

Ambiguities in Solvation Free Energies from Cluster-Continuum Quasichemical Theory: Lithium Cation in Protic and Aprotic Solvents

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Computational details

Identification procedure of 20 most stable and geometrically diverse conformers from the molecular dynamic trajectory

First, we filled up the Python¹ list A with the 3000 most stable geometries from the MD trajectory and sorted it out based on respective energy values. Second, we consequently populated another list B of maximum length of 20 with the most structurally and energetically diverse geometries. Each new structure was allowed to join the list B if a) its QUATFIT² calculated RMSD structural deviation against all already found structure in list B was larger than certain threshold (0.5 Å); b) its PBE/ λ 1 energy deviates by certain threshold (0.001 Hartree) from that of already found structures in list A. If at the end of procedure the number of structures was less than 20, the RMSD threshold was further relaxed and the procedure was repeated until the total number of structures was 20.

Internal SMD parameters for DME and GBL solvents

DME

```
%cpcm
```

```
epsilon = 7.55
```

```
Refrac = 1.37702
```

```
smd true # turn on SMD
```

```
SMDsolvent "THF" # specify the name of solvent from the list
```

```
soln 1.37945 # index of refraction at optical frequencies at 293 K
```

```
soln25 1.37702 # index of refraction at optical frequencies at 298 K
```

```
sola 0.0 # Abraham's hydrogen bond acidity
```

solb 0.68 # Abraham's hydrogen bond basicity
solg 35.4216652 # relative macroscopic surface tension
solc 0.0 # aromaticity, fraction of non-hydrogenic solvent atoms
that are aromatic carbon atoms
solh 0.0 # electronegative halogenicity, fraction of non-hydrogenic
solvent atoms that are F, Cl, or Br
end

GBL

epsilon = 41.7
Refrac = 1.4358
smd true # turn on SMD
SMDsolvent "METHANOL" # specify the name of solvent from the list
soln 1.4374 # index of refraction at optical frequencies at 293 K
soln25 1.4358 # index of refraction at optical frequencies at 298 K
sola 0.0 # Abraham's hydrogen bond acidity
solb 0.59 # Abraham's hydrogen bond basicity
solg 62.524 # relative macroscopic surface tension
solc 0.0 # aromaticity, fraction of non-hydrogenic solvent atoms
that are aromatic carbon atoms
solh 0.0 # electronegative halogenicity, fraction of non-hydrogenic
solvent atoms that are F, Cl, or Br
end

Tables

Table S1. Li⁺ solvation free energies in kcal/mol from pure continuum solvation models with no explicit solvent molecules introduced.

	1 ^a	2 ^a	3 ^a	Expt. ³
MeCN	-88.7	-87.8	-115	-110.1
DMA	-88.8	-87.8	-115.1	-122.1
DMF	-88.8	-87.7	-115.2	-122.2
DMSO	-89.3	-87.9	-115.7	-121.0
H₂O	-90.0	-90.0	-116.8	-116.9
MeOH	-88.4	-87.7	-114.6	-116.2
TMS	-89.1	-87.2	-115.6	-115.4
MSE ^{b,c}	28.7	29.7	2.3	
MUE ^{c,d}	28.7	29.7	3.7	
ρ ^{c,e}	0.10	-0.01	0.08	
DME	-79.1	-78.4	-102.6	
GBL	-89.0	-87.7	-115.4	
Py	-84.2	-83.2	-108.8	

^a Strategies: 1 SMD_SP; 2 SMD_SP_PBE; 3 CPCM_SP_PBE; ^b Mean signed error in kcal/mol; ^c With respect to experimental values comprised in compilation of Marcus.;³ ^d Mean unsigned error in kcal/mol; ^e Pearson correlation coefficient.

Table S2. Monomer cycle Li⁺ solvation free energies $\Delta G_{solv}^*(Li^+)$ in kcal/mol obtained with four continuum model strategies: SMD_OPT, SMD_SP, SMD_SP_PBE, CPCM_SP_PBE.

	SMD_OPT	SMD_SP	SMD_SP_PBE	CPCM_SP_PBE
MeCN₄	-112.0	-112.0	-115.2	-110.6
MeCN₅	-103.1	-102.1	-105.5	-101.0
DMA₄	-129.1	-128.6	-124.5	-119.8
DMA₅	-122.3	-124.8	-120.4	-115.0
DME₃	-127.1	-127.7	-126.1	-123.4
DME₄	-123.8	-122.7	-120.2	-118.1
DMF₄	-124.6	-125.2	-121.9	-117.8
DMF₅	-122.7	-120.5	-116.6	-112.9
DMF₆	-117.0	-117.1	-113.7	-107.9
DMSO₃	-123.7	-125.0	-124.0	-120.9
DMSO₄	-129.2	-129.3	-127.8	-121.2
DMSO₅	-125.5	-125.0	-122.6	-115.8
GBL₄	-123.4	-121.3	-118.1	-115.2
GBL₅	-122.2	-122.9	-118.8	-115.8
GBL₆	-118.2	-119.7	-114.7	-111.8
H₂O₄	-119.4	-118.2	-115.8	-117.0
H₂O₅	-112.4	-114.4	-112.3	-114.1
MeOH₃	-111.7	-111.8	-114.3	-115.5
MeOH₄	-114.2	-113.8	-117.4	-115.6
Py₃	-112.4	-112.4	-114.2	-113.5
Py₄	-117.5	-117.5	-120.4	-117.0
TMS₄	-118.8	-118.0	-115.6	-111.8

Table S3. Cluster cycle Li⁺ solvation free energies $\Delta G_{solv}^*(Li^+)$ in kcal/mol obtained with four continuum model strategies: SMD_OPT, SMD_SP, SMD_SP_PBE, CPCM_SP_PBE.

	SMD_OPT	SMD_SP	SMD_SP_PBE	CPCM_SP_PBE
MeCN₄	-130.0	-130.6	-132.9	-128.7
MeCN₅	-127.7	-129.2	-131.8	-127.3
DMA₄	-141.6	-141.6	-140.1	-136.0
DMA₅	-140.6	-142.1	-141.1	-136.3
DME₃	-137.9	-138.2	-138.3	-134.8
DME₄	-140.0	-139.4	-139.0	-136.3
DMF₄	-136.7	-136.3	-133.5	-130.6
DMF₅	-140.0	-137.4	-135.1	-133.0
DMF₆	-140.0	-139.6	-139.6	-134.5
DMSO₃	-132.5	-134.0	-134.3	-132.2
DMSO₄	-142.0	-143.5	-143.7	-138.9
DMSO₅	-143.7	-141.7	-142.0	-137.5
GBL₄	-131.7	-129.0	-128.4	-124.7
GBL₅	-132.5	-131.7	-131.2	-127.1
GBL₆	-131.8	-131.9	-130.8	-126.8
H₂O₄	-128.8	-128.4	-126.4	-125.9
H₂O₅	-126.2	-130.5	-128.4	-128.1
MeOH₃	-120.5	-121.2	-123.1	-123.0
MeOH₄	-124.0	-124.4	-126.9	-123.0
Py₃	-123.6	-123.5	-125.4	-124.0
Py₄	-132.2	-133.1	-135.9	-131.6
TMS₄	-131.2	-129.5	-128.8	-125.5

Table S4. Individual contributions to monomer cycle predicted Li⁺ solvation free energies.

Complex	$\Delta E_{clust}(Li^+(S)_n)$	$\Delta G_{clust}^*(Li^+(S)_n)$	$\Delta G_{solv}^*(Li^+(S)_n)$	$\Delta G_{solv}^*(S)$	$nRT \ln[S]$
MeCN₄	-123.0	-89.3	-45.1/-45.2/ 45.5/-42.1	-7.4/-7.4/ 6.7/-7.0	7.0
MeCN₅	-130.8	-85.5	-45.6/-44.8/ 44.6/-41.6	-7.4/-7.4/ 6.7/-7.0	8.75
DMA₄	-148.9	-107.9	-40.8/-39.2/ 39.8/-36.7	-6.3/-6.0/ 7.2/-7.6	5.63
DMA₅	-164.4	-108.5	-38.4/-39.5/ 41.0/-37.4	-6.3/-6.0/ 7.2/-7.6	7.04
DME₃	-132.3	-96.1	-37.3/-37.6/ 38.1/-35.0	-3.5/-3.3/ 4.1/-3.9	4.03
DME₄	-144.1	-95.6	-36.7/-35.2/ 35.5/-32.9	-3.5/-3.3/ 4.1/-3.9	5.37
DMF₄	-143.1	-102.4	-41.7/-40.9/ 39.5/-38.8	-6.4/-6.1/ 6.5/-7.4	6.07
DMF₅	-154.1	-103.3	-43.8/-39.9/ 38.3/-38.9	-6.4/-6.1/ 6.5/-7.4	7.59
DMF₆	-170.1	-103.8	-42.5/-40.6/ 39.9/-39.3	-6.4/-6.1/ 6.5/-7.4	9.11
DMSO₃	-129.3	-99.1	-43.8/-44.9/ 42.8/-45.8	-8.0/-7.9/ 7.5/-9.6	4.7
DMSO₄	-154.2	-110.9	-44.0/-43.8/ 40.8/-42.3	-8.0/-7.9/ 7.5/-9.6	6.27
DMSO₅	-167.0	-112.1	-45.5/-44.7/ 40.4/-43.7	-8.0/-7.9/ 7.5/-9.6	7.83
GBL₄	-135.3	-94.4	-46.1/-43.1/ 45.7/-41.8	-7.4/-7.1/ 8.6/-8.3	12.38
GBL₅	-154.9	-100.7	-42.9/-42.4/ 45.5/-41.2	-7.4/-7.1/ 8.6/-8.3	15.47

GBL₆	-167.3	-101.4	-42.5/-42.6/ 46.3/-41.7	-7.4/-7.1/ 8.6/-8.3	18.57
H₂O₄	-105.2	-76.1	-68.0/-67.0/ 61.9/-60.9	-8.5/-8.6/ 7.9/-7.4	9.51
H₂O₅	-120.1	-80.0	-63.2/-65.5/ 60.0/-59.0	-8.5/-8.6/ 7.9/-7.4	11.89
MeOH₃	-95.1	-69.6	-56.1/-55.8/ 53.9/-55.1	-6.6/-6.4/ 5.0/-5.0	5.7
MeOH₄	-113.9	-78.5	-54.4/-53.4/ 51.2/-49.3	-6.6/-6.4/ 5.0/-5.0	7.6
Py₃	-112.3	-82.0	-42.0/-41.9/ 46.1/-40.4	-5.3/-5.3/ 6.1/-4.5	4.48
Py₄	-136.2	-93.4	-39.5/-39.5/ 45.6/-35.5	-5.3/-5.3/ 6.1/-4.5	5.97
TMS₄	-148.4	-104.2	-47.5/-46.5/ 46.9/-46.5	-9.6/-9.5/ 10.2/-11.1	5.57

Table S5. Individual contributions to cluster cycle predicted Li⁺ solvation free energies.

Complex	$\Delta E_{bind}(Li^+(S)_n)$	$\Delta G_{bind}^*(Li^+(S)_n)$	$\Delta G_{solv}^*(Li^+(S)_n)$	$\Delta G_{solv}^*(S_n)$	$RT\ln(\frac{[S]}{n})$
MeCN₄	-100.6	-96.8	-45.1/-45.2/ 45.5/-42.1	-12.9/ 12.4/ 10.4/-11.2	0.93
MeCN₅	-102.5	-98.1	-45.6/-44.8/ 44.6/-41.6	-16.9/ 14.5/ 11.7/-13.2	0.79
DMA₄	-116.7	-112.2	-40.8/-39.2/ 39.8/-36.7	-12.1/ 10.4/ 12.5/-13.5	0.59
DMA₅	-121.5	-114.8	-38.4/-39.5/ 41.0/-37.4	-13.0/ 12.6/ 15.1/-16.3	0.45
DME₃	-117.5	-105.8	-37.3/-37.6/ 38.1/-35.0	-5.9/-5.9/ 6.3/-6.7	0.69
DME₄	-123.3	-111.3	-36.7/-35.2/ 35.5/-32.9	-8.5/-7.6/ 8.3/-8.5	0.52
DMF₄	-113.0	-106.0	-41.7/-40.9/ 39.5/-38.8	-11.7/ 11.3/ 12.8/-15.0	0.70
DMF₅	-113.7	-108.7	-43.8/-39.9/ 38.3/-38.9	-13.0/ 11.7/ 12.4/-15.2	0.56
DMF₆	-117.6	-110.9	-42.5/-40.6/ 39.9/-39.3	-13.9/ 12.3/ 11.6/16.1	0.46
DMSO₃	-106.4	-99.1	-43.8/-44.9/ 42.8/-45.8	-11.4/ 11.0/-8.5/ 13.6	0.92
DMSO₄	-118.6	-110.8	-44.0/-43.8/ 40.8/-42.3	-13.6/ 11.8/-8.6/ 15.0	0.75

DMSO₅	-120.1	-112.4	-45.5/-44.7/ 40.4/-43.7	-14.8/ 16.0/ 11.5/-19.2	0.61
GBL₄	-102.3	-95.6	-46.1/-43.1/ 45.7/-41.8	-12.3/ 11.9/ 15.1/-14.9	2.27
GBL₅	-107.4	-99.8	-42.9/-42.4/ 45.5/-41.2	-12.3/ 12.7/ 16.3/-16.1	2.14
GBL₆	-110.6	-103.0	-42.5/-42.6/ 46.3/-41.7	-15.7/ 15.7/ 20.4/-20.0	2.03
H₂O₄	-78.4	-76.2	-68.0/-67.0/ 61.9/-60.9	-16.9/ 16.4/ 13.3/-12.7	1.57
H₂O₅	-85.7	-82.9	-63.2/-65.5/ 60.0/-59.0	-21.2/ 19.3/ 15.8/-15.2	1.42
MeOH₃	-77.7	-71.8	-56.1/-55.8/ 53.9/-55.1	-8.6/-7.7/ 3.8/-5.1	1.25
MeOH₄	-83.4	-78.1	-54.4/-53.4/ 51.2/-49.3	-9.5/-8.2/ 3.5/-5.5	1.08
Py₃	-99.6	-91.4	-42.0/-41.9/ 46.1/-40.4	-10.6/ 10.6/ 13.0/-8.7	0.84
Py₄	-115.4	-105.9	-39.5/-39.5/ 45.6/-35.5	-13.9/ 13.0/ 16.3/-10.5	0.67
TMS₄	-107.6	-99.6	-47.5/-46.5/ 46.9/-46.5	-16.5/ 17.2/ 18.2/-21.2	0.57

Table S6. $\Delta G_{solv}^*(S_n)$ obtained from continuum solvation models and their equation 3 counterparts in kcal/mol.

Complex	SMD_OPT		SMD_SP		SMD_SP_PBE		CPCM_SP_PBE	
	Continuum	Eq. 3	Continuum	Eq. 3	Continuum	Eq. 3	Continuum	Eq. 3
MeCN ₄	-12.9	-31.2	-12.4	-31.3	-10.4	-28.5	-11.2	-29.7
MeCN ₅	-16.9	-41.5	-14.5	-41.6	-11.7	-38.0	-13.2	-39.6
DMA ₄	-12.1	-24.6	-10.4	-23.5	-12.5	-28.2	-13.5	-29.7
DMA ₅	-13.0	-31.2	-12.6	-29.9	-15.1	-35.8	-16.3	-37.7
DME ₃	-5.9	-16.7	-5.9	-16.4	-6.3	-18.5	-6.7	-18.2
DME ₄	-8.5	-24.7	-7.6	-24.2	-8.3	-27.1	-8.5	-26.6
DMF ₄	-11.7	-23.8	-11.3	-22.5	-12.8	-24.3	-15.0	-27.8
DMF ₅	-13.0	-30.3	-11.7	-28.6	-12.4	-30.9	-15.2	-35.2
DMF ₆	-13.9	-36.9	-12.3	-34.8	-11.6	-37.6	-16.1	-42.7
DMSO ₃	-11.4	-20.2	-11.0	-20.0	-8.5	-18.8	-13.6	-24.9
DMSO ₄	-13.6	-26.3	-11.8	-26.0	-8.6	-24.5	-15.0	-32.6
DMSO ₅	-14.8	-33.0	-16.0	-32.7	-11.5	-30.8	-19.2	-40.9
GBL ₄	-12.3	-20.6	-11.9	-19.6	-15.1	-25.4	-14.9	-24.4
GBL ₅	-12.3	-22.6	-12.7	-21.4	-16.3	-28.7	-16.1	-27.3
GBL ₆	-15.7	-29.3	-15.7	-27.8	-20.4	-36.5	-20.0	-34.9
H ₂ O ₄	-16.9	-26.3	-16.4	-26.6	-13.3	-23.9	-12.7	-21.6
H ₂ O ₅	-21.2	-35.0	-19.3	-35.4	-15.8	-32.0	-15.2	-29.2
MeOH ₃	-8.6	-17.4	-7.7	-17.0	-3.8	-12.6	-5.1	-12.6
MeOH ₄	-9.5	-19.4	-8.2	-18.9	-3.5	-13.0	-5.5	-12.9
Py ₃	-10.6	-21.8	-10.6	-21.8	-13.0	-24.2	-8.7	-19.2
Py ₄	-13.9	-28.6	-13.0	-28.6	-16.3	-31.8	-10.5	-25.1
TMS ₄	-16.5	-28.9	-17.2	-28.6	-18.2	-31.4	-21.2	-34.9
MAD	13.9		14.0		15.3		15.2	
MSD	13.9		14.0		15.3		15.2	

Table S7. Experimental $\Delta G_{solv}^*(S)$ in comparison with their counterparts from continuum solvation models in kcal/mol.

Solvent	Expt.	SMD_OPT	SMD_SP	SMD_SP_PBE	CPCM_SP_PCM
H₂O	-6.3 (3146 Pa) ^{a4}	-8.5	-8.6	-7.9	-7.4
MeCN	-4.9 (11825 Pa) ^{a5}	-7.4	-7.4	-6.7	-7.0
DMA	-6.8 (266.7 Pa) ^{a6}	-6.3	-6.0	-7.2	-7.6
DME	-4.9 (6399.5 Pa) ^{a7}	-3.5	-3.3	-4.1	-3.9
DMF	-6.6 (500.0 Pa) ^{a8}	-6.4	-6.1	-6.5	-7.4
DMSO	-7.7 (82.0 Pa) ^{a9}	-8.0	-7.9	-7.5	-9.6
GBL	-9.4 (60.0 Pa) ^{a10}	-7.4	-7.1	-8.6	-8.3
MeOH	-4.9 (16931.9 Pa) ^{a11}	-6.6	-6.4	-5.0	-5.0
Py	-5.5 (2773.1 Pa) ^{a6}	-5.3	-5.3	-6.1	-4.5
TMS	-10.2 (0.8 Pa) ^{a6}	-9.6	-9.5	-10.2	-11.1
MUE		1.2	1.2	0.6	1.1
MSE		-0.2	-0.1	-0.3	-0.4

^a See equation (3) in main paper for relation between $\Delta G_{solv}^*(S)$ and pressure.

Table S8. Equation 3 $\Delta G_{sol}^*(S_n)$ calculated from the DLPNO-CCSD(T) $\Delta G_{bind}^*((S)_n)$ and experimental $\Delta G_{sol}^*(S)$ against their counterparts from continuum solvation models in kcal/mol.

	Eq. 3	SMD_OPT	SMD_SP	SMD_SP_PBE	CPCM_SP_PBE
MeCN ₄	-21.4	-12.9	-12.4	-10.4	-11.2
MeCN ₅	-29.3	-16.9	-14.5	-11.7	-13.2
DMA ₄	-26.6	-12.1	-10.4	-12.5	-13.5
DMA ₅	-33.8	-13.0	-12.6	-15.1	-16.3
DME ₃	-21.0	-5.9	-5.9	-6.3	-6.7
DME ₄	-30.3	-8.5	-7.6	-8.3	-8.5
DMF ₄	-24.5	-11.7	-11.3	-12.8	-15.0
DMF ₅	-31.1	-13.0	-11.7	-12.4	-15.2
DMF ₆	-37.8	-13.9	-12.3	-11.6	-16.1
DMSO ₃	-19.3	-11.4	-11.0	-8.5	-13.6
DMSO ₄	-25.1	-13.6	-11.8	-8.6	-15.0
DMSO ₅	-31.5	-14.8	-16.0	-11.5	-19.2
GBL ₄	-28.7	-12.3	-11.9	-15.1	-14.9
GBL ₅	-32.7	-12.3	-12.7	-16.3	-16.1
GBL ₆	-41.4	-15.7	-15.7	-20.4	-20.0
H ₂ O ₄	-17.5	-16.9	-16.4	-13.3	-12.7
H ₂ O ₅	-24.0	-21.2	-19.3	-15.8	-15.2
MeOH ₃	-12.3	-8.6	-7.7	-3.8	-5.1
MeOH ₄	-12.5	-9.5	-8.2	-3.5	-5.5
Py ₃	-22.3	-10.6	-10.6	-13.0	-8.7
Py ₄	-29.3	-13.9	-13.0	-16.3	-10.5
TMS ₄	-31.4	-16.5	-17.2	-18.2	-21.2
MUE		13.6	14.3	14.5	13.2
MSE		13.6	14.3	14.5	13.2

Table S9. Experimental-based monomer/cluster (EB MC) $\Delta G_{solv,n}^*(Li^+)$.

	SMD_opt	SMD_SP	SMD_SP_PBE	CPCM_SP_PBE
MeCN₄	-121.8	-121.9	-122.2	-118.9
MeCN₅	-115.4	-114.5	-114.3	-111.3
DMA₄	-127.0	-125.4	-126.0	-122.9
DMA₅	-119.8	-120.9	-122.4	-118.8
DME₃	-122.8	-123.1	-123.6	-120.5
DME₄	-118.2	-116.6	-116.9	-114.4
DMF₄	-124.0	-123.2	-121.8	-121.1
DMF₅	-122.0	-118.0	-116.5	-117.1
DMF₆	-116.1	-114.2	-113.5	-112.9
DMSO₃	-124.6	-125.7	-123.6	-126.6
DMSO₄	-130.4	-130.3	-127.2	-128.8
DMSO₅	-127.0	-126.2	-121.9	-125.2
GBL₄	-115.3	-112.3	-114.8	-110.9
GBL₅	-112.1	-111.6	-114.8	-110.4
GBL₆	-106.0	-106.2	-109.9	-105.3
H₂O₄	-128.2	-127.3	-122.2	-121.2
H₂O₅	-123.4	-125.8	-120.2	-119.3
MeOH₃	-116.8	-116.5	-114.7	-115.8
MeOH₄	-121.0	-120.1	-117.8	-116.0
Py₃	-111.9	-111.8	-116.0	-110.3
Py₄	-116.7	-116.8	-122.8	-112.8
TMS₄	-116.3	-115.3	-115.7	-115.3

Table S10. MSE, MUE in kcal/mol and the Person correlation coefficient between Marcus experimental-based “bulk” scale $\Delta G_{solv,n}^*(Li^+)$ and their counterparts obtained from “monomer”, “cluster” and “experimental-based monomer/cluster” cycles.

Cycle	SMD_OPT	SMD_SP	SMD_SP_PBE	CPCM_SP_PBE
Monomer				
MSE	-3.4	-3.0	-2.0	1.4
MUE	3.9	3.7	2.4	1.7
ρ	0.91	0.91	0.82	0.89
Cluster (n=4)				
MSE	-15.8	-15.8	-15.5	-12.1
MUE	15.8	15.8	15.5	12.1
ρ	0.71	0.69	0.53	0.60
Cluster ^a				
MSE	-16.5	-16.6	-16.8	-13.3
MUE	16.5	16.6	16.8	13.3
ρ	0.75	0.75	0.68	0.72
EB M/C				
MSE	-6.4	-5.6	-4.2	-2.9
MUE	6.4	5.7	4.3	3.3
ρ	0.55	0.48	0.49	0.59
^a Number of explicitly coordinated solvent molecules n correspond to lowest Li+ solvation Gibbs free energy obtained (in some cases n larger than 4).				

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Cartesian Coordinates (Å) and Absolute Energies (Hartree) of All Species Studied in Present Work

MeCN

E (PBE-D3/ma-def2-svp GAS_OPT) =	-132.4932441391
E (PBE-D3/ma-def2-svp SMD_OPT) =	-132.5039012660
ΔG_{corr} (ID-RR-HR GAS) =	0.0186445809
E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT GAS) =	-132.5363959498
E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT SMD) =	-132.5481456865
E (DLPNO-CCSDT/cc-p(wC)VTZ SMD_OPT SMD) =	-132.5481131465
E (PBE-D3/ma-def2-tzvp GAS_OPT GAS) =	-132.6381795565
E (PBE-D3/ma-def2-tzvp GAS_OPT SMD) =	-132.6487938268
E (PBE-D3/ma-def2-tzvp GAS_OPT CPCM) =	-132.6492806100
GAS_OPT	SMD_OPT
C 2.985925 -0.526925 -3.017894	C 2.993737 -0.529528 -3.016186
N 1.918333 -0.132856 -3.293685	N 1.924608 -0.135657 -3.291820
C 4.314793 -1.017305 -2.674641	C 4.315955 -1.017472 -2.674409
H 4.719016 -1.644385 -3.493927	H 4.713912 -1.643769 -3.497436
H 4.274599 -1.628211 -1.751041	H 4.268201 -1.627355 -1.750450
H 5.008029 -0.169500 -2.505806	H 5.004284 -0.165400 -2.506694

(MeCN)₄

E (PBE-D3/ma-def2-svp GAS_OPT) =	-530.0099892320
E (PBE-D3/ma-def2-svp SMD_OPT) =	-530.0275452086
ΔG_{corr} (ID-RR-HR GAS) =	0.1313758392

E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT GAS) =	-530.1813785753
E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT SMD) =	-530.2011244816
E (DLPNO-CCSDT/cc-p(wC)VTZ SMD_OPT SMD) =	-530.2018602264
E (PBE-D3/ma-def2-tzvp GAS_OPT GAS) =	-530.5883226935
E (PBE-D3/ma-def2-tzvp GAS_OPT SMD) =	-530.6048281048
E (PBE-D3/ma-def2-tzvp GAS_OPT CPCM) =	-530.6060947060
GAS_OPT	SMD_OPT
C 1.427630 -0.656319 2.342283	C 0.565472 -0.988133 2.811184
N 2.228319 -0.917514 3.157454	N 1.488095 -0.411176 3.247337
C 0.428588 -0.318906 1.341367	C -0.570661 -1.708139 2.269695
H 0.673795 0.668352 0.900043	H -0.265989 -2.743633 2.016055
H -0.567564 -0.247688 1.823713	H -0.933119 -1.208190 1.349885
H 0.404056 -1.087095 0.543862	H -1.389776 -1.743285 3.015036
C -1.320739 2.135309 3.652148	C 1.348049 -1.793397 -1.126376
N -1.679124 1.019258 3.653208	N 0.507921 -0.999263 -0.931676
C -0.857673 3.513313 3.644981	C 2.391404 -2.771552 -1.365350
H -1.711743 4.209671 3.534159	H 2.459476 -2.997057 -2.448038
H -0.145821 3.655094 2.805908	H 2.169689 -3.706420 -0.813702
H -0.322570 3.724625 4.592569	H 3.364983 -2.369759 -1.019553
C 2.718124 2.487243 2.634089	C 3.302904 0.641499 0.469350
N 1.903164 2.755912 1.835696	N 4.141668 -0.169876 0.356010
C 3.717441 2.147867 3.633803	C 2.262239 1.641636 0.602953
H 3.844191 1.046705 3.664099	H 2.102762 1.881237 1.672495
H 3.368127 2.486184 4.630386	H 1.316295 1.251376 0.176644
H 4.685868 2.628049 3.392263	H 2.550190 2.564711 0.061696
C 0.911519 1.045111 5.990089	C 2.892764 -3.501417 2.285975
N 1.282651 2.156773 5.975137	N 1.970236 -4.119438 1.909253
C 0.451779 -0.334270 5.993122	C 4.035474 -2.731232 2.735489
H -0.519960 -0.394869 5.462143	H 4.932560 -3.379815 2.788260
H 0.331231 -0.700220 7.031510	H 3.837407 -2.306098 3.738991
H 1.185092 -0.967998 5.454508	H 4.228638 -1.899453 2.026732

Li⁺(MeCN)₄

E (PBE-D3/ma-def2-svp GAS_OPT) =	-537.4258365340
E (PBE-D3/ma-def2-svp SMD_OPT) =	-537.4979479113
ΔG_{corr} (ID-RR-HR GAS) =	0.1276162193

E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT GAS) =	-537.6152972849
E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT SMD) =	-537.6872989455
E (DLPNO-CCSDT/cc-p(wC)VTZ SMD_OPT SMD) =	-537.6871119807
E (PBE-D3/ma-def2-tzvp GAS_OPT GAS) =	-538.0074629541
E (PBE-D3/ma-def2-tzvp GAS_OPT SMD) =	-538.0799573534
E (PBE-D3/ma-def2-tzvp GAS_OPT CPCM) =	-538.0745953591
GAS_OPT	SMD_OPT
C -1.360835 2.001590 2.102683	C -1.380632 1.997945 2.071490
N -0.864527 1.272297 1.336659	N -0.845402 1.287772 1.311637
C -1.977753 2.908101 3.055098	C -2.045412 2.874082 3.010450
H -1.239417 3.657950 3.402020	H -1.351492 3.144349 3.831003
H -2.351925 2.343795 3.932208	H -2.930569 2.362592 3.437795
H -2.828565 3.437649 2.582376	H -2.374353 3.797972 2.494687
Li 0.001180 0.000635 -0.000335	Li 0.034394 0.031967 -0.007795
C 1.721392 1.684036 -2.119004	C 1.748990 1.675868 -2.139826
N 1.094665 1.070924 -1.346807	N 1.114675 1.081416 -1.357230
C 2.500537 2.446229 -3.078916	C 2.533242 2.406508 -3.110599
H 2.811330 1.796144 -3.920681	H 2.777471 1.746925 -3.966874
H 3.407113 2.858714 -2.593376	H 3.474687 2.759933 -2.645146
H 1.897808 3.285089 -3.479918	H 1.959726 3.280654 -3.477666
C -2.279652 -1.643290 -1.542438	C -2.265709 -1.621768 -1.482644
N -1.448326 -1.044250 -0.981160	N -1.413966 -1.016355 -0.957080
C -3.313011 -2.387942 -2.240352	C -3.320990 -2.370644 -2.128342
H -3.859745 -1.721562 -2.936624	H -4.122662 -1.681251 -2.459998
H -4.033725 -2.813368 -1.514158	H -3.747435 -3.106548 -1.417980
H -2.860762 -3.216339 -2.820874	H -2.917803 -2.908846 -3.009020
C 1.920776 -2.041684 1.557534	C 1.944395 -2.006215 1.539378
N 1.222347 -1.297521 0.988848	N 1.250129 -1.253115 0.974535
C 2.789138 -2.966798 2.264323	C 2.802220 -2.938627 2.236406
H 3.371396 -2.428544 3.038291	H 3.252381 -2.447402 3.121812
H 3.494305 -3.445451 1.556226	H 3.611774 -3.281502 1.561881
H 2.186749 -3.756194 2.756002	H 2.212340 -3.815708 2.569125

Li⁺ in MeCN

E (PBE-D3/ma-def2-svp GAS_OPT) =	-7.2519251623
E (PBE-D3/ma-def2-svp SMD_OPT) =	-7.3917970144

ΔG_{corr} (ID-RR-HR GAS) =	-0.0127326619
E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT GAS) =	-7.2736440090
E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT SMD) =	-7.4149214430
E (DLPNO-CCSDT/cc-p(wC)VTZ SMD_OPT SMD) =	-7.4149214430
E (PBE-D3/ma-def2-tzvp GAS_OPT GAS) =	-7.2566456293
E (PBE-D3/ma-def2-tzvp GAS_OPT SMD) =	-7.3964999510
E (PBE-D3/ma-def2-tzvp GAS_OPT CPCM) =	-7.4399355109
GAS_OPT	SMD_OPT
Li 0.0 0.0 0.0	Li 0.0 0.0 0.0

(MeCN)₅

E (PBE-D3/ma-def2-svp GAS_OPT) =	-662.5145186803
E (PBE-D3/ma-def2-svp SMD_OPT) =	-662.5362702156
ΔG_{corr} (ID-RR-HR GAS) =	0.1705267200
E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT GAS) =	-662.7270254144
E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT SMD) =	-662.7501386194
E (DLPNO-CCSDT/cc-p(wC)VTZ SMD_OPT SMD) =	-662.7539816331
E (PBE-D3/ma-def2-tzvp GAS_OPT GAS) =	-663.2369149863
E (PBE-D3/ma-def2-tzvp GAS_OPT SMD) =	-663.2556383866
E (PBE-D3/ma-def2-tzvp GAS_OPT CPCM) =	-663.2579799476
GAS_OPT	SMD_OPT
C 0.132099 1.090059 3.278800	C 0.509758 1.486293 2.169892

N	-0.532563	1.532575	2.421221	N	1.658679	1.372027	2.373203
C	0.966720	0.525205	4.325006	C	-0.911851	1.606581	1.911952
H	0.337139	0.132479	5.147661	H	-1.273510	0.686918	1.407969
H	1.646176	1.299202	4.733201	H	-1.107992	2.480669	1.260578
H	1.570020	-0.305372	3.894941	H	-1.462068	1.736538	2.865125
C	-1.218846	0.159729	-3.221230	C	-3.123727	0.198304	-2.372640
N	-1.891032	1.058147	-2.882999	N	-3.135432	-0.646478	-3.185620
C	-0.377115	-0.956670	-3.621133	C	-3.087367	1.242784	-1.367696
H	-0.627104	-1.839899	-2.999354	H	-3.777885	2.063075	-1.647731
H	0.685051	-0.691902	-3.445788	H	-2.056466	1.646766	-1.289824
H	-0.530480	-1.197734	-4.691046	H	-3.396775	0.834595	-0.385353
C	1.082007	1.647421	-1.224207	C	1.398118	1.628883	-1.144177
N	1.780258	0.800503	-1.634970	N	0.300407	2.003393	-1.315399
C	0.202130	2.687885	-0.718075	C	2.748222	1.146509	-0.932208
H	-0.051378	2.483839	0.343649	H	3.310087	1.159457	-1.887477
H	-0.730833	2.696981	-1.317674	H	2.721393	0.107753	-0.542189
H	0.694180	3.677495	-0.792623	H	3.270884	1.788759	-0.196385
C	-2.030886	-1.091379	-0.178231	C	-0.691578	-1.531979	-0.761878
N	-1.435852	-2.027091	-0.557698	N	-1.288189	-1.399532	0.238534
C	-2.760404	0.079376	0.279646	C	0.047663	-1.694383	-1.998471
H	-2.139812	0.653502	0.999984	H	0.101459	-0.730993	-2.542555
H	-3.703394	-0.223662	0.775647	H	-0.453404	-2.441182	-2.645573
H	-2.994130	0.724991	-0.591116	H	1.075734	-2.043920	-1.775799
C	2.124962	-1.950958	1.209650	C	1.947873	-2.075884	1.482661
N	2.281784	-1.696799	2.342663	N	2.561504	-2.025619	0.484857
C	1.924793	-2.262704	-0.195256	C	1.180218	-2.137282	2.710499
H	2.568208	-3.112703	-0.496002	H	1.293780	-3.135015	3.179200
H	2.169077	-1.373016	-0.812845	H	0.107870	-1.965236	2.487986
H	0.859225	-2.519496	-0.371824	H	1.532596	-1.361798	3.418519

Li⁺(MeCN)₅

E (PBE-D3/ma-def2-svp GAS_OPT) =	-669.9325182730
E (PBE-D3/ma-def2-svp SMD_OPT) =	-670.2353950389
ΔG_{corr} (ID-RR-HR GAS) =	0.1678198000
E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT GAS) =	-670.1640757362
E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT SMD) =	-670.2353950389
E (DLPNO-CCSDT/cc-p(wC)VTZ SMD_OPT SMD) =	-670.2368147974
E (PBE-D3/ma-def2-tzvp GAS_OPT GAS) =	-670.6586676812
E (PBE-D3/ma-def2-tzvp GAS_OPT SMD) =	-670.7297892800

E (PBE-D3/ma-def2-tzvp GAS_OPT CPCM) =	-670.7249423088
GAS_OPT	SMD_OPT
C -3.829553 -1.679885 0.772141	C -0.904026 1.539039 2.741138
N -2.957956 -1.300017 1.450801	N -0.589416 0.977056 1.764382
C -4.913268 -2.150333 -0.072780	C -1.293279 2.235087 3.949618
H -5.600526 -1.314872 -0.312338	H -0.412003 2.373448 4.606841
H -5.484637 -2.945192 0.446276	H -2.058643 1.646218 4.492964
H -4.508619 -2.561838 -1.018602	H -1.715066 3.227777 3.695855
Li -1.439391 -0.668370 2.645001	Li -0.010617 -0.008436 0.010978
C -2.608243 0.197567 5.496131	C -2.138624 1.914440 -1.788282
N -2.181401 -0.115724 4.454877	N -1.406610 1.251428 -1.160140
C -3.138937 0.587972 6.790593	C -3.043167 2.736424 -2.566861
H -2.852846 -0.155906 7.560328	H -4.081516 2.610638 -2.200995
H -4.244359 0.649401 6.747203	H -3.000551 2.441288 -3.634088
H -2.737977 1.578251 7.084280	H -2.757713 3.803438 -2.477972
C 0.624895 1.336737 1.318395	C 2.486633 1.148638 -1.744818
N -0.297757 0.785479 1.777374	N 1.593327 0.733451 -1.113563
C 1.793200 1.988045 0.756387	C 3.591808 1.662508 -2.526456
H 2.042878 2.896365 1.339380	H 3.784889 0.995772 -3.390260
H 1.601297 2.278655 -0.295276	H 4.505311 1.715700 -1.901704
H 2.651138 1.282789 0.791462	H 3.350594 2.676685 -2.902016
C 5.368747 -0.463003 0.762913	C -1.598686 -2.683159 -0.972924
N 4.241710 -0.497002 1.081575	N -1.030116 -1.723371 -0.620224
C 6.768525 -0.419914 0.368405	C -2.301472 -3.870934 -1.410543
H 6.869903 0.028362 -0.639839	H -3.375857 -3.642972 -1.557284
H 7.191856 -1.443620 0.343454	H -2.202137 -4.671426 -0.650872
H 7.352311 0.187482 1.088155	H -1.875766 -4.229205 -2.368836
C 1.123153 -2.531728 2.710092	C 2.134181 -1.931999 1.786945
N 0.064696 -2.043178 2.792939	N 1.389593 -1.267729 1.175129
C 2.451019 -3.103599 2.589109	C 3.058044 -2.753646 2.542883
H 2.422344 -4.006678 1.948065	H 3.894215 -2.133128 2.921873
H 2.839464 -3.385467 3.587586	H 3.469761 -3.553926 1.896392
H 3.128136 -2.350991 2.131091	H 2.536908 -3.219104 3.402842

DMA

E (PBE-D3/ma-def2-svp GAS_OPT) =	-287.2839327722
E (PBE-D3/ma-def2-svp SMD_OPT) =	-287.2959546690
ΔG_{corr} (ID-RR-HR GAS) =	0.0945535400
E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT GAS) =	-287.3732181847
E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT SMD) =	-287.3828292206

E (DLPNO-CCSDT/cc-p(wC)VTZ SMD_OPT SMD) =	-287.3832678615
E (PBE-D3/ma-def2-tzvp GAS_OPT GAS) =	-287.5920600082
E (PBE-D3/ma-def2-tzvp GAS_OPT SMD) =	-287.6035466029
E (PBE-D3/ma-def2-tzvp GAS_OPT CPCM) =	-287.6041503305
GAS_OPT	SMD_OPT
H -1.932162 0.308822 1.531288	H -1.917858 0.303299 1.525426
O 1.722814 -0.334211 -0.601590	O 1.733666 -0.341430 -0.608059
C 0.493988 -0.405542 -0.502366	C 0.493806 -0.407108 -0.503102
N -0.223905 0.474449 0.288806	N -0.212427 0.469377 0.283389
C 0.486504 1.507793 1.022023	C 0.484175 1.508470 1.022834
H 1.565371 1.412365 0.805957	H 1.567076 1.436395 0.821398
H 0.318828 1.400335 2.116231	H 0.307599 1.396821 2.114725
H 0.137044 2.518326 0.716164	H 0.121835 2.514178 0.717957
C -1.663136 0.459672 0.461473	C -1.655631 0.453092 0.455182
H -2.132125 -0.347017 -0.125102	H -2.127035 -0.352318 -0.130261
H -2.110430 1.426155 0.136908	H -2.096069 1.421096 0.130410
C -0.289496 -1.475038 -1.254042	C -0.293000 -1.470538 -1.249829
H -1.020488 -1.036328 -1.963547	H -1.026036 -1.026116 -1.953595
H 0.439516 -2.076082 -1.824544	H 0.421253 -2.084555 -1.826841
H -0.843893 -2.147054 -0.567576	H -0.852923 -2.134019 -0.559550

(DMA)₄

E (PBE-D3/ma-def2-svp GAS_OPT) =	-1149.1852821713
E (PBE-D3/ma-def2-svp SMD_OPT) =	-1149.2106422178
ΔG_{corr} (ID-RR-HR GAS) =	0.4455471200
E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT GAS) =	-1149.5442039514
E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT SMD) =	-1149.5607800158
E (DLPNO-CCSDT/cc-p(wC)VTZ SMD_OPT SMD) =	-1149.5634200077
E (PBE-D3/ma-def2-tzvp GAS_OPT GAS) =	-1150.4102376568
E (PBE-D3/ma-def2-tzvp GAS_OPT SMD) =	-1150.4302364297

E (PBE-D3/ma-def2-tzvp GAS_OPT CPCM) =				-1150.4317374931			
GAS_OPT				SMD_OPT			
H	1.242681	2.973889	0.945646	H	2.014211	-2.021571	-0.692350
O	1.166875	-0.671169	2.248811	O	-1.130718	-0.435566	-2.431398
C	1.317231	0.458824	1.740290	C	-0.229793	-1.038515	-1.810634
N	1.500672	1.573363	2.515696	N	0.922877	-1.448295	-2.427793
C	1.648505	1.444241	3.958625	C	1.088244	-1.266982	-3.860112
H	1.623669	0.373419	4.224102	H	1.125868	-2.250391	-4.378506
H	0.827744	1.981288	4.477860	H	2.036330	-0.730454	-4.076072
H	2.618708	1.882786	4.278558	H	0.238681	-0.685214	-4.255943
C	1.522793	2.936522	2.010700	C	1.950403	-2.245173	-1.771343
H	2.530302	3.393281	2.134293	H	2.932738	-2.007774	-2.224712
H	0.784790	3.542086	2.577607	H	1.769865	-3.335631	-1.906914
H	1.852072	-2.638538	1.221048	H	-1.416177	2.377391	-5.636386
O	-0.383119	-2.642044	-2.006620	O	-1.870469	4.751961	-2.332074
C	0.212881	-2.810958	-0.929903	C	-1.815258	3.685914	-2.978063
N	1.587328	-2.903371	-0.870207	N	-0.812025	3.432299	-3.878373
C	2.357397	-2.907321	-2.101087	C	0.165948	4.461986	-4.188930
H	1.662894	-2.799998	-2.952295	H	0.030526	4.831639	-5.229670
H	2.923728	-3.858092	-2.210246	H	1.196633	4.062639	-4.095425
H	3.087002	-2.068176	-2.113880	H	0.039771	5.306171	-3.489650
C	2.323380	-3.152247	0.363211	C	-0.789397	2.246107	-4.725327
H	3.344497	-2.734908	0.259967	H	-1.127225	1.349726	-4.174958
H	2.421191	-4.241337	0.576554	H	0.249694	2.063224	-5.059844
H	0.503924	-0.622352	-5.449437	H	-0.352542	1.674243	-1.356706
O	-1.144523	1.376351	-1.917189	O	2.885228	4.536982	-1.597675
C	-1.253522	0.531569	-2.824240	C	1.824137	4.147251	-1.072259
N	-0.228570	0.278792	-3.704516	N	1.374761	2.860048	-1.218738
C	1.056355	0.925458	-3.502512	C	2.143445	1.904270	-1.997608
H	0.927287	1.741152	-2.769749	H	2.254322	0.955419	-1.436617
H	1.434819	1.342798	-4.458766	H	3.139723	2.324412	-2.217597
H	1.810830	0.207142	-3.110120	H	1.632977	1.672128	-2.956813
C	-0.281048	-0.795328	-4.688589	C	0.143911	2.348882	-0.634105
H	-1.254370	-0.812420	-5.213694	H	-0.559819	3.161919	-0.393685
H	-0.119376	-1.786622	-4.212237	H	0.342089	1.767076	0.292040
H	-3.574168	0.351115	1.151103	H	5.439369	2.410479	1.585183
O	-1.381147	2.837101	3.622855	O	2.657897	-0.669681	1.328180
C	-1.701784	1.774626	3.064711	C	3.560114	0.084982	0.910487
N	-2.038645	1.724866	1.731372	N	3.585969	1.421676	1.213061
C	-2.168810	2.962930	0.975645	C	2.624102	1.972370	2.153422
H	-3.240032	3.186293	0.768242	H	2.155008	2.886507	1.736128
H	-1.645454	2.875258	0.002851	H	3.122325	2.250590	3.108828
H	-1.747617	3.787819	1.576136	H	1.844255	1.220256	2.362524
C	-2.474031	0.509718	1.058020	C	4.651878	2.324190	0.802739
H	-1.954295	-0.376636	1.460448	H	4.229345	3.332574	0.627058
H	-2.220958	0.593553	-0.016515	H	5.124875	1.996152	-0.138035
C	-0.536300	-2.918884	0.383841	C	-2.864894	2.605057	-2.801791
H	-0.360455	-3.901836	0.867200	H	-3.429175	2.438923	-3.743349
H	-0.207004	-2.137237	1.100583	H	-2.422752	1.629464	-2.512112
H	-1.614142	-2.811102	0.172467	H	-3.572887	2.929412	-2.018577
C	-2.521755	-0.282090	-2.993639	C	0.963662	5.090911	-0.252280
H	-3.274962	0.098998	-2.282435	H	-0.009605	5.270476	-0.756732

H	-2.935836	-0.219045	-4.019727	H	0.745397	4.700426	0.762286
H	-2.307070	-1.348250	-2.771608	H	1.498728	6.052194	-0.155477
C	1.308347	0.633139	0.232182	C	-0.371962	-1.348721	-0.333093
H	2.128095	1.284319	-0.129059	H	0.482374	-0.973725	0.267437
H	1.418638	-0.365133	-0.225668	H	-1.305799	-0.886063	0.032981
H	0.353646	1.059974	-0.138248	H	-0.430869	-2.444709	-0.164410
C	-1.722411	0.461051	3.831117	C	4.681925	-0.452142	0.039827
H	-2.694082	-0.063853	3.735214	H	5.678628	-0.238148	0.476438
H	-0.926300	-0.225869	3.473927	H	4.562325	-1.546019	-0.046861
H	-1.541774	0.689666	4.895687	H	4.669597	-0.014454	-0.979657

Li⁺(DMA)₄

E (PBE-D3/ma-def2-svp GAS_OPT) =	-1156.6263758706						
E (PBE-D3/ma-def2-svp SMD_OPT) =	-1156.6942422775						
ΔG_{corr} (ID-RR-HR GAS) =	0.4428523800						
E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT GAS) =	-1157.0037431027						
E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT SMD) =	-1157.0661684321						
E (DLPNO-CCSDT/cc-p(wC)VTZ SMD_OPT SMD) =	-1157.0687960074						
E (PBE-D3/ma-def2-tzvp GAS_OPT GAS) =	-1157.8559297903						
E (PBE-D3/ma-def2-tzvp GAS_OPT SMD) =	-1157.9193643836						
E (PBE-D3/ma-def2-tzvp GAS_OPT CPCM) =	-1157.9143920821						
GAS_OPT	SMD_OPT						
Li	-0.055867	-0.157118	-0.069582	Li	-0.585696	-0.523674	-1.132167
H	4.496950	3.008417	-0.445757	H	1.350804	2.350033	3.332910
O	1.329712	1.014526	0.601212	O	0.669750	0.401746	0.043530
C	2.312844	1.659739	0.177347	C	0.752779	1.039462	1.118978
N	3.203494	2.224640	1.044977	N	1.588966	0.627477	2.110763
C	3.005046	2.083916	2.481275	C	2.378491	-0.584399	1.933723
H	2.079070	1.511803	2.660703	H	3.419063	-0.343602	1.624890
H	2.922656	3.083301	2.958138	H	1.914895	-1.214556	1.157612
H	3.864673	1.551127	2.940254	H	2.420620	-1.143327	2.889560
C	4.376735	2.988387	0.648897	C	1.809721	1.348645	3.355653
H	5.292195	2.539895	1.089777	H	2.899036	1.476454	3.524120
H	4.302168	4.035856	1.012863	H	1.392544	0.785732	4.218603
H	1.529168	-4.383825	2.991551	H	3.524710	-4.783820	-0.353924

O	0.535536	-1.997709	0.088089	O	0.102103	-2.373423	-1.087530
C	0.809093	-2.711013	1.079704	C	1.338711	-2.589867	-1.043772
N	1.431698	-3.915068	0.922322	N	1.862784	-3.479570	-0.155870
C	1.775853	-4.387488	-0.412375	C	0.990876	-4.224963	0.741086
H	1.527874	-3.603185	-1.146986	H	1.101381	-3.869108	1.788578
H	1.211491	-5.313028	-0.654975	H	1.259579	-5.300824	0.714176
H	2.860190	-4.617442	-0.468309	H	-0.058555	-4.102254	0.425100
C	1.778501	-4.817081	2.010225	C	3.284754	-3.754462	-0.010671
H	2.867336	-5.035283	1.993826	H	3.572099	-3.675223	1.058789
H	1.236579	-5.781542	1.904530	H	3.898236	-3.040951	-0.583731
H	-1.353903	-0.111177	-6.052754	H	0.142637	3.952021	-4.113898
O	-0.499252	0.314025	-1.908598	O	-0.526968	0.303988	-2.867757
C	-1.016665	-0.288979	-2.877361	C	-0.327289	1.410079	-3.424891
N	-1.406101	0.391310	-3.994106	N	-1.074026	2.509206	-3.130540
C	-1.207097	1.832095	-4.078962	C	-2.211238	2.413736	-2.225698
H	-0.721759	2.184846	-3.153670	H	-3.153118	2.644472	-2.769050
H	-2.181066	2.350227	-4.205371	H	-2.108030	3.146548	-1.398670
H	-0.566435	2.081276	-4.950902	H	-2.276586	1.395017	-1.808011
C	-2.014662	-0.221258	-5.165915	C	-0.901870	3.795396	-3.794632
H	-2.980080	0.276248	-5.396638	H	-1.162128	4.604327	-3.084710
H	-2.210339	-1.293344	-5.007460	H	-1.567201	3.887459	-4.681490
H	-5.030881	2.252807	2.464425	H	-3.055421	1.023405	3.323803
O	-1.597645	0.153117	1.076551	O	-2.309945	-0.425114	-0.225876
C	-2.252996	1.192865	1.309083	C	-2.712196	0.003260	0.883313
N	-3.179284	1.225073	2.310766	N	-2.205553	-0.462668	2.058035
C	-3.442815	0.024163	3.092868	C	-1.279189	-1.587617	2.074578
H	-2.913119	-0.827893	2.634445	H	-1.752731	-2.464467	2.566423
H	-4.532827	-0.182164	3.112182	H	-0.368376	-1.324753	2.648973
H	-3.094471	0.152081	4.140273	H	-0.996832	-1.860001	1.044627
C	-3.951899	2.399068	2.688610	C	-2.657456	-0.004390	3.365558
H	-3.602353	3.301340	2.162038	H	-1.799309	-0.007299	4.066267
H	-3.852754	2.579822	3.779492	H	-3.441921	-0.674512	3.781098
C	0.457574	-2.247223	2.480462	C	2.280665	-1.857606	-1.974374
H	-0.173766	-2.984129	3.015555	H	1.675449	-1.213443	-2.636438
H	1.367817	-2.076515	3.090409	H	2.990003	-1.214173	-1.416068
H	-0.101087	-1.298806	2.397445	H	2.876131	-2.558818	-2.592900
C	-1.219722	-1.790351	-2.828113	C	0.766899	1.552168	-4.459923
H	-0.785440	-2.164691	-1.884402	H	1.207093	0.556234	-4.642513
H	-2.296171	-2.055246	-2.857051	H	0.384532	1.957374	-5.418217
H	-0.724527	-2.302223	-3.677295	H	1.570500	2.231718	-4.107849
C	2.535931	1.830541	-1.313438	C	-0.074301	2.287329	1.341918
H	3.478816	1.348747	-1.642721	H	0.568115	3.191186	1.377962
H	1.689331	1.353965	-1.838266	H	-0.768529	2.396972	0.491439
H	2.585218	2.898473	-1.606167	H	-0.653487	2.254119	2.285416
C	-2.028536	2.443800	0.480397	C	-3.784613	1.069331	0.943336
H	-1.500463	3.220329	1.070957	H	-4.630636	0.773488	1.595020
H	-1.395841	2.171852	-0.382220	H	-3.385258	2.028340	1.333548
H	-2.973722	2.884104	0.107743	H	-4.165467	1.242166	-0.078212

Li⁺ in DMA

E (PBE-D3/ma-def2-svp GAS_OPT) =	-7.2519251623
E (PBE-D3/ma-def2-svp SMD_OPT) =	-7.3917970144
ΔG_{corr} (ID-RR-HR GAS) =	-0.0127326619
E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT GAS) =	-7.2736440090
E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT SMD) =	-7.4151470685
E (DLPNO-CCSDT/cc-p(wC)VTZ SMD_OPT SMD) =	-7.4151470685
E (PBE-D3/ma-def2-tzvp GAS_OPT GAS) =	-7.2566456293
E (PBE-D3/ma-def2-tzvp GAS_OPT SMD) =	-7.3965055394
E (PBE-D3/ma-def2-tzvp GAS_OPT CPCM) =	-7.4400964517
GAS_OPT	SMD_OPT
Li 0.000000 0.000000 0.000000	Li 0.000000 0.000000 0.000000

(DMA)₅

E (PBE-D3/ma-def2-svp GAS_OPT) =	-1436.4871646214
E (PBE-D3/ma-def2-svp SMD_OPT) =	-1436.5137231692
ΔG_{corr} (ID-RR-HR GAS) =	0.5631541700
E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT GAS) =	-1436.9343810755
E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT SMD) =	-1436.9545379897
E (DLPNO-CCSDT/cc-p(wC)VTZ SMD_OPT SMD) =	-1436.9550228148
E (PBE-D3/ma-def2-tzvp GAS_OPT GAS) =	-1438.0169501172
E (PBE-D3/ma-def2-tzvp GAS_OPT SMD) =	-1438.0410503756

E (PBE-D3/ma-def2-tzvp GAS_OPT CPCM) =				-1438.0429294882			
GAS_OPT				SMD_OPT			
H	2.643867	0.621594	3.024577	H	3.702114	2.137286	1.745733
O	-1.519291	-0.383506	2.303434	O	-0.388270	1.498637	1.908923
C	-0.429534	0.058978	1.887640	C	0.771029	1.251738	1.513686
N	0.569722	0.413991	2.764954	N	1.844319	1.298810	2.363496
C	0.330219	0.327327	4.194048	C	1.652246	1.700060	3.746982
H	-0.665468	-0.118873	4.361942	H	0.571738	1.773576	3.959217
H	0.365427	1.334848	4.665507	H	2.126451	2.687297	3.942371
H	1.106053	-0.301572	4.681778	H	2.112893	0.957435	4.431892
C	1.839196	1.000972	2.362227	C	3.227360	1.147547	1.935614
H	1.821205	2.111312	2.452496	H	3.316524	0.529266	1.025211
H	2.111583	0.721197	1.330012	H	3.804706	0.646179	2.738645
H	-0.728866	-2.837789	2.814351	H	-0.187844	-0.988805	3.122877
O	-0.731201	-3.275294	-1.050220	O	-0.819037	-2.634249	-0.384688
C	-0.834485	-3.272531	0.189026	C	-0.757420	-2.189536	0.780683
N	0.275989	-3.272862	1.000262	N	0.393567	-2.261615	1.520792
C	1.600815	-3.368473	0.403934	C	1.562106	-2.939941	0.981325
H	1.486209	-3.581821	-0.673414	H	1.320236	-3.321138	-0.025501
H	2.172140	-4.192330	0.883381	H	1.851080	-3.792093	1.634211
H	2.168664	-2.420004	0.518497	H	2.425219	-2.246339	0.900784
C	0.232138	-3.238561	2.451860	C	0.491968	-1.830427	2.908165
H	1.029657	-2.563537	2.825476	H	1.525126	-1.485017	3.106418
H	0.403487	-4.247297	2.893079	H	0.268695	-2.663240	3.612669
H	-3.227507	-0.940894	-3.219940	H	-3.164267	0.019272	-2.510372
O	0.420264	0.948027	-4.049484	O	0.615374	1.201260	-3.868219
C	-0.291374	0.043172	-3.575828	C	-0.190958	0.453798	-3.279606
N	-1.518040	0.312581	-3.020108	N	-1.249509	0.954239	-2.563656
C	-2.033660	1.675498	-3.046227	C	-1.475868	2.387743	-2.506742
H	-3.039580	1.688748	-3.519597	H	-0.768248	2.896549	-3.184246
H	-1.343657	2.300766	-3.639328	H	-1.324326	2.774534	-1.475179
H	-2.111220	2.099017	-2.021518	H	-2.515547	2.627272	-2.816206
C	-2.416701	-0.701236	-2.493292	C	-2.244213	0.127221	-1.893123
H	-2.901635	-0.320206	-1.570456	H	-2.538895	0.605720	-0.939166
H	-1.884159	-1.632008	-2.228266	H	-1.848653	-0.874880	-1.654332
H	-2.919128	1.315400	3.402193	H	-2.532477	1.485746	3.144495
O	-1.973016	3.164070	0.054297	O	-5.461302	0.927278	-0.021564
C	-2.531843	2.676494	1.048402	C	-5.057237	0.708201	1.137310
N	-2.107176	2.955265	2.330080	N	-4.065625	1.458531	1.714933
C	-1.026823	3.904530	2.531353	C	-3.514882	2.605735	1.009075
H	-1.377420	4.799693	3.090335	H	-2.407387	2.549913	1.012498
H	-0.653571	4.221233	1.541098	H	-3.821459	3.554806	1.503957
H	-0.196663	3.439460	3.105257	H	-3.894561	2.610563	-0.027192
C	-2.755699	2.404586	3.511677	C	-3.624743	1.307811	3.094086
H	-3.723445	2.906894	3.737470	H	-3.821170	0.291982	3.476154
H	-2.091232	2.551641	4.383677	H	-4.131900	2.038759	3.764278
H	4.028931	-0.315096	-4.085233	H	3.289513	-1.657797	-4.331817
O	3.095078	-0.372305	-0.310140	O	4.005416	-0.981925	-0.552644
C	3.437483	-0.417469	-1.508725	C	3.815524	-1.282746	-1.750368
N	3.280947	0.649136	-2.348650	N	3.699936	-0.328721	-2.723741
C	2.681158	1.883299	-1.858204	C	3.828681	1.080923	-2.388656
H	1.713333	2.062307	-2.370927	H	2.909095	1.624637	-2.688482

H	3.358287	2.739498	-2.064707	H	4.693471	1.528286	-2.925712
H	2.521915	1.799165	-0.770637	H	3.987419	1.185818	-1.302227
C	3.608007	0.652490	-3.767726	C	3.570813	-0.608531	-4.145836
H	4.356656	1.445577	-3.985472	H	4.527406	-0.404445	-4.677405
H	2.685696	0.852284	-4.353709	H	2.782332	0.043861	-4.572955
C	4.043148	-1.693358	-2.077153	C	3.702894	-2.737257	-2.171453
H	4.181959	-2.399581	-1.240596	H	3.832804	-3.368134	-1.274770
H	3.370707	-2.161267	-2.825044	H	2.716267	-2.964159	-2.624759
H	5.023613	-1.520804	-2.563665	H	4.479666	-3.014561	-2.912766
C	-2.196590	-3.252866	0.858545	C	-1.958677	-1.526407	1.426338
H	-2.316625	-4.072705	1.595012	H	-2.208340	-1.980781	2.406097
H	-2.351062	-2.288108	1.386966	H	-1.770647	-0.444904	1.588889
H	-2.959838	-3.365122	0.069040	H	-2.821482	-1.644229	0.748150
C	0.169810	-1.404146	-3.596085	C	-0.038859	-1.054952	-3.320600
H	1.158686	-1.433104	-4.085566	H	0.816621	-1.301425	-3.971188
H	0.239301	-1.848023	-2.582173	H	0.131108	-1.482001	-2.310684
H	-0.527491	-2.047683	-4.170169	H	-0.945584	-1.546885	-3.728294
C	-0.160202	0.225423	0.407890	C	1.030653	0.904268	0.062643
H	0.795296	-0.233543	0.089147	H	1.701163	0.036410	-0.076451
H	-0.990042	-0.243357	-0.143495	H	0.061039	0.695341	-0.415328
H	-0.125157	1.298442	0.129124	H	1.494972	1.765388	-0.460365
C	-3.701393	1.718441	0.914256	C	-5.655790	-0.412758	1.970349
H	-3.385557	0.699609	1.222630	H	-6.430732	-0.916998	1.366033
H	-4.565964	2.010768	1.542854	H	-4.899691	-1.165693	2.272086
H	-4.014330	1.703602	-0.144030	H	-6.123941	-0.027109	2.899226

Li⁺(DMA)₅

E (PBE-D3/ma-def2-svp GAS_OPT) =	-1443.9330915087
E (PBE-D3/ma-def2-svp SMD_OPT) =	-1443.9996813027
ΔG_{corr} (ID-RR-HR GAS) =	0.5641638400
E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT GAS) =	-1444.4016751848
E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT SMD) =	-1444.4645659387
E (DLPNO-CCSDT/cc-p(wC)VTZ SMD_OPT SMD) =	-1444.4628059089
E (PBE-D3/ma-def2-tzvp GAS_OPT GAS) =	-1445.4660570978
E (PBE-D3/ma-def2-tzvp GAS_OPT SMD) =	-1445.5313170723
E (PBE-D3/ma-def2-tzvp GAS_OPT CPCM) =	-1445.5256698258

GAS_OPT				SMD_OPT			
Li	-1.279902	0.398179	0.461406	Li	-0.852545	1.539367	1.006083
H	3.999357	2.085344	1.455704	H	-1.063304	-1.989677	-3.303955
O	-0.018150	1.480134	1.455971	O	-1.527821	0.898617	-0.738235
C	1.034204	2.109427	1.196067	C	-1.462011	-0.039723	-1.567486
N	1.999385	2.288925	2.139145	N	-0.305747	-0.316827	-2.231913
C	1.866278	1.663438	3.446265	C	0.881476	0.491587	-1.993221
H	2.574818	0.813428	3.548247	H	1.623558	-0.060296	-1.379738
H	0.835557	1.289227	3.562574	H	0.600589	1.411817	-1.456441
H	2.086148	2.400872	4.244762	H	1.351624	0.755414	-2.961822
C	3.302859	2.864628	1.836177	C	-0.128727	-1.426400	-3.155487
H	3.728446	3.303672	2.758537	H	0.642264	-2.127986	-2.769655
H	3.224583	3.671281	1.086821	H	0.213800	-1.052693	-4.143329
H	2.580257	-3.337432	1.537266	H	5.046608	1.867268	1.410310
O	-0.533803	-1.398461	0.241640	O	1.005937	2.066646	0.942364
C	0.360810	-2.057017	0.812951	C	2.141407	1.546504	1.074185
N	0.964013	-3.110102	0.181593	N	3.203347	1.970943	0.336047
C	0.499522	-3.536563	-1.128609	C	3.067769	3.093948	-0.580116
H	-0.325899	-2.875386	-1.442646	H	3.326487	2.786267	-1.615180
H	0.138597	-4.586446	-1.092843	H	3.749565	3.918931	-0.283089
H	1.324082	-3.476994	-1.870287	H	2.027658	3.460639	-0.558671
C	2.025153	-3.909265	0.774809	C	4.547287	1.430525	0.517696
H	2.744876	-4.200906	-0.016151	H	5.157463	1.685868	-0.368609
H	1.633879	-4.842405	1.237514	H	4.525904	0.328841	0.609169
H	-2.940860	-0.907607	-4.493610	H	-1.862893	-4.137949	1.770360
O	-1.410951	0.940701	-1.426980	O	-1.097875	-0.111938	2.049602
C	-2.006828	0.342738	-2.348451	C	-1.813824	-1.117426	1.831494
N	-1.747171	0.638106	-3.658576	N	-1.345555	-2.176344	1.112909
C	-0.825141	1.714314	-3.993833	C	0.043522	-2.192302	0.673375
H	-0.414405	2.139298	-3.063135	H	0.442799	-1.166724	0.673631
H	-1.350621	2.512165	-4.560433	H	0.108025	-2.615275	-0.346897
H	0.004828	1.331948	-4.625045	H	0.667068	-2.815713	1.349306
C	-2.420203	0.017248	-4.789792	C	-2.085855	-3.420889	0.949475
H	-1.674860	-0.244478	-5.568787	H	-1.792426	-3.897664	-0.005810
H	-3.160561	0.709984	-5.247630	H	-3.174774	-3.244764	0.918378
H	-4.910960	1.731977	4.863535	H	-5.368331	4.816289	3.638939
O	-2.995556	0.348952	1.308451	O	-1.956042	2.981361	1.677140
C	-4.002033	0.599737	2.002961	C	-3.195330	3.162471	1.754333
N	-3.989445	1.568623	2.963470	N	-3.714307	4.152619	2.532268
C	-2.780532	2.342609	3.218244	C	-2.834883	5.077563	3.232057
H	-2.512377	2.276141	4.293600	H	-3.024501	5.040635	4.325421
H	-2.949048	3.412462	2.971094	H	-3.013751	6.117061	2.882911
H	-1.943831	1.960154	2.609590	H	-1.784430	4.803700	3.035154
C	-5.133004	1.923089	3.791579	C	-5.139297	4.440783	2.622557
H	-6.031267	1.349066	3.514975	H	-5.749115	3.537081	2.452734
H	-5.364095	3.003665	3.679640	H	-5.444077	5.221479	1.890273
H	4.677099	-2.141658	-2.630689	H	3.084200	-2.894178	-4.029871
O	2.962860	-0.170385	0.250954	O	3.487934	-1.887445	-0.255989
C	3.561698	-0.840499	-0.606306	C	3.483449	-2.158909	-1.472954
N	3.049987	-1.008021	-1.872657	N	2.966570	-3.337584	-1.950627
C	1.801066	-0.346793	-2.225199	C	2.525799	-4.364945	-1.019377
H	1.209282	-0.148383	-1.317196	H	1.505364	-4.715524	-1.279329
H	1.214191	-0.999553	-2.901992	H	2.526855	-3.954613	0.004474
H	1.986486	0.616060	-2.751031	H	3.207519	-5.243138	-1.055932

C	3.765898	-1.627291	-2.976097	C	3.061688	-3.756548	-3.342245
H	4.063870	-0.868665	-3.734046	H	2.178098	-4.373540	-3.600428
H	3.119805	-2.374513	-3.484495	H	3.971665	-4.372465	-3.521032
C	4.888588	-1.507995	-0.278398	C	4.064068	-1.192539	-2.488911
H	5.075238	-1.371218	0.800787	H	4.340427	-0.260537	-1.966541
H	4.895734	-2.591645	-0.509832	H	4.974979	-1.616812	-2.960300
H	5.725964	-1.041886	-0.837303	H	3.360274	-0.946286	-3.308221
C	0.818267	-1.708051	2.210751	C	2.379400	0.421467	2.053976
H	0.860021	-2.588253	2.880910	H	2.741297	-0.488573	1.532699
H	1.824261	-1.243532	2.160449	H	3.145762	0.700077	2.806168
H	0.119307	-0.962326	2.623557	H	1.428691	0.194975	2.566660
C	-3.032471	-0.730369	-2.038968	C	-3.229410	-1.185192	2.359757
H	-3.173412	-0.765805	-0.944857	H	-3.972341	-1.266607	1.540221
H	-4.007853	-0.523637	-2.522560	H	-3.375659	-2.059911	3.025415
H	-2.690612	-1.728315	-2.380887	H	-3.431451	-0.264417	2.933425
C	1.255393	2.715461	-0.172723	C	-2.685664	-0.879491	-1.866297
H	0.393512	2.448373	-0.807978	H	-2.984184	-0.797477	-2.931192
H	1.337534	3.820015	-0.117281	H	-2.522984	-1.953980	-1.651497
H	2.183701	2.322241	-0.629459	H	-3.517764	-0.517191	-1.238108
C	-5.281076	-0.188829	1.785515	C	-4.156741	2.288439	0.978731
H	-6.112781	0.460217	1.444088	H	-3.565758	1.602249	0.346438
H	-5.083761	-0.946439	1.008167	H	-4.806555	1.695068	1.653581
H	-5.613948	-0.706775	2.706999	H	-4.822263	2.891988	0.328792

DME

E (PBE-D3/ma-def2-svp GAS_OPT) =	-308.2661632815
E (PBE-D3/ma-def2-svp SMD_OPT) =	-308.2729971294
ΔG_{corr} (ID-RR-HR GAS) =	0.1040877592
E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT GAS) =	-308.3909223370
E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT SMD) =	-308.3962524010
E (DLPNO-CCSDT/cc-p(wC)VTZ SMD_OPT SMD) =	-308.3964229470
E (PBE-D3/ma-def2-tzvp GAS_OPT GAS) =	-308.6047305582
E (PBE-D3/ma-def2-tzvp GAS_OPT SMD) =	-308.6111893030
E (PBE-D3/ma-def2-tzvp GAS_OPT CPCM) =	-308.6109937200
GAS_OPT	SMD_OPT

H	-1.686365	0.646589	-1.218292	H	-1.564909	0.559736	-1.115482
C	-1.394064	-0.521564	0.534455	C	-1.413385	-0.786505	0.529433
H	-1.723766	0.336152	1.170111	H	-1.580625	0.079548	1.214849
H	-0.293517	-0.461048	0.457498	H	-0.320138	-0.925731	0.431445
O	-1.670604	-1.757414	1.186599	O	-1.908303	-1.985029	1.124385
C	-3.026034	-1.966967	1.508982	C	-3.274860	-1.940054	1.480477
H	-3.664946	-2.116453	0.607161	H	-3.954822	-1.933641	0.596176
H	-3.080274	-2.885415	2.126240	H	-3.494497	-2.851068	2.072989
H	-3.447331	-1.115793	2.099161	H	-3.512279	-1.045235	2.106566
O	0.754830	1.159402	-2.176539	O	0.776701	1.216702	-2.243031
C	1.474380	-0.025858	-2.469420	C	1.419728	-0.002391	-2.567610
H	2.486641	0.207507	-2.882575	H	2.504127	0.155256	-2.791515
H	1.594226	-0.659701	-1.562977	H	1.342568	-0.743665	-1.741137
H	0.899151	-0.584857	-3.230837	H	0.932079	-0.414985	-3.472161
C	1.374979	1.916374	-1.155057	C	1.260390	1.768058	-1.026806
H	2.374939	2.288434	-1.497725	H	2.351852	2.000687	-1.114991
H	1.539921	1.288918	-0.247379	H	1.141955	1.040405	-0.189423
C	0.516830	3.111958	-0.800742	C	0.531068	3.052790	-0.705357
H	0.194348	3.628462	-1.738437	H	0.546480	3.729402	-1.595704
H	1.131318	3.839763	-0.211950	H	1.080152	3.579841	0.114027
O	-0.609778	2.699050	-0.047610	O	-0.804692	2.782608	-0.311746
C	-1.515201	3.744999	0.217143	C	-1.536984	3.956530	-0.027719
H	-1.928718	4.185052	-0.722736	H	-1.610471	4.628157	-0.917138
H	-2.349913	3.322987	0.810065	H	-2.560025	3.653114	0.270933
H	-1.040980	4.569405	0.804676	H	-1.081073	4.540195	0.808942
O	1.779244	-2.111878	0.351273	O	1.800951	-2.088992	0.399380
C	1.093894	-3.215501	-0.218414	C	1.212790	-3.293736	-0.057962
H	0.008106	-3.187622	0.022419	H	0.197017	-3.448249	0.373746
H	1.213756	-3.146004	-1.316163	H	1.119103	-3.225879	-1.159121
H	1.528586	-4.183663	0.130919	H	1.846758	-4.179067	0.190640
C	1.703386	-2.090462	1.764883	C	2.005721	-2.078181	1.802909
H	2.245622	-2.969758	2.197393	H	2.745569	-2.864535	2.094338
H	0.640332	-2.144901	2.101260	H	1.052879	-2.302388	2.341680
C	2.339194	-0.823019	2.297952	C	2.532554	-0.732032	2.247290
H	3.351773	-0.686600	1.842816	H	3.394808	-0.432059	1.601724
H	2.478207	-0.929674	3.403225	H	2.920268	-0.829269	3.291777
O	1.510230	0.288255	2.010917	O	1.503850	0.242662	2.190044
C	2.003636	1.509598	2.508225	C	1.949486	1.532328	2.553695
H	3.001364	1.765527	2.073329	H	2.762252	1.900905	1.882136
H	1.276455	2.295657	2.226000	H	1.084234	2.219698	2.481310
H	2.106652	1.494353	3.620764	H	2.335365	1.558931	3.601901

Li⁺(DME)₃

E (PBE-D3/ma-def2-svp GAS_OPT) =	-932.2660978654
E (PBE-D3/ma-def2-svp SMD_OPT) =	-932.3265943452
ΔG_{corr} (ID-RR-HR GAS) =	0.3662557700

E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT GAS) =	-932.6572162484
E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT SMD) =	-932.7171608941
E (DLPNO-CCSDT/cc-p(wC)VTZ SMD_OPT SMD) =	-932.7167204400
E (PBE-D3/ma-def2-tzvp GAS_OPT GAS) =	-933.2718368106
E (PBE-D3/ma-def2-tzvp GAS_OPT SMD) =	-933.3325937209
E (PBE-D3/ma-def2-tzvp GAS_OPT CPCM) =	-933.3276881664
GAS_OPT	SMD_OPT
Li 0.023422 0.011009 0.029569	Li 0.023786 0.012337 0.030254
O -0.327943 2.147685 -0.235090	O -0.348378 2.143295 -0.195691
C 0.867389 2.714691 -0.763751	C 0.843126 2.717797 -0.726131
H 0.975750 2.432530 -1.837308	H 0.956590 2.434772 -1.798926
H 0.837312 3.827153 -0.703161	H 0.806346 3.830088 -0.667967
C -1.501634 2.687304 -0.827664	C -1.527137 2.687647 -0.768975
H -2.370744 2.211987 -0.338092	H -2.394246 2.194090 -0.293279
H -1.557961 3.787392 -0.670185	H -1.593130 3.783046 -0.577256
H -1.533670 2.481197 -1.921484	H -1.564284 2.521398 -1.869541
O -1.947530 -0.716364 -0.385847	O -1.928016 -0.696262 -0.434200
C -2.261537 -0.720437 -1.775401	C -2.209850 -0.693057 -1.831584
H -2.622320 0.288557 -2.083517	H -2.569726 0.315485 -2.141732
H -3.073239 -1.450837 -1.997667	H -3.011078 -1.427180 -2.078025
C -3.093432 -0.567340 0.446503	C -3.091739 -0.559163 0.371048
H -2.730276 -0.472614 1.485001	H -2.757403 -0.406985 1.413465
H -3.673242 0.345471 0.179206	H -3.706785 0.315117 0.056811
H -3.765688 -1.449498 0.358289	H -3.727154 -1.472002 0.311576
O -0.368534 0.130274 2.114541	O -0.405806 0.079967 2.097467
C -0.380575 1.329676 2.882346	C -0.404421 1.253899 2.898103
H -0.751405 2.134253 2.223780	H -0.749091 2.088333 2.261465
H -1.045034 1.227100 3.768768	H -1.089542 1.142132 3.769202
H 0.643669 1.590125 3.234619	H 0.616484 1.483597 3.281285
C 0.148098 -0.987361 2.830374	C 0.049828 -1.074225 2.797846
H -0.424120 -1.153777 3.772457	H -0.583328 -1.269215 3.694373
H 1.212871 -0.801472 3.106589	H 1.097299 -0.917649 3.147999
C -1.019557 -1.109237 -2.551864	C -0.950139 -1.071792 -2.580514
H -1.197548 -0.929314 -3.637050	H -1.104277 -0.877798 -3.666889
H -0.793930 -2.193424 -2.422386	H -0.725605 -2.157141 -2.460496
C 2.036261 2.204890 0.050287	C 2.011706 2.222827 0.094256
H 2.987295 2.581216 -0.393056	H 2.960619 2.602209 -0.351121
H 1.976673 2.580959 1.098905	H 1.947709 2.608796 1.138896
C 0.033864 -2.213233 1.951162	C -0.026475 -2.261637 1.865931
H -1.034825 -2.467542 1.758591	H -1.084329 -2.503200 1.608229
H 0.504521 -3.080241 2.469703	H 0.413101 -3.149774 2.375692
O 0.694366 -1.943305 0.717888	O 0.701225 -1.945629 0.681906
C 0.784440 -3.087818 -0.119921	C 0.871741 -3.062421 -0.177231
H 1.332057 -2.790385 -1.032385	H 1.449535 -2.727688 -1.058114

H	1.343841	-3.907331	0.383676	H	1.440608	-3.873000	0.333087
H	-0.225446	-3.464366	-0.399702	H	-0.105787	-3.477910	-0.512139
O	2.003087	0.780995	0.044228	O	1.989026	0.798155	0.100475
C	3.110522	0.192774	0.719456	C	3.064060	0.228510	0.834677
H	2.961074	-0.900771	0.698989	H	3.046872	0.556874	1.899505
H	4.067477	0.455358	0.216396	H	2.948498	-0.869275	0.792576
H	3.161113	0.534022	1.778691	H	4.044929	0.517567	0.393275
O	0.075458	-0.329443	-2.080144	O	0.132583	-0.295914	-2.072693
C	1.244310	-0.462000	-2.882929	C	1.319097	-0.416614	-2.846777
H	1.546632	-1.529095	-2.986550	H	1.594137	-1.483606	-3.011797
H	1.076944	-0.043406	-3.900124	H	1.197174	0.069898	-3.841271
H	2.051743	0.093997	-2.374737	H	2.131643	0.081300	-2.287052

Li⁺ in DME

E (PBE-D3/ma-def2-svp GAS_OPT) =	-7.2519251623
E (PBE-D3/ma-def2-svp SMD_OPT) =	-7.3917970144
ΔG_{corr} (ID-RR-HR GAS) =	-0.0127326619
E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT GAS) =	-7.2736440090
E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT SMD) =	-7.3997425591
E (DLPNO-CCSDT/cc-p(wC)VTZ SMD_OPT SMD) =	-7.3997425591
E (PBE-D3/ma-def2-tzvp GAS_OPT GAS) =	-7.2566456293
E (PBE-D3/ma-def2-tzvp GAS_OPT SMD) =	-7.3815222019
E (PBE-D3/ma-def2-tzvp GAS_OPT CPCM) =	-7.4201253171
GAS_OPT	SMD_OPT
Li 0.000000 0.000000 0.000000	Li 0.000000 0.000000 0.000000

(DME)₄

E (PBE-D3/ma-def2-svp GAS_OPT) =	-1233.1001152192
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E (PBE-D3/ma-def2-svp SMD_OPT) =	-1233.1170715630
ΔG_{corr} (ID-RR-HR GAS) =	0.4836008500
E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT GAS) =	-1233.5968068721
E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT SMD) =	-1233.6089680784
E (DLPNO-CCSDT/cc-p(wC)VTZ SMD_OPT SMD) =	-1233.6104066100
E (PBE-D3/ma-ma-def2-tzvp GAS_OPT GAS) =	-1234.4467290682
E (PBE-D3/ma-ma-def2-tzvp GAS_OPT SMD) =	-1234.4599872972
E (PBE-D3/ma-def2-tzvp GAS_OPT CPCM) =	-1234.4602519874
GAS_OPT	SMD_OPT
O 3.692032 -0.376620 -1.229053	O 3.891746 -0.384148 -1.187013
C 3.351950 -1.709296 -1.559296	C 3.585088 -1.727326 -1.508536
H 4.222429 -2.399994 -1.441843	H 4.463103 -2.402954 -1.364160
H 2.509530 -2.078741 -0.928980	H 2.739107 -2.113333 -0.892154
H 3.037962 -1.716302 -2.620903	H 3.291213 -1.759282 -2.576393
C 4.103524 -0.227052 0.114018	C 4.258463 -0.209111 0.172219
H 5.130560 -0.646997 0.264866	H 5.300206 -0.573711 0.351963
H 3.415445 -0.778298 0.798773	H 3.583011 -0.798040 0.837244
C 4.108213 1.240532 0.491235	C 4.172570 1.253168 0.551048
H 4.684199 1.821800 -0.271045	H 4.745878 1.873079 -0.182388
H 4.635266 1.360526 1.471803	H 4.656620 1.392794 1.549892
O 2.778518 1.710441 0.578615	O 2.814282 1.649457 0.591906
C 2.677574 3.080911 0.905446	C 2.625845 3.008725 0.927074
H 3.197986 3.720735 0.151947	H 3.106137 3.690324 0.183154
H 1.602456 3.344100 0.913998	H 1.535364 3.203204 0.932659
H 3.121506 3.297855 1.907863	H 3.047276 3.249321 1.933931
O -1.948827 -2.241732 -1.903542	O -2.449817 -1.670470 -1.982602
C -1.957645 -2.011007 -3.291676	C -2.675134 -0.751903 -3.032351
H -2.968914 -2.184559 -3.735968	H -3.766382 -0.607043 -3.228327
H -1.645271 -0.968431 -3.544430	H -2.225340 0.244599 -2.813203
H -1.241913 -2.717659 -3.756036	H -2.207278 -1.162610 -3.949400
C -2.835884 -1.388052 -1.199113	C -2.954783 -1.204275 -0.740430
H -3.873087 -1.503292 -1.606000	H -4.046508 -0.975043 -0.833498
H -2.546374 -0.316407 -1.335404	H -2.449356 -0.253452 -0.445295
C -2.786574 -1.684230 0.293233	C -2.698306 -2.222037 0.357886
H -3.477146 -0.961862 0.798822	H -3.043872 -1.768809 1.319338
H -1.768741 -1.496107 0.683361	H -1.609664 -2.401911 0.451843
O -3.109129 -3.016875 0.663281	O -3.302766 -3.499926 0.171746
C -4.426283 -3.415237 0.364575	C -4.715571 -3.482675 0.157006
H -4.609481 -3.518827 -0.731260	H -5.135505 -3.011617 -0.762860
H -4.585586 -4.405637 0.834869	H -5.062026 -4.535428 0.188899
H -5.180955 -2.700818 0.778314	H -5.134973 -2.946308 1.043357

O	-0.557237	1.338327	-1.054660	O	-0.414091	1.160240	-1.230648
C	0.377503	0.367733	-1.510001	C	0.515372	0.143773	-1.573412
H	0.281842	0.204905	-2.611386	H	0.490496	-0.080636	-2.668538
H	1.420684	0.674196	-1.280671	H	1.551209	0.431056	-1.289097
H	0.157680	-0.577738	-0.982650	H	0.230529	-0.766956	-1.015725
C	-0.370480	2.604356	-1.645697	C	-0.134812	2.406145	-1.837981
H	-0.651220	2.583836	-2.730266	H	-0.273574	2.350107	-2.947330
H	0.701135	2.915779	-1.589634	H	0.925091	2.708163	-1.655131
C	-1.231150	3.628554	-0.935148	C	-1.071216	3.457990	-1.283688
H	-2.265300	3.219946	-0.821095	H	-2.120167	3.076056	-1.325877
H	-1.300835	4.555901	-1.557152	H	-1.024399	4.371438	-1.926650
O	-0.673923	3.925585	0.334142	O	-0.711911	3.769324	0.054651
C	-1.519015	4.704568	1.149766	C	-1.715762	4.475602	0.752755
H	-2.483495	4.182423	1.361104	H	-2.662225	3.887308	0.825659
H	-0.991701	4.878714	2.107770	H	-1.340398	4.672533	1.776526
H	-1.753077	5.693572	0.685692	H	-1.954612	5.454527	0.270333
O	0.547901	-2.260174	0.693816	O	0.716478	-2.441594	0.882267
C	0.282643	-3.615398	0.382614	C	0.914320	-3.837567	0.800058
H	-0.527564	-4.026690	1.026929	H	0.255889	-4.393276	1.510573
H	-0.070364	-3.641642	-0.665335	H	0.664605	-4.154631	-0.231799
H	1.195985	-4.249886	0.493793	H	1.972109	-4.124349	1.016396
C	0.897496	-2.027938	2.045673	C	1.018085	-1.912242	2.164795
H	1.947714	-2.361739	2.247002	H	2.106867	-2.036143	2.388830
H	0.227043	-2.604936	2.727463	H	0.457928	-2.467389	2.957112
C	0.764759	-0.548983	2.349673	C	0.667274	-0.442111	2.223865
H	1.258963	0.050304	1.550480	H	1.073615	0.082826	1.330335
H	1.296762	-0.322157	3.309543	H	1.173256	0.005892	3.116952
O	-0.608326	-0.220029	2.453722	O	-0.739406	-0.276124	2.320152
C	-0.851425	1.173059	2.405835	C	-1.135575	1.071804	2.125670
H	-0.535872	1.613761	1.434983	H	-0.859958	1.439690	1.113353
H	-1.943499	1.318251	2.526154	H	-2.237174	1.115702	2.245052
H	-0.330968	1.710670	3.237071	H	-0.676470	1.749583	2.887987

Li⁺(DME)₄

E (PBE-D3/ma-def2-svp GAS_OPT) =	-1240.5516629293
E (PBE-D3/ma-def2-svp SMD_OPT) =	-1240.6111378351
ΔG_{corr} (ID-RR-HR GAS) =	0.4930091000
E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT GAS) =	-1241.0670083397
E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT SMD) =	-1241.1230475676
E (DLPNO-CCSDT/cc-p(wC)VTZ SMD_OPT SMD) =	-1241.1254624266

E (PBE-D3/ma-def2-tzvp GAS_OPT GAS) =	-1241.8928591184
E (PBE-D3/ma-def2-tzvp GAS_OPT SMD) =	-1241.9493970807
E (PBE-D3/ma-def2-tzvp GAS_OPT CPCM) =	-1241.9452731665
GAS_OPT	SMD_OPT
Li -0.148838 -0.608536 1.366561	Li -0.568124 -0.769829 0.998946
O 1.823250 1.613048 -3.795322	O 2.253952 0.887517 -2.753825
C 2.923245 2.461721 -4.073161	C 3.400160 0.097703 -2.506098
H 3.418154 2.191729 -5.035006	H 3.956019 -0.132326 -3.446478
H 2.614242 3.532362 -4.126028	H 4.107309 0.596923 -1.800915
H 3.654551 2.340851 -3.251174	H 3.063420 -0.855851 -2.056001
C 0.805315 1.685301 -4.776205	C 2.565477 2.129885 -3.367401
H 1.204149 1.418909 -5.786493	H 3.020543 1.963414 -4.374439
H 0.413677 2.729909 -4.856367	H 3.312583 2.692535 -2.755811
C -0.307180 0.702599 -4.439301	C 1.314513 2.961377 -3.535413
H 0.119627 -0.318676 -4.367741	H 0.517496 2.350999 -4.028083
H -1.046259 0.707159 -5.277026	H 1.545599 3.813680 -4.220558
O -0.960768 0.933926 -3.198235	O 0.869335 3.444938 -2.277192
C -1.775941 2.090154 -3.159569	C -0.312441 4.215068 -2.379308
H -2.338478 2.060959 -2.206088	H -0.560812 4.593261 -1.368338
H -1.183415 3.033463 -3.188143	H -0.176966 5.091473 -3.057785
H -2.506392 2.108182 -4.002231	H -1.172817 3.615099 -2.762126
O 1.390823 -1.186235 0.019858	O 0.149761 -1.469236 -0.883362
C 1.768565 -2.517339 -0.304791	C 0.745586 -2.729670 -1.148225
H 1.184548 -2.906867 -1.169962	H -0.008371 -3.477579 -1.487139
H 2.850595 -2.573143 -0.560167	H 1.525770 -2.649921 -1.939266
H 1.558740 -3.144419 0.580196	H 1.205735 -3.083696 -0.207780
C 1.469150 -0.297350 -1.098440	C -0.582550 -0.954332 -1.993244
H 0.688785 -0.558214 -1.845701	H -1.458732 -1.612045 -2.201681
H 2.459567 -0.374380 -1.600362	H 0.051642 -0.928225 -2.907898
C 1.270913 1.120984 -0.614407	C -1.024400 0.455231 -1.670075
H 1.126942 1.764930 -1.508465	H -1.746837 0.789259 -2.450610
H 2.164831 1.483164 -0.053557	H -0.157814 1.151038 -1.676906
O 0.128408 1.157716 0.242883	O -1.642289 0.453321 -0.380097
C -0.276509 2.478623 0.567524	C -2.268735 1.687768 -0.062772
H -0.610066 3.028194 -0.341083	H -3.137089 1.879324 -0.734174
H -1.111459 2.398392 1.286446	H -2.617015 1.625462 0.984275
H 0.553298 3.056388 1.037260	H -1.562576 2.543854 -0.151419
O -0.084284 -2.468856 2.406797	O 0.729044 -2.090295 2.017881
C -1.162294 -3.394190 2.487701	C 0.348097 -3.194657 2.825573
H -0.786531 -4.431234 2.634791	H 1.126733 -3.991047 2.804230
H -1.845289 -3.140972 3.330932	H 0.187164 -2.888634 3.885066
H -1.721170 -3.325712 1.538138	H -0.598187 -3.591720 2.416222
C 0.694464 -2.410271 3.596635	C 1.928053 -1.457772 2.455995
H 1.103053 -3.415340 3.853642	H 2.765761 -2.191277 2.509893
H 0.059857 -2.072043 4.449830	H 1.781601 -1.030604 3.476216
C 1.837559 -1.444954 3.371420	C 2.281764 -0.368838 1.468826
H 2.531191 -1.827085 2.586108	H 2.540938 -0.801838 0.474727
H 2.417285 -1.334765 4.317268	H 3.174234 0.183912 1.844059
O 1.291564 -0.194696 2.964494	O 1.162493 0.501279 1.344896

C	2.277762	0.820456	2.838507	C	1.447093	1.664685	0.574061
H	2.807470	0.983147	3.803642	H	2.275860	2.248942	1.036201
H	3.026129	0.559500	2.056814	H	1.719571	1.410865	-0.472434
H	1.759763	1.753218	2.552128	H	0.538311	2.292429	0.568609
O	-1.896571	-1.238520	0.219212	O	-2.252862	-2.136094	1.227425
C	-1.857877	-1.661132	-1.142694	C	-2.766087	-2.901953	0.148087
H	-1.636485	-0.812038	-1.826695	H	-3.258442	-2.256687	-0.614218
H	-1.060540	-2.421885	-1.226162	H	-1.921173	-3.440994	-0.317552
H	-2.825755	-2.127442	-1.434270	H	-3.508204	-3.650221	0.509112
C	-2.911424	-0.274393	0.468436	C	-3.270391	-1.430740	1.932553
H	-3.894418	-0.623053	0.074734	H	-4.063396	-2.129779	2.286241
H	-2.657289	0.683895	-0.042407	H	-3.750181	-0.682392	1.258943
C	-3.021710	-0.076901	1.965192	C	-2.639841	-0.755212	3.127900
H	-3.378051	-1.013371	2.456054	H	-2.254498	-1.512993	3.850535
H	-3.765071	0.725765	2.181234	H	-3.411801	-0.145849	3.652683
O	-1.737509	0.274276	2.468861	O	-1.571356	0.067286	2.668946
C	-1.731364	0.525123	3.869066	C	-0.963280	0.822736	3.707371
H	-2.088513	-0.364054	4.437843	H	-0.553299	0.161331	4.505151
H	-0.687329	0.742558	4.155327	H	-0.135121	1.397998	3.256549
H	-2.382687	1.391466	4.121714	H	-1.695928	1.521715	4.171451

DMF

E (PBE-D3/ma-def2-svp GAS_OPT) =	-248.0475159115
E (PBE-D3/ma-def2-svp SMD_OPT) =	-248.0584061985
ΔG_{corr} (ID-RR-HR GAS) =	0.0700846500
E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT GAS) =	-248.1260204285
E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT SMD) =	-248.1356854812
E (DLPNO-CCSDT/cc-p(wC)VTZ SMD_OPT SMD) =	-248.1362261054
E (PBE-D3/ma-def2-tzvp GAS_OPT GAS) =	-248.3148701326
E (PBE-D3/ma-def2-tzvp GAS_OPT SMD) =	-248.3252689787
E (PBE-D3/ma-def2-tzvp GAS_OPT CPCM) =	-248.3266359656
GAS_OPT	SMD_OPT
H -0.789837 2.747682 -4.462181	H -0.783811 2.751721 -4.449112
O 2.001055 1.589271 -1.426955	O 2.017420 1.577771 -1.431907
C 1.353416 1.460005 -2.460581	C 1.350425 1.457828 -2.468564

H	1.730626	0.875412	-3.345713	H	1.722575	0.875647	-3.353035
N	0.109009	1.988375	-2.696619	N	0.117743	1.986898	-2.690895
C	-0.554945	2.778465	-1.677087	C	-0.556495	2.778654	-1.678205
H	-1.520606	2.313216	-1.382513	H	-1.522249	2.308784	-1.393898
H	-0.761379	3.806743	-2.045535	H	-0.767152	3.801144	-2.058079
H	0.108505	2.833117	-0.794255	H	0.089666	2.849372	-0.784571
C	-0.580150	1.781200	-3.952976	C	-0.576163	1.781222	-3.949599
H	-1.548640	1.255889	-3.799927	H	-1.543937	1.260385	-3.786495
H	0.048891	1.163578	-4.623484	H	0.047921	1.163527	-4.623464

(DMF)₄

E (PBE-D3/ma-def2-svp GAS_OPT) =	-992.2337306912
E (PBE-D3/ma-def2-svp SMD_OPT) =	-992.2570285916
ΔG_{corr} (ID-RR-HR GAS) =	0.3430621700
E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT GAS) =	-992.5520271386
E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT SMD) =	-992.5700594319
E (DLPNO-CCSDT/cc-p(wC)VTZ SMD_OPT SMD) =	-992.5707507098
E (PBE-D3/ma-def2-tzvp GAS_OPT GAS) =	-993.2975435311
E (PBE-D3/ma-def2-tzvp GAS_OPT SMD) =	-993.3179122004
E (PBE-D3/ma-def2-tzvp GAS_OPT CPCM) =	-993.3213760498
GAS_OPT	SMD_OPT
H 1.108407 -1.180395 -2.672012	H 1.237439 -1.299618 -2.663998
O -0.751353 0.429819 0.192637	O -0.087417 0.842666 0.151184
C -0.153140 -0.118109 -0.735847	C 0.318950 0.140985 -0.784675
H 0.878134 0.195675 -1.054482	H 1.324975 0.298034 -1.256698
N -0.627087 -1.148665 -1.492282	N -0.358858 -0.887122 -1.359868
C -1.957504 -1.685555 -1.264937	C -1.680515 -1.260846 -0.888634
H -2.595942 -1.507608 -2.156401	H -2.374915 -1.361779 -1.746963
H -2.390060 -1.174525 -0.386081	H -2.044238 -0.471594 -0.207689
H -1.906418 -2.777233 -1.066376	H -1.650657 -2.229351 -0.343489
C 0.139445 -1.709509 -2.589316	C 0.232147 -1.690155 -2.415186
H -0.416016 -1.592628 -3.543840	H -0.400712 -1.662564 -3.326700
H 0.340200 -2.789510 -2.419686	H 0.337726 -2.748064 -2.091932
H -0.864053 3.017308 -2.300661	H -0.974975 2.925781 -2.317289
O -2.224220 0.023706 -4.140585	O -2.308345 -0.058737 -4.191073

C	-1.751122	0.995661	-3.536339	C	-1.841210	0.916478	-3.582333
H	-2.266697	1.475671	-2.667029	H	-2.357394	1.377070	-2.702534
N	-0.571271	1.612175	-3.833208	N	-0.677698	1.554354	-3.880581
C	0.230798	1.188271	-4.966481	C	0.158287	1.126301	-4.985871
H	-0.261199	0.318700	-5.439212	H	-0.299964	0.243100	-5.466046
H	1.253123	0.901788	-4.636990	H	1.175286	0.861076	-4.626131
H	0.311790	2.014532	-5.704382	H	0.257456	1.939696	-5.735689
C	-0.120260	2.771667	-3.082275	C	-0.236225	2.704560	-3.110597
H	-0.007819	3.643799	-3.760447	H	-0.133042	3.593620	-3.767771
H	0.860674	2.569497	-2.598466	H	0.751014	2.508899	-2.639688
H	-2.506088	1.615529	2.293608	H	-2.918389	1.269213	2.302032
O	-3.010615	3.100369	-1.130167	O	-3.069385	2.997128	-1.049348
C	-2.871667	2.619808	0.000956	C	-3.036308	2.415559	0.046427
H	-2.036717	2.920960	0.682784	H	-2.314271	2.702648	0.850925
N	-3.686274	1.684665	0.562625	N	-3.840504	1.385635	0.417341
C	-4.801780	1.134067	-0.182670	C	-4.859244	0.864068	-0.475519
H	-5.735934	1.194142	0.414161	H	-5.870989	1.002186	-0.038054
H	-4.620288	0.068506	-0.443497	H	-4.706308	-0.221073	-0.654878
H	-4.923227	1.712471	-1.116204	H	-4.807193	1.401725	-1.438968
C	-3.389995	1.111693	1.860894	C	-3.754187	0.804837	1.745406
H	-3.146031	0.031858	1.769933	H	-3.576299	-0.290018	1.687437
H	-4.252971	1.230178	2.550783	H	-4.695738	0.970605	2.311751
H	-4.390118	2.150778	-4.906752	H	-4.437361	2.289276	-4.933328
O	-1.298627	4.043238	-5.965100	O	-1.411623	4.232698	-6.104215
C	-2.333158	3.458617	-5.634344	C	-2.405540	3.611390	-5.700725
H	-2.656330	2.491641	-6.106107	H	-2.751669	2.662087	-6.187856
N	-3.207433	3.870196	-4.670177	N	-3.198119	3.966568	-4.656123
C	-2.976956	5.100734	-3.932358	C	-2.936561	5.166570	-3.880802
H	-2.045870	5.562618	-4.308326	H	-2.000130	5.632066	-4.237123
H	-2.884546	4.884522	-2.847738	H	-2.841423	4.910079	-2.805578
H	-3.821124	5.808055	-4.084646	H	-3.768489	5.895013	-3.995962
C	-4.388796	3.097636	-4.333363	C	-4.373641	3.192171	-4.297110
H	-5.317005	3.663906	-4.568687	H	-5.298320	3.792035	-4.441393
H	-4.386504	2.856035	-3.249898	H	-4.317738	2.883839	-3.232581

Li⁺(DMF)₄

E (PBE-D3/ma-def2-svp GAS_OPT) =	-999.6690542039
E (PBE-D3/ma-def2-svp SMD_OPT) =	-999.7344970487
ΔG_{corr} (ID-RR-HR GAS) =	0.3444332400
E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT GAS) =	-1000.0057375926
E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT SMD) =	-1000.0709323329
E (DLPNO-CCSDT/cc-p(wC)VTZ SMD_OPT SMD) =	-1000.0722542146

E (PBE-D3/ma-def2-tzvp GAS_OPT GAS) =	-1000.7371609942
E (PBE-D3/ma-def2-tzvp GAS_OPT SMD) =	-1000.8001751533
E (PBE-D3/ma-def2-tzvp GAS_OPT CPCM) =	-1000.7990051739
GAS_OPT	SMD_OPT
Li -0.241261 0.062903 0.050157	Li -0.151080 0.222746 1.072496
H 1.289674 3.375498 -4.631327	H -0.525722 1.406226 -3.939175
O 0.757116 0.414514 -1.595360	O 0.580948 1.376132 -0.327568
C 1.008713 1.547438 -2.043229	C 0.223766 1.402623 -1.524529
H 0.778922 2.471216 -1.455385	H -0.479458 0.640074 -1.937739
N 1.571645 1.796744 -3.246871	N 0.623012 2.316138 -2.429029
C 1.927176 0.708718 -4.145826	C 1.530746 3.393615 -2.069319
H 1.644103 -0.248727 -3.674046	H 1.791249 3.310290 -0.999387
H 3.018459 0.714858 -4.349196	H 1.050825 4.376989 -2.255156
H 1.391156 0.816411 -5.111609	H 2.456792 3.335678 -2.678402
C 1.840575 3.154685 -3.693159	C 0.161099 2.262994 -3.806730
H 2.924956 3.297790 -3.883398	H 1.019723 2.143653 -4.500017
H 1.520013 3.874674 -2.916935	H -0.376798 3.196978 -4.071791
H 4.260499 -2.464613 -0.057093	H 1.680370 -4.753976 1.073093
O 0.763286 -1.380477 0.890835	O 1.139994 -1.086341 1.785707
C 1.915757 -1.741284 0.591192	C 1.366279 -2.285690 1.530155
H 2.454083 -1.304496 -0.286673	H 1.348924 -3.064798 2.331622
N 2.631985 -2.671829 1.260151	N 1.647654 -2.791938 0.310617
C 2.084191 -3.335021 2.434644	C 1.779441 -1.940109 -0.860468
H 2.741013 -3.165456 3.312748	H 1.729343 -0.881162 -0.554666
H 2.006992 -4.428839 2.261570	H 0.971658 -2.147506 -1.592974
H 1.081432 -2.921313 2.641271	H 2.752292 -2.134193 -1.356718
C 3.974144 -3.043893 0.840725	C 1.834830 -4.220873 0.116326
H 4.022657 -4.125535 0.595459	H 2.859086 -4.434797 -0.253841
H 4.708475 -2.835684 1.646791	H 1.109249 -4.607956 -0.629242
H -3.239477 3.309684 2.705842	H -1.461101 4.079196 4.926847
O -0.242142 1.780343 0.979608	O -0.929772 1.255071 2.484681
C -1.219551 2.290134 1.556013	C -1.091365 2.212067 3.265853
H -2.241880 1.843237 1.475199	H -1.797146 2.138439 4.129098
N -1.172697 3.404699 2.319613	N -0.476684 3.409711 3.190462
C 0.082319 4.108283 2.539297	C 0.478010 3.718395 2.137544
H 0.889305 3.567771 2.013905	H 0.511214 2.892504 1.404991
H 0.313965 4.152720 3.623735	H 1.491171 3.870342 2.566646
H 0.017157 5.146955 2.152967	H 0.177514 4.652168 1.618577
C -2.366152 3.941374 2.954588	C -0.726857 4.442556 4.183580
H -2.565488 4.975876 2.604435	H -1.128855 5.357108 3.699804
H -2.246893 3.963450 4.058086	H 0.213077 4.709228 4.710682
H -5.151931 -2.414716 -1.061703	H -3.175248 -4.716988 -0.715710
O -2.113335 -0.371205 -0.135911	O -1.369701 -0.952758 0.053714
C -3.098144 -1.068084 -0.427306	C -1.561425 -2.176105 0.205001
H -4.055545 -0.602422 -0.772361	H -1.474812 -2.666984 1.205600
N -3.161682 -2.417459 -0.369471	N -1.883517 -3.039941 -0.779012
C -2.023360 -3.214319 0.065705	C -2.067444 -2.594045 -2.150809
H -2.319557 -3.862446 0.916346	H -1.826604 -1.518740 -2.221046
H -1.199918 -2.549692 0.382527	H -3.118923 -2.752350 -2.470538

H	-1.671343	-3.865867	-0.761836	H	-1.406698	-3.167117	-2.833165
C	-4.369754	-3.133261	-0.752542	C	-2.120953	-4.446745	-0.495998
H	-4.754848	-3.733316	0.098146	H	-1.915717	-4.655059	0.570776
H	-4.164812	-3.820019	-1.600320	H	-1.462381	-5.084752	-1.120847

Li⁺ in DMF

E (PBE-D3/ma-def2-svp GAS_OPT) =	-7.2519251623
E (PBE-D3/ma-def2-svp SMD_OPT) =	-7.3917970144
ΔG_{corr} (ID-RR-HR GAS) =	-0.0127326619
E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT GAS) =	-7.2736440090
E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT SMD) =	-7.4150889774
E (DLPNO-CCSDT/cc-p(wC)VTZ SMD_OPT SMD) =	-7.4150889774
E (PBE-D3/ma-def2-tzvp GAS_OPT GAS) =	-7.2566456293
E (PBE-D3/ma-def2-tzvp GAS_OPT SMD) =	-7.3963804330
E (PBE-D3/ma-def2-tzvp GAS_OPT CPCM) =	-7.4401640391
GAS_OPT	SMD_OPT
Li 0.000000 0.000000 0.000000	Li 0.000000 0.000000 0.000000

(DMF)₅

E (PBE-D3/ma-def2-svp GAS_OPT) =	-1240.2974060660
E (PBE-D3/ma-def2-svp SMD_OPT) =	-1240.3239013672
ΔG_{corr} (ID-RR-HR GAS) =	0.4353376200
E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT GAS) =	-1240.6944901651

E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT SMD) =	-1240.7131902924
E (DLPNO-CCSDT/cc-p(wC)VTZ SMD_OPT SMD) =	-1240.7152610060
E (PBE-D3/ma-def2-tzvp GAS_OPT GAS) =	-1241.6266571738
E (PBE-D3/ma-def2-tzvp GAS_OPT SMD) =	-1241.6464485680
E (PBE-D3/ma-def2-tzvp GAS_OPT CPCM) =	-1241.6508558572
GAS_OPT	SMD_OPT
H 0.211764 4.862966 -1.877429	Li -2.148080 1.984135 -0.455481
O 2.777315 1.908524 -0.145675	H 0.527577 3.283310 -4.609499
C 1.781443 2.319262 -0.755336	O -1.473863 3.523555 -1.416263
H 0.788204 1.803117 -0.718559	C -0.814575 3.464566 -2.475298
N 1.745711 3.441308 -1.533612	H -0.544408 2.486238 -2.942734
C 2.934643 4.249209 -1.724657	N -0.360469 4.528829 -3.165321
H 3.763328 3.792675 -1.152649	C -0.612959 5.888463 -2.717049
H 2.767479 5.288512 -1.367445	H -1.170164 6.451488 -3.494599
H 3.210991 4.293658 -2.800229	H 0.345349 6.414575 -2.524175
C 0.521215 3.845240 -2.202184	H -1.208443 5.861575 -1.787483
H -0.285032 3.126702 -1.955676	C 0.402804 4.360368 -4.391250
H 0.661770 3.867447 -3.305230	H 1.406512 4.823537 -4.290225
H 2.010961 -0.328106 0.140214	H -0.120517 4.840513 -5.244446
O 1.390586 -1.703929 -3.339994	H -3.389357 -2.011480 -3.420407
C 1.574220 -1.268715 -2.198509	O -1.386150 0.367961 -1.275994
H 1.894341 -0.211523 -2.003604	C -2.036999 -0.431368 -1.980839
N 1.422124 -1.974103 -1.041851	H -2.966043 -0.119820 -2.516596
C 1.035856 -3.374786 -1.071890	N -1.719647 -1.727163 -2.172023
H 0.972616 -3.697587 -2.127052	C -0.542557 -2.317756 -1.556147
H 0.054232 -3.521039 -0.574514	H 0.183543 -2.633899 -2.334279
H 1.799076 -3.991720 -0.548828	H -0.827665 -3.213682 -0.967399
C 1.594790 -1.347987 0.258874	H -0.063369 -1.574783 -0.894849
H 2.306802 -1.939272 0.875129	C -2.532639 -2.584737 -3.019295
H 0.630165 -1.280875 0.805053	H -2.919423 -3.449434 -2.440650
H -1.077499 -2.416285 -3.195901	H -1.934059 -2.972929 -3.869534
O -1.335771 1.273109 -1.067591	H -6.405212 1.616328 2.401241
C -1.592466 0.077494 -1.292643	O -4.086905 1.664335 -0.580681
H -1.810093 -0.648182 -0.469480	C -4.854819 1.624867 0.401933
N -1.630106 -0.498312 -2.520671	H -4.736152 2.319466 1.268716
C -1.331536 0.264652 -3.720513	N -5.886638 0.768996 0.546738
H -1.167053 1.320015 -3.439277	C -6.203606 -0.214639 -0.475987
H -2.179376 0.203752 -4.435574	H -6.250183 -1.229412 -0.030550
H -0.419175 -0.140624 -4.207014	H -5.425644 -0.189777 -1.259479
C -1.926229 -1.913099 -2.687518	H -7.189687 0.007374 -0.935560
H -2.839699 -2.045436 -3.307030	C -6.729148 0.796756 1.732556
H -2.088318 -2.382788 -1.698356	H -6.650825 -0.163074 2.283895
H -0.041969 3.946487 2.907729	H -7.788768 0.966109 1.450415
O -1.076429 -0.114107 2.242767	H -0.319915 0.361462 5.118762
C -1.038678 1.097452 2.002687	O -1.827430 1.884527 1.459276
H -1.890425 1.639921 1.520678	C -1.182893 1.094273 2.177875

N	0.014048	1.922268	2.269186	H	-0.231569	0.621743	1.829567
C	1.232773	1.411007	2.874651	N	-1.534925	0.721630	3.424537
H	1.088897	0.335908	3.085853	C	-2.748819	1.223730	4.048937
H	1.447789	1.945513	3.824924	H	-3.429307	0.384581	4.300253
H	2.090972	1.540330	2.181691	H	-3.259374	1.907607	3.348555
C	-0.051295	3.340039	1.974842	H	-2.501921	1.772491	4.981405
H	-0.980916	3.557827	1.414862	C	-0.693392	-0.162666	4.214161
H	0.813035	3.652686	1.352915	H	0.175331	-0.491118	3.613548
H	-2.309881	-3.207527	4.811254	H	-1.264583	-1.055023	4.542768
O	-2.009956	-3.138709	0.478624	H	-0.751851	-2.564168	2.034587
C	-2.407717	-2.787776	1.593764	O	-4.744296	-1.802875	3.477083
H	-3.371887	-2.233147	1.738274	C	-3.675827	-2.419787	3.364773
N	-1.773931	-3.027723	2.774084	H	-3.283657	-3.088913	4.175134
C	-0.462458	-3.645760	2.789264	N	-2.846237	-2.374680	2.288718
H	-0.268525	-4.090245	1.796777	C	-3.189221	-1.577614	1.124714
H	-0.417881	-4.437609	3.565552	H	-2.302468	-1.020173	0.769038
H	0.324460	-2.890348	3.005655	H	-3.981572	-0.863056	1.405536
C	-2.248251	-2.440091	4.010881	H	-3.556797	-2.218785	0.293986
H	-3.255551	-2.009936	3.853018	C	-1.649482	-3.192420	2.216351
H	-1.573506	-1.619733	4.337288	H	-1.726611	-3.936437	1.394595
				H	-1.510464	-3.739139	3.168333

Li⁺(DMF)₅

E (PBE-D3/ma-def2-svp GAS_OPT) =	-1247.7333543943
E (PBE-D3/ma-def2-svp SMD_OPT) =	-1247.8035333343
ΔG_{corr} (ID-RR-HR GAS) =	0.4336469900
E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT GAS) =	-1248.1493216593
E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT SMD) =	-1248.2128851299
E (DLPNO-CCSDT/cc-p(wC)VTZ SMD_OPT SMD) =	-1248.2191775468
E (PBE-D3/ma-def2-tzvp GAS_OPT GAS) =	-1249.0679870866
E (PBE-D3/ma-def2-tzvp GAS_OPT SMD) =	-1249.1290669326
E (PBE-D3/ma-def2-tzvp GAS_OPT CPCM) =	-1249.1300283377
GAS_OPT	SMD_OPT
Li 0.794781 1.185159 -0.227211	Li -2.148080 1.984135 -0.455481
H 1.351051 2.884095 -5.034820	H 0.527577 3.283310 -4.609499

O	1.761478	2.522489	-1.295129	O	-1.473863	3.523555	-1.416263
C	1.639662	2.645607	-2.525316	C	-0.814575	3.464566	-2.475298
H	0.870817	2.066475	-3.095825	H	-0.544408	2.486238	-2.942734
N	2.389567	3.464086	-3.300020	N	-0.360469	4.528829	-3.165321
C	3.443766	4.281791	-2.719602	C	-0.612959	5.888463	-2.717049
H	3.499035	4.071895	-1.636768	H	-1.170164	6.451488	-3.494599
H	3.232371	5.360100	-2.878890	H	0.345349	6.414575	-2.524175
H	4.420039	4.043473	-3.190620	H	-1.208443	5.861575	-1.787483
C	2.175004	3.558525	-4.734547	C	0.402804	4.360368	-4.391250
H	3.091577	3.267075	-5.289353	H	1.406512	4.823537	-4.290225
H	1.907000	4.596196	-5.025298	H	-0.120517	4.840513	-5.244446
H	1.277479	-3.949334	1.243413	H	-3.389357	-2.011480	-3.420407
O	1.834539	-0.353783	0.280904	O	-1.386150	0.367961	-1.275994
C	1.662579	-1.539082	0.614912	C	-2.036999	-0.431368	-1.980839
H	0.645594	-1.991076	0.726857	H	-2.966043	-0.119820	-2.516596
N	2.662616	-2.414198	0.878111	N	-1.719647	-1.727163	-2.172023
C	4.056393	-2.009269	0.792416	C	-0.542557	-2.317756	-1.556147
H	4.097191	-0.942247	0.509705	H	0.183543	-2.633899	-2.334279
H	4.590825	-2.614140	0.030053	H	-0.827665	-3.213682	-0.967399
H	4.562387	-2.152470	1.770081	H	-0.063369	-1.574783	-0.894849
C	2.372489	-3.789633	1.248973	C	-2.532639	-2.584737	-3.019295
H	2.767153	-4.017220	2.262076	H	-2.919423	-3.449434	-2.440650
H	2.838464	-4.495670	0.529440	H	-1.934059	-2.972929	-3.869534
H	-2.693621	-2.537233	-1.227423	H	-6.405212	1.616328	2.401241
O	-0.631495	0.604677	-1.448512	O	-4.086905	1.664335	-0.580681
C	-1.335004	-0.419998	-1.376401	C	-4.854819	1.624867	0.401933
H	-1.195186	-1.189519	-0.578355	H	-4.736152	2.319466	1.268716
N	-2.338540	-0.727539	-2.231910	N	-5.886638	0.768996	0.546738
C	-2.690765	0.159111	-3.328373	C	-6.203606	-0.214639	-0.475987
H	-2.058934	1.063140	-3.269920	H	-6.250183	-1.229412	-0.030550
H	-3.759067	0.452207	-3.259541	H	-5.425644	-0.189777	-1.259479
H	-2.528864	-0.343373	-4.305424	H	-7.189687	0.007374	-0.935560
C	-3.094059	-1.962000	-2.083962	C	-6.729148	0.796756	1.732556
H	-3.011718	-2.581518	-3.002021	H	-6.650825	-0.163074	2.283895
H	-4.169234	-1.745080	-1.908099	H	-7.788768	0.966109	1.450415
H	-0.330580	6.115437	2.947097	H	-0.319915	0.361462	5.118762
O	0.182516	2.195875	1.322948	O	-1.827430	1.884527	1.459276
C	0.509626	3.366222	1.577260	C	-1.182893	1.094273	2.177875
H	1.180312	3.947954	0.895931	H	-0.231569	0.621743	1.829567
N	0.112015	4.061907	2.669039	N	-1.534925	0.721630	3.424537
C	-0.762168	3.455206	3.660650	C	-2.748819	1.223730	4.048937
H	-0.995581	2.424167	3.340905	H	-3.429307	0.384581	4.300253
H	-1.703564	4.036054	3.754395	H	-3.259374	1.907607	3.348555
H	-0.264843	3.431215	4.652955	H	-2.501921	1.772491	4.981405
C	0.542586	5.431255	2.895528	C	-0.693392	-0.162666	4.214161
H	1.199082	5.758883	2.067476	H	0.175331	-0.491118	3.613548
H	1.106887	5.514398	3.848334	H	-1.264583	-1.055023	4.542768
H	-4.655476	-4.687235	2.959718	H	-0.751851	-2.564168	2.034587
O	-1.345771	-3.077699	0.781675	O	-4.744296	-1.802875	3.477083
C	-2.016380	-3.334123	1.791780	C	-3.675827	-2.419787	3.364773
H	-2.026956	-2.657964	2.686731	H	-3.283657	-3.088913	4.175134
N	-2.805070	-4.427415	1.958212	N	-2.846237	-2.374680	2.288718
C	-2.917930	-5.429973	0.910359	C	-3.189221	-1.577614	1.124714
H	-2.247309	-5.150904	0.078002	H	-2.302468	-1.020173	0.769038
H	-3.962604	-5.492360	0.538611	H	-3.981572	-0.863056	1.405536

H	-2.626270	-6.428378	1.297551	H	-3.556797	-2.218785	0.293986
C	-3.567670	-4.638352	3.177681	C	-1.649482	-3.192420	2.216351
H	-3.387008	-3.803851	3.881618	H	-1.726611	-3.936437	1.394595
H	-3.268778	-5.587115	3.671280	H	-1.510464	-3.739139	3.168333

(DMF)₆

E (PBE-D3/ma-def2-svp GAS_OPT) =	-1488.3642538444
E (PBE-D3/ma-def2-svp SMD_OPT) =	-1488.3887889211
ΔG_{corr} (ID-RR-HR GAS) =	0.5304941700
E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT GAS) =	-1488.8398073824
E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT SMD) =	-1488.8594609522
E (DLPNO-CCSDT/cc-p(wC)VTZ SMD_OPT SMD) =	-1488.8618975566
E (PBE-D3/ma-def2-tzvp GAS_OPT GAS) =	-1489.9586201319
E (PBE-D3/ma-def2-tzvp GAS_OPT SMD) =	-1489.9771403817
E (PBE-D3/ma-def2-tzvp GAS_OPT CPCM) =	-1489.9842294831
GAS_OPT	SMD_OPT
H 0.241785 1.869890 -3.631963	H 1.710180 -1.812161 -5.609057
O 3.194570 0.617759 -1.650449	O -1.485722 -2.484101 -3.718943
C 2.242169 1.043343 -2.317456	C -0.420719 -2.263812 -4.313652
H 1.542898 0.370717 -2.879411	H -0.393195 -1.784807 -5.327919
N 1.911093 2.359491 -2.454396	N 0.824504 -2.552224 -3.853684
C 2.696793 3.398130 -1.808581	C 1.020937 -3.168147 -2.553934
H 3.597062 2.930383 -1.369525	H 0.043678 -3.270806 -2.053114
H 2.114065 3.888569 -1.000203	H 1.691279 -2.548168 -1.923098
H 3.006161 4.161648 -2.553554	H 1.484396 -4.172370 -2.660781
C 0.767505 2.766355 -3.249446	C 2.010411 -2.244842 -4.635289
H 1.085244 3.396476 -4.109000	H 2.601695 -3.165604 -4.826105
H 0.059071 3.361718 -2.633814	H 2.648526 -1.508399 -4.101384
H 3.339866 -1.874479 1.379115	H -2.001415 0.143207 -0.399285
O 0.330610 -3.196400 -0.464223	O 0.187829 -2.597029 1.039521
C 1.334399 -2.763469 0.122909	C -0.543853 -1.718602 0.559286
H 1.326160 -2.525342 1.217554	H -0.302782 -0.626746 0.648014
N 2.538732 -2.510004 -0.453134	N -1.699737 -1.927574 -0.119686
C 2.757620 -2.715071 -1.874623	C -2.204244 -3.267184 -0.362795
H 1.819933 -3.083041 -2.328230	H -2.276151 -3.451282 -1.455246

H	3.559157	-3.467420	-2.038751	H	-3.215710	-3.388325	0.079928
H	3.063331	-1.758012	-2.344973	H	-1.518644	-4.003774	0.092780
C	3.649532	-1.983513	0.322037	C	-2.469148	-0.823686	-0.667093
H	3.954079	-0.993963	-0.076687	H	-3.504389	-0.837090	-0.265496
H	4.518697	-2.675347	0.278137	H	-2.519493	-0.905393	-1.773681
H	-1.877240	-2.698311	-0.969799	H	0.176410	3.377064	-2.019012
O	-0.602020	-0.364023	-3.638244	O	3.254968	0.468571	-2.838623
C	-1.050064	-1.167199	-2.807222	C	2.702909	1.578821	-2.872978
H	-0.423552	-1.960896	-2.326596	H	3.287026	2.529676	-2.986494
N	-2.333705	-1.182255	-2.348352	N	1.369061	1.808877	-2.771919
C	-3.304670	-0.220778	-2.832746	C	0.417198	0.719675	-2.621334
H	-2.841128	0.369758	-3.644448	H	0.964917	-0.219338	-2.435652
H	-3.626325	0.461220	-2.015339	H	-0.193014	0.600116	-3.542566
H	-4.205997	-0.739945	-3.222284	H	-0.261531	0.938181	-1.774362
C	-2.744322	-2.086563	-1.285552	C	0.822252	3.150449	-2.892016
H	-3.563647	-2.754489	-1.630432	H	0.209647	3.244971	-3.814993
H	-3.101361	-1.503744	-0.410147	H	1.646796	3.887286	-2.939111
H	-1.229633	3.988782	-0.002810	H	-1.682337	2.824646	3.539873
O	-3.142761	0.350702	1.251261	O	-1.156543	2.393564	-0.169546
C	-3.086025	1.528256	0.876818	C	-1.310666	2.550824	1.054670
H	-3.873118	2.280100	1.156133	H	-1.817433	1.783450	1.693246
N	-2.107724	2.073825	0.108185	N	-0.921490	3.642067	1.760546
C	-0.982619	1.277646	-0.361365	C	-0.263782	4.765254	1.119998
H	-1.007512	0.290315	0.131932	H	0.741326	4.937047	1.560459
H	-0.036883	1.800133	-0.123212	H	-0.859742	5.693360	1.252230
H	-1.035445	1.133888	-1.458755	H	-0.156785	4.555155	0.040890
C	-2.155650	3.463344	-0.316737	C	-1.150762	3.729620	3.191578
H	-3.031723	3.962088	0.141150	H	-1.768974	4.620219	3.433908
H	-2.251157	3.531476	-1.422461	H	-0.189681	3.806236	3.741203
H	0.695264	2.226390	4.563879	H	0.055478	-1.197109	4.719667
O	0.861497	3.672431	1.075228	O	-2.952468	0.144442	2.884112
C	0.853022	3.196893	2.217906	C	-1.957371	-0.322357	3.462105
H	0.324457	3.705958	3.068983	H	-1.125883	0.325588	3.841732
N	1.441399	2.036084	2.606706	N	-1.727737	-1.638364	3.701861
C	2.192935	1.215233	1.668908	C	-2.659512	-2.659870	3.262039
H	2.229138	1.712841	0.685769	H	-3.437888	-2.191613	2.633460
H	1.717701	0.218790	1.569727	H	-3.143048	-3.155073	4.131739
H	3.232292	1.072084	2.033563	H	-2.124131	-3.433906	2.675658
C	1.352728	1.556002	3.977236	C	-0.538849	-2.077719	4.410114
H	2.357756	1.542135	4.453212	H	0.084314	-2.724805	3.757705
H	0.940095	0.525178	3.987546	H	-0.815503	-2.652437	5.319684
H	-3.116753	-3.404228	1.395104	H	2.262701	-0.260331	-0.534239
O	0.313394	-1.455796	3.033702	O	1.162276	1.163549	3.400108
C	-0.899232	-1.593801	2.810395	C	1.596990	0.359685	2.562002
H	-1.598041	-0.725868	2.707617	H	1.577172	-0.748632	2.727083
N	-1.532295	-2.786973	2.648429	N	2.141452	0.679511	1.358887
C	-0.794426	-4.036805	2.699313	C	2.267569	2.061691	0.931261
H	0.208639	-3.838802	3.119049	H	1.625446	2.259914	0.048576
H	-0.681217	-4.463105	1.678976	H	3.320536	2.286383	0.660295
H	-1.326410	-4.766666	3.344137	H	1.955404	2.720725	1.760569
C	-2.950405	-2.851744	2.344419	C	2.684410	-0.347766	0.486064
H	-3.353442	-1.828192	2.228868	H	2.432336	-1.346888	0.887713
H	-3.504348	-3.379794	3.151016	H	3.788306	-0.251489	0.402526

Li⁺(DMF)₆

E (PBE-D3/ma-def2-svp GAS_OPT) =	-1495.8062663450
E (PBE-D3/ma-def2-svp SMD_OPT) =	-1495.8727190791
ΔG_{corr} (ID-RR-HR GAS) =	0.5314964500
E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT GAS) =	-1496.3008727727
E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT SMD) =	-1496.3655638450
E (DLPNO-CCSDT/cc-p(wC)VTZ SMD_OPT SMD) =	-1496.3685913342
E (PBE-D3/ma-def2-tzvp GAS_OPT GAS) =	-1497.4036698883
E (PBE-D3/ma-def2-tzvp GAS_OPT SMD) =	-1497.4672903903
E (PBE-D3/ma-def2-tzvp GAS_OPT CPCM) =	-1497.4662445481
GAS_OPT	SMD_OPT
Li 1.244388 0.320435 -1.654907	Li 1.327935 0.215548 -1.525172
H 3.806560 2.068413 -5.711476	H 3.390016 1.387523 -6.035581
O 2.226517 -0.275357 -3.202683	O 2.342493 -0.566905 -2.978600
C 2.750413 0.486528 -4.033249	C 2.695784 0.062781 -3.996985
H 2.663219 1.597931 -3.941322	H 2.497610 1.157090 -4.104424
N 3.463546 0.082178 -5.109713	N 3.336790 -0.472828 -5.054857
C 3.674759 -1.332533 -5.375817	C 3.680430 -1.884539 -5.098493
H 3.178040 -1.918787 -4.582629	H 3.342899 -2.371250 -4.166409
H 4.759831 -1.566511 -5.384346	H 4.778515 -2.009802 -5.201699
H 3.248820 -1.608624 -6.363094	H 3.190295 -2.373393 -5.966354
C 4.045059 1.038399 -6.037047	C 3.710486 0.341671 -6.199617
H 3.642407 0.888207 -7.060944	H 3.226606 -0.040024 -7.122979
H 5.149063 0.926116 -6.076905	H 4.810566 0.323579 -6.347578
H -0.017119 -1.622414 3.035870	H 0.383157 -1.348368 3.437623
O 1.892198 -0.264162 0.089901	O 2.012142 -0.206678 0.234006
C 1.263926 -0.695924 1.072265	C 1.464680 -0.549337 1.303038
H 0.224700 -1.097588 0.989017	H 0.484610 -1.086160 1.324408
N 1.750747 -0.732738 2.336493	N 1.979986 -0.326985 2.530324
C 3.085231 -0.243394 2.642252	C 3.237406 0.377704 2.714085
H 3.574061 0.063651 1.700722	H 3.658137 0.636247 1.726684
H 3.687863 -1.039406 3.126542	H 3.959544 -0.261619 3.263196
H 3.034215 0.624553 3.333439	H 3.078252 1.306003 3.301974
C 0.948317 -1.254096 3.430295	C 1.295404 -0.794411 3.724783
H 0.750320 -0.462518 4.184716	H 1.017841 0.061025 4.375129
H 1.473832 -2.091195 3.936203	H 1.953755 -1.473259 4.305911
H -4.373127 0.412071 0.421412	H -4.419445 -0.233139 0.236237

O	-0.674306	-0.073476	-1.591447	O	-0.581563	-0.175149	-1.606587
C	-1.578673	0.574719	-1.032569	C	-1.494446	0.230315	-0.857282
H	-1.367497	1.481970	-0.413729	H	-1.290833	0.761426	0.105761
N	-2.892595	0.258130	-1.083551	N	-2.813386	0.087233	-1.110526
C	-3.352009	-0.916922	-1.805214	C	-3.289150	-0.556030	-2.322719
H	-2.512219	-1.319871	-2.398251	H	-2.427552	-0.954352	-2.886036
H	-4.187462	-0.646198	-2.482317	H	-3.834903	0.172909	-2.958838
H	-3.707583	-1.694394	-1.096113	H	-3.986993	-1.381557	-2.073173
C	-3.882045	1.035662	-0.356192	C	-3.811627	0.596342	-0.183930
H	-4.665618	1.414859	-1.044643	H	-4.496598	1.298704	-0.703146
H	-3.390218	1.893835	0.138174	H	-3.310108	1.132113	0.643009
H	-1.964163	-0.773789	5.028201	H	-1.299167	-0.824271	5.701258
O	-1.224213	2.077963	1.898671	O	-1.530041	1.674535	2.234465
C	-1.690419	1.049319	2.409249	C	-1.787540	0.687636	2.946314
H	-1.890950	0.121018	1.816640	H	-2.016985	-0.316769	2.506895
N	-2.012112	0.893750	3.722250	N	-1.815266	0.683677	4.302509
C	-1.836182	1.980462	4.669801	C	-1.520041	1.880886	5.068393
H	-1.416724	2.851369	4.134823	H	-1.259453	2.699300	4.373514
H	-1.145594	1.681094	5.486789	H	-0.668582	1.701486	5.758673
H	-2.808159	2.263492	5.126077	H	-2.399079	2.183588	5.676132
C	-2.582755	-0.352523	4.206731	C	-2.141498	-0.522851	5.042143
H	-2.621324	-1.085669	3.377691	H	-2.354931	-1.348587	4.337522
H	-3.609092	-0.191708	4.600819	H	-3.036655	-0.362146	5.679523
H	-0.325136	5.349582	-0.285902	H	-1.269848	4.664277	-0.649603
O	1.323335	2.283110	-1.761048	O	1.336449	2.182691	-1.805636
C	0.815507	3.301569	-1.260722	C	0.499216	3.017141	-1.403379
H	0.166247	3.985653	-1.865131	H	-0.244700	3.479050	-2.099386
N	0.969073	3.716528	0.014834	N	0.378027	3.459709	-0.136152
C	1.791695	2.972789	0.957734	C	1.267857	3.002975	0.921321
H	2.326417	2.171589	0.419280	H	2.022408	2.322401	0.492123
H	1.144894	2.519727	1.736925	H	0.683393	2.468133	1.697566
H	2.520412	3.657636	1.438158	H	1.773174	3.872903	1.390270
C	0.238111	4.862934	0.532795	C	-0.658822	4.409212	0.236709
H	0.938466	5.604169	0.970221	H	-0.206814	5.339742	0.639446
H	-0.475830	4.531524	1.315190	H	-1.313446	3.965851	1.014567
H	-2.020452	-5.724093	-1.142799	H	-1.551313	-3.386421	-2.676557
O	-1.814886	-2.156050	1.252020	O	-1.421454	-2.316150	1.451288
C	-1.973304	-3.362476	1.012381	C	-1.910343	-2.816626	0.424153
H	-2.643450	-4.007130	1.639870	H	-3.016915	-2.846749	0.250504
N	-1.391274	-4.053866	0.000388	N	-1.213567	-3.391016	-0.585329
C	-0.482206	-3.402670	-0.934040	C	0.237354	-3.462830	-0.558651
H	-0.620627	-2.307596	-0.898025	H	0.597341	-3.247554	0.462717
H	-0.693508	-3.754723	-1.963529	H	0.683704	-2.728735	-1.262007
H	0.576620	-3.643185	-0.696924	H	0.567136	-4.479689	-0.852876
C	-1.591273	-5.487150	-0.146875	C	-1.881451	-3.921077	-1.761007
H	-2.286011	-5.852450	0.633008	H	-2.976566	-3.806482	-1.655257
H	-0.628699	-6.031748	-0.044691	H	-1.650318	-4.999666	-1.887353

DMSO

E (PBE-D3/ma-def2-svp GAS_OPT) =

-552.6078871743

E (PBE-D3/ma-def2-svp SMD_OPT) =	-552.6212804088
ΔG_{corr} (ID-RR-HR GAS) =	0.0480126100
E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT GAS) =	-552.5203312602
E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT SMD) =	-552.5329364308
E (DLPNO-CCSDT/cc-p(wC)VTZ SMD_OPT SMD) =	-552.5330471425
E (PBE-D3/ma-def2-tzvp GAS_OPT GAS) =	-552.9372162962
E (PBE-D3/ma-def2-tzvp GAS_OPT SMD) =	-552.9492238183
E (PBE-D3/ma-def2-tzvp GAS_OPT CPCM) =	-552.9524468482
GAS_OPT	SMD_OPT
O 0.713931 -3.064997 -4.214221	O 0.725478 -3.068289 -4.219531
S 1.110585 -1.831941 -3.402686	S 1.101017 -1.818449 -3.390307
C -0.070958 -0.495164 -3.852844	C -0.072177 -0.501231 -3.855099
C 0.478321 -2.092359 -1.694446	C 0.476615 -2.096601 -1.699059
H 0.101751 0.390609 -3.209694	H 0.106404 0.384352 -3.212865
H -1.105758 -0.876377 -3.747805	H -1.110761 -0.870569 -3.741697
H 0.132399 -0.241131 -4.909977	H 0.133673 -0.241940 -4.911310
H 1.058347 -2.933736 -1.271280	H 1.059568 -2.935165 -1.272253
H -0.595562 -2.359919 -1.742975	H -0.600665 -2.353365 -1.737369
H 0.641061 -1.177551 -1.090538	H 0.644965 -1.181309 -1.096979

(DMSO)₃

E (PBE-D3/ma-def2-svp GAS_OPT) =	-1657.8645153296
E (PBE-D3/ma-def2-svp SMD_OPT) =	-1657.8803383988
ΔG_{corr} (ID-RR-HR GAS) =	0.1865310700
E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT GAS) =	-1657.5974284791
E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT SMD) =	-1657.6149771979
E (DLPNO-CCSDT/cc-p(wC)VTZ SMD_OPT SMD) =	-1657.6155200580

E (PBE-D3/ma-def2-tzvp GAS_OPT GAS) =	-1658.8407174717
E (PBE-D3/ma-def2-tzvp GAS_OPT SMD) =	-1658.8542470794
E (PBE-D3/ma-def2-tzvp GAS_OPT CPCM) =	-1658.8624043137
GAS_OPT	SMD_OPT
O 1.982075 0.716842 -0.219025	O 2.362998 0.430301 0.076553
S 2.427732 2.150582 0.144711	S 2.592609 1.961783 0.172612
C 0.948106 3.217659 -0.025514	C 1.049545 2.761403 -0.383490
C 2.525117 2.209053 1.973195	C 2.448463 2.397128 1.936665
O -0.541385 1.320847 2.068599	O -0.647232 1.229966 2.216802
S -0.869373 0.095268 1.178126	S -0.880685 -0.014965 1.315302
C 0.275855 -1.235606 1.677716	C 0.288655 -1.290800 1.870270
C -2.398182 -0.633625 1.867923	C -2.414137 -0.802430 1.902655
O -1.502715 -2.260979 -0.748821	O -1.336106 -2.419665 -0.783016
S -1.369418 -1.327811 -1.968368	S -1.373809 -1.269286 -1.822492
C 0.416059 -1.126853 -2.296761	C 0.356047 -0.861592 -2.215695
C -1.755219 -2.374234 -3.426051	C -1.806649 -2.037208 -3.419257
H 0.664257 3.188556 -1.094250	H 0.890482 2.465474 -1.438032
H 1.224792 4.251594 0.262034	H 1.186367 3.859931 -0.325144
H 0.147370 2.806752 0.626612	H 0.211292 2.431554 0.262405
H 3.344975 1.525637 2.263713	H 3.298033 1.915767 2.457894
H 1.546730 1.875431 2.379363	H 1.473292 2.022911 2.313361
H 2.769534 3.244547 2.282804	H 2.525280 3.498619 2.035475
H 1.270590 -0.910409 1.318832	H 1.289327 -0.920098 1.573090
H -0.043202 -2.162288 1.163474	H 0.048488 -2.225649 1.327600
H 0.250072 -1.330042 2.780748	H 0.205657 -1.417958 2.967715
H -3.199628 0.113323 1.716513	H -3.243493 -0.101309 1.687725
H -2.254943 -0.826893 2.948587	H -2.343444 -0.997171 2.990917
H -2.609612 -1.556173 1.293444	H -2.549127 -1.738098 1.325250
H 0.845697 -0.479754 -1.503522	H 0.828540 -0.436959 -1.305527
H 0.541192 -0.635729 -3.282534	H 0.365457 -0.109750 -3.030770
H 0.891457 -2.127642 -2.288580	H 0.884755 -1.783352 -2.531269
H -2.819679 -2.660577 -3.337475	H -2.846504 -2.405887 -3.332059
H -1.114005 -3.276877 -3.401641	H -1.114112 -2.875713 -3.631279
H -1.594250 -1.790602 -4.353853	H -1.749988 -1.266948 -4.214261

Li⁺(DMSO)₃

E (PBE-D3/ma-def2-svp GAS_OPT) =	-1665.2879688474
E (PBE-D3/ma-def2-svp SMD_OPT) =	-1665.3556613467
ΔG_{corr} (ID-RR-HR GAS) =	0.1884216000

E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT GAS) =	-1665.0406642053
E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT SMD) =	-1665.1122368574
E (DLPNO-CCSDT/cc-p(wC)VTZ SMD_OPT SMD) =	-1665.1105277461
E (PBE-D3/ma-def2-tzvp GAS_OPT GAS) =	-1666.2634708505
E (PBE-D3/ma-def2-tzvp GAS_OPT SMD) =	-1666.3316347308
E (PBE-D3/ma-def2-tzvp GAS_OPT CPCM) =	-1666.3364273997
GAS_OPT	SMD_OPT
Li -0.265322 0.030769 0.194557	Li 0.187685 0.495268 -1.575746
O 1.028263 1.010904 -0.726552	O 0.979816 2.075071 -0.967044
S 1.285069 2.546692 -0.565649	S 2.350600 2.364357 -0.276885
C 1.411676 2.832216 1.226744	C 1.940514 3.164047 1.297674
C 3.029441 2.769321 -1.022099	C 2.930193 0.773489 0.377568
O -1.140396 0.713433 1.685611	O -1.514582 -0.008492 -0.970879
S -2.299856 0.082933 2.519343	S -2.607485 0.752367 -0.148789
C -3.574624 -0.381129 1.302131	C -3.371950 -0.517112 0.890877
C -1.733042 -1.596714 2.942131	C -1.716132 1.669327 1.137246
O -0.789121 -1.656686 -0.420302	O 1.247067 -0.956286 -2.159932
S -0.281126 -2.416890 -1.686935	S 1.014680 -2.471788 -1.853977
C -0.432541 -1.223592 -3.056350	C 0.689075 -2.571952 -0.069658
C 1.536296 -2.417366 -1.550684	C -0.657207 -2.855976 -2.446219
H 0.434821 2.533481 1.657666	H 1.448503 4.125406 1.056303
H 1.598008 3.910262 1.400816	H 2.887503 3.356297 1.840061
H 2.226461 2.210878 1.646576	H 1.272241 2.514149 1.894407
H 3.107040 2.566531 -2.106456	H 3.865897 0.952077 0.944024
H 3.653464 2.060580 -0.444497	H 3.135150 0.119906 -0.491257
H 3.316105 3.819214 -0.816087	H 2.154468 0.335246 1.035647
H -3.966056 0.562104 0.877353	H -4.105751 -0.022867 1.557643
H -4.388199 -0.918697 1.827682	H -2.592192 -1.041553 1.476342
H -3.110204 -1.012578 0.518676	H -3.895109 -1.218940 0.214034
H -0.878713 -1.478335 3.634545	H -1.067690 0.975304 1.706486
H -1.426972 -2.118210 2.013220	H -2.462262 2.148140 1.802043
H -2.556535 -2.130915 3.455562	H -1.116892 2.442141 0.620429
H -1.514321 -1.058104 -3.216746	H 0.393901 -3.611735 0.174523
H 0.014408 -1.667914 -3.967348	H -0.117385 -1.859056 0.193324
H 0.076905 -0.282033 -2.768841	H 1.632482 -2.324419 0.452742
H 1.789842 -3.055057 -0.683295	H -0.635679 -2.767701 -3.549198
H 1.886655 -1.377073 -1.397495	H -1.373127 -2.135573 -2.003009
H 1.962577 -2.858024 -2.473280	H -0.896329 -3.899141 -2.158782

Li⁺ in DMSO

E (PBE-D3/ma-def2-svp GAS_OPT) =	-7.2519251623
E (PBE-D3/ma-def2-svp SMD_OPT) =	-7.3917970144
ΔG_{corr} (ID-RR-HR GAS) =	-0.0127326619
E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT GAS) =	-7.2736440090
E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT SMD) =	-7.4158901969
E (DLPNO-CCSDT/cc-p(wC)VTZ SMD_OPT SMD) =	-7.4158901969
E (PBE-D3/ma-def2-tzvp GAS_OPT GAS) =	-7.2566456293
E (PBE-D3/ma-def2-tzvp GAS_OPT SMD) =	-7.3967595445
E (PBE-D3/ma-def2-tzvp GAS_OPT CPCM) =	-7.4410917657
GAS_OPT	SMD_OPT
Li 0.000000 0.000000 0.000000	Li 0.000000 0.000000 0.000000

(DMSO)₄

E (PBE-D3/ma-def2-svp GAS_OPT) =	-2210.4955298611
E (PBE-D3/ma-def2-svp SMD_OPT) =	-2210.5133528928
ΔG_{corr} (ID-RR-HR GAS) =	0.2576870600
E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT GAS) =	-2210.1380758661
E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT SMD) =	-2210.1569256905
E (DLPNO-CCSDT/cc-p(wC)VTZ SMD_OPT SMD) =	-2210.1596862713
E (PBE-D3/ma-def2-tzvp GAS_OPT GAS) =	-2211.7949020496
E (PBE-D3/ma-def2-tzvp GAS_OPT SMD) =	-2211.8086437208

E (PBE-D3/ma-def2-tzvp GAS_OPT CPCM) =				-2211.8187475426			
GAS_OPT				SMD_OPT			
C	0.243199	-0.522197	2.300675	C	1.606287	-3.309595	2.677016
S	-0.394361	-2.227817	2.232464	S	-0.093372	-3.437461	2.029634
O	-1.081313	-2.391342	0.853856	O	-0.499879	-2.009424	1.567067
C	1.229162	-3.069180	2.105555	C	0.313274	-4.375847	0.520776
O	0.230302	1.643460	-1.665316	O	0.289301	2.117088	-0.954408
S	0.596284	1.984381	-0.198242	S	-0.121710	3.568590	-1.328965
C	2.338256	2.545643	-0.235139	C	0.569507	3.880495	-2.983991
C	-0.178890	3.605381	0.134527	C	-1.879051	3.506612	-1.789962
O	-2.226950	1.406779	1.323227	O	-3.213709	2.478560	1.020388
S	-3.382518	0.852241	0.460459	S	-2.784384	1.050949	1.457436
C	-2.607860	-0.068695	-0.913925	C	-2.324110	0.139967	-0.051998
C	-4.047134	-0.610089	1.346373	C	-1.104569	1.190984	2.147411
O	2.397667	-0.708608	-0.218932	O	2.897712	-2.390685	-0.297190
S	2.266330	-1.476753	-1.557724	S	2.522732	-0.960654	-0.781551
C	0.483589	-1.599416	-1.922671	C	0.846631	-1.065908	-1.488075
C	2.676864	-0.276332	-2.880678	C	2.078235	-0.000535	0.700358
H	-0.632292	0.149958	2.177059	H	1.569914	-2.631395	3.551037
H	0.961266	-0.382185	1.468297	H	2.268845	-2.914221	1.879496
H	0.723655	-0.370971	3.288457	H	1.929297	-4.318680	3.003312
H	1.022453	-4.133234	1.885861	H	-0.611257	-4.432097	-0.085292
H	1.746811	-2.977627	3.081133	H	0.623270	-5.397067	0.820796
H	1.821750	-2.589258	1.300827	H	1.127738	-3.852298	-0.021675
H	2.935453	1.627191	-0.389353	H	1.671434	3.892439	-2.880847
H	2.590923	2.999187	0.743585	H	0.215055	4.868799	-3.338571
H	2.473020	3.271286	-1.061201	H	0.251571	3.074482	-3.674310
H	-1.258882	3.398348	0.250765	H	-2.439154	3.244712	-0.865752
H	0.028559	4.289131	-0.711387	H	-2.029456	2.743351	-2.579303
H	0.217867	4.004833	1.088629	H	-2.178423	4.510235	-2.153510
H	-1.982740	0.657617	-1.470247	H	-1.537745	0.705237	-0.589600
H	-3.410067	-0.475213	-1.561993	H	-3.241152	0.036367	-0.663256
H	-1.983082	-0.875588	-0.481088	H	-1.950464	-0.854006	0.268639
H	-4.425627	-0.246633	2.319947	H	-1.184232	1.768444	3.088262
H	-3.236729	-1.356045	1.472663	H	-0.460075	1.708231	1.409271
H	-4.880761	-1.031962	0.750369	H	-0.739006	0.163165	2.347975
H	0.360785	-2.169254	-2.865461	H	0.914558	-1.690996	-2.399065
H	0.081414	-0.569165	-1.999178	H	0.526071	-0.034146	-1.740665
H	0.019179	-2.137158	-1.069971	H	0.173091	-1.519671	-0.735379
H	3.742205	-0.006514	-2.753362	H	2.999353	0.114076	1.303522
H	2.013557	0.605803	-2.767372	H	1.294505	-0.553794	1.254283
H	2.528654	-0.770001	-3.861488	H	1.703366	0.985698	0.356685

Li⁺(DMSO)₄

E (PBE-D3/ma-def2-svp GAS_OPT) =				-2217.9389799558			
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E (PBE-D3/ma-def2-svp SMD_OPT) =	-2218.0043019898
ΔG_{corr} (ID-RR-HR GAS) =	0.2604922600
E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT GAS) =	-2217.6007728249
E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT SMD) =	-2217.6706320276
E (DLPNO-CCSDT/cc-p(wC)VTZ SMD_OPT SMD) =	-2217.6709004169
E (PBE-D3/ma-def2-tzvp GAS_OPT GAS) =	-2219.2348444772
E (PBE-D3/ma-def2-tzvp GAS_OPT SMD) =	-2219.2999010173
E (PBE-D3/ma-def2-tzvp GAS_OPT CPCM) =	-2219.3023047522
GAS_OPT	SMD_OPT
C -0.102864 -0.356594 3.983529	C 2.388730 -0.516397 2.052990
S 0.037110 -1.771327 2.840896	S 0.894166 -1.383555 2.617160
O -0.734397 -1.342315 1.554991	O -0.314422 -0.676567 1.927628
C 1.804625 -1.590371 2.430926	C 1.150528 -2.930892 1.699594
Li -0.206549 0.040837 0.292299	Li -0.254858 0.162208 0.168586
O 0.682747 1.391380 1.381133	O 0.557451 1.923020 0.270706
S 1.427548 2.652608 0.848088	S 1.200841 2.449466 -1.048450
C 2.962648 2.022405 0.089222	C 1.525999 4.208678 -0.747266
C 0.563764 3.118501 -0.688903	C 2.917592 1.856892 -1.044661
O -1.779948 0.387575 -0.812313	O -2.078613 0.181981 -0.543547
S -3.253145 -0.059004 -0.562551	S -3.347612 0.364207 0.349736
C -3.197195 -1.876864 -0.427057	C -3.509305 -1.181437 1.291367
C -3.587689 0.316219 1.189578	C -2.850532 1.447412 1.721177
O 1.057425 -0.308262 -1.178073	O 0.932598 -0.803545 -1.071083
S 0.445042 -1.130120 -2.353922	S 0.474795 -1.586882 -2.344523
C -0.130010 0.097995 -3.568838	C -0.895134 -2.652311 -1.805586
C 1.885469 -1.767772 -3.266852	C -0.487744 -0.406952 -3.334264
H -1.156172 -0.321954 4.319324	H 2.335373 0.516053 2.444607
H 0.174164 0.563552 3.430147	H 2.420891 -0.525413 0.947283
H 0.557351 -0.535534 4.854649	H 3.268057 -1.037391 2.481490
H 2.023002 -2.331346 1.639882	H 0.253779 -3.558580 1.861530
H 2.404203 -1.815195 3.334559	H 2.043950 -3.439988 2.112640
H 1.975163 -0.558752 2.067293	H 1.285254 -2.688485 0.628223
H 3.611403 1.681631 0.917797	H 0.543816 4.711004 -0.660899
H 3.459682 2.850445 -0.453104	H 2.081216 4.617207 -1.614646
H 2.694925 1.181550 -0.582211	H 2.108002 4.323429 0.187957
H -0.461719 3.414161 -0.400372	H 2.863548 0.762643 -1.196518
H 0.540399 2.241805 -1.363192	H 3.395269 2.106725 -0.077051
H 1.091563 3.978145 -1.146262	H 3.457333 2.333462 -1.887025
H -2.941157 -2.260770 -1.432088	H -3.813966 -1.971063 0.578423
H -4.201058 -2.241544 -0.133503	H -4.299421 -1.046251 2.056328
H -2.420488 -2.148615 0.316129	H -2.528468 -1.411147 1.753629

H	-3.562788	1.417369	1.288129	H	-2.617998	2.436788	1.284597
H	-2.797450	-0.161692	1.800506	H	-1.966479	1.013989	2.228871
H	-4.596107	-0.061292	1.448819	H	-3.709086	1.538332	2.415975
H	-0.958561	0.632406	-3.066301	H	-1.639278	-2.026188	-1.275429
H	-0.498431	-0.431940	-4.469236	H	-0.469643	-3.424674	-1.137465
H	0.700594	0.784227	-3.824097	H	-1.335350	-3.136241	-2.699780
H	2.379323	-2.508771	-2.611378	H	-0.933161	-0.952704	-4.189807
H	2.574280	-0.931551	-3.493922	H	0.220483	0.355271	-3.710033
H	1.533301	-2.261231	-4.193724	H	-1.268601	0.047894	-2.692465

(DMSO)₅

E (PBE-D3/ma-def2-svp GAS_OPT) =	-2763.1237470859
E (PBE-D3/ma-def2-svp SMD_OPT) =	-2763.1446869000
ΔG_{corr} (ID-RR-HR GAS) =	0.3273942900
E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT GAS) =	-2762.6763640437
E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT SMD) =	-2762.7018418562
E (DLPNO-CCSDT/cc-p(wC)VTZ SMD_OPT SMD) =	-2762.6999660541
E (PBE-D3/ma-def2-tzvp GAS_OPT GAS) =	-2764.7459011055
E (PBE-D3/ma-def2-tzvp GAS_OPT SMD) =	-2764.7641728541
E (PBE-D3/ma-def2-tzvp GAS_OPT CPCM) =	-2764.7765645039
GAS_OPT	SMD_OPT
C -1.390951 -1.120271 1.981691	C -1.389612 -2.826849 3.610784
S 0.033071 -2.241648 2.180496	S -1.682443 -2.298527 1.890327
O 0.469992 -2.150403 3.661207	O -1.901084 -0.758493 1.956648
C -0.870217 -3.819116 1.991600	C 0.012826 -2.584846 1.280577
O -2.490386 2.455408 -1.099065	O 1.104104 2.790884 -2.888900
S -1.323047 1.911393 -0.243517	S 1.414298 2.999332 -1.385843
C 0.202464 2.705270 -0.854681	C 2.875531 1.975167 -1.014561
C -1.415733 2.789352 1.359280	C 2.222394 4.628376 -1.241302
O -0.338926 0.512665 -3.246904	O -2.371246 -1.169637 -2.669000
S -1.692202 0.080976 -3.867100	S -2.299195 -0.890783 -1.139910
C -2.744209 -0.527220 -2.501242	C -1.465671 0.718868 -0.952178
C -2.603428 1.628646 -4.208897	C -3.967011 -0.367623 -0.625532
O -0.636322 -2.450654 -0.910247	O 1.282204 -0.947991 -1.326888
S 0.898316 -2.449640 -1.120261	S 1.560315 -1.428534 -2.780863

C	1.155329	-2.560531	-2.932556	C	0.576613	-2.944797	-3.009156
C	1.463358	-0.724885	-0.935399	C	0.602425	-0.346521	-3.890023
H	-1.755828	-1.219347	0.941785	H	-1.154120	-3.910030	3.611568
H	-0.982386	-0.107918	2.150945	H	-2.325879	-2.647892	4.173006
H	-2.161730	-1.376538	2.734054	H	-0.547280	-2.233830	4.022662
H	-0.135565	-4.626620	2.168616	H	0.107413	-2.118577	0.279228
H	-1.247010	-3.853444	0.950482	H	0.155003	-3.682019	1.200337
H	-1.681772	-3.867694	2.743131	H	0.735948	-2.140545	1.993973
H	1.029662	2.396363	-0.185115	H	3.255257	2.230987	-0.005489
H	0.061678	3.803733	-0.865725	H	3.652448	2.170395	-1.780738
H	0.342366	2.307127	-1.878265	H	2.538170	0.918882	-1.049859
H	-1.453993	3.880356	1.173948	H	1.470100	5.389628	-1.523342
H	-0.527927	2.487911	1.949833	H	3.095458	4.674105	-1.921776
H	-2.346873	2.453104	1.852440	H	2.531167	4.782018	-0.187943
H	-2.137288	-1.293435	-1.973248	H	-0.390152	0.522229	-1.117975
H	-3.651118	-0.981593	-2.948312	H	-1.643159	1.088828	0.074057
H	-2.999252	0.321209	-1.835364	H	-1.873922	1.416898	-1.709132
H	-2.058511	2.149011	-5.018458	H	-4.645381	-1.224593	-0.800895
H	-2.619871	2.223279	-3.271203	H	-4.288869	0.509361	-1.220862
H	-3.627292	1.368771	-4.543919	H	-3.921926	-0.133507	0.455875
H	0.690227	-3.508946	-3.259677	H	0.982953	-3.707082	-2.317246
H	2.244833	-2.584495	-3.133112	H	0.700215	-3.288143	-4.055859
H	0.680878	-1.682145	-3.414092	H	-0.486914	-2.717855	-2.789918
H	1.333195	-0.428809	0.123279	H	0.934058	0.693902	-3.688821
H	0.854089	-0.099947	-1.618620	H	-0.480003	-0.463372	-3.675300
H	2.537598	-0.688943	-1.208684	H	0.839213	-0.633739	-4.934534
O	1.247453	0.985137	1.909645	O	1.451251	-0.920980	3.819272
S	2.115605	1.096518	3.185221	S	1.327495	0.611283	3.599708
C	3.067677	-0.451238	3.318177	C	0.935127	0.860575	1.834538
C	3.501726	2.206332	2.727680	C	-0.305954	1.097795	4.249925
H	2.314679	-1.240366	3.546665	H	1.779730	0.451024	1.252450
H	3.790816	-0.346988	4.151107	H	0.832662	1.948785	1.653827
H	3.583708	-0.644909	2.357241	H	-0.006556	0.325102	1.606771
H	3.068031	3.209085	2.554577	H	-0.289359	0.918923	5.342047
H	3.974118	1.827823	1.800127	H	-1.081840	0.485409	3.745689
H	4.230968	2.248268	3.560435	H	-0.456802	2.178011	4.050574

Li⁺(DMSO)₅

E (PBE-D3/ma-def2-svp GAS_OPT) =	-2770.5697690941
E (PBE-D3/ma-def2-svp SMD_OPT) =	-2770.6362333428
ΔG_{corr} (ID-RR-HR GAS) =	0.3299401700
E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT GAS) =	-2770.1414439347
E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT SMD) =	-2770.2126210677

E (DLPNO-CCSDT/cc-p(wC)VTZ SMD_OPT SMD) =	-2770.2139010531
E (PBE-D3/ma-def2-tzvp GAS_OPT GAS) =	-2772.1895074900
E (PBE-D3/ma-def2-tzvp GAS_OPT SMD) =	-2772.2538942960
E (PBE-D3/ma-def2-tzvp GAS_OPT CPCM) =	-2772.2591981931
GAS_OPT	SMD_OPT
C 0.841570 -1.739482 3.191864	C 0.697496 -1.735772 3.167676
S 0.975921 -2.003701 1.395327	S 0.798793 -1.933021 1.364286
O -0.238687 -1.254120 0.764477	O -0.364849 -1.074326 0.775622
C 2.432198 -0.950708 1.098988	C 2.319999 -0.978079 1.096785
Li -0.240924 -0.054020 -0.774670	Li -0.352665 0.095649 -0.793027
O -0.367350 1.778972 -0.251705	O -0.370496 1.953198 -0.282541
S 0.465307 3.020117 -0.672761	S 0.605204 3.095218 -0.690999
C 2.207396 2.577306 -0.362208	C 2.283225 2.488519 -0.340202
C 0.514717 2.972039 -2.496824	C 0.698890 3.038962 -2.506330
O -1.837754 -0.659321 -1.742909	O -1.945658 -0.518377 -1.751138
S -3.128571 -0.601359 -0.876119	S -3.188753 -0.763061 -0.839383
C -4.499979 -0.754620 -2.063220	C -4.606244 -0.803633 -1.969953
C -3.254249 -2.237080 -0.083317	C -3.150436 -2.523095 -0.396123
O 1.299590 -0.348365 -1.969448	O 1.179083 -0.271620 -1.968338
S 1.181998 -1.230223 -3.251159	S 1.001097 -1.253085 -3.172987
C 2.860707 -1.883968 -3.518844	C 2.686629 -1.739483 -3.629054
C 0.363144 -2.767478 -2.721762	C 0.446592 -2.827297 -2.460083
H -0.110680 -2.201695 3.512778	H -0.296378 -2.107989 3.481574
H 0.869581 -0.647106 3.387871	H 0.840779 -0.666767 3.425883
H 1.691407 -2.259534 3.676646	H 1.490067 -2.365355 3.619434
H 2.539870 -0.882700 -0.000414	H 2.445271 -0.890161 0.000778
H 3.314266 -1.444331 1.552672	H 3.164173 -1.545246 1.537879
H 2.236545 0.042000 1.554144	H 2.200889 0.012499 1.581339
H 2.292255 2.401962 0.728510	H 2.350945 2.343986 0.755503
H 2.850055 3.425597 -0.669684	H 3.007057 3.262195 -0.665657
H 2.447662 1.656340 -0.927553	H 2.445796 1.536009 -0.880049
H -0.516020 3.163452 -2.848449	H -0.294958 3.334337 -2.892876
H 0.857444 1.965898 -2.806601	H 0.953584 2.004864 -2.810846
H 1.192033 3.769873 -2.859336	H 1.464941 3.764160 -2.845338
H -4.513335 0.176503 -2.659414	H -4.733920 0.219625 -2.371101
H -5.449523 -0.859246 -1.502816	H -5.506908 -1.097277 -1.395511
H -4.318500 -1.629921 -2.716200	H -4.404842 -1.522525 -2.787991
H -2.344376 -2.312602 0.543697	H -2.246023 -2.654707 0.226898
H -3.268086 -3.028117 -0.857830	H -3.106761 -3.143859 -1.312215
H -4.170068 -2.268399 0.539065	H -4.059141 -2.756887 0.193528
H 3.504206 -1.021893 -3.775130	H 3.188139 -0.838234 -4.029573
H 2.834109 -2.597289 -4.365696	H 2.626043 -2.516710 -4.416248
H 3.218434 -2.374310 -2.593121	H 3.219218 -2.119173 -2.735553
H -0.654888 -2.457042 -2.413115	H -0.560790 -2.636048 -2.046467
H 0.917272 -3.209749 -1.871291	H 1.152215 -3.156732 -1.673208
H 0.321266 -3.462348 -3.583295	H 0.388445 -3.577305 -3.273695
O 1.286791 1.445219 2.818747	O 1.455244 1.527354 3.048650

S	0.106939	2.444440	2.750176	S	0.246973	2.482440	2.833982
C	-1.422585	1.447849	2.773500	C	-1.244378	1.442854	2.803681
C	-0.031358	3.160092	4.427158	C	-0.046953	3.294211	4.438669
H	-1.372472	0.811345	1.871810	H	-1.109441	0.729065	1.968410
H	-2.291946	2.131825	2.716624	H	-2.118847	2.096268	2.612557
H	-1.454496	0.834515	3.694729	H	-1.355491	0.910271	3.768891
H	0.868996	3.782643	4.583719	H	0.812321	3.965122	4.629193
H	-0.065093	2.342139	5.172585	H	-0.126367	2.528574	5.235550
H	-0.940741	3.790597	4.479802	H	-0.978812	3.890442	4.369719

GBL

E (PBE-D3/ma-def2-svp GAS_OPT) =	-305.9341008593
E (PBE-D3/ma-def2-svp SMD_OPT) =	-305.9486384456
ΔG_{corr} (ID-RR-HR GAS) =	0.0668101500
E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT GAS) =	-306.0344394527
E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT SMD) =	-306.0458051277
E (DLPNO-CCSDT/cc-p(wC)VTZ SMD_OPT SMD) =	-306.0461809580
E (PBE-D3/ma-def2-tzvp GAS_OPT GAS) =	-306.2674665634
E (PBE-D3/ma-def2-tzvp GAS_OPT SMD) =	-306.2811441284
E (PBE-D3/ma-def2-tzvp GAS_OPT CPCM) =	-306.2807123831
GAS_OPT	SMD_OPT
H -2.725680 2.401573 -3.602773	H -2.712566 2.398510 -3.602011
O -2.517059 1.120890 -1.975517	O -2.509953 1.114986 -1.971470
C -1.308842 0.469849 -1.976147	C -1.312279 0.468511 -1.985121
C -0.910106 0.172376 -3.420933	C -0.912386 0.173256 -3.419704
C -2.220412 0.333535 -4.195185	C -2.223716 0.329671 -4.193334
C -2.972808 1.352534 -3.326062	C -2.972200 1.352009 -3.334970
H -0.431468 -0.822065 -3.490265	H -0.428334 -0.818290 -3.495476
H -0.148195 0.926239 -3.717111	H -0.159385 0.938065 -3.712539
H -2.773410 -0.627858 -4.221589	H -2.776254 -0.631710 -4.214566
H -2.094035 0.681014 -5.238651	H -2.093376 0.678963 -5.234805
H -4.073545 1.236111 -3.335590	H -4.072540 1.240803 -3.338136
O -0.709643 0.217045 -0.957577	O -0.712216 0.216468 -0.955268

(GBL)₄

E (PBE-D3/ma-def2-svp GAS_OPT) =	-1223.7876355697
E (PBE-D3/ma-def2-svp SMD_OPT) =	-1223.8156291751
ΔG_{corr} (ID-RR-HR GAS) =	0.3308218000
E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT GAS) =	-1224.1903764430
E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT SMD) =	-1224.2093733705
E (DLPNO-CCSDT/cc-p(wC)VTZ SMD_OPT SMD) =	-1224.2099022556
E (PBE-D3/ma-def2-tzvp GAS_OPT GAS) =	-1225.1119689620
E (PBE-D3/ma-def2-tzvp GAS_OPT SMD) =	-1225.1359956994
E (PBE-D3/ma-def2-tzvp GAS_OPT CPCM) =	-1225.1357680619
GAS_OPT	SMD_OPT
H 4.469547 -1.147477 -5.337321	H 0.256106 -1.510246 -2.207474
O 3.225282 0.466029 -4.949796	O -0.424651 0.432128 -1.893286
C 1.930577 0.078235 -4.774771	C -1.780349 0.499398 -1.990725
C 1.606646 -1.062032 -5.724947	C -2.262209 -0.442231 -3.077479
C 2.763430 -1.039830 -6.730173	C -0.988588 -0.762619 -3.864678
C 3.890108 -0.394159 -5.908808	C 0.095326 -0.585631 -2.798554
H 0.600259 -0.921960 -6.163037	H -3.077081 0.023297 -3.662753
H 1.592485 -2.002254 -5.129223	H -2.678914 -1.337627 -2.568761
H 2.513005 -0.409248 -7.608100	H -0.844115 -0.029531 -4.683884
H 3.045906 -2.044003 -7.099331	H -0.975109 -1.778486 -4.302011
H 4.582089 0.237725 -6.496999	H 1.064613 -0.221717 -3.186038
O 1.209557 0.618019 -3.957172	O -2.434266 1.236002 -1.271652
H 3.461568 2.257388 -3.241162	H -1.998867 -0.285573 1.097176
O 4.476271 1.511953 -1.599204	O -1.445226 -1.879969 -0.110344
C 4.118041 1.326119 -0.289336	C -1.252876 -3.208319 0.124479
C 2.971779 2.266168 0.055294	C -1.018587 -3.433878 1.605022
C 2.450459 2.715355 -1.312474	C -1.486347 -2.125301 2.249191
C 3.689351 2.568867 -2.205591	C -1.271554 -1.116807 1.116721
H 3.391785 3.101371 0.657716	H 0.072432 -3.597255 1.749949
H 2.229375 1.733270 0.676769	H -1.545770 -4.344632 1.945490
H 2.044307 3.745171 -1.325833	H -0.923742 -1.849288 3.160422
H 1.660488 2.022097 -1.660175	H -2.562425 -2.181267 2.510396
H 4.316735 3.487321 -2.223983	H -0.246374 -0.697393 1.111355
O 4.684543 0.515836 0.412995	O -1.277991 -4.021941 -0.782282
H 4.459656 -0.757699 -2.132949	H 1.697906 -0.131953 -0.393608
O 3.501521 -2.239490 -3.236496	O 2.153454 -2.000740 0.417825

C	2.671856	-3.262503	-2.890472	C	2.477363	-1.916746	1.738591
C	2.909667	-3.632502	-1.436273	C	3.187425	-0.605352	2.004534
C	3.613106	-2.393976	-0.873108	C	3.654321	-0.169731	0.613841
C	4.342929	-1.855236	-2.107178	C	2.581929	-0.792511	-0.281878
H	3.558224	-4.536965	-1.423817	H	3.984696	-0.735613	2.759448
H	1.952318	-3.893048	-0.950541	H	2.428464	0.095462	2.422190
H	4.307447	-2.596754	-0.036910	H	4.648653	-0.602662	0.383047
H	2.864784	-1.655816	-0.522550	H	3.707653	0.926868	0.485141
H	5.336957	-2.330283	-2.256514	H	2.938399	-1.097918	-1.282877
O	1.896094	-3.747881	-3.695404	O	2.185575	-2.806319	2.520115
H	-1.603952	-2.953746	-1.841553	H	0.830581	2.521116	-1.018107
O	0.203389	-1.962702	-1.583199	O	1.375200	2.280265	0.977509
C	0.068998	-0.653003	-1.222753	C	0.290047	2.111988	1.781353
C	-1.158049	-0.065327	-1.903632	C	-0.866577	2.931945	1.249303
C	-1.478698	-1.075753	-3.008716	C	-0.184392	3.945453	0.325875
C	-0.877865	-2.377102	-2.455046	C	1.046172	3.162385	-0.138773
H	-0.929844	0.954584	-2.263212	H	-1.461477	3.360194	2.077162
H	-1.961258	0.012217	-1.138629	H	-1.521489	2.242860	0.669167
H	-0.954205	-0.777472	-3.936690	H	0.123728	4.846913	0.894097
H	-2.558473	-1.175707	-3.230321	H	-0.813160	4.268474	-0.525049
H	-0.439293	-3.047471	-3.218185	H	1.938158	3.782533	-0.344717
O	0.844704	-0.122092	-0.454981	O	0.333053	1.377363	2.755065

Li⁺(GBL)₄

E (PBE-D3/ma-def2-svp GAS_OPT) =	-1231.2078200895
E (PBE-D3/ma-def2-svp SMD_OPT) =	-1231.2862310505
ΔG_{corr} (ID-RR-HR GAS) =	0.3317891600
E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT GAS) =	-1231.6269968141
E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT SMD) =	-1231.6957099730
E (DLPNO-CCSDT/cc-p(wC)VTZ SMD_OPT SMD) =	-1231.7004768049
E (PBE-D3/ma-def2-tzvp GAS_OPT GAS) =	-1232.5379505069
E (PBE-D3/ma-def2-tzvp GAS_OPT SMD) =	-1232.6107488153
E (PBE-D3/ma-def2-tzvp GAS_OPT CPCM) =	-1232.6044998883
GAS_OPT	SMD_OPT
Li 0.065712 0.062281 -0.015773	Li -0.998779 -0.587634 0.922876

H	-2.905424	1.313678	-5.095172	H	1.525493	2.124070	-2.401805
O	-2.321913	0.289051	-3.387486	O	-0.170806	1.159491	-1.669279
C	-1.175490	0.255122	-2.688332	C	-0.099860	-0.178065	-1.811491
C	-0.010309	0.687164	-3.555753	C	0.616229	-0.534629	-3.091889
C	-0.695907	1.364670	-4.748744	C	0.592180	0.775609	-3.885781
C	-2.065135	0.672107	-4.772530	C	0.523433	1.823897	-2.773254
H	0.547841	-0.230706	-3.844781	H	0.133820	-1.399990	-3.583081
H	0.681938	1.321777	-2.970143	H	1.647129	-0.847370	-2.814009
H	-0.151970	1.248056	-5.704574	H	-0.317748	0.826865	-4.516548
H	-0.815696	2.450118	-4.557807	H	1.475520	0.920363	-4.534571
H	-2.069628	-0.258196	-5.378511	H	-0.053572	2.732070	-3.025252
O	-1.165977	-0.094206	-1.512599	O	-0.568739	-0.934226	-0.965970
H	4.408109	3.870767	-0.011139	H	3.691051	0.835254	-1.021851
O	3.089552	2.672187	-1.084343	O	2.140746	0.349721	0.280360
C	2.432963	1.794569	-0.308097	C	1.440836	1.069037	1.181452
C	3.328769	1.297177	0.808458	C	2.226807	2.287304	1.603021
C	4.730743	1.704966	0.338807	C	3.286955	2.416619	0.504505
C	4.433077	2.908900	-0.565143	C	3.450046	0.965628	0.049064
H	3.167536	0.213792	0.967141	H	2.675315	2.057409	2.594800
H	3.018619	1.817800	1.741284	H	1.560770	3.160331	1.732917
H	5.192566	0.886105	-0.248698	H	4.242252	2.848513	0.855307
H	5.422865	1.961729	1.162283	H	2.908323	3.045028	-0.327094
H	5.105846	3.014490	-1.435794	H	4.188871	0.405669	0.658315
O	1.266267	1.497166	-0.542487	O	0.332482	0.708706	1.563577
H	2.030669	-3.452349	3.830486	H	1.320563	-5.657590	3.234423
O	2.291928	-2.851618	1.856540	O	0.046781	-4.036065	2.955927
C	1.190712	-2.297500	1.322886	C	0.173048	-2.881986	2.279786
C	-0.054808	-2.971789	1.862451	C	1.633819	-2.544652	2.079137
C	0.484768	-4.272167	2.470199	C	2.338422	-3.877289	2.350627
C	1.930933	-3.890847	2.815372	C	1.368187	-4.556691	3.318391
H	-0.810407	-3.094524	1.063975	H	1.894572	-1.768816	2.832618
H	-0.494205	-2.281929	2.616231	H	1.806279	-2.104423	1.080119
H	0.470213	-5.087075	1.718744	H	3.348126	-3.767308	2.787532
H	-0.077887	-4.619427	3.356723	H	2.423636	-4.465129	1.414587
H	2.666148	-4.708705	2.703808	H	1.551874	-4.277178	4.376628
O	1.274915	-1.364418	0.532159	O	-0.818044	-2.248007	1.927989
H	-4.317348	1.382687	3.536380	H	-5.211888	3.090270	0.049304
O	-2.890706	0.017827	2.880935	O	-4.686317	1.309942	0.995599
C	-2.301660	0.393169	1.732323	C	-3.588396	0.757955	0.452060
C	-3.297668	1.093020	0.828932	C	-3.559301	1.000319	-1.040484
C	-4.651507	0.721855	1.446486	C	-5.004029	1.398817	-1.356820
C	-4.279690	0.464666	2.913019	C	-5.460762	2.011809	-0.032111
H	-3.142381	0.776967	-0.220225	H	-3.180852	0.110868	-1.576632
H	-3.085367	2.183721	0.880681	H	-2.839902	1.828630	-1.221218
H	-5.046253	-0.203328	0.980360	H	-5.608346	0.500342	-1.594776
H	-5.422905	1.507516	1.342628	H	-5.095757	2.113444	-2.195482
H	-4.867395	-0.329117	3.409364	H	-6.529956	1.864476	0.205945
O	-1.115054	0.162802	1.529475	O	-2.770509	0.168590	1.152533

Li⁺ in GBL

E (PBE-D3/ma-def2-svp GAS_OPT) =	-7.2519251623
E (PBE-D3/ma-def2-svp SMD_OPT) =	-7.3917970144
ΔG_{corr} (ID-RR-HR GAS) =	-0.0127326619
E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT GAS) =	-7.2736440090
E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT SMD) =	-7.4155086302
E (DLPNO-CCSDT/cc-p(wC)VTZ SMD_OPT SMD) =	-7.4155086302
E (PBE-D3/ma-def2-tzvp GAS_OPT GAS) =	-7.2566456293
E (PBE-D3/ma-def2-tzvp GAS_OPT SMD) =	-7.3963522720
E (PBE-D3/ma-def2-tzvp GAS_OPT CPCM) =	-7.4405651965
GAS_OPT	SMD_OPT
Li 0.0 0.0 0.0	Li 0.0 0.0 0.0

(GBL)₅

E (PBE-D3/ma-def2-svp GAS_OPT) =	-1529.7430284144
E (PBE-D3/ma-def2-svp SMD_OPT) =	-1529.7745740099
ΔG_{corr} (ID-RR-HR GAS) =	0.4203686600
E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT GAS) =	-1530.2478813412
E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT SMD) =	-1530.2681033191
E (DLPNO-CCSDT/cc-p(wC)VTZ SMD_OPT SMD) =	-1530.2675148320
E (PBE-D3/ma-def2-tzvp GAS_OPT GAS) =	-1531.3964538869
E (PBE-D3/ma-def2-tzvp GAS_OPT SMD) =	-1531.4224945321

E (PBE-D3/ma-def2-tzvp GAS_OPT CPCM) =				-1531.4220642321			
GAS_OPT				SMD_OPT			
H	2.298686	3.180896	-2.311891	H	6.848510	-0.640796	2.825646
O	1.395273	4.445993	-0.934236	O	7.391079	-0.651238	0.822187
C	0.351023	5.143082	-1.467231	C	7.577789	0.338421	-0.096167
C	0.671441	5.509010	-2.909932	C	6.827474	1.581251	0.339657
C	2.179069	5.263995	-3.026673	C	6.539294	1.325506	1.821904
C	2.423100	4.214469	-1.931043	C	6.490353	-0.204597	1.876451
H	0.339952	6.542271	-3.125216	H	5.902166	1.616077	-0.277816
H	0.097649	4.814112	-3.556599	H	7.416373	2.491129	0.119783
H	2.745955	6.192938	-2.810004	H	5.600660	1.784651	2.184383
H	2.489314	4.894621	-4.022300	H	7.370203	1.704241	2.450711
H	3.401990	4.309276	-1.422836	H	5.482972	-0.608786	1.650129
O	-0.650039	5.393015	-0.826438	O	8.253765	0.155186	-1.093104
H	-2.962417	4.357798	-0.958686	H	1.269082	2.606911	-2.745792
O	-4.351486	3.111753	-1.890594	O	2.808722	1.952423	-1.507656
C	-3.831617	2.559030	-3.024056	C	3.347902	0.775708	-1.925573
C	-2.960899	3.579808	-3.735087	C	2.258572	-0.121303	-2.481022
C	-3.320641	4.907299	-3.059543	C	0.957989	0.544130	-2.022657
C	-3.800485	4.443107	-1.679051	C	1.386351	2.001897	-1.822327
H	-3.137885	3.536887	-4.826469	H	2.403328	-1.160768	-2.131083
H	-1.902668	3.281234	-3.567766	H	2.366417	-0.124957	-3.587246
H	-4.138185	5.418063	-3.608846	H	0.606852	0.106133	-1.067924
H	-2.471163	5.609083	-2.966512	H	0.132330	0.457614	-2.753013
H	-4.603349	5.064489	-1.239293	H	0.876719	2.522586	-0.990183
O	-4.060883	1.404309	-3.333188	O	4.546639	0.567088	-1.855108
H	1.399086	-0.848209	-1.392802	H	4.968477	-1.493901	-0.563762
O	1.275630	0.801687	-2.649553	O	5.329710	-3.116328	0.703014
C	0.257722	1.290866	-3.409900	C	6.586906	-3.610658	0.549321
C	-0.724384	0.179444	-3.732686	C	7.000036	-3.506953	-0.906735
C	-0.349534	-0.930469	-2.747293	C	5.672736	-3.284287	-1.638515
C	1.123093	-0.629819	-2.440765	C	4.829547	-2.592567	-0.564355
H	-0.555862	-0.111400	-4.793072	H	7.570712	-4.402308	-1.216200
H	-1.766645	0.543900	-3.655137	H	7.674459	-2.626851	-0.987473
H	-0.493960	-1.953578	-3.143333	H	5.217758	-4.255353	-1.921938
H	-0.938511	-0.831722	-1.816912	H	5.763522	-2.665343	-2.550988
H	1.824818	-1.143488	-3.133265	H	3.746748	-2.808910	-0.599387
O	0.238033	2.456101	-3.763383	O	7.215342	-4.052961	1.496607
H	0.094689	1.900629	3.674530	H	3.128877	1.522880	1.201661
O	-0.729467	0.693696	2.198295	O	2.724068	-0.485850	0.885009
C	0.147043	0.357965	1.205235	C	1.605575	-1.244091	1.039777
C	1.078732	1.527172	0.930444	C	0.653699	-0.560596	2.004321
C	0.404375	2.710862	1.630276	C	1.190194	0.871675	2.089442
C	-0.442665	2.022225	2.708731	C	2.674147	0.681165	1.755694
H	1.203468	1.655053	-0.160588	H	0.732571	-1.098450	2.972926
H	2.073066	1.271704	1.358094	H	-0.390604	-0.655323	1.652496
H	-0.241615	3.254452	0.915997	H	1.048503	1.343353	3.079764
H	1.117150	3.440673	2.057458	H	0.699782	1.517487	1.332977
H	-1.412370	2.520504	2.895256	H	3.279944	0.453845	2.657007
O	0.116110	-0.737905	0.679476	O	1.466299	-2.302811	0.450740
H	-5.053367	2.236646	0.767106	H	3.279736	-3.682060	2.183957
O	-2.984364	2.344270	0.685377	O	3.096760	-2.207867	3.640689

C	-2.477807	1.494653	-0.254214	C	4.303430	-1.870112	4.170106
C	-3.266802	0.199844	-0.256406	C	5.185017	-3.099800	4.254082
C	-4.085280	0.267522	1.036451	C	4.195093	-4.259394	4.106108
C	-4.178917	1.781111	1.278816	C	3.081366	-3.620211	3.272134
H	-2.572228	-0.658772	-0.315686	H	5.773533	-3.092804	5.190594
H	-3.888976	0.207335	-1.178171	H	5.900461	-3.066663	3.402495
H	-3.532013	-0.219612	1.863687	H	3.806232	-4.569183	5.097300
H	-5.084142	-0.201896	0.958539	H	4.623190	-5.149208	3.607437
H	-4.189998	2.072332	2.346573	H	2.066655	-4.005440	3.483842
O	-1.535249	1.813116	-0.954091	O	4.552050	-0.720670	4.496150

Li⁺(GBL)₅

E (PBE-D3/ma-def2-svp GAS_OPT) =	-1537.1706459253
E (PBE-D3/ma-def2-svp SMD_OPT) =	-1537.2464714381
ΔG_{corr} (ID-RR-HR GAS) =	0.4226732600
E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT GAS) =	-1537.6926577839
E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT SMD) =	-1537.7601866618
E (DLPNO-CCSDT/cc-p(wC)VTZ SMD_OPT SMD) =	-1537.7609915785
E (PBE-D3/ma-def2-tzvp GAS_OPT GAS) =	-1538.8281023429
E (PBE-D3/ma-def2-tzvp GAS_OPT SMD) =	-1538.9006650168
E (PBE-D3/ma-def2-tzvp GAS_OPT CPCM) =	-1538.8937010835
GAS_OPT	SMD_OPT
H -1.740329 -1.290490 2.381078	H -3.222373 0.021759 0.783693
O -0.956591 -0.209309 0.785488	O -1.877761 0.502937 -0.732521
C -0.393220 -0.990888 -0.159661	C -1.432654 -0.580076 -1.393814
C 0.265537 -2.194905 0.481204	C -1.302594 -1.755784 -0.454437
C 0.376385 -1.792151 1.955475	C -1.324778 -1.102431 0.931035
C -0.783513 -0.798339 2.106864	C -2.129203 0.173557 0.672649
H 1.223268 -2.418374 -0.023663	H -0.395658 -2.341970 -0.687122
H -0.402487 -3.067241 0.310353	H -2.184783 -2.410683 -0.627955
H 1.343624 -1.283754 2.140203	H -0.295880 -0.853449 1.259573
H 0.295353 -2.639518 2.661629	H -1.790426 -1.731243 1.711913
H -0.593336 0.030194 2.814060	H -1.823782 1.048507 1.275360
O -0.466100 -0.698514 -1.345068	O -1.209547 -0.526177 -2.600451
Li 0.609044 -1.459391 -2.819094	Li 0.005681 -1.538655 -3.755292

H	0.948907	3.076118	-6.582870	H	0.335012	2.158165	-8.447954
O	0.225936	1.291047	-5.814569	O	0.420127	0.421562	-7.304473
C	0.826578	0.286040	-5.152626	C	0.163159	0.169324	-6.010541
C	2.296613	0.224596	-5.512146	C	0.242558	1.437734	-5.193662
C	2.566615	1.612075	-6.102012	C	0.194811	2.543646	-6.253086
C	1.186098	1.998230	-6.651925	C	0.766817	1.834868	-7.483393
H	2.421317	-0.590425	-6.259273	H	1.199189	1.420863	-4.624999
H	2.891195	-0.049641	-4.622179	H	-0.575452	1.458073	-4.450944
H	3.346584	1.625050	-6.886151	H	0.781153	3.442918	-5.987185
H	2.862610	2.310626	-5.295507	H	-0.852663	2.853791	-6.440017
H	1.025714	1.662714	-7.698290	H	1.873461	1.895580	-7.539648
O	0.192077	-0.446653	-4.403824	O	-0.087226	-0.970539	-5.625228
H	3.839806	0.598124	1.137508	H	2.485757	-1.613560	0.607510
O	2.464984	0.106981	-0.341979	O	1.715665	-0.604480	-1.044001
C	2.984380	-0.184623	-1.551636	C	2.397475	-0.898840	-2.170400
C	4.254406	0.605367	-1.779002	C	3.867696	-1.059482	-1.868134
C	4.160090	1.732766	-0.745544	C	4.016345	-0.442615	-0.474132
C	3.266832	1.116850	0.340394	C	2.614746	-0.630058	0.109950
H	4.312194	0.943794	-2.829388	H	4.482163	-0.598579	-2.663536
H	5.111422	-0.080732	-1.598787	H	4.082971	-2.150929	-1.876158
H	3.652467	2.606637	-1.195600	H	4.252820	0.636301	-0.553412
H	5.139145	2.055731	-0.345554	H	4.789293	-0.929227	0.148406
H	2.559308	1.833263	0.796084	H	2.294895	0.170780	0.799871
O	2.458995	-1.011178	-2.287918	O	1.826214	-1.028998	-3.246878
H	-2.577961	-5.914950	-1.217665	H	1.792106	-4.687200	0.049606
O	-0.996858	-4.649638	-1.677419	O	1.195860	-3.838596	-1.754077
C	-0.332661	-4.393589	-2.826545	C	0.384328	-4.265960	-2.742184
C	-0.468519	-5.564996	-3.778721	C	0.274766	-5.770315	-2.716993
C	-1.654816	-6.348816	-3.205782	C	0.779546	-6.133732	-1.316620
C	-1.594159	-5.981272	-1.717684	C	1.739261	-4.981886	-1.014279
H	0.484130	-6.138189	-3.737164	H	0.941918	-6.156071	-3.519669
H	-0.586488	-5.208514	-4.818943	H	-0.755071	-6.094887	-2.955381
H	-1.592657	-7.440797	-3.369558	H	1.284890	-7.115739	-1.266464
H	-2.604971	-5.992572	-3.652155	H	-0.059664	-6.135012	-0.592319
H	-0.936204	-6.658283	-1.132930	H	2.764527	-5.161754	-1.398185
O	0.278879	-3.350956	-2.993034	O	-0.144558	-3.473333	-3.516365
H	-0.563228	3.895517	0.210453	H	1.339491	3.513473	1.171897
O	0.692546	2.757124	-0.985797	O	2.176840	2.608419	-0.501893
C	0.632814	2.381158	-2.291151	C	1.823947	2.571942	-1.816500
C	-0.803667	2.425192	-2.772920	C	0.349908	2.902322	-1.955271
C	-1.512576	3.274148	-1.712882	C	-0.003468	3.541256	-0.610597
C	-0.643652	3.028769	-0.471862	C	1.009506	2.881061	0.327319
H	-1.162219	1.373576	-2.787649	H	-0.191740	1.945420	-2.113441
H	-0.860275	2.799415	-3.811223	H	0.174149	3.538354	-2.842343
H	-2.566647	2.984898	-1.543408	H	-1.046366	3.361131	-0.289829
H	-1.495060	4.346773	-1.993943	H	0.164748	4.636292	-0.644952
H	-0.967075	2.134535	0.098881	H	0.645308	1.912017	0.730120
O	1.637114	2.050806	-2.900123	O	2.634245	2.299620	-2.685320

(GBL)₆

E (PBE-D3/ma-def2-svp GAS_OPT) =	-1835.6931033583
E (PBE-D3/ma-def2-svp SMD_OPT) =	-1835.7295103332
Δ Gcorr (ID-RR-HR GAS) =	0.5088087400
E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT GAS) =	-1836.2969961829
E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT SMD) =	-1836.3220560268
E (DLPNO-CCSDT/cc-p(wC)VTZ SMD_OPT SMD) =	-1836.3220017422
E (PBE-D3/ma-def2-tzvp GAS_OPT GAS) =	-1837.6767032445
E (PBE-D3/ma-def2-tzvp GAS_OPT SMD) =	-1837.7092163747
E (PBE-D3/ma-def2-tzvp GAS_OPT CPCM) =	-1837.7084988048
GAS_OPT	SMD_OPT
H -3.354272 2.679582 1.062434	H 0.816153 4.599100 -0.920322
O -2.143059 4.358756 0.921705	O 1.322789 2.611066 -0.558821
C -0.875542 4.037714 0.561571	C 0.766788 1.758564 -1.459519
C -0.459490 2.739727 1.234288	C -0.599253 2.268970 -1.871497
C -1.529630 2.525647 2.310417	C -0.948340 3.279834 -0.776746
C -2.723228 3.299939 1.732407	C 0.437374 3.745499 -0.320170
H 0.582493 2.811624 1.598303	H -1.311377 1.433534 -1.993015
H -0.476283 1.950549 0.454675	H -0.480884 2.749006 -2.867644
H -1.207865 2.978577 3.270787	H -1.485623 2.774979 0.050960
H -1.771557 1.462013 2.502039	H -1.570123 4.124443 -1.127958
H -3.366985 3.783314 2.491334	H 0.507740 4.003423 0.752906
O -0.230488 4.735044 -0.204263	O 1.358126 0.761078 -1.840217
H -0.436036 2.128453 -2.349506	H -5.663039 0.185974 -0.508049
O -2.299482 2.277560 -1.469353	O -5.009959 -0.126396 -2.459201
C -3.565418 2.022252 -1.902893	C -4.100556 0.803173 -2.856143
C -3.593023 2.071481 -3.424898	C -4.440587 2.147015 -2.239811
C -2.113997 1.973350 -3.812654	C -5.893469 1.974638 -1.788267
C -1.419424 2.573942 -2.583540	C -5.972473 0.466043 -1.536022
H -4.052216 3.041571 -3.716186	H -4.258078 2.965314 -2.961070
H -4.243699 1.269486 -3.820760	H -3.751845 2.290988 -1.379849
H -1.856584 2.512705 -4.744261	H -6.587811 2.264962 -2.602635
H -1.809503 0.913877 -3.921965	H -6.154062 2.558047 -0.885400
H -1.315861 3.678662 -2.637983	H -6.958680 0.015269 -1.752608
O -4.475802 1.804790 -1.128723	O -3.171721 0.508799 -3.589784
H -0.057125 -1.468283 3.957944	H 2.532144 -2.194970 1.874808
O 0.781886 -2.167125 2.201831	O 3.860440 -2.950004 0.461886
C 0.588603 -3.315435 1.497548	C 3.576752 -2.559221 -0.810351
C 0.122523 -4.415061 2.438718	C 2.074576 -2.451921 -0.991007
C -0.331222 -3.654739 3.688229	C 1.511931 -3.229739 0.201955

C	0.494206	-2.361460	3.611706	C	2.633731	-3.096834	1.236666
H	0.991870	-5.082861	2.626484	H	1.778898	-2.836924	-1.985069
H	-0.662170	-5.020471	1.948889	H	1.817277	-1.369662	-0.978304
H	-0.160381	-4.202934	4.634298	H	1.363229	-4.294390	-0.068587
H	-1.406620	-3.404257	3.611800	H	0.555576	-2.837499	0.593231
H	1.466872	-2.433557	4.144644	H	2.758738	-3.979451	1.891434
O	0.800829	-3.372940	0.300950	O	4.461211	-2.340675	-1.620298
H	1.675443	-0.674869	0.601138	H	2.093772	0.312035	3.877744
O	0.529267	0.122802	-0.936506	O	0.232852	-0.618809	3.839773
C	0.496302	-0.683422	-2.031206	C	-0.206654	-0.822166	2.571889
C	1.836249	-1.379801	-2.187355	C	0.220978	0.333527	1.687211
C	2.775098	-0.545719	-1.309502	C	0.608473	1.427389	2.685516
C	1.817189	0.015889	-0.252533	C	1.024809	0.608079	3.911052
H	2.111353	-1.457174	-3.255609	H	-0.596364	0.591482	0.989204
H	1.703638	-2.407020	-1.785100	H	1.096901	-0.000213	1.092296
H	3.226375	0.285206	-1.889949	H	-0.266892	2.065235	2.924624
H	3.594040	-1.132442	-0.851934	H	1.428544	2.077184	2.329284
H	2.090400	1.023829	0.108258	H	0.802435	1.087871	4.882173
O	-0.501932	-0.780093	-2.723651	O	-0.839924	-1.820198	2.267760
H	0.907587	4.562802	-2.482502	H	4.174080	2.049352	0.443827
O	2.288793	3.273807	-1.626378	O	3.595583	0.264526	1.342913
C	2.750094	3.785412	-0.445934	C	4.545148	-0.209817	2.193912
C	2.906000	5.291986	-0.571348	C	5.923570	0.093158	1.639226
C	2.836063	5.538769	-2.081645	C	5.655161	0.434721	0.170885
C	1.992772	4.346279	-2.554484	C	4.218775	0.963000	0.221760
H	3.835274	5.626746	-0.073926	H	6.608242	-0.757798	1.814078
H	2.042033	5.740297	-0.038081	H	6.320024	0.961554	2.210238
H	3.848834	5.501960	-2.533606	H	5.706022	-0.477995	-0.455509
H	2.373451	6.506165	-2.354688	H	6.353162	1.184017	-0.247201
H	2.238023	3.983839	-3.571086	H	3.604069	0.760627	-0.673836
O	2.975718	3.074917	0.513231	O	4.242052	-0.763819	3.237369
H	-3.082758	-3.708247	-0.509414	H	-4.402820	-2.972348	-1.195743
O	-2.353070	-2.688321	1.142028	O	-3.826190	-1.613852	0.272382
C	-2.407183	-1.374433	1.520609	C	-2.833053	-0.792888	-0.145924
C	-2.639100	-0.507568	0.302754	C	-1.886361	-1.550450	-1.057268
C	-3.123936	-1.489631	-0.766520	C	-2.230075	-3.018341	-0.793492
C	-2.480378	-2.802886	-0.304520	C	-3.691931	-2.928188	-0.344059
H	-1.663002	-0.056119	0.025789	H	-0.838871	-1.262720	-0.852893
H	-3.336920	0.319031	0.523781	H	-2.114129	-1.238968	-2.099949
H	-2.794626	-1.215673	-1.785653	H	-1.604883	-3.418316	0.027825
H	-4.230206	-1.563627	-0.753878	H	-2.108411	-3.671134	-1.677850
H	-1.460564	-2.943076	-0.719355	H	-3.986401	-3.680478	0.410782
O	-2.258765	-1.042071	2.681801	O	-2.797294	0.382707	0.184526

Li⁺(GBL)₆

E (PBE-D3/ma-def2-svp GAS_OPT) =	-1843.1251675176
E (PBE-D3/ma-def2-svp SMD_OPT) =	-1843.2007983958

ΔG_{corr} (ID-RR-HR GAS) =	0.5112249800
E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT GAS) =	-1843.7468538377
E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT SMD) =	-1843.8147222833
E (DLPNO-CCSDT/cc-p(wC)VTZ SMD_OPT SMD) =	-1843.8145091525
E (PBE-D3/ma-def2-tzvp GAS_OPT GAS) =	-1845.1124093926
E (PBE-D3/ma-def2-tzvp GAS_OPT SMD) =	-1845.1861272772
E (PBE-D3/ma-def2-tzvp GAS_OPT CPCM) =	-1845.1788989239
GAS_OPT	SMD_OPT
H -2.236481 2.632738 -4.162972	H -0.491176 5.272406 -2.648439
O -1.299387 2.530356 -2.317147	O -0.929993 3.740807 -1.303267
C -0.015277 2.300556 -1.927574	C -0.179367 2.637446 -1.522223
C 0.730634 1.593217 -3.049647	C 0.091352 2.477699 -3.001166
C -0.168404 1.800975 -4.272862	C -0.978843 3.363237 -3.646232
C -1.551917 1.951169 -3.624632	C -1.203103 4.424795 -2.567360
H 0.798231 0.524613 -2.758994	H 0.069020 1.411014 -3.284868
H 1.755059 1.999896 -3.142700	H 1.120378 2.856028 -3.186983
H -0.139040 0.965939 -4.997974	H -1.909161 2.782931 -3.813132
H 0.109859 2.730068 -4.810635	H -0.671289 3.810754 -4.609539
H -2.054863 0.975889 -3.462425	H -2.234178 4.819258 -2.511392
O 0.392768 2.637114 -0.832929	O 0.189490 1.937294 -0.588353
Li 0.855516 -1.701255 -0.506689	Li 0.626512 -0.154561 -0.703401
H -4.661916 -1.368948 -1.552366	H -4.288617 -2.200729 -3.198110
O -2.913386 -0.262446 -1.367864	O -3.176390 -0.535447 -2.617796
C -1.891476 -0.923592 -0.791154	C -2.236833 -0.849421 -1.703063
C -2.404818 -1.870993 0.270771	C -2.746544 -1.932171 -0.777209
C -3.843004 -1.399822 0.511400	C -4.260542 -1.905629 -1.009243
C -4.187833 -0.694694 -0.808718	C -4.354574 -1.387683 -2.445569
H -1.745237 -1.831279 1.157130	H -2.428184 -1.732347 0.263473
H -2.340432 -2.898680 -0.148953	H -2.290820 -2.890289 -1.109433
H -3.860510 -0.675941 1.347625	H -4.746278 -1.194388 -0.310498
H -4.548893 -2.220560 0.737568	H -4.746975 -2.891181 -0.890113
H -4.817025 0.207953 -0.694230	H -5.243006 -0.765330 -2.657345
O -0.737896 -0.746009 -1.167966	O -1.152368 -0.281273 -1.700387
H 5.088781 1.769389 -0.198219	H 6.196051 -0.315774 -1.983067
O 3.494732 0.533157 -0.686334	O 4.248133 -0.503659 -2.702205
C 3.304760 -0.396709 -1.642756	C 3.335884 -0.480158 -1.709182
C 4.284792 -0.187041 -2.780544	C 3.892992 -1.150826 -0.471570
C 5.320062 0.776833 -2.187904	C 5.076887 -1.955797 -1.014398
C 4.509979 1.493670 -1.098801	C 5.486159 -1.130796 -2.236470
H 3.717690 0.255325 -3.628811	H 3.107078 -1.731792 0.042157
H 4.680839 -1.157362 -3.134558	H 4.217264 -0.342321 0.219874
H 5.747941 1.482831 -2.923768	H 4.745381 -2.966854 -1.326708
H 6.159269 0.212129 -1.734464	H 5.908708 -2.069164 -0.294880

H	3.977042	2.394042	-1.471159	H	5.892914	-1.719567	-3.078916
O	2.429554	-1.245222	-1.550693	O	2.242533	0.046903	-1.872302
H	0.020381	-7.257065	0.951064	H	0.891291	-5.863935	0.930179
O	-0.674144	-5.406074	0.302435	O	0.312606	-4.473970	-0.512581
C	0.278801	-4.453622	0.339533	C	0.409109	-3.201175	-0.060721
C	1.188012	-4.662763	1.534684	C	0.079998	-3.152125	1.416071
C	0.392092	-5.634099	2.414372	C	-0.661838	-4.471205	1.651524
C	-0.479089	-6.364352	1.383207	C	-0.042936	-5.374345	0.583519
H	1.424800	-3.685201	1.995436	H	-0.462894	-2.226133	1.678942
H	2.139624	-5.100216	1.160900	H	1.050136	-3.118651	1.958470
H	-0.243803	-5.071496	3.127421	H	-1.749095	-4.346128	1.468900
H	1.021467	-6.330826	2.999039	H	-0.529415	-4.882164	2.669584
H	-1.481345	-6.657138	1.746560	H	-0.724041	-6.141269	0.171733
O	0.325539	-3.576360	-0.511629	O	0.735088	-2.295021	-0.815169
H	0.463466	0.521396	5.169232	H	3.303252	0.837590	4.414331
O	0.282855	-0.541096	3.397692	O	1.682387	0.039476	3.378241
C	0.844165	-0.406275	2.188586	C	1.573399	0.516760	2.122518
C	1.408501	0.981762	2.003691	C	2.032033	1.956705	2.068601
C	1.369323	1.577783	3.416854	C	2.001499	2.391986	3.536190
C	0.281423	0.738067	4.100658	C	2.226903	1.064921	4.266169
H	0.757955	1.520601	1.283613	H	1.400616	2.534134	1.369892
H	2.406491	0.923423	1.531953	H	3.064502	1.954959	1.653546
H	1.114555	2.653336	3.426564	H	1.008933	2.810766	3.795946
H	2.343817	1.445895	3.929025	H	2.772019	3.141253	3.796040
H	-0.728312	1.174595	3.970487	H	1.700831	0.975648	5.234290
O	0.860231	-1.349359	1.399236	O	1.182202	-0.200442	1.211701
H	-0.711205	5.023457	1.676395	H	-0.790965	3.222027	1.633009
O	-1.303950	3.082825	2.093677	O	-1.451693	1.588408	2.746359
C	-2.044247	2.191866	1.383501	C	-2.156140	0.707655	1.990621
C	-2.993910	2.932283	0.460088	C	-2.948313	1.460564	0.935763
C	-2.419010	4.350959	0.412028	C	-2.960079	2.898916	1.459906
C	-1.653930	4.448373	1.740691	C	-1.659732	2.951077	2.266092
H	-4.006459	2.889394	0.918184	H	-3.944131	1.002373	0.791993
H	-3.035382	2.423610	-0.520201	H	-2.387166	1.374654	-0.017841
H	-3.185736	5.142270	0.314949	H	-3.832763	3.061274	2.123749
H	-1.717602	4.435620	-0.439413	H	-2.978592	3.664065	0.662225
H	-2.270978	4.860139	2.567400	H	-1.695363	3.613331	3.150855
O	-1.914117	0.990983	1.544034	O	-2.108713	-0.493479	2.197804

H₂O

E (PBE-D3/ma-def2-svp GAS_OPT) =	-76.2921257766
E (PBE-D3/ma-def2-svp SMD_OPT) =	-76.3053257742
ΔG_{corr} (ID-RR-HR GAS) =	0.0030616600
E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT GAS) =	-76.3422877820

E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT SMD) =	-76.3560054732
E (DLPNO-CCSDT/cc-p(wC)VTZ SMD_OPT SMD) =	-76.3558980996
E (PBE-D3/ma-def2-tzvp GAS_OPT GAS) =	-76.3795881584
E (PBE-D3/ma-def2-tzvp GAS_OPT SMD) =	-76.3922213778
E (PBE-D3/ma-def2-tzvp GAS_OPT CPCM) =	-76.3913308078
GAS_OPT	SMD_OPT
O -0.083652 1.675603 -0.841151 H -0.040395 0.793723 -1.250306 H 0.728248 2.117674 -1.145094	O -0.087856 1.677775 -0.837642 H -0.036941 0.795012 -1.251856 H 0.728998 2.114214 -1.147054

(H₂O)₄

E (PBE-D3/ma-def2-svp GAS_OPT) =	-305.2290002952
E (PBE-D3/ma-def2-svp SMD_OPT) =	-305.2518032108
ΔG_{corr} (ID-RR-HR GAS) =	0.0641993892
E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT GAS) =	-305.4119450751
E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT SMD) =	-305.4380807683
E (DLPNO-CCSDT/cc-p(wC)VTZ SMD_OPT SMD) =	-305.4388171705
E (PBE-D3/ma-def2-tzvp GAS_OPT GAS) =	-305.5738230130
E (PBE-D3/ma-def2-tzvp GAS_OPT SMD) =	-305.5949714827
E (PBE-D3/ma-def2-tzvp GAS_OPT CPCM) =	-305.5940726429
GAS_OPT	SMD_OPT
O 0.149225 1.772058 -0.636810 H 0.091873 0.929199 -1.185923 H 0.957900 2.223191 -0.933944 O -0.149006 -1.771663 0.638483	O -0.175085 1.739333 -0.757914 H -0.308647 0.839812 -1.191127 H 0.595542 2.118429 -1.222857 O 0.144591 -1.741380 0.774657

H	0.566722	-2.331939	0.984284	H	1.030461	-2.152540	0.774688
H	-0.121776	-0.926987	1.187460	H	0.291892	-0.836959	1.193489
O	0.012482	-0.639634	-1.773856	O	-0.462173	-0.783605	-1.678417
H	-0.747976	-0.909772	-2.316459	H	-1.396213	-1.002642	-1.860764
H	-0.043428	-1.191377	-0.932617	H	-0.266125	-1.241505	-0.803298
O	-0.016523	0.639041	1.773821	O	0.497248	0.778986	1.671745
H	0.064945	1.186489	0.931706	H	-0.209432	1.042871	2.291752
H	-0.764437	1.021395	2.263854	H	0.257940	1.239200	0.808048

Li⁺(H₂O)₄

E (PBE-D3/ma-def2-svp GAS_OPT) =	-312.5993006491
E (PBE-D3/ma-def2-svp SMD_OPT) =	-312.6983015054
ΔG_{corr} (ID-RR-HR GAS) =	0.0579799092
E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT GAS) =	-312.8104575750
E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT SMD) =	-312.9173065434
E (DLPNO-CCSDT/cc-p(wC)VTZ SMD_OPT SMD) =	-312.9187598073
E (PBE-D3/ma-def2-tzvp GAS_OPT GAS) =	-312.9486412885
E (PBE-D3/ma-def2-tzvp GAS_OPT SMD) =	-313.0472788331
E (PBE-D3/ma-def2-tzvp GAS_OPT CPCM) =	-313.0456678392
GAS_OPT	SMD_OPT
O	O
H	H
H	H
O	O
H	H
H	H
O	O
H	H
H	H
O	O
H	H
Li	Li
O	O
H	H
H	H

Li⁺ in water

E (PBE-D3/ma-def2-svp GAS_OPT) =	-7.2519251623
E (PBE-D3/ma-def2-svp SMD_OPT) =	-7.3917970144
ΔG_{corr} (ID-RR-HR GAS) =	-0.0127326619
E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT GAS) =	-7.2736440090
E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT SMD) =	-7.4171392254
E (DLPNO-CCSDT/cc-p(wC)VTZ SMD_OPT SMD) =	-7.4171392254
E (PBE-D3/ma-def2-tzvp GAS_OPT GAS) =	-7.2566456293
E (PBE-D3/ma-def2-tzvp GAS_OPT SMD) =	-7.4001426722
E (PBE-D3/ma-def2-tzvp GAS_OPT CPCM) =	-7.4427403487
GAS_OPT	SMD_OPT
Li 0.0 0.0 0.0	Li 0.0 0.0 0.0

(H₂O)₅

E (PBE-D3/ma-def2-svp GAS_OPT) =	-381.5369147408
E (PBE-D3/ma-def2-svp SMD_OPT) =	-381.5679720272
ΔG_{corr} (ID-RR-HR GAS) =	0.0866924000
E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT GAS) =	-381.7662566160
E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT SMD) =	-381.7969821942
E (DLPNO-CCSDT/cc-p(wC)VTZ SMD_OPT SMD) =	-381.8000537734
E (PBE-D3/ma-def2-tzvp GAS_OPT GAS) =	-381.9679383247

E (PBE-D3/ma-def2-tzvp GAS_OPT SMD) =	-381.9931864352
E (PBE-D3/ma-def2-tzvp GAS_OPT CPCM) =	-381.9921451287
GAS_OPT	SMD_OPT
O -1.655995 1.389299 -0.101931 H -1.189293 0.865845 -0.802393 H -1.518982 2.321088 -0.345654 O 1.909923 0.936158 -0.077237 H 2.809948 0.575042 -0.148042 H 1.379358 0.464980 -0.770399 O -0.262552 -2.015880 0.505066 H -1.065048 -2.501299 0.762064 H -0.183395 -1.234199 1.159363 O -0.050868 -0.397345 -1.517981 H -0.097594 -0.786023 -2.408084 H -0.187700 -1.158264 -0.849222 O -0.008624 0.232164 1.835153 H -0.702474 0.760699 1.361237 H 0.823296 0.547736 1.398061	O -0.455794 2.208457 0.295140 H -1.246929 2.511047 -0.190717 H 0.150188 1.835103 -0.422630 O 1.166696 1.181297 -1.564466 H 2.094739 1.368612 -1.325457 H 1.097471 0.173658 -1.527963 O -0.267605 -2.078037 0.860590 H -1.074912 -2.612421 0.734791 H -0.597162 -1.224085 1.289019 O 0.915359 -1.480216 -1.463152 H 0.294852 -1.746603 -2.168352 H 0.440471 -1.725085 -0.605441 O -1.088928 0.215600 1.964005 H -0.850886 0.980384 1.347908 H -0.577560 0.392289 2.776725

Li⁺(H₂O)₅

E (PBE-D3/ma-def2-svp GAS_OPT) =	-388.9196432701
E (PBE-D3/ma-def2-svp SMD_OPT) =	-389.0128404189
ΔG_{corr} (ID-RR-HR GAS) =	0.0815238592
E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT GAS) =	-389.1764837508
E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT SMD) =	-389.2808595015
E (DLPNO-CCSDT/cc-p(wC)VTZ SMD_OPT SMD) =	-389.2771483304
E (PBE-D3/ma-def2-tzvp GAS_OPT GAS) =	-389.3546950101
E (PBE-D3/ma-def2-tzvp GAS_OPT SMD) =	-389.4502852187
E (PBE-D3/ma-def2-tzvp GAS_OPT CPCM) =	-389.4487858307
GAS_OPT	SMD_OPT

O	1.067201	-1.901946	1.362058	O	-0.883602	-2.319535	0.706175
H	0.368350	-2.419237	1.801844	H	-1.755088	-2.627456	0.391496
H	1.891493	-2.130313	1.827904	H	-0.330917	-3.124515	0.701198
O	2.262456	-0.496870	-1.140658	O	1.503473	-0.086532	1.136051
H	2.583407	0.289412	-1.618251	H	1.591835	0.843392	0.792289
H	2.775458	-1.244155	-1.497161	H	1.521439	0.004396	2.107499
O	-1.135064	-0.845217	-0.576562	O	0.463204	-0.245679	-1.696945
H	-1.531535	-1.527051	-1.145535	H	-0.168892	-0.210149	-2.441387
H	-1.771687	-0.092608	-0.549893	H	1.213353	-0.765114	-2.047092
O	0.393173	1.384953	0.525035	O	-1.380834	0.960925	0.449674
H	0.866102	2.017517	1.092377	H	-1.731661	1.142853	1.343512
H	-0.515073	1.744990	0.391842	H	-2.146154	1.108040	-0.140067
Li	0.694907	-0.493375	0.043843	Li	-0.158893	-0.599754	0.175507
O	-2.327106	1.673930	-0.152888	O	1.073931	2.207683	-0.359283
H	-2.600240	2.255323	-0.889255	H	1.038652	1.558426	-1.102074
H	-3.021844	1.784651	0.525300	H	0.150152	2.153021	-0.016552

MeOH

E (PBE-D3/ma-def2-svp GAS_OPT) =	-115.5030080367						
E (PBE-D3/ma-def2-svp SMD_OPT) =	-115.5120824906						
ΔG_{corr} (ID-RR-HR GAS) =	0.0268633300						
E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT GAS) =	-115.5617284993						
E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT SMD) =	-115.5719838921						
E (DLPNO-CCSDT/cc-p(wC)VTZ SMD_OPT SMD) =	-115.5721769088						
E (PBE-D3/ma-def2-tzvp GAS_OPT GAS) =	-115.6332033383						
E (PBE-D3/ma-def2-tzvp GAS_OPT SMD) =	-115.6411190977						
E (PBE-D3/ma-def2-tzvp GAS_OPT CPCM) =	-115.6410977397						
GAS_OPT	SMD_OPT						
C	0.706967	1.762320	-1.349702	C	0.706306	1.760385	-1.357218
O	-0.290233	2.179645	-0.430862	O	-0.293760	2.182255	-0.428898
H	0.190658	1.498268	-2.293520	H	0.193563	1.493905	-2.302802
H	1.264054	0.860440	-1.002836	H	1.259673	0.864784	-0.994860
H	1.446031	2.565461	-1.579538	H	1.441225	2.568439	-1.573298
H	0.140365	2.417351	0.408252	H	0.150834	2.413717	0.408869

(MeOH)₃

E (PBE-D3/ma-def2-svp GAS_OPT) =	-346.5457860949
E (PBE-D3/ma-def2-svp SMD_OPT) =	-346.5540708996
ΔG_{corr} (ID-RR-HR GAS) =	0.1178318100
E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT GAS) =	-346.7129184523
E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT SMD) =	-346.7251199717
E (DLPNO-CCSDT/cc-p(wC)VTZ SMD_OPT SMD) =	-346.7266803922
E (PBE-D3/ma-def2-tzvp GAS_OPT GAS) =	-346.9310502759
E (PBE-D3/ma-def2-tzvp GAS_OPT SMD) =	-346.9371715367
E (PBE-D3/ma-def2-tzvp GAS_OPT CPCM) =	-346.9392281605
GAS_OPT	SMD_OPT
C 1.344819 0.510981 -2.190878	C 0.873282 -0.228112 -2.101421
O 0.119977 0.533892 -1.475980	O 1.228082 -1.020284 -0.966304
H 1.177891 -0.039231 -3.138189	H -0.044697 0.376242 -1.922298
H 2.156454 -0.006478 -1.628356	H 0.673562 -0.914338 -2.948360
H 1.692436 1.537218 -2.447936	H 1.698373 0.458676 -2.392525
H 0.246363 0.996915 -0.600949	H 1.468836 -0.408899 -0.214680
C -2.261120 -1.650162 0.093406	C -2.064803 -1.055912 0.524860
O -0.902636 -1.262901 0.234976	O -0.740748 -1.444664 0.895797
H -2.387170 -2.432785 -0.688442	H -2.091398 -0.041029 0.067837
H -2.921977 -0.789515 -0.158758	H -2.684542 -1.038060 1.443287
H -2.597511 -2.075179 1.059975	H -2.515276 -1.779348 -0.189718
H -0.584420 -0.825895 -0.604172	H -0.180593 -1.518523 0.074825
C 1.093343 1.055774 2.119000	C 0.773542 1.798846 1.250504
O 0.045879 1.069037 1.163039	O 1.189814 0.434492 1.339594
H 1.574220 2.054425 2.114599	H 1.679364 2.423478 1.119974
H 1.871695 0.291949 1.887457	H 0.251350 2.124690 2.176929
H 0.712236 0.864774 3.147761	H 0.099712 1.976200 0.382372
H -0.380479 0.167182 1.113450	H 0.386142 -0.143456 1.459327

Li⁺(MeOH)₃

E (PBE-D3/ma-def2-svp GAS_OPT) =	-353.9189050673
E (PBE-D3/ma-def2-svp SMD_OPT) =	-354.0055267312
ΔG_{corr} (ID-RR-HR GAS) =	0.1175581400
E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT GAS) =	-354.1103906105
E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT SMD) =	-354.1992896646
E (DLPNO-CCSDT/cc-p(wC)VTZ SMD_OPT SMD) =	-354.1997650276
E (PBE-D3/ma-def2-tzvp GAS_OPT GAS) =	-354.3073470861
E (PBE-D3/ma-def2-tzvp GAS_OPT SMD) =	-354.3933147708
E (PBE-D3/ma-def2-tzvp GAS_OPT CPCM) =	-354.3951076954
GAS_OPT	SMD_OPT
Li -0.011339 -0.472753 0.056642	Li 0.078187 -0.364687 -0.449487
C 2.904700 0.097518 -0.357786	C 2.781641 0.069224 0.750651
O 1.841623 -0.426895 0.469083	O 1.937889 -0.014783 -0.406979
H 2.433714 0.520512 -1.264267	H 3.065519 1.121551 0.965300
H 3.607604 -0.706293 -0.656685	H 3.701763 -0.537159 0.615734
H 3.454666 0.903409 0.168801	H 2.215148 -0.335380 1.610618
H 2.228008 -0.803207 1.280887	H 2.442429 0.276488 -1.190290
C -1.740892 -0.005046 -2.346581	C -2.329641 -0.775341 -2.166648
O -0.588955 -0.637187 -1.744548	O -0.916442 -0.910348 -1.957276
H -1.440318 0.632014 -3.202756	H -2.759172 -0.308170 -1.260014
H -2.203930 0.633471 -1.571753	H -2.806219 -1.766428 -2.320735
H -2.479183 -0.762118 -2.680184	H -2.542590 -0.124331 -3.040775
H -0.157679 -1.206793 -2.407474	H -0.513916 -1.316970 -2.748227
C -1.141362 0.609827 2.616319	C -0.559453 1.140895 2.054137
O -1.291540 -0.208118 1.434333	O -0.848699 0.067210 1.147209
H -1.176302 -0.010554 3.534715	H -0.125694 0.760115 3.003021
H -1.926234 1.391745 2.658970	H -1.475422 1.726239 2.280462
H -0.152681 1.100248 2.549461	H 0.173884 1.808491 1.563201
H -2.159902 -0.649777 1.462824	H -1.519214 -0.516614 1.550095

Li⁺ in methanol

E (PBE-D3/ma-def2-svp GAS_OPT) =	-7.2519251623
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E (PBE-D3/ma-def2-svp SMD_OPT) =	-7.3917970144
ΔG_{corr} (ID-RR-HR GAS) =	-0.0127326619
E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT GAS) =	-7.2736440090
E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT SMD) =	-7.4145374283
E (DLPNO-CCSDT/cc-p(wC)VTZ SMD_OPT SMD) =	-7.4145374283
E (PBE-D3/ma-def2-tzvp GAS_OPT GAS) =	-7.2566456293
E (PBE-D3/ma-def2-tzvp GAS_OPT SMD) =	-7.3964434016
E (PBE-D3/ma-def2-tzvp GAS_OPT CPCM) =	-7.4393090945
GAS_OPT	SMD_OPT
Li 0.0 0.0 0.0	Li 0.0 0.0 0.0

(MeOH)₄

E (PBE-D3/ma-def2-svp GAS_OPT) =	-462.0778869072
E (PBE-D3/ma-def2-svp SMD_OPT) =	-462.0867950301
ΔG_{corr} (ID-RR-HR GAS) =	0.1645356200
E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT GAS) =	-462.2955145584
E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT SMD) =	-462.3086470814
E (DLPNO-CCSDT/cc-p(wC)VTZ SMD_OPT SMD) =	-462.3106864603
E (PBE-D3/ma-def2-tzvp GAS_OPT GAS) =	-462.5890097990
E (PBE-D3/ma-def2-tzvp GAS_OPT SMD) =	-462.5945255833
E (PBE-D3/ma-def2-tzvp GAS_OPT CPCM) =	-462.5978008157

GAS_OPT				SMD_OPT			
C	0.744946	-1.860554	-2.215677	C	1.592976	-0.764949	-2.236786
O	1.073793	-0.892831	-1.231125	O	0.280136	-1.138911	-1.813749
H	1.069448	-1.476228	-3.203518	H	2.042864	0.009886	-1.576554
H	-0.350145	-2.060964	-2.261920	H	1.521116	-0.349218	-3.261690
H	1.270698	-2.824099	-2.031946	H	2.272263	-1.645204	-2.263701
H	0.768687	-1.214299	-0.320801	H	0.332623	-1.514931	-0.876760
C	0.859824	2.540297	-1.280487	C	-0.683340	2.048160	-1.170843
O	-0.066528	1.475719	-1.129925	O	-1.411252	0.818699	-1.216210
H	1.265302	2.584637	-2.315975	H	-1.352401	2.834036	-0.766972
H	1.715266	2.459340	-0.571165	H	-0.351767	2.358010	-2.186268
H	0.330777	3.493341	-1.078804	H	0.212318	1.980139	-0.513004
H	0.402398	0.592032	-1.285714	H	-0.787951	0.098173	-1.556407
C	-2.538294	0.989065	1.224653	C	-1.635600	0.723529	2.223857
O	-1.124773	0.865033	1.200027	O	-1.780247	-0.252780	1.190454
H	-2.855560	2.053601	1.155878	H	-0.664742	1.264020	2.159336
H	-2.906607	0.583597	2.188397	H	-1.679252	0.202290	3.201033
H	-3.026635	0.422784	0.398585	H	-2.459421	1.469939	2.188938
H	-0.766962	1.211192	0.318275	H	-1.739768	0.211007	0.292879
C	0.939329	-1.664132	2.276062	C	1.401371	-1.380609	1.464281
O	0.103461	-1.461250	1.147273	O	0.270855	-1.876831	0.743652
H	1.537326	-2.581903	2.105976	H	2.292804	-1.963307	1.157360
H	0.342928	-1.809410	3.204428	H	1.264923	-1.501532	2.561474
H	1.642095	-0.815057	2.439273	H	1.596015	-0.305753	1.248987
H	-0.430773	-0.609915	1.268230	H	-0.534524	-1.323864	1.006691

Li⁺(MeOH)₄

E (PBE-D3/ma-def2-svp GAS_OPT) =	-469.4530716512
E (PBE-D3/ma-def2-svp SMD_OPT) =	-469.5364995368
ΔG_{corr} (ID-RR-HR GAS) =	0.1632704800
E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT GAS) =	-469.7021210318
E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT SMD) =	-469.7872767126
E (DLPNO-CCSDT/cc-p(wC)VTZ SMD_OPT SMD) =	-469.7887479127
E (PBE-D3/ma-def2-tzvp GAS_OPT GAS) =	-469.9693239943
E (PBE-D3/ma-def2-tzvp GAS_OPT SMD) =	-470.0508611175
E (PBE-D3/ma-def2-tzvp GAS_OPT CPCM) =	-470.0479381207

GAS_OPT				SMD_OPT			
Li	0.029893	-0.266851	-0.367414	Li	-0.233531	0.025859	-0.528562
C	1.637168	-2.848779	-0.380433	C	2.285054	-0.240037	1.059096
O	1.038521	-1.762829	-1.109333	O	1.205264	-0.897149	0.387800
H	2.719870	-2.938264	-0.607075	H	3.226817	-0.300639	0.472441
H	1.132850	-3.812345	-0.602635	H	2.460377	-0.678563	2.065027
H	1.517359	-2.621559	0.695308	H	2.009685	0.825410	1.180110
H	1.156247	-1.913098	-2.064259	H	1.444623	-1.830799	0.237992
C	0.416101	2.389631	-1.797438	C	1.859037	0.849706	-2.460757
O	-0.316438	1.159339	-1.655055	O	0.487778	0.983717	-2.062524
H	-0.260766	3.267663	-1.752282	H	2.156932	-0.201117	-2.284824
H	0.990428	2.411155	-2.746827	H	2.520983	1.518491	-1.869427
H	1.122169	2.442681	-0.948549	H	1.983989	1.076756	-3.540573
H	-0.985230	1.100833	-2.360431	H	0.189015	1.888320	-2.275894
C	-2.849377	0.025635	0.585234	C	-2.525738	-1.698721	0.004199
O	-1.731563	-0.820415	0.265104	O	-1.599061	-1.284897	-1.009590
H	-3.113048	-0.041845	1.661533	H	-3.294089	-0.919033	0.196354
H	-3.738168	-0.229915	-0.028286	H	-1.948935	-1.875449	0.932239
H	-2.546381	1.063650	0.353333	H	-3.032027	-2.645279	-0.279562
H	-1.977471	-1.749855	0.419541	H	-2.080108	-1.196960	-1.854672
C	0.719954	0.971999	2.335096	C	-1.004746	0.947626	2.236201
O	1.153150	0.405977	1.085539	O	-0.904345	1.240159	0.837911
H	1.141397	0.415039	3.197212	H	-2.050652	0.714372	2.529025
H	-0.381595	0.886028	2.365217	H	-0.637501	1.797518	2.850496
H	0.999117	2.043464	2.411991	H	-0.371396	0.064078	2.441064
H	2.125814	0.422663	1.044909	H	-1.496757	1.986865	0.628728

Py

E (PBE-D3/ma-def2-svp GAS_OPT) =	-247.8083843741
E (PBE-D3/ma-def2-svp SMD_OPT) =	-247.8182773601
ΔG_{corr} (ID-RR-HR GAS) =	0.0580347592
E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT GAS) =	-247.8475501993
E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT SMD) =	-247.8560500167
E (DLPNO-CCSDT/cc-p(wC)VTZ SMD_OPT SMD) =	-247.8560499457
E (PBE-D3/ma-def2-tzvp GAS_OPT GAS) =	-248.0677900702
E (PBE-D3/ma-def2-tzvp GAS_OPT SMD) =	-248.0775520951

E (PBE-D3/ma-def2-tzvp GAS_OPT CPCM) =	-248.0749123824
GAS_OPT	SMD_OPT
C -2.455164 2.402807 -2.384806	C -2.455462 2.401935 -2.383719
C -3.765914 2.246837 -1.909749	C -3.766918 2.246483 -1.909119
C -3.966822 1.502266 -0.734635	C -3.970743 1.502903 -0.734912
N -2.970827 0.929319 -0.038055	N -2.970727 0.929554 -0.038263
C -1.719752 1.085438 -0.502584	C -1.715836 1.084609 -0.502094
C -1.406760 1.809282 -1.666151	C -1.406138 1.808485 -1.665490
H -2.253877 2.978508 -3.301700	H -2.254169 2.978014 -3.300417
H -4.622305 2.692920 -2.437590	H -4.623402 2.692594 -2.436707
H -4.986401 1.360554 -0.333772	H -4.991459 1.363285 -0.337262
H -0.917481 0.605793 0.086164	H -0.911188 0.606721 0.084064
H -0.361535 1.902646 -1.997526	H -0.360796 1.901785 -1.996485

(Py)₃

E (PBE-D3/ma-def2-svp GAS_OPT) =	-743.4452750476
E (PBE-D3/ma-def2-svp SMD_OPT) =	-743.4664301858
ΔG_{corr} (ID-RR-HR GAS) =	0.2155179000
E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT GAS) =	-743.5630182006
E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT SMD) =	-743.5799836236
E (DLPNO-CCSDT/cc-p(wC)VTZ SMD_OPT SMD) =	-743.5799092055
E (PBE-D3/ma-def2-tzvp GAS_OPT GAS) =	-744.2203808864
E (PBE-D3/ma-def2-tzvp GAS_OPT SMD) =	-744.2410756614
E (PBE-D3/ma-def2-tzvp GAS_OPT CPCM) =	-744.2341680634
GAS_OPT	SMD_OPT
C -2.664871 2.261744 -2.426662	C -2.707317 2.312571 -2.444579
C -3.641986 2.413020 -1.430354	C -3.703911 2.462252 -1.467649
C -3.392100 1.866462 -0.160595	C -3.482352 1.911089 -0.194668
N -2.264010 1.204749 0.151020	N -2.359065 1.246548 0.137870
C -1.335271 1.066169 -0.812036	C -1.409625 1.110044 -0.806612
C -1.483161 1.573523 -2.114215	C -1.533276 1.620751 -2.108864
H -2.822809 2.675250 -3.435019	H -2.843834 2.728444 -3.454999

H	-4.584558	2.944980	-1.629104	H	-4.641113	2.997280	-1.682648
H	-4.139120	1.966282	0.646675	H	-4.248443	2.009711	0.594385
H	-0.418178	0.519695	-0.530790	H	-0.498108	0.561351	-0.509542
H	-0.679774	1.422394	-2.851674	H	-0.719448	1.472286	-2.834944
C	2.366505	-0.639390	-0.155400	C	2.475601	-0.684855	-0.161904
C	2.614026	0.700890	-0.485927	C	2.710819	0.660194	-0.483670
C	2.238933	1.155986	-1.761753	C	2.289255	1.132543	-1.737769
N	1.654004	0.374744	-2.686205	N	1.666549	0.360268	-2.648713
C	1.428581	-0.910902	-2.359904	C	1.445970	-0.930131	-2.329709
C	1.762974	-1.467155	-1.113833	C	1.830086	-1.499323	-1.104493
H	2.627696	-1.034310	0.838286	H	2.787962	-1.091462	0.812143
H	3.081782	1.390216	0.233032	H	3.212899	1.338261	0.222464
H	2.411726	2.208171	-2.050217	H	2.458089	2.186937	-2.018964
H	0.943474	-1.531956	-3.133746	H	0.928747	-1.543614	-3.088373
H	1.536103	-2.519580	-0.887305	H	1.617880	-2.558006	-0.893732
C	0.466041	-0.586787	3.199386	C	0.482185	-0.571812	3.148885
C	1.367585	-1.629820	3.464727	C	1.389331	-1.602748	3.439164
C	1.285575	-2.798478	2.687328	C	1.283355	-2.808870	2.726332
N	0.388233	-2.972874	1.701273	N	0.355555	-3.027414	1.774694
C	-0.471918	-1.966536	1.463694	C	-0.509478	-2.030478	1.505592
C	-0.479214	-0.755150	2.176699	C	-0.490824	-0.788347	2.161248
H	0.500395	0.347102	3.782304	H	0.533749	0.389498	3.683997
H	2.125068	-1.545191	4.258910	H	2.170226	-1.480700	4.204766
H	1.981390	-3.637427	2.868418	H	1.983033	-3.637849	2.932530
H	-1.196922	-2.125755	0.645776	H	-1.256313	-2.228623	0.716400
H	-1.206196	0.029934	1.907206	H	-1.224217	-0.012464	1.884875

Li⁺(Py)₃

E (PBE-D3/ma-def2-svp GAS_OPT) =	-750.8627292733
E (PBE-D3/ma-def2-svp SMD_OPT) =	-750.9355072366
ΔG_{corr} (ID-RR-HR GAS) =	0.2187829900
E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT GAS) =	-750.9953231314
E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT SMD) =	-751.0621242554
E (DLPNO-CCSDT/cc-p(wC)VTZ SMD_OPT SMD) =	-751.0622126182
E (PBE-D3/ma-def2-tzvp GAS_OPT GAS) =	-751.6398922433
E (PBE-D3/ma-def2-tzvp GAS_OPT SMD) =	-751.7134014280
E (PBE-D3/ma-def2-tzvp GAS_OPT CPCM) =	-751.7042731010

GAS_OPT				SMD_OPT			
C	3.792200	0.645611	-2.900545	C	3.803401	0.639056	-2.879245
C	3.530213	-0.610086	-2.331886	C	3.547246	-0.608239	-2.289559
C	2.413904	-0.748070	-1.496547	C	2.418488	-0.743687	-1.469919
N	1.577443	0.274728	-1.210641	N	1.566401	0.274688	-1.221714
C	1.838138	1.481266	-1.761842	C	1.818743	1.473010	-1.792079
C	2.928690	1.712816	-2.610362	C	2.921771	1.701024	-2.626059
H	4.659539	0.790834	-3.562341	H	4.680288	0.782148	-3.529353
H	4.180167	-1.474438	-2.530018	H	4.210051	-1.469221	-2.459378
H	2.178051	-1.720736	-1.032585	H	2.186233	-1.709225	-0.990101
H	1.138998	2.297289	-1.512306	H	1.104964	2.284370	-1.571488
H	3.093935	2.713739	-3.034220	H	3.081816	2.696133	-3.066056
Li	-0.001540	0.005515	-0.004867	Li	-0.029187	0.015747	-0.037417
C	-1.499943	3.579775	2.854594	C	-1.496190	3.580808	2.842861
C	-0.138041	3.429100	2.552412	C	-0.134290	3.413877	2.548857
C	0.250305	2.374980	1.715187	C	0.245491	2.363567	1.702206
N	-0.627458	1.493410	1.186117	N	-0.642360	1.503422	1.157498
C	-1.937362	1.645362	1.483459	C	-1.951886	1.669387	1.444536
C	-2.418434	2.670212	2.308833	C	-2.423832	2.691446	2.279361
H	-1.841691	4.396823	3.508034	H	-1.830877	4.394780	3.504280
H	0.617338	4.117140	2.958376	H	0.629027	4.086332	2.966709
H	1.312465	2.226772	1.456680	H	1.307026	2.202556	1.449745
H	-2.631139	0.912746	1.037482	H	-2.652437	0.952132	0.984979
H	-3.495008	2.750337	2.517098	H	-3.501117	2.782860	2.480766
C	-2.287599	-4.233271	0.052632	C	-2.270826	-4.240089	0.082538
C	-1.714229	-3.748103	-1.132554	C	-1.730910	-3.751463	-1.116989
C	-1.059088	-2.510027	-1.102502	C	-1.088188	-2.506081	-1.105233
N	-0.955743	-1.758859	0.016656	N	-0.966688	-1.754466	0.010665
C	-1.512317	-2.233288	1.153584	C	-1.489407	-2.229980	1.161941
C	-2.184295	-3.460918	1.219491	C	-2.147829	-3.464377	1.245398
H	-2.809112	-5.202382	0.066697	H	-2.781252	-5.215135	0.111015
H	-1.771850	-4.318260	-2.070851	H	-1.802755	-4.324004	-2.053189
H	-0.596965	-2.098218	-2.015637	H	-0.652285	-2.090882	-2.029357
H	-1.412409	-1.600118	2.051407	H	-1.373951	-1.594045	2.055639
H	-2.617158	-3.801684	2.170968	H	-2.554679	-3.806449	2.208141

Li⁺ in pyridine

E (PBE-D3/ma-def2-svp GAS_OPT) =	-7.2519251623
E (PBE-D3/ma-def2-svp SMD_OPT) =	-7.3917970144
ΔG_{corr} (ID-RR-HR GAS) =	-0.0127326619
E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT GAS) =	-7.2736440090
E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT SMD) =	-7.4077945060

E (DLPNO-CCSDT/cc-p(wC)VTZ SMD_OPT SMD) =	-7.4077945060
E (PBE-D3/ma-def2-tzvp GAS_OPT GAS) =	-7.2566456293
E (PBE-D3/ma-def2-tzvp GAS_OPT SMD) =	-7.3892671107
E (PBE-D3/ma-def2-tzvp GAS_OPT CPCM) =	-7.4300089998
GAS_OPT	SMD_OPT
Li 0.0 0.0 0.0	Li 0.0 0.0 0.0

(Py)₄

E (PBE-D3/ma-def2-svp GAS_OPT) =	-991.2660452356
E (PBE-D3/ma-def2-svp SMD_OPT) =	-991.2930748849
ΔG_{corr} (ID-RR-HR GAS) =	0.2944698900
E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT GAS) =	-991.4234659777
E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT SMD) =	-991.4442405503
E (DLPNO-CCSDT/cc-p(wC)VTZ SMD_OPT SMD) =	-991.4455914176
E (PBE-D3/ma-def2-tzvp GAS_OPT GAS) =	-992.2981765643
E (PBE-D3/ma-def2-tzvp GAS_OPT SMD) =	-992.3241746836
E (PBE-D3/ma-def2-tzvp GAS_OPT CPCM) =	-992.3149284708
GAS_OPT	SMD_OPT
C -0.367494 0.452757 -0.653119	C -0.577339 0.419265 -0.372853
C -1.498735 0.204098 -1.443883	C -1.880078 0.724874 -0.796663
C -2.751210 0.117163 -0.813188	C -2.833056 1.093153 0.166401
N -2.928349 0.255331 0.512085	N -2.562693 1.170604 1.484013
C -1.835909 0.488463 1.260447	C -1.309887 0.875913 1.881076
C -0.539107 0.596392 0.731353	C -0.287179 0.498694 0.996407
H 0.630642 0.512686 -1.110597	H 0.189312 0.107667 -1.100699
H -1.411477 0.072028 -2.532994	H -2.164172 0.672377 -1.858615
H -3.661980 -0.076487 -1.408530	H -3.866151 1.336029 -0.139230

H	-2.002062	0.583761	2.348167	H	-1.109668	0.937396	2.965341
H	0.320776	0.772740	1.394166	H	0.711029	0.253754	1.384377
C	4.151338	1.321947	1.491197	C	3.408642	1.383892	1.725398
C	3.550833	0.305094	2.248752	C	3.423829	0.097387	2.286577
C	2.915766	-0.752578	1.574746	C	3.290575	-1.009072	1.430594
N	2.856656	-0.835825	0.231831	N	3.148296	-0.898548	0.096376
C	3.431733	0.145022	-0.488998	C	3.128774	0.339868	-0.431947
C	4.087687	1.243615	0.091664	C	3.253915	1.509395	0.336161
H	4.656823	2.166986	1.984537	H	3.509154	2.276274	2.362732
H	3.568946	0.325695	3.348817	H	3.534171	-0.052722	3.371047
H	2.404823	-1.554171	2.138479	H	3.289645	-2.032537	1.843018
H	3.341129	0.057858	-1.586888	H	2.992376	0.404247	-1.525858
H	4.536987	2.019680	-0.546008	H	3.225953	2.496046	-0.150215
C	-2.364835	-3.004401	1.240268	C	-2.085661	-2.697437	0.322119
C	-2.173009	-2.920991	2.627424	C	-2.127801	-2.528497	1.713364
C	-0.864852	-2.760229	3.112730	C	-0.929150	-2.643800	2.437545
N	0.216436	-2.673663	2.318536	N	0.261940	-2.902232	1.866101
C	0.020540	-2.751973	0.989333	C	0.292421	-3.053418	0.528157
C	-1.244086	-2.923832	0.402921	C	-0.849069	-2.964825	-0.283952
H	-3.376149	-3.109646	0.819461	H	-3.000985	-2.610935	-0.283433
H	-3.022550	-2.968970	3.324977	H	-3.069883	-2.304660	2.235616
H	-0.679383	-2.693117	4.199687	H	-0.931997	-2.516593	3.534610
H	0.920727	-2.643056	0.360435	H	1.281756	-3.241185	0.077623
H	-1.343278	-2.961085	-0.691577	H	-0.764730	-3.096704	-1.372347
C	-0.254111	-2.874742	-4.124272	C	0.269489	-3.529357	-4.143692
C	0.526231	-3.039993	-2.970537	C	1.371879	-3.406459	-3.283995
C	1.377078	-1.993088	-2.576170	C	1.690281	-2.136252	-2.774499
N	1.487275	-0.836884	-3.257940	N	0.992870	-1.023994	-3.078228
C	0.740376	-0.690372	-4.365854	C	-0.060680	-1.151033	-3.907375
C	-0.147520	-1.671781	-4.839046	C	-0.466882	-2.376964	-4.460228
H	-0.935443	-3.670883	-4.462862	H	-0.015496	-4.509425	-4.557131
H	0.481531	-3.965781	-2.377220	H	1.975568	-4.281594	-3.000136
H	1.981733	-2.069561	-1.654319	H	2.525627	-2.010672	-2.063296
H	0.851239	0.266133	-4.907085	H	-0.615788	-0.225886	-4.143060
H	-0.738196	-1.493260	-5.750156	H	-1.341580	-2.420952	-5.126434

Li⁺(Py)₄

E (PBE-D3/ma-def2-svp GAS_OPT) =	-998.7081917678
E (PBE-D3/ma-def2-svp SMD_OPT) =	-998.7799741149
ΔG_{corr} (ID-RR-HR GAS) =	0.2997691200
E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT GAS) =	-998.8809595026
E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT SMD) =	-998.9439494420

E (DLPNO-CCSDT/cc-p(wC)VTZ SMD_OPT SMD) =	-998.9438281017
E (PBE-D3/ma-def2-tzvp GAS_OPT GAS) =	-999.7412526452
E (PBE-D3/ma-def2-tzvp GAS_OPT SMD) =	-999.8138691632
E (PBE-D3/ma-def2-tzvp GAS_OPT CPCM) =	-999.7977979346
GAS_OPT	SMD_OPT
Li -0.001584 0.000573 0.001247	Li 0.020111 -0.003539 -0.007723
C -3.812008 0.921379 -2.874916	C -3.816965 0.912761 -2.844602
C -3.963514 0.106767 -1.742681	C -3.958204 0.081333 -1.723216
C -2.838308 -0.151084 -0.946556	C -2.829754 -0.173392 -0.930431
N -1.614844 0.347474 -1.219041	N -1.613045 0.342840 -1.198622
C -1.476547 1.127662 -2.311811	C -1.483388 1.138939 -2.280511
C -2.542205 1.443166 -3.166310	C -2.553687 1.453202 -3.129805
H -4.672574 1.145953 -3.523324	H -4.680863 1.136510 -3.489179
H -4.938478 -0.326403 -1.476795	H -4.927468 -0.367362 -1.461416
H -2.916487 -0.789547 -0.050690	H -2.903219 -0.823347 -0.042763
H -0.461304 1.510574 -2.512391	H -0.474489 1.539423 -2.476663
H -2.375529 2.084193 -4.044115	H -2.393516 2.108398 -3.998393
C 3.727033 -0.960024 -2.967522	C 3.683724 -1.055534 -3.025791
C 3.910958 -0.129854 -1.851517	C 3.881386 -0.156609 -1.966769
C 2.809086 0.139454 -1.027036	C 2.801273 0.129572 -1.119184
N 1.578323 -0.362307 -1.257378	N 1.579389 -0.419691 -1.275929
C 1.408674 -1.157334 -2.334947	C 1.395755 -1.282086 -2.297849
C 2.449383 -1.485181 -3.215203	C 2.414972 -1.630765 -3.195405
H 4.568702 -1.193988 -3.637073	H 4.508370 -1.304390 -3.711310
H 4.893149 0.306598 -1.619814	H 4.857141 0.320779 -1.795160
H 2.913005 0.790051 -0.142589	H 2.919108 0.833942 -0.279139
H 0.387957 -1.542165 -2.501211	H 0.384315 -1.709240 -2.404024
H 2.257523 -2.138165 -4.078943	H 2.212026 -2.339644 -4.011482
C 0.991196 3.789257 2.881735	C 1.027210 3.812599 2.827973
C 1.515520 2.515989 3.152907	C 1.610736 2.557778 3.060831
C 1.177669 1.457026 2.298641	C 1.274415 1.494566 2.211006
N 0.373506 1.604927 1.224633	N 0.415642 1.622843 1.177848
C -0.127472 2.831564 0.971667	C -0.143243 2.830993 0.961162
C 0.151751 3.950670 1.769215	C 0.131150 3.952457 1.757356
H 1.233002 4.644789 3.530602	H 1.267994 4.671148 3.473549
H 2.175502 2.341561 4.015021	H 2.316964 2.399198 3.888856
H 1.562007 0.439372 2.483692	H 1.708817 0.492588 2.366176
H -0.785858 2.917557 0.091057	H -0.844935 2.902759 0.113696
H -0.284317 4.928636 1.519587	H -0.351751 4.915557 1.536933
C -0.903262 -3.751639 2.958608	C -0.926708 -3.661200 3.051695
C -0.098196 -3.926901 1.822981	C -0.097661 -3.870388 1.939286
C 0.154509 -2.818226 1.002445	C 0.164368 -2.789473 1.085116
N -0.340530 -1.588930 1.254293	N -0.342165 -1.555762 1.285543
C -1.111622 -1.427715 2.350371	C -1.136127 -1.360501 2.359350
C -1.421167 -2.475582 3.228776	C -1.457523 -2.380017 3.266743
H -1.123463 -4.598736 3.625979	H -1.155722 -4.486342 3.743501
H 0.331511 -4.907614 1.573106	H 0.343244 -4.855955 1.730808

H	0.785946	-2.915077	0.103428	H	0.812507	-2.916475	0.202309
H	-1.492052	-0.408241	2.533470	H	-1.528852	-0.339394	2.500811
H	-2.054591	-2.290480	4.108405	H	-2.111506	-2.168428	4.125378

TMS

E (PBE-D3/ma-def2-svp GAS_OPT) =	-704.9740293780
E (PBE-D3/ma-def2-svp SMD_OPT) =	-704.9921572598
ΔG_{corr} (ID-RR-HR GAS) =	0.0874757200
E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT GAS) =	-704.9410165271
E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT SMD) =	-704.9562194056
E (DLPNO-CCSDT/cc-p(wC)VTZ SMD_OPT SMD) =	-704.9563158596
E (PBE-D3/ma-def2-tzvp GAS_OPT GAS) =	-705.4885023715
E (PBE-D3/ma-def2-tzvp GAS_OPT SMD) =	-705.5048317128
E (PBE-D3/ma-def2-tzvp GAS_OPT CPCM) =	-705.5062004972
GAS_OPT	SMD_OPT
H 3.586927 2.116087 -0.781404	H 3.588949 2.119484 -0.789095
S 1.235130 2.601058 -0.808546	S 1.242219 2.591537 -0.818382
C 0.600042 1.308370 -1.973317	C 0.603171 1.308189 -1.974235
C 1.848542 0.721645 -2.631143	C 1.851685 0.720319 -2.629077
C 2.837641 1.887101 -2.846886	C 2.835788 1.885495 -2.849148
C 2.945466 2.636433 -1.519176	C 2.943197 2.638456 -1.524225
H 0.002713 0.599227 -1.371115	H -0.004389 0.599307 -1.381358
H -0.052531 1.845118 -2.689288	H -0.042972 1.845764 -2.695554
H 1.596846 0.217011 -3.585591	H 1.588083 0.221159 -3.582286
H 2.305037 -0.043026 -1.967410	H 2.308032 -0.046104 -1.967959
H 2.453931 2.566326 -3.637489	H 2.454555 2.560607 -3.643698
H 3.830180 1.524270 -3.181845	H 3.833070 1.524908 -3.169563
H 3.238958 3.699555 -1.596441	H 3.241317 3.700548 -1.602381
O 1.286072 2.049258 0.574381	O 1.282826 2.058453 0.583207
O 0.549679 3.894733 -1.084359	O 0.539105 3.895046 -1.055872

(TMS)₄

E (PBE-D3/ma-def2-svp GAS_OPT) =	-2819.9655123684
E (PBE-D3/ma-def2-svp SMD_OPT) =	-2819.9997183874
ΔG_{corr} (ID-RR-HR GAS) =	0.4168278200
E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT GAS) =	-2819.8292060678
E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT SMD) =	-2819.8565368229
E (DLPNO-CCSDT/cc-p(wC)VTZ SMD_OPT SMD) =	-2819.8554262230
E (PBE-D3/ma-def2-tzvp GAS_OPT GAS) =	-2822.0040533856
E (PBE-D3/ma-def2-tzvp GAS_OPT SMD) =	-2822.0331109070
E (PBE-D3/ma-def2-tzvp GAS_OPT CPCM) =	-2822.0377741407
GAS_OPT	SMD_OPT
H 1.158686 0.545460 -2.778668	H 1.579285 0.358278 -2.908655
S 2.085097 -0.242683 -0.735400	S 2.376638 -0.388093 -0.789422
C 2.906142 -1.842327 -1.092459	C 2.972906 -2.091500 -1.142221
C 2.620102 -2.076212 -2.574633	C 2.450314 -2.400041 -2.544460
C 1.142809 -1.686390 -2.797235	C 1.048275 -1.770208 -2.652455
C 0.898085 -0.322126 -2.144293	C 1.148108 -0.329178 -2.155931
H 3.969608 -1.723642 -0.814846	H 4.073790 -2.080854 -1.035790
H 2.401962 -2.603373 -0.464621	H 2.525258 -2.743658 -0.363938
H 2.797077 -3.138414 -2.835501	H 2.418458 -3.495130 -2.709381
H 3.293302 -1.456341 -3.204722	H 3.125668 -1.967669 -3.312076
H 0.496235 -2.447428 -2.316978	H 0.325765 -2.342417 -2.035612
H 0.886680 -1.653006 -3.874981	H 0.670896 -1.789136 -3.693719
H -0.116669 -0.197676 -1.724590	H 0.208972 0.091087 -1.754298
O 3.075711 0.861307 -0.960344	O 3.475699 0.605690 -1.022687
O 1.373596 -0.284113 0.586684	O 1.687501 -0.356918 0.549404
H 2.611278 5.085768 -0.909511	H 2.608483 5.217161 -0.034962
S 0.941598 3.581791 -0.122647	S 0.853566 3.605288 0.100721
C 1.437417 2.908766 1.510634	C 1.144133 2.700634 1.671916
C 2.727837 3.663798 1.818986	C 2.473031 3.255551 2.180530
C 3.565165 3.659258 0.519502	C 3.394302 3.396585 0.951782
C 2.653618 4.006794 -0.666697	C 2.607179 4.115503 -0.145903
H 0.597445 3.104850 2.202904	H 0.272977 2.880031 2.329220
H 1.585349 1.818019 1.373652	H 1.216584 1.628842 1.394681
H 3.278652 3.176638 2.648197	H 2.909440 2.571643 2.935448
H 2.495275 4.701601 2.139481	H 2.321327 4.239295 2.673118
H 3.976238 2.644362 0.356565	H 3.694360 2.392848 0.589535
H 4.412820 4.369616 0.585450	H 4.314341 3.963191 1.196450
H 2.855662 3.403110 -1.569823	H 2.887276 3.842003 -1.179889
O 0.168818 4.843773 0.098645	O 0.007840 4.819285 0.356767

O	0.330946	2.524623	-0.990800	O	0.404212	2.660630	-0.977230
H	-1.719511	-5.923049	1.201117	H	-0.542865	-5.302250	2.583226
S	0.014743	-4.312361	0.865567	S	-0.086494	-4.205545	0.504918
C	-0.621356	-2.783003	1.668281	C	-0.811904	-2.539873	0.792929
C	-2.055719	-3.134958	2.059498	C	-1.662459	-2.699109	2.053037
C	-2.647352	-3.935522	0.881006	C	-2.297407	-4.101704	1.998698
C	-1.651778	-5.043339	0.531705	C	-1.173711	-5.091045	1.697640
H	0.067629	-2.553168	2.501641	H	0.024365	-1.816891	0.861398
H	-0.566220	-1.987951	0.900108	H	-1.418740	-2.324334	-0.107715
H	-2.655279	-2.222132	2.243736	H	-2.439831	-1.911753	2.093315
H	-2.064552	-3.742508	2.989600	H	-1.031081	-2.598771	2.960386
H	-2.783521	-3.253438	0.017483	H	-3.067337	-4.139693	1.199675
H	-3.641114	-4.356710	1.131744	H	-2.796205	-4.363444	2.952546
H	-1.655657	-5.368107	-0.525069	H	-1.485285	-6.039409	1.221684
O	0.740403	-5.149698	1.864749	O	1.340599	-4.247864	0.972562
O	0.691146	-3.979586	-0.430389	O	-0.370791	-4.654416	-0.898401
H	-0.866119	1.088240	0.564283	H	-0.989698	1.090741	0.223283
S	-2.933169	0.013620	0.017591	S	-3.016833	0.110235	-0.561362
C	-3.709677	1.349197	-0.997123	C	-3.899823	1.604819	-1.175580
C	-2.958417	2.627480	-0.617147	C	-3.141025	2.782941	-0.566508
C	-2.535625	2.505715	0.862146	C	-2.684078	2.351988	0.839749
C	-1.875168	1.135833	1.018131	C	-1.992481	0.998834	0.682870
H	-3.618216	1.045481	-2.056275	H	-3.900068	1.559078	-2.280408
H	-4.774622	1.353178	-0.693329	H	-4.936113	1.516518	-0.794941
H	-3.589535	3.522175	-0.786613	H	-3.787855	3.681373	-0.530679
H	-2.045147	2.737931	-1.235044	H	-2.252715	3.029477	-1.182961
H	-3.417520	2.586169	1.532680	H	-3.554670	2.262192	1.522505
H	-1.836760	3.322476	1.130634	H	-1.996064	3.097740	1.282828
H	-1.858173	0.723661	2.044162	H	-1.948508	0.378308	1.596450
O	-2.088631	-0.879627	-0.840242	O	-2.137826	-0.464819	-1.635233
O	-3.971622	-0.611805	0.893415	O	-3.979142	-0.818145	0.120007

Li⁺(TMS)₄

E (PBE-D3/ma-def2-svp GAS_OPT) =	-2827.3949729456
E (PBE-D3/ma-def2-svp SMD_OPT) =	-2827.4745075234
ΔG_{corr} (ID-RR-HR GAS) =	0.4197485300
E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT GAS) =	-2827.2742541102
E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT SMD) =	-2827.3482905134
E (DLPNO-CCSDT/cc-p(wC)VTZ SMD_OPT SMD) =	-2827.3499407970
E (PBE-D3/ma-def2-tzvp GAS_OPT GAS) =	-2829.4316861564

E (PBE-D3/ma-def2-tzvp GAS_OPT SMD) =	-2829.5063859289
E (PBE-D3/ma-def2-tzvp GAS_OPT CPCM) =	-2829.5057147119
GAS_OPT	SMD_OPT
H 2.713377 2.247942 0.834034	H 1.270981 4.290026 0.264377
S 1.778553 1.078206 2.720355	S 0.780776 2.854637 2.098783
C 2.250145 1.898340 4.290231	C 2.045483 3.394577 3.315400
C 3.738083 2.193063 4.106793	C 3.063606 4.184227 2.491645
C 3.911409 2.715876 2.664629	C 3.154495 3.512055 1.108431
C 3.166320 1.766360 1.718790	C 1.724844 3.337599 0.602452
H 1.630065 2.814236 4.357024	H 1.522494 3.966957 4.103826
H 1.991514 1.199463 5.107392	H 2.463284 2.461493 3.740331
H 4.332282 1.268089 4.261202	H 4.042714 4.196358 3.008646
H 4.086298 2.933757 4.853332	H 2.729891 5.236625 2.380720
H 4.980196 2.784966 2.382616	H 3.655340 2.524530 1.188641
H 3.486104 3.737971 2.586905	H 3.738798 4.123545 0.393329
H 3.754009 0.886797 1.392723	H 1.582320 2.556768 -0.167486
O 0.456076 1.624011 2.243795	O -0.486606 3.641893 2.227357
O 1.919731 -0.400937 2.856243	O 0.658758 1.347579 2.179179
Li -0.556379 0.838306 0.783152	Li 0.051389 0.187925 0.757906
H 0.510228 -1.861957 -2.183979	H 3.116136 -2.405957 -1.414167
S 1.858209 0.020695 -1.510842	S 2.005156 -0.301582 -1.602258
C 1.734369 1.401007 -2.711918	C 0.713219 -0.671519 -2.856186
C 1.800214 0.703301 -4.070910	C 1.154113 -1.993951 -3.481720
C 0.931957 -0.568267 -3.957922	C 2.693097 -1.990165 -3.541319
C 1.332115 -1.304627 -2.674473	C 3.191115 -1.586068 -2.155189
H 0.746785 1.869791 -2.533565	H -0.255354 -0.711425 -2.328136
H 2.562487 2.099057 -2.488555	H 0.735885 0.178221 -3.565218
H 2.850373 0.444323 -4.322390	H 0.704998 -2.107158 -4.487612
H 1.426114 1.376598 -4.866977	H 0.795254 -2.842773 -2.863097
H 1.060900 -1.228667 -4.837712	H 3.046887 -1.265148 -4.303504
H -0.135723 -0.278434 -3.901367	H 3.095301 -2.984787 -3.815260
H 2.228779 -1.944124 -2.791835	H 4.201989 -1.139280 -2.118511
O 0.833103 0.187737 -0.417381	O 1.511457 -0.667707 -0.218240
O 3.267883 -0.182927 -1.073258	O 2.566280 1.073024 -1.779534
H -3.602638 -0.145382 -0.277017	H -2.721885 -0.442423 -1.151966
S -2.448331 1.482118 -1.575719	S -1.979766 1.846806 -1.236024
C -3.816867 2.650108 -1.963352	C -2.793617 3.057555 -0.117620
C -5.097693 1.863886 -1.670389	C -4.074953 2.362356 0.360702
C -4.828258 0.389698 -2.040221	C -3.849054 0.837152 0.311213
C -3.511007 -0.002998 -1.371704	C -3.233767 0.534485 -1.051321
H -3.658088 3.554105 -1.346921	H -2.059214 3.248497 0.691103
H -3.691318 2.893618 -3.036453	H -2.956947 3.982723 -0.700851
H -5.949966 2.281812 -2.241349	H -4.919279 2.630464 -0.305924
H -5.354577 1.943345 -0.593537	H -4.334667 2.701103 1.382288
H -4.749706 0.275263 -3.141945	H -4.799107 0.281571 0.434842
H -5.649616 -0.272281 -1.702144	H -3.165927 0.507391 1.122244
H -2.962849 -0.858974 -1.807686	H -3.952237 0.676112 -1.883255
O -1.832794 1.867026 -0.254963	O -0.700600 1.379905 -0.573238
O -1.540850 1.333717 -2.752156	O -1.851742 2.334038 -2.640522
H 1.244737 -1.807345 1.315515	H 0.980306 -3.077956 1.376259
S -1.022124 -2.250034 0.606420	S -1.153217 -2.579326 0.431612

C	-1.898985	-3.537733	1.589529	C	-2.291515	-3.747610	1.258817
C	-0.794373	-4.484594	2.065484	C	-1.366835	-4.694424	2.020930
C	0.456152	-3.624421	2.340425	C	-0.153029	-4.959404	1.110177
C	0.674230	-2.733759	1.118446	C	0.361202	-3.603508	0.624772
H	-2.386443	-2.987814	2.417943	H	-2.989510	-3.150417	1.874349
H	-2.661666	-3.988095	0.927502	H	-2.842511	-4.253906	0.442003
H	-0.574119	-5.238142	1.280687	H	-1.903370	-5.630554	2.270117
H	-1.120280	-5.039268	2.967246	H	-1.041977	-4.230480	2.975355
H	1.351938	-4.248667	2.527114	H	-0.457380	-5.583453	0.244720
H	0.308828	-2.990835	3.239882	H	0.651844	-5.499409	1.645484
H	1.091171	-3.282059	0.250694	H	0.881272	-3.615920	-0.349883
O	-1.396955	-0.903320	1.174054	O	-1.042879	-1.329824	1.280071
O	-1.223129	-2.458927	-0.861515	O	-1.513736	-2.382065	-1.010037

Li⁺ in TMS

E (PBE-D3/ma-def2-svp GAS_OPT) =	-7.2519251623
E (PBE-D3/ma-def2-svp SMD_OPT) =	-7.3917970144
ΔG_{corr} (ID-RR-HR GAS) =	-0.0127326619
E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT GAS) =	-7.2736440090
E (DLPNO-CCSDT/cc-p(wC)VTZ GAS_OPT SMD) =	-7.4156879765
E (DLPNO-CCSDT/cc-p(wC)VTZ SMD_OPT SMD) =	-7.4156879765
E (PBE-D3/ma-def2-tzvp GAS_OPT GAS) =	-7.2566456293
E (PBE-D3/ma-def2-tzvp GAS_OPT SMD) =	-7.3956692142
E (PBE-D3/ma-def2-tzvp GAS_OPT CPCM) =	-7.4407977109
GAS_OPT	SMD_OPT
Li 0.0 0.0 0.0	Li 0.0 0.0 0.0