

Supporting Information

Theoretical Evidence of Charge Transfer Interaction between SO₂ and
Deep Eutectic Solvents formed by ChCl and Glycerol

Hongping Li,^a Yonghui Chang,*^b Wenshuai Zhu,^a Changwei Wang,^c Chao Wang,^a

Siwen Zhu,^a Ming Zhang,^d and Huaming Li*^{a,d}

^a *School of Chemistry and Chemical Engineering, Jiangsu University, Zhenjiang
212013, P. R. China*

^b *College of Chemistry and Chemical Engineering, Hainan Normal University,
Haikou, Hainan 571158, P. R. China*

^c *Department of Chemistry, School of Science, China University of Petroleum (East
China), Tsingtao 266580, P. R. China.*

^d *Institute for Energy Research, Jiangsu University, Zhenjiang 212013, P. R. China*

***Corresponding author:** Tel.:+86-511-88791800; Fax: +86-511-88791708;

E-mail address: lihm@ujs.edu.cn (H. M. Li), qqchang@sohu.com (Y. H. Chang)

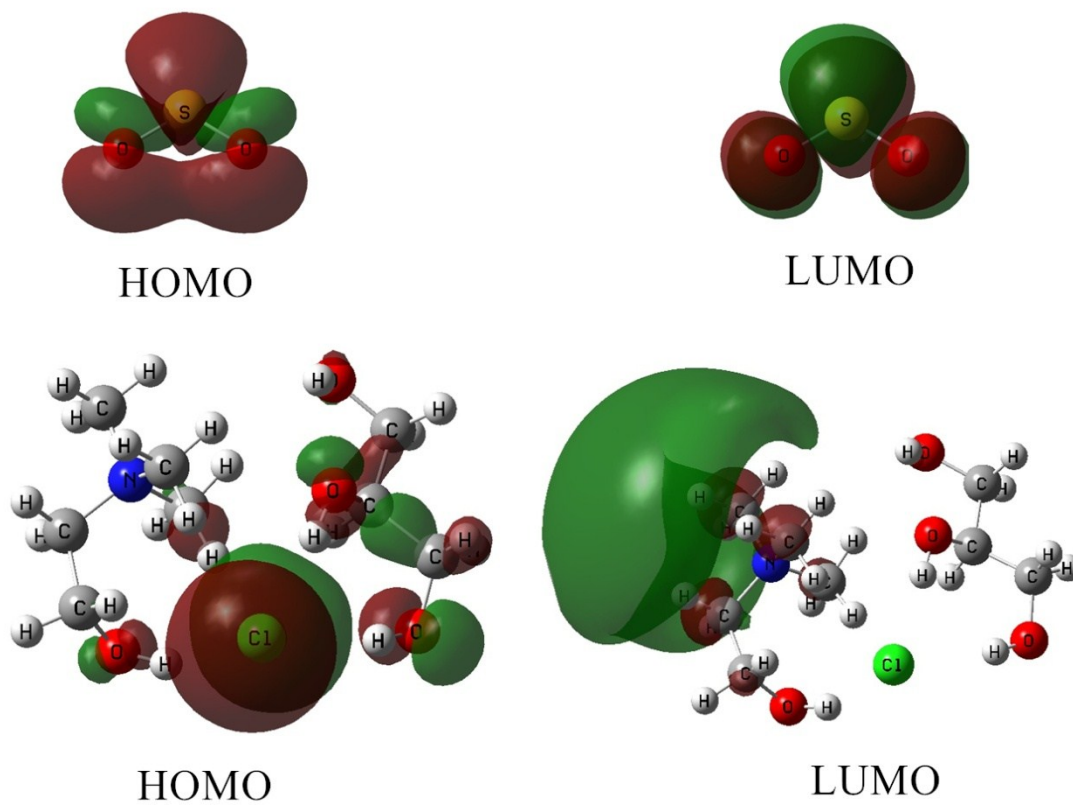


Figure S1. Frontier orbitals for SO₂ and DES.

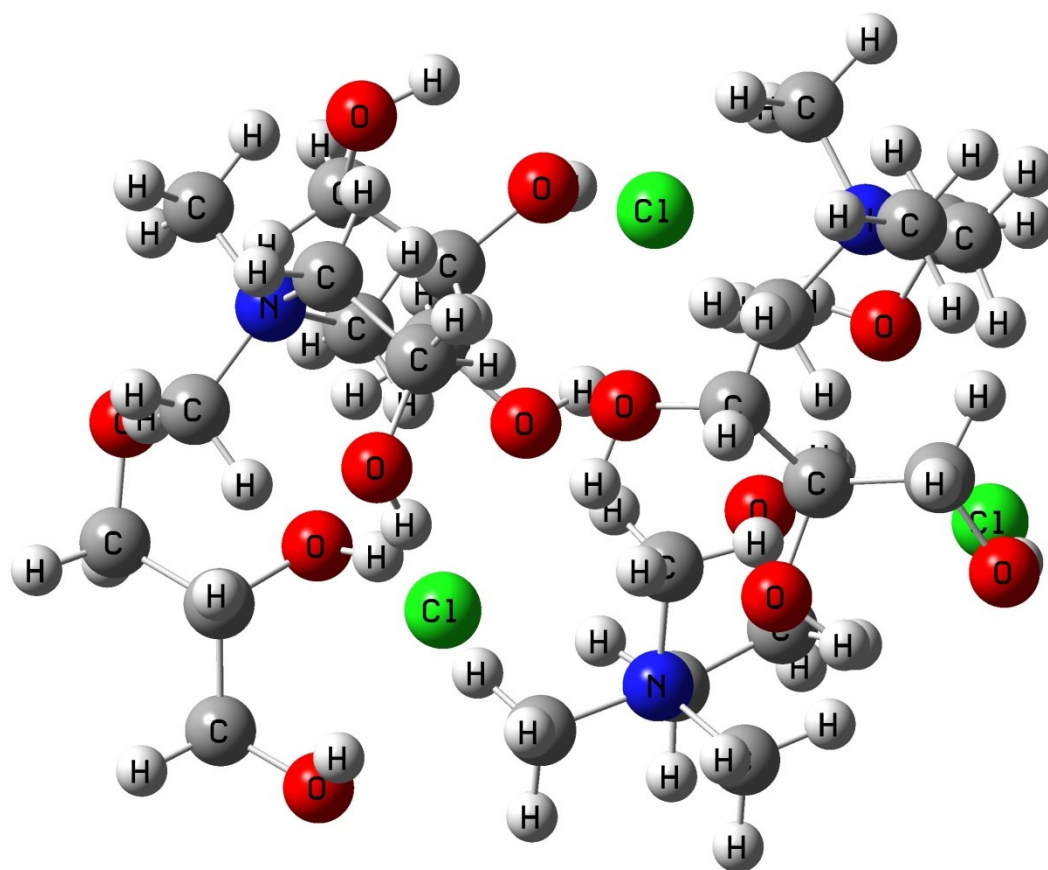


Figure S2. Optimized configuration of pure solvents (cluster-3)

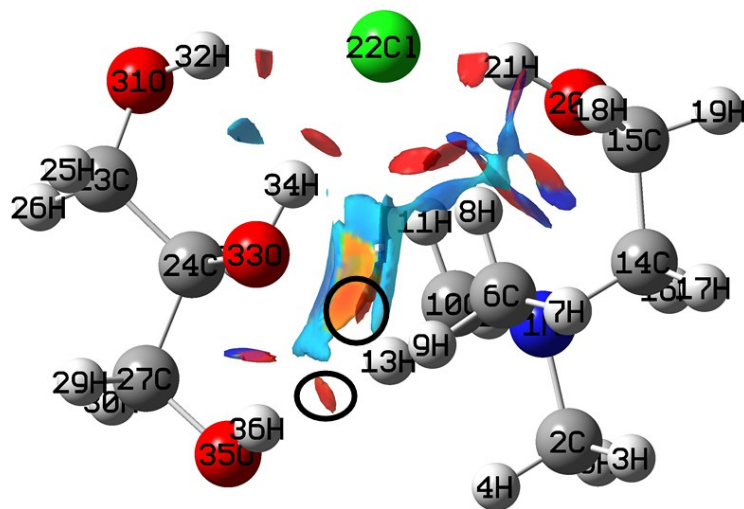


Figure S3. Gradient isosurfaces ($s = 0.35$ au) for complex-c. The surface is colored on a red-green-blue scale according to values of $\sin(\lambda_2)\rho$, ranging from -0.02 to 0.02 au. Red indicates strong attractive interactions, and blue indicates strong nonbonded overlap.

* The colors in the black cycles are red, which means a strong attractive interaction between O33...H9 and O35...H13. These results should be a direct evidence for the hydrogen bonding between C-H groups and O atoms.

Table S1. Charge analysis on interaction of SO₂ for different Ch-cation-based species
(MK charge was used)

	before	after	Δ_Q	SO ₂ (Δ_Q)
Ch ⁺	1.000	0.975	-0.025	0.025
[Ch ₂ Cl] ⁺	1.000	1.104	0.104	-0.104
[ChCl ₂] ⁻	-1.000	-0.731	0.269	-0.269

Table S2. Calculated entropies for different clusters.

	entropy (unit: cal/mol*K)
cluster-2-a	261.61
cluster-2-b	250.63
cluster-2-c	248.87

* Strictly speaking, the definition of the compactness in the current manuscript is difficult. Generally, the compactness can be estimated by the volumes of the clusters. Lower volume value means higher compactness of the cluster. According to the Glasser's theory, the values of the volumes for ionic liquids are linearly correlated to the entropies.[1-3] Because of the similarity with ionic liquids, the DESs may possess the same relationship between entropies and volumes. Hence, the entropies of three clusters have been calculated (**Table S2**). These results show the order of the entropy follows: cluster-2-a < cluster-2-b < cluster-2-c. According to the Glasser's theory, it can be roughly known that the volume of the clusters also follow the same order.

[1] L. Glasser, *Thermochim Acta*, 2004, 421, 87-93.

[2] J. Wei, C. Chang, Y. Y. Zhang, S. Y. Hou, D. W. Fang and W. Guan, *J Chem Thermodyn*, 2015, 90, 310-316.

[3] Q. S. Liu, J. Liu, X. X. Liu and S. T. Zhang, *J Chem Thermodyn*, 2015, 90, 39-45.

The optimized geometries of the crucial structure reported in the paper

	abs-com-a		
N	-2.16658900	-1.12067700	0.55704100
C	-2.29277800	-2.38501700	1.33975300
H	-2.73318800	-3.15559500	0.70487500
H	-1.29729400	-2.68740800	1.66828100
H	-2.93010000	-2.19963000	2.20580300
C	-1.27155300	-1.37306000	-0.61949000
H	-1.73127100	-2.13438900	-1.25274600
H	-1.12427000	-0.44199500	-1.16785400
H	-0.30996000	-1.71596200	-0.23895000
C	-1.53450700	-0.08450100	1.44509300
H	-1.32215700	0.80273700	0.85035000
H	-2.24017800	0.15627300	2.24154000
H	-0.60861100	-0.51339000	1.83668100
C	-3.54885200	-0.70851600	0.10322600
C	-3.64585900	0.58446200	-0.69857300
H	-4.15135900	-0.60963800	1.01142200
H	-3.92877600	-1.54741500	-0.48904900
H	-2.94187700	0.59241700	-1.53866600
H	-4.66010500	0.58597200	-1.12068100
O	-3.47759300	1.70974200	0.11893800
H	-2.69449100	2.19716000	-0.20231800
Cl	-0.69279300	2.23443200	-1.21347400
C	2.69177400	2.06703000	0.79273800
C	1.74596300	0.90808400	1.08996300
H	3.38039800	1.74636200	-0.00627800
H	3.29023700	2.28910100	1.68415600
C	2.41911200	-0.19159500	1.90107200
H	0.88998700	1.30639300	1.65633600
H	3.35585400	-0.49473700	1.41101200
H	2.66903900	0.19683600	2.89295900
O	2.02790200	3.26082400	0.46167800
H	1.33321000	3.09863600	-0.19919400
O	1.25974200	0.31293300	-0.10899400
H	0.64597500	0.94788200	-0.57569200
O	1.57108500	-1.31229400	2.08357100
H	1.70731200	-1.89490800	1.32302900
S	2.27213700	-1.33477600	-1.57551900
O	1.10054300	-1.43615000	-2.42413400
O	2.34472500	-2.31133200	-0.49101300

abs-com-b

N	-1.98738300	-1.78918200	-0.27062900
C	-3.44381300	-1.74618700	-0.59070100
H	-3.72518700	-0.70809800	-0.77725400
H	-3.62770200	-2.35218900	-1.47903200
H	-4.00353300	-2.14616900	0.25649200
C	-1.22519100	-1.20269400	-1.42336200
H	-1.45989500	-0.13907600	-1.48277600
H	-0.16029500	-1.37212100	-1.26335600
H	-1.54564200	-1.72110300	-2.32913400
C	-1.55883700	-3.21368400	-0.07908700
H	-0.47469400	-3.24708900	0.02591300
H	-2.04239100	-3.60653700	0.81616400
H	-1.86746100	-3.77448700	-0.96346800
C	-1.78687200	-0.96851300	0.99233500
C	-0.34990500	-0.76384900	1.43875100
H	-2.34584000	-1.48665000	1.77748500
H	-2.24597000	0.00143800	0.78851100
H	0.25235200	-0.36980200	0.60993100
H	-0.40145100	0.02153700	2.20482900
O	0.20638900	-1.92926500	1.98727800
H	0.94048000	-2.21793800	1.40726800
Cl	1.99425000	-2.46372800	-0.47976100
C	3.18250700	0.65381500	0.62098600
C	2.38145800	1.37445200	-0.45838100
H	2.49351400	0.09429800	1.27251500
H	3.69025300	1.40791500	1.23585800
C	1.42245200	2.39020900	0.16173100
H	3.08364900	1.88077100	-1.13566800
H	0.92094000	1.95143400	1.03740900
H	1.94324800	3.30062400	0.46799800
O	4.16669000	-0.18457300	0.07544100
H	3.77039400	-1.05706400	-0.09557200
O	1.56065500	0.50064800	-1.21999100
H	1.88563000	-0.42466900	-1.17536200
O	0.43027300	2.75972800	-0.79989500
H	0.37882800	2.00764200	-1.42043900
S	-1.76088700	2.87601200	0.08010300
O	-1.40230900	2.37977600	1.40077600
O	-2.33749900	1.87462100	-0.81651500

abs-com-e

N	2.64010300	0.16562700	1.17227900
C	3.55771800	1.04560500	1.95134100
H	3.49144400	2.05729100	1.54929200
H	3.24784500	1.03842700	2.99737200
H	4.57706900	0.66836400	1.85704800
C	1.22964100	0.65261800	1.37472900
H	1.17143600	1.68431400	1.03375600
H	0.53785000	0.03755000	0.79978500
H	0.99371300	0.58499100	2.43810200
C	2.76676300	-1.24026800	1.65913700
H	2.00906500	-1.85312200	1.17140200
H	3.77196800	-1.59995200	1.42952900
H	2.60112400	-1.24604000	2.73787800
C	3.02359200	0.26360900	-0.28808100
C	2.32808000	-0.74102900	-1.21220300
H	4.10856200	0.13215000	-0.34268900
H	2.75431900	1.27322300	-0.61068500
H	2.73878000	-1.74683300	-1.07934400
H	1.25462200	-0.78100800	-0.99741600
O	2.58359100	-0.35745600	-2.53504800
H	2.00103000	0.40130000	-2.72546800
Cl	0.46226200	1.93772900	-1.85318900
C	-2.50537100	2.14370100	0.93773100
C	-2.95530100	0.72393200	0.60826000
H	-2.86242400	2.39875400	1.93945300
H	-2.97503100	2.83725600	0.22592500
C	-2.55991800	0.27154400	-0.80062200
H	-2.49646200	0.02585700	1.32490000
H	-3.24724300	-0.52404400	-1.11528700
H	-2.64425800	1.09613700	-1.52050000
O	-1.09969800	2.27791800	0.94239400
H	-0.76553300	2.35958100	0.03068000
O	-4.36764300	0.73693100	0.73391000
H	-4.69020100	-0.17131000	0.70693300
O	-1.23960800	-0.25265100	-0.82766100
H	-0.62806500	0.39417300	-1.28011100
S	-1.13719200	-2.56599100	-0.35686200
O	-2.44105600	-2.54818200	0.28297900
O	0.01380000	-2.46034100	0.53539400

abs-com-d

N	-1.03583100	-2.14251600	-0.18200500
C	-0.91849700	-3.43090800	-0.92465300
H	-1.75672800	-3.51954100	-1.61750200
H	0.02626300	-3.43157700	-1.47034800
H	-0.93315900	-4.25348100	-0.20774600
C	-1.04208600	-1.00795700	-1.16104900
H	-1.94958200	-1.06165000	-1.76478300
H	-1.01081900	-0.07772200	-0.60065400
H	-0.14474400	-1.07162200	-1.77627800
C	0.16070200	-2.00613600	0.71756100
H	0.14954300	-1.01360500	1.16460900
H	0.09238600	-2.76891500	1.49457200
H	1.05437900	-2.13850100	0.10312900
C	-2.32981500	-2.16982800	0.60459400
C	-2.68093200	-0.90863500	1.38418200
H	-2.24608800	-3.01417100	1.29570500
H	-3.11741100	-2.37914000	-0.12622700
H	-2.68816600	-0.02554100	0.73613200
H	-3.71470800	-1.06297900	1.72263700
O	-1.84347400	-0.74429700	2.49856800
H	-1.38623900	0.11172800	2.41441200
Cl	-0.33695700	1.70751200	1.16260500
C	3.58237100	1.22249100	0.65973200
C	2.82573700	0.01090000	0.12666300
H	3.72462000	1.93132000	-0.17010600
H	4.57201900	0.90466800	1.00922000
C	3.72805300	-0.91353900	-0.68314600
H	2.42325400	-0.53610700	0.99441000
H	4.31901800	-0.31943300	-1.39595800
H	4.41512800	-1.45082400	-0.02506000
O	2.96023300	1.82814400	1.76874400
H	2.03951900	2.05429700	1.56210400
O	1.77698800	0.36587000	-0.76161900
H	1.12376300	0.92518100	-0.30187900
O	2.96029700	-1.88816500	-1.37365700
H	2.34808700	-1.37811200	-1.92180900
S	-1.86282100	2.47770400	-1.09950300
O	-2.99691300	1.59786600	-0.83596700
O	-0.92079400	1.98108500	-2.09107800

abs-com-e

N	2.53840300	0.92476900	-0.35271900
C	3.41289900	-0.14822500	0.22088400
H	2.77524900	-0.85909300	0.74955600
H	3.93429800	-0.64064300	-0.60132000
H	4.12909300	0.31510200	0.90166900
C	1.54712600	0.27317200	-1.27376500
H	0.88368800	-0.33921900	-0.66824100
H	0.96587200	1.02677700	-1.79987500
H	2.09053700	-0.35389300	-1.98290800
C	3.37328200	1.90387500	-1.10011300
H	2.72609200	2.65809100	-1.54809200
H	4.07531200	2.37207000	-0.40731800
H	3.91582000	1.37324100	-1.88413600
C	1.80379700	1.60264000	0.78270500
C	0.94346100	2.80054000	0.35965800
H	2.56041300	1.90755700	1.51202400
H	1.17335400	0.82938500	1.22878400
H	1.54741300	3.71052800	0.28581800
H	0.47610300	2.61785200	-0.61670100
O	-0.02968000	3.02680900	1.34180900
H	-0.69405200	2.32690500	1.20987400
C	-3.66952100	0.98306500	-0.21154000
C	-2.27270200	0.77859900	-0.78861800
H	-3.93768400	0.10788300	0.40169100
H	-4.40015500	1.06905900	-1.02090700
C	-2.20386800	-0.50652400	-1.60248900
H	-2.01999300	1.63345900	-1.42888100
H	-2.31471200	-1.36425000	-0.92517400
H	-3.04536100	-0.51544200	-2.30948200
O	-3.76051000	2.17493500	0.53781100
H	-3.11049100	2.12438700	1.24881600
O	-1.31197300	0.79545000	0.27053500
H	-1.35235000	-0.06546900	0.73874800
O	-0.98635900	-0.58992500	-2.31768300
H	-0.57862900	-1.44784800	-2.11821900
Cl	0.49441400	-3.01294800	-0.79275300
S	-0.07819100	-2.38189300	1.49058000
O	0.95633300	-1.35500100	1.72758100
O	-1.40899500	-1.77130100	1.29126000

cluster-2-c

N	-0.96491400	0.42731800	2.94942000
C	-0.88487000	-0.90123100	3.62651800
H	-1.00539200	-0.75872200	4.70250600
H	-1.67473400	-1.54145700	3.23004600
H	0.09622200	-1.32485500	3.40246100
C	-2.31218700	1.02853900	3.16738600
H	-2.47956000	1.14731500	4.23957200
H	-2.35062300	1.99500500	2.66026300
H	-3.05316000	0.35840900	2.72871500
C	-0.77081800	0.21448500	1.47772800
H	-0.95906700	1.16094200	0.96542500
H	0.26101900	-0.10641100	1.34080300
H	-1.48032300	-0.55185100	1.15764000
C	0.11986900	1.31526300	3.53061200
C	0.45570200	2.54507500	2.70144900
H	1.01871800	0.69467700	3.59289900
H	-0.22399700	1.58410800	4.53355100
H	-0.43268000	3.00518500	2.24582000
H	0.90111900	3.27927100	3.38765400
O	1.37822000	2.13968800	1.72307500
H	1.45748000	2.79544100	1.00918600
Cl	-1.11542900	3.30998900	-0.38540800
C	-3.98967300	1.61762100	-1.35781700
C	-3.46518800	0.25945400	-0.87007600
H	-5.01445700	1.49910900	-1.73053300
H	-3.35805500	1.99953700	-2.16960600
C	-3.89678100	-0.88583100	-1.77762100
H	-2.36580200	0.28875600	-0.79438300
H	-4.94559600	-0.74904800	-2.07567800
H	-3.27436000	-0.92228700	-2.67744900
O	-4.04581400	2.52357000	-0.27952400
H	-3.15708500	2.94256900	-0.20443700
O	-4.01153700	-0.00241000	0.41968700
H	-4.27732000	0.87278400	0.75376200
O	-3.75794300	-2.13913900	-1.12471900
H	-4.10902100	-2.02348000	-0.22791600
S	-1.39546700	-3.09040800	-0.95326300
O	-1.40910500	-2.91427500	0.49272600
O	-0.87828600	-1.95992600	-1.71818100
N	1.29959600	1.05864200	-2.41262500
C	-0.00548400	1.01042400	-3.14264400
H	0.16190700	1.29945100	-4.18253700
H	-0.39301200	-0.00858600	-3.08216700

H	-0.68562500	1.71090000	-2.64872800
C	2.26269100	0.10072500	-3.02947900
H	2.46859100	0.41630000	-4.05482400
H	3.17466000	0.07949200	-2.42964700
H	1.80534800	-0.89008700	-3.00966800
C	1.03976800	0.64011900	-0.99671300
H	1.98724900	0.56015600	-0.46602900
H	0.40757800	1.40644600	-0.55317600
H	0.53793000	-0.32861600	-1.03945600
C	1.80007800	2.48680300	-2.48070800
C	3.10842600	2.78538100	-1.76143400
H	0.99944600	3.10154900	-2.05350500
H	1.90580000	2.70922700	-3.54808800
H	3.88846700	2.05393300	-2.00433300
H	3.43905600	3.75779800	-2.14849100
O	2.94081700	2.88344800	-0.36972000
H	3.45946500	2.16543100	0.04842700
Cl	4.40161500	0.18746600	0.13697500
C	2.52114700	-2.14923200	1.83452300
C	1.84273500	-2.49635700	0.50950400
H	3.60226300	-2.32139300	1.75372500
H	2.12852100	-2.81110200	2.61803400
C	1.48562800	-3.97248200	0.42597400
H	0.90661500	-1.92088200	0.46038400
H	2.37839300	-4.59043600	0.59763500
H	0.72241900	-4.22498400	1.16819700
O	2.24511800	-0.82428400	2.25545300
H	2.85628400	-0.21923400	1.78923700
O	2.62458800	-2.22544300	-0.64209900
H	3.26059500	-1.49860200	-0.46048800
O	0.93225200	-4.26331100	-0.85102000
H	1.52150000	-3.83956700	-1.49543900

cluster-2-e

N	-0.54809800	-2.30038800	1.85426900
C	0.45491000	-2.41725900	2.95880700
H	1.44339100	-2.51236400	2.51072600
H	0.42163400	-1.50739000	3.55951600
H	0.20402100	-3.29352000	3.56028700
C	-0.15174800	-1.15018700	0.98267700
H	0.80165500	-1.38843600	0.51055400
H	-0.92811700	-0.98726400	0.23555700
H	-0.03755800	-0.27966200	1.62685400
C	-1.89546000	-2.02295100	2.44442800
H	-2.62621000	-1.96688400	1.63942600
H	-2.14390900	-2.83425700	3.13148100
H	-1.83357400	-1.07479700	2.97974800
C	-0.55282000	-3.60340500	1.07677100
C	-1.10478500	-3.49995300	-0.33132100
H	-1.13894300	-4.30790300	1.67471600
H	0.48826500	-3.93016100	1.02253700
H	-0.47825200	-2.83467300	-0.94178000
H	-1.02848800	-4.51058400	-0.75914100
O	-2.43981200	-3.05121900	-0.30256700
H	-2.64592500	-2.69036500	-1.19033700
Cl	0.19320400	-0.54299100	-2.44108600
C	-3.63677700	-0.71797100	-2.58569200
C	-3.23587800	0.32712900	-1.55152400
H	-3.78186000	-0.21847600	-3.55302900
H	-4.58414600	-1.18325600	-2.28930500
C	-4.41980700	1.20320600	-1.16702800
H	-2.86047200	-0.18901000	-0.65113200
H	-4.91193100	1.59380900	-2.06796400
H	-5.14531100	0.64202100	-0.57203000
O	-2.70193400	-1.77635700	-2.70250200
H	-1.80424700	-1.42372100	-2.87411300
O	-2.25531000	1.22681600	-2.04357900
H	-1.42273100	0.72842900	-2.21459200
O	-3.96662200	2.29290500	-0.36980500
H	-3.13117500	2.57541500	-0.78049300
N	1.35145400	2.82218000	-0.69950900
C	0.63286000	3.28372800	-1.92451500
H	1.32337900	3.86209900	-2.54102900
H	0.28793200	2.40171400	-2.46818600
H	-0.21694400	3.89931300	-1.62396800
C	2.48296200	1.92977600	-1.12421600
H	3.21093800	2.52008500	-1.68243800

H	2.93457400	1.48929000	-0.23526600
H	2.06405500	1.14457800	-1.75599400
C	0.38840400	2.04087200	0.14614600
H	0.94020100	1.58724100	0.96716900
H	-0.37139300	2.72185600	0.53069500
H	-0.05414100	1.27076400	-0.48788300
C	1.87294700	4.02851700	0.04086500
C	2.68653000	3.75147400	1.30279000
H	0.99932800	4.63340900	0.30303800
H	2.48628500	4.58017600	-0.67904500
H	3.49338500	3.03562200	1.10620700
H	3.15762400	4.71023000	1.55765700
O	1.88378900	3.33579500	2.37383400
H	2.12637700	2.41487700	2.59549600
Cl	2.76935600	0.32330800	2.22102000
C	2.81441800	-2.83926900	-0.82167600
C	3.37088700	-1.42170500	-0.78910800
H	3.54015500	-3.52077600	-1.28804900
H	1.88225000	-2.86394400	-1.39603500
C	3.94050700	-0.99084300	-2.13377000
H	2.56858800	-0.73430400	-0.49307700
H	4.63272000	-1.76190300	-2.50435200
H	3.13205200	-0.86306100	-2.86029100
O	2.52693700	-3.27333700	0.50170500
H	3.31419100	-3.03817100	1.01765600
O	4.41411800	-1.36441700	0.17625900
H	4.10226600	-0.80730700	0.91963300
O	4.61207700	0.25086000	-2.00941300
H	5.21383800	0.14308200	-1.25857000
S	-3.52167200	1.48364400	1.93378100
O	-2.09388800	1.25562600	1.76031800
O	-4.37272100	0.31645000	1.77757800

cluster-3-a

N	-0.86484100	1.08040400	-3.13686900
C	0.40290900	1.15389600	-3.92590200
H	0.15442200	1.29597300	-4.97945800
H	0.99774300	1.98915600	-3.55396000
H	0.96419300	0.23586900	-3.76908800
C	-1.62206500	2.35376700	-3.33169100
H	-1.88002400	2.44677500	-4.38880600
H	-2.51250000	2.35626600	-2.70022500
H	-0.95731600	3.16418200	-3.03004000
C	-0.52605900	0.91470600	-1.68254800
H	-1.44617200	0.99177300	-1.10514200
H	-0.07140100	-0.06576500	-1.55725200
H	0.17240600	1.70633700	-1.40468000
C	-1.64443400	-0.11416500	-3.62510400
C	-2.89269100	-0.47708500	-2.83677800
H	-0.94833100	-0.95910600	-3.60352700
H	-1.90595500	0.10238200	-4.66510400
H	-3.46904300	0.41514600	-2.55803900
H	-3.50855700	-1.09306100	-3.50543400
O	-2.53565900	-1.21877000	-1.68132300
H	-3.35885900	-1.39813200	-1.17738300
Cl	-3.86910800	2.27237900	-0.66774200
C	-1.80739000	4.78588100	0.73290700
C	-0.68739400	3.75806300	0.53247800
H	-1.37790300	5.74386600	1.05094200
H	-2.50091200	4.43598900	1.50843000
C	0.33736500	3.84546600	1.64538700
H	-1.12411300	2.74608900	0.50768700
H	0.75319600	4.86084000	1.68568000
H	-0.13846400	3.61683500	2.60621400
O	-2.46735600	5.03139300	-0.48836900
H	-3.05186800	4.26255400	-0.65755200
O	-0.02580200	4.01165800	-0.69735500
H	-0.65359800	4.54568500	-1.21296900
O	1.39460400	2.91062900	1.48971800
H	1.73708400	2.91458600	0.57405100
S	0.74198100	0.67546900	2.18409800
O	0.25325500	0.25359000	0.88152900
O	-0.28579800	1.12440700	3.11710500
N	-4.12302600	-0.09068700	2.23920800
C	-3.99125800	1.32796000	2.70232400
H	-4.85415800	1.57340200	3.32431800
H	-3.06434200	1.40470100	3.27496300

H	-3.94861200	1.96909300	1.81816000
C	-4.28050100	-0.98673500	3.42315100
H	-5.23344100	-0.75999000	3.90620600
H	-4.23639000	-2.03006500	3.09942000
H	-3.45608900	-0.78049000	4.10837200
C	-2.86305400	-0.45248100	1.50812800
H	-2.91520600	-1.50602100	1.24624400
H	-2.79978400	0.18586800	0.62536800
H	-2.02471300	-0.25729900	2.17723400
C	-5.32266400	-0.16342500	1.31684200
C	-5.67653200	-1.53231800	0.75579700
H	-5.11581200	0.54325700	0.50745100
H	-6.16990400	0.20834500	1.90373300
H	-5.82367300	-2.27304800	1.55033000
H	-6.63974000	-1.39247200	0.24980000
O	-4.73947200	-2.02543300	-0.17966400
H	-4.34918300	-2.84195600	0.22869000
Cl	-3.67822400	-4.07414000	1.68805300
C	-0.51355500	-3.90065100	-0.35509700
C	-0.40008400	-3.24279300	1.01717700
H	-1.53020600	-4.28752500	-0.49541300
H	0.18745400	-4.74064300	-0.41160700
C	0.98742600	-2.68411300	1.23250600
H	-1.09508800	-2.39164600	1.07066500
H	1.72963000	-3.49072600	1.12017700
H	1.18215900	-1.90154000	0.49312400
O	-0.15122400	-2.97710300	-1.37628000
H	-0.89467000	-2.35972600	-1.48812000
O	-0.63005300	-4.14300300	2.07393700
H	-1.59507300	-4.31132300	2.11105400
O	1.09178700	-2.10299300	2.53097400
H	0.57950000	-2.68921900	3.11209600
N	5.00708100	-0.81784300	1.52335200
C	5.52143200	-2.09573200	2.10050400
H	4.90395200	-2.36787600	2.95738700
H	5.45341600	-2.87175100	1.33706600
H	6.55884900	-1.95368000	2.40803400
C	3.59546000	-1.04315700	1.06945200
H	2.99702000	-1.29576400	1.94709200
H	3.22938000	-0.13602000	0.58312400
H	3.57558100	-1.86576800	0.34874100
C	5.85411100	-0.44342100	0.34454700
H	5.38403300	0.38985800	-0.17651400
H	6.84326700	-0.15180800	0.69938400

H	5.91241800	-1.31900000	-0.30490400
C	5.05220200	0.23124900	2.61646600
C	4.52003900	1.61003400	2.25640000
H	6.09986500	0.31070800	2.92201100
H	4.46472900	-0.18625100	3.44013000
H	3.50673700	1.54985200	1.84600100
H	4.45253800	2.16001200	3.20424200
O	5.38895000	2.27983400	1.38180300
H	4.88508900	2.50356100	0.57918500
Cl	3.24540300	1.93413000	-0.90781200
C	3.53665200	-0.60287500	-3.92146100
C	3.27566500	-1.20421400	-2.54138600
H	2.80958900	-1.01926900	-4.63166800
H	4.53828800	-0.90838300	-4.26289300
C	3.17910200	-2.72483300	-2.59701000
H	4.10246700	-0.90936200	-1.87428000
H	2.44979400	-3.01465200	-3.36754600
H	4.14771800	-3.16405300	-2.85636100
O	3.38911900	0.79884700	-3.96575400
H	3.64701500	1.20932000	-3.12136800
O	2.05428100	-0.74972100	-1.99465800
H	2.21962500	0.11970500	-1.57753000
O	2.81513200	-3.24096300	-1.33954300
H	1.92040500	-2.90278700	-1.15609300