Supporting Information

For

Unravelling the structural and dynamical complexity of the equilibrium liquid grain-binding layer in highly conductive organic crystalline electrolytes

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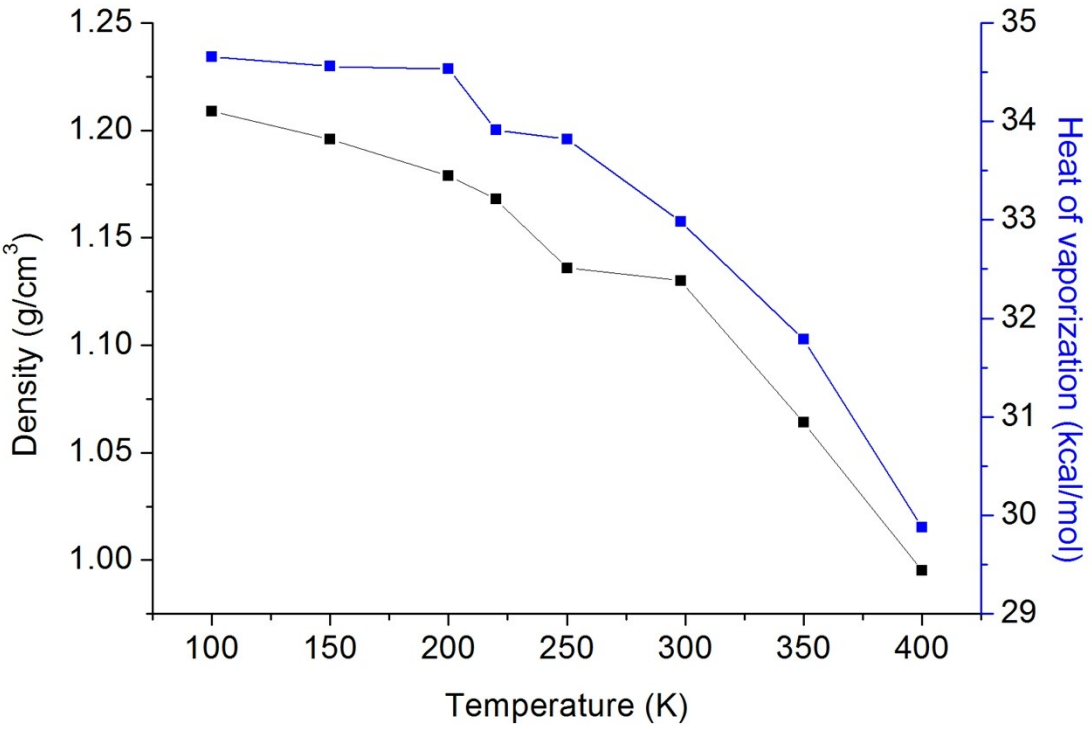

Figure S1. Calculated density and ΔH_{vap} at different temperatures.

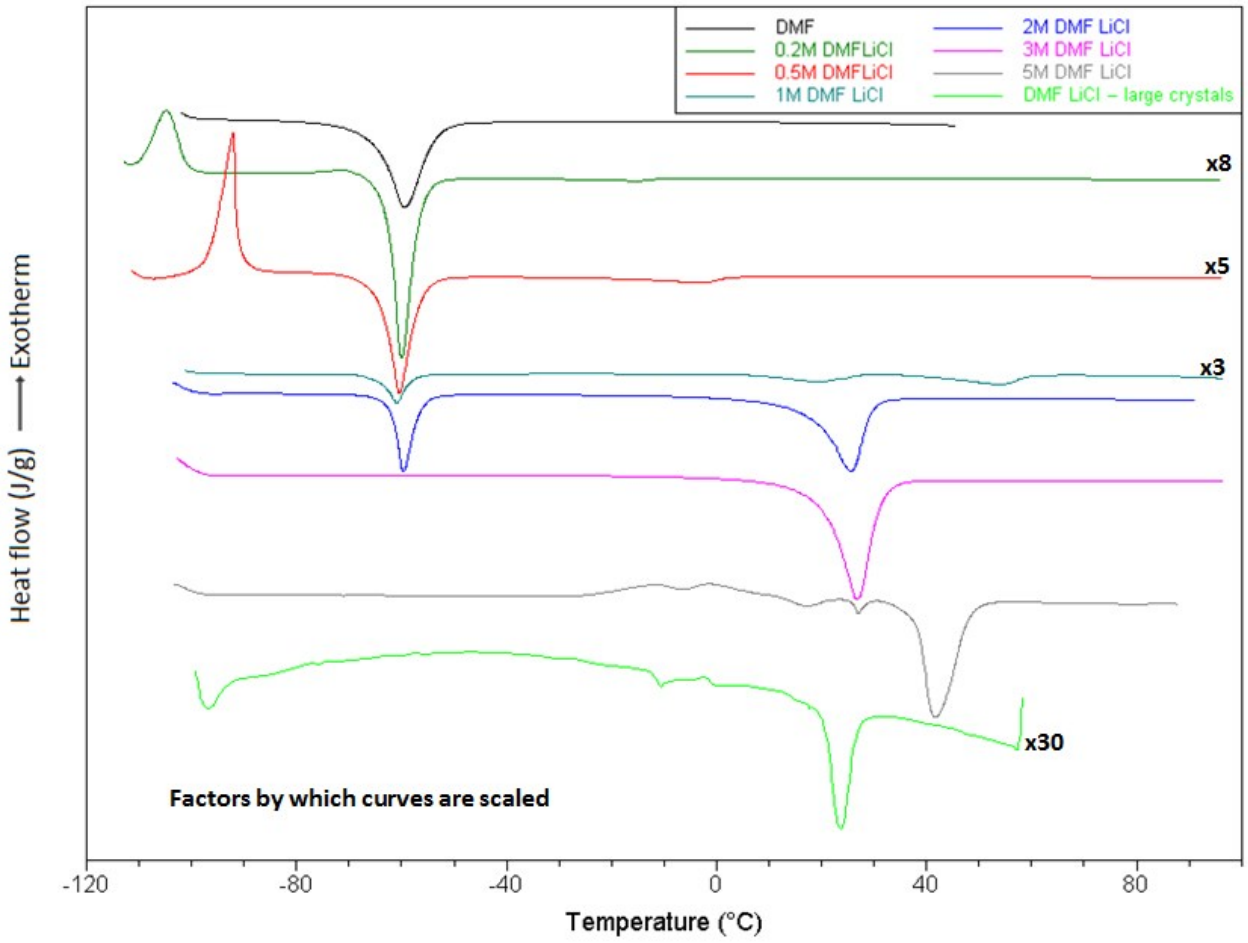

Figure S2. DSC data (second heating cycle) of solutions of DMF (—); LiCl in DMF (0.2 M —,0.5 M —,1.0 M —, 2.0 M—, 3M —); and cocrystals of DMF·LiCl (—). The melt transitions observed are new crystalline phases of DMF and LiCl located at the surface of the co-crystal, and so are very weak, and are not from the bulk co-crystal of DMF·LiCl, which has no melt transition. Instead they correspond to new phases found in the crystallized solutions of DMF and LiCl.

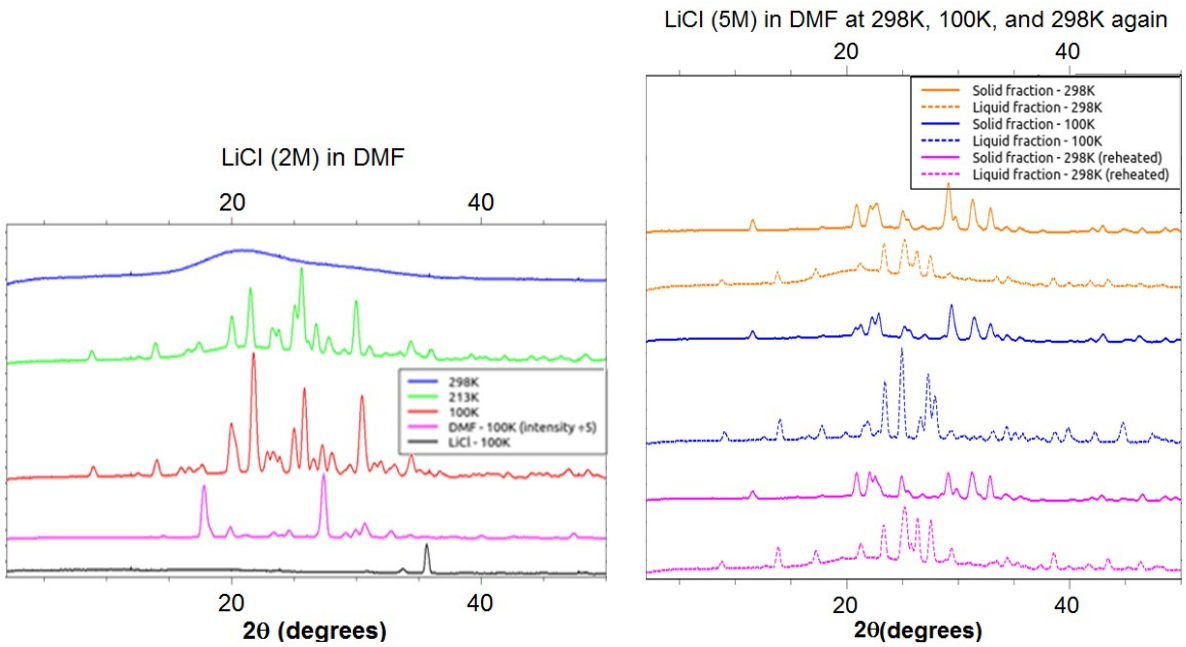

Figure S3. XRD of (**left**) 2M LiCl in DMF at room temperature (—), showing amorphous liquid; at 213 K, just above melt temperature (212K) of DMF (—), showing crystal and small amount of underlying liquid DMF; and at 100 K (—) below the melt temperature of DMF, showing only crystal phase. Note: none of the peaks correspond to either pure DMF (—) or pure LiCl (—), measured separately, or to the co-crystal of DMF·LiCl (not shown); (**right**) 5M LiCl in DMF, where the solution phase separates with time; here the solution and solid phases are distinct, and distinct from LiCl, DMF or DMF·LiCl; (**bottom)**

Force field for LiCl·DMF

Bonded parameters: From OPLA-AA force field

vdW parameters in the form of Lennard Jones potential: OPLA-AA force field

Electrostatic charges for Coulombic potential: hybrid B3LYP functional with aug-cc-PVQZ basis set using CHELPG method.

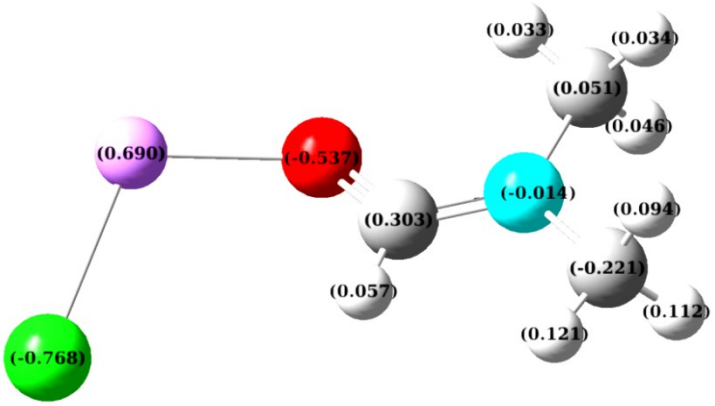

Figure S4. Distribution of partial charges from electrostatic potential on LiCl·DMF single molecule Dipole moment: 10.9 Debye from B3LYP functional with aug-cc-PVQZ basis set using CHELPG method.

Table S1. Dipole moment (in Debye) of DMF determined using different quantum calculations:

Experimental	3.82[1]
PBE/6-311++G(d,p)	4.069
B3LYP/6-311++G(d,p)	4.174
CCSD/6-311++G(d,p)	4.399
M06-2X/6-311++G(d,p)	4.205
B3LYP/aug-cc-PVQZ	4.069[1]

[1] Computational Chemistry Comparison and Benchmark DataBase Release 18 (October 2016) Standard Reference Database 101 National Institute of Standards and Technology. http://cccbdb.nist.gov/diplistx.asp#NSRDS-NBS10

Heat of vaporization of DMF and LiCl·DMF

Heat of vaporization from simulation can be calculated from enthalpy of bulk system using the relation:

$$\Delta H_{vap} = < h_{gas}(T) > \; - \; < h_{liq}(p,T) >$$

$$= \Delta H_{gas}(T) - \frac{1}{N}\Delta H_{liq}(p,T)$$

ΔH_{vap} for DMF, at 298 K:

10.492 kcal/mol (our force field) 11.10 kcal/mol (from experiments)[2]

Ionic charge density of the system *V* at different temperatures

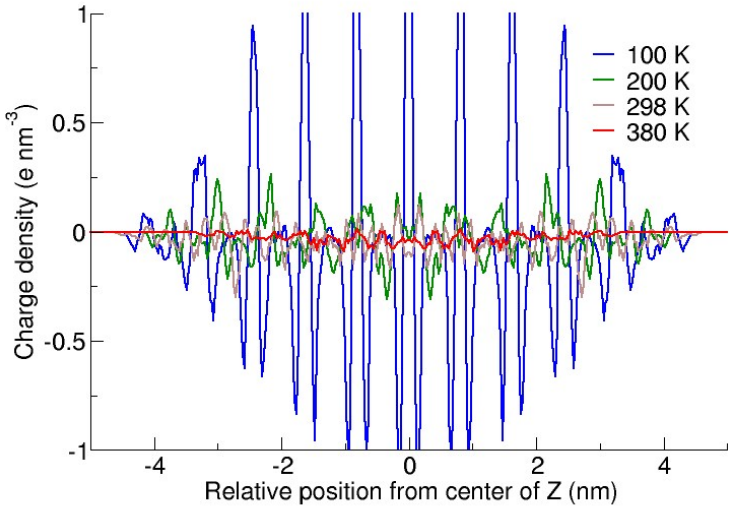

Figure S5. Distribution of charges carried by Li^+ and Cl^- in *z*-dimension of the crystal structure modeled as system *V*

[2] Chickos, J. S.; Acree, W. E. Enthalpies of Vaporization of Organic and Organometallic Compounds, 1880-2002. *J. Phys. Chem. Ref. Data* **2003**, *32*, 519–878.

Calculation of density gradients in simulated crystal

Since the interatomic distances correspond to only to O--Li—Cl networks, the density at the interfacial regions cannot be calculated. Further, the density in the interfacial regions is also not uniform in all directions of the simulation box. However, a density distribution can be obtained by using very fine grids perpendicular to the X, Y and Z directions of the simulation box. The density distribution in System V (T = 298 K) is shown in Figure S6. The density distribution (in each direction) shows a gradual decrease from the bulk to the interfacial regions. The dotted lines in Figure S6 represent the interfacial regions where the change in density is lower by at-least 30 % compared to the bulk mass density.

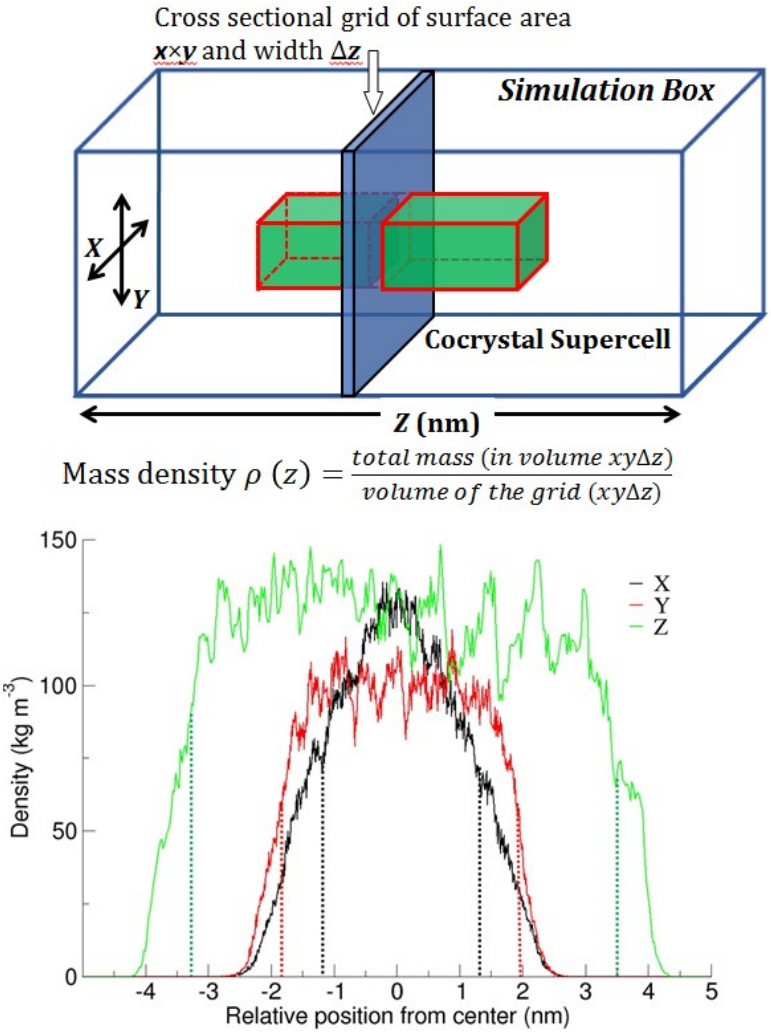

Figure S6. The mass density distribution in System V (T = 298 K) in fine grids perpendicular to X, Y and Z directions. Schematic diagram shows how the mass density distribution is calculated across the box (System V) in Z direction.

Calculation of interaction energy of different fragments using DFT:

(i) Fragment relaxations: Li^+---Cl^-DMF and LiCl---DMF

fCP method[3]: Fragment Counterpoise method the correction to incompleteness of the basis sets and the interaction energies are calculated as:

$$\Delta E_{AB} = E^{a \cup b}_{AB}(AB) - \left[E^{a \cup b}_{AB}(A) + E^{a \cup b}_{AB}(B)\right] \quad (1)$$

where, subscript is the geometry of structure, superscript is the basis set used and the entity for which energy is calculated is in parenthesis (). '*a'*, '*b'* and '*ab'* are basis functions for A, B, and AB respectively.

rig-fCP method[4]: Rigorous fragment Counterpoise method provides the additional correction to errors associated to fCP method- Basis Set Superposition Error and takes care of fragment relaxation for monomer to dimer optimizations. The interaction energy in this method is calculated as:

$$\Delta E_{AB} = E^{a \cup b}_{AB}(AB) - \left[E^{a}_{A}(A) + E^{b}_{B}(B)\right] + \left[E^{a}_{AB}(A) - E^{a \cup b}_{AB}(A) + E^{b}_{AB}(B) - E^{a \cup b}_{AB}(B)\right] \quad (2)$$

The last four energy terms in square bracket are the correction to BSSE.

(ii) Tetramerization: If 4A (in optimized structure- A_1, A_2, A_3 and A_4 form a tetramer 'T', then energy of tetramerization is calculated as:

$$\Delta E_{tet}(fCP) = E^{4a}_{T}(T) - \sum_{i=1}^{4} E^{4a}_{T}(A_i) \quad (3)$$

and

$$\Delta E_{tet}(rig - fCP) = E^{4a}_{T}(T) - \sum_{i=1}^{4} E^{a}_{A_i}(A_i) + \sum_{i=1}^{4} E^{a}_{T}(A_i) - \sum_{i=1}^{4} E^{4a}_{T}(A_i) \quad (4)$$

[3] Boys, S.; Bernardi, F. The Calculation of Small Molecular Interactions by the Differences of Separate Total Energies. Some Procedures with Reduced Errors. *Mol. Phys.* **1970**, *19*, 553–566.

[4] Kirschner, K. N.; Sorensen, J. B.; Bowen, J. P. Calculating Interaction Energies Using First Principle Theories: Consideration of Basis Set Superposition Error and Fragment Relaxation. *J. Chem. Educ.* **2007**, *84*, 1225–1229.

Since without optimization, ΔE(fCP) → ΔE(rig-fCP), hence for D1 and D2 dimers, single point interaction energies (Table 1) are calculated using fCP method only (equation 1)

Table S2. Important structural parameters of single point and optimized geometries for Interaction energy analysis (B3LYP/6-311++G(d,p) for both single point and optimization)

Structure	**O-Li-Cl angle (deg)**	**Li-O distance (Å)**	**Li-Cl distance (Å)**
LiCl·DMF monomer-sp **M0**	111.77	1.96	2.33
LiCl·DMF monomer-opt **M1/M2**	179.97	1.84	2.08
LiCl·DMF dimer-opt **D0**	157.01	1.88	2.14
two dimer configurations (unoptimized)			
LiCl·DMF dimer-conf-1-sp Normal **D1**	118.11 118.11	1.96 1.96	2.34 2.34
LiCl·DMF dimer-conf-2-sp Invert **D2**	114.32 114.32	1.96 1.96	2.34 2.34
two dimer config started from optimized dimer geometry			
LiCl·DMF opt-conf-1-opt Normal **D3**	110.70 110.70	2.04 2.04	2.14 2.14
LiCl·DMF opt-conf-2-opt Invert **D4**	157.89 157.89	1.88 1.88	2.14 2.14
Tetramer Analysis			
tetra-dmli-1-cp-4-1 **T1**	139.23 118.47 139.23 118.47	1.92 1.99 1.92 1.99	2.14 2.30 2.14 2.30
tetra-dmli-1-cp-4-2 **T2**	118.62 117.52 139.19 121.76	1.99 1.95 2.04 1.92	2.30 2.14 2.30 2.14
tetra-dmli-2-cp-4-1 **T3**	146.06 163.26 163.20 143.05	1.90 1.79 1.79 1.90	2.15 2.12 2.12 2.15
tetra-dmli-2-cp-4-2 **T4**	121.98 163.64 163.64 121.97	1.95 1.80 1.80 1.95	2.16 2.12 2.12 2.16
tetra-dmli-1-cp-2-two-dimers **T5**	118.30 138.73 118.30 138.73	1.99 1.92 1.99 1.92	2.30 2.14 2.30 2.14

The colors for parameters are based on color codes for fragments defined for Counterpoise calculation of interaction energy from fCP and rig-fCP methods.

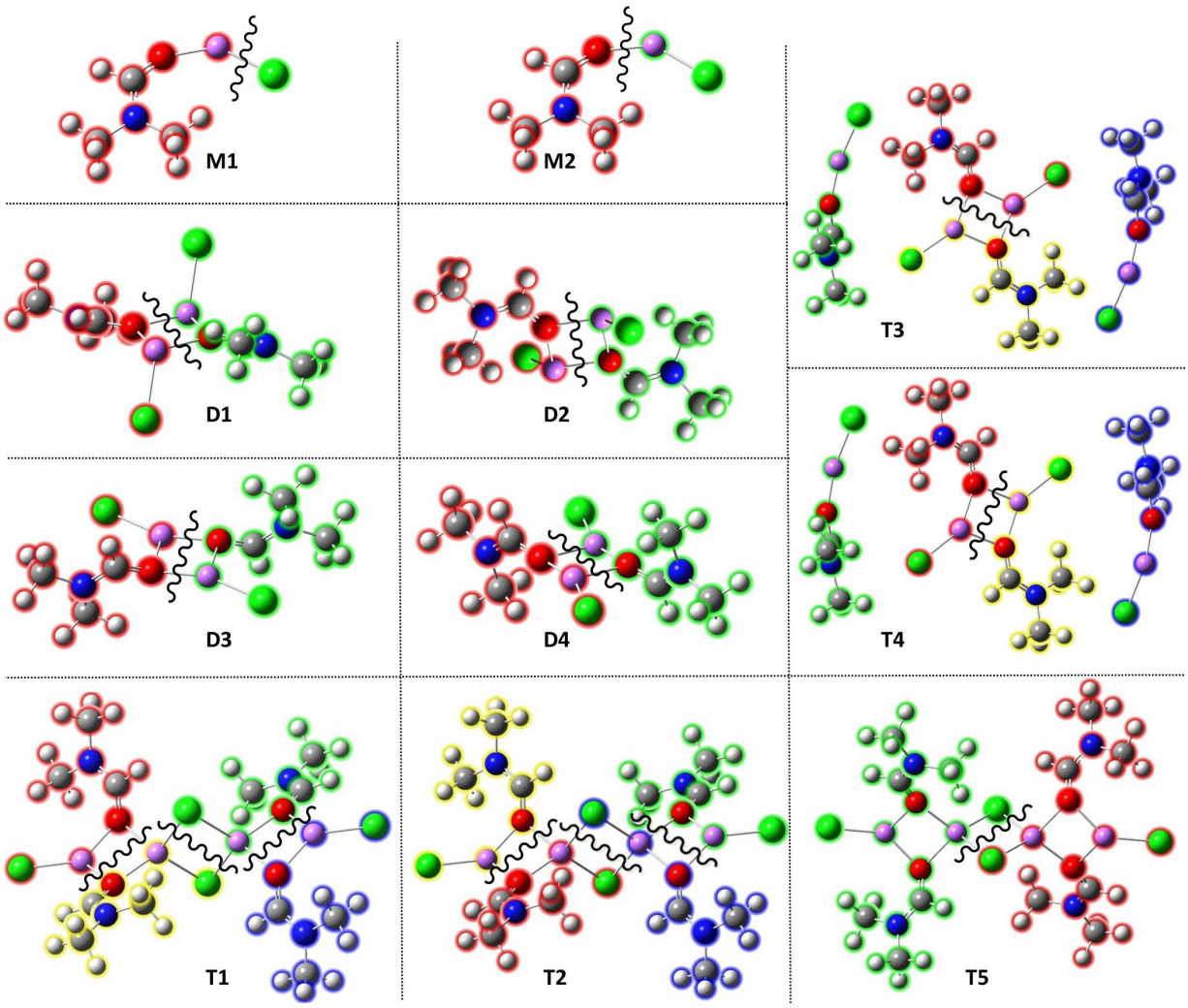

Figure S7. Replica of Figure 14 placed for convenience, and illustrating single point (D1 and D2) and optimized geometries (all other) of structures with the color clouds indicating fragments. E.g. values in table with yellow text correspond to yellow fragment in the system. Squiggly lines are used to show the fragments with clarity.

Absolute electronic energies (in Hartree) and coordinates of electronic structures

(The fragment number follows the color code of Figure S6 as – Fragment 1: Red, Fragment 2: Green, Fragment 3: Blue and Fragment 4: Yellow; All geometries accept D1 and D2 are optimized stationary point structures)

M1 **-716.467571 Hartree**

Cl(Fragment=2)	3.05566200	-0.35075600	-0.00369500
O(Fragment=1)	-0.12183800	1.53540900	0.00585200
N(Fragment=1)	-1.66579000	-0.16597100	-0.00063700
C(Fragment=1)	-1.28423800	1.11497600	-0.00119600
H(Fragment=1)	-2.12485300	1.82239300	-0.00885900
C(Fragment=1)	-3.08107100	-0.52141300	-0.00683700
H(Fragment=1)	-3.69321300	0.38056900	-0.01324500
H(Fragment=1)	-3.31757800	-1.11504300	-0.89407800
H(Fragment=1)	-3.32705500	-1.10873800	0.88205700
C(Fragment=1)	-0.71157900	-1.27781500	0.00938200
H(Fragment=1)	-0.86760100	-1.88482500	0.90499400
H(Fragment=1)	-0.87138800	-1.90278100	-0.87299100
H(Fragment=1)	0.31525900	-0.91584100	0.00326900
Li(Fragment=1)	1.67891500	1.22372300	0.00374200

M2 **-716.466371 Hartree**

Cl(Fragment=2)	-3.19392100	0.35594400	0.00015000
O(Fragment=1)	-0.04664800	-1.23962100	-0.00032200
N(Fragment=1)	1.74395100	0.17901000	-0.00031200
C(Fragment=1)	0.43442700	-0.09445800	-0.00047100
H(Fragment=1)	-0.22051600	0.78697700	-0.00070200

C(Fragment=1)	2.22528700	1.55546700	0.00005500
H(Fragment=1)	1.37835400	2.24113300	0.00009800
H(Fragment=1)	2.83373100	1.74568900	-0.88866900
H(Fragment=1)	2.83345000	1.74528100	0.88906000
C(Fragment=1)	2.74187300	-0.88537400	0.00042800
H(Fragment=1)	3.37298100	-0.80695400	0.89021700
H(Fragment=1)	3.37459700	-0.80665100	-0.88816000
H(Fragment=1)	2.23228700	-1.84582200	-0.00018700
Li(Fragment=2)	-1.91740800	-1.30020800	0.00015900

D1 **-1432.842801 Hartree**

Cl(Fragment=2)	-1.19700000	1.91700000	9.11700000
Cl(Fragment=1)	4.58700000	4.47300000	6.65500000
O(Fragment=1)	1.75800000	2.12500000	7.04200000
O(Fragment=2)	1.63200000	4.26500000	8.73000000
N(Fragment=1)	1.27800000	0.54900000	5.46200000
N(Fragment=2)	2.11200000	5.84100000	10.31000000
C(Fragment=1)	2.02300000	1.06600000	6.42200000
C(Fragment=2)	1.36700000	5.32400000	9.35000000
H(Fragment=1)	2.81600000	0.60200000	6.66400000
H(Fragment=2)	0.57400000	5.78800000	9.10800000
C(Fragment=1)	0.01500000	1.16700000	5.06000000
C(Fragment=2)	3.37500000	5.22300000	10.71200000
H(Fragment=1)	-0.73200000	0.65700000	5.43700000
H(Fragment=2)	4.12200000	5.73300000	10.33500000
H(Fragment=1)	-0.05000000	1.16900000	4.08200000
H(Fragment=2)	3.44100000	5.22100000	11.69000000

H(Fragment=1)	-0.01800000	2.08800000	5.39200000
H(Fragment=2)	3.40800000	4.30200000	10.38000000
Li(Fragment=1)	3.10000000	3.22400000	7.96200000
Li(Fragment=2)	0.29000000	3.16600000	7.81000000
C(Fragment=1)	1.43900000	-0.82400000	5.01000000
H(Fragment=1)	0.73500000	-1.02700000	4.22900000
H(Fragment=1)	1.26600000	-1.49100000	5.82800000
H(Fragment=1)	2.43300000	-0.96400000	4.64000000
C(Fragment=2)	1.91438547	7.26023163	10.58987512
H(Fragment=2)	0.95038547	7.56223163	10.23787512
H(Fragment=2)	2.67038547	7.83023163	10.09087512
H(Fragment=2)	1.97938547	7.42823163	11.64387512

D2 **-1432.843028 Hartree**

Cl(Fragment=1)	-1.19700000	1.91700000	9.11700000
Cl(Fragment=2)	4.58700000	4.47300000	6.65500000
O(Fragment=1)	1.75800000	2.12500000	7.04200000
O(Fragment=2)	1.63200000	4.26500000	8.73000000
N(Fragment=1)	1.27800000	0.54900000	5.46200000
N(Fragment=2)	2.11200000	5.84100000	10.31000000
C(Fragment=1)	2.02300000	1.06600000	6.42200000
C(Fragment=2)	1.36700000	5.32400000	9.35000000
H(Fragment=1)	2.81600000	0.60200000	6.66400000
H(Fragment=2)	0.57400000	5.78800000	9.10800000
C(Fragment=1)	0.01500000	1.16700000	5.06000000
C(Fragment=2)	3.37500000	5.22300000	10.71200000
H(Fragment=1)	-0.73200000	0.65700000	5.43700000

H(Fragment=2)	4.12200000	5.73300000	10.33500000
H(Fragment=1)	-0.05000000	1.16900000	4.08200000
H(Fragment=2)	3.44100000	5.22100000	11.69000000
H(Fragment=1)	-0.01800000	2.08800000	5.39200000
H(Fragment=2)	3.40800000	4.30200000	10.38000000
Li(Fragment=2)	3.10000000	3.22400000	7.96200000
Li(Fragment=1)	0.29000000	3.16600000	7.81000000
C(Fragment=1)	1.43900000	-0.82400000	5.01000000
H(Fragment=1)	0.73500000	-1.02700000	4.22900000
H(Fragment=1)	1.26600000	-1.49100000	5.82800000
H(Fragment=1)	2.43300000	-0.96400000	4.64000000
C(Fragment=2)	1.91438547	7.26023163	10.58987512
H(Fragment=2)	0.95038547	7.56223163	10.23787512
H(Fragment=2)	2.67038547	7.83023163	10.09087512
H(Fragment=2)	1.97938547	7.42823163	11.64387512

D3 **-1432.967356 Hartree**

Cl(Fragment=1)	-2.43536100	2.41932000	0.07251000
Cl(Fragment=2)	2.43542900	-2.41931700	-0.07241200
O(Fragment=1)	-1.15660800	-0.77792700	0.20673400
O(Fragment=2)	1.15660600	0.77788300	-0.20699200
N(Fragment=1)	-3.42503600	-0.92692000	-0.01577000
N(Fragment=2)	3.42500400	0.92693000	0.01577500
C(Fragment=1)	-2.30523000	-0.92304800	0.68603500
C(Fragment=2)	2.30528400	0.92297300	-0.68616600
H(Fragment=1)	-2.44216800	-1.06832300	1.76314400
H(Fragment=2)	2.44235000	1.06814300	-1.76327200

C(Fragment=1)	-3.41370300	-0.69219900	-1.46044900
C(Fragment=2)	3.41350100	0.69234400	1.46047400
H(Fragment=1)	-3.54246200	0.37595400	-1.65425000
H(Fragment=2)	3.54227500	-0.37578700	1.65438900
H(Fragment=1)	-4.22622400	-1.26160000	-1.91395100
H(Fragment=2)	4.22594500	1.26181400	1.91402500
H(Fragment=1)	-2.46329900	-1.02487200	-1.87190300
H(Fragment=2)	2.46303500	1.02502000	1.87178000
Li(Fragment=2)	0.69149800	-1.18766000	0.11501100
Li(Fragment=1)	-0.69149100	1.18762000	-0.11520700
C(Fragment=1)	-4.72162400	-0.85916700	0.65424400
H(Fragment=1)	-5.40245800	-1.59302200	0.21857900
H(Fragment=1)	-5.13733300	0.14507900	0.53931200
H(Fragment=1)	-4.60086500	-1.07086300	1.71633700
C(Fragment=2)	4.72167400	0.85912500	-0.65407600
H(Fragment=2)	4.60104200	1.07073500	-1.71620100
H(Fragment=2)	5.13736700	-0.14511300	-0.53901400
H(Fragment=2)	5.40245500	1.59301500	-0.21838800

D4 **-1432.967600 Hartree**

Cl(Fragment=1)	-2.43016300	-2.41931200	0.06639800
O(Fragment=1)	1.15494800	-0.78493400	-0.21235000
O(Fragment=2)	-1.15491800	0.78495700	0.21258900
N(Fragment=1)	3.42342900	-0.92487300	0.01314600
N(Fragment=2)	-3.42338700	0.92481400	-0.01297000
C(Fragment=1)	2.30518300	-0.91656100	-0.69112400
C(Fragment=2)	-2.30517000	0.91648400	0.69134400

H(Fragment=1)	2.44542300	-1.04540600	-1.76988800
H(Fragment=2)	-2.44545900	1.04515000	1.77012300
C(Fragment=1)	3.40744500	-0.70509500	1.45995700
C(Fragment=2)	-3.40731700	0.70509800	-1.45978800
H(Fragment=1)	3.53121100	0.36174900	1.66429800
H(Fragment=2)	-3.53103300	-0.36174200	-1.66418900
H(Fragment=1)	4.22110900	-1.27552500	1.91004600
H(Fragment=2)	-4.22098100	1.27551100	-1.90989700
H(Fragment=1)	2.45713300	-1.04521200	1.86543800
H(Fragment=2)	-2.45699700	1.04527100	-1.86520400
Li(Fragment=1)	-0.67956600	-1.20015900	-0.11110600
Li(Fragment=2)	0.67956500	1.20021000	0.11112500
C(Fragment=1)	4.72170200	-0.84893600	-0.65259600
H(Fragment=1)	5.39985300	-1.59147400	-0.22741800
H(Fragment=1)	5.14005800	0.15209100	-0.52058600
H(Fragment=1)	4.60291700	-1.04295700	-1.71826800
C(Fragment=2)	-4.72168200	0.84872600	0.65271400
H(Fragment=2)	-4.60295700	1.04269700	1.71840000
H(Fragment=2)	-5.13994400	-0.15233200	0.52063500
H(Fragment=2)	-5.39988100	1.59122800	0.22754800

T1 **-2865.980901 Hartree**

Cl(Fragment=4)	0.37788900	-1.38121300	-1.11114900
O(Fragment=4)	-2.92031400	-1.32803700	0.54633900
N(Fragment=4)	-3.12931200	-2.13712400	2.67712800
C(Fragment=4)	-3.55389900	-1.93421800	1.43057900
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H(Fragment=4)	-4.86316000	-3.22189200	3.13865900
H(Fragment=4)	-4.17560900	-2.30453700	4.49455000
H(Fragment=4)	-3.38837600	-3.79999700	3.94251800
C(Fragment=4)	-1.84192200	-1.63114100	3.15270600
H(Fragment=4)	-1.10470100	-2.43886500	3.18989600
H(Fragment=4)	-1.48082700	-0.83962000	2.49882500
Li(Fragment=4)	-1.40418900	-0.26185800	-0.17558800
H(Fragment=4)	-4.55241800	-2.32758400	1.20852700
H(Fragment=4)	-1.97144000	-1.22420800	4.15757200
O(Fragment=1)	-2.78514300	0.72018900	-1.34386500
N(Fragment=1)	-3.80357700	2.67242800	-1.93039900
C(Fragment=1)	-2.86331600	1.96516800	-1.31045300
H(Fragment=1)	-2.12520600	2.54155000	-0.74153600
C(Fragment=2)	-3.89433600	4.11844800	-1.75185500
H(Fragment=1)	-3.07053000	4.46342500	-1.12722300
H(Fragment=1)	-3.84413900	4.62373800	-2.71973500
H(Fragment=1)	-4.83728900	4.38113600	-1.26497400
C(Fragment=1)	-4.84329200	2.00123400	-2.72142300
H(Fragment=1)	-5.60481500	1.55050200	-2.07903000
H(Fragment=1)	-5.30309100	2.73493700	-3.38285900
H(Fragment=1)	-4.39139300	1.21158400	-3.32139300
Li(Fragment=1)	-4.01923700	-0.69594400	-0.95031700
Cl(Fragment=1)	-6.13372600	-1.01779600	-0.82625600
Cl(Fragment=3)	6.13366500	1.01788200	0.82634800
O(Fragment=3)	2.78512100	-0.72018400	1.34387900
N(Fragment=3)	3.80362700	-2.67236700	1.93038800
C(Fragment=3)	2.86332000	-1.96515900	1.31045800

C(Fragment=3)	3.89445500	-4.11838400	1.75185700
H(Fragment=3)	3.07064800	-4.46341000	1.12725400
H(Fragment=3)	3.84431200	-4.62366400	2.71974500
H(Fragment=3)	4.83740700	-4.38102900	1.26495100
C(Fragment=3)	4.84333200	-2.00110000	2.72136400
H(Fragment=3)	5.60479200	-1.55031800	2.07893300
H(Fragment=3)	4.39140600	-1.21147800	3.32135100
Li(Fragment=3)	4.01918400	0.69597700	0.95036000
H(Fragment=3)	2.12523200	-2.54156700	0.74153900
H(Fragment=3)	5.30321400	-2.73476800	3.38278200
O(Fragment=2)	2.92027400	1.32803500	-0.54632200
N(Fragment=2)	3.12926900	2.13705300	-2.67712200
C(Fragment=2)	3.55386000	1.93420500	-1.43056700
H(Fragment=2)	4.55237500	2.32758700	-1.20852600
C(Fragment=2)	3.93497100	2.91014700	-3.61693600
H(Fragment=2)	4.86309600	3.22183200	-3.13870800
H(Fragment=2)	4.17555600	2.30440500	-4.49455600
H(Fragment=2)	3.38829800	3.79987500	-3.94258600
C(Fragment=2)	1.84188700	1.63102100	-3.15266800
H(Fragment=2)	1.10464900	2.43872800	-3.18989500
H(Fragment=2)	1.97140600	1.22403500	-4.15751300
H(Fragment=2)	1.48081500	0.83952900	-2.49873800
Li(Fragment=2)	1.40415300	0.26185200	0.17560600
Cl(Fragment=2)	-0.37792400	1.38120500	1.11117200

T2 **-2865.980650 Hartree**

Cl(Fragment=1)	0.37591600	-1.38353200	-1.10944700

O(Fragment=1)	-2.92427900	-1.33107400	0.54984700
N(Fragment=1)	-3.13857600	-2.13943600	2.68036000
C(Fragment=1)	-3.56094200	-1.93522300	1.43329600
C(Fragment=1)	-3.94785700	-2.91008500	3.61911400
H(Fragment=1)	-4.87629000	-3.21896100	3.13965400
H(Fragment=1)	-4.18776500	-2.30360400	4.49640600
H(Fragment=1)	-3.40431100	-3.80146000	3.94547500
C(Fragment=1)	-1.85003000	-1.63765200	3.15734900
H(Fragment=1)	-1.11475600	-2.44722100	3.19300000
H(Fragment=1)	-1.48683900	-0.84558900	2.50527500
Li(Fragment=1)	-1.40507300	-0.26704000	-0.16933300
H(Fragment=1)	-4.56042300	-2.32542700	1.20998700
H(Fragment=1)	-1.97890000	-1.23257400	4.16303300
O(Fragment=4)	-2.78163800	0.71811600	-1.33908300
N(Fragment=4)	-3.79358000	2.67165500	-1.93208600
C(Fragment=4)	-2.85704000	1.96327300	-1.30779800
H(Fragment=4)	-2.11955200	2.53891600	-0.73730800
C(Fragment=4)	-3.88146900	4.11822400	-1.75668100
H(Fragment=4)	-3.05879800	4.46248900	-1.13015900
H(Fragment=4)	-3.82700700	4.62146800	-2.72539600
H(Fragment=4)	-4.82531100	4.38415100	-1.27329900
C(Fragment=4)	-4.83210800	2.00125300	-2.72538400
H(Fragment=4)	-5.59563000	1.55159600	-2.08461000
H(Fragment=4)	-5.28957300	2.73519300	-3.38816200
H(Fragment=4)	-4.37962100	1.21090900	-3.32402500
Li(Fragment=4)	-4.01941200	-0.69552700	-0.94801800
Cl(Fragment=4)	-6.13503500	-1.01130000	-0.82822700

Cl(Fragment=2)	6.13451300	1.00809000	0.81870300
O(Fragment=3)	2.78369800	-0.72457800	1.33744900
N(Fragment=3)	3.81315000	-2.67071300	1.92532200
C(Fragment=3)	2.87167100	-1.96899600	1.30176800
C(Fragment=3)	3.91390600	-4.11595800	1.74573000
H(Fragment=3)	3.09544500	-4.46557700	1.11664900
H(Fragment=3)	3.86183500	-4.62244600	2.71286900
H(Fragment=3)	4.86094100	-4.37221200	1.26340700
C(Fragment=3)	4.84330100	-1.99371400	2.72406900
H(Fragment=3)	5.59968300	-1.52809000	2.08619200
H(Fragment=3)	4.38072300	-1.21472000	3.32996200
Li(Fragment=2)	4.01670200	0.70264300	0.94672000
H(Fragment=3)	2.14105300	-2.54975300	0.72744000
H(Fragment=3)	5.31094400	-2.72761300	3.37969500
O(Fragment=2)	2.92234700	1.33507500	-0.54171000
N(Fragment=2)	3.11997700	2.14034200	-2.67573000
C(Fragment=2)	3.55214300	1.93664800	-1.43200700
H(Fragment=2)	4.55370600	2.32685500	-1.21799600
C(Fragment=2)	3.92430800	2.90646600	-3.62236500
H(Fragment=2)	4.85739100	3.21371500	-3.15092700
H(Fragment=2)	4.15560900	2.29726400	-4.50010700
H(Fragment=2)	3.38073300	3.79858700	-3.94666700
C(Fragment=2)	1.82733200	1.64043300	-3.14285500
H(Fragment=2)	1.09775400	2.45468100	-3.18785300
H(Fragment=2)	1.95075700	1.22054900	-4.14320100
H(Fragment=2)	1.46094400	0.85989000	-2.47906300
Li(Fragment=3)	1.40290800	0.24994600	0.18801900

Cl(Fragment=3)	-0.37757600	1.37164300	1.12270800

T3 **-2865.956047 Hartree**

Cl(Fragment=4)	2.65241800	2.01993300	0.97009700
Cl(Fragment=2)	5.62261600	-3.46267800	-0.64572700
Cl(Fragment=1)	-2.65341300	-2.01945300	-0.97089500
Cl(Fragment=3)	-5.62183500	3.46250000	0.64874500
O(Fragment=1)	0.64043900	-1.21691200	0.20427700
O(Fragment=3)	-6.47392700	-0.29493300	1.02913300
O(Fragment=4)	-0.64091000	1.21685900	-0.20544400
O(Fragment=2)	6.47601000	0.29422000	-1.02883200
N(Fragment=1)	1.99068500	-2.98133500	0.77219800
N(Fragment=3)	-6.14562900	-2.32247500	0.02537900
N(Fragment=4)	-1.99119900	2.98165500	-0.77208300
N(Fragment=2)	6.14596900	2.32222000	-0.02654900
C(Fragment=1)	0.94838400	-2.43601000	0.17471600
C(Fragment=3)	-6.21208000	-1.50844500	1.07222800
C(Fragment=4)	-0.94863700	2.43600300	-0.17535700
C(Fragment=2)	6.21337200	1.50753000	-1.07282800
H(Fragment=1)	0.31188000	-3.13249100	-0.38028400
H(Fragment=3)	-6.02342500	-2.00275400	2.03387500
H(Fragment=4)	-0.31171200	3.13221200	0.37950300
H(Fragment=2)	6.02480000	2.00108200	-2.03488100
C(Fragment=3)	-5.70631900	-3.70805400	0.17322300
C(Fragment=2)	5.70551900	3.70734700	-0.17544600
H(Fragment=3)	-5.62516800	-3.95639000	1.23169300
H(Fragment=2)	5.62482500	3.95502800	-1.23410300

H(Fragment=3)	-4.72849400	-3.83061300	-0.29826700
H(Fragment=2)	4.72730200	3.82921500	0.29540800
H(Fragment=3)	-6.43295400	-4.37797600	-0.29353700
H(Fragment=2)	6.43126900	4.37815600	0.29140700
C(Fragment=1)	2.93988800	-2.20897800	1.57831000
C(Fragment=3)	-6.30489200	-1.82587400	-1.34059000
C(Fragment=4)	-2.94095000	2.20968300	-1.57790600
C(Fragment=2)	6.30482600	1.82659900	1.33983400
H(Fragment=1)	3.95034800	-2.45944000	1.25058900
H(Fragment=3)	-6.95480500	-2.50687400	-1.89474300
H(Fragment=4)	-3.95118300	2.45982500	-1.24923600
H(Fragment=2)	6.95385100	2.50847700	1.89394000
H(Fragment=1)	2.81869200	-2.47154100	2.63332300
H(Fragment=3)	-5.32444000	-1.77628800	-1.82099000
H(Fragment=4)	-2.82063900	2.47294600	-2.63284600
H(Fragment=2)	5.32412700	1.77658700	1.81968200
H(Fragment=1)	2.76617200	-1.14318200	1.45132600
H(Fragment=3)	-6.75501700	-0.83663900	-1.31202800
H(Fragment=4)	-2.76696800	1.14383400	-1.45173600
H(Fragment=2)	6.75576400	0.83770900	1.31218300
Li(Fragment=1)	-1.10458600	-0.62512700	-0.42183300
Li(Fragment=2)	6.28780300	-1.49037300	-1.03007300
Li(Fragment=4)	1.10412200	0.62514000	0.42063700
Li(Fragment=3)	-6.28580300	1.48964900	1.03225300
C(Fragment=1)	2.26648200	-4.41549400	0.64398300
H(Fragment=1)	3.24912800	-4.55091700	0.18736600
H(Fragment=1)	2.25610600	-4.88008700	1.63346600

H(Fragment=1)	1.50193000	-4.88181600	0.02314400
C(Fragment=4)	-2.26667800	4.41582600	-0.64334400
H(Fragment=4)	-3.24918000	4.55127500	-0.18642100
H(Fragment=4)	-1.50190500	4.88179100	-0.02250700
H(Fragment=4)	-2.25644200	4.88075100	-1.63267400

T4 **-2865.956290 Hartree**

Cl(Fragment=1)	-2.61277200	-2.06291600	0.97317100
Cl(Fragment=2)	-5.66521000	3.44878900	-0.62761600
Cl(Fragment=4)	2.61296900	2.06463300	-0.97720900
Cl(Fragment=3)	5.66338100	-3.44864800	0.62934300
O(Fragment=1)	-0.66796000	1.20448700	0.19675700
O(Fragment=3)	6.48297600	0.31126300	1.02874100
O(Fragment=4)	0.66706600	-1.20266100	-0.20358400
O(Fragment=2)	-6.48156100	-0.31269800	-1.02128700
N(Fragment=1)	-2.01950600	2.96754600	0.76400400
N(Fragment=3)	6.12386900	2.33746400	0.03250900
N(Fragment=4)	2.01927400	-2.96601600	-0.76849200
N(Fragment=2)	-6.12308400	-2.34002200	-0.02724000
C(Fragment=1)	-0.97764400	2.42293300	0.16469700
C(Fragment=3)	6.21487200	1.52326400	1.07731100
C(Fragment=4)	0.97646800	-2.42116100	-0.17102900
C(Fragment=2)	-6.21346000	-1.52463900	-1.07117200
H(Fragment=1)	-0.34334400	3.11879900	-0.39346300
H(Fragment=3)	6.04072100	2.01580200	2.04262200
H(Fragment=4)	0.34100300	-3.11689400	0.38598700
H(Fragment=2)	-6.03879900	-2.01608000	-2.03694400

C(Fragment=3)	5.68187900	3.72134900	0.18952300
C(Fragment=2)	-5.68151900	-3.72384600	-0.18556200
H(Fragment=3)	5.61542400	3.96732400	1.24957800
H(Fragment=2)	-5.61347400	-3.96834700	-1.24584800
H(Fragment=3)	4.69708600	3.84121300	-0.26792700
H(Fragment=2)	-4.69749100	-3.84490800	0.27321200
H(Fragment=3)	6.39930700	4.39468300	-0.28648500
H(Fragment=2)	-6.39996500	-4.39757700	0.28837900
C(Fragment=1)	-2.96457600	2.19468000	1.57458400
C(Fragment=3)	6.26457100	1.84431100	-1.33688500
C(Fragment=4)	2.96628800	-2.19337300	-1.57700400
C(Fragment=2)	-6.26394800	-1.84820000	1.34259400
H(Fragment=1)	-3.97685800	2.45151900	1.25774600
H(Fragment=3)	6.90845200	2.52575700	-1.89758700
H(Fragment=4)	3.97777800	-2.44815400	-1.25593900
H(Fragment=2)	-6.90750800	-2.53040900	1.90272700
H(Fragment=1)	-2.83231500	2.44971300	2.63013700
H(Fragment=3)	5.27784100	1.79837500	-1.80458800
H(Fragment=4)	2.83842700	-2.45080900	-2.63250800
H(Fragment=2)	-5.27718400	-1.80223800	1.81022300
H(Fragment=1)	-2.79720800	1.12883900	1.43940400
H(Fragment=3)	6.71346000	0.85432900	-1.31686400
H(Fragment=4)	2.79669900	-1.12754300	-1.44463300
H(Fragment=2)	-6.71319300	-0.85836100	1.32350200
Li(Fragment=4)	1.09571600	0.63716000	-0.42740800
Li(Fragment=2)	-6.31692300	1.47393300	-1.02009400
Li(Fragment=1)	-1.09649100	-0.63522000	0.42124800

Li(Fragment=3)	6.31729500	-1.47529000	1.02560200
C(Fragment=1)	-2.29729000	4.40134100	0.63555500
H(Fragment=1)	-3.28152700	4.53563500	0.18208200
H(Fragment=1)	-2.28428600	4.86669800	1.62465600
H(Fragment=1)	-1.53499900	4.86784300	0.01210600
C(Fragment=4)	2.29670300	-4.39980700	-0.63921500
H(Fragment=4)	3.28013300	-4.53409900	-0.18398200
H(Fragment=4)	1.53328000	-4.86609800	-0.01699200
H(Fragment=4)	2.28541300	-4.86538700	-1.62823100

T5 **-2865.985676 Hartree**

Cl(Fragment=1)	0.37484400	-1.37574600	-1.11999000
O(Fragment=1)	-2.91875500	-1.33084000	0.53883600
N(Fragment=1)	-3.13000200	-2.13019100	2.67357500
C(Fragment=1)	-3.55520200	-1.92852200	1.42725000
C(Fragment=1)	-3.94000000	-2.89432000	3.61700000
H(Fragment=1)	-4.87131900	-3.20050300	3.14140300
H(Fragment=1)	-4.17439300	-2.28419200	4.49326400
H(Fragment=1)	-3.39937100	-3.78711400	3.94438800
C(Fragment=1)	-1.83886200	-1.63156100	3.14656900
H(Fragment=1)	-1.10902100	-2.44558500	3.19139200
H(Fragment=1)	-1.47035300	-0.84830100	2.48697700
Li(Fragment=1)	-1.40338000	-0.25830400	-0.17773800
H(Fragment=1)	-4.55700400	-2.31561000	1.20851400
H(Fragment=1)	-1.96602600	-1.21539000	4.14798400
O(Fragment=1)	-2.77176400	0.71939300	-1.33924200
N(Fragment=1)	-3.80177300	2.66681400	-1.92153000

C(Fragment=1)	-2.86126400	1.96375300	-1.29779500
H(Fragment=1)	-2.13318800	2.54250500	-0.71837400
C(Fragment=1)	-3.90602700	4.11091900	-1.73529500
H(Fragment=1)	-3.09066900	4.45906200	-1.10139500
H(Fragment=1)	-3.85142800	4.62223600	-2.69977900
H(Fragment=1)	-4.85545600	4.36301100	-1.25546200
C(Fragment=1)	-4.82802700	1.99206800	-2.72703600
H(Fragment=1)	-5.58963900	1.52784300	-2.09436600
H(Fragment=1)	-5.28989700	2.72701100	-3.38567900
H(Fragment=1)	-4.36269000	1.21256800	-3.33010800
Li(Fragment=1)	-4.00610500	-0.69948500	-0.95451800
Cl(Fragment=1)	-6.12367200	-1.00126000	-0.82539500
Cl(Fragment=2)	6.12369500	1.00133900	0.82539400
O(Fragment=2)	2.77179500	-0.71935900	1.33923600
N(Fragment=2)	3.80178500	-2.66680800	1.92152600
C(Fragment=2)	2.86129200	-1.96372100	1.29779300
C(Fragment=2)	3.90600600	-4.11091400	1.73528000
H(Fragment=2)	3.09065000	-4.45902900	1.10136400
H(Fragment=2)	3.85137700	-4.62223700	2.69975900
H(Fragment=2)	4.85543700	-4.36302800	1.25546300
C(Fragment=2)	4.82803600	-1.99209700	2.72706700
H(Fragment=2)	5.58964400	-1.52782800	2.09442300
H(Fragment=2)	4.36269600	-1.21263800	3.33018800
Li(Fragment=2)	4.00613000	0.69953000	0.95451600
H(Fragment=2)	2.13320700	-2.54246200	0.71837400
H(Fragment=2)	5.28991500	-2.72707600	3.38566400
O(Fragment=2)	2.91878100	1.33087600	-0.53883900

N(Fragment=2)	3.13000000	2.13018200	-2.67358300
C(Fragment=2)	3.55522100	1.92855100	-1.42726100
H(Fragment=2)	4.55702300	2.31565100	-1.20854200
C(Fragment=2)	3.93997100	2.89429700	-3.61704400
H(Fragment=2)	4.87129800	3.20049800	-3.14147500
H(Fragment=2)	4.17434800	2.28415100	-4.49329900
H(Fragment=2)	3.39932700	3.78707900	-3.94444000
C(Fragment=2)	1.83885400	1.63152600	-3.14653300
H(Fragment=2)	1.10899900	2.44553800	-3.19135400
H(Fragment=2)	1.96599700	1.21533400	-4.14794200
H(Fragment=2)	1.47037500	0.84827600	-2.48691000
Li(Fragment=2)	1.40340600	0.25833500	0.17773200
Cl(Fragment=2)	-0.37482100	1.37577300	1.11998900