H	2.218332	-3.484752	-1.959743
H	3.165194	-2.981531	0.660500
H	1.038496	-1.483205	-1.728994
H	1.172113	0.104017	-0.984596
H	3.445710	-0.866163	1.457351
H	2.832696	0.507962	0.550180
H	-0.208724	-0.881011	2.191810
H	0.257867	0.450327	1.154355
H	-1.136522	1.304496	-0.350530
H	-2.801664	0.681917	-0.495927
H	-3.502153	-0.998153	0.847658
H	-2.459508	-1.633111	2.101312
Cl	-5.013620	-0.129570	-0.691577

GdmCl_Orientation12

C	1.681646	-3.764497	-0.508858
C	1.730825	-2.248170	-0.501173
O	2.269481	-1.644124	-1.444099
O	1.191714	-1.670017	0.501820
N	-1.394412	-2.152580	1.387050
C	-2.007600	-1.142525	0.774646
N	-1.291272	-0.291565	0.045533
N	-3.322299	-0.961617	0.889458
N	1.535192	1.019835	-1.247171
C	1.816217	1.645357	-0.100606
N	1.808684	2.976192	-0.028991
C	1.988401	3.713299	1.212930
N	2.079315	0.910953	0.976144
H	2.179208	-4.144396	0.385158
H	1.830552	4.767555	1.005074
H	0.638503	-4.085513	-0.462702
H	2.154394	-4.170252	-1.400115
H	1.256156	3.394735	1.957506
H	2.997278	3.583039	1.610392
H	1.694730	3.495465	-0.885326
H	2.283963	1.348909	1.858799
H	1.862191	-0.096426	0.936498
H	1.370329	1.571036	-2.074617
H	1.828851	0.029927	-1.364058
H	-1.765699	0.449863	-0.460790
H	-0.296978	-0.464625	-0.060215
H	-0.381981	-2.242785	1.270243
H	-1.910504	-2.797610	1.961432
H	-3.890922	-1.607796	1.410706
H	-3.761485	-0.200941	0.377222
Cl	-3.702443	1.644331	-1.055456

GdmCl_Orientation13

C	-3.355436	-2.880319	-0.659625
C	-2.389823	-1.752574	-0.354264
O	-2.548106	-1.120978	0.725843
O	-1.463981	-1.516772	-1.175065
N	-0.000065	-0.412398	1.784856
C	1.140768	-0.640785	1.138945
N	1.141160	-1.342555	0.009375
N	2.295680	-0.185268	1.624173
N	-2.272693	1.689034	0.523246
C	-1.190646	2.041744	-0.174206
N	-0.695788	3.275264	-0.070011
C	0.458960	3.742878	-0.821893
N	-0.632779	1.166143	-1.002315
H	-3.322323	-3.146453	-1.713986
H	0.624056	4.786574	-0.570402
H	-3.065892	-3.750512	-0.065389
H	-4.365445	-2.597951	-0.364736
H	1.355294	3.176513	-0.558221
H	0.278763	3.669880	-1.896471
H	-1.127329	3.902539	0.589893
H	0.214809	1.399958	-1.493103
H	-0.990817	0.202766	-1.084718
H	-2.648856	2.325856	1.207455
H	-2.507444	0.694027	0.604394
H	2.021309	-1.447412	-0.487014
H	0.256683	-1.549461	-0.457111
H	-0.903159	-0.731219	1.414698
H	0.001362	0.153730	2.617846
H	2.334731	0.283637	2.513682
H	3.152417	-0.355416	1.103082
Cl	4.350412	-1.077192	-0.742655

GdmCl_Orientation14

C	-3.281005	-3.258468	0.158135
N	-2.292030	-2.550323	-0.640337
C	-2.106096	-1.231287	-0.580077
N	-2.799894	-0.486385	0.272164
N	-1.230408	-0.630772	-1.394729
O	-2.688528	2.253895	0.048954
C	-1.493390	2.591790	-0.022130
O	-0.526803	1.766672	-0.112715
C	-1.131751	4.064817	0.009006
N	1.974050	0.563451	-0.013632
C	1.673978	-0.359266	0.893566
N	0.464249	-0.355032	1.452580
N	2.580638	-1.273561	1.233304
Cl	5.057117	-0.373247	-0.695397
H	-2.023438	4.688581	-0.013855
H	-3.262580	-4.305279	-0.132980
H	-0.564309	4.269395	0.919845
H	-0.486175	4.298539	-0.838916
H	-3.051076	-3.189671	1.224124
H	-4.282736	-2.865290	-0.028257
H	-1.694325	-3.085022	-1.250579
H	-3.489883	-0.915811	0.866598
H	-2.773655	0.553206	0.200196
H	-0.612223	-1.200134	-1.951285
H	-0.905079	0.299788	-1.106244
H	-0.195776	0.362898	1.160440
H	0.225973	-1.004190	2.183025
H	2.347490	-2.023691	1.862584
H	3.488836	-1.260622	0.775434
H	2.896737	0.554080	-0.437070
H	1.287227	1.286729	-0.217670

GdmCl_Orientation15

C	4.080671	-0.212919	-0.825869
C	2.676655	-0.729858	-0.574924
O	2.119844	-1.431586	-1.438719
O	2.135878	-0.396042	0.530859
N	-0.503697	-1.851761	-0.768755
C	-0.766366	-2.288171	0.459243
N	-1.976440	-2.748983	0.776861
C	-3.077287	-2.836168	-0.170965
N	0.212563	-2.274366	1.368705
N	1.702155	2.342044	0.996495
C	0.436727	2.379100	0.583510
N	-0.164551	1.246342	0.235607
N	-0.241537	3.525787	0.541363
H	4.477630	-0.593577	-1.764316
H	-3.905216	-3.338544	0.321349
H	4.054904	0.879056	-0.852805
H	4.727308	-0.503964	0.003252
H	-3.407793	-1.845256	-0.491300
H	-2.786787	-3.427566	-1.040999
H	-2.167128	-2.935009	1.749118
H	-1.227271	-1.856873	-1.469447
H	0.486311	-1.699873	-1.062044
H	0.007943	-2.545360	2.317378
H	1.021289	-1.665689	1.189531
H	0.396953	0.399577	0.216939
H	-1.097241	1.284105	-0.166939
H	-1.179550	3.522119	0.150058
H	0.217593	4.403615	0.720847
H	2.171406	3.176454	1.305808
H	2.173846	1.437157	1.015397
Cl	-3.018342	2.375605	-0.809227

Trimethylamine N-oxide

TMAO_Orientation1

C	3.849076	0.274333	0.179855
C	2.653836	-0.623919	-0.119447
O	2.148484	-0.553549	-1.267870
O	2.224939	-1.338177	0.822467
N	-0.567529	-1.085960	-0.905584
C	-0.949270	-2.005698	-0.026056
N	-0.040583	-2.861488	0.468303
N	-2.236206	-2.105101	0.316636
C	-3.289835	-1.338151	-0.337262
C	-0.308937	1.368829	1.324363
N	-0.707949	2.133988	0.106860
C	-1.367416	3.404073	0.513220
O	-1.607102	1.408720	-0.646187
C	0.501395	2.431397	-0.712149
H	4.481700	-0.162144	0.951047
H	4.425951	0.470814	-0.722586
H	3.467569	1.229278	0.553462
H	0.446040	-1.024983	-1.099264
H	-1.070856	-0.169225	-0.919482
H	-3.286027	-1.532563	-1.412481
H	-3.150409	-0.269398	-0.167955
H	-4.243636	-1.654032	0.077572
H	-2.492635	-2.788025	1.011640
H	-0.345739	-3.533659	1.155441

H	0.907347	-2.455181	0.578755
H	0.165947	2.969776	-1.595261
H	0.955655	1.481267	-0.993703
H	1.200668	3.035071	-0.132363
H	0.241660	0.482594	1.011855
H	0.316557	1.993998	1.961886
H	-1.224480	1.085274	1.838941
H	-0.678576	4.018481	1.092458
H	-2.242120	3.139846	1.102430
H	-1.672407	3.911603	-0.398321

TMAO_Orientation2

C	3.572097	1.932761	0.206577
H	4.560723	1.671011	0.584169
H	3.657087	2.574908	-0.668239
H	3.050086	2.477415	0.997933
C	2.780421	0.668599	-0.110703
O	2.846369	-0.263363	0.729572
O	2.097217	0.652147	-1.165660
H	0.842745	-0.551399	-1.005044
N	0.002393	-1.127314	-0.814527
H	-0.908086	-0.618039	-0.828039
H	-2.228252	-2.936623	-1.337071
C	-2.220508	-2.748735	-0.260160
H	-2.561731	-1.729439	-0.073488
H	-2.894827	-3.448123	0.227209
N	-0.886709	-2.950572	0.291841
H	-0.715141	-3.773735	0.847083
H	1.503156	-3.345307	0.939600
H	2.069407	-1.765086	0.436179
N	1.405032	-2.557065	0.318891
C	0.166058	-2.202159	-0.056095
O	-2.192540	0.484911	-0.643955
N	-1.810160	1.577223	0.105065
C	-1.179083	1.131680	1.380660
H	-0.270394	0.586019	1.133274
H	-1.889230	0.476404	1.880099
H	-0.944710	1.997484	1.999895
C	-3.025709	2.381175	0.404087
H	-3.705288	1.742757	0.963157
H	-2.759903	3.267096	0.980477
H	-3.470282	2.654467	-0.549521
C	-0.838002	2.400426	-0.669812
H	-0.566943	3.287806	-0.096600
H	-1.325334	2.675798	-1.602068
H	0.043015	1.788640	-0.864861

TMAO_Orientation3

C	2.560397	-2.448346	-0.240930
H	2.903420	-3.078573	0.578467
H	2.850052	-2.871827	-1.201746
H	3.011771	-1.455209	-0.136077
C	1.060945	-2.228177	-0.170269
O	0.521427	-2.253962	0.965606
O	0.462161	-1.964127	-1.246755
H	-0.903629	-1.046079	-1.077362
N	-1.711122	-0.392152	-0.938059
H	-2.001151	0.207041	-1.692882
H	-4.223710	0.739779	-1.531487
C	-3.927533	1.314565	-0.651346
H	-3.190076	2.068722	-0.937202
H	-4.805852	1.821646	-0.262248
N	-3.412065	0.441006	0.390485
H	-3.848356	0.463324	1.298306
H	-2.400031	-1.101774	2.107570
H	-1.030587	-1.653770	1.122241
N	-1.946294	-1.155965	1.210131
C	-2.356576	-0.363928	0.222119
O	2.900349	0.947060	0.478613
N	1.759998	1.619979	0.123124
C	0.645765	1.218401	1.025566
H	0.939564	1.492638	2.036408
H	0.547396	0.137335	0.951306
H	-0.281095	1.720405	0.740183
C	1.401780	1.297595	-1.285937
H	1.228580	0.224494	-1.341909
H	0.509653	1.849834	-1.586239
H	2.255287	1.576195	-1.899821
C	2.000791	3.082816	0.250421
H	1.106826	3.647073	-0.017909
H	2.828913	3.328499	-0.409893
H	2.284497	3.270849	1.283075

TMAO_Orientation4

C	5.274272	-1.487750	0.080552
C	3.922327	-0.782251	0.016450
O	2.959994	-1.402110	-0.492058
O	3.882094	0.385984	0.483866
N	0.472060	-0.185979	-0.295302
C	0.460374	1.139490	-0.141655
N	1.591710	1.781914	0.133628
N	-0.700771	1.793141	-0.253246
C	-0.826399	3.227495	-0.088314
O	-2.308650	-0.374838	-0.893561
N	-3.166854	-0.876585	0.060682
C	-3.340580	-2.336313	-0.173283
C	-4.480691	-0.187655	-0.064126
C	-2.601508	-0.647885	1.420442
H	5.210795	-2.501871	-0.309139
H	6.004245	-0.917208	-0.497069
H	5.622770	-1.508237	1.114721
H	2.482238	1.245177	0.270798
H	1.582929	2.780954	0.252472
H	-0.266608	3.774024	-0.852727
H	-0.485099	3.546167	0.900159
H	-1.877918	3.488187	-0.183147
H	-1.505000	1.209149	-0.513571
H	-0.410276	-0.609427	-0.580798
H	1.380552	-0.675288	-0.372841
H	-2.476041	0.425158	1.548903
H	-1.633705	-1.142790	1.460418
H	-3.274648	-1.050715	2.176337
H	-2.360942	-2.798986	-0.079688
H	-4.037639	-2.751186	0.554407
H	-3.715322	-2.456569	-1.186420
H	-5.183477	-0.585530	0.667350
H	-4.835560	-0.354968	-1.077731
H	-4.308586	0.873456	0.100867

Glycerol

Glycerol_Orientation1

C	-4.214049	-0.162151	-0.006207
C	-2.826075	-0.769126	-0.067934
O	-2.666791	-1.905790	-0.538106
O	-1.873522	-0.047281	0.387990
O	0.323864	0.836893	-0.946420
C	0.718716	1.822358	-0.000211
C	2.085854	2.288845	-0.466033
O	2.954737	1.179093	-0.623580
C	-0.290226	2.957712	0.090303
O	-1.427047	2.630078	0.865549
N	0.074121	-2.302979	-0.859540
C	0.920459	-1.900073	0.081877
N	0.432952	-1.410507	1.224503
N	2.239658	-2.015968	-0.095626
C	3.220341	-1.628969	0.910944
H	-4.459389	0.061201	1.033722
H	4.208825	-1.779168	0.485165
H	-4.213754	0.783826	-0.551087
H	-4.956980	-0.835831	-0.427001
H	3.114948	-0.568944	1.145067
H	3.130394	-2.236545	1.814329
H	2.554750	-2.570202	-0.877327
H	1.068685	-1.082074	1.933500
H	-0.497862	-0.981399	1.175470
H	0.425534	-2.521679	-1.778082
H	-0.948264	-2.194351	-0.729333
H	0.817932	1.364073	0.994491
H	1.975746	2.831906	-1.414416
H	2.533655	2.958831	0.269212
H	0.178622	3.824376	0.566200
H	-0.569906	3.240189	-0.933857
H	-1.715271	1.726061	0.644913
H	-0.477420	0.397187	-0.608041
H	2.422589	0.493208	-1.048180

Gycerol_Orientation2

C	-2.956464	-2.003022	0.622771
C	-1.456905	-1.870200	0.418360
O	-0.788954	-1.321576	1.347327
O	-0.969332	-2.315954	-0.640716
O	-1.779843	1.199472	1.064641
C	-1.069193	1.440484	-0.141625
C	-0.047522	2.551492	0.034642
O	0.899544	2.262661	1.048433
C	-2.102382	1.771136	-1.208077
O	-3.073041	0.741851	-1.277296
N	1.459548	-1.343897	-1.319997
C	2.258709	-0.816634	-0.405586
N	3.494113	-0.420134	-0.708299
C	4.335823	0.340528	0.205270
N	1.791166	-0.629045	0.842223
H	-3.320507	-1.261750	1.333752
H	5.207663	0.681286	-0.345869
H	-3.471203	-1.905865	-0.332009
H	-3.165828	-2.997203	1.025381
H	3.794699	1.210921	0.581378
H	4.674548	-0.273094	1.042778
H	3.842437	-0.619286	-1.633327
H	2.464426	-0.591918	1.594638
H	0.839084	-0.999270	1.069550
H	1.745065	-1.355003	-2.286567
H	0.537500	-1.759505	-1.048117
H	-0.550128	0.520630	-0.445929
H	-2.573673	2.733912	-0.967615
H	-1.634293	1.850777	-2.190544
H	0.446944	2.735794	-0.928496
H	-0.560438	3.468320	0.337160
H	1.197731	1.351835	0.929848
H	-1.437294	0.366641	1.433881
H	-3.329906	0.579985	-0.361039

Glycerol_Orientation3

C	-4.503011	-0.776160	-0.775513
C	-3.190905	-0.174575	-0.303482
O	-3.211829	0.720381	0.563039
O	-2.131881	-0.639661	-0.835677
O	1.744788	-0.412688	0.963686
C	1.510729	-1.387338	-0.045446
C	2.868479	-1.942716	-0.422464
O	3.758170	-0.891140	-0.764423
C	0.542560	-2.439424	0.478995
O	-0.573458	-1.806806	1.077003
N	-0.695158	1.608069	1.238037
C	0.096307	1.857762	0.192595
N	-0.230493	1.345290	-0.988840
N	1.197838	2.600839	0.327314
C	2.272080	2.570898	-0.655959
H	-4.505575	-1.843980	-0.548119
H	3.121055	3.109238	-0.243862
H	-5.352682	-0.294520	-0.296492
H	-4.576147	-0.674381	-1.859517
H	2.570911	1.539921	-0.866905
H	1.971287	3.069103	-1.579593
H	1.422685	2.919375	1.256990
H	0.376831	1.478794	-1.780577
H	-0.963989	0.613012	-1.027096
H	-0.503432	2.069660	2.113533
H	-1.658806	1.260114	1.053645

H	1.067205	-0.896854	-0.922474
H	3.266294	-2.525760	0.418148
H	2.787554	-2.595164	-1.293173
H	0.245201	-3.114235	-0.331791
H	1.031463	-3.026882	1.261145
H	-1.117401	-1.403635	0.369497
H	0.895845	-0.284929	1.410997
H	3.752631	-0.289632	-0.011304

Glycerol_Orientation4

C	-4.123718	-0.398423	-0.446593
C	-2.891521	0.443136	-0.158909
O	-1.897380	-0.169276	0.343494
O	-2.913491	1.661059	-0.410712
O	-1.134123	-2.652478	0.894504
C	-0.203155	-2.954871	-0.126785
C	0.862653	-1.866427	-0.207276
C	2.086035	-2.278378	-1.000125
O	3.101448	-1.290030	-0.906209
O	1.317054	-1.546778	1.107856
N	-0.497982	3.051463	-0.256318
C	0.581617	2.369532	0.132624
N	1.804222	2.879880	-0.037806
C	3.015952	2.146335	0.295085
N	0.422296	1.198471	0.736957
H	-4.523510	-0.774149	0.497697
H	3.869771	2.752565	0.005972
H	-4.886385	0.183121	-0.959721
H	-3.842187	-1.263978	-1.048840
H	3.074360	1.953576	1.368729
H	3.055246	1.200479	-0.251431
H	1.885891	3.786343	-0.469984
H	1.212710	0.603747	0.950425
H	-0.500760	0.722491	0.663239
H	-0.376085	3.867721	-0.833908
H	-1.415719	2.571328	-0.271526
H	0.420963	-0.967967	-0.656061
H	2.455141	-3.240904	-0.625021
H	1.836628	-2.386647	-2.056722
H	-0.686202	-3.067050	-1.104420
H	0.262422	-3.907722	0.140964
H	-1.561871	-1.796595	0.665597
H	0.568189	-1.731089	1.692574
H	3.296428	-1.199371	0.033016

Glycerol_Orientation5

C	-3.363575	1.907487	0.376882
C	-1.854975	1.768171	0.277922
O	-1.383518	1.523379	-0.875863
O	-1.172222	1.858824	1.317710
O	-2.314582	-0.933830	-1.663509
C	-1.055095	-1.552388	-1.454721
C	-0.734336	-1.587988	0.032573
C	0.565455	-2.306809	0.327526
O	0.965885	-2.164111	1.679314
O	-1.792234	-2.232925	0.726991
N	1.396067	0.899857	1.362916
C	2.010198	0.870854	0.162660
N	3.317593	0.625652	0.092332
C	4.050730	0.536919	-1.161725
N	1.290328	1.043000	-0.934250
H	-3.806188	0.919123	0.224323
H	5.099015	0.375789	-0.928276
H	-3.660545	2.286212	1.352248
H	-3.731930	2.559220	-0.415432
H	3.696384	-0.299933	-1.768138
H	3.960901	1.466737	-1.726624
H	3.807819	0.435501	0.952693
H	1.725595	0.953118	-1.838804
H	0.267287	1.271402	-0.889273
H	1.977987	1.083917	2.168318
H	0.436432	1.307394	1.382275
H	-0.642242	-0.554595	0.394514
H	0.435345	-3.376290	0.145083
H	1.342416	-1.934170	-0.355117
H	-0.259994	-1.034678	-2.002576
H	-1.131238	-2.576010	-1.832616
H	-2.163383	0.017842	-1.511907
H	-2.600532	-1.890179	0.326501
H	1.081895	-1.218144	1.831972

Glycerol_Orientation6

C	-3.792866	-1.555598	0.185559
C	-2.296030	-1.318584	0.132930
O	-1.718957	-1.446106	-0.979432
O	-1.721183	-0.943332	1.189071
N	1.002514	-2.054198	-1.062890
C	1.678785	-1.440355	-0.087025
N	1.057015	-1.129681	1.045477
N	2.985813	-1.202606	-0.223140
H	3.438497	-1.549740	-1.054403
O	-0.115754	0.884054	-1.103986
C	-0.183458	1.754295	0.013106
C	1.016665	2.673236	-0.115088
O	2.208710	1.908988	-0.205637
C	-1.499532	2.507645	0.071653
O	-2.598130	1.624628	0.228325
H	-4.102158	-2.263898	-0.580828
H	-4.097342	-1.895790	1.173767
H	-4.278500	-0.596179	-0.014226
C	3.818340	-0.668450	0.846953
H	1.451705	-2.146078	-1.961024
H	-0.021379	-1.936710	-1.066054
H	1.552497	-0.585633	1.734201
H	0.019613	-1.111398	1.086239
H	-0.078816	1.176725	0.941199
H	0.895723	3.306213	-1.004118
H	1.104557	3.315881	0.761870
H	-1.460770	3.237604	0.890854
H	-1.657149	3.045984	-0.866268
H	-2.358862	0.966072	0.896652
H	-0.767412	0.166004	-1.014717
H	2.029751	1.227350	-0.865810
H	4.836566	-0.599340	0.474407
H	3.480301	0.333477	1.116331
H	3.806860	-1.324126	1.720552

Glycerol_Orientation7

C	3.511689	1.948528	-0.120488
C	2.042197	1.573234	-0.108239
O	1.467226	1.478330	1.006451
O	1.497639	1.318772	-1.217571
N	-1.258241	1.067299	-1.301424
C	-1.950264	1.060685	-0.165857
N	-3.271036	0.860701	-0.182580
C	-4.076129	0.763562	1.024478
N	-1.319226	1.292538	0.982512
O	0.872133	-1.399757	-1.293188
C	0.519027	-1.649882	0.061012
C	1.707400	-2.139370	0.869527
O	2.708697	-1.141180	0.980231
C	-0.634075	-2.633630	0.024351
O	-1.718448	-2.076049	-0.699772
H	-3.675265	0.537258	-1.047451
H	3.771273	2.466532	-1.042060
H	3.766255	2.551775	0.749175
H	4.081587	1.016222	-0.075791
H	-1.738995	1.002775	-2.184098
H	-0.231562	1.195680	-1.287610
H	-1.796297	1.138221	1.855736
H	-0.288884	1.400409	0.995903
H	0.154114	-0.722518	0.518513
H	-0.296332	-3.571035	-0.438131
H	-0.987941	-2.851151	1.033628
H	1.365931	-2.466370	1.860437
H	2.166317	-2.992247	0.363526
H	2.287369	-0.335238	1.313307
H	1.227665	-0.497271	-1.343992
H	-1.312186	-1.628932	-1.453457
H	-5.118303	0.681426	0.728673
H	-3.807772	-0.114549	1.617882
H	-3.964509	1.665564	1.628345

Glycerol_Orientation8

C	-3.347852	-2.283545	0.388358
C	-1.881441	-1.909185	0.253043
O	-1.158052	-1.986719	1.268812
O	-1.491044	-1.511570	-0.886638
O	-0.347071	0.942080	-0.958247
C	-0.787192	1.426573	0.307255
C	0.219625	2.485116	0.728771
O	1.544297	1.978419	0.639084
C	-2.195009	1.990275	0.159136
H	-2.507477	2.502176	1.072391
N	1.274693	-1.840308	-1.262586
C	1.903568	-1.116869	-0.332941
N	3.072452	-0.528553	-0.603920
C	3.981594	-0.041290	0.430035
N	1.391485	-1.036626	0.892802
H	-2.888347	1.160056	-0.027759
H	3.414908	-0.584806	-1.550669
H	-3.736497	-2.661415	-0.555908
H	-3.486392	-3.014715	1.183024
H	-3.908080	-1.381995	0.651116
H	1.688138	-1.923133	-2.178256
H	0.250358	-1.904157	-1.188776
H	1.650382	-0.221423	1.434609
H	0.438634	-1.427696	1.052508
H	-0.797364	0.609089	1.038096
H	0.101537	3.367742	0.090459
H	0.049448	2.777070	1.765925
O	-2.245022	2.931504	-0.898669
H	-0.737843	0.049946	-1.064076
H	1.607447	1.597269	-0.247194
H	4.950431	0.131442	-0.030817
H	3.621739	0.893536	0.861371
H	4.090740	-0.789423	1.217175
H	-1.756780	2.522668	-1.623960

Glycerol_Orientation9

C	-3.163149	-1.784688	0.351738
C	-1.648955	-1.872032	0.242525
O	-1.135180	-1.787807	-0.911466
O	-0.999762	-1.975999	1.307795
H	-2.730658	0.641971	-1.090001
C	-2.317671	1.540597	-0.615878
C	-0.865831	1.268197	-0.263203
C	-0.113225	2.516681	0.158234
O	1.256870	2.210122	0.379281
O	-0.173765	0.747808	-1.386519
N	1.659979	-1.866568	-0.979371
C	2.091086	-0.945735	-0.114339
N	1.449490	-0.785713	1.039990
N	3.192477	-0.229471	-0.365139
C	3.924089	0.490149	0.674888
H	3.652434	-0.380029	-1.249741
H	-3.641588	-1.993705	-0.603455
H	-3.526851	-2.466038	1.120391
H	-3.415399	-0.765027	0.661119
H	2.163356	-1.997074	-1.843022
H	0.646439	-2.059951	-0.974862
H	1.545820	0.114500	1.492111
H	0.551644	-1.297260	1.176677
H	-0.843390	0.548655	0.565151
H	-0.213296	3.279197	-0.625253
H	-0.521607	2.913052	1.087367
O	-2.996685	1.846606	0.592434
H	-2.376080	2.369515	-1.331845
H	-0.450037	-0.182751	-1.457349

H	1.542882	1.744173	-0.418126
H	4.875077	0.806574	0.255327
H	3.374202	1.374350	0.999939
H	4.108018	-0.161488	1.531083
H	-3.904477	2.078747	0.380138

Glycerol_Orientation10

C	2.789657	-2.870436	-0.464960
C	1.427317	-2.240106	-0.232317
O	1.200192	-1.779003	0.925775
O	0.626174	-2.189882	-1.191442
N	-1.686452	-0.824794	-0.827610
C	-2.180252	-0.722492	0.414203
N	-1.490668	-1.229614	1.433119
N	-3.348772	-0.118530	0.618710
C	-4.114613	0.533095	-0.434321
O	-1.064159	2.127663	-0.744679
C	0.315883	2.450889	-0.717426
C	1.172052	1.280331	-0.266398
C	2.653806	1.639341	-0.234305
H	3.231847	0.730452	-0.022710
O	0.764806	0.915780	1.044610
H	-3.701480	-0.082026	1.562408
H	3.085167	-3.457225	0.404193
H	2.785920	-3.487171	-1.361483
H	3.523023	-2.069708	-0.590788
H	-1.726017	-0.933852	2.368215
H	-0.515467	-1.528949	1.264158
H	-2.337091	-0.782844	-1.599037
H	-0.809297	-1.383711	-0.968436
H	1.019572	0.438147	-0.957169
H	0.443415	3.278774	-0.017049
H	0.662178	2.779019	-1.705582
H	2.985777	2.043745	-1.193026
O	2.893677	2.626173	0.754663
H	0.982404	-0.028130	1.149530
H	-1.138719	1.219014	-1.059975
H	-4.964076	1.027270	0.028670
H	-3.505980	1.285201	-0.940087
H	-4.492343	-0.191109	-1.159345
H	2.403798	2.324085	1.529715

Glycerol_Orientation11

C	2.509608	2.421721	-0.362885
C	1.042440	2.044294	-0.427562
O	0.659559	1.364612	-1.427000
O	0.308978	2.370253	0.532231
O	2.289423	-0.788910	-0.924005
C	1.490420	-1.255991	0.145696
C	0.744340	-2.524038	-0.255707
O	-0.026465	-2.341602	-1.428065
C	2.376911	-1.501408	1.347963
O	2.807120	-0.243309	1.844727
C	-2.460843	0.268044	-0.131223
N	-3.664893	-0.293786	-0.022792
C	-4.488977	-0.198324	1.172344
N	-1.916704	0.923127	0.878986
N	-1.766482	0.139686	-1.279902
H	1.817378	-2.051266	2.114224
H	-3.968395	-0.897888	-0.770591
H	2.927145	2.528254	-1.363154
H	2.647049	3.335159	0.213418
H	3.019231	1.599085	0.147193
H	-2.300836	-0.019399	-2.122592
H	-0.881317	0.689770	-1.376012
H	-2.368541	0.923364	1.779441
H	-1.048474	1.501936	0.734711
H	0.754110	-0.486899	0.425569
H	1.470421	-3.310545	-0.480527
H	0.120626	-2.862536	0.581994
H	3.230771	-2.112577	1.031011
H	1.783939	-0.085762	-1.363899
H	-0.645567	-1.616666	-1.270781
H	-5.454258	-0.645985	0.953789
H	-4.038212	-0.731305	2.012811
H	-4.646395	0.847547	1.441890
H	3.425564	-0.401617	2.562590

Glycerol_Orientation12

C	3.539253	-1.738933	-0.458958
C	2.044855	-1.526852	-0.310891
O	1.624966	-1.197545	0.846028
O	1.320449	-1.650574	-1.317834
O	0.071346	1.002335	1.100438
C	0.515843	1.670549	-0.075185
C	1.850399	2.349224	0.177629
H	2.128499	2.965401	-0.681198
C	-0.581954	2.656779	-0.441059
O	-1.840719	1.999497	-0.464882
N	-1.120375	-1.977296	1.105509
C	-1.824073	-1.246248	0.234551
N	-1.310221	-0.982751	-0.962919
N	-3.058888	-0.835795	0.534970
C	-4.005716	-0.354822	-0.467881
O	2.894960	1.408322	0.367442
H	-3.405690	-1.033669	1.460946
H	3.943520	-2.230947	0.424905
H	3.766023	-2.310535	-1.356611
H	4.000357	-0.750888	-0.538028
H	-1.529743	-2.202484	1.998659
H	-0.098458	-1.916256	1.054933
H	-1.666029	-0.164681	-1.440650
H	-0.317143	-1.248217	-1.134179
H	0.641299	0.939599	-0.885028
H	-0.595847	3.477526	0.287677
H	-0.409830	3.075691	-1.432892
H	1.748321	3.000646	1.055191
H	0.516923	0.133924	1.115324
H	-1.884722	1.520250	0.374073
H	-4.990754	-0.324743	-0.010399
H	-3.743658	0.647984	-0.808286
H	-4.028687	-1.035109	-1.320998
H	2.552365	0.672952	0.894870

Two guanidinium ions

2Gdm$^+$_Orientation1

C	-2.152655	-1.101450	2.395184
C	-0.896339	-0.858136	1.590761
O	0.222664	-1.027402	2.113069
O	-1.045627	-0.482016	0.377397
N	1.201360	1.199163	-0.306584
C	2.161872	1.551958	0.543856
N	2.116766	1.119491	1.803279
N	3.149662	2.348590	0.141171
C	3.246096	2.897628	-1.203846
N	0.705355	-1.897143	-1.422352
C	1.946654	-2.107066	-0.995097
N	2.242832	-1.908632	0.283979
N	2.885174	-2.517240	-1.847921
H	-2.789814	-0.215691	2.355617
H	4.107624	3.558171	-1.233357
H	-2.707958	-1.926138	1.943253
H	-1.911771	-1.343350	3.427311
H	3.388059	2.107985	-1.944996
H	2.355858	3.479862	-1.448850
H	3.889361	2.550429	0.795151
H	1.246230	1.475542	-1.273576
H	0.413215	0.617373	-0.012392
H	2.838926	1.377711	2.455817
H	1.438589	0.408100	2.073242
H	0.476608	-2.020988	-2.395328
H	0.013614	-1.462713	-0.809183
H	1.517232	-1.647190	0.957942
H	3.178719	-2.068282	0.620966
H	3.814157	-2.741704	-1.531706
H	2.675778	-2.650912	-2.823757
C	-3.925999	0.663570	-0.779767
N	-3.608489	-0.622940	-0.874459
N	-3.079776	1.486429	-0.167413
N	-5.072546	1.121930	-1.275693
H	-2.705247	-0.917769	-0.508285
H	-4.193458	-1.270515	-1.376176
H	-5.735773	0.502221	-1.711494
H	-5.311901	2.097984	-1.211558
H	-3.282549	2.467328	-0.068980
H	-2.191930	1.111342	0.152031

2Gdm$^+$_Orientation2

C	2.118779	-0.292536	2.520412
C	0.901692	-0.270139	1.623706
O	-0.213216	-0.589939	2.083141
O	1.072688	0.093085	0.410460
N	-2.410292	0.771028	0.863301
C	-2.218804	1.634423	-0.129154
N	-3.257138	2.250391	-0.691153
C	-4.635236	2.052655	-0.266572
N	-0.978502	1.890828	-0.546676
N	-1.785865	-2.506507	0.657851
C	-1.739083	-2.287362	-0.651254
N	-2.563327	-2.940247	-1.469497
N	-0.864902	-1.415781	-1.145287
H	1.891598	-0.775411	3.467354
H	-5.269420	2.685427	-0.880549
H	2.940885	-0.806570	2.019490
H	2.436794	0.736259	2.705878
H	-4.942836	1.014302	-0.406766
H	-4.766616	2.340157	0.778593
H	-3.073249	2.890306	-1.447791
H	-3.336334	0.589796	1.214395
H	-1.616956	0.326375	1.335057
H	-0.831398	2.473671	-1.354875
H	-0.198719	1.323318	-0.210923
H	-2.486184	-3.116133	1.047924
H	-1.207179	-1.949883	1.286735
H	-0.188059	-0.934516	-0.549905
H	-0.783552	-1.291282	-2.141745
H	-2.543720	-2.781043	-2.463443
H	-3.233901	-3.601289	-1.112888
C	4.152961	0.409590	-0.775378
N	5.393406	0.529837	-1.241703
N	3.540599	1.440494	-0.202928
N	3.503286	-0.746680	-0.868464
H	5.900772	1.394249	-1.145539
H	5.876820	-0.258084	-1.641404
H	3.909671	-1.538405	-1.338661
H	2.544041	-0.784254	-0.534905
H	2.583590	1.310760	0.116033
H	3.995467	2.333749	-0.109539

2Gdm$^+$_Orientation3

C	1.149432	4.149129	-0.082848
C	1.047640	2.638447	-0.089789
O	0.842450	2.044729	1.002951
O	1.203579	2.041607	-1.189940
N	2.546396	-0.414553	-0.754205
C	2.943719	-0.811811	0.450026
N	2.717992	-0.034418	1.509066
N	3.576748	-1.975446	0.596654
C	3.898944	-2.862611	-0.510656
N	-0.651891	-0.017093	-1.670904
C	-0.902499	-0.774891	-0.612336
N	-0.518892	-0.374270	0.597497
N	-1.581386	-1.917166	-0.747730
H	2.208784	4.418858	-0.072251
H	4.428804	-3.721248	-0.108525
H	0.709614	4.560404	-0.990326
H	0.673317	4.566626	0.801572
H	2.992685	-3.216621	-1.006880

H	4.546582	-2.364029	-1.234668
H	3.839778	-2.255028	1.528643
H	2.722772	-0.987772	-1.563199
H	2.102643	0.501962	-0.898584
H	2.968060	-0.354629	2.430567
H	2.114856	0.787340	1.420219
H	-1.025130	-0.265772	-2.572692
H	-0.038805	0.801610	-1.584300
H	-0.024998	0.522469	0.731228
H	-0.539330	-1.027427	1.365299
H	-1.801515	-2.481864	0.057241
H	-1.773091	-2.301843	-1.658995
C	-4.000085	-0.325855	0.398303
N	-4.855703	-1.032281	-0.329449
N	-3.586210	-0.789933	1.578764
N	-3.527392	0.828723	-0.057242
H	-5.185031	-1.930836	-0.013583
H	-5.101968	-0.747195	-1.264148
H	-3.076133	-0.186484	2.205472
H	-4.033816	-1.595286	1.988979
H	-3.837748	1.209151	-0.937549
H	-2.899119	1.387541	0.499035

2Gdm$^+$_Orientation4

C	-1.136497	-2.365479	0.646777
C	-0.522026	-0.981853	0.593329
O	-1.267687	-0.002482	0.319969
O	0.717291	-0.875177	0.790554
N	-3.571226	-0.573620	-1.283453
C	-4.471913	-0.454602	-0.313655
N	-4.055955	-0.132117	0.906935
N	-5.764566	-0.655621	-0.559821
N	2.919185	-1.207101	-1.001964
C	3.393958	-2.300944	-0.412220
N	4.490482	-2.893584	-0.881349
N	2.761184	-2.784626	0.649737
N	1.794432	1.703927	1.199714
C	1.299430	2.613541	0.360046
N	1.927122	3.775678	0.175992
C	1.413439	4.840669	-0.672187
N	0.161012	2.354196	-0.273445
H	-2.200709	-2.316710	0.874596
H	2.081294	5.692201	-0.583678
H	-1.013765	-2.828014	-0.336735
H	-0.622743	-2.985980	1.379512
H	1.379925	4.532956	-1.720143
H	0.417980	5.146960	-0.345503
H	2.832512	3.894957	0.603045
H	-0.207100	3.002483	-0.949612
H	-0.371297	1.499584	-0.059068
H	2.655633	1.882675	1.689384
H	1.412334	0.753030	1.182458
H	3.121994	-3.579067	1.151377
H	1.931279	-2.290095	0.980260
H	2.064330	-0.795007	-0.643042
H	3.335027	-0.847507	-1.845074
H	4.979069	-2.524649	-1.680760
H	4.853058	-3.729141	-0.452640
H	-6.079627	-0.942275	-1.472527
H	-6.445493	-0.618197	0.181066
H	-4.707402	0.003615	1.662368
H	-3.062358	0.041718	1.043355
H	-2.598459	-0.383063	-1.057495
H	-3.842340	-0.807127	-2.224301

Two molecules of trimethylamine N-oxide

2TMAO_Orientation1

C	-1.931051	-3.090485	-1.579821
C	-1.290894	-1.740829	-1.886962
O	-0.039318	-1.721414	-2.001741
O	-2.047911	-0.742447	-1.986047
C	-3.107153	-0.982402	1.406156
N	-2.476448	0.342225	1.660421
C	-2.973524	1.314601	0.648585
O	-1.111938	0.229408	1.557228
C	-2.821391	0.812754	3.028081
N	-0.865426	1.773120	-2.112722
C	0.322746	1.819437	-1.484187
N	1.089072	0.744111	-1.466356
N	0.735973	2.968233	-0.932393
C	2.097827	3.171653	-0.456308
O	3.185154	0.223716	0.191444
N	2.891982	-0.923525	0.899281
C	3.998186	-1.168088	1.861152
C	2.776892	-2.074012	-0.041438
C	1.605686	-0.751331	1.632546
H	-3.013819	-3.046841	-1.684518
H	-1.519125	-3.856244	-2.237938
H	-1.680821	-3.370832	-0.553074
H	0.661816	-0.143658	-1.785885
H	1.922239	0.653117	-0.840801
H	2.807054	3.207613	-1.288517
H	2.388513	2.366095	0.218836
H	2.129712	4.116602	0.080644
H	0.156798	3.781798	-1.067776
H	-1.477238	2.569103	-2.019367
H	-1.316754	0.841683	-2.179256
H	3.705170	-2.118599	-0.606136
H	1.930973	-1.887317	-0.702794
H	2.619800	-2.996052	0.519545
H	0.810377	-0.577950	0.912584
H	1.394324	-1.642711	2.224315
H	1.709875	0.120521	2.274269
H	3.808854	-2.079858	2.427344
H	4.047618	-0.304536	2.519771
H	4.915753	-1.249751	1.283601
H	-4.050698	1.453684	0.752733
H	-2.440877	2.248094	0.816708
H	-2.722554	0.902985	-0.326773
H	-4.189419	-0.917479	1.527634
H	-2.847241	-1.261193	0.386863
H	-2.677809	-1.684138	2.117366
H	-3.901877	0.907488	3.142390
H	-2.417889	0.084535	3.727590
H	-2.330663	1.772804	3.169134

2TMAO_Orientation2

C	2.990330	3.210115	-0.888595
C	2.024643	2.601430	0.125151
O	2.519318	2.120243	1.176085
O	0.807362	2.583079	-0.182992
C	-4.612850	1.318137	-1.026342
N	-3.833479	0.100319	-0.673062
C	-2.570914	0.065198	-1.465216
O	-3.547465	0.133868	0.674842
C	-4.641705	-1.116087	-0.962081
N	-0.997563	1.191950	1.432800
C	-0.419588	-0.019276	1.546772
N	0.892818	-0.111787	1.762265
N	-1.184123	-1.109223	1.498514
C	-0.683889	-2.442664	1.792162
O	2.250213	-2.118557	0.452374
N	2.698468	-1.578014	-0.733127
C	3.193265	-2.687329	-1.592359
C	3.807818	-0.622884	-0.455022
C	1.588890	-0.865669	-1.431170
H	2.494868	3.972765	-1.487957
H	3.867595	3.623110	-0.392569
H	3.324301	2.414091	-1.561155
H	1.427615	0.766458	1.686591
H	1.390111	-0.953363	1.406483
H	-0.294528	-2.489772	2.812796
H	0.112971	-2.726341	1.101405
H	-1.512058	-3.141565	1.700321
H	-2.164953	-0.943506	1.245304
H	-1.985751	1.155036	1.173860
H	-0.398851	1.886472	0.962297
H	4.577060	-1.174391	0.080110
H	3.409786	0.178428	0.167902
H	4.198440	-0.225441	-1.392662
H	1.284262	-0.018136	-0.818470
H	1.929489	-0.521395	-2.407988
H	0.770577	-1.575221	-1.534865
H	3.576356	-2.293514	-2.533557
H	2.357961	-3.361523	-1.765018
H	3.975028	-3.198165	-1.036016
H	-4.864517	1.306230	-2.086576
H	-5.508851	1.315724	-0.411286
H	-3.995240	2.179632	-0.783717
H	-2.801542	0.040244	-2.529876
H	-1.997567	0.956271	-1.216697
H	-2.021261	-0.825692	-1.168860
H	-4.899805	-1.151593	-2.020242
H	-4.042046	-1.978745	-0.680330
H	-5.533716	-1.063696	-0.343230

2TMAO_Orientation3

C	-2.680517	4.410723	-0.020539
C	-1.814061	3.153126	-0.020557
O	-2.408283	2.065940	0.221224
O	-0.592429	3.279615	-0.254985
N	-0.765244	-0.117615	-0.134811
C	0.546724	-0.088552	-0.297177
N	1.242576	-1.220377	-0.472444
C	0.589407	-2.509037	-0.607901
N	1.208110	1.076309	-0.262907
O	-2.516613	-2.208153	-0.040082
N	-3.759335	-1.640515	0.146461
C	-4.763956	-2.734525	0.210561
C	-4.073837	-0.729529	-0.991245
C	-3.776396	-0.862283	1.418373
O	3.757658	-0.064821	-0.859018
N	4.666407	-0.234788	0.162918
C	3.974778	-0.139084	1.479511
C	5.301633	-1.574435	0.025194
C	5.704630	0.826442	0.060130
H	-2.093605	5.296220	-0.256960
H	-3.484958	4.295114	-0.749240
H	-3.144828	4.527644	0.960674
H	-1.282934	0.767279	0.014837
H	-1.323463	-0.995704	-0.127493
H	-0.055660	-2.544873	-1.490574
H	-0.029817	-2.727042	0.265077
H	1.358081	-3.273402	-0.696436
H	2.235712	-1.090741	-0.692876
H	2.197039	1.047313	-0.505187
H	0.652777	1.939018	-0.262509
H	-3.972293	-1.311492	-1.903988
H	-3.356547	0.089534	-0.968546
H	-5.087898	-0.342741	-0.886284
H	-3.080964	-0.031469	1.309552
H	-4.782312	-0.486923	1.608394
H	-3.457412	-1.537034	2.208840
H	-5.762669	-2.322547	0.353636
H	-4.484269	-3.377262	1.041475
H	-4.698906	-3.284529	-0.724717
H	6.446078	0.703688	0.849312
H	6.160851	0.733872	-0.922191
H	5.198144	1.784378	0.148270
H	4.691530	-0.285777	2.286924
H	3.519051	0.846322	1.540776
H	3.203412	-0.906297	1.501080
H	6.047715	-1.717894	0.806134
H	4.512161	-2.318771	0.104055
H	5.755301	-1.614706	-0.961767

2TMAO_Orientation4

C	-4.014516	-1.382131	-1.757382

C	-2.744247	-1.795951	-1.032159
O	-2.850885	-2.103512	0.185493
O	-1.664708	-1.738483	-1.671089
N	-0.675725	-1.415999	1.676153
C	0.522170	-1.294695	1.107140
N	0.673310	-1.576647	-0.186944
N	1.583984	-0.893340	1.811638
C	1.524840	-0.569500	3.223733
C	-3.018448	1.135690	1.205649
N	-2.409380	1.955897	0.121558
C	-2.245242	3.356483	0.597019
O	-3.222158	1.950137	-0.982251
C	-1.078618	1.395819	-0.242005
H	-3.929067	-1.555832	-2.829433
H	-4.884456	-1.897419	-1.351927
H	-4.124604	-0.305657	-1.583017
H	-1.492959	-1.748490	1.120104
H	-0.789307	-1.221125	2.656946
H	1.237270	-1.438090	3.822275
H	0.823203	0.247015	3.417503
H	2.514561	-0.249493	3.539964
H	2.451699	-0.790709	1.270495
H	1.602344	-1.411980	-0.576137
H	-0.164507	-1.736248	-0.771703
H	-0.667173	2.039923	-1.016925
H	-1.245419	0.396950	-0.641566
H	-0.421829	1.366355	0.630770
H	-3.117607	0.117776	0.832721
H	-2.389097	1.158273	2.096994
H	-3.997669	1.562695	1.410539
H	-1.599077	3.392644	1.474901
H	-3.238585	3.732603	0.829403
H	-1.817925	3.925543	-0.224901
O	3.406119	-0.834541	-0.279159
N	3.770512	0.366861	-0.846971
C	5.063563	0.806501	-0.254041
C	3.928536	0.172717	-2.315095
C	2.718359	1.389459	-0.586263
H	4.242724	1.105628	-2.782854
H	4.673330	-0.606392	-2.457583
H	2.966728	-0.153034	-2.705264
H	5.381747	1.746270	-0.705032
H	4.907314	0.923076	0.816152
H	5.787177	0.017109	-0.441929
H	2.991973	2.334899	-1.053927
H	1.786223	1.008993	-1.000297
H	2.628758	1.506146	0.492167

2TMAO_Orientation5

C	-3.268680	0.169628	2.501968
C	-2.102077	-0.649403	1.977630
O	-2.352512	-1.786097	1.503770
O	-0.963594	-0.108598	1.991143
N	0.908404	-1.304989	0.351817
C	0.638726	-2.404633	-0.331859
N	1.540152	-2.922724	-1.182081
C	2.713857	-2.186498	-1.630851
N	-0.537922	-3.014306	-0.163654
C	-1.482553	2.064254	-0.514168
N	-2.394526	1.244676	-1.359931
C	-1.812234	-0.113144	-1.543959
C	-2.568470	1.899676	-2.684306
O	-3.617019	1.135510	-0.750031
H	-4.083479	-0.473610	2.831862
H	-2.951671	0.832551	3.306428
H	-3.611687	0.771868	1.653348
H	0.189555	-0.943411	1.007046
H	1.860732	-0.877768	0.411263
H	3.282602	-1.806671	-0.782511
H	2.433554	-1.340805	-2.265831
H	3.340128	-2.868171	-2.201286
H	1.240620	-3.704659	-1.743588
H	-0.798547	-3.782755	-0.759155
H	-1.229805	-2.609979	0.497169
H	-2.495302	-0.671141	-2.180710
H	-1.766176	-0.573386	-0.560351
H	-0.820398	-0.051047	-1.997143
H	-1.337239	1.524915	0.421370
H	-0.531961	2.223274	-1.026309
H	-1.984734	3.012748	-0.338330
H	-1.611618	1.989954	-3.200118
H	-3.005322	2.878669	-2.502075
H	-3.261955	1.286565	-3.254629
O	3.236218	0.040830	0.718090
N	2.946310	1.370635	0.499432
C	4.188734	2.161678	0.708586
C	2.464165	1.551730	-0.897752
C	1.896514	1.817417	1.460331
H	2.240226	2.601792	-1.086451
H	3.250722	1.197798	-1.560265
H	1.574437	0.935503	-1.014871
H	3.992785	3.221529	0.547454
H	4.518203	1.975309	1.727586
H	4.928359	1.789790	0.004057
H	1.671815	2.872587	1.302147
H	1.007257	1.206798	1.306648
H	2.289347	1.651308	2.460678

Salt-bridge

C	3.924674	-0.241763	0.042018
C	2.407409	-0.100140	0.008700
O	1.945283	1.051416	0.207187
O	1.727104	-1.133376	-0.207096
N	-0.941428	-0.896455	0.048803
C	-1.496920	0.305084	-0.042477
N	-2.829415	0.439721	-0.021843
C	-3.745272	-0.682352	0.098169
N	-0.712815	1.372337	-0.174537
H	4.233503	-1.256945	-0.199199
H	-4.759927	-0.296744	0.051679
H	4.369361	0.461436	-0.664105
H	4.285039	0.024413	1.037698
H	-3.608144	-1.388325	-0.723851
H	-3.614574	-1.201836	1.050566
H	-3.209223	1.372278	-0.037907
H	-1.522027	-1.712495	0.145178
H	0.100408	-1.001247	-0.047204
H	-1.128497	2.289367	-0.185581
H	0.321236	1.271585	-0.033425

XYZ Coordinates of the optimized geometries obtained at the CPCM(water)/M06-2X/6-311++G** level of theory

Guanidinium ion

Gdm$^+$_Orientation1

C	2.965287	-2.702375	-0.130493
C	1.948221	-1.586029	-0.034767
O	1.809208	-0.975188	1.058480
O	1.284853	-1.302085	-1.071941
N	-1.520694	-1.198453	-0.722407
C	-1.886770	-0.562551	0.386679
N	-0.965172	-0.237735	1.293391
N	-3.167281	-0.249394	0.587129
C	-4.223021	-0.526924	-0.375976
C	1.007597	2.298943	-0.217541
N	0.647734	1.455783	-1.178033
N	0.680463	3.591426	-0.302917
N	1.693378	1.851549	0.829187
H	3.810166	-2.350134	-0.727068
H	-5.152161	-0.130084	0.022981
H	3.321118	-2.997775	0.853922
H	2.528983	-3.555942	-0.649465
H	-4.018115	-0.035095	-1.328905
H	-4.343680	-1.601399	-0.530640
H	-3.417737	0.177043	1.465734
H	-2.204590	-1.464918	-1.411470
H	-0.526913	-1.344677	-0.923675
H	-1.231404	0.264109	2.125584
H	0.008998	-0.544396	1.204053
H	0.105332	1.784949	-1.960762
H	0.920156	0.463632	-1.151366
H	1.828920	0.844242	0.963383
H	1.966943	2.483665	1.564189
H	0.952606	4.243636	0.414885
H	0.252012	3.962699	-1.135553

Gdm$^+$_Orientation2

C	2.556471	-2.864438	-0.355237
C	1.257505	-2.153223	-0.036409
O	0.394191	-2.718322	0.662353
O	1.111601	-0.981652	-0.519941
N	-1.644394	-0.880709	1.199283
C	-2.206102	-0.278365	0.147213
N	-3.383626	0.335718	0.259821
C	-3.997428	1.104506	-0.813372
N	-1.555981	-0.285052	-1.013973
N	2.506127	1.385199	-0.779340
C	1.871584	2.077529	0.159411
N	2.183192	3.353744	0.390017
N	0.918527	1.478480	0.869042
H	2.615695	-3.026826	-1.433288
H	-4.910129	1.548745	-0.426321
H	3.396609	-2.227123	-0.073815
H	2.622392	-3.818671	0.162607
H	-3.333314	1.906676	-1.140871
H	-4.255670	0.466743	-1.661789
H	-3.891044	0.225738	1.124156
H	-1.943656	0.169474	-1.824472
H	-0.573229	-0.585575	-1.018461
H	-2.141407	-0.899955	2.076361
H	-0.895297	-1.578937	1.041650
H	2.889839	3.820181	-0.155568
H	1.677806	3.898429	1.069971
H	2.241291	0.406513	-0.922670
H	3.212846	1.818494	-1.350967
H	0.456530	1.951506	1.628666
H	0.725287	0.496663	0.681923

Gdm$^+$_Orientation3

C	-4.788720	-0.762550	-0.334774
C	-3.392676	-0.212870	-0.093175
O	-2.945387	-0.234910	1.082269
O	-2.753037	0.208874	-1.093581
N	-0.376907	1.402625	-0.614149
C	0.298686	1.042734	0.467413
N	-0.266169	0.185727	1.330933
N	1.544384	1.480837	0.676203
C	2.247543	2.368847	-0.237169
C	2.472413	-1.370579	-0.266775
N	1.482699	-1.269418	-1.149221
N	3.704489	-0.998439	-0.601251
N	2.222031	-1.831394	0.954911
H	-5.291497	-0.202165	-1.122256
H	3.239755	2.548511	0.167695
H	-4.694945	-1.799168	-0.669188
H	-5.378482	-0.747938	0.580134
H	2.356554	1.907176	-1.221737
H	1.731311	3.326265	-0.334998
H	1.994359	1.227683	1.542745
H	0.066567	1.968532	-1.319807
H	-1.309206	0.961724	-0.814013
H	0.148467	0.103399	2.247849
H	-1.298236	0.024413	1.257257
H	1.650265	-0.946950	-2.089702
H	0.548950	-1.571148	-0.915155
H	1.278220	-2.047461	1.238719
H	2.952119	-1.900826	1.646706
H	4.469035	-1.097991	0.048080
H	3.926996	-0.728816	-1.546935

Gdm$^+$_Orientation4

C	3.654998	-1.751330	-0.245099
C	2.335245	-1.018082	-0.145427
O	1.798283	-0.573374	-1.195595
O	1.823741	-0.880051	1.001018
N	-1.040279	-0.712959	-0.895544
C	-1.640401	-1.188717	0.191405
N	-2.971071	-1.211213	0.265591
C	-3.847104	-0.763492	-0.807224
N	-0.902696	-1.661129	1.197881
N	0.377443	1.545691	1.197233
C	0.272426	2.390633	0.178174
N	-0.408754	3.530545	0.318658
N	0.853091	2.100833	-0.982017
H	3.976693	-1.848733	-1.279276
H	-4.873200	-0.936071	-0.494950
H	4.408121	-1.204916	0.325804
H	3.552238	-2.738056	0.209490
H	-3.718117	0.303729	-0.999859
H	-3.664104	-1.330815	-1.722035
H	-3.388188	-1.557389	1.115650
H	-1.584835	-0.350244	-1.661295
H	-0.018046	-0.722385	-0.994168
H	-1.351555	-1.965662	2.047122
H	0.105899	-1.486545	1.209911
H	0.769415	2.732542	-1.762491
H	1.270008	1.177028	-1.132309
H	0.939695	0.686208	1.127102
H	-0.070896	1.756361	2.074749
H	-0.805564	3.793931	1.206125
H	-0.528875	4.161974	-0.456538

Gdm$^+$_Orientation5

C	-2.310541	3.037794	-0.114424
C	-1.067401	2.173350	-0.153479
O	-1.102632	1.082193	0.505170
O	-0.071605	2.549647	-0.802900
N	1.860541	0.563810	-0.758717
C	2.194986	0.045191	0.419743
N	1.433067	0.323214	1.483394
N	3.272495	-0.728812	0.542630
C	4.199548	-0.999147	-0.546546
H	-2.231645	3.872588	-0.807269
H	5.012756	-1.601893	-0.152341
H	-3.185440	2.431209	-0.354105
H	-2.442689	3.418597	0.900585
H	3.712730	-1.556062	-1.350027
H	4.616222	-0.069621	-0.939076
H	3.440567	-1.163867	1.436552
H	2.438482	0.391223	-1.565881
H	1.146426	1.317688	-0.807564
H	1.630679	-0.123014	2.365422
H	0.482942	0.669705	1.308753
C	-2.102618	-1.923850	-0.125350
N	-2.537219	-3.159559	-0.374100
N	-0.940679	-1.506058	-0.621776
N	-2.814444	-1.093394	0.627826
H	-0.664726	-0.541875	-0.444459
H	-0.401410	-2.082991	-1.246341
H	-2.000890	-3.795970	-0.941657
H	-3.419424	-3.481921	-0.010358
H	-3.687622	-1.385206	1.035964
H	-2.453241	-0.147742	0.779177

Gdm$^+$_Orientation6

C	3.915163	-1.084325	-0.122616
C	2.401980	-1.154857	-0.096324
O	1.777711	-0.095940	0.234826
O	1.828565	-2.218899	-0.408276
N	-0.898534	-1.740889	-0.523440
C	-1.480462	-1.100595	0.482960
N	-0.714838	-0.636201	1.481525
N	-2.802390	-0.939541	0.516312
C	-3.706562	-1.493530	-0.480924
N	-0.814304	3.602271	-0.348775
C	-0.013055	2.542034	-0.242254
N	-0.176439	1.490543	-1.039095
N	0.957939	2.517238	0.665126
H	4.353659	-2.072416	-0.248891
H	-4.723969	-1.268808	-0.172985
H	4.216833	-0.446950	-0.957434
H	4.280937	-0.620881	0.794261
H	-3.533873	-1.045083	-1.461839
H	-3.594777	-2.577689	-0.544137
H	-3.189727	-0.387261	1.265570
H	-1.452895	-2.097202	-1.285346
H	0.119059	-1.953340	-0.494116
H	-1.140483	-0.056073	2.188470
H	0.269665	-0.463925	1.255852
H	-0.913418	1.462124	-1.724703
H	0.437039	0.687441	-0.906123
H	-0.687551	4.409426	0.240083
H	-1.540444	3.637346	-1.046214
H	1.564056	1.697811	0.711598
H	1.123250	3.307882	1.266929

Gdm$^+$ ion

C	-0.000225	0.000054	-0.000058
N	-1.296030	0.296591	-0.000700
N	0.904915	0.973813	0.000372
N	0.391099	-1.270362	-0.000115
H	1.891445	0.767953	-0.003276
H	0.628727	1.943090	0.002653
H	-1.612242	1.253324	-0.000885
H	-1.995962	-0.427975	0.003578
H	-0.279279	-2.022803	0.000023
H	1.368779	-1.514213	0.001357

Urea

Urea_Orientation1

C	4.175093	-0.283820	-0.317455
C	2.672649	-0.381931	-0.131690
O	2.220107	-0.999844	0.863706
O	1.943409	0.180131	-0.998766
N	-0.703254	-0.720271	-1.100350
C	-1.225480	-1.359055	-0.056022
N	-0.409080	-1.972947	0.806713
N	-2.547868	-1.421063	0.099603
C	-3.488510	-0.726760	-0.768786
N	0.049974	2.376917	-0.611226
C	-0.710141	1.946279	0.440159
N	-0.036124	1.226910	1.390292
O	-1.898792	2.238020	0.564044
H	4.447617	-0.739328	-1.271288
H	-4.490603	-0.910356	-0.391340
H	4.464232	0.767699	-0.363135
H	4.707370	-0.778978	0.491827
H	-3.298941	0.349773	-0.751035
H	-3.429943	-1.104982	-1.791510
H	-2.906285	-1.926348	0.895167
H	-1.309391	-0.195415	-1.711423
H	0.301441	-0.471257	-1.101921
H	-0.800782	-2.339606	1.660773
H	0.584578	-1.691146	0.823430
H	-0.475791	2.752988	-1.385384
H	0.880984	1.840886	-0.848085
H	0.811724	0.728648	1.142457
H	-0.621217	0.775847	2.077136

Urea_Orientation2

C	4.131547	-0.429146	-0.117575
C	2.636768	-0.679038	-0.047603
O	1.900720	0.306654	0.256865
O	2.197635	-1.826561	-0.290824
N	-0.548537	-1.823091	-0.415974
C	-1.229243	-1.137792	0.492736
N	-0.549962	-0.459464	1.430604
N	-2.562453	-1.145007	0.495735
C	-3.362471	-1.925599	-0.435954
N	-0.365240	1.436300	-1.270032
C	-0.705904	2.356452	-0.315617
O	-1.819139	2.878048	-0.265835
N	0.307818	2.701242	0.530516
H	4.674163	-1.335876	-0.376239
H	-4.408367	-1.793070	-0.173940
H	4.328923	0.344282	-0.862389
H	4.479146	-0.051114	0.845534
H	-3.216196	-1.582128	-1.462563
H	-3.118049	-2.987209	-0.362549
H	-3.036488	-0.571230	1.175921
H	-1.034227	-2.321974	-1.143995
H	0.493500	-1.850603	-0.381334
H	-1.063902	0.161027	2.038131
H	0.405850	-0.176506	1.175944
H	-1.136401	1.032133	-1.778563
H	0.435200	0.839649	-1.084381
H	1.118324	2.095469	0.604264
H	0.049215	3.252895	1.332641

Urea_Orientation3

C	4.198809	-0.799390	-0.582441
N	3.265495	-0.597486	0.515740
C	2.157656	0.138925	0.415734
N	1.394485	0.369337	1.488934
N	1.801314	0.671689	-0.748456
O	-0.275045	2.482453	-0.817207
C	-1.234570	2.075079	-0.125384
C	-2.563959	2.801808	-0.193888
O	-1.172863	1.064649	0.640228
N	-2.670293	-1.386543	0.751510
C	-1.999149	-2.140931	-0.163260
N	-0.795422	-1.621302	-0.559165
O	-2.407577	-3.232834	-0.558338
H	-2.511956	3.666889	-0.851418
H	5.041150	-1.373054	-0.206331
H	-3.325748	2.108638	-0.557681
H	-2.858858	3.113597	0.809402
H	3.735162	-1.358875	-1.397905
H	4.570218	0.157252	-0.954978
H	3.458250	-1.041917	1.399901
H	2.362237	0.511336	-1.569451
H	1.028322	1.368582	-0.791730
H	1.617474	-0.087538	2.359188
H	0.425696	0.679936	1.324201
H	-0.624920	-0.635001	-0.397563
H	-0.380342	-2.042944	-1.374659
H	-3.613850	-1.668857	0.960316
H	-2.400729	-0.414992	0.886731

Urea_Orientation4

C	1.831548	2.395407	-0.079087
C	0.540024	1.598136	-0.010149
O	0.640486	0.334819	-0.081022
O	-0.542484	2.214882	0.087363
N	-2.884430	0.778151	0.169149
C	-2.866387	-0.533229	-0.041851
N	-1.697833	-1.148133	-0.215120
N	-4.008741	-1.227102	-0.080006
C	-5.322566	-0.623081	0.078706
N	3.151664	-0.760153	-1.134515
C	3.790831	-0.977038	0.052787
O	4.994418	-1.223641	0.127374
N	2.969396	-0.967065	1.144298
H	1.687695	3.407197	0.294670
H	-6.067602	-1.405061	-0.039564
H	2.621736	1.892477	0.480414
H	2.148411	2.448214	-1.124356
H	-5.438750	-0.181002	1.070805
H	-5.496369	0.136671	-0.686210
H	-3.949159	-2.226525	-0.194383
H	-3.756786	1.252722	0.334057
H	-2.000305	1.325370	0.148539
H	-1.673568	-2.131774	-0.430151
H	-0.812606	-0.611682	-0.167894
H	2.054352	-0.536189	1.050258
H	3.422267	-0.950155	2.043602
H	3.741467	-0.584410	-1.931768
H	2.228786	-0.335405	-1.106819

Urea_Orientation5

C	2.649843	-2.688258	-0.271550
C	1.297823	-2.037755	-0.048673
O	1.042311	-0.999834	-0.735190
O	0.505964	-2.534829	0.781010
N	-1.603462	-0.789248	1.241485
C	-2.223926	-0.269820	0.180308
N	-3.397119	0.351322	0.313153
C	-4.078737	1.029714	-0.779405
N	-1.643576	-0.372568	-1.012885
N	2.513854	1.470414	-0.882574
C	1.973176	2.156368	0.162903
O	2.434691	3.220760	0.574631
N	0.830583	1.604936	0.678453
H	2.699742	-3.063092	-1.295920
H	-4.957830	1.520462	-0.371223
H	3.434628	-1.937775	-0.159121
H	2.814940	-3.507120	0.425287
H	-3.433344	1.790172	-1.223004
H	-4.400993	0.322908	-1.547241
H	-3.843469	0.326072	1.216641
H	-2.072685	0.038412	-1.825784
H	-0.652223	-0.660253	-1.049067
H	-2.045081	-0.737215	2.146080
H	-0.823639	-1.460381	1.102002
H	0.528664	1.968531	1.568286
H	0.636020	0.630716	0.476575
H	2.219755	0.511615	-1.053711
H	3.420735	1.772679	-1.198331

Urea_Orientation6

C	-1.973895	2.404104	-0.175289
C	-0.606037	1.750403	-0.079332
O	0.406933	2.476359	-0.003009
O	-0.576575	0.480449	-0.104968
N	1.884783	-0.749825	-0.259796
C	2.971831	-0.058883	0.066384
N	4.167829	-0.654784	0.101998
C	4.373723	-2.068238	-0.173035
N	2.852542	1.232545	0.369949
N	-2.941726	-0.934051	-1.109365
C	-3.549922	-1.188065	0.087129
N	-2.737361	-1.036339	1.174659
O	-4.712736	-1.581855	0.174218
H	-2.304964	2.362640	-1.216616
H	5.422224	-2.294055	0.001966
H	-2.700790	1.853612	0.424018
H	-1.933696	3.445033	0.139403
H	3.772454	-2.684930	0.497913
H	4.135034	-2.311168	-1.211022
H	4.974184	-0.078824	0.285541
H	1.958432	-1.715626	-0.534207
H	0.949521	-0.299535	-0.218541
H	3.666898	1.763416	0.633893
H	1.945122	1.716721	0.240382
H	-3.189278	-1.046387	2.074496
H	-1.883325	-0.498116	1.062300
H	-2.079895	-0.395546	-1.098150
H	-3.549574	-0.855619	-1.908558

Urea_Orientation7

C	4.184959	0.294118	-0.151008
C	2.773738	-0.263667	-0.124054
O	1.825217	0.536364	-0.380521
O	2.608383	-1.469054	0.173772
N	-0.050071	-1.977259	0.748930
C	-0.977427	-1.468364	-0.056367
N	-0.583652	-0.736454	-1.104084
N	-2.273752	-1.694186	0.159335
C	-3.338888	-1.084289	-0.626857
N	-0.300664	2.485241	-0.621811
C	-1.097378	1.968112	0.359261
N	-0.423486	1.341410	1.372995
O	-2.320014	2.108135	0.364845
H	4.292716	1.023377	-0.953261
H	-4.288079	-1.401694	-0.203331
H	4.365717	0.809707	0.795889
H	4.918644	-0.502718	-0.257876
H	-3.276497	0.005412	-0.570933
H	-3.298501	-1.415109	-1.666954
H	-2.524335	-2.323433	0.906373
H	-1.278547	-0.265066	-1.662357
H	0.345434	-0.298172	-1.030504
H	-0.324730	-2.491008	1.570918
H	0.957836	-1.826786	0.545175
H	-0.777149	2.803542	-1.450820
H	0.635905	2.110526	-0.732904
H	0.493694	0.963895	1.155019
H	-0.999435	0.797259	1.997394

Urea_Orientation8

C	-4.931068	-1.434352	-0.107548
C	-3.575114	-0.746828	-0.035460
O	-3.574022	0.513323	-0.017290
O	-2.544515	-1.464893	-0.016402

N	-1.173321	1.814374	-0.096054
C	-0.035830	1.135392	0.023914
N	1.138507	1.769199	0.074465
C	1.260819	3.215204	0.002607
N	-0.079184	-0.197820	0.093084
C	3.353788	-1.102087	-0.013912
N	2.713729	-1.474556	1.145720
N	3.825547	-2.097877	-0.792762
O	3.442980	0.085737	-0.333137
H	-5.617944	-0.983705	0.609659
H	2.311842	3.468297	0.118510
H	-5.349156	-1.278970	-1.105160
H	-4.843578	-2.503219	0.077671
H	0.915928	3.605687	-0.958918
H	0.702884	3.693543	0.810336
H	1.985089	1.204814	-0.006278
H	-1.150970	2.807350	-0.260094
H	-2.091585	1.317971	-0.070990
H	0.741378	-0.707220	0.395180
H	-0.996531	-0.680955	0.069193
H	4.150025	-1.857901	-1.715528
H	3.678269	-3.070271	-0.576491
H	2.834881	-2.417072	1.489019
H	2.721404	-0.768908	1.869747

Urea_Orientation9

C	-5.076216	-1.551208	-0.064573
C	-3.735036	-0.832655	-0.013590
O	-2.689314	-1.523884	-0.096302
O	-3.761582	0.423349	0.086490
N	-1.392574	1.778060	-0.132623
C	-0.243790	1.127225	0.040666
N	-0.257857	-0.194686	0.210223
N	0.920339	1.782927	0.048534
C	1.027144	3.223324	-0.097978
N	4.805358	-0.388226	-0.200696
C	3.658797	-1.070801	0.044697
N	3.712193	-2.419482	-0.090189
O	2.616112	-0.492352	0.376730
H	-5.770686	-1.109250	0.650103
H	2.080321	3.488832	-0.052996
H	-5.501357	-1.420332	-1.063094
H	-4.961276	-2.616023	0.129910
H	0.630801	3.557267	-1.060235
H	0.507243	3.745035	0.709433
H	1.757127	1.216675	0.161089
H	-1.393782	2.781362	-0.213251
H	-2.298913	1.267721	-0.055906
H	0.633391	-0.672577	0.283099
H	-1.145060	-0.715150	0.103520
H	4.493820	-2.868910	-0.540253
H	2.833243	-2.911820	-0.091009
H	4.826040	0.580240	0.076471
H	5.689761	-0.865434	-0.274291

Urea_Orientation10

C	0.907719	3.998861	-0.166476
C	0.128511	2.715071	0.069047
O	0.786322	1.714463	0.473501
O	-1.106143	2.712102	-0.149359
N	-2.647442	0.402192	-0.103651
C	-1.966952	-0.714837	0.144509
N	-0.700962	-0.627062	0.537941
N	-2.557736	-1.908323	0.016928
C	-3.940594	-2.083256	-0.396635
H	0.249702	4.817957	-0.449137
H	-4.141358	-3.149505	-0.454689
H	1.460203	4.260905	0.737294
H	1.640279	3.829656	-0.958644
H	-4.631678	-1.639442	0.323874
H	-4.108825	-1.648157	-1.384003
H	-2.027389	-2.720982	0.289149
H	-3.615993	0.366340	-0.374710
H	-2.139000	1.303858	-0.105766
H	-0.080608	-1.431845	0.559191
H	-0.231221	0.294856	0.549825
O	1.770686	-2.046682	0.582358
C	2.732814	-1.550418	-0.012213
N	3.829994	-2.305119	-0.329747
N	2.784281	-0.245245	-0.370002
H	2.077449	0.404579	-0.030934
H	3.636200	0.148667	-0.736009
H	4.479901	-1.980341	-1.028896
H	3.699487	-3.303230	-0.278217

Urea_Orientation11

C	3.689573	-2.056225	-0.077977
C	2.701360	-0.911000	0.076724
O	3.073435	0.249451	-0.216702
O	1.548674	-1.207435	0.503626
N	-0.144064	0.981147	0.446265
C	0.146168	2.188258	-0.014764
N	1.425748	2.518643	-0.220845
N	-0.829482	3.075127	-0.234610
C	-2.229289	2.789229	0.041383
H	3.828207	-2.544153	0.888753
H	-2.811850	3.666744	-0.225303
H	3.275699	-2.799250	-0.762396
H	4.648958	-1.705442	-0.452809
H	-2.578250	1.942020	-0.552719
H	-2.382090	2.571533	1.100979
H	-0.573587	3.996510	-0.552430
H	-1.100179	0.629138	0.487413
H	0.594874	0.258960	0.507783
H	1.650143	3.396759	-0.660249
H	2.118704	1.755104	-0.223523
O	-2.427542	-0.685965	0.487020
C	-2.276155	-1.809037	-0.008096
N	-3.354312	-2.595685	-0.302439
N	-1.059327	-2.340538	-0.273041
H	-3.253847	-3.385408	-0.920752
H	-4.246314	-2.127026	-0.319000
H	-0.210902	-1.882485	0.051408
H	-0.975984	-3.299631	-0.569629

Urea_Orientation12

C	5.017403	-1.210354	0.105980
C	3.628186	-0.594872	0.023092
O	3.554602	0.662845	0.016626
O	2.639942	-1.370849	-0.008134
N	1.075579	1.796152	0.134983
C	-0.007557	1.058851	-0.094012
N	-1.219657	1.622572	-0.110906
C	-1.444596	3.044603	0.086550
N	0.132335	-0.247607	-0.314920
N	-3.822803	-0.119851	-0.360135
C	-3.316319	-1.293857	0.160338
N	-2.535540	-2.018609	-0.710462
O	-3.442449	-1.594493	1.334337
H	5.730332	-0.623380	-0.472500
H	-2.511593	3.229987	-0.011437
H	5.339712	-1.192170	1.150525
H	5.010392	-2.243778	-0.236298
H	-1.129746	3.365455	1.082570
H	-0.922106	3.633855	-0.670389
H	-2.031089	1.026133	-0.234306
H	0.984149	2.778975	0.332217
H	2.025966	1.363997	0.098496
H	-0.679948	-0.824642	-0.496252
H	1.066234	-0.688107	-0.210172
H	-2.315891	-2.952961	-0.394730
H	-2.706381	-1.939936	-1.703505
H	-4.536997	0.306740	0.214138
H	-4.011895	-0.075018	-1.352583

Urea molecule

C	0.000000	0.000000	0.133907
N	0.000000	1.156243	-0.597847
O	0.000000	0.000000	1.359804
N	0.000000	-1.156243	-0.597847
H	0.277295	-1.137135	-1.567245
H	0.233393	-1.994502	-0.088763
H	-0.277295	1.137135	-1.567245
H	-0.233393	1.994502	-0.088763

Guanidinium Chloride

GdmCl_Orientation1

C	4.153513	-1.134332	-0.170179
C	2.646432	-0.964450	-0.158600
O	2.030982	-1.265208	0.910055
O	2.082584	-0.512471	-1.182328
N	-0.668289	-0.612729	-1.115314
C	-1.199869	-1.662500	-0.502549
N	-0.388760	-2.513301	0.140983
N	-2.513522	-1.886898	-0.550587
C	-3.444508	-1.050860	-1.293375
N	0.536134	1.135547	1.267283
C	-0.767933	1.030776	1.504105
N	-1.598562	1.983514	1.091098
N	-1.235926	-0.029771	2.169836
Cl	0.360086	3.466823	-1.013775
H	4.535004	-1.177545	-1.189055
H	-4.432503	-1.495386	-1.211391
H	4.598972	-0.272178	0.334293
H	4.438720	-2.028592	0.384249
H	-3.484313	-0.039052	-0.882346
H	-3.169810	-1.010499	-2.349302
H	-2.882940	-2.649103	-0.003743
H	-1.255562	0.054806	-1.589469
H	0.366557	-0.502882	-1.148627
H	-0.799753	-3.259602	0.680301
H	0.531507	-2.163519	0.439863
H	-2.586504	1.928492	1.280520
H	-1.248427	2.679347	0.433512
H	0.812607	1.854109	0.598867
H	1.102631	0.280265	1.294241
H	-0.592147	-0.669917	2.608921
H	-2.207379	-0.089630	2.432024

GdmCl_Orientation2

C	-4.585569	0.215641	-0.611609
C	-3.089538	0.119430	-0.387361
O	-2.689059	-0.579741	0.586963
O	-2.312674	0.735173	-1.162059
N	-0.210438	-1.845194	-0.034925
C	0.677043	-1.250506	-0.832252
N	1.979958	-1.496100	-0.697945
C	2.527721	-2.315262	0.372410
N	0.251424	-0.446507	-1.817235
C	0.292601	0.850739	1.634750
N	1.577085	0.823563	1.992013
N	-0.053499	1.483117	0.517910
N	-0.646790	0.289216	2.402389
Cl	2.812666	1.670655	-1.057526
H	-5.006938	-0.788540	-0.675610
H	3.606868	-2.347925	0.249826
H	-5.041691	0.706959	0.250159
H	-4.816167	0.775641	-1.514758
H	2.298941	-1.896135	1.356423
H	2.145917	-3.335321	0.307607
H	2.598932	-0.833247	-1.153170
H	0.119178	-2.400745	0.739522
H	-1.165265	-1.471347	0.048345
H	0.943244	0.181401	-2.210855
H	-0.696699	-0.067967	-1.732326
H	-0.354509	-0.304391	3.163913
H	-1.532380	0.053201	1.946500

H	-0.964523	1.311168	0.086322
H	0.701637	1.775953	-0.101083
H	2.275230	1.208636	1.363317
H	1.869027	0.411153	2.863520

GdmCl_Orientation3

C	-4.578124	-0.641903	0.513803
C	-3.199527	-0.040264	0.314260
O	-3.073181	1.203688	0.294805
O	-2.231174	-0.851474	0.178401
N	-0.495006	2.144919	-0.214093
C	0.452833	1.450548	0.406128
N	1.745285	1.703943	0.211339
C	2.229752	2.733820	-0.693146
N	0.088688	0.500559	1.285307
C	0.596580	-1.419350	-1.271701
N	0.281766	-2.207263	-0.241006
N	-0.382295	-0.835842	-1.960035
N	1.873186	-1.292455	-1.641338
Cl	2.997976	-1.175171	1.425531
H	-5.334118	0.130821	0.636334
H	3.311333	2.783797	-0.599083
H	-4.824216	-1.266109	-0.347440
H	-4.563924	-1.289227	1.392533
H	1.979648	2.504349	-1.732664
H	1.815727	3.706971	-0.422688
H	2.400469	1.028693	0.598277
H	-0.256784	2.784121	-0.955272
H	-1.483083	1.868967	-0.069958
H	0.834449	-0.102906	1.621899
H	-0.809130	0.046179	1.096475
H	2.584861	-1.511483	-0.949656
H	2.117156	-0.609888	-2.342956
H	-0.159741	-0.169813	-2.683659
H	-1.287490	-0.767370	-1.492601
H	-0.666420	-2.135738	0.117589
H	1.020057	-2.435301	0.415920

GdmCl_Orientation4

C	0.048019	3.881238	-0.099743
C	0.828055	2.582307	-0.101713
O	0.233689	1.552766	0.353907
O	2.000850	2.566438	-0.528845
N	2.916330	-0.045503	-0.555875
C	2.767689	-0.776783	0.544365
N	1.994442	-0.306612	1.529779
N	3.386566	-1.950788	0.669555
C	4.315779	-2.478262	-0.319112
H	0.590846	4.669433	-0.616891
H	4.719968	-3.410779	0.064474
H	-0.924558	3.723641	-0.568863
H	-0.132447	4.181320	0.934838
H	3.810872	-2.682346	-1.265802
H	5.141754	-1.783389	-0.482389
H	3.189366	-2.503923	1.489353
H	3.517660	-0.370128	-1.296137
H	2.586353	0.940780	-0.573171
H	1.798322	-0.893667	2.325493
H	1.320657	0.429043	1.286488
C	-1.778836	-0.801762	-0.611764
N	-2.208162	0.212704	0.129262
N	-2.626456	-1.765799	-0.970101
N	-0.498303	-0.842613	-0.985465
H	-2.308527	-2.571887	-1.482963
H	-3.587537	-1.722932	-0.636719
H	-3.179171	0.222580	0.429295
H	-1.543679	0.945711	0.379733
H	0.097493	-0.057159	-0.734195
H	-0.163820	-1.552058	-1.616543
Cl	-5.332060	-0.709884	0.504190

GdmCl_Orientation5

C	-4.608753	0.010769	-0.410148
C	-3.132250	-0.308107	-0.275100
O	-2.698718	-1.403095	-0.694450
O	-2.398513	0.572170	0.276018
N	-0.338015	-0.726769	1.771134
C	0.525547	-1.241142	0.882992
N	0.049326	-1.821556	-0.218524
N	1.836191	-1.221210	1.118109
C	2.435343	-0.552619	2.263012
H	-5.039086	0.122764	0.587199
H	3.514803	-0.643884	2.175003
H	-4.727876	0.965079	-0.925477
H	-5.136317	-0.772986	-0.949514
H	2.178621	0.510022	2.290621
H	2.125387	-1.029569	3.194317
H	2.430555	-1.439087	0.324260
H	0.031383	-0.206931	2.552855
H	-1.226570	-0.383308	1.389969
H	0.700830	-1.995880	-0.973974
H	-0.954275	-1.713058	-0.440992
C	0.552620	1.896565	-0.186799
N	0.050137	1.114768	-1.139558
N	1.868156	2.099011	-0.128923
N	-0.282352	2.497915	0.662896
H	2.274897	2.709788	0.561312
H	2.477104	1.531430	-0.711782
H	0.700100	0.538386	-1.669848
H	-0.902636	0.785435	-0.993620
H	-1.243632	2.167283	0.688070
H	0.075036	3.004574	1.457342
Cl	2.740022	-0.584151	-1.959292

GdmCl_Orientation6

C	3.661170	-1.758566	-0.833168
C	2.199473	-1.497194	-0.521060
O	1.884969	-1.355256	0.703118
O	1.385829	-1.404998	-1.465747
N	-1.256886	-0.903022	-0.777382
C	-1.678193	-1.573380	0.290669
N	-0.820742	-2.378115	0.934030
N	-2.945426	-1.478784	0.689860
C	-3.973730	-0.778686	-0.070565
H	3.785106	-2.129889	-1.848406
H	-4.931187	-0.970089	0.406481
H	4.208471	-0.816736	-0.735133
H	4.080908	-2.462461	-0.114904
H	-3.789768	0.297427	-0.084867
H	-4.006154	-1.156487	-1.094184
H	-3.201627	-1.921766	1.558539
H	-1.756100	-0.070530	-1.075008
H	-0.273941	-1.032096	-1.080879
H	-1.144410	-2.913769	1.724407
H	0.181137	-2.173315	0.870930
C	1.458334	1.928041	0.642392
N	1.170256	3.160748	0.224631
N	0.474388	1.070036	0.893046
N	2.718412	1.552549	0.864477
H	0.745241	0.085936	0.962305
H	-0.451277	1.313658	0.543429
H	0.223684	3.349112	-0.093285
H	1.903787	3.805582	-0.022354
H	3.492655	2.158802	0.647041
H	2.897847	0.588401	1.119862
Cl	-1.971358	2.414416	-0.731364

GdmCl_Orientation7

C	-4.619029	-0.015197	-0.375253
C	-3.134690	-0.310804	-0.281208
O	-2.697147	-1.403013	-0.703385
O	-2.399636	0.582930	0.246967
N	-0.341103	-0.704467	1.753303
C	0.524394	-1.234763	0.877258
N	0.052706	-1.815734	-0.225937
N	1.832833	-1.229406	1.126038
C	2.428342	-0.559122	2.271788
H	-5.028856	0.042410	0.635632
H	3.507241	-0.666411	2.197235
H	-4.769613	0.957953	-0.844544
H	-5.142926	-0.787194	-0.935134
H	2.185966	0.506982	2.287005
H	2.101250	-1.023373	3.203622
H	2.432450	-1.460550	0.340292
H	0.024697	-0.191124	2.540759
H	-1.225942	-0.358412	1.365959
H	0.708659	-1.997738	-0.975680
H	-0.949225	-1.705520	-0.454569
C	0.551806	1.898237	-0.192348
N	0.057085	1.120166	-1.152354
N	1.868186	2.086825	-0.111512
N	-0.291161	2.511086	0.640987
H	2.268666	2.687577	0.591121
H	2.481201	1.509954	-0.681266
H	0.710603	0.537693	-1.671604
H	-0.899024	0.795513	-1.016484
H	-1.255066	2.187785	0.653663
H	0.058562	3.017299	1.439003
Cl	2.753580	-0.584798	-1.943457

GdmCl_Orientation8

C	4.913123	0.203557	-0.102225
C	3.486087	-0.306004	0.024013
O	2.970440	-0.329949	1.170880
O	2.895913	-0.645453	-1.035870
N	0.332999	-1.531833	-0.849276
C	-0.313717	-1.459691	0.308064
N	0.320776	-0.993755	1.380850
N	-1.593701	-1.848011	0.396613
C	-2.337481	-2.421873	-0.712566
C	-2.779561	0.945793	0.065590
N	-2.203140	1.029328	-1.130906
N	-4.003269	0.428979	0.190513
N	-2.105810	1.347288	1.137115
Cl	0.488608	2.600968	-0.335956
H	5.436516	-0.309090	-0.908536
H	-3.357537	-2.594123	-0.378731
H	4.872994	1.268040	-0.349600
H	5.452921	0.089629	0.836409
H	-2.365717	-1.728236	-1.556099
H	-1.908155	-3.373444	-1.035984
H	-2.013286	-1.866806	1.313234
H	-0.129355	-1.903103	-1.662750
H	1.318550	-1.186201	-0.925989
H	-0.178960	-0.881327	2.248067
H	1.323241	-0.715879	1.316809
H	-2.734248	0.856090	-1.969869
H	-1.297899	1.496748	-1.199628
H	-1.180418	1.757169	1.010744
H	-2.502868	1.272947	2.060040
H	-4.469448	0.419294	1.083936
H	-4.549180	0.190408	-0.622497

GdmCl_Orientation9

C	-4.451022	0.853201	-0.757193
C	-2.999699	0.537825	-0.456460
O	-2.122421	0.796036	-1.318715
O	-2.735471	0.016541	0.665719
N	0.511091	1.663499	-0.532825
C	0.781967	1.373312	0.744688
N	2.009481	1.574032	1.220606
C	3.071649	2.222015	0.460622
N	-0.185546	0.926405	1.544106
N	-1.116547	-2.254707	1.204621
C	-0.064614	-2.054316	0.407248
N	1.131088	-2.563089	0.708197
N	-0.213299	-1.395938	-0.738401
H	-5.038997	-0.063465	-0.683802

H	3.898121	2.412561	1.140215
H	-4.830164	1.545961	-0.003704
H	-4.565008	1.287418	-1.747986
H	3.416761	1.577275	-0.349992
H	2.718570	3.173967	0.060124
H	2.202846	1.278763	2.165159
H	1.276569	1.597823	-1.191865
H	-0.421844	1.422898	-0.884493
H	-0.023288	0.852033	2.536300
H	-1.106957	0.644958	1.182057
H	0.637929	-1.147131	-1.243331
H	-1.042286	-0.829170	-0.909035
H	-1.918403	-1.635185	1.078274
H	-0.969625	-2.654737	2.118444
H	1.290016	-3.012144	1.595729
H	1.929765	-2.294014	0.139254
Cl	2.848563	-0.817769	-1.530290

GdmCl_Orientation10

C	4.420700	0.348807	-0.996202
C	3.007862	0.216666	-0.464681
O	2.068718	0.696969	-1.154537
O	2.827976	-0.387396	0.629000
N	-0.418436	-0.751799	-0.894604
C	-0.429876	-1.842701	-0.134825
N	-1.579288	-2.458739	0.134828
C	-2.859413	-2.039839	-0.420263
N	0.728414	-2.340893	0.318496
N	0.015159	2.034394	0.348983
C	-0.351708	1.294378	1.398781
N	0.553994	0.572771	2.053429
N	-1.619441	1.346865	1.821962
H	4.556004	1.319840	-1.471449
H	-3.611164	-2.759846	-0.108637
H	5.153685	0.204374	-0.205136
H	4.571427	-0.419819	-1.758709
H	-3.140621	-1.047869	-0.060591
H	-2.814191	-2.024863	-1.511237
H	-1.559745	-3.239849	0.771938
H	-1.272854	-0.228535	-1.081156
H	0.474611	-0.276889	-1.069646
H	0.710360	-3.160137	0.906007
H	1.535825	-1.715939	0.407814
H	-1.928562	0.708272	2.538914
H	-2.318121	1.666064	1.156404
H	-0.740862	2.346035	-0.256137
H	0.875743	1.763821	-0.133507
H	1.455049	0.351111	1.611027
H	0.253624	-0.024157	2.809038
Cl	-2.815410	1.610573	-1.242304

GdmCl_Orientation11

C	1.483788	3.951052	-0.453189
C	1.740981	2.482591	-0.181976
O	0.753155	1.690030	-0.311031
O	2.882422	2.107816	0.155666
N	2.794134	-0.611493	0.759200
C	2.221114	-1.428107	-0.126326
N	1.489311	-0.898992	-1.106720
N	2.369751	-2.749497	-0.033784
C	1.706190	-3.697029	-0.917466
N	-1.858165	0.712618	-0.081015
C	-1.642029	-0.109640	0.939057
N	-2.606687	-0.939012	1.336922
N	-0.458536	-0.092718	1.554606
Cl	-4.980456	-0.049481	-0.698640
H	1.043638	4.066267	-1.444919
H	1.994418	-4.698729	-0.611857
H	0.757178	4.323149	0.272143
H	2.401181	4.531407	-0.382386
H	0.620543	-3.608779	-0.838697
H	2.015999	-3.549360	-1.954209
H	2.984132	-3.105919	0.681825
H	0.978588	-1.495430	-1.737515
H	1.205058	0.083753	-1.011279
H	3.400054	-0.999799	1.465127
H	2.855704	0.404458	0.556954
H	-0.231597	-0.776554	2.258183
H	0.273161	0.497917	1.165603
H	-1.102490	1.323391	-0.385967
H	-2.776153	0.720015	-0.517759
H	-3.515730	-0.888086	0.880743
H	-2.489468	-1.508835	2.158742

GdmCl_Orientation12

C	1.849417	-3.733425	-0.485166
C	1.804689	-2.218442	-0.491865
O	1.204911	-1.655327	0.481405
O	2.353106	-1.590076	-1.419262
N	-1.372518	-2.163014	1.405638
C	-2.013975	-1.190738	0.760488
N	-3.335234	-1.049526	0.860680
N	-1.321856	-0.338817	0.008674
N	1.556086	1.075779	-1.256549
C	1.789992	1.699077	-0.097971
N	2.043331	0.962114	0.981094
N	1.751989	3.028763	-0.017413
C	1.882983	3.763070	1.232829
Cl	-3.754843	1.551384	-1.060838
H	2.573970	-4.056511	0.267193
H	1.720350	4.816173	1.022006
H	0.875677	-4.134442	-0.198685
H	2.148201	-4.122002	-1.456949
H	1.130754	3.434468	1.952552
H	2.881075	3.643554	1.659953
H	1.646620	3.550345	-0.874121
H	2.204411	1.399173	1.873920
H	1.848057	-0.047778	0.934345
H	1.395130	1.627401	-2.084825
H	1.863710	0.092075	-1.369434
H	-1.817493	0.392381	-0.494953
H	-0.324177	-0.488816	-0.100466
H	-0.362591	-2.248511	1.267258
H	-1.878257	-2.842213	1.950031
H	-3.879979	-1.660709	1.446526
H	-3.788473	-0.289245	0.357995

GdmCl_Orientation13

C	-2.854219	-3.330029	-0.671810
C	-2.068182	-2.074431	-0.358352
O	-2.296618	-1.494779	0.739889
O	-1.210143	-1.667703	-1.186996
N	0.150162	-0.426517	1.777362
C	1.306773	-0.495597	1.121161
N	1.378553	-1.133414	-0.043273
N	2.407194	0.064057	1.626558
N	-2.532031	1.332672	0.604526
C	-1.569107	1.894164	-0.130908
N	-1.314782	3.198871	-0.027196
C	-0.329084	3.893838	-0.842188
N	-0.885250	1.147601	-0.992115
H	-2.717562	-3.633541	-1.707279
H	-0.365434	4.948594	-0.584597
H	-2.505802	-4.129416	-0.013627
H	-3.911030	-3.166753	-0.459709
H	0.678929	3.523267	-0.642288
H	-0.558966	3.788184	-1.904355
H	-1.835800	3.728971	0.653819
H	-0.126397	1.546681	-1.520973
H	-1.057966	0.136924	-1.080816
H	-3.004886	1.879495	1.306620
H	-2.575443	0.311028	0.674188
H	2.266189	-1.123613	-0.540250
H	0.523408	-1.439570	-0.508905
H	-0.704403	-0.862035	1.412722
H	0.098942	0.063286	2.656256
H	2.396079	0.507609	2.530284
H	3.273525	0.016657	1.094209
Cl	4.519806	-0.553322	-0.771582

GdmCl_Orientation14

C	-2.988091	-3.420657	0.173707
N	-2.090570	-2.630226	-0.656220
C	-2.008443	-1.301239	-0.594368
N	-2.700045	-0.618936	0.310927
N	-1.238825	-0.626609	-1.458212
O	-2.774965	2.138311	0.119548
C	-1.610109	2.566735	-0.020872
O	-0.598068	1.808971	-0.158464
C	-1.358603	4.060939	-0.019728
N	1.951021	0.661565	0.012326
C	1.644343	-0.284260	0.893718
N	0.435266	-0.286183	1.455330
N	2.547948	-1.210916	1.209744
Cl	5.020893	-0.257145	-0.668192
H	-2.292713	4.618150	0.000176
H	-2.922898	-4.454761	-0.152479
H	-0.763206	4.316183	0.859868
H	-0.775675	4.335403	-0.900221
H	-2.701303	-3.369977	1.226406
H	-4.020067	-3.084911	0.054099
H	-1.496437	-3.109474	-1.315086
H	-3.291313	-1.104698	0.966001
H	-2.752411	0.418983	0.256977
H	-0.644324	-1.137212	-2.092101
H	-0.958899	0.321681	-1.186905
H	-0.242872	0.403159	1.137105
H	0.159038	-1.012680	2.095368
H	2.331387	-1.944481	1.864531
H	3.464319	-1.175903	0.767250
H	2.878265	0.661353	-0.404020
H	1.250058	1.362428	-0.218376

GdmCl_Orientation15

C	4.601514	0.042884	-0.680895
C	3.150485	-0.344094	-0.475139
O	2.741084	-1.444666	-0.902437
O	2.411495	0.490138	0.136677
N	0.049044	-1.881416	-0.382802
C	-0.421546	-1.501641	0.799387
N	-1.667720	-1.797948	1.164600
C	-2.576187	-2.593093	0.349768
N	0.392313	-0.845670	1.637322
N	0.690302	2.538064	1.031551
C	-0.366344	2.128256	0.327679
N	-0.181830	1.319408	-0.712155
N	-1.595240	2.548279	0.623428
H	5.143586	-0.728568	-1.223383
H	-3.472345	-2.780812	0.935353
H	4.647513	0.984992	-1.229987
H	5.068529	0.208263	0.291819
H	-2.856791	-2.051325	-0.556307
H	-2.120644	-3.553443	0.100065
H	-2.010215	-1.406763	2.028500
H	-0.561625	-2.321873	-1.052070
H	1.050027	-1.734725	-0.618486
H	0.024185	-0.498611	2.509509
H	1.211251	-0.375423	1.236069
H	0.727465	0.869753	-0.791203
H	-1.004897	0.913901	-1.155598
H	-2.381370	2.151246	0.113244
H	-1.762923	3.147160	1.415334
H	0.566442	3.087658	1.866444
H	1.588415	2.094929	0.853769
Cl	-3.247814	0.592410	-1.415023

GdmCl

N	-0.585681	1.145407	-0.004403

C	-1.258936	0.000001	-0.000528
N	-0.585673	-1.145398	-0.004331
N	-2.592374	-0.000005	0.013135
Cl	2.434341	-0.000001	0.001008
H	-1.064545	-2.031008	0.005762
H	0.433411	-1.115991	-0.000962
H	0.433401	1.116000	-0.001001
H	-1.064549	2.031009	0.006194
H	-3.110913	0.862770	-0.027536
H	-3.110899	-0.862801	-0.027243

Trimethyl N-oxide

TMAO_Orientation1

C	3.337496	2.103835	0.237409
C	2.688999	0.773763	-0.120262
O	2.900198	-0.211682	0.632253
O	1.947654	0.752772	-1.138047
N	1.492248	-2.596778	0.284515
C	0.227220	-2.292489	-0.044455
N	-0.778783	-3.104174	0.292329
C	-2.138012	-2.923755	-0.202179
N	-0.017001	-1.199560	-0.757186
O	-2.238575	0.341814	-0.280032
N	-1.793891	1.589344	0.110514
C	-1.120445	2.265924	-1.035103
C	-0.829153	1.455204	1.241028
C	-2.965256	2.394335	0.550949
H	4.124494	1.978700	0.978914
H	3.734738	2.581674	-0.658443
H	2.565829	2.761985	0.646672
H	0.783421	-0.579156	-0.961971
H	-0.937318	-0.720928	-0.664836
H	-2.143333	-2.911136	-1.294156
H	-2.569732	-1.992226	0.167640
H	-2.735566	-3.762258	0.145780
H	-0.576204	-3.897753	0.879614
H	1.664102	-3.417839	0.843679
H	2.137855	-1.794396	0.380181
H	-1.835367	2.302830	-1.854070
H	-0.245441	1.675735	-1.305274
H	-0.818828	3.271291	-0.739267
H	0.027157	0.885281	0.883847
H	-0.515332	2.444237	1.574872
H	-1.336416	0.919638	2.040528
H	-2.637057	3.384633	0.865928
H	-3.436022	1.861421	1.373751
H	-3.648316	2.462314	-0.292306

TMAO_Orientation2

C	3.534334	2.709395	0.076512
H	4.594305	2.542751	-0.107422
H	3.137956	3.442389	-0.626030
H	3.414839	3.116192	1.084217
C	2.747655	1.408711	-0.012719
O	3.378718	0.328150	0.110150
O	1.502101	1.499483	-0.180020
H	0.806500	-0.105497	-0.137273
N	0.243064	-0.973653	-0.095787
H	-0.790871	-0.856012	-0.055922
H	-1.684905	-2.970908	-0.934269
C	-1.311269	-3.290750	0.041518
H	-1.724329	-2.631870	0.806643
H	-1.641809	-4.307708	0.235864
N	0.143419	-3.272606	0.084290
H	0.638712	-4.148338	0.023561
H	2.663183	-3.059909	0.111657
H	2.708297	-1.304995	-0.022440
N	2.191797	-2.195626	-0.101556
C	0.853410	-2.141973	-0.032150
O	-2.405443	-0.298271	0.020781
N	-2.473984	1.080762	0.012929
C	-1.772165	1.626990	1.209881
H	-0.722572	1.345730	1.137876
H	-2.233239	1.180150	2.087457
H	-1.871638	2.712416	1.229653
C	-3.905563	1.484298	0.042692
H	-4.341126	1.070038	0.948938
H	-3.985999	2.571001	0.034643
H	-4.382277	1.053391	-0.834554
C	-1.827356	1.612605	-1.221381
H	-1.939684	2.696422	-1.255158
H	-2.320758	1.146248	-2.070858
H	-0.771937	1.345835	-1.189130

TMAO_Orientation3

C	2.516928	-2.616172	-0.274955
H	2.815911	-3.279527	0.534970
H	2.738159	-3.068347	-1.241482
H	3.075316	-1.677725	-0.194337
C	1.048778	-2.248812	-0.176803
O	0.476688	-2.359616	0.938071
O	0.496005	-1.797704	-1.217494
H	-0.918781	-0.921796	-1.080744
N	-1.767110	-0.325052	-0.947868
H	-2.093071	0.254910	-1.703622
H	-4.335850	0.722194	-1.515014
C	-4.043886	1.298736	-0.634557
H	-3.331279	2.075486	-0.921886
H	-4.930935	1.777712	-0.229526
N	-3.490535	0.434342	0.396008
H	-3.937995	0.413199	1.298893
H	-2.403116	-1.070653	2.104719
H	-1.059005	-1.623984	1.097571
N	-1.951478	-1.097617	1.204732
C	-2.404878	-0.326359	0.217161
O	2.938439	0.863322	0.449388
N	1.836411	1.621716	0.131176
C	0.682141	1.195802	0.970323
H	0.958491	1.357937	2.010118
H	0.525615	0.135598	0.786027
H	-0.206534	1.773730	0.710206
C	1.495084	1.428964	-1.306590
H	1.302198	0.367288	-1.452754
H	0.617880	2.024170	-1.564498
H	2.358825	1.745391	-1.887774
C	2.126961	3.059569	0.383121
H	1.258224	3.668458	0.130857
H	2.981388	3.331551	-0.232457
H	2.377723	3.162293	1.436467

TMAO_Orientation4

C	5.308690	-1.514247	0.108093
C	3.969213	-0.795597	0.015987
O	2.927068	-1.496213	-0.015982
O	3.990724	0.464419	0.005206
N	0.519302	-0.136133	-0.473781
C	0.475399	1.160614	-0.162212
N	1.592564	1.789464	0.203551
N	-0.692477	1.803779	-0.225886
C	-0.847804	3.214762	0.071741
O	-2.304547	-0.367247	-0.883360
N	-3.199966	-0.878008	0.031730
C	-3.710920	-2.184948	-0.465930
C	-4.334167	0.074048	0.192287
C	-2.518655	-1.071714	1.343281
H	5.234131	-2.531889	-0.271890
H	6.079695	-0.963421	-0.429763
H	5.601886	-1.559384	1.160512
H	2.507854	1.296649	0.142007
H	1.574862	2.780661	0.378759
H	-0.243132	3.832885	-0.597034
H	-0.581758	3.438726	1.108234
H	-1.892921	3.476556	-0.076275
H	-1.499176	1.217367	-0.471788
H	-0.372953	-0.589801	-0.664700
H	1.388887	-0.669166	-0.315624
H	-2.128591	-0.105155	1.656875
H	-1.703911	-1.775789	1.189259
H	-3.228091	-1.457800	2.074553
H	-2.855437	-2.845621	-0.583970
H	-4.424809	-2.596442	0.247006
H	-4.183177	-2.003971	-1.428480
H	-5.057501	-0.329688	0.900101
H	-4.783872	0.211643	-0.788051
H	-3.924450	1.014737	0.554590

TMAO molecule

C	0.379996	-1.350809	-0.417936
N	-0.000146	-0.000008	0.081435
C	-1.359237	0.346691	-0.419614
C	0.980602	1.003867	-0.417619
O	-0.001627	0.000219	1.455375
H	0.386508	-1.361336	-1.507953
H	1.367696	-1.576322	-0.022632
H	-0.348832	-2.057717	-0.028447
H	-1.370339	0.347709	-1.509661
H	-2.048873	-0.396334	-0.025958
H	-1.607334	1.330917	-0.029249
H	0.990338	1.011834	-1.507641
H	0.680619	1.973180	-0.026370
H	1.956084	0.727881	-0.024116

Glycerol

Glycerol_Orientation1

C	-4.251762	-0.128956	0.008717
C	-2.857969	-0.714846	-0.082422
O	-2.689673	-1.848554	-0.568930
O	-1.903572	0.007630	0.361598
O	0.337654	0.858858	-0.950661
C	0.771971	1.824205	-0.000638
C	2.134763	2.281750	-0.489795
O	2.996857	1.168253	-0.663203
C	-0.210618	2.979121	0.130233
O	-1.349567	2.656244	0.908413
N	0.055789	-2.311600	-0.895397
C	0.885345	-1.940817	0.075751
N	0.375133	-1.450927	1.209673
N	2.205321	-2.083880	-0.062855
C	3.166976	-1.715906	0.968667
H	-4.476364	0.102736	1.051478
H	4.163443	-1.874226	0.564940
H	-4.281145	0.809574	-0.548413
H	-4.995715	-0.816893	-0.386829
H	3.067937	-0.657503	1.215304
H	3.048782	-2.331074	1.863596
H	2.535892	-2.615446	-0.854172
H	0.995851	-1.145820	1.942541
H	-0.546957	-1.008087	1.149196
H	0.424949	-2.539590	-1.805117
H	-0.964505	-2.177643	-0.788006
H	0.890966	1.347224	0.983049
H	2.015845	2.826673	-1.435337
H	2.599372	2.945178	0.240685
H	0.280559	3.820004	0.627620
H	-0.500761	3.299514	-0.878808
H	-1.681996	1.774102	0.658967
H	-0.468707	0.428788	-0.611239
H	2.473035	0.490597	-1.110212

Glycerol_Orientation2

C	-2.747690	-2.389377	0.715843
C	-1.306191	-2.012236	0.428072
O	-0.703844	-1.318100	1.304197
O	-0.783308	-2.405733	-0.637555
O	-1.979374	1.079565	1.024074

C	-1.237324	1.454823	-0.126958
C	-0.330077	2.638912	0.164238
O	0.613580	2.357203	1.184479
C	-2.240379	1.767428	-1.226438
O	-3.091514	0.655646	-1.449166
N	1.543150	-1.164838	-1.370867
C	2.341785	-0.657334	-0.439742
N	3.588029	-0.284835	-0.726782
C	4.473627	0.373156	0.223713
N	1.854991	-0.462044	0.798158
H	-3.257451	-1.578072	1.236821
H	5.364772	0.687749	-0.312195
H	-3.274270	-2.645673	-0.201693
H	-2.750398	-3.260702	1.375903
H	3.991275	1.255792	0.647226
H	4.772892	-0.305196	1.025911
H	3.942288	-0.494737	-1.647548
H	2.515778	-0.390698	1.559332
H	0.915196	-0.857534	1.020897
H	1.872403	-1.243805	-2.320538
H	0.656063	-1.639922	-1.099707
H	-0.622709	0.602977	-0.452331
H	-2.828091	2.649326	-0.940564
H	-1.728828	1.979301	-2.166398
H	0.173918	2.943759	-0.761465
H	-0.930681	3.478697	0.521822
H	1.080083	1.542558	0.956366
H	-1.564127	0.278688	1.390812
H	-3.398128	0.378614	-0.576810

C	0.268883	-3.002361	-0.004757
C	1.180241	-1.792481	-0.186291
O	1.601935	-1.303196	1.087787
C	2.431193	-2.118164	-0.976801
O	3.283627	-0.987194	-1.074545
N	0.246076	1.245419	0.591143
C	0.224314	2.462479	0.060955
N	1.334340	3.206509	0.033948
C	2.624681	2.722659	0.501005
N	-0.924522	2.937703	-0.420957
H	-4.061400	-1.737546	0.437885
H	3.353939	3.515998	0.361643
H	-5.089753	-0.412060	-0.185321
H	-4.104262	-1.384408	-1.290802
H	2.587045	2.468310	1.562635
H	2.944626	1.851305	-0.075532
H	1.275567	4.134562	-0.354710
H	1.112604	0.804735	0.871448
H	-0.574019	0.622610	0.455373
H	-0.953836	3.842660	-0.861523
H	-1.769464	2.342062	-0.416064
H	0.625204	-0.997667	-0.701029
H	2.956264	-2.953194	-0.497903
H	2.166248	-2.407950	-1.995207
H	-0.187018	-3.261001	-0.967121
H	0.853386	-3.858489	0.343793
H	-1.268201	-1.998574	0.670483
H	0.913124	-1.551083	1.720347
H	3.529750	-0.743840	-0.175426

C	1.665926	-1.471118	-0.101425
N	1.033289	-1.120755	1.014216
N	2.983335	-1.286386	-0.209860
H	3.437043	-1.636425	-1.039839
O	-0.135787	0.960929	-1.123768
C	-0.167333	1.809626	0.011669
C	1.058054	2.697431	-0.101190
O	2.231635	1.903417	-0.193285
C	-1.459234	2.602576	0.100817
O	-2.585115	1.748054	0.227880
H	-4.018299	-2.432817	-0.628015
H	-3.934598	-2.311717	1.157334
H	-4.403528	-0.910352	0.193981
C	3.816695	-0.784321	0.875383
H	1.452173	-2.201472	-1.974327
H	-0.032261	-1.913887	-1.119738
H	1.535297	-0.596197	1.713898
H	0.000789	-1.083220	1.050224
H	-0.073880	1.207284	0.924937
H	0.962689	3.343019	-0.983478
H	1.158785	3.326262	0.784289
H	-1.397942	3.294026	0.950580
H	-1.604840	3.184927	-0.812472
H	-2.361272	1.035357	0.845167
H	-0.773343	0.229164	-1.024982
H	2.049364	1.236809	-0.868028
H	4.845073	-0.768934	0.524965
H	3.524384	0.234593	1.136148
H	3.754641	-1.434657	1.750668

Glycerol_Orientation3

C	-4.493587	-0.812557	-0.860802
C	-3.187495	-0.266760	-0.316196
O	-3.213422	0.577717	0.604902
O	-2.116833	-0.712744	-0.838611
O	1.810174	-0.383143	0.940144
C	1.556710	-1.400362	-0.022058
C	2.899417	-1.992846	-0.396211
O	3.782620	-0.990370	-0.875457
C	0.597188	-2.433028	0.554647
O	-0.528950	-1.788564	1.121441
N	-0.729094	1.643633	1.262277
C	0.049475	1.908671	0.210058
N	-0.246292	1.351017	-0.960350
N	1.110421	2.709271	0.328123
C	2.157292	2.773372	-0.681449
H	-4.519526	-1.893040	-0.706199
H	2.968220	3.380229	-0.288576
H	-5.349957	-0.350843	-0.373977
H	-4.537071	-0.635936	-1.936873
H	2.536728	1.771853	-0.901945
H	1.791658	3.243393	-1.596407
H	1.308131	3.084057	1.243094
H	0.350899	1.500975	-1.757382
H	-0.954484	0.599511	-0.997446
H	-0.561092	2.126545	2.131517
H	-1.662686	1.223844	1.095870
H	1.104447	-0.943879	-0.913353
H	3.329829	-2.494471	0.479214
H	2.779566	-2.725170	-1.196137
H	0.306195	-3.146598	-0.223998
H	1.089449	-2.979348	1.363776
H	-1.082756	-1.423681	0.400580
H	0.976888	-0.228844	1.407726
H	3.837616	-0.318163	-0.187102

Glycerol_Orientation5

C	-3.422367	1.977788	0.358650
C	-1.921531	1.784607	0.254977
O	-1.467071	1.429025	-0.876456
O	-1.213404	1.951860	1.271979
O	-2.246936	-1.081917	-1.693596
C	-0.968531	-1.639809	-1.437485
C	-0.687032	-1.650497	0.059197
C	0.651159	-2.283640	0.381418
O	1.008745	-2.136075	1.745818
O	-1.710830	-2.366148	0.736732
N	1.365439	0.951946	1.353018
C	1.976983	0.927267	0.150370
N	3.288235	0.707590	0.073819
C	4.014530	0.610080	-1.184101
N	1.247176	1.072359	-0.945106
H	-3.904726	1.002433	0.249962
H	5.063788	0.449593	-0.953967
H	-3.700243	2.410169	1.317400
H	-3.772979	2.609863	-0.457841
H	3.656702	-0.232993	-1.779483
H	3.922892	1.534887	-1.756973
H	3.794142	0.567964	0.935239
H	1.681516	0.998378	-1.851965
H	0.217523	1.248890	-0.896773
H	1.948059	1.140889	2.157393
H	0.409366	1.359200	1.373394
H	-0.676459	-0.611734	0.418606
H	0.605052	-3.356689	0.181835
H	1.419354	-1.846998	-0.270989
H	-0.183486	-1.086570	-1.963794
H	-0.984210	-2.666770	-1.813036
H	-2.163534	-0.125583	-1.518185
H	-2.546464	-2.057970	0.364573
H	1.084447	-1.188977	1.918511

Glycerol_Orientation7

C	3.497961	2.158403	-0.217495
C	2.108468	1.556728	-0.161610
O	1.550657	1.456600	0.964403
O	1.596757	1.142563	-1.237902
N	-1.210800	1.110257	-1.313240
C	-1.896344	1.151508	-0.172032
N	-3.221656	0.994032	-0.174452
C	-4.033679	1.003336	1.032843
N	-1.249887	1.382516	0.968212
O	0.905866	-1.557412	-1.239304
C	0.431460	-1.734848	0.087807
C	1.535174	-2.191535	1.028112
O	2.572247	-1.231159	1.130414
C	-0.712495	-2.728431	0.009792
O	-1.735503	-2.234950	-0.840111
H	-3.662904	0.751932	-1.047896
H	3.701867	2.577979	-1.200958
H	3.623942	2.912818	0.557584
H	4.216449	1.355185	-0.029814
H	-1.689031	0.930058	-2.181331
H	-0.181023	1.145698	-1.307352
H	-1.741864	1.333515	1.845707
H	-0.217496	1.432917	0.982234
H	0.033344	-0.782754	0.459969
H	-0.333135	-3.689062	-0.361874
H	-1.154157	-2.884454	0.995273
H	1.102320	-2.405528	2.013685
H	1.989398	-3.108299	0.643948
H	2.174785	-0.369375	1.330807
H	1.263867	-0.655360	-1.312229
H	-1.284096	-1.870185	-1.611476
H	-5.073847	0.899046	0.737211
H	-3.773442	0.172476	1.692959
H	-3.922043	1.949651	1.565405

Glycerol_Orientation4

C	-4.141460	-0.934808	-0.294966
C	-2.971742	0.023867	-0.163466
O	-3.156839	1.240555	-0.376582
O	-1.844779	-0.478582	0.134938
O	-0.708659	-2.742956	0.985154

Glycerol_Orientation6

C	-3.760037	-1.794595	0.214612
C	-2.322277	-1.324947	0.125444
O	-1.747274	-1.357165	-0.996436
O	-1.778232	-0.876831	1.171444
N	0.984396	-2.055275	-1.092907

Glycerol_Orientation8

C	-3.153676	-1.923938	0.321615
C	-1.638350	-1.939825	0.220605
O	-1.115629	-1.786840	-0.921953
O	-0.983859	-2.067460	1.283118
H	-2.813667	0.668496	-0.960143

C	-2.364181	1.576940	-0.542028
C	-0.894455	1.303309	-0.265908
C	-0.128510	2.555871	0.118648
O	1.249301	2.260701	0.303361
O	-0.265945	0.787835	-1.428785
N	1.699368	-1.847601	-1.002404
C	2.123774	-0.946763	-0.109270
N	1.456336	-0.802156	1.030951
N	3.231276	-0.231975	-0.329560
C	3.929258	0.500364	0.723399
H	3.704975	-0.367647	-1.209714
H	-3.619226	-2.043307	-0.655043
H	-3.494066	-2.703885	1.002939
H	-3.455012	-0.960823	0.745458
H	2.211341	-1.957309	-1.864233
H	0.688244	-2.042355	-1.013546
H	1.587578	0.054074	1.551411
H	0.567163	-1.324057	1.161279
H	-0.821159	0.577090	0.554013
H	-0.255191	3.311090	-0.667623
H	-0.506940	2.959543	1.057334
O	-2.977380	1.932168	0.688992
H	-2.457841	2.382544	-1.280038
H	-0.521338	-0.150012	-1.483316
H	1.532230	1.800838	-0.498043
H	4.879054	0.839818	0.319090
H	3.354001	1.371424	1.040768
H	4.117544	-0.149896	1.579840
H	-3.901610	2.139518	0.526423

Glycerol_Orientation9

C	-2.097418	3.358575	-0.365793
C	-0.927192	2.410150	-0.186341
O	-0.804272	1.841909	0.939967
O	-0.161334	2.214863	-1.158566
O	-1.372481	-0.824359	1.207000
C	-1.527469	-1.090553	-0.180466
C	-0.841293	-2.405833	-0.511645
O	0.561249	-2.352382	-0.304518
C	-3.016833	-1.125167	-0.507715
O	-3.692791	-2.040841	0.340235
N	1.873924	0.398076	-0.877294
C	2.417233	0.321940	0.348716
N	1.761258	0.849536	1.376324
N	3.577659	-0.306233	0.528127
C	4.343112	-0.916829	-0.549625
H	-3.430940	-0.116927	-0.387702
H	3.947041	-0.352168	1.465327
H	-2.309313	3.886271	0.563079
H	-1.907833	4.063564	-1.173108
H	-2.978899	2.765451	-0.624655
H	2.087987	0.684991	2.315782
H	0.815663	1.246520	1.236360
H	2.480217	0.249939	-1.671546
H	1.089257	1.075558	-1.009578
H	-1.058272	-0.288809	-0.768303
H	-1.225552	-3.194605	0.137840
H	-1.068727	-2.672315	-1.550822
H	-3.186120	-1.448398	-1.536804
H	-1.243376	0.136309	1.295658
H	0.898614	-1.567879	-0.754697
H	5.200315	-1.416523	-0.107248
H	3.742956	-1.660132	-1.078028
H	4.705913	-0.164835	-1.253366
H	-3.392632	-1.842880	1.235981

Glycerol_Orientation10

C	3.302180	-2.463708	-0.332273
C	1.869827	-1.969802	-0.251869
O	1.479303	-1.531085	0.873544
O	1.151729	-2.014021	-1.275634
O	0.454581	0.984146	0.992279
C	0.774848	1.493683	-0.297689
C	-0.244425	2.581275	-0.593616
O	-1.567644	2.078712	-0.467445
C	2.206285	2.016874	-0.298090
O	2.416519	2.926387	0.769930
N	-1.404502	-1.029644	-0.900535
C	-1.941153	-1.123536	0.311697
N	-1.310006	-1.833322	1.254279
N	-3.122919	-0.554963	0.565200
C	-4.003310	-0.042743	-0.480374
H	2.895391	1.167114	-0.217985
H	-3.491499	-0.640994	1.500275
H	3.458828	-3.239919	0.418705
H	3.533654	-2.852029	-1.321732
H	3.976184	-1.638355	-0.093556
H	-1.724309	-1.900360	2.171137
H	-0.286459	-1.894704	1.187366
H	-1.723102	-0.280990	-1.499782
H	-0.451257	-1.412707	-1.062478
H	0.686577	0.697052	-1.046053
H	-0.088700	3.422680	0.090626
H	-0.128772	2.936727	-1.618438
H	2.422013	2.548271	-1.227635
H	0.810470	0.073023	1.044872
H	-1.610104	1.662111	0.403142
H	-4.962947	0.186463	-0.024975
H	-3.596253	0.868937	-0.920086
H	-4.149975	-0.796063	-1.256765
H	2.030822	2.513873	1.552642

Glycerol_Orientation11

C	-2.682981	-2.525346	-0.366901
C	-1.226024	-2.115327	-0.427334
O	-0.441126	-2.548959	0.447940
O	-0.885603	-1.311485	-1.347337
N	1.810265	-1.090320	0.816820
C	2.355610	-0.398341	-0.169916
N	1.633843	-0.166499	-1.286822
N	3.581808	0.110763	-0.059340
C	4.432832	-0.088978	1.104406
O	-2.073633	1.117968	-0.983536
C	-1.306654	1.444940	0.159285
C	-2.203977	1.568461	1.375941
O	-2.713977	0.275537	1.673738
C	-0.534578	2.736060	-0.081500
O	0.328238	2.648498	-1.202229
H	-1.631315	1.961816	2.223420
H	3.898042	0.733460	-0.786980
H	-3.100028	-2.619131	-1.368986
H	-2.806011	-3.453491	0.188366
H	-3.214598	-1.725609	0.157221
H	2.146489	0.010505	-2.139940
H	0.725517	-0.664666	-1.377661
H	2.300101	-1.186354	1.692588
H	0.936410	-1.648848	0.662307
H	-0.585570	0.638148	0.357247
H	-1.236163	3.548446	-0.289863
H	0.030705	2.993008	0.822345
H	-3.019653	2.264587	1.147664
H	-1.793853	0.232404	-1.275819
H	0.804890	1.809020	-1.154327
H	5.398346	0.363325	0.896446
H	4.009307	0.386031	1.992150
H	4.582094	-1.154076	1.290135
H	-3.342675	0.352524	2.396590

Glycerol_Orientation12

C	3.617688	-1.748631	-0.404534
C	2.122475	-1.537500	-0.273613
O	1.702004	-1.086209	0.839791
O	1.384539	-1.791088	-1.249502
O	0.046424	1.051294	1.097747
C	0.426225	1.742575	-0.086431
C	1.745427	2.468799	0.113969
H	1.956606	3.106963	-0.747775
C	-0.712299	2.697229	-0.405617
O	-1.947753	1.998743	-0.440540
N	-1.051437	-1.964072	1.160324
C	-1.774954	-1.303342	0.246209
N	-1.253317	-1.080975	-0.953552
N	-3.023693	-0.915547	0.520123
C	-3.977650	-0.517874	-0.511838
O	2.837045	1.569283	0.235508
H	-3.380010	-1.113797	1.442923
H	4.006442	-2.240806	0.487015
H	3.858379	-2.326987	-1.294152
H	4.092730	-0.766479	-0.476416
H	-1.447422	-2.122569	2.074227
H	-0.033439	-1.881542	1.102031
H	-1.671746	-0.367371	-1.533465
H	-0.259161	-1.340208	-1.116752
H	0.538572	1.021002	-0.907194
H	-0.747301	3.492750	0.349564
H	-0.566536	3.152726	-1.385547
H	1.666322	3.102266	1.006172
H	0.542029	0.210867	1.112293
H	-1.986251	1.496377	0.384573
H	-4.950128	-0.406263	-0.040020
H	-3.695716	0.437671	-0.956496
H	-4.043443	-1.282423	-1.288467
H	2.559659	0.808270	0.766321

Glycerol molecule

C	1.218130	-0.125399	0.685056
C	0.026885	0.800107	0.446008
O	0.137613	1.409561	-0.833956
O	1.407622	-1.012505	-0.411004
C	-1.309362	0.079149	0.572487
O	-1.408333	-1.016812	-0.337109
H	2.132672	0.464728	0.759487
H	1.079393	-0.674064	1.622446
H	0.050069	1.598424	1.194245
H	-2.125166	0.787764	0.405959
H	-1.409650	-0.337795	1.576491
H	-1.623657	-0.668563	-1.208106
H	0.597385	0.782694	-1.406342
H	0.589826	-1.518281	-0.508939

Two guanidinium ions

2Gdm$^+$_Orientation1

C	-2.123731	-1.166154	2.419213
C	-0.885741	-0.867455	1.606943
O	0.246135	-1.033753	2.108148
O	-1.053303	-0.465536	0.405488
N	1.203213	1.217340	-0.292268
C	2.170720	1.563264	0.552918
N	2.116700	1.145161	1.818868
N	3.171786	2.338290	0.140679
C	3.268282	2.887757	-1.204482
N	0.675073	-1.895404	-1.419223
C	1.923805	-2.117750	-1.018464
N	2.244402	-1.940408	0.258007
N	2.845843	-2.519270	-1.894789
H	-2.871969	-0.386638	2.267130
H	4.138321	3.537355	-1.236374
H	-2.548344	-2.107932	2.061510
H	-1.884042	-1.262221	3.475471
H	3.398191	2.096823	-1.946279
H	2.384402	3.481645	-1.444410
H	3.913249	2.537415	0.794227
H	1.251370	1.483121	-1.262791
H	0.404125	0.655255	0.010577
H	2.855737	1.380872	2.461998
H	1.451027	0.419071	2.082176

H	0.427714	-2.001802	-2.390154
H	0.001592	-1.450079	-0.792947
H	1.534759	-1.668130	0.944819
H	3.189133	-2.093570	0.573578
H	3.774415	-2.769474	-1.594812
H	2.614687	-2.651888	-2.866385
C	-3.931639	0.684860	-0.781411
N	-3.603804	-0.598166	-0.887619
N	-3.080334	1.513525	-0.183507
N	-5.089853	1.136725	-1.258884
H	-2.707899	-0.895159	-0.504319
H	-4.201232	-1.255627	-1.361908
H	-5.745475	0.517488	-1.707611
H	-5.325664	2.114879	-1.207506
H	-3.304188	2.485542	-0.045906
H	-2.203930	1.135674	0.163669

2Gdm$^+$_Orientation2

C	2.044031	-0.094434	2.614656
C	0.859344	-0.169928	1.680499
O	-0.261247	-0.504629	2.121735
O	1.052758	0.134635	0.455585
N	-2.462078	0.798387	0.837708
C	-2.261103	1.627279	-0.181979
N	-3.294838	2.212211	-0.784502
C	-4.678566	2.025988	-0.371643
N	-1.014599	1.880300	-0.588479
N	-1.652518	-2.578014	0.708076
C	-1.607692	-2.390367	-0.606058
N	-2.367067	-3.128133	-1.417378
N	-0.808061	-1.455893	-1.111616
H	1.832542	-0.601230	3.553113
H	-5.305229	2.631735	-1.020049
H	2.926977	-0.524887	2.139801
H	2.255650	0.958752	2.817708
H	-4.980289	0.981791	-0.475493
H	-4.826068	2.355414	0.658827
H	-3.101010	2.834270	-1.553958
H	-3.393590	0.618058	1.176264
H	-1.673396	0.369639	1.331834
H	-0.859527	2.434300	-1.415837
H	-0.234733	1.332429	-0.222032
H	-2.243173	-3.291874	1.104139
H	-1.157113	-1.939623	1.331121
H	-0.152079	-0.935296	-0.524937
H	-0.800807	-1.277141	-2.103387
H	-2.256754	-3.077543	-2.417646
H	-2.982086	-3.836243	-1.049990
C	4.118682	0.420678	-0.799358
N	5.361941	0.529006	-1.263866
N	3.487375	1.476737	-0.297318
N	3.483859	-0.747317	-0.830069
H	5.842230	1.414346	-1.256817
H	5.854739	-0.272172	-1.624653
H	3.904169	-1.562300	-1.246099
H	2.536982	-0.789088	-0.464110
H	2.543899	1.344016	0.060834
H	3.950286	2.366314	-0.201790

2Gdm$^+$_Orientation3

C	1.078044	4.156909	-0.092783
C	1.038421	2.644680	-0.093109
O	0.869325	2.043742	1.003480
O	1.204555	2.041234	-1.189277
N	2.619515	-0.393932	-0.752174
C	3.011506	-0.791708	0.454131
N	2.788218	-0.008772	1.511742
N	3.639770	-1.957530	0.603632
C	3.976119	-2.841909	-0.502180
N	-0.660046	-0.031862	-1.677855
C	-0.903949	-0.790061	-0.616534
N	-0.485367	-0.404136	0.584675
N	-1.603787	-1.922589	-0.746021
H	2.122928	4.468208	-0.011044
H	4.500844	-3.701255	-0.094458
H	0.681629	4.549631	-1.027942
H	0.531286	4.559896	0.757602
H	3.075505	-3.195479	-1.008690
H	4.632656	-2.341552	-1.216879
H	3.911560	-2.229130	1.535981
H	2.784766	-0.974160	-1.559023
H	2.155172	0.511913	-0.895227
H	3.018614	-0.339006	2.435584
H	2.164130	0.797172	1.423614
H	-1.023137	-0.290386	-2.581485
H	-0.047006	0.785901	-1.596123
H	-0.011693	0.499972	0.725832
H	-0.582695	-1.023523	1.374315
H	-1.753108	-2.525787	0.047624
H	-1.805855	-2.299053	-1.659038
C	-4.069074	-0.338195	0.400426
N	-4.898409	-1.058395	-0.345986
N	-3.708513	-0.774364	1.607170
N	-3.574397	0.805436	-0.063073
H	-5.253837	-1.943316	-0.018876
H	-5.100225	-0.796765	-1.298449
H	-3.218802	-0.165881	2.245291
H	-4.132611	-1.602069	1.997388
H	-3.868673	1.176365	-0.953388
H	-2.977784	1.383213	0.509307

2Gdm$^+$_Orientation4

C	-0.751499	-2.483131	0.805021
C	-0.313260	-1.046186	0.618168
O	-1.169983	-0.192658	0.259596
O	0.902717	-0.769263	0.803529
N	-3.449501	-0.968568	-1.290420
C	-4.350828	-0.855889	-0.319883
N	-3.949303	-0.449950	0.880498
N	-5.631717	-1.142474	-0.547330
N	3.105978	-0.990292	-1.023614
C	3.649863	-2.047097	-0.424895
N	4.748849	-2.611754	-0.924873
N	3.083372	-2.523771	0.676815
N	1.448737	1.986065	1.252313
C	0.887739	2.790696	0.346281
N	1.297969	4.051924	0.214417
C	0.681118	5.008202	-0.693262
N	-0.095822	2.318227	-0.413213
H	-1.833604	-2.560162	0.902619
H	1.173749	5.966604	-0.556392
H	-0.436647	-3.051379	-0.074612
H	-0.262780	-2.917578	1.676780
H	0.804991	4.700383	-1.733850
H	-0.379917	5.129480	-0.466060
H	2.088437	4.350265	0.764611
H	-0.545567	2.911906	-1.090894
H	-0.503211	1.394135	-0.208143
H	2.230168	2.313983	1.797431
H	1.275629	0.977030	1.191973
H	3.478589	-3.310409	1.165574
H	2.230097	-2.072387	1.012806
H	2.242830	-0.609833	-0.647198
H	3.476756	-0.632870	-1.889016
H	5.200977	-2.235881	-1.742670
H	5.178667	-3.401331	-0.470414
H	-5.938320	-1.470856	-1.449064
H	-6.315657	-1.085557	0.190152
H	-4.599632	-0.345894	1.642391
H	-2.962956	-0.233921	1.009327
H	-2.483015	-0.733718	-1.076620
H	-3.710191	-1.272065	-2.214451

Two molecules of trimethylamine N-oxide

2TMAO_Orientation1

C	2.325796	-1.687168	2.891809
C	1.535615	-0.470535	2.428095
O	0.282558	-0.530816	2.526722
O	2.173779	0.510141	1.964021
C	3.317440	-1.397622	-0.823485
N	2.431227	-0.604711	-1.720812
C	2.621388	0.843978	-1.429670
O	1.118094	-0.954296	-1.500390
C	2.783094	-0.880544	-3.140231
N	0.794963	2.754883	1.030894
C	-0.367110	2.407699	0.449192
N	-0.972851	1.294934	0.822702
N	-0.913695	3.207765	-0.474274
C	-2.257264	3.006091	-0.998944
O	-3.133782	0.023726	-0.308776
N	-2.968191	-1.345359	-0.247958
C	-4.232373	-1.996627	-0.685445
C	-2.653230	-1.756713	1.149975
C	-1.852612	-1.752527	-1.149328
H	3.398839	-1.516776	2.821144
H	2.056161	-1.928125	3.921798
H	2.051457	-2.545921	2.274248
H	-0.490519	0.679885	1.500445
H	-1.810079	0.908630	0.337899
H	-3.008188	3.124060	-0.213336
H	-2.355775	2.010185	-1.431839
H	-2.429789	3.750010	-1.772566
H	-0.451466	4.082764	-0.666027
H	1.304831	3.536111	0.648047
H	1.342270	1.990840	1.462474
H	-3.462227	-1.399104	1.783309
H	-1.708688	-1.297501	1.439231
H	-2.575192	-2.842874	1.201985
H	-0.943988	-1.244240	-0.828815
H	-1.724459	-2.834632	-1.106239
H	-2.120355	-1.438825	-2.156234
H	-4.122290	-3.080481	-0.653240
H	-4.438403	-1.658566	-1.698184
H	-5.020195	-1.667018	-0.012056
H	3.652588	1.131729	-1.638972
H	1.931307	1.397303	-2.063489
H	2.384181	0.991469	-0.377848
H	4.361808	-1.152342	-1.020086
H	3.048217	-1.141559	0.199105
H	3.124213	-2.449384	-1.022668
H	3.825523	-0.621611	-3.326477
H	2.610440	-1.939523	-3.317854
H	2.119957	-0.283317	-3.762044

2TMAO_Orientation2

C	3.238525	3.194265	-0.851856
C	2.221556	2.611417	0.121957
O	2.671420	1.980515	1.114364
O	1.001088	2.754952	-0.144579
C	-4.827243	1.299820	-1.034767
N	-3.986003	0.128507	-0.663826
C	-2.800808	0.058708	-1.566251
O	-3.569062	0.270836	0.642720
C	-4.785408	-1.122176	-0.787444
N	-0.935836	1.256906	1.282775
C	-0.426802	0.030752	1.489991
N	0.878057	-0.120820	1.741234
N	-1.242792	-1.021093	1.498463
C	-0.815817	-2.353010	1.897211
O	2.097826	-2.216948	0.365099
N	2.729943	-1.663636	-0.729280
C	3.141491	-2.760636	-1.646988
C	3.932140	-0.902666	-0.284756
C	1.800284	-0.741036	-1.445080
H	2.804275	3.995671	-1.447502
H	4.120848	3.549680	-0.319914
H	3.556200	2.393443	-1.527022
H	1.464779	0.718379	1.628348
H	1.322430	-0.993541	1.405122

H	-0.387452	-2.331965	2.902548
H	-0.073420	-2.754202	1.204455
H	-1.690903	-2.999041	1.901646
H	-2.214928	-0.826400	1.232616
H	-1.921499	1.273605	1.017577
H	-0.291457	1.935020	0.853255
H	4.577105	-1.598142	0.247490
H	3.594305	-0.104206	0.375308
H	4.444481	-0.487910	-1.153736
H	1.553917	0.081700	-0.775569
H	2.281049	-0.363665	-2.347833
H	0.906241	-1.310287	-1.691442
H	3.648885	-2.347063	-2.518398
H	2.240872	-3.295535	-1.939366
H	3.803745	-3.418088	-1.088740
H	-5.166242	1.199512	-2.065447
H	-5.670713	1.324519	-0.349102
H	-4.216549	2.191426	-0.912555
H	-3.129355	-0.057454	-2.598643
H	-2.239277	0.982447	-1.443297
H	-2.198344	-0.793171	-1.256458
H	-5.138187	-1.237730	-1.811851
H	-4.141384	-1.951763	-0.503843
H	-5.620683	-1.041751	-0.096142

2TMAO_Orientation3

C	-2.563690	4.473229	0.189542
C	-1.774103	3.190091	-0.045395
O	-2.427004	2.112295	-0.069390
O	-0.527810	3.279658	-0.175962
N	-0.785718	-0.135093	-0.395390
C	0.535635	-0.116199	-0.507266
N	1.236057	-1.254083	-0.578506
C	0.603360	-2.558087	-0.660137
N	1.190593	1.049284	-0.559132
O	-2.571961	-2.211420	0.023216
N	-3.805503	-1.626294	0.226424
C	-4.815897	-2.698500	0.431872
C	-4.177933	-0.807671	-0.962844
C	-3.756312	-0.747100	1.430036
O	3.796178	-0.117679	-0.810498
N	4.680161	-0.251985	0.238964
C	4.021848	0.181799	1.504169
C	5.093625	-1.678725	0.354068
C	5.876019	0.595627	-0.021678
H	-1.979950	5.352119	-0.079288
H	-3.496925	4.452485	-0.373859
H	-2.818926	4.532052	1.251197
H	-1.299596	0.754731	-0.294799
H	-1.331176	-1.006105	-0.270284
H	0.019672	-2.663362	-1.579208
H	-0.059472	-2.728925	0.191025
H	1.385720	-3.314310	-0.651115
H	2.245186	-1.138523	-0.713338
H	2.205045	1.015273	-0.634116
H	0.657569	1.916566	-0.431209
H	-4.159180	-1.465695	-1.828418
H	-3.441353	-0.012319	-1.064149
H	-5.171881	-0.383364	-0.819714
H	-3.043741	0.052112	1.231515
H	-4.745960	-0.330415	1.618804
H	-3.429887	-1.361163	2.266145
H	-5.799233	-2.255778	0.590209
H	-4.506770	-3.276554	1.299774
H	-4.811233	-3.324748	-0.457177
H	6.583014	0.502856	0.802089
H	6.318099	0.253755	-0.954441
H	5.531162	1.621853	-0.123209
H	4.708188	0.053863	2.340994
H	3.745806	1.227805	1.388888
H	3.131467	-0.430345	1.636177
H	5.813104	-1.792076	1.164689
H	4.199180	-2.266453	0.551094
H	5.532413	-1.967757	-0.597921

2TMAO_Orientation4

C	-4.111937	-2.441080	-1.313984
C	-2.840643	-2.092877	-0.554355
O	-2.975609	-1.599907	0.598474
O	-1.737905	-2.281254	-1.125894
N	-0.735264	-0.849350	2.013465
C	0.458416	-0.900048	1.420065
N	0.584712	-1.501132	0.236578
N	1.537740	-0.369664	1.998665
C	1.499958	0.319762	3.274803
O	3.359610	-0.923943	-0.033195
N	3.848697	0.029594	-0.899981
C	4.080670	-0.598836	-2.230102
C	2.860933	1.137709	-1.035147
C	5.132147	0.564346	-0.366682
C	-2.948290	1.766573	0.935874
N	-2.371844	2.096246	-0.398554
O	-3.297908	1.832675	-1.380232
C	-1.157168	1.265045	-0.625822
C	-2.001080	3.537440	-0.437604
H	-3.910910	-3.151818	-2.113777
H	-4.867605	-2.835531	-0.635158
H	-4.506715	-1.521937	-1.755933
H	-1.582796	-1.168779	1.502595
H	-0.843407	-0.341938	2.876584
H	1.152098	-0.340822	4.073003
H	0.859471	1.205644	3.234348
H	2.510671	0.640158	3.515245
H	2.402640	-0.426900	1.448391
H	1.509741	-1.472712	-0.192778
H	-0.253086	-1.828493	-0.269921
H	-0.768374	1.524092	-1.608790
H	-1.468322	0.222268	-0.605038
H	-0.415519	1.465751	0.150224
H	-3.195903	0.706214	0.926199
H	-2.223350	1.989697	1.720202
H	-3.844318	2.371974	1.056582
H	-1.261205	3.756019	0.332755
H	-2.910442	4.111494	-0.274810
H	-1.600399	3.743341	-1.427872
H	4.471334	0.142462	-2.926309
H	4.791765	-1.408722	-2.086714
H	3.127442	-0.991448	-2.576657
H	5.528523	1.317039	-1.047586
H	4.925159	0.995621	0.610142
H	5.818775	-0.273200	-0.271172
H	2.705918	1.565275	-0.046304
H	3.242234	1.890387	-1.724528
H	1.934757	0.706220	-1.409640

2TMAO_Orientation5

C	-3.312084	-0.137921	2.538805
C	-2.128370	-0.855953	1.915873
O	-2.332420	-1.977612	1.381688
O	-1.016692	-0.261114	1.919768
N	0.969011	-1.388454	0.314555
C	0.712189	-2.421997	-0.469782
N	1.655336	-2.906234	-1.289681
C	2.960356	-2.283645	-1.448924
N	-0.501531	-2.984618	-0.448194
C	-1.586320	2.178080	-0.405186
N	-2.411055	1.335250	-1.315623
C	-1.729455	0.026316	-1.520419
C	-2.569740	2.023341	-2.625803
O	-3.646999	1.125462	-0.751421
H	-4.063755	-0.845573	2.886543
H	-2.991716	0.511161	3.353456
H	-3.748512	0.480563	1.747338
H	0.221802	-1.045381	0.943717
H	1.886856	-0.898303	0.348541
H	3.463227	-2.193049	-0.485239
H	2.875937	-1.287307	-1.889505
H	3.557022	-2.916228	-2.101472
H	1.390700	-3.639968	-1.927621
H	-0.678020	-3.817339	-0.986128
H	-1.197912	-2.666102	0.249333
H	-2.364877	-0.573230	-2.168840
H	-1.636310	-0.442551	-0.544282
H	-0.747538	0.175934	-1.973164
H	-1.484102	1.633647	0.532996
H	-0.610904	2.367622	-0.856340
H	-2.122947	3.112212	-0.254057
H	-1.595235	2.186798	-3.086748
H	-3.071138	2.969785	-2.438074
H	-3.192129	1.388176	-3.252299
O	3.217496	0.140094	0.675221
N	2.873839	1.469812	0.549255
C	4.042246	2.307433	0.934087
C	2.502686	1.750887	-0.865370
C	1.720099	1.780367	1.441897
H	2.230646	2.800381	-0.979164
H	3.362926	1.503680	-1.483348
H	1.665266	1.102372	-1.116904
H	3.794350	3.362940	0.824357
H	4.285435	2.071260	1.967246
H	4.867666	2.032581	0.282018
H	1.462453	2.836595	1.357935
H	0.878162	1.155796	1.146442
H	2.022723	1.537158	2.457972

Salt-bridge

C	3.955290	-0.253965	-0.042088
C	2.443915	-0.094195	0.016265
O	1.745805	-1.141719	0.020894
O	1.981462	1.075736	0.027541
N	-0.961340	-0.895211	0.026842
C	-1.520667	0.309283	0.009680
N	-0.739947	1.388053	0.008194
N	-2.852907	0.435533	-0.009671
C	-3.765602	-0.696496	-0.031713
H	4.264123	-1.204329	0.390621
H	-4.778173	-0.310008	-0.109033
H	4.259572	-0.241776	-1.092280
H	4.451458	0.574219	0.462303
H	-3.572914	-1.333318	-0.897622
H	-3.688954	-1.287059	0.884103
H	-3.239188	1.365842	0.016129
H	-1.538329	-1.718022	0.087125
H	0.080547	-0.993801	0.029232
H	-1.151993	2.304202	-0.065124
H	0.297456	1.285517	0.016639

XYZ Coordinates of the optimized geometries obtained at the CPCM(water)/MP2/6-311G** level of theory

Guanidinium ion

Gdm^+_Orientation2

C	-1.886857	2.566838	-0.184809
C	-0.540875	1.860307	-0.091137
O	-0.582710	0.574327	-0.028786
O	0.503557	2.539867	-0.084332
N	1.817845	-0.754018	-0.234944
C	2.939026	-0.104988	0.081726
N	4.116301	-0.743404	0.084675
C	4.253746	-2.169311	-0.173342
N	2.885539	1.200109	0.379682
C	-3.320835	-1.142274	0.066676
N	-4.556891	-1.658345	0.098679
N	-2.687588	-0.945917	-1.090945
N	-2.676806	-0.839604	1.195857
H	-2.393426	2.264900	-1.105982
H	5.315784	-2.392485	-0.256063
H	-2.521825	2.265837	0.652852
H	-1.759237	3.649153	-0.179142
H	3.825716	-2.774138	0.631890
H	3.772181	-2.424671	-1.119678
H	4.903068	-0.254267	0.483584
H	1.808209	-1.759543	-0.167069
H	0.911580	-0.253127	-0.149474
H	3.741788	1.727238	0.297336
H	1.999385	1.705637	0.199826
H	-3.184382	-0.819913	2.066233
H	-1.847079	-0.252547	1.081473
H	-1.859375	-0.347200	-1.038734
H	-3.197560	-1.019683	-1.957042
H	-4.924927	-2.090762	-0.734617
H	-4.910699	-2.013155	0.973849

Gdm^+_Orientation4

C	3.665692	-1.644549	-0.233046
C	2.330630	-0.931895	-0.113045
O	1.762409	-0.552759	-1.182056
O	1.837967	-0.786887	1.046651
N	-1.023523	-0.854711	-0.994239
C	-1.583383	-1.244060	0.154385
N	-2.909217	-1.213424	0.298383
C	-3.821380	-0.743990	-0.735561
N	-0.810867	-1.779428	1.113365
N	0.269729	1.523049	1.196593
C	0.216400	2.377719	0.179315
N	-0.532600	3.491582	0.269077
N	0.868618	2.105720	-0.952466
H	4.199295	-1.315234	-1.125163
H	-4.835932	-0.961625	-0.408099
H	4.269463	-1.481350	0.660253
H	3.471658	-2.718065	-0.324828
H	-3.725843	0.333801	-0.895901
H	-3.635297	-1.274773	-1.671970
H	-3.287480	-1.443239	1.204594
H	-1.560570	-0.277634	-1.622413
H	0.002951	-0.787547	-1.061487
H	-1.243466	-1.983042	2.001843
H	0.174439	-1.493587	1.138929
H	0.644714	2.643317	-1.775820
H	1.244907	1.159228	-1.089492
H	0.882243	0.693486	1.152675
H	-0.079915	1.810259	2.097426
H	-0.826562	3.800619	1.183034
H	-0.380344	4.223686	-0.407623

Gdm^+ ion

C	0.000581	0.000633	-0.003096
N	1.297298	0.307083	0.039683
N	-0.915569	0.969149	0.043208
N	-0.383462	-1.277255	-0.051957
H	-1.883254	0.747276	-0.131388
H	-0.636532	1.926226	-0.103709
H	1.594093	1.258212	-0.114154
H	1.986786	-0.414052	-0.103952
H	0.293888	-2.003955	0.119366
H	-1.346335	-1.510348	0.135872

Urea

Urea_Orientation1

C	4.120740	0.350911	-0.153435
C	2.730757	-0.269924	-0.100763
O	1.760039	0.494196	-0.429281
O	2.614623	-1.466175	0.254788
N	-0.023649	-2.142418	0.674052
C	-0.952586	-1.535079	-0.071529
N	-0.550506	-0.796962	-1.115772
N	-2.252337	-1.721092	0.181771
C	-3.320825	-1.097378	-0.589956
N	-0.274630	2.572016	-0.614918
C	-1.094471	2.038482	0.354589
N	-0.406006	1.421819	1.380766
O	-2.316578	2.182353	0.356991
H	4.310344	0.725799	-1.162583
H	-4.265037	-1.355245	-0.113472
H	4.156531	1.207465	0.525262
H	4.888430	-0.371596	0.124081
H	-3.210858	-0.010613	-0.572451
H	-3.335906	-1.460696	-1.621633
H	-2.497909	-2.449974	0.834889
H	-1.253764	-0.281303	-1.622457
H	0.369524	-0.329371	-0.985650
H	-0.298099	-2.489527	1.580284
H	0.977090	-1.899274	0.520763
H	-0.760536	2.820209	-1.463363
H	0.624581	2.118132	-0.739986
H	0.475205	0.998791	1.105504
H	-0.996067	0.838602	1.956095

Urea_Orientation7

C	-1.941390	2.319390	-0.352518
C	-0.569950	1.680673	-0.160923
O	0.440013	2.420333	-0.148750
O	-0.556348	0.408773	-0.019470
N	1.886920	-0.818065	-0.034170
C	2.970132	-0.057414	0.143199
N	4.194218	-0.591516	0.051161
C	4.438791	-1.991975	-0.259586
N	2.811975	1.214571	0.530658
N	-2.819364	-1.170938	-1.034704
C	-3.608468	-1.126226	0.096886
N	-2.887212	-0.875144	1.246864
O	-4.810214	-1.380826	0.094809
H	-2.429047	1.887308	-1.230378
H	5.496039	-2.191677	-0.094502
H	-2.571537	2.094924	0.512460
H	-1.855947	3.399341	-0.473513
H	3.855228	-2.630189	0.407653
H	4.193060	-2.227743	-1.299329
H	4.980742	0.038611	0.076240
H	1.986546	-1.675777	-0.553879
H	0.953712	-0.354613	-0.028202
H	3.639565	1.786004	0.606227
H	1.917772	1.686119	0.286002
H	-3.458901	-0.587604	2.026460
H	-2.025924	-0.352949	1.106889
H	-1.966135	-0.619225	-0.982281
H	-3.343215	-1.097811	-1.893559

Urea molecule

C	-0.000017	-0.142566	-0.000018
N	1.155797	0.610410	-0.083185
O	0.000003	-1.367002	0.000019
N	-1.155758	0.610362	0.083078
H	-1.127255	1.534133	-0.323116
H	-1.986231	0.089022	-0.154995
H	1.127197	1.533940	0.323595
H	1.986098	0.088916	0.155225

Trimethylamine N-oxide

TMAO_Orientation4

C	5.324993	-1.453587	-0.136533
C	3.954487	-0.783125	-0.008955
O	2.941508	-1.466368	-0.319753
O	3.959665	0.419431	0.383608
N	0.493189	-0.241413	0.067564
C	0.492205	1.100896	0.004699
N	1.607635	1.778806	0.308880
N	-0.655070	1.731302	-0.259599
C	-0.796423	3.174789	-0.236896
O	-2.227819	-0.407826	-0.840709
N	-3.218034	-0.839396	0.021032
C	-3.332352	-2.320656	-0.088147
C	-4.507584	-0.205004	-0.370849
C	-2.871533	-0.462344	1.421302
H	5.229176	-2.529136	-0.290539
H	5.855075	-1.016210	-0.988365
H	5.920848	-1.254096	0.757341
H	2.508938	1.248003	0.343999
H	1.648272	2.747717	0.033309
H	-0.234289	3.654709	-1.045419
H	-0.463780	3.586249	0.720991
H	-1.852332	3.410395	-0.366589
H	-1.442385	1.105797	-0.504513
H	-0.367520	-0.662146	-0.284648
H	1.403982	-0.721155	-0.068768
H	-2.796837	0.623226	1.458366
H	-1.906514	-0.912225	1.648206
H	-3.643482	-0.823521	2.103045
H	-2.371911	-2.741300	0.204864
H	-4.132436	-2.678844	0.561898
H	-3.540376	-2.546070	-1.132219
H	-5.305943	-0.547925	0.289680
H	-4.699672	-0.488822	-1.403769
H	-4.372448	0.872558	-0.294894

TMAO molecule

C	1.385329	-0.227144	-0.418685
N	0.000079	-0.000042	0.078924
C	-0.889679	-1.086169	-0.417765
C	-0.496277	1.313196	-0.418099
O	0.000705	0.000157	1.448408
H	1.408551	-0.230769	-1.510838
H	1.999476	0.575231	-0.014181
H	1.711363	-1.183598	-0.014253
H	-0.906362	-1.103503	-1.509913
H	-0.501106	-2.019477	-0.014532
H	-1.880359	-0.890662	-0.011563
H	-0.506035	1.334781	-1.510267
H	-1.497708	1.444083	-0.012283
H	0.169758	2.073657	-0.014614

Glycerol

Glycerol_Orientation1

C	-4.136257	-0.405848	-0.025097
C	-2.711322	-0.929618	-0.094113
O	-2.470685	-2.005668	-0.675324
O	-1.820873	-0.201201	0.487040
O	0.224882	0.866254	-0.907378
C	0.544562	1.922729	-0.001810
C	1.836687	2.517628	-0.531693
O	2.821754	1.498865	-0.675658
C	-0.586030	2.936619	0.105537
O	-1.641109	2.506189	0.953362
N	0.279352	-2.426598	-0.850523
C	1.080430	-1.913884	0.089520
N	0.538586	-1.476587	1.234907
N	2.406937	-1.920794	-0.082326
C	3.350651	-1.444896	0.922708
H	-4.457854	-0.393282	1.020056
H	4.351537	-1.548918	0.507854
H	-4.159332	0.625752	-0.385628
H	-4.814991	-1.025298	-0.611012
H	3.176352	-0.387167	1.126825
H	3.287016	-2.030168	1.844323
H	2.766023	-2.481050	-0.841152
H	1.147401	-1.032065	1.904730
H	-0.408867	-1.080352	1.143361
H	0.654717	-2.509677	-1.783525
H	-0.744569	-2.286940	-0.766168
H	0.733954	1.512178	1.001410
H	1.639173	3.008572	-1.495307
H	2.230673	3.258425	0.167734
H	-0.199950	3.867777	0.534645
H	-0.945684	3.146282	-0.912172
H	-1.823640	1.571830	0.746633
H	-0.520370	0.379223	-0.505783
H	2.330220	0.760834	-1.057904

Glycerol_Orientation6

C	-3.989539	-0.463696	-0.576816
C	-2.845987	0.459245	-0.173546
O	-1.953400	-0.053653	0.585639
O	-2.836525	1.636146	-0.597381
O	-1.133536	-2.529669	1.035282
C	-0.302078	-2.862640	-0.066399
C	0.824472	-1.840603	-0.205684
C	1.974489	-2.325228	-1.065736
O	3.057938	-1.398580	-1.044957
O	1.366784	-1.556931	1.089342
N	-0.476952	3.070697	-0.242570
C	0.591435	2.359247	0.156842
N	1.828456	2.810384	-0.074862
C	3.024276	2.068904	0.301017
N	0.397394	1.260748	0.889488
H	-4.433752	-0.908346	0.317435
H	3.890086	2.663308	0.015797
H	-4.750000	0.075139	-1.142664
H	-3.591595	-1.281084	-1.185885
H	3.050967	1.909025	1.381838
H	3.067493	1.106402	-0.215770
H	1.930148	3.633455	-0.648929
H	1.162339	0.610616	1.025491
H	-0.545909	0.819236	0.835098
H	-0.310292	3.787423	-0.932983
H	-1.377314	2.561361	-0.323219
H	0.415853	-0.914361	-0.628984
H	2.303357	-3.308270	-0.703040
H	1.655878	-2.420163	-2.106571
H	-0.864485	-2.919536	-1.007108
H	0.123443	-3.847926	0.149252
H	-1.547050	-1.659248	0.828443
H	0.627471	-1.743419	1.687845
H	3.278584	-1.306289	-0.111905

Glycerol_Orientation18

C	3.423129	-1.969742	-0.419312
C	1.950723	-1.609922	-0.300394
O	1.548775	-1.241210	0.860519
O	1.236355	-1.664807	-1.328323
O	0.168472	1.037599	1.088159
C	0.615248	1.720236	-0.084574
C	1.982067	2.335818	0.156847
H	2.276212	2.951570	-0.698618
C	-0.457275	2.749248	-0.407069
O	-1.737764	2.121325	-0.427235
N	-1.189788	-1.990835	1.079254
C	-1.888970	-1.222467	0.224830
N	-1.388312	-0.978399	-0.990039
N	-3.115300	-0.796838	0.538799
C	-4.054053	-0.264390	-0.444956
O	2.990385	1.340805	0.310186
H	-3.450422	-0.979142	1.472845
H	3.754031	-2.514913	0.466494
H	3.612531	-2.552516	-1.321181
H	3.988556	-1.034488	-0.472948
H	-1.588908	-2.146725	1.993357
H	-0.168600	-1.874215	1.046780
H	-1.710174	-0.128759	-1.435196
H	-0.389707	-1.235088	-1.143594
H	0.692962	1.007225	-0.915703
H	-0.435371	3.550607	0.344376
H	-0.288218	3.185314	-1.393675
H	1.921496	2.974510	1.048741
H	0.582589	0.149488	1.049351
H	-1.726218	1.593417	0.382628
H	-5.042637	-0.254082	0.010501
H	-3.786072	0.752860	-0.738174
H	-4.072513	-0.906954	-1.328474
H	2.609279	0.642023	0.857709

Glycerol molecule

C	1.230301	-0.100657	0.685218
C	0.022259	0.802335	0.446717
O	0.107324	1.369851	-0.860234
O	1.405206	-1.002204	-0.408247
C	-1.301211	0.061658	0.597989
O	-1.412337	-1.007724	-0.348916
H	2.138326	0.505071	0.727798
H	1.117588	-0.634765	1.636639
H	0.042808	1.621077	1.175305
H	-2.130319	0.767950	0.476565
H	-1.367733	-0.392557	1.589706
H	-1.489459	-0.578573	-1.207617
H	0.616751	0.723626	-1.365301
H	0.562402	-1.471224	-0.473454

Salt-bridge

C	3.921394	-0.239929	0.009408
C	2.399787	-0.096208	0.031723
O	1.722775	-1.134909	-0.214770
O	1.938809	1.056998	0.260664
N	-0.932455	-0.898168	0.116087
C	-1.491758	0.299662	-0.045011
N	-0.709912	1.371908	-0.229063
N	-2.826566	0.444539	-0.001528
C	-3.746990	-0.678781	0.091485
H	4.219372	-1.262459	0.246865
H	-4.747172	-0.279698	0.250740
H	4.278700	-0.002625	-0.998075
H	4.383731	0.462190	0.705543
H	-3.748092	-1.287737	-0.818099
H	-3.486221	-1.303019	0.948755
H	-3.196830	1.330877	-0.308749
H	-1.506019	-1.715310	-0.020750
H	0.107366	-0.990393	-0.018032
H	-1.123985	2.272654	-0.040368
H	0.314413	1.262389	-0.039085