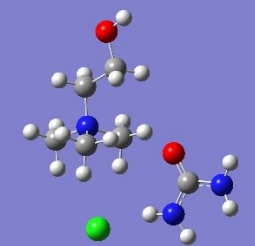
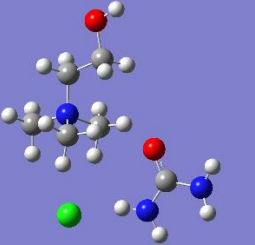
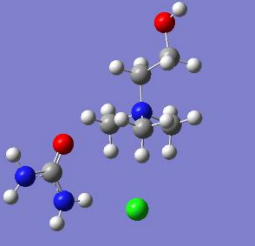
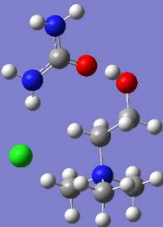
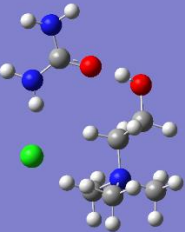
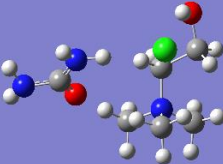


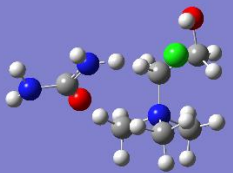
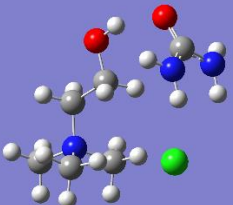
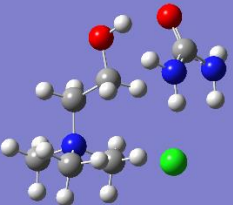
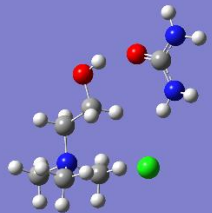
Supplementary material
Summary of research work

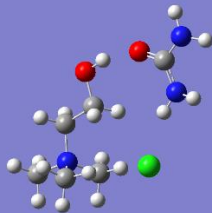
Model systems of choline chloride, and urea 1:1 ratio

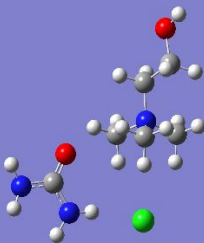
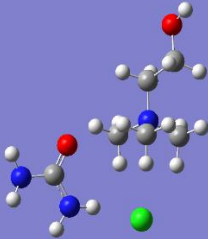
Table 1: Optimized systems of choline chloride (Trans) + 1 urea (1:1 ratio)

SYSTEM	LEVEL OF THEORY	BASIS FUNCTIONS	ENERGY (ZPE CORRECTED)	SPECIFICATIONS	REPRESENTATION
Choline chloride Trans + Urea (Conformer 1) C1	RHF	6-31+G(d,p)	-1010.30761702 H	Positive frequencies	
Choline chloride Trans + Urea (Conformer 1) C1	RB3LYP	6-31+G(d,p)	-1014.45096580 H (-1014.188386 H)	Positive frequencies	
Choline chloride Trans + Urea (Conformer 2) C1	RHF	6-31+G(d,p)	-1010,30540078 H	Positive frequencies	

Choline chloride Trans + Urea (Conformer 2) C1	RB3LYP	6-31+G(d,p)	-1014.44886138 H (-1014.186290 H)	Positive frequencies	
Choline chloride Trans + Urea (Conformer 3) C1	RHF	6-31+G(d,p)	-1010.31238812 H	Positive frequencies	
Choline chloride Trans + Urea (Conformer 3) C1	RB3LYP	6-31+G(d,p)	-1014.45772776 H (-1014.194848 H)	Positive frequencies	
Choline chloride Trans + Urea (Conformer 4) C1	RHF	6-31+G(d,p)	-1010.31126056 H	Positive frequencies	

Choline chloride Trans + Urea (Conformer 4) C1	RB3LYP	6-31+G(d,p)	-1014.45592300 H (-1014.192932 H)	Positive frequencies	
Choline chloride Trans + Urea (Conformer 5) C1	RHF	6-31+G(d,p)	-1010.30895608 H	Positive frequencies	
Choline chloride Trans + Urea (Conformer 5) C1	RB3LYP	6-31+G(d,p)	-1014.45288666 H (-1014.189257 H)	Positive frequencies	
Choline chloride Trans + Urea (Conformer 6) C1	RHF	6-31+G(d,p)	-1010.30828544 H	Positive frequencies	

Choline chloride Trans + Urea (Conformer 6) C1	RB3LYP	6-31+G(d,p)	-1014.45181167 H (-1014.188919 H)	Positive frequencies	
Choline chloride Trans + Urea (Conformer 7) C1	RHF	6-31+G(d,p)	-1010.30562100 H	Positive frequencies	
Choline chloride Trans + Urea (Conformer 7) C1	RB3LYP	6-31+G(d,p)	-1014.44949340 H (-1014.186938 H)	Positive frequencies	

Choline chloride Trans + Urea (Conformer 8) C1	RHF	6-31+G(d,p)	-1010.30536908 H	Positive frequencies	
Choline chloride Trans + Urea (Conformer 8) C1	RB3LYP	6-31+G(d,p)	-1014.44882721 H (-1014.186325 H)	Positive frequencies	
Choline chloride Trans + Urea (Conformer 9) C1	RHF	6-31+G(d,p)	-1010.31422157 H	Positive frequencies	

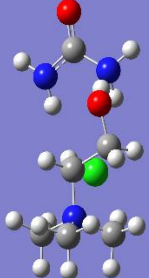
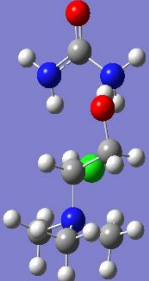
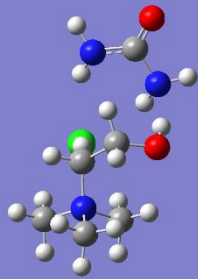
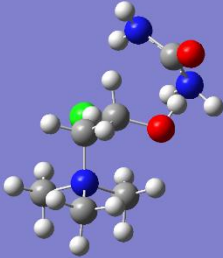
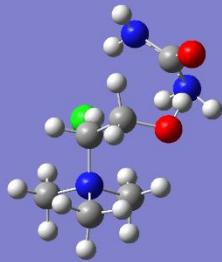
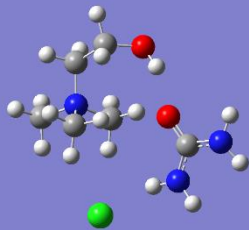
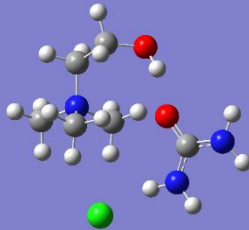
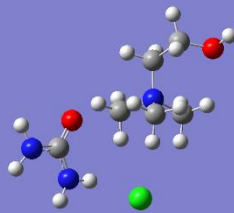
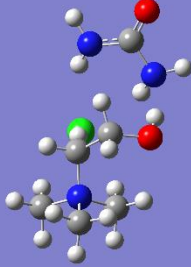
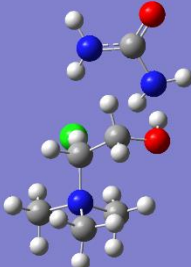
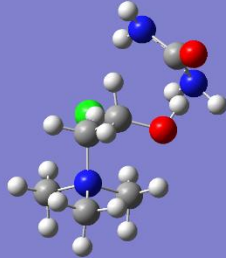
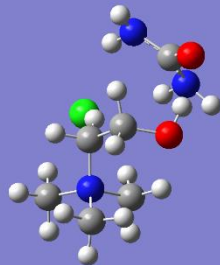
Choline chloride Trans + Urea (Conformer 9) C1	RB3LYP	6-31+G(d,p)	-1014.45840232 H (-1014.194805 H)	Positive frequencies	
Choline chloride Trans + Urea (Conformer 10) C1	RHF	6-31+G(d,p)	-1010.31112408 H	Positive frequencies	
Choline chloride Trans + Urea (Conformer 10) C1	RB3LYP	6-31+G(d,p)	-1014.5813634 H (-1014.193708 H)	Positive frequencies	

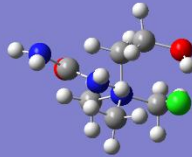
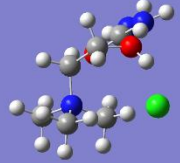
Table 2: Optimized systems of choline chloride Gauche + 1 urea (1:1 ratio)

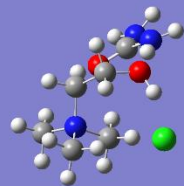
SYSTEM	LEVEL OF THEORY	BASIS FUNCTIONS	ENERGY (ZPE CORRECTED)	SPECIFICATIONS	REPRESENTATION
Choline chloride Gauche + Urea (Conformer 1) C1	RHF	6-31+G(d,p)	-1010.31563775 H	Positive frequencies	
Choline chloride Gauche + Urea (Conformer 1) C1	RB3LYP	6-31+G(d,p)	-1014.46331118 H (-1014.198607 H)	Positive frequencies	
Choline chloride Gauche + Urea (Conformer 2) C1	RHF	6-31+G(d,p)	-1010.31695749 H	Positive frequencies	

Choline chloride Gauche + Urea (Conformer 2) C1	RB3LYP	6-31+G(d,p)	-1014.46311559 H (-1014.198793 H)	Positive frequencies	
Choline chloride Gauche + Urea (Conformer 3) C1	RHF	6-31+G(d,p)	-1010.31238224 H	Positive frequencies	
Choline chloride Gauche + Urea (Conformer 3) C1	RB3LYP	6-31+G(d,p)	-1014.45801036 H (-1014.194460 H)	Positive frequencies	
Choline chloride Gauche + Urea (Conformer 4) C1	RHF	6-31+G(d,p)	-1010.30714332 H	Positive frequencies	

Choline chloride Gauche + Urea (Conformer 4) C1	RB3LYP	6-31+G(d,p)	-1014.45123504 H (-1014.188262 H)	Positive frequencies	
Choline chloride Gauche + Urea (Conformer 5) C1	RHF	6-31+G(d,p)	-1010.31563743 H	Positive frequencies	
Choline chloride Gauche + Urea (Conformer 5) C1	RB3LYP	6-31+G(d,p)	-1014.46331111 H (-1014.198610 H)	Positive frequencies	
Choline chloride Gauche + Urea (Conformer 6) C1	RHF	6-31+G(d,p)	-1010,.1695746 H	Positive frequencies	

Choline chloride Gauche + Urea (Conformer 6) C1	RB3LYP	6-31+G(d,p)	-1014.46311559 H (-1014.198793 H)	Positive frequencies	
Choline chloride Gauche + Urea (Conformer 7) C1	RHF	6-31+G(d,p)	-1010.31422557 H	Positive frequencies	
Choline chloride Gauche + Urea (Conformer 7) C1	RB3LYP	6-31+G(d,p)	-1014.45836385 H (-1014.194860 H)	Positive frequencies	
Choline chloride Gauche + Urea (Conformer 8) C1	RHF	6-31+G(d,p)	-1010.30790786 H	Positive frequencies	

Choline chloride Gauche + Urea (Conformer 8) C1	RB3LYP	6-31+G(d,p)	-1014.45813351 H (-1014.195181 H)	Positive frequencies	
Choline chloride Gauche + Urea (Conformer 9) C1	RHF	6-31+G(d,p)	-1010.31605054 H	Positive frequencies	
Choline chloride Gauche + Urea (Conformer 9) C1	RB3LYP	6-31+G(d,p)	-1014.46223652 H (-1014.199087 H)	Positive frequencies	
Choline chloride Gauche + Urea (Conformer 10) C1	RHF	6-31+G(d,p)	-1010.31306885 H	Positive frequencies	

Choline chloride Gauche + Urea (Conformer 10) C1	RB3LYP	6-31+G(d,p)	-1014.46068570 H (-1014.197101 H)	Positive frequencies	
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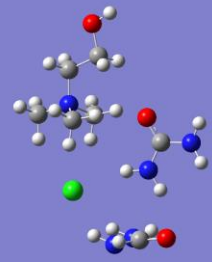
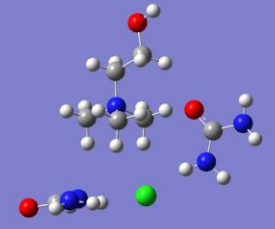
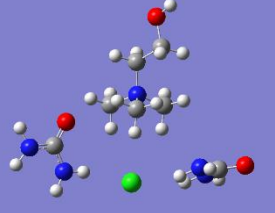
Model systems of choline chloride and urea in 1:2 ratio

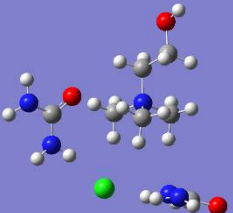
Conformers resulting from interaction of choline chloride (Trans and Gauche) with two molecules of urea.

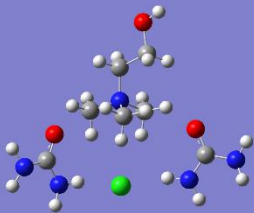
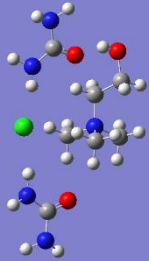
Table 3: Optimized systems of choline chloride (Trans) + 2 urea (1:2 ratio)

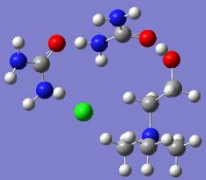
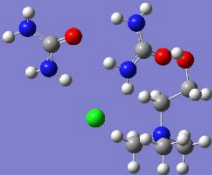
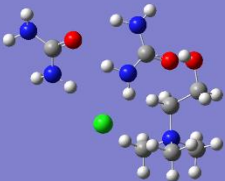
30 conformers of C1 symmetry

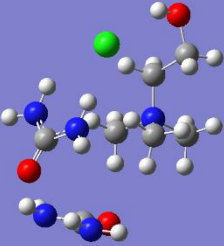
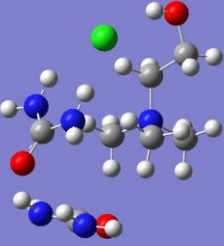
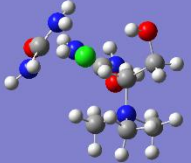
SYSTEM	LEVEL OF THEORY	BASIS FUNCTIONS	ENERGIES (ZPE CORRECTED)	SPECIFICATIONS	REPRESENTATION
Choline chloride Trans + 2 Ureas C1	RHF	6-31+G(d,p)	-1234.33991059 H	Positive frequencies	
Choline chloride Trans + 2 Ureas C1	RB3LYP	6-31+G(d,p)	-1239.76596945 H (-1239.437993 H)	Positive frequencies	
Choline chloride Trans + 2 Ureas C1	RHF	6-31+G(d,p)	-1234.34002130 H	Positive frequencies	

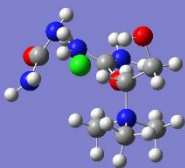
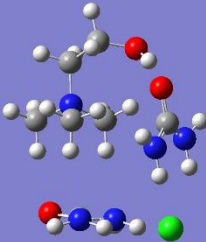
Choline chloride Trans + 2 Ureas C1	RB3LYP	6-31+G(d,p)	-1239.76489073 H (-1239.436547 H)	Positive frequencies	
Choline chloride Trans + 2 Ureas C1	RHF	6-31+G(d,p)	-1234.33908442 H	Positive frequencies	
Choline chloride Trans + 2 Ureas C1	RB3LYP	6-31+G(d,p)	-1239.76466761 H (-1239.436682 H)	Positive frequencies	
Choline chloride Trans + 2 Ureas C1	RHF	6-31+G(d,p)	-1234.33730030 H	Positive frequencies	

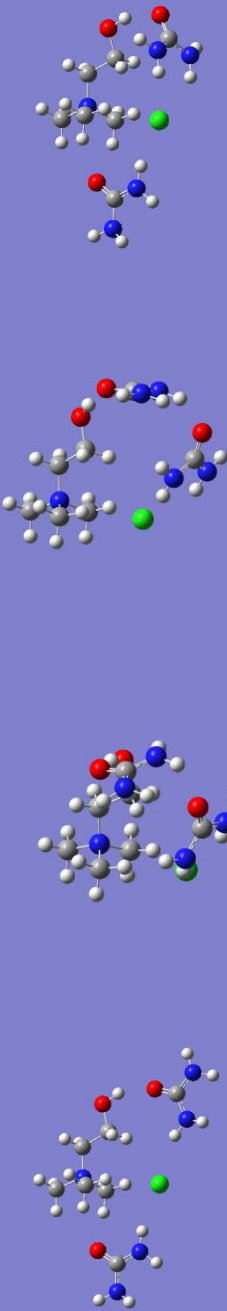
Choline chloride Trans + 2 Ureas C1	RB3LYP	6-31+G(d,p)	-1239.76305206 H (-1239.434975 H)	Positive frequencies	
Choline chloride Trans + 2 Ureas C1	RHF	6-31+G(d,p)	-1234.33664418 H	Positive frequencies	
Choline chloride Trans + 2 Ureas C1	RB3LYP	6-31+G(d,p)	-1239,6296646 H (-1239.435057 H)	Positive frequencies	
Choline chloride Trans + 2 Ureas C1	RHF	6-31+G(d,p)	-1234.33759912 H	Positive frequencies	

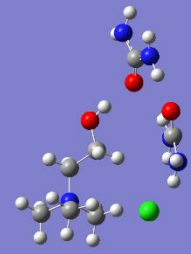
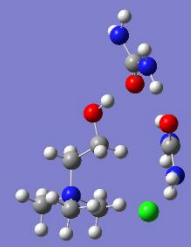
Choline chloride Trans + 2 Ureas C1	RB3LYP	6-31+G(d,p)	-1239.76258402 H (-1239.435049 H)	Positive frequencies	
Choline chloride Trans + 2 Ureas C1	RHF	6-31+G(d,p)	-1234.34488077 H	Positive frequencies	
Choline chloride Trans + 2 Ureas C1	RB3LYP	6-31+G(d,p)	-1239.77180571 H (-1239.443640 H)	Positive frequencies	
Choline chloride Trans + 2 Ureas C1	RHF	6-31+G(d,p)	-1234.34346814 H	Positive frequencies	

Choline chloride Trans + 2 Ureas C1	RB3LYP	6-31+G(d,p)	-1239,77170000 H (-1239.443142 H)	Positive frequencies	
Choline chloride Trans + 2 Ureas C1	RHF	6-31+G(d,p)	-1234.34340362 H	Positive frequencies	
Choline chloride Trans + 2 Ureas C1	RB3LYP	6-31+G(d,p)	-1239.77123671 H (-1239.442485 H)	Positive frequencies	
Choline chloride Trans + 2 Ureas C1	RHF	6-31+G(d,p)	-1234.34537396 H	Positive frequencies	

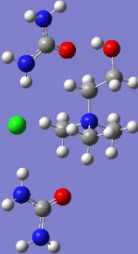
Choline chloride Trans + 2 Ureas C1	RB3LYP	6-31+G(d,p)	-1239.77275458 H (-1239.443663 H)	Positive frequencies	
Choline chloride Trans + 2 Ureas C1	RHF	6-31+G(d,p)	-1234.34430842 H	Positive frequencies	
Choline chloride Trans + 2 Ureas C1	RB3LYP	6-31+G(d,p)	-1239.77153877 H (-1239.442294 H)	Positive frequencies	
Choline chloride Trans + 2 Ureas C1	RHF	6-31+G(d,p)	-1234.34379501 H	Positive frequencies	

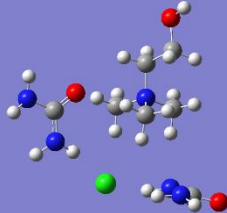
Choline chloride Trans + 2 Ureas C1	RB3LYP	6-31+G(d,p)	-1239.77134248 H (-1239.442433 H)	Positive frequencies	
Choline chloride Trans + 2 Ureas C1	RHF	6-31+G(d,p)	-1234,.3692961 H	Positive frequencies	
Choline chloride Trans + 2 Ureas C1	RB3LYP	6-31+G(d,p)	-1239.77546043 H (-1239.446594 H)	Positive frequencies	
Choline chloride Trans + 2 Ureas C1	RHF	6-31+G(d,p)	-1234.34498645 H	Positive frequencies	

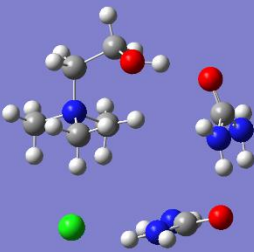
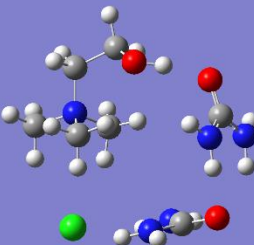
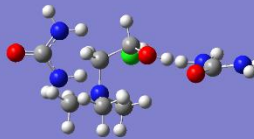
Choline chloride Trans + 2 Ureas C1	RB3LYP	6-31+G(d,p)	-1239.77119649 H (-1239.442508)	Positive frequencies	
Choline chloride Trans + 2 Ureas C1	RHF	6-31+G(d,p)	-1234,.4113812 H	Positive frequencies	
Choline chloride Trans + 2 Ureas C1	RB3LYP	6-31+G(d,p)	-1239.77021662 H (-1239.440637)	Positive frequencies	
Choline chloride Trans + 2 Ureas C1	RHF	6-31+G(d,p)	-1234,.4321657 H	Positive frequencies	

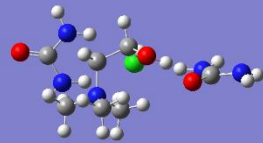
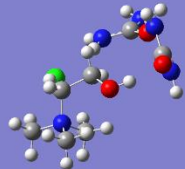
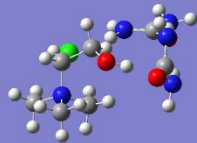
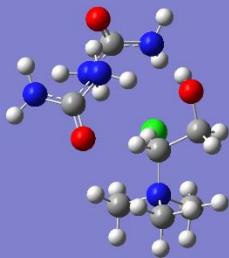
Choline chloride Trans + 2 Ureas C1	RB3LYP	6-31+G(d,p)	-1239.76868606 H (-1239.440774 H)	Positive frequencies	
Choline chloride Trans + 2 Ureas C1	RHF	6-31+G(d,p)	-1234.4017710 H	Positive frequencies	
Choline chloride Trans + 2 Ureas C1	RB3LYP	6-31+G(d,p)	-1239.76864098 H (-1239.439749 H)	Positive frequencies	
Choline chloride Trans + 2 Ureas C1	RHF	6-31+G(d,p)	-1234.34125219 H	Positive frequencies	

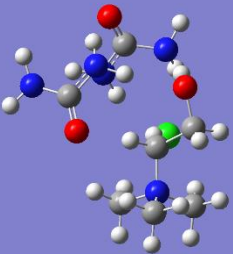
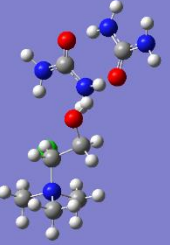
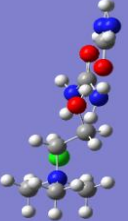
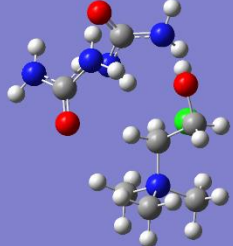
Choline chloride Trans + 2 Ureas C1	RB3LYP	6-31+G(d,p)	-1239.76664853 H (-1239.438203 H)	Positive frequencies	
Choline chloride Trans + 2 Ureas C1	RHF	6-31+G(d,p)	-1234.33991057 H	Positive frequencies	
Choline chloride Trans + 2 Ureas C1	RB3LYP	6-31+G(d,p)	-1239.76596945 H (-1239.437993 H)	Positive frequencies	
Choline chloride Trans + 2 Ureas C1	RHF	6-31+G(d,p)	-1234.34002140 H	Positive frequencies	

Choline chloride Trans + 2 Ureas C1	RB3LYP	6-31+G(d,p)	-1239,.6489073 H (-1239.436547 H)	Positive frequencies	
Choline chloride Trans + 2 Ureas C1	RHF	6-31+G(d,p)	-1234.33958011 H	Positive frequencies	
Choline chloride Trans + 2 Ureas C1	RB3LYP	6-31+G(d,p)	-1239.76481065 H (-1239.436887 H)	Positive frequencies	
Choline chloride Trans + 2 Ureas C1	RHF	6-31+G(d,p)	-1234.34488079 H	Positive frequencies	

Choline chloride Trans + 2 Ureas C1	RB3LYP	6-31+G(d,p)	-1239.77180571 H (-1239.443640 H)	Positive frequencies	
Choline chloride Trans + 2 Ureas C1	RHF	6-31+G(d,p)	-1234.33730788 H	Positive frequencies	
Choline chloride Trans + 2 Ureas C1	RB3LYP	6-31+G(d,p)	-1239.76303760 H (-1239.434973 H)	Positive frequencies	
Choline chloride Trans + 2 Ureas C1	RHF	6-31+G(d,p)	-1234.33659722 H	Positive frequencies	

Choline chloride Trans + 2 Ureas C1	RB3LYP	6-31+G(d,p)	-1239.76291764 H (-1239.434972 H)	Positive frequencies	
Choline chloride Trans + 2 Ureas C1	RHF	6-31+G(d,p)	-1234.35016976 H	Positive frequencies	
Choline chloride Trans + 2 Ureas C1	RB3LYP	6-31+G(d,p)	-1239.77947578 H (-1239.450107 H)	Positive frequencies	
Choline chloride Trans + 2Ureas C1	RHF	6-31+G(d,p)	-1234.34659867 H	Positive frequencies	

Choline chloride Trans + 2 Ureas C1	RB3LYP	6-31+G(d,p)	-1239.77499024 H (-1239.445587 H)	Positive frequencies	
Choline chloride Trans + 2 Ureas C1	RHF	6-31+G(d,p)	-1234.34733258 H	Positive frequencies	
Choline chloride Trans + 2 Ureas C1	RB3LYP	6-31+G(d,p)	-1239.77450874 H (-1239.445622 H)	Positive frequencies	
Choline chloride Trans + 2 Ureas C1	RHF	6-31+G(d,p)	-1234.34373431 H	Positive frequencies	

Choline chloride Trans + 2 Ureas C1	RB3LYP	6-31+G(d,p)	-1239.77315830 H (-1239.442770 H)	Positive frequencies	
Choline chloride Trans + 2 Ureas C1	RHF	6-31+G(d,p)	-1234.34226373 H	Positive frequencies	
Choline chloride Trans + 2 Ureas C1	RB3LYP	6-31+G(d,p)	-1239.77242726 H (-1239.443599 H)	Positive frequencies	
Choline chloride Trans + 2 Ureas C1	RHF	6-31+G(d,p)	-1234.34321273 H	Positive frequencies	

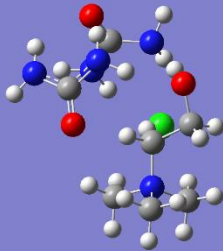
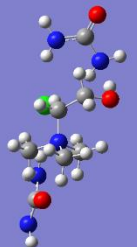
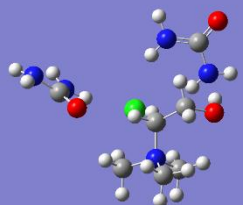
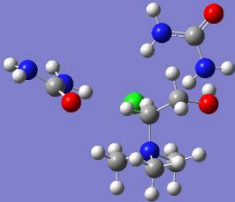
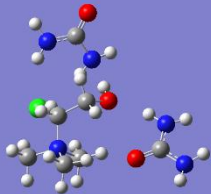
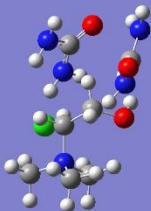
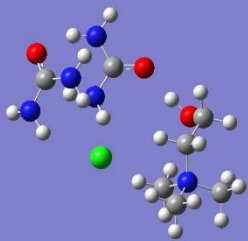
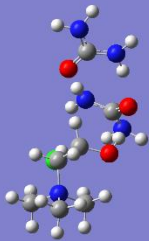
Choline chloride Trans + 2 Ureas C1	RB3LYP	6-31+G(d,p)	-1239.77211248 H (-1239.441883 H)	Positive frequencies	
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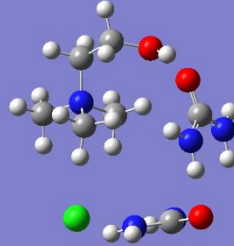
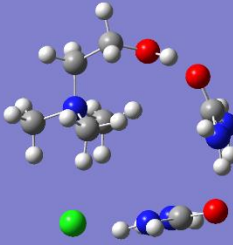
Table 4: Optimized systems of choline chloride (Gauche) + 2 ureas (1:2 ratio)

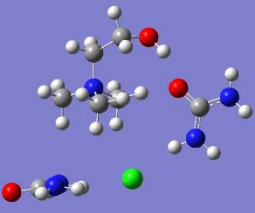
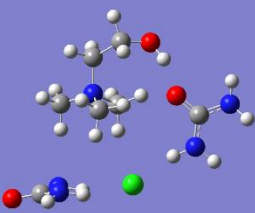
24 conformers of C1 symmetry

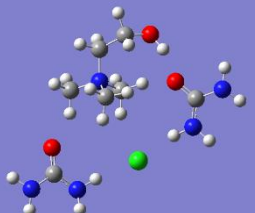
SYSTEM	Level of theory	BASIS FUNCTIONS	ENERGIES (ZPE CORRECTED)	SPECIFICATIONS	REPRESENTATION
Choline chloride Gauche + 2 Ureas C1	RHF	6-31+G(d,p)	-1234.34649304 H	Positive frequencies	
Choline chloride Gauche + 2 Ureas C1	RB3LYP	6-31+G(d,p)	-1239.77522375 H (-1239.445795 H)	Positive frequencies	
Choline chloride Gauche + 2 Ureas C1	RHF	6-31+G(d,p)	-1234.34574908 H	Positive frequencies	

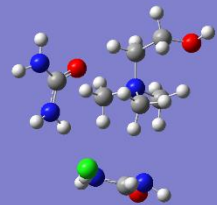
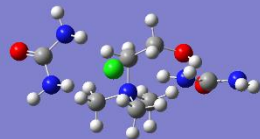
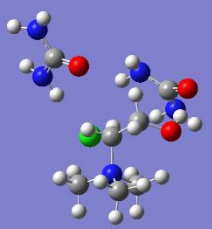
Choline chloride Gauche + 2 Ureas C1	RB3LYP	6-31+G(d,p)	-1239.77460645 H (-1239.445269 H)	Positive frequencies	
Choline chloride Gauche + 2 Ureas C1	RHF	6-31+G(d,p)	-1234.34386688 H	Positive frequencies	
Choline chloride Gauche + 2 Ureas C1	RB3LYP	6-31+G(d,p)	-1239.77450134 H (-1239.444645)	Positive frequencies	
Choline chloride Gauche + 2 Ureas C1	RHF	6-31+G(d,p)	-1234.34903984 H	Positive frequencies	

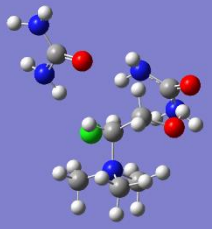
Choline chloride Gauche + 2 Ureas C1	RB3LYP	6-31+G(d,p)	-1239.77752056 H (-1239.447589 H)	Positive frequencies	
Choline chloride Gauche + 2 Ureas C1	RHF	6-31+G(d,p)	-1234.34851685 H	Positives frequencies	
Choline chloride Gauche + 2 Ureas C1	RB3LYP	6-31+G(d,p)	-1239.77729932 H (-1239.4458759 H)	Positive frequencies	
Choline chloride Gauche + 2 Ureas C1	RHF	6-31+G(d,p)	-1234.4640858 H	Positive frequencies	

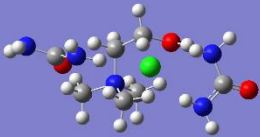
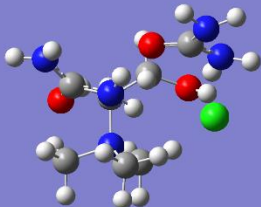
Choline chloride Gauche + 2 Ureas C1	RB3LYP	6-31+G(d,p)	-1239.77663143 H (-1239.446815 H)	Positive frequencies	
Choline chloride Gauche + 2 Ureas C1	RHF	6-31+G(d,p)	-1234.35017009 H	Positive frequencies	
Choline chloride Gauche + 2 Ureas C1	RB3LYP	6-31+G(d,p)	-1239.77947555 H (-1239.450108 H)	Positive frequencies	
Choline chloride Gauche + 2 Ureas C1	RHF	6-31+G(d,p)	-1234.34635988 H	Positive frequencies	

Choline chloride Gauche + 2 Ureas C1	RB3LYP	6-31+G(d,p)	-1239.77509677 H (-1239.445958 H)	Positive frequencies	
Choline chloride Guache + 2 Ureas C1	RHF	6-31+G(d,p)	-1234.34550937 H	Positive frequencies	
Choline chloride Gauche + 2 Ureas C1	RB3LYP	6-31+G(d,p)	-1239.77373195 H (-1239.444815 H)	Positive frequencies	
Choline chloride Gauche + 2 Ureas C1	RHF	6-31+G(d,p)	-1234.34314622 H	Positive frequencies	

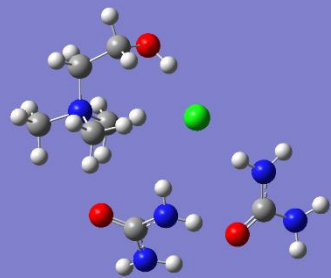
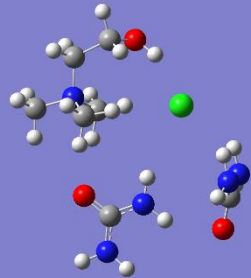
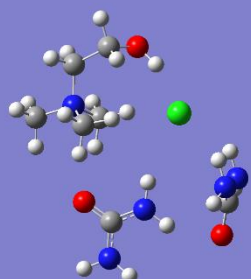
Choline chloride + 2 Ureas C1	RB3LYP	6-31+G(d,p)	-1239.77038824 H (-1239.442527 H)	Positive frequencies	
Choline chloride + 2 Ureas C1	RHF	6-31+G(d,p)	-1234.34080851 H	Positive frequencies	
Choline chloride Gauche + 2 Ureas C1	RB3LYP	6-31+G(d,p)	-1239.76717355 H (-1239.439435 H)	Positive frequencies	
Choline chloride Gauche + 2 Ureas C1	RHF	6-31+G(d,p)	-1234.34060947 H	Positive frequencies	

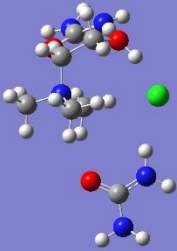
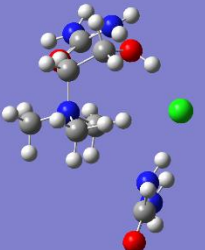
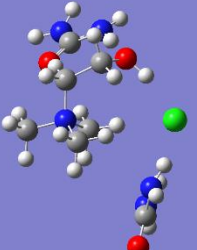
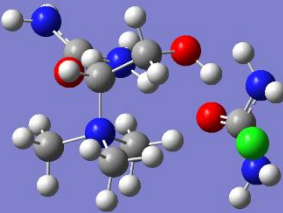
Choline chloride Gauche + 2 Ureas C1	RB3LYP	6-31+G(d,p)	-1239.76680049 H (-1239.438120 H)	Positive frequencies	
Choline chloride Gauche + 2 Ureas C1	RHF	6-31+G(d,p)	-1234.34659868 H	Positive frequencies	
Choline chloride Gauche + 2 Ureas C1	RB3LYP	6-31+G(d,p)	-1239.77499025 H (-1239.445588 H)	Positive frequencies	
Choline chloride Gauche + 2 Ureas C1	RHF	6-31+G(d,p)	-1234.34700389 H	Positive frequencies	

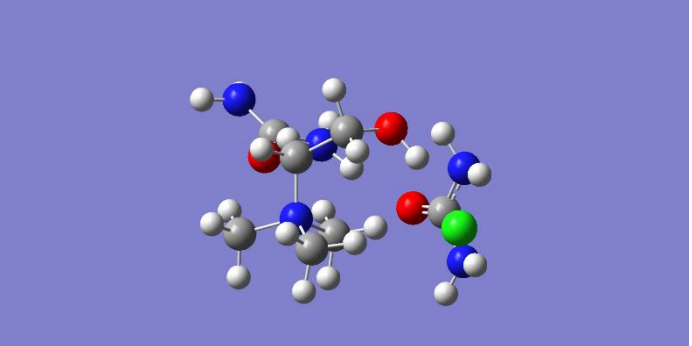
Choline chloride Gauche + 2 Ureas C1	RB3LYP	6-31+G(d,p)	-1239.77463632 H (-1239.445450 H)	Positive frequencies	
Choline chloride Gauche + 2 Ureas C1	RHF	6-31+G(d,p)	-1234.34638136 H	Positive frequencies	
Choline chloride Gauche + 2 Ureas C1	RB3LYP	6-31+G(d,p)	-1239.77387743 H (-1239.445029 H)	Positive frequencies	
Choline chloride Gauche + 2 Ureas C1	RHF	6-31+G(d,p)	-1234.34497767 H	Positive frequencies	

Choline chloride Gauche + 2 Ureas C1	RB3LYP	6-31+G(d,p)	-1239.77437127 H (-1239.444786 H)	Positive frequencies	
Choline chloride Gauche + 2 Ureas C1	RHF	6-31+G(d,p)	-1234.34542801 H	Positive frequencies	
Choline chloride Gauche + 2 Ureas C1	RB3LYP	6-31+G(d,p)	-1239.77320182 H (-1239.444743 H)	Positive frequencies	
Choline chloride Gauche + 2 Ureas C1	RHF	6-31+G(d,p)	-1234.34421004 H	Positive frequencies	

Choline chloride Gauche + 2 Ureas C1	RB3LYP	6-31+G(d,p)	-1239.77276864 H (-1239.444332 H)	Positive frequencies	
Choline chloride Gauche + 2 Ureas C1	RHF	6-31+G(d,p)	-1234.34753003 H	Positive frequencies	
Choline chloride Gauche + 2 Ureas C1	RB3LYP	6-31+G(d,p)	-1239.77620479 H (-1239.447730 H)	Positive frequencies	
Choline chloride Gauche + 2 Ureas C1	RHF	6-31+G(d,p)	-1234.34720717 H	Positive frequencies	

Choline chloride Gauche + 2 Ureas C1	RB3LYP	6-31+G(d,p)	-1239.77592049 H (-1239.446891 H)	Positive frequencies	
Choline chloride Gauche + 2 Ureas C1	RHF	6-31+G(d,p)	-1234.34741917 H	Positive frequencies	
Choline chloride Gauche + 2 Ureas C1	RB3LYP	6-31+G(d,p)	-1239.77483634 H (-1239.445945 H)	Positive frequencies	
Choline chloride Gauche + 2 Ureas C1	RHF	6-31+G(d,p)	-1234.34527097 H	Positive frequencies	

Choline chloride Gauche + 2 Ureas C1	RB3LYP	6-31+G(d,p)	-1239.77453473 H (-1239.445981 H)	Positive frequencies	
Choline chloride Gauche + 2 Ureas C1	RHF	6-31+G(d,p)	-1234.4509263 H	Positive frequencies	
Choline chloride Gauche + 2 Ureas C1	RB3LYP	6-31+G(d,p)	-1239.77390186 H (-1239.444800 H)	Positive frequencies	
Choline chloride Gauche + 2 Ureas C1	RHF	6-31+G(d,p)	-1234.34464822 H	Positive frequencies	

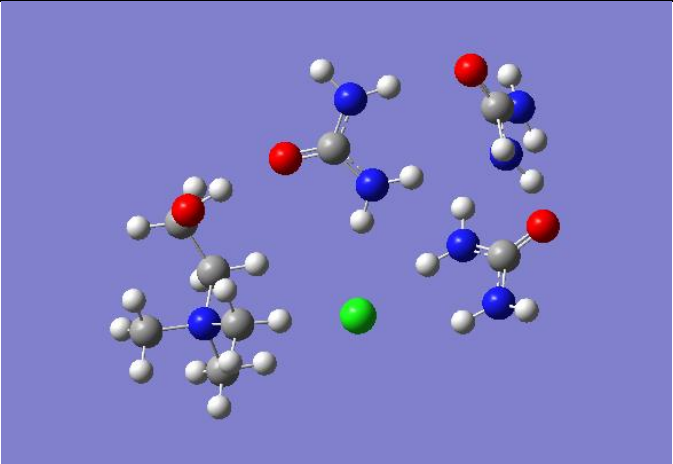
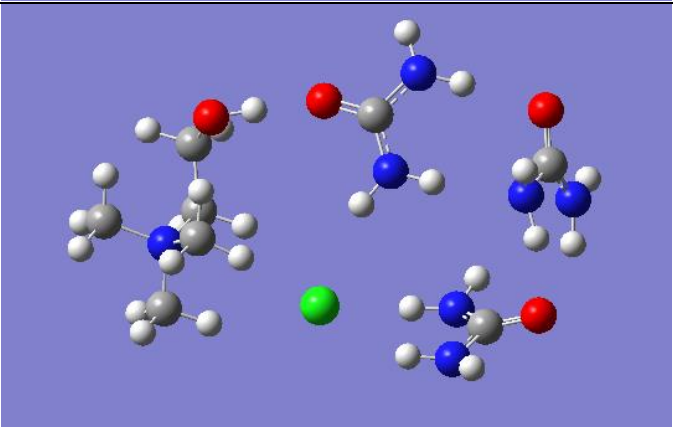
Choline chloride Gauche + 2 Ureas C1	RB3LYP	6-31+G(d,p)	-1239.77333900 H (-1239.444807 H)	Positive frequencies	
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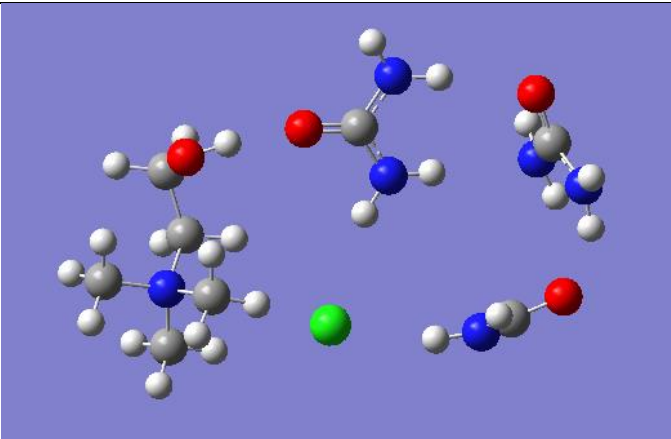
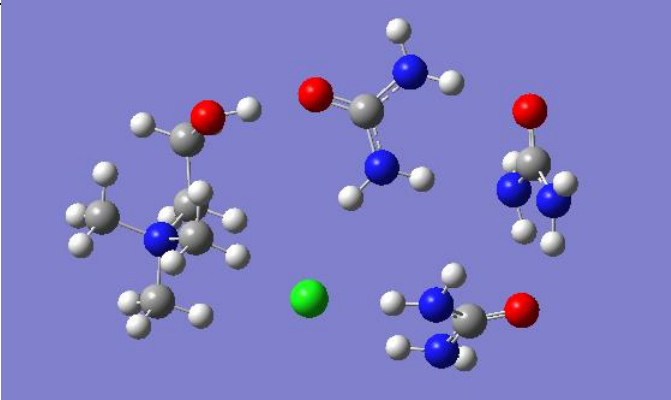
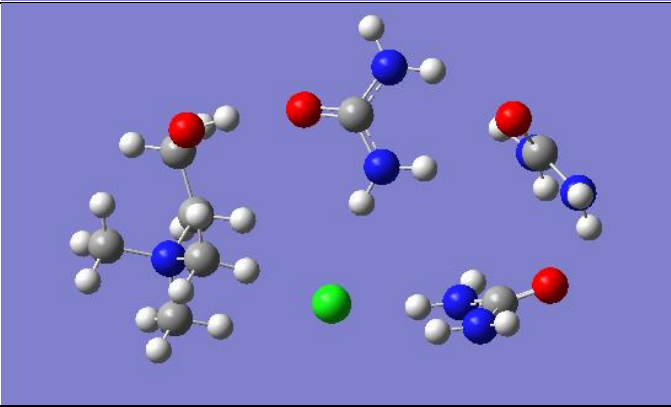
Model systems of choline chloride and urea in 1:3 ratio

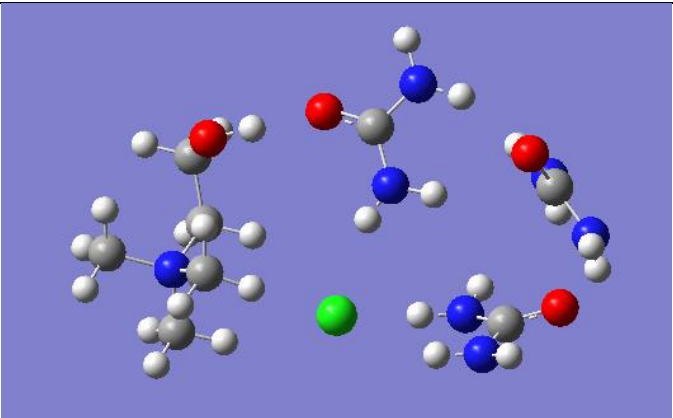
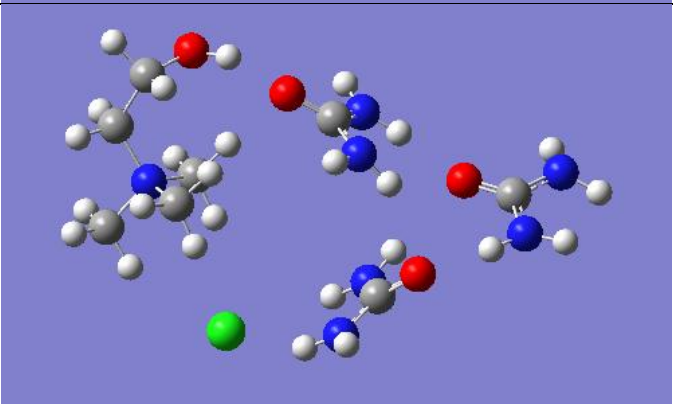
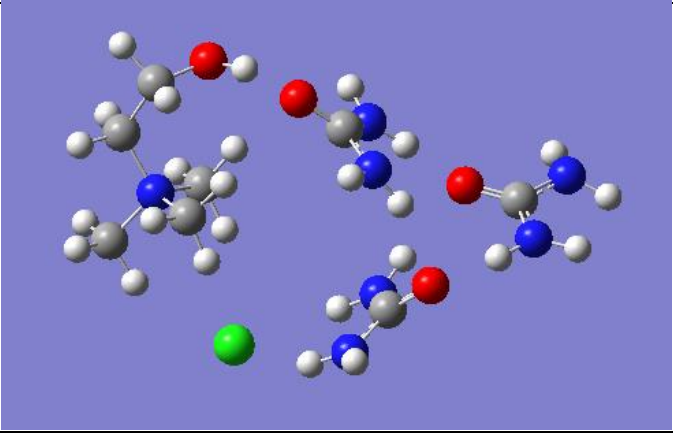
Conformers resulting from interaction of choline chloride (Trans and Gauche) with three molecules of urea.

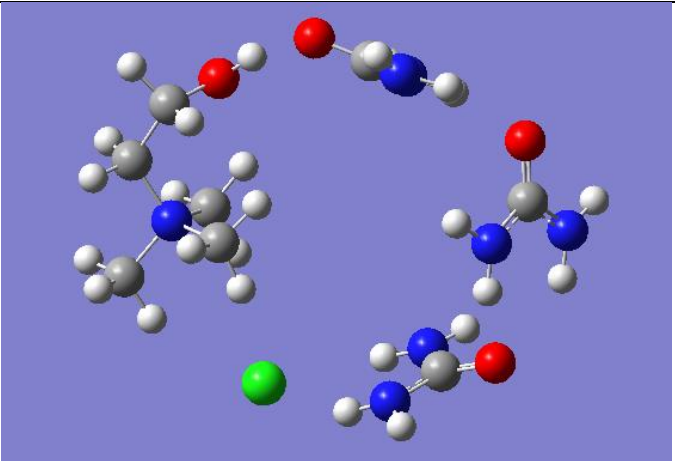
Table 5: Optimized systems of choline chloride + 3 ureas (ratio of 1:3)

5 Conformers of C1 symmetry

SYSTEM	Level of theory	Basis functions	Energies (ZPE Corrected)	Specifications	REPRESENTATION	
Choline chloride + 3 Ureas C1	RHF	6-31+G(d,p)	-1458.38448463 H	Positive frequencies		
Choline chloride + 3 Ureas C1	RB3LYP	6-31+G(d,p)	-1465.09649002 H (-1464.701126 H)	Positive frequencies		

Choline chloride + 3 Ureas C1	RHF	6-31+G(d,p)	-1458.38417220 H	Positive frequencies			
Choline chloride + 3 Ureas C1	RB3LYP	6-31+G(d,p)	-1465.09611181 H (-1464.700720 H)	Positive frequencies			
Choline chloride + 3 Ureas C1	RHF	6-31+G(d,p)	-1458.38428362 H	Positive frequencies			

Choline chloride + 3 Ureas C1	RB3LYP	6-31+G(d,p)	-1465.09514050 H (-1464.700478 H)	Positive frequencies	
Choline chloride + 3 Ureas C1	RHF	6-31+G(d,p)	-1458.38117028 H	Positive frequencies	
Choline chloride + 3 Ureas C1	RB3LYP	6-31+G(d,p)	-1465.09469003 H (-1464.700157 H)	Positive frequencies	

Choline chloride + 3 Ureas C1	RHF	6-31+G(d,p)	-1458.38232017 H	Positive frequencies		
Choline chloride + 3 Ureas C1	RB3LYP	6-31+G(d,p)	-1465.09452841 H (-1464.699833 H)	Positive frequencies		