Supporting information for

Understanding the Solvation-Dependent Properties of Cyclic Ether Multivalent Electrolytes Using High Field NMR and Quantum Chemistry

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Relationship between ^{43}Ca (^{67}Zn) chemical shielding and the number of the H_2O molecules:

To establish the relationship between the calculated ^{43}Ca (^{67}Zn) absolute chemical shielding and the number of H_2O molecules, a large number of calculations were carried out focusing on (1) finding out the impact of the number of H_2O molecules, and how the initial coordination setup affects the fully geometry-optimized solvation structures as there is always a chance the optimized structure lands on a local energy minimum rather than a global energy minimum given the large number of H_2O molecules involved in the process of geometry optimization; (2) establishing the relationship between the calculated chemical shielding and the number of H_2O molecules via statistical analysis by fitting the data in (1); and (3) establishing the relationship between the calculated chemical shielding and the number of H_2O molecules by first optimizing a solvation structures with a large number of H_2O molecules, e.g., 27 H_2O, and then systematically removing one H_2O at a time from the most outer shells and calculating the absolute chemical shielding using a single point calculation. The following results are obtained:

(1) The fully optimized geometries for, e.g., Ca, for a given number of H_2O molecules depend on the initial geometry setup and thus, the calculated ^{43}Ca absolute chemical shielding varies accordingly. The results are summarized in Figure S1 and Table S1.

(2) It is found by statistical analysis, see Figure S1, that the relationship between the calculated chemical shielding and the number of H_2O molecules approximately follows the equation of

$f = y0+(a/x)$, where "f" is the calculated ^{43}Ca chemical shielding and "x" is the number of H_2O molecules, "y0" is the chemical shielding of Ca in vacuum and "a" is the water molecule scaling factor. Regression analysis reveals y0=1093.3 ± 2.7 ppm with R = 0.91 and p value of <0.0001. This confirms that the initial selection of 1092.8 ppm as the ^{43}Ca reference is valid.

To further consolidate the selection of the reference, we further employed COSMO (A., Klamt; G., Schüürmann (1993). "COSMO: a new approach to dielectric screening in solvents with explicit expressions

for the screening energy and its gradient". *J. Chem. Soc*. Perkin Trans.2. **2** (5): 799–805. doi:10.1039/P29930000799) to include the electrostatic interaction of the solvation cluster with the solvent H_2O as a continuum to simulate the case with an infinite number of H_2O molecules. The results Figure S2 and Table S1 indicate a ^{43}Ca chemical shielding of 1094.5 ± 2.7 ppm, in excellent agreement with that extrapolated from the cluster model calculations above.

The calculated ^{43}Ca chemical shielding for the Ca^{2+} solvation structure with 27 H_2O molecules is 1105.8 ppm. By removing one of the most outer shell H_2O molecules, the calculated ^{43}Ca shielding becomes 1105.5 ppm based on the remaining intact structures. By subsequently removing outer shell molecules one at a time, a relationship between the calculated chemical shielding and the number of H_2O molecules is obtained with the shielding value reaching 1114.2 ppm for 6 H_2O molecules, the fully coordinated 1st shell solvation structure (See Figure S3 and Table S1). Apparently, the ^{43}Ca chemical shielding is relatively insensitive to the number of H_2O molecules in the 2nd and 3rd solvation shells as long as the geometries of the first shell structures remain the same. This supports the typical view that NMR is a local structure probe. However, care must be taken as the longer-range structures affect the local structure of a cluster and thus the calculated chemical shielding. For example, the calculated ^{43}Ca chemical shielding for a fully optimized structure, $Ca^{2+}(H_2O)_6$, is 1139 ppm when constructed, rather than from removal of waters from a larger cluster. An extension of the study from this practice is that for a system with known crystal structure, NMR calculations on crystal structures with only up to 3rd shells should be sufficiently accurate (though this is not the focus of this work).

Table S1: The relationship between ^{43}Ca chemical shielding and the number of the H_2O molecules with different calculation strategies.

	Geometry optimization 1 ^{43}Ca chemical shift (ppm)	Geometry optimization 2 ^{43}Ca chemical shift (ppm)	Single point calculation by removing H2O ^{43}Ca chemical shift (ppm)	COSMO Effect ^{43}Ca chemical shift (ppm)
$6H_2O$	1134.50	1139.37	1114.15	1121.70
$7H_2O$		1132.82		
$8H_2O$		1129.37	1112.29	1118.27
$9H_2O$		1129.79		
$10H_2O$	1124.35	1128.20	1110.10	1116.74
$12H_2O$	1118.48	1112.39	1109.98	
$13H_2O$		1121.20		
$14H_2O$		1120.81	1108.11	
$15H_2O$		1114.80		
$16H_2O$	1108.24	1106.30	1106.06	
$17H_2O$		1107.57		
$18H_2O$		1108.23	1105.78	1101.39
$19H_2O$		1108.92		
$20H_2O$	1092.61	1109.75		1104.03
$24H_2O$		1105.87		
$25H_2O$			1105.75	
$26H_2O$			1105.47	
$27H_2O$		1105.81	1105.81	

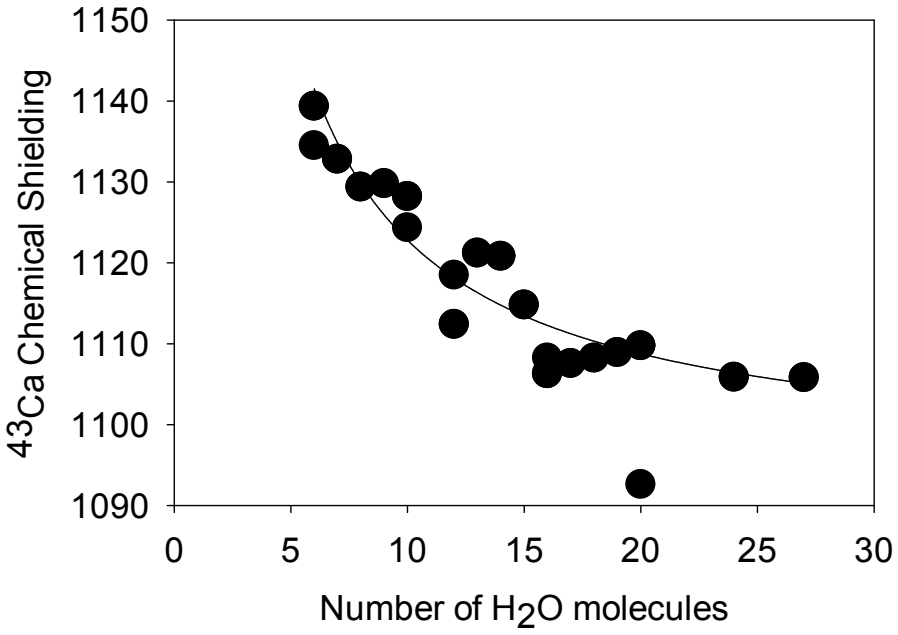


Figure S1: The relationship between ^{43}Ca chemical shielding and the number of the H_2O molecules with all the data from Geometry Optimization 1 and Geometry Optimization 2 from Table S1, highlighting the impact of initial geometry setup, thus the possibilities of landing at a local energy minimum for geometry optimization and the chemical shielding. However, the statistical results extrapolated to infinite number of water molecules converges to the value of 1093.3 ± 2.7 ppm that is independent of the initial geometry set up.

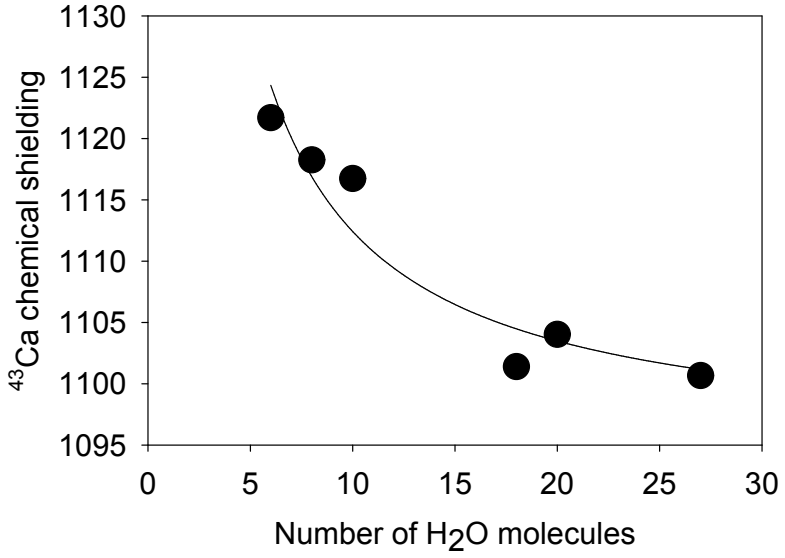


Figure S2: The relationship between ^{43}Ca chemical shielding and the number of the H_2O molecules with COSMO effect. The chemical shielding at infinite number of water molecules is 1094.5 ± 2.7 ppm, in excellent agreement with that extrapolated from cluster model calculations in Figure S1.

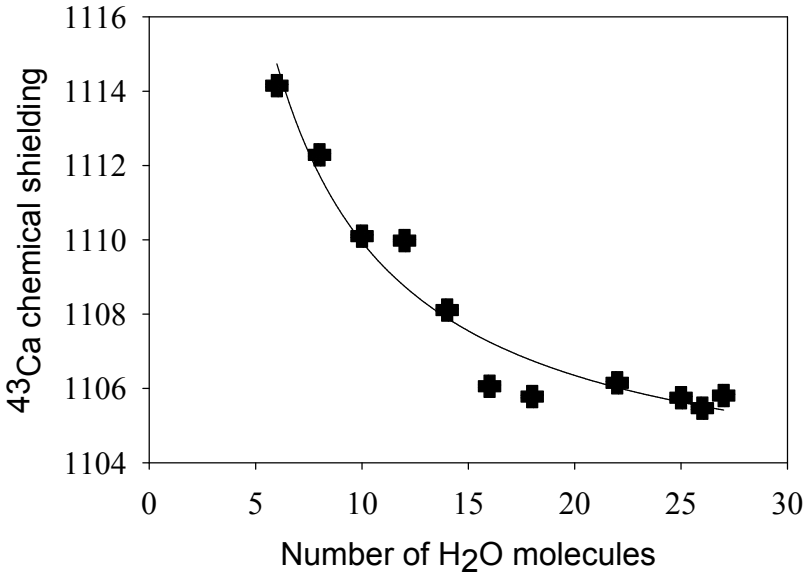


Figure S3: The relationship between ^{43}Ca chemical shielding and the number of the H_2O molecules by removing H_2O sequentially with single point calculations (fourth column, Table S1). The calculated ^{43}Ca chemical shielding for the solvation structures with 27 H_2O molecules is 1105.8 ppm. By removing one of

the most outer shell H_2O molecules, the calculated ^{43}Ca shielding becomes 1105.5 ppm based on the remaining intact structures. By subsequently removing outer shell molecules one at a time, a relationship between the calculated chemical shielding and the number of H_2O molecules is also obtained with the shielding lands at 1114.2 ppm for 6 H_2O molecules, the fully coordinated 1st shell solvation structure. Apparently, the ^{43}Ca chemical shielding is insensitive to the number of H_2O molecules in the 2nd and the 3rd solvation shells as long as the geometries of the first shell structures remain the same. This supports the claim in the literatures "NMR is a local structure probe". However, care must be taken as the longer range structure affects the local structures in a cluster and thus the calculated chemical shielding. For example, the calculated ^{43}Ca chemical shielding for a fully optimized structure, Ca $(H_2O)_6$, is 1139 ppm.

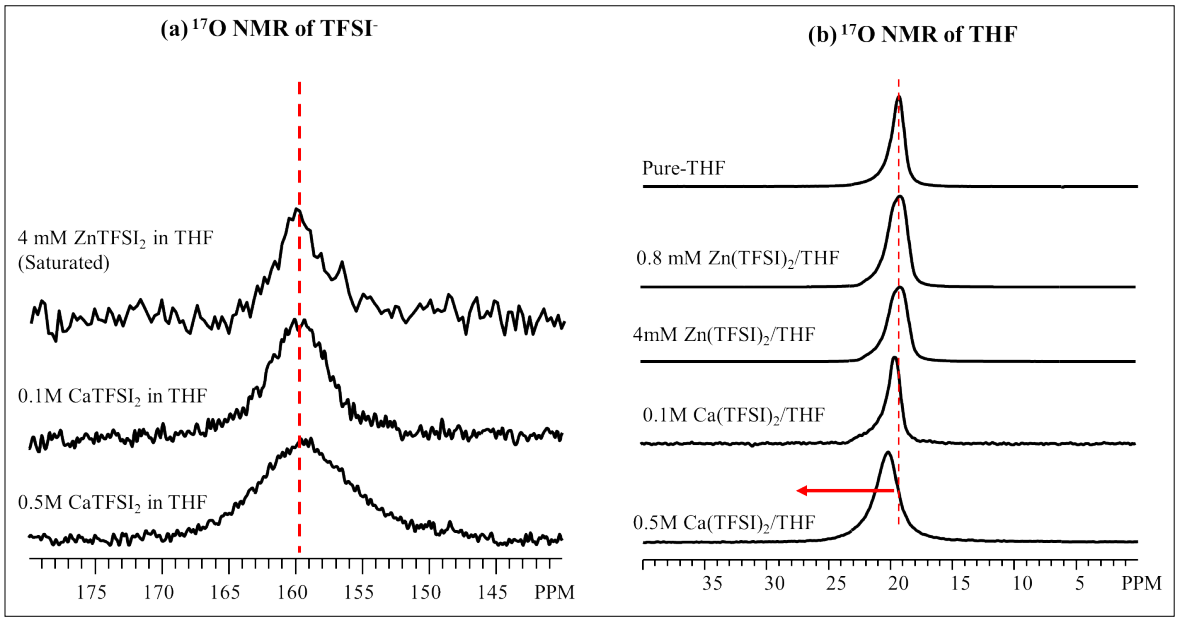


Figure S4. ^{17}O NMR spectra (with reference to D_2O) of the $TFSI^-$ anion (a) and THF solvent (b) in electrolytes with two different concentrations of $Ca(TFSI)_2$ and $Zn(TFSI)_2$ in THF, showing the increased line broadening of both the anions and the solvents at increased concentration and the trend of the chemical shifts.

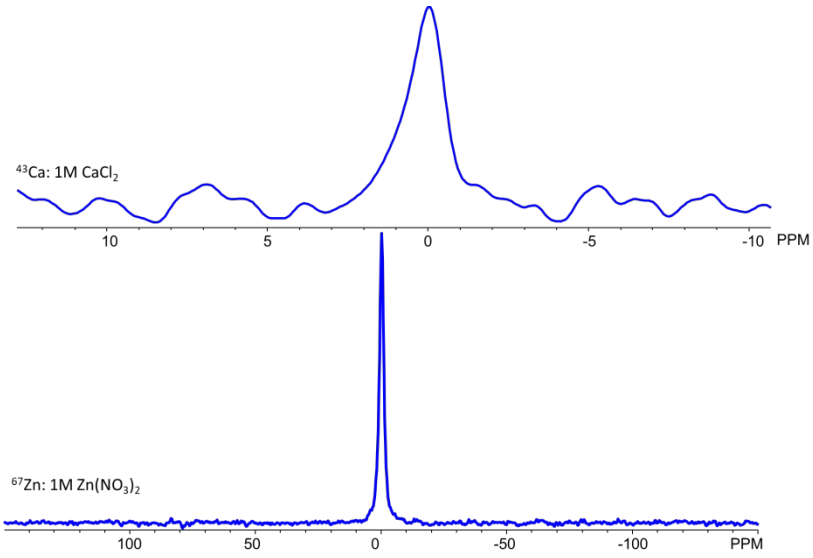


Figure S5: Representative reference NMR spectra. ^{43}Ca $\nu_{1/2}$: 62 Hz ^{67}Zn $\nu_{1/2}$: 85 Hz

Calculated Model Shielding

References:

$14H_2O_{center}$: 247.82

Ca-20 H_2O: NoFC: 1092.8 ppm

Zn-10 H_2O-NoFC: 1789.6 ppm

Zn-12 H_2O-NoFC: 1788.33 ppm

Zn-20 H_2O-NoFC: 1785.8 ppm

Model Equations

$\delta_{17O} = 247.82 - \sigma_{calc}$

$\delta_{43Ca} = 1093 - \sigma_{calc}$

$\delta_{79Zn} = 1788 - \sigma_{calc}$

Additional description of theoretical calculations:

Given the experimental values of ~20 ppm (THF, of which a vast majority are free in solution), 160 ppm ($TFSI^-$) and -19 ppm (^{43}Ca) for ^{17}O in the case of $Ca(TFSI)_2$ dissolved in THF, the probable solvation

structures, based on best agreement with experimental values, consist of contact ion pairs solvated by 4 THF molecules, i.e., the $Ca(TFSI)^+$ with a Ca-O coordination number of six (cluster formation energy derived from 0 K geometry optimization energies of -391 kcal/mol), neutral species of $Ca(TFSI)_2$ with 1 and 2 THF molecules (-440 and -454 kcal/mol), and pure THF solvated species of Ca^{2+} with 5 and 6 THF molecules (-260, and -277 kcal/mol). The free energy trend of neutral < +1 < +2 is likely a result of decreased energy from the ionic bonding. For comparison of these cluster models, it may be prudent to compare energies only across a given charge. Taking this into account, it may be possible to narrow the solvation structures which match the observed chemical shift by preferring those with lower energies. The results clearly suggest that neutral clusters are the most prevalent species in solutions for $Ca(TFSI)_2$ in THF, a result consistent with those from Raman studies of $TFSI^-$ coordination.[25]

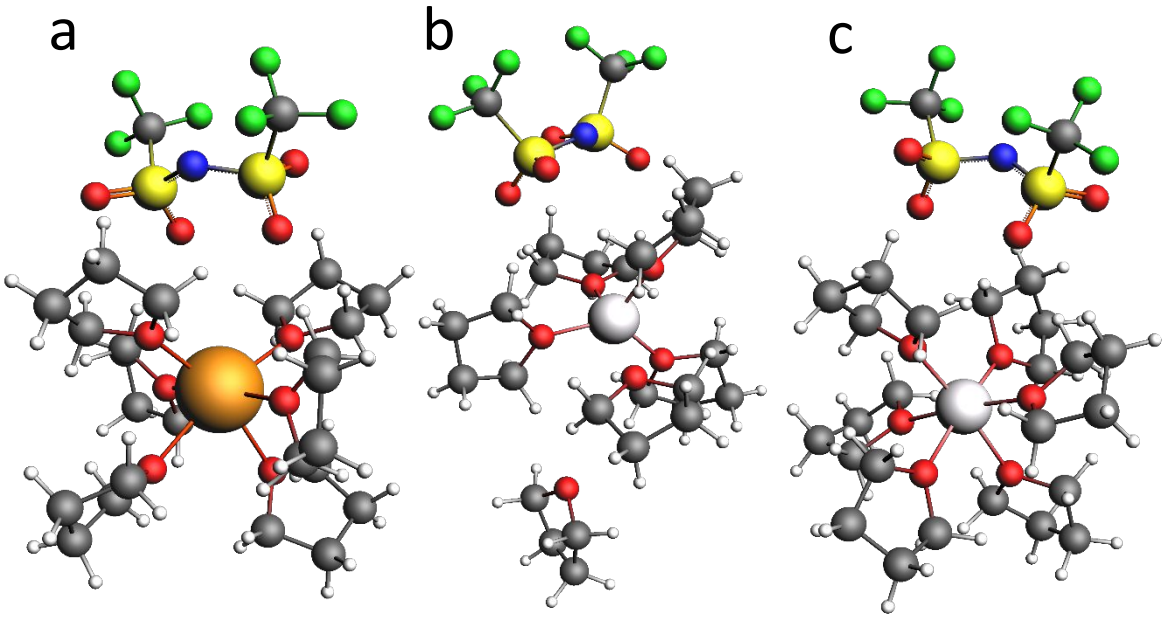
For the cases of $Ca(TFSI)_2$ in 2-MeTHF, the experimental values are ~47 ppm (2-MeTHF), 160 ppm ($TFSI^-$) and -23 ppm (^{43}Ca.). The most probable solvation structures include contact ion pairs solvated by four 2-MeTHF molecules, i.e., the $Ca(TFSI)^+$ with a Ca-O coordination number of six (-382 kcal/mol), neutral species of $Ca(TFSI)_2$ with two 2-MeTHF molecules (-452 kcal/mol), and pure 2-MeTHF solvated species of Ca^{2+} with six 2-MeTHF molecules (-262 kcal/mol compared to -254 kcal/mol with only five 2-MeTHF molecules). The neutral species of $Ca(TFSI)_2$ with two 2-MeTHF molecules would be the most abundant solvation species based upon their lowest formation energy. Furthermore, the possibility of monodentate neutral $Ca(TFSI)_2$ solvation structures, where each $TFSI^-$ anion donates only one oxygen atom for the bonding with Ca^{2+}, derived from the study of Mg^{2+} systems,[34] has also been investigated with quantum chemistry calculations on models of $Ca(TFSI)_2$ coordinated with 4 solvent molecules of either THF or 2-MeTHF. The quantum chemistry predicted chemical shifts of 173.3 ppm ($TFSI^-$), 29.1 ppm (THF-O) and -43.8 ppm (Ca^{2+}) for $THF_4Ca(TFSI)_2$-monodentate, and 173.6 ppm ($TFSI^-$), 52.8 ppm (2-MeTHF-O) and -58.7 ppm (Ca^{2+}) for 2-$MeTHF_4Ca(TFSI)_2$-monodentate both are also close to experimental

values, suggesting these are also possible solvation structures. The relative energies are also low (-459 kcal/mol for the THF analog, and -449.2 kcal/mol for the 2-MeTHF analog), making them good contenders with the other reported structures. Though these predicted values are near those observed, the $TFSI^-$ and Ca chemical shift values are still 10 to 20 ppm disparate, so it is also possible that Ca with coordination number of 5 provides the best overall agreement (-458 kcal/mol for THF). The possible solvation structures justified by quantum chemistry calculations based on the best agreement with experimental results are summarized in Table 4. It is apparent that the solvation structures in the studied electrolytes contain multiple structures, indicating the co-existence of a range of complex solvation structures in the cases of $Ca(TFSI)_2$ dissolved in either THF or 2-MeTHF. Measured Raman spectra reveal noticeable differences in the $TFSI^-$ coordination structures of THF or 2-MeTHF that assist in identifying the most prevalent structures.[19] In particular, the reported line-shapes for the $TFSI^-$ breathing mode region suggest that THF tends to allow a mixture of monodentate (slight blue-shift) and bidentate (large blue-shift) coordinated $TFSI^-$ populations while 2-MeTHF primarily favors a bidentate coordinated population. This observation could be consistent with the relative free energy differences found among the computed clusters from quantum chemistry and with the slightly different $^{17}O_{TFSI}$ chemical shift values in THF vs. 2-MeTHF.

In contrast, for the cases of $Zn(TFSI)_2$ dissolved in THF or 2-MeTHF with increasing Zn-O coordination number the ^{17}O chemical shifts of $TFSI^-$ anion and the solvents shift downfield (increased chemical shift values) while the chemical shift of ^{67}Zn shifts upfield (decreased chemical shift values) for each of the three types of model solvation structures: Zn^{2+} solvated by solvents only, bidentate $ZnTFSI^+$ contact ion pairs, and neutral species of $Zn(TFSI)_2$. This distinct difference with respect to the cases of Ca^{2+} highlights the cation size effect. Given the experimental values of about 45 ppm (2-MeTHF), 154 ppm ($TFSI^-$) and -50 ppm (^{67}Zn) for $Zn(TFSI)_2$ dissolved in 2-MeTHF, the most probable solvation structures, based on best agreement with experimental values, include contact ion pairs solvated by four 2-MeTHF molecules, i.e.,

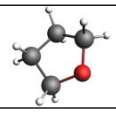
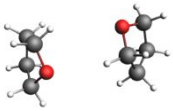
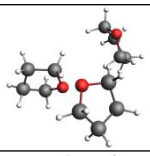
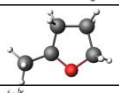
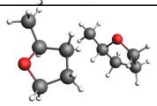
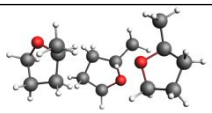
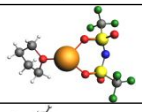
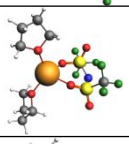
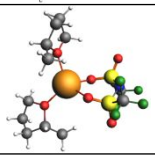
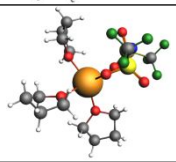
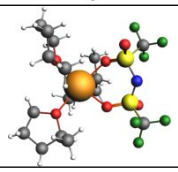
the bidentate $ZnTFSI^+$ with Zn-O coordination number of 6 (-483 kcal/mol), neutral $Zn(TFSI)_2$ solvated by two 2-MeTHF also with a Zn-O coordination number of 6 (-560 kcal/mol), the Zn solvated only by five 2-MeTHF molecules with a Zn-O coordination number of 5 (-362 kcal/mol), and monodentate $TFSI^-$ neutral species with $Zn(TFSI)_2$ coordinated by four 2-MeTHF molecules (-549.6 kcal/mol). Since it is not presently possible to obtain ^{67}Zn NMR spectra on $Zn(TFSI)_2$ dissolved in THF due to the low solubility (4 mM and lower), no experimental shift is available to compare with computed values. If the experimental ^{67}Zn chemical shift in THF were to be close to that of ^{67}Zn of $Zn(TFSI)_2$ in 2-MeTHF, there might be some agreement with quantum chemistry calculations which indicate that they would be similar (compare Table 3 and Figure 4); however, this is only speculation. Experimentally, we do know that the ^{17}O chemical shift of the $TFSI^-$ oxygen is located at about 154 ppm while that of the THF oxygen is at about 19 ppm, the latter of which is the same as from pure THF. This is quite reasonable as for a solution of 4 mM $Zn(TFSI)_2$ in THF, most of the THF molecules do not participate in the solvation structure of Zn^{2+} on the timescale of an NMR experiment. The weighted average of the chemical shifts will be nearly the same as that of pure THF assuming fast molecular exchange between the Zn-bonded and the free THF molecules. Therefore, one must rely on the $^{17}O_{TFSI}$ chemical shift of 160 ppm to deduce the solvation structures. The most likely solvation structures are, therefore, the neutral bidentate $Zn(TFSI)_2$ species solvated by two THF molecules (Zn-O cordination number = 6), where the predicted chemical shifts are about 158 ppm (^{17}O in $TFSI^-$), 4 ppm (^{17}O in THF) and -58 ppm (^{67}Zn), and the monodentate $Zn(TFSI)_2$ with four THF molecules (Zn-O coordination number = 6), where the predicted chemical shifts are about 166 ppm (^{17}O in $TFSI^-$), 16.8 ppm (^{17}O in THF) and -87.5 ppm (^{67}Zn). It is thus apparent that the range of accessible solvation structures of $Zn(TFSI)_2$ in THF is much narrower the range present in 2-MeTHF, restricted to predominantly monodentate and bidentate neutral species. This small number of accessible solvation structures and the attendant lower entropy gain for dissolution may be the reason why the solubility of $Zn(TFSI)_2$ in THF is much lower than that in 2-MeTHF.

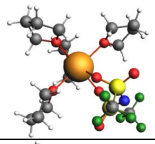
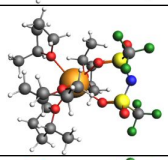
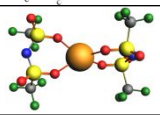
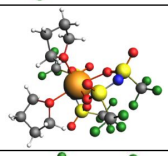
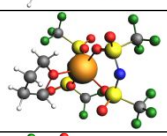
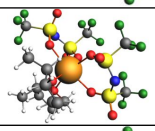
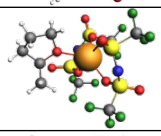
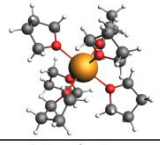
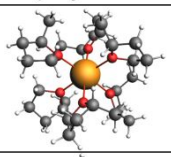
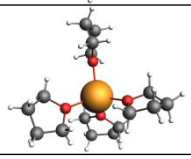
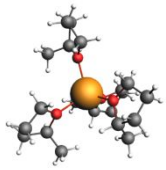
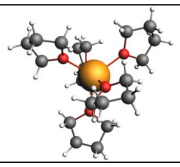
The preferred THF cluster also has a formation energy about 10 kcal/mol lower in magnitude than the 2-MeTHF analog, suggesting the latter is more strongly solvated. Further, these two structures also exhibit relatively tighter binding compared to most other clusters models presented at -563 kcal/mol. The results suggest that monodentate $TFSI^-$ is preferred in THF while bidentate $TFSI^-$ is preferred in 2-MeTHF, a result consistent with differences in the Raman spectra of these solutions in our previous works. A possible explanation is that the monodentate configuration allows more solvent molecules to coordinate to Zn^{2+}, which increases the formation energy in THF but not in 2-MeTHF due to the steric effect of the latter solvent's additional methyl group adjacent to the coordinating oxygen atom. It is worth considering why the monodentate-type structure could limit solubility. Perhaps this structure favors aggregation by allowing the $TFSI^-$ to bridge between Zn^{2+} species more easily. Table 4 summarizes the probable solvation structures for both Ca/Zn $(TFSI)_2$ in solvents of THF/2-MeTHF from this study.

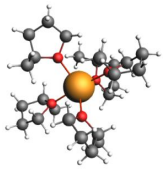
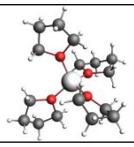
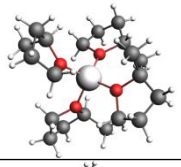
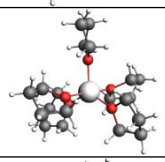
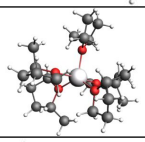
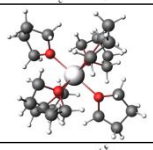
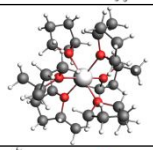
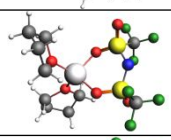
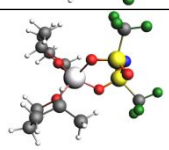
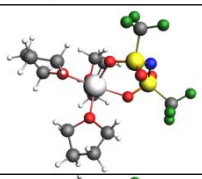
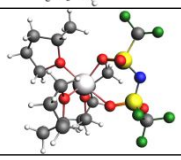


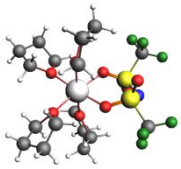
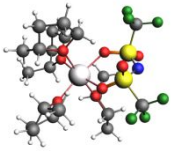
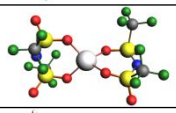
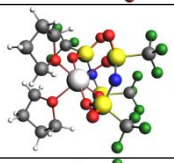
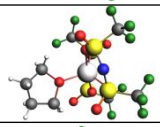
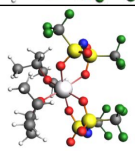
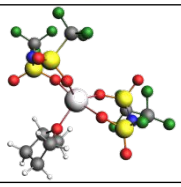
Scheme S1: Possible solvent-shared ion pairs (SIP) (a): $THF_6Ca(TFSI)^+$ (b) $THF_6Zn(TFSI)^+$ (c) $THF_6Zn(TFSI)^+$ Isomer

Table S2: Calculated Model Chemical Shift, where the reported chemical shifts are average values among the chemically equivalent sites between different molecules due to fast exchanging of the molecules in the models as explained in details in the text.

Structure	Model	δ $^{17}O_{TFSI}$	δ $^{17}O_{THF\ or\ 2\text{-}MeTHF}$	δ ^{43}Ca or ^{79}Zn
	THF_1		-2.29	
	THF_2		24.055	
	THF_3		20.12	
	2MeTHF		29.93	
	2-$MeTHF_2$		52.135	
	2-$MeTHF_3$		39.38	
	$THFCa(TFSI)^+$	183.735	50.61	-45.46
	$THF_2Ca(TFSI)^+$ (Coordination number 4)	178.975	38.505	-6.35
	2-$MeTHF_2Ca(TFSI)^+$NoFC (Coordination number 4)	178.4225	72.645	0.24
	$THF_3Ca(TFSI)^+$ (Coordination number 5)	173.2225	30.32	-12.89
	2-$MeTHF_3Ca(TFSI)^+$ (Coordination number 5)	173.2925	61.503	-9.83

	$THF_4Ca(TFSI)^+$ (Coordination number 6)	170.5225	22.275	-35.89
	2-$MeTHF_4Ca(TFSI)^+$ (Coordination number 6)	173.14	51.9625	-47.42
	$Ca(TFSI)_2$ (Coordination number 4)	167.97125		-35.06
	$THF_2Ca(TFSI)_2$ (Coordination number 6)	166.489	19.205	-41.03
	$THFCa(TFSI)_2$ (Coordination number 5)	165.045	29.43	-35.46
	2-$MeTHF_2Ca(TFSI)_2$ (Coordination number 6)	166.391	52.395	-42.3
	2-$MeTHFCa(TFSI)_2$ (Coordination number 5)	166.031	63.49	-30.84
	THF_6Ca^{2+} (Coordination number 6)		26.972	-37.78
	2-$MeTHF_6Ca^{2+}$ (Coordination number 6)		58.44	-60.01
	THF_4Ca^{2+} (Coordination number 4)		49.275	6.48
	2-$MeTHF_4Ca^{2+}$ (Coordination number 4)		82.487	12.13
	THF_5Ca^{2+} (Coordination number 5)		35.346	-13.92

	2-MeTHF$_5$Ca^{2+} (Coordination number 5)		67.156	-19.28
	THF$_4$Zn^{2+} (Coordination number 4)		-2.253	71.13
	2-MeTHF$_4$Zn^{2+} (Coordination number 4)		31.0576	71.43
	THF$_5$Zn^{2+} (Coordination number 5)		7.634	-16.15
	2-MeTHF$_5$Zn^{2+} (Coordination number 5)		43.898	-63.39
	THF$_6$Zn^{2+} (Coordination number 6)		15.262	-105.29
	2-MeTHF$_6$Zn^{2+} (Coordination number 6)		46.388	-185.33
	THF$_2$Zn(TFSI)$^+$ (Coordination number 4)	155.84	-5.605	101.93
	2-MeTHF$_2$Zn(TFSI)$^+$ (Coordination number 4)	155.335	27.425	94.73
	THF$_3$Zn(TFSI)$^+$ (Coordination number 5)	161.755	1.873	9.25
	2-MeTHF$_3$Zn(TFSI)$^+$ (Coordination number 5)	162.175	34.773	3.18

	$THF_4Zn(TFSI)^+$ (Coordination number 6)	163.665	8.4925	-82.72
	2-$MeTHF_4Zn(TFSI)^+$ (Coordination number 6)	171.51	43.1325	-140.33
	$Zn(TFSI)_2$ (Coordination number 4)	143.125		95.87
	$THF_2Zn(TFSI)_2$ (Coordination number 6)	158.29	4.135	-57.92
	$THFZn(TFSI)_2$ (Coordination number 5)	152.781	-2.01	9.22
	2-$MeTHF_2Zn(TFSI)_2$ (Coordination number 6)	159.284	38.98	-74.14
	2-$MeTHFZn(TFSI)_2$ (Coordination number 5)	153.344	31.99	5.34

Neat Solvents: It is shown in Table S2 that the average of the predicted ^{17}O chemical shift value of 22 ppm (using a cluster containing two (24 ppm) and three (20 ppm) THF molecules) is in excellent agreement with the experimental value for neat THF of 19.5 ppm. Likewise, the average of the predicted values of 45.8 ppm for cluster models containing two (52.1 ppm) and three (39.4 ppm) 2-MeTHF molecules are also close to the experimental value of 46.7 ppm for neat 2-MeTHF. Using a cluster model with more than one THF or 2-MeTHF molecule is needed for taking account of the hydrogen bonding and nearest neighbor effects in bulk solvents; however, it is noted that these effects are less prominent for non-polar and/or aprotic solvents in contrast to water, alcohol, etc. These results suggest that ^{17}O NMR chemical shift prediction is accurate with the basis set of TZ2P and the method of BLYP and can be employed for

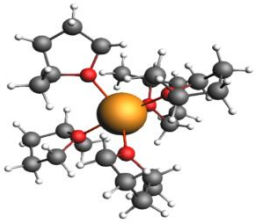
identifying solvation structures based on the best value agreement between the theory predicted and the experimentally observed chemical shift values.

Table S3: DFT total bonding energies of the cluster models

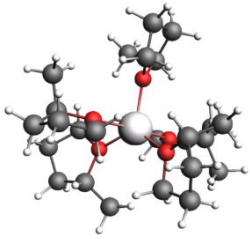
Model	**DFT Energy (0 K)**	
Zn^{2+}	651.16	kcal/mol
Ca^{2+}	417.59	kcal/mol
TFSI-cis	-1872.05	kcal/mol
TFSI-trans	-1872.93	kcal/mol
THF	-1580.92	kcal/mol
THF_2	-3162.62	kcal/mol
THF_3	-4743.77	kcal/mol
2-MeTHF	-1947.01	kcal/mol
2-$MeTHF_2$	-3894.42	kcal/mol
2-$MeTHF_3$	-5840.59	kcal/mol
2-$MeTHF_2$-TFSI	-5772.15	kcal/mol
2-$MeTHF_3$-TFSI	-7720.59	kcal/mol
THF_2-TFSI	-5040.09	kcal/mol
THF_3-TFSI	-6622.93	kcal/mol
$THFCa(TFSI)^+$	-3354.57	kcal/mol
$THF_2Ca(TFSI)^+$	-4968.81	kcal/mol
$THFZn(TFSI)^+$	-3246.19	kcal/mol
$THF_2Zn(TFSI)^+$	-4860.40	kcal/mol
THF_5Ca	-7746.50	kcal/mol
THF_6Ca	-9344.94	kcal/mol
$THF_4Ca(TFSI)^+$	-8169.24	kcal/mol
$THF_3Ca(TFSI)^+$	-6572.13	kcal/mol
$THFCa(TFSI)_2$	-5347.22	kcal/mol
$THF_2Ca(TFSI)_2$	-6942.24	kcal/mol
$THF_4Ca(TFSI)_2$	-10109	kcal/mol
2-$MeTHF_5Ca$	-9571.20	kcal/mol
2-$MeTHF_6Ca$	-11526.06	kcal/mol
2-$MeTHF_3Ca(TFSI)^+$	-7668.58	kcal/mol
2-$MeTHF_4Ca(TFSI)^+$	-9624.53	kcal/mol
2-$MeTHFCa(TFSI)_2$	-5712.78	kcal/mol
2-$MeTHF_2Ca(TFSI)_2$	-7672.75	kcal/mol
THF_5Zn	-7627.47	kcal/mol
THF_6Zn	-9216.06	kcal/mol
$THF_4Zn(TFSI)^+$	-8044.25	kcal/mol

$THF_3Zn(TFSI)^+$	-6455.91	kcal/mol
$THFZn(TFSI)_2$	-5228.08	kcal/mol
$THF_2Zn(TFSI)_2$	-6817.63	kcal/mol
$THF_4Zn(TFSI)_2$	-9980.01	kcal/mol
2-$MeTHF_5Zn$	-9446.34	kcal/mol
2-$MeTHF_6Zn$	-11385.08	kcal/mol
2-$MeTHF_3Zn(TFSI)^+$	-7552.41	kcal/mol
2-$MeTHF_4Zn(TFSI)^+$	-9492.04	kcal/mol
2-$MeTHFZn(TFSI)_2$	-7546.71	kcal/mol
2-$MeTHF_2Zn(TFSI)_2$	-7546.71	kcal/mol

Table S4: Cation size effect on metal-oxygen distance



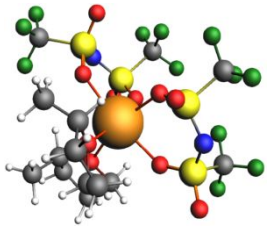
2-$MeTHF_5Ca^{2+}$



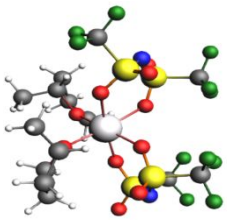
2-$MeTHF_5Zn^{2+}$

Ca-MeTHF	Zn-MeTHF
2.389	2.224
2.440	2.114
2.367	2.081

2.403	2.345
2.428	2.102
2.405 (average)	2.173(average)



2-MeTHF$_2$Ca(TFSI)$_2$

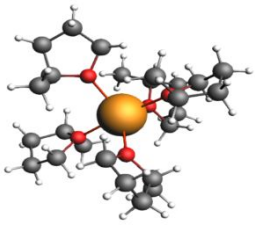
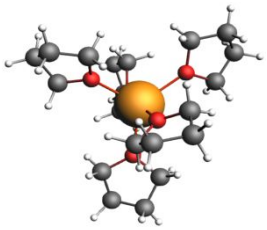


2-MeTHF$_2$Zn(TFSI)$_2$

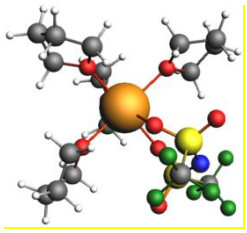
Ca-MeTHF	Ca-TFSI	Zn-MeTHF	Zn-TFSI
2.420	2.359	2.149	2.131
2.412	2.372	2.156	2.202

	2.356		2.134
	2.357		2.159
2.416(average)	2.361 (average)	2.153 (average)	2.157 (average)

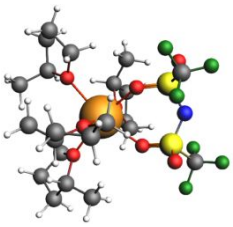
Table S5: Solvent effect on metal-oxygen distance

	
2-MeTHF$_5$Ca^{2+}	THF$_5$Ca^{2+}
Ca-MeTHF	Ca-THF

2.389	2.396
2.440	2.343
2.367	2.365
2.403	2.393
2.428	2.363
2.405 (average)	2.372 (average)



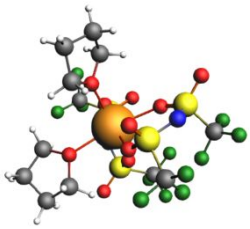
$THF_4Ca(TFSI)^+$



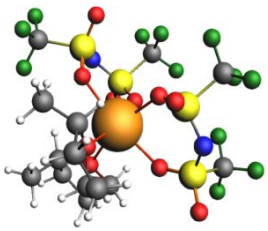
$2\text{-}MeTHF_4Ca(TFSI)^+$

Ca-THF	Ca-TFSI	Ca-MeTHF	Ca-TFSI
2.418	2.352	2.473	2.372
2.419	2.374	2.453	2.382
2.436		2.488	

2.42		2.455	
2.423(average)	2.363 (average)	2.467(average)	2.377 (average)

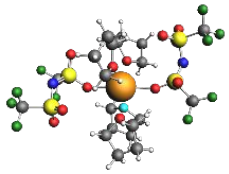


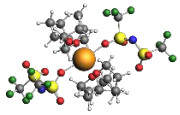
$THF_2Ca(TFSI)_2$



$2\text{-}MeTHF_2Ca(TFSI)_2$

Ca-THF	Ca-TFSI	Ca-MeTHF	Ca-TFSI
2.396	2.355	2.420	2.359
2.411	2.351	2.412	2.372
	2.359		2.356
	2.358		2.357
2.403(average)	2.355 (average)	2.416(average)	2.361 (average)





$THF_4Ca(TFSI)_2$-monodentate		$2\text{-}MeTHF_4Ca(TFSI)_2$-monodendate	
Ca-THF	Ca-TFSI	Ca-MeTHF	Ca-TFSI
2.389	2.359	2.478	2.347
2.427	2.335	2.494	2.38
2.433		2.475	
2.469		2.452	
2.429(average)	2.347 (average)	2.475(average)	2.363 (average)

Optimized Coordinates

1THF

1.H	-1.120215	0.169623	0.958222
2.O	-0.226159	-1.937256	2.716135
3.C	-1.555753	-2.300205	2.249755
4.C	-2.396008	-1.010661	2.283578
5.C	-1.328863	0.079573	2.032107
6.C	-0.105404	-0.488534	2.773727
7.H	-0.094587	-0.172285	3.829340
8.H	0.850135	-0.205833	2.314197
9.H	-1.478134	-2.700795	1.226085
10.H	-1.945591	-3.089204	2.905282
11.H	-2.854401	-0.875814	3.271840
12.H	-3.194689	-1.011637	1.533334
13.H	-1.625174	1.065781	2.406922

2THF

1.H	1.297281	-2.397355	0.250724
2.O	-0.530403	-2.004799	2.544985

3.C	-1.861902	-2.272979	3.032945
4.C	-2.651717	-0.961975	2.814765
5.C	-1.546768	0.142835	2.858758
6.C	-0.221681	-0.657878	2.974597
7.H	0.102590	-1.931414	-3.760199
8.H	-1.069547	-1.270058	-2.609853
9.H	0.607684	-3.676253	-2.194256
10.H	-0.601131	-2.991470	-1.096263
11.H	2.397989	-2.484898	-1.160967
12.O	1.288234	-0.722427	-0.946573
13.C	0.958142	-0.489188	-2.331956
14.C	-0.035064	-1.612878	-2.720504
15.C	0.280794	-2.754465	-1.699901
16.C	1.402428	-2.158098	-0.811099
17.H	-2.252111	-3.129637	2.473891
18.H	-1.823414	-2.536890	4.105532
19.H	-3.421927	-0.818078	3.580993
20.H	-3.147439	-0.973045	1.837985
21.H	-1.676454	0.822473	3.708534
22.H	-1.560480	0.744117	1.944084
23.H	0.137597	-0.676334	4.018395
24.H	0.577851	-0.283692	2.328300
25.H	1.872632	-0.542593	-2.950066
26.H	0.542324	0.521012	-2.406219
3THF			
1.H	0.761758	-2.390522	-0.107955
2.O	-0.717400	-1.681322	2.661908
3.C	-2.155721	-1.765970	2.583974
4.C	-2.665620	-0.755090	3.622193
5.C	-1.644557	0.405047	3.477937
6.C	-0.366580	-0.288198	2.920714
7.O	2.655306	-0.235519	5.097065
8.C	3.597530	-0.868675	4.201783
9.C	3.492550	-2.385205	4.494118
10.C	2.958282	-2.444015	5.962593
11.C	2.766561	-0.953520	6.346153
12.O	1.674256	-1.022050	-1.407405
13.C	0.545219	-0.782786	-2.274468
14.C	0.300425	-2.114826	-3.033738
15.C	1.011223	-3.185999	-2.144055
16.C	1.505254	-2.374230	-0.923017
17.H	3.317475	-0.590073	3.181367
18.H	4.615763	-0.493259	4.407246
19.H	4.460276	-2.886685	4.380650
20.H	2.784116	-2.858435	3.806932
21.H	3.658698	-2.943350	6.641524
22.H	2.006562	-2.983574	6.005852
23.H	3.635985	-0.578513	6.914479
24.H	1.856661	-0.753732	6.921223
25.H	0.802739	0.059561	-2.924766
26.H	-0.337177	-0.508117	-1.669499
27.H	0.745079	-2.082162	-4.034054
28.H	-0.770229	-2.316971	-3.151285
29.H	1.858012	-3.630546	-2.678196
30.H	0.337295	-3.997374	-1.846668
31.H	2.471955	-2.703711	-0.529131
32.H	-2.506848	-1.499329	1.569406
33.H	-2.435961	-2.804994	2.790201

34.H	-2.615401	-1.196327	4.625312
35.H	-3.698776	-0.437987	3.437694
36.H	-1.453887	0.909247	4.431029
37.H	-2.014110	1.158388	2.772033
38.H	0.464307	-0.292333	3.633738
39.H	-0.029748	0.182634	1.984727

4THF

1.H	1.658828	-2.695323	1.811821
2.O	-1.818631	-0.734815	2.885149
3.C	-3.010410	-0.101933	2.359239
4.C	-2.623840	1.362417	2.108717
5.C	-1.673182	1.643102	3.295921
6.C	-0.969122	0.284828	3.513414
7.O	2.680099	-0.623240	3.297503
8.C	3.945256	-0.625274	2.591647
9.C	4.933390	-1.419534	3.487306
10.C	4.253106	-1.418498	4.894570
11.C	3.011584	-0.518990	4.701499
12.O	2.532604	-2.871444	-0.064611
13.C	2.004912	-2.227147	-1.248995
14.C	0.698148	-1.556063	-0.803449
15.C	0.144513	-2.583372	0.212326
16.C	1.426512	-3.167641	0.849586
17.H	3.771063	-1.083921	1.613774
18.H	4.290213	0.414341	2.452054
19.H	5.921268	-0.945581	3.505921
20.H	5.061516	-2.441264	3.115660
21.H	4.914843	-1.036640	5.680390
22.H	3.948348	-2.432219	5.176295
23.H	3.245662	0.532030	4.951077
24.H	2.134070	-0.836802	5.272522
25.H	1.815194	-2.978096	-2.036764
26.H	2.766678	-1.526856	-1.611880
27.H	0.012516	-1.365444	-1.637469
28.H	0.914203	-0.601321	-0.307797
29.H	-0.415234	-3.366792	-0.315073
30.H	-0.516330	-2.133102	0.960492
31.H	1.366163	-4.256133	0.988643
32.H	-3.303840	-0.646028	1.453613
33.H	-3.832836	-0.172780	3.093156
34.H	-3.490774	2.032761	2.085201
35.H	-2.090500	1.455020	1.153957
36.H	-2.253107	1.924656	4.184067
37.H	-0.960817	2.449584	3.090981
38.H	-0.849115	0.036301	4.575081
39.H	0.015561	0.237180	3.032837
40.O	-0.118129	-2.032322	6.465942
41.C	-0.715590	-3.079463	5.654035
42.C	-1.731927	-3.766140	6.574866
43.C	-0.998133	-3.739946	7.937012
44.C	-0.163571	-2.435819	7.865740
45.H	-1.155234	-2.601450	4.773163
46.H	0.062842	-3.790052	5.325185
47.H	-1.984819	-4.780920	6.247229
48.H	-2.657247	-3.177790	6.619315
49.H	-0.339681	-4.612555	8.029291
50.H	-1.683382	-3.746601	8.791561
51.H	0.861709	-2.580723	8.236111

52.H	-0.623438	-1.613667	8.430991

1-2MeTHF

1.H	-2.283914	-2.961116	4.226218
2.O	-2.312403	-1.542669	2.692528
3.C	-2.476971	-1.887372	4.096975
4.C	-1.488463	-1.004776	4.892809
5.C	-1.250431	0.182273	3.934901
6.C	-1.308140	-0.492984	2.552737
7.H	-0.925841	1.179776	1.228566
8.H	-2.654316	0.896720	1.570192
9.H	-3.521087	-1.684782	4.377770
10.C	-1.690841	0.407001	1.381464
11.H	-1.774947	-0.177495	0.457939
12.H	-0.548652	-1.542553	5.071087
13.H	-1.892543	-0.701212	5.865070
14.H	-0.296313	0.692133	4.112314
15.H	-2.058295	0.922123	4.022305
16.H	-0.334395	-0.972347	2.341035

2-2MeTHF

1.H	-3.368413	-2.542106	3.294933
2.O	-3.851345	-0.795713	2.246481
3.C	-3.919751	-1.595910	3.442906
4.C	-3.259335	-0.742274	4.555461
5.C	-2.328324	0.229764	3.765527
6.C	-2.552266	-0.147363	2.274639
7.O	3.551285	-0.115609	4.713577
8.C	3.866951	-1.245484	3.859944
9.C	4.854997	-2.099618	4.696186
10.C	4.504447	-1.753049	6.176194
11.C	3.419833	-0.648294	6.047558
12.H	-2.709770	-1.365492	5.270037
13.H	-4.017646	-0.183958	5.114954
14.H	-1.274489	0.125351	4.047549
15.H	-2.617751	1.273166	3.938403
16.H	-1.790842	-0.890643	1.969941
17.H	2.938033	-1.824836	3.693094
18.C	4.393721	-0.731469	2.525358
19.H	5.886820	-1.810128	4.463171
20.H	4.749597	-3.168304	4.476670
21.H	5.384783	-1.377731	6.708581
22.H	4.126251	-2.619948	6.729825
23.H	3.545719	0.183658	6.748073
24.H	2.409594	-1.073689	6.183003
25.C	-2.553994	1.014187	1.287625
26.H	-2.768896	0.661060	0.272320
27.H	4.622120	-1.572149	1.858039
28.H	5.308902	-0.145217	2.674924
29.H	3.649439	-0.095138	2.032682
30.H	-1.573797	1.507387	1.279834
31.H	-3.314948	1.753362	1.567818
32.H	-4.973826	-1.829430	3.624950

3-2MeTHF

1.H	0.695144	-3.272347	-0.374360
2.O	-2.880581	-1.472680	2.597958
3.C	-2.934990	-1.833352	4.005079
4.C	-1.798438	-1.059414	4.706754
5.C	-1.589603	0.150088	3.771168
6.C	-1.856928	-0.452888	2.379698

7.O	3.383578	0.364373	4.786157
8.C	3.356615	-0.515840	3.614827
9.C	2.940659	-1.923040	4.143611
10.C	3.045714	-1.795575	5.682491
11.C	2.748191	-0.304418	5.894858
12.O	1.989452	-1.636931	-0.543301
13.C	1.501176	-1.067339	-1.787667
14.C	1.931986	-2.085362	-2.875542
15.C	2.034059	-3.442742	-2.113686
16.C	1.745158	-3.056303	-0.637867
17.H	2.592916	-0.133617	2.919725
18.C	4.724603	-0.459102	2.933740
19.H	3.580631	-2.715754	3.740640
20.H	1.908333	-2.147929	3.848897
21.H	4.062252	-2.024807	6.025716
22.H	2.347742	-2.452692	6.214375
23.H	3.171616	0.110615	6.816647
24.H	1.659312	-0.113408	5.891815
25.H	3.146417	0.330213	-1.978300
26.H	0.395931	-1.032621	-1.741380
27.H	2.905822	-1.797887	-3.290352
28.H	1.213353	-2.118686	-3.702412
29.H	3.035404	-3.874082	-2.217131
30.H	1.314223	-4.183393	-2.479966
31.H	2.397699	-3.551719	0.088411
32.H	-3.922875	-1.548363	4.398746
33.H	-2.828461	-2.923067	4.097187
34.H	-0.886377	-1.668501	4.751489
35.H	-2.061016	-0.772852	5.731301
36.H	-0.588245	0.587989	3.850719
37.H	-2.325814	0.937378	3.985916
38.H	-0.942589	-0.955144	2.016159
39.C	-2.348659	0.522840	1.312995
40.C	2.049813	0.345994	-1.944663
41.H	4.697117	-1.007226	1.983171
42.H	5.499684	-0.898093	3.575287
43.H	5.000959	0.580462	2.722156
44.H	-1.572078	1.265865	1.088655
45.H	-3.250673	1.046654	1.653408
46.H	-2.589284	-0.010767	0.386174
47.H	1.736125	0.980878	-1.108092
48.H	1.678968	0.795851	-2.874248

4-2MeTHF

1.H	-3.932012	0.459861	1.308693
2.O	0.749984	0.038902	0.599555
3.C	0.026745	1.237901	1.178131
4.C	1.080560	1.980732	2.035071
5.C	2.403788	1.713375	1.255748
6.C	2.252582	0.247688	0.769864
7.O	1.030637	0.215536	5.078669
8.C	-0.308222	-0.504086	4.884888
9.C	-0.790654	-0.826397	6.322485
10.C	-0.214417	0.343543	7.174517
11.C	1.178844	0.578903	6.536475
12.O	-2.782705	-1.299996	1.686140
13.C	-2.116570	-1.849254	0.416191
14.C	-3.002386	-1.330904	-0.753512
15.C	-4.414390	-1.149762	-0.114152

16.C	-4.079354	-0.633232	1.304484
17.H	-0.989355	0.220684	4.411397
18.C	-0.086071	-1.701172	3.959936
19.H	-0.359765	-1.784916	6.654608
20.H	-1.886125	-0.896860	6.383567
21.H	-0.152647	0.101835	8.245517
22.H	-0.843571	1.239386	7.055071
23.H	1.944501	-0.078238	6.977841
24.H	1.516271	1.622735	6.584318
25.H	-3.063249	-3.821632	0.533176
26.H	-1.108141	-1.419534	0.393277
27.H	-3.012408	-2.028115	-1.603754
28.H	-2.625153	-0.358830	-1.107612
29.H	-4.936318	-2.116809	-0.055798
30.H	-5.045583	-0.449137	-0.680392
31.H	-4.818946	-0.909225	2.066826
32.H	-0.330988	1.859327	0.340615
33.H	-0.826015	0.849411	1.746993
34.H	1.141762	1.536715	3.039410
35.H	0.859141	3.054424	2.129830
36.H	3.294882	1.846937	1.885981
37.H	2.482159	2.389145	0.387605
38.H	2.576774	-0.449775	1.558633
39.C	2.935999	-0.091259	-0.559788
40.C	-2.054632	-3.380388	0.535353
41.H	-1.050221	-2.175931	3.726094
42.H	0.586989	-2.431093	4.435141
43.H	0.360637	-1.370768	3.012531
44.H	4.030021	0.006271	-0.466106
45.H	2.582818	0.584976	-1.352855
46.H	2.701018	-1.124186	-0.855420
47.H	-1.558367	-3.661822	1.475011
48.H	-1.477129	-3.805776	-0.302269
49.O	3.579798	-5.527695	7.930009
50.C	3.262468	-4.035048	7.915577
51.C	3.513217	-3.564318	6.445880
52.C	4.410746	-4.682255	5.826811
53.C	3.883115	-5.957065	6.520660
54.H	2.202314	-3.934752	8.194524
55.C	4.157679	-3.369426	8.970519
56.H	3.989676	-2.574875	6.405629
57.H	2.562076	-3.506983	5.896607
58.H	5.465889	-4.519649	6.093758
59.H	4.328224	-4.724654	4.731094
60.H	4.613935	-6.770435	6.597319
61.H	2.959830	-6.325377	6.041052
62.H	3.877683	-2.312230	9.107829
63.H	5.214887	-3.423368	8.669615
64.H	4.047789	-3.891038	9.932393

Ca-1THF-1TFSI

1.Ca	-0.770617	-0.216399	1.292009
2.O	-1.780180	-1.419471	2.937948
3.C	-3.262446	-1.688531	2.986810
4.C	-3.568446	-1.922001	4.463656
5.C	-2.278871	-2.600376	4.980112
6.C	-1.169283	-1.845812	4.247119
7.F	1.733323	3.740620	3.375868
8.F	-0.435936	3.653471	3.751797

9.H	-3.765168	-0.818738	2.552382
10.H	-3.448257	-2.578212	2.374430
11.H	-4.454109	-2.551287	4.594283
12.H	-3.745057	-0.970225	4.978069
13.H	-2.264706	-3.663325	4.712983
14.H	-2.167160	-2.519354	6.065731
15.H	-0.293166	-2.458691	4.013319
16.H	-0.864769	-0.933300	4.772170
17.C	-1.875890	2.891145	-1.826669
18.S	-2.252753	2.634027	0.040091
19.O	-3.584200	3.123312	0.292462
20.O	-2.064026	1.128482	0.182400
21.F	-0.640685	2.399593	-2.089835
22.F	-1.921621	4.194928	-2.111733
23.F	-2.791540	2.218365	-2.543299
24.N	-1.155459	3.450911	0.843258
25.S	0.325066	3.017413	1.252822
26.O	1.390424	3.386268	0.348777
27.O	0.378565	1.575044	1.746624
28.C	0.518996	4.025823	2.874366
29.F	0.418808	5.328799	2.602124

Ca-2THF-1TFSI

1.Ca	-0.450007	-0.548774	1.070077
2.O	-1.530838	-1.530082	2.861446
3.C	-3.008904	-1.803420	2.862335
4.C	-3.342022	-2.231303	4.294225
5.C	-2.275411	-1.499356	5.140676
6.C	-1.026423	-1.599723	4.266838
7.H	1.979792	-3.288511	0.540799
8.H	3.160059	-3.928833	-1.473690
9.H	0.564815	-3.657257	-0.499493
10.H	2.135683	0.115372	-0.835659
11.H	1.208812	-0.624867	-2.181289
12.O	1.051101	-1.617153	-0.328342
13.C	1.856593	-0.824950	-1.319966
14.C	3.033296	-1.729537	-1.675973
15.C	2.410709	-3.142633	-1.607167
16.C	1.470784	-3.050541	-0.401025
17.C	-2.498964	2.757062	-1.627740
18.S	-2.394057	2.204015	0.206108
19.O	-3.693218	2.435935	0.792303
20.O	-1.963714	0.758721	0.080257
21.F	-1.306967	2.538679	-2.228337
22.F	-2.805893	4.059028	-1.681702
23.F	-3.451483	2.027887	-2.239209
24.N	-1.272428	3.114822	0.873689
25.S	0.282760	2.771707	1.006861
26.O	1.133875	3.090457	-0.123840
27.O	0.511056	1.395896	1.599241
28.C	0.731171	3.950017	2.448908
29.F	0.522698	5.216868	2.073803
30.F	2.035171	3.755107	2.726911
31.F	-0.012545	3.654365	3.532505
32.H	-3.510187	-0.872817	2.573610
33.H	-3.198093	-2.578938	2.113644
34.H	-3.245819	-3.317722	4.405600
35.H	-4.362900	-1.948948	4.568573
36.H	-2.122600	-1.964870	6.119270

37.H	-2.552963	-0.450508	5.298447
38.H	-0.510127	-2.560022	4.385375
39.H	-0.317899	-0.775662	4.402674
40.H	1.845411	-3.361018	-2.520611
41.H	3.841417	-1.620507	-0.942862
42.H	3.435940	-1.495282	-2.666283

Ca-2-2MeTHF-TFSI (NoFC)

1.Ca	-0.338984	-0.375760	1.007957
2.O	-1.344234	-1.353286	2.848305
3.C	-2.831745	-1.499757	2.981273
4.C	-3.083874	-1.830951	4.459584
5.C	-1.841383	-1.259707	5.175702
6.C	-0.706981	-1.559249	4.194466
7.H	1.562259	-3.540483	0.521996
8.H	2.468778	-4.378244	-1.575192
9.H	0.114534	-3.398190	-0.527340
10.H	2.929663	-0.465614	-0.254905
11.C	1.839478	-0.103124	-2.093423
12.O	1.174980	-1.613555	-0.229955
13.C	2.355347	-1.030283	-0.998125
14.C	3.124231	-2.269842	-1.490861
15.C	2.045229	-3.369606	-1.605854
16.C	1.157923	-3.091473	-0.394515
17.C	-3.232226	2.298842	-1.706683
18.S	-2.794364	1.910397	0.120759
19.O	-4.032907	1.943929	0.864881
20.O	-2.115369	0.564129	0.014238
21.F	-2.105122	2.273231	-2.451735
22.F	-3.800252	3.509652	-1.777411
23.F	-4.087451	1.356768	-2.148167
24.N	-1.796617	3.058537	0.587184
25.S	-0.199148	3.010314	0.537258
26.O	0.438738	3.396849	-0.705911
27.O	0.348358	1.747628	1.168306
28.C	0.184203	4.350105	1.850662
29.F	-0.316555	5.526107	1.456701
30.F	1.525133	4.427251	1.958353
31.F	-0.344626	3.991693	3.038502
32.H	-3.277137	-0.546701	2.678837
33.H	-3.151135	-2.289849	2.294655
34.H	-3.147967	-2.915048	4.607468
35.H	-4.018291	-1.386086	4.814490
36.H	-1.666590	-1.727789	6.149836
37.H	-1.935493	-0.176337	5.327190
38.H	-0.432857	-2.622619	4.243247
39.C	0.537146	-0.686076	4.289765
40.H	1.473809	-3.268762	-2.535302
41.H	3.888825	-2.561212	-0.761208
42.H	3.625472	-2.074528	-2.443573
43.H	2.694259	0.363462	-2.598587
44.H	1.230708	0.713970	-1.688556
45.H	1.253100	-0.647656	-2.842389
46.H	1.290351	-0.958136	3.534612
47.H	1.018431	-0.835278	5.263517
48.H	0.290574	0.379054	4.198321

Ca-3THF-1TFSI

1.Ca	0.407882	-0.587830	1.670205
2.O	-1.306623	-1.387663	3.071436

3.C	-2.537104	-2.062387	2.552465
4.C	-3.593407	-1.903083	3.652298
5.C	-3.161842	-0.602695	4.368713
6.C	-1.638065	-0.709859	4.356110
7.O	2.154141	-1.344070	3.094480
8.C	2.160961	-2.567813	3.933417
9.C	3.112134	-2.256983	5.089306
10.C	4.175458	-1.362434	4.412343
11.C	3.350542	-0.513666	3.438919
12.O	1.203961	-1.614191	-0.286924
13.C	0.954035	-1.058128	-1.654541
14.C	2.037341	-1.675006	-2.537772
15.C	2.250528	-3.064684	-1.896723
16.C	2.136066	-2.769186	-0.398373
17.C	-2.187014	2.476387	-1.151856
18.S	-1.922996	1.849341	0.638210
19.O	-3.238548	1.777878	1.239787
20.O	-1.199935	0.548708	0.433116
21.F	-0.992241	2.582322	-1.776332
22.F	-2.793722	3.671194	-1.124819
23.F	-2.957061	1.583083	-1.809485
24.N	-1.015852	2.949168	1.349132
25.S	0.577973	2.869705	1.489067
26.O	1.368527	3.334329	0.364840
27.O	1.027824	1.564739	2.097119
28.C	0.801448	4.116260	2.922328
29.F	0.372665	5.327751	2.548473
30.F	2.120007	4.161455	3.209843
31.F	0.121433	3.699440	4.011902
32.H	-2.822004	-1.549416	1.627135
33.H	-2.273806	-3.103802	2.341175
34.H	-3.565378	-2.754324	4.342937
35.H	-4.601853	-1.836068	3.233185
36.H	-3.555807	-0.532083	5.387495
37.H	-3.489833	0.278645	3.806222
38.H	-1.257812	-1.336826	5.172842
39.H	-1.121857	0.256193	4.365549
40.H	1.127388	-2.761974	4.237010
41.H	2.525197	-3.401428	3.318149
42.H	3.538285	-3.166413	5.524419
43.H	2.589724	-1.709395	5.883038
44.H	4.905451	-1.976186	3.871228
45.H	4.721208	-0.739188	5.127324
46.H	3.871039	-0.278443	2.505579
47.H	2.981080	0.412231	3.891508
48.H	1.001400	0.031189	-1.579267
49.H	-0.055499	-1.362722	-1.953035
50.H	2.957585	-1.079998	-2.494500
51.H	1.719911	-1.736345	-3.583372
52.H	3.219732	-3.505458	-2.149934
53.H	1.465394	-3.761328	-2.213806
54.H	3.094981	-2.464237	0.038260
55.H	1.713047	-3.595576	0.182550

Ca-3-2MeTHF-1TFSI

1.Ca	0.422817	-0.266264	1.825508
2.O	-1.294904	-1.439638	2.966790
3.C	-2.321156	-2.183978	2.189610
4.C	-3.428124	-2.533293	3.191039

5.C	-3.345078	-1.375426	4.205800	34.H	-3.220299	-3.493300	3.678670
6.C	-1.839117	-1.123200	4.335023	35.H	-4.405710	-2.604412	2.704228
7.O	2.115487	-1.076135	3.293791	36.H	-3.793672	-1.627352	5.172203
8.C	2.167097	-2.478522	3.771307	37.H	-3.846183	-0.479105	3.818398
9.C	3.326859	-2.536295	4.767363	38.H	-1.386897	-1.861683	5.012329
10.C	4.301006	-1.475086	4.210418	39.C	-1.427935	0.287177	4.738109
11.C	3.375203	-0.350905	3.713406	40.H	1.191096	-2.718279	4.204662
12.O	1.088694	-1.294702	-0.175585	41.H	2.348446	-3.127498	2.903615
13.C	0.754433	-0.732410	-1.545145	42.H	3.772195	-3.534850	4.815865
14.C	1.931079	-1.185969	-2.424691	43.H	2.987559	-2.268925	5.774440
15.C	2.375011	-2.523128	-1.792120	44.H	4.882547	-1.890083	3.378238
16.C	2.211969	-2.256398	-0.294526	45.H	5.005878	-1.112662	4.964794
17.C	-2.323928	2.869338	-0.780206	46.H	3.754006	0.122642	2.801456
18.S	-1.671647	2.473691	0.976540	47.C	3.038536	0.711986	4.755974
19.O	-2.763860	2.763288	1.881554	48.H	0.740846	0.354744	-1.417234
20.O	-1.248050	1.037219	0.860784	49.C	-0.617204	-1.238724	-1.982212
21.F	-1.350790	2.639987	-1.692133	50.H	2.743826	-0.451686	-2.380034
22.F	-2.708447	4.151807	-0.841128	51.H	1.632099	-1.295296	-3.471720
23.F	-3.375462	2.061393	-1.039871	52.H	3.406061	-2.787818	-2.046448
24.N	-0.438352	3.457160	1.201457	53.H	1.726179	-3.346156	-2.112297
25.S	1.093503	3.029845	1.007743	54.H	3.106510	-1.787231	0.135358
26.O	1.623115	3.058138	-0.345241	55.H	1.949222	-3.147797	0.285153
27.O	1.442032	1.800445	1.804666	56.H	-0.622083	-2.325386	-2.126934
28.C	1.915068	4.450743	1.988748	57.H	-0.335952	0.399602	4.774316
29.F	1.635711	5.625531	1.410252	58.H	-1.795341	0.497573	5.750025
30.F	3.248100	4.231054	1.965664	59.H	-1.858042	1.037752	4.064613
31.F	1.483069	4.447087	3.265609	60.H	3.942448	1.289746	4.986048
32.H	-2.682861	-1.519187	1.395580	61.H	2.672314	0.265252	5.687759
33.H	-1.835018	-3.060271	1.747697	62.H	2.289620	1.414633	4.377082

63.H	-0.890699	-0.764082	-2.932627
64.H	-1.388345	-0.974469	-1.250755

Ca-4THF-1TFSI-NoFC

1.O	0.427625	-1.857355	-0.687559
2.C	-0.135049	-3.195115	-1.018593
3.C	-0.160596	-3.267446	-2.548666
4.C	1.043985	-2.386067	-2.951204
5.C	0.982771	-1.250527	-1.926828
6.H	0.522339	-3.953343	-0.578152
7.H	-1.125273	-3.258857	-0.555491
8.H	-1.095775	-2.849361	-2.941877
9.H	-0.069510	-4.297925	-2.907180
10.H	0.972161	-2.012931	-3.978142
11.H	1.985156	-2.938728	-2.849162
12.H	0.299619	-0.448773	-2.237705
13.H	1.964179	-0.833552	-1.681078
14.O	-1.243807	-1.595455	2.315482
15.C	-1.589227	-2.586031	3.368560
16.C	-2.944674	-3.150093	2.946844
17.C	-3.644044	-1.910680	2.340884
18.C	-2.496306	-1.157742	1.645444
19.H	-0.778252	-3.317978	3.397602
20.H	-1.650274	-2.056189	4.329166
21.H	-3.495515	-3.572593	3.793525
22.H	-2.816083	-3.938365	2.194664
23.H	-4.082981	-1.294254	3.134610
24.H	-4.441294	-2.173214	1.638252
25.H	-2.575635	-0.069557	1.746910
26.H	-2.402819	-1.414768	0.583582
27.O	1.851347	-0.365811	3.678111
28.C	1.611905	-0.970703	5.016560
29.C	2.457005	-0.150218	5.996061
30.C	3.661830	0.276553	5.126303
31.C	3.013336	0.556373	3.766915
32.H	0.535592	-0.915806	5.210790
33.H	1.932912	-2.018186	4.972233
34.H	2.753029	-0.740232	6.869516
35.H	1.901658	0.728490	6.348447
36.H	4.388449	-0.540135	5.044757
37.H	4.178111	1.158361	5.519835
38.H	3.666647	0.350531	2.914120
39.H	2.629021	1.583316	3.699347
40.O	0.733151	1.176513	1.036897
41.C	1.500042	1.977568	0.046628
42.C	1.388053	3.429244	0.520389
43.C	-0.016517	3.464822	1.165023
44.C	-0.115766	2.092801	1.842332
45.H	2.523007	1.588847	0.029523
46.H	1.034568	1.832193	-0.936573
47.H	1.491999	4.138250	-0.307437
48.H	2.163228	3.656184	1.262683
49.H	-0.790788	3.573253	0.395435
50.H	-0.135212	4.282950	1.882938
51.H	-1.131493	1.684525	1.853442
52.H	0.282025	2.101385	2.864803
53.Ca	1.016376	-1.185981	1.560253
54.O	4.402323	-2.663466	-0.961215
55.O	1.448661	-3.444851	2.148305

56.N	3.743075	-3.959987	1.090500
57.S	2.753084	-4.161881	2.335414
58.S	4.145732	-2.552979	0.460940
59.O	3.263150	-1.426148	0.907429
60.O	3.341000	-4.061730	3.662114
61.C	5.835057	-2.098771	1.261176
62.C	2.317641	-6.009632	2.056883
63.F	6.757236	-3.020165	0.938287
64.F	5.702230	-2.036517	2.611100
65.F	6.220490	-0.883751	0.800224
66.F	1.757385	-6.185450	0.836741
67.F	1.422763	-6.362920	3.010732
68.F	3.422840	-6.762909	2.169413

Ca-4-2MeTHF-1TFSI-NoFC

1.O	0.509096	-1.805558	-0.579055
2.C	0.134088	-3.193634	-0.936206
3.C	-0.749042	-3.056947	-2.174005
4.C	-0.047576	-1.914442	-2.937262
5.C	0.456344	-0.964832	-1.829581
6.H	1.047773	-3.758670	-1.150504
7.H	-0.359433	-3.635425	-0.065873
8.H	-1.773294	-2.776414	-1.895794
9.H	-0.794991	-3.987101	-2.750702
10.H	-0.713595	-1.394971	-3.634368
11.H	0.801803	-2.305723	-3.511912
12.H	-0.298174	-0.194411	-1.621917
13.C	1.811224	-0.323514	-2.105914
14.O	-1.015693	-2.047391	2.485671
15.C	-1.403789	-2.754280	3.764673
16.C	-2.866358	-3.165780	3.546897
17.C	-3.417164	-2.070123	2.613382
18.C	-2.233560	-1.822631	1.673034
19.C	-0.437397	-3.892170	4.063605
20.H	-1.346016	-1.986994	4.549071
21.H	-3.408594	-3.229045	4.496302
22.H	-2.914497	-4.150320	3.062583
23.H	-3.662159	-1.162733	3.179711
24.H	-4.313848	-2.382019	2.067569
25.H	-2.190932	-0.804295	1.273644
26.H	-2.225595	-2.535941	0.839268
27.O	1.902562	-0.813100	4.057854
28.C	1.179932	-0.327272	5.275602
29.C	2.294516	0.089209	6.242048
30.C	3.404436	-0.939262	5.955598
31.C	3.315199	-1.125194	4.435717
32.C	0.190127	0.767329	4.903453
33.H	0.644008	-1.196382	5.686139
34.H	1.953558	0.072350	7.282954
35.H	2.632877	1.108993	6.011112
36.H	3.201074	-1.883033	6.475728
37.H	4.397711	-0.593752	6.260462
38.H	3.536269	-2.145665	4.113095
39.H	3.955191	-0.421773	3.894055
40.O	0.812843	1.062511	1.329824
41.C	2.003832	1.951279	1.435011
42.C	1.536039	3.345003	1.000147
43.C	0.359420	3.036167	0.046396
44.C	-0.316494	1.817616	0.700518

45.H	2.358373	1.908062	2.469784
46.H	2.778926	1.546939	0.773813
47.H	2.337712	3.905613	0.508831
48.H	1.196286	3.932222	1.861301
49.H	0.732566	2.777388	-0.951741
50.H	-0.331993	3.878600	-0.059489
51.H	-0.740460	1.138170	-0.048065
52.C	-1.385098	2.177247	1.736452
53.Ca	1.209768	-1.345419	1.728585
54.O	4.948410	-1.596733	-0.782223
55.O	1.962281	-3.604819	1.663352
56.N	4.355665	-3.547465	0.694479
57.S	3.306500	-4.264013	1.673084
58.S	4.589485	-1.977525	0.568993
59.O	3.525487	-1.164108	1.243080
60.O	3.808979	-4.649850	2.981908
61.C	6.168715	-1.627255	1.615179
62.C	3.063940	-5.888882	0.681033
63.F	7.231894	-2.201760	1.029159
64.F	6.024231	-2.118285	2.872303
65.F	6.353637	-0.284432	1.684191
66.F	2.633859	-5.622953	-0.577411
67.F	2.122988	-6.621041	1.324523
68.F	4.217852	-6.572279	0.628715
69.H	2.588857	-1.080635	-2.254467
70.H	2.124839	0.335610	-1.289539
71.H	1.743863	0.282910	-3.019236
72.H	0.591372	-3.538907	4.190719
73.H	-0.450137	-4.644241	3.267186
74.H	-0.738932	-4.377812	5.000881
75.H	-0.342648	1.094181	5.805638
76.H	-0.556808	0.413161	4.185520
77.H	0.705245	1.635448	4.476937
78.H	-1.009890	2.889702	2.479640
79.H	-1.744890	1.288276	2.265642
80.H	-2.242992	2.635134	1.227239

Ca-2TFSI(NoFC)

1.Ca	-0.770284	-0.077759	1.820072
2.S	-1.723422	2.452558	-0.442710
3.O	-2.982761	2.876537	-1.009076
4.O	-1.668460	1.050594	0.094414
5.F	0.742863	1.980512	-1.396618
6.F	-0.340176	3.582144	-2.457606
7.F	-1.522940	4.075664	4.359487
8.F	-3.000660	3.353805	2.889909
9.F	-0.893858	1.476843	-2.785238
10.N	-1.058206	3.544266	0.507046
11.C	-0.463109	2.378013	-1.878559
12.S	-0.474426	3.438822	1.981311
13.O	0.657492	4.312353	2.182855
14.O	-0.337642	2.031188	2.488236
15.C	-1.894377	4.122465	3.063356
16.F	-2.170364	5.389176	2.715614
17.S	-1.563675	-3.123252	3.421781
18.O	-2.667470	-4.053038	3.402954
19.O	-1.838921	-1.741014	2.901683
20.F	-0.245968	-1.816339	5.373620
21.F	-0.757203	-3.903066	5.872681

22.F	3.533963	-2.842423	2.334517
23.F	2.685387	-4.608240	3.340709
24.F	-2.323692	-2.355801	5.868259
25.N	-0.230795	-3.772258	2.847863
26.S	0.918559	-3.164451	1.924977
27.O	0.810213	-1.680887	1.707414
28.O	1.171954	-3.966431	0.749444
29.C	2.477840	-3.318797	3.024397
30.F	2.321099	-2.594481	4.156778
31.C	-1.194577	-2.784924	5.269837

Ca-2TFSI-2THF-NoFC

1.Ca	-0.861621	-0.021715	1.766809
2.S	-1.614189	3.444324	1.328127
3.O	-2.420952	4.128648	2.320568
4.O	-1.897332	1.994087	1.113860
5.F	-1.349796	3.661204	-1.359187
6.F	-1.826446	5.553619	-0.337029
7.F	2.311683	3.258034	4.447526
8.F	0.185965	3.841597	4.462436
9.F	-3.378678	4.010240	-0.577530
10.N	-0.048289	3.788500	1.332445
11.C	-2.061203	4.229398	-0.353725
12.S	1.095094	2.970231	2.081967
13.O	2.361532	3.099423	1.385548
14.O	0.680676	1.603315	2.504634
15.C	1.332365	3.875495	3.748538
16.F	1.683987	5.158344	3.526903
17.S	-2.110319	-1.359134	4.907660
18.O	-3.430595	-1.544194	5.471083
19.O	-1.968814	-0.362095	3.812666
20.F	0.198494	-0.353487	5.873683
21.F	-0.991465	-1.471388	7.354318
22.F	2.006244	-4.199026	3.385728
23.F	0.773571	-4.860658	5.087217
24.F	-1.624080	0.542969	6.727330
25.N	-1.430042	-2.772683	4.593684
26.S	-0.452443	-3.164005	3.397253
27.O	0.071010	-2.016252	2.601487
28.O	-0.946666	-4.301590	2.639327
29.C	1.096735	-3.808435	4.311000
30.F	1.638563	-2.835686	5.076414
31.C	-1.055966	-0.610833	6.317564
32.O	-2.664190	-1.145564	0.659406
33.C	-2.621136	-2.428908	-0.082886
34.C	-4.069085	-2.711112	-0.503655
35.C	-4.891067	-2.016327	0.605774
36.C	-4.075331	-0.751327	0.880529
37.H	-1.934374	-2.300586	-0.926324
38.H	-2.228074	-3.195579	0.594135
39.H	-4.268325	-3.785464	-0.570899
40.H	-4.285190	-2.260218	-1.480400
41.H	-4.938808	-2.644664	1.503235
42.H	-5.914581	-1.782902	0.294504
43.H	-4.158003	-0.380972	1.906472
44.H	-4.313208	0.059027	0.179572
45.O	0.601984	-0.259229	-0.134359
46.C	2.006535	-0.697400	0.054071
47.C	2.807637	0.047302	-1.015675

48.C	1.795724	0.153044	-2.179059
49.C	0.469911	0.405222	-1.450675
50.H	2.298067	-0.446170	1.077866
51.H	2.037649	-1.786271	-0.078329
52.H	3.719066	-0.492590	-1.293059
53.H	3.088753	1.043588	-0.655137
54.H	1.755162	-0.787445	-2.742903
55.H	2.033808	0.961482	-2.877909
56.H	-0.401551	-0.025929	-1.954790
57.H	0.295810	1.472962	-1.275605

Ca-2TFSI-1THF-NoFC

1.Ca	-0.231302	0.297605	0.193414
2.S	-1.277813	3.717272	0.489900
3.O	-2.028216	4.479740	1.461275
4.O	-1.424535	2.229787	0.531483
5.F	-1.347390	3.475203	-2.189219
6.F	-1.946788	5.465200	-1.451064
7.F	3.663835	2.991658	1.705118
8.F	1.740139	3.120789	2.774569
9.F	-3.319232	3.757065	-1.242782
10.N	0.221609	4.232785	0.353594
11.C	-2.025526	4.144909	-1.215520
12.S	1.567804	3.416693	0.106025
13.O	2.406959	4.023742	-0.904903
14.O	1.392994	1.934151	0.031088
15.C	2.482274	3.644782	1.767710
16.F	2.702590	4.949304	2.006723
17.S	-2.159945	-2.579969	1.163194
18.O	-3.029670	-3.525234	0.498615
19.O	-1.913207	-1.282418	0.465127
20.F	-2.374341	-1.096664	3.402669
21.F	-3.282574	-3.099912	3.554087
22.F	2.362218	-2.521928	3.795980
23.F	1.074594	-4.306988	3.879789
24.F	-4.287881	-1.520327	2.395025
25.N	-0.832720	-3.291225	1.688070
26.S	0.651515	-2.708485	1.763466
27.O	0.746865	-1.222122	1.614553
28.O	1.596966	-3.491223	0.989787
29.C	1.111690	-2.991616	3.597036
30.F	0.253859	-2.331613	4.405227
31.C	-3.093493	-2.040844	2.744379
32.O	0.340494	-0.583473	-1.904507
33.C	1.756615	-0.694405	-2.357555
34.C	1.693054	-1.371527	-3.731115
35.C	0.408856	-2.227245	-3.639155
36.C	-0.535930	-1.323235	-2.845982
37.H	2.176745	0.315103	-2.373969
38.H	2.288146	-1.306649	-1.619249
39.H	2.588300	-1.970148	-3.926861
40.H	1.600988	-0.622265	-4.526787
41.H	0.600244	-3.157212	-3.090599
42.H	-0.001589	-2.484214	-4.621027
43.H	-1.280395	-1.858561	-2.250195
44.H	-1.036806	-0.586285	-3.487413

Ca-2TFSI-2-2MeTHF-NoFC

1.Ca	-0.859967	-0.040791	1.577190
2.S	-1.402143	3.485930	1.538067

3.O	-2.070889	4.055394	2.692556
4.O	-1.783361	2.090254	1.161147
5.F	-1.397243	4.051548	-1.109706
6.F	-1.654648	5.808800	0.194168
7.F	2.764440	2.780096	4.228457
8.F	0.703934	3.516978	4.495121
9.F	-3.312459	4.385253	-0.075002
10.N	0.173048	3.757388	1.421245
11.C	-1.968427	4.511271	0.030339
12.S	1.322448	2.800269	1.974261
13.O	2.522866	2.916004	1.167105
14.O	0.850231	1.429352	2.311991
15.C	1.781177	3.529610	3.680450
16.F	2.216873	4.797553	3.533575
17.S	-2.294258	-1.500042	4.512305
18.O	-3.699901	-1.851747	4.411841
19.O	-1.832387	-0.341137	3.702207
20.F	-0.746689	-0.618164	6.540950
21.F	-2.421945	-1.903888	7.165445
22.F	2.529578	-3.067635	3.759747
23.F	1.423182	-3.492024	5.616962
24.F	-2.803856	0.169460	6.528648
25.N	-1.359633	-2.798729	4.425475
26.S	-0.129027	-3.076137	3.452775
27.O	0.007601	-2.097382	2.335775
28.O	-0.058620	-4.479642	3.100947
29.C	1.440120	-2.743955	4.495747
30.F	1.511534	-1.434702	4.831503
31.C	-2.043259	-0.926201	6.317998
32.O	-2.711930	-1.186306	0.539479
33.C	-2.552364	-2.542491	-0.011843
34.C	-3.722035	-3.337703	0.567169
35.C	-4.861811	-2.296856	0.548803
36.C	-4.166835	-0.952502	0.853594
37.H	-2.599687	-2.484828	-1.108875
38.H	-1.566368	-2.908579	0.287899
39.H	-3.498568	-3.656140	1.591781
40.H	-3.949591	-4.229121	-0.027520
41.H	-5.640781	-2.514007	1.286256
42.H	-5.332237	-2.261499	-0.442946
43.H	-4.197836	-0.740685	1.928209
44.C	-4.685107	0.241109	0.059192
45.O	0.531934	-0.293739	-0.385977
46.C	1.883293	-0.878291	-0.219800
47.C	2.585868	-0.659358	-1.559997
48.C	1.982306	0.680773	-2.036061
49.C	0.510209	0.599374	-1.585115
50.H	2.389313	-0.344717	0.594342
51.H	1.751058	-1.927715	0.057625
52.H	2.351499	-1.470751	-2.259811
53.H	3.673718	-0.612811	-1.445247
54.H	2.066923	0.825354	-3.118194
55.H	2.482245	1.518459	-1.537023
56.C	-0.453977	0.027608	-2.625140
57.H	0.146623	1.572692	-1.236294
58.H	-0.094857	-0.930506	-3.019984
59.H	-1.448832	-0.124694	-2.191973
60.H	-4.124354	1.151305	0.293816

61.H	-5.737712	0.417950	0.316370
62.H	-4.623970	0.051942	-1.019854
63.H	-0.554059	0.732065	-3.460684

Ca-2TFSI-1-2MeTHF-NoFC

1.Ca	-1.159957	-0.026963	2.471390
2.S	-0.785995	3.513691	2.267555
3.O	-0.081107	4.343919	3.222192
4.O	-1.370204	2.239815	2.793032
5.F	-3.057520	3.777193	0.836085
6.F	-1.969182	5.665730	1.163205
7.F	3.286936	1.356536	0.340270
8.F	2.612263	2.422445	2.148921
9.F	-3.083051	4.736300	2.819204
10.N	-0.069813	3.356335	0.845027
11.C	-2.329775	4.497925	1.723290
12.S	0.714651	2.099394	0.271706
13.O	0.709610	2.093692	-1.175769
14.O	0.381085	0.811848	0.955094
15.C	2.531384	2.379169	0.797069
16.F	2.986092	3.537474	0.284631
17.S	-2.992263	-1.974829	4.783885
18.O	-4.059038	-2.777379	4.213708
19.O	-2.689074	-0.688824	4.086018
20.F	-2.692781	-0.668334	7.124766
21.F	-3.928784	-2.487159	7.248445
22.F	2.002741	-1.738639	5.898364
23.F	0.492861	-2.534748	7.289757
24.F	-4.740152	-0.666163	6.311266
25.N	-1.711483	-2.851032	5.156245
26.S	-0.197252	-2.671661	4.689842
27.O	-0.015645	-1.679010	3.586631
28.O	0.454096	-3.952262	4.532673
29.C	0.682240	-1.822483	6.163069
30.F	0.186016	-0.570809	6.335483
31.C	-3.628667	-1.412036	6.495892
32.O	-2.320822	-1.104608	0.743123
33.C	-1.618214	-1.711992	-0.410402
34.C	-2.715064	-1.980496	-1.438341
35.C	-3.919123	-2.361383	-0.547642
36.C	-3.786738	-1.443812	0.685999
37.H	-0.853508	-1.002041	-0.736786
38.H	-1.139486	-2.641062	-0.071576
39.H	-2.435662	-2.777968	-2.134568
40.H	-2.923541	-1.075864	-2.021622
41.H	-3.849588	-3.413131	-0.245523
42.H	-4.879866	-2.218939	-1.052537
43.H	-4.008566	-1.980767	1.613980
44.C	-4.592831	-0.148106	0.619463
45.H	-4.369142	0.506212	1.470649
46.H	-5.663611	-0.382946	0.664231
47.H	-4.394618	0.403751	-0.307007

Ca-6THF-NoFC

1.O	1.469511	-1.252766	0.163495
2.C	2.156666	-2.533813	-0.168703
3.C	2.368270	-2.516791	-1.685624
4.C	2.519079	-1.009563	-1.991928
5.C	1.507165	-0.371068	-1.037261
6.H	3.108649	-2.552789	0.377333

7.H	1.520920	-3.352354	0.181824	36.H	1.443731	-4.706044	5.414087
8.H	1.496613	-2.933005	-2.205066	37.H	1.419464	-5.962695	4.163959
9.H	3.247008	-3.099116	-1.980905	38.H	-0.287488	-3.775988	3.997283
10.H	2.303063	-0.766339	-3.036934	39.H	0.450142	-4.464667	2.520564
11.H	3.536535	-0.666275	-1.767750	40.O	-0.470567	1.326000	1.340811
12.H	0.498137	-0.348017	-1.468880	41.C	0.053317	2.708317	1.527890
13.H	1.781274	0.633422	-0.701883	42.C	-1.051835	3.642939	1.029116
14.O	-1.557569	-1.919863	1.675755	43.C	-1.708813	2.814796	-0.098268
15.C	-2.804988	-2.022527	2.486287	44.C	-1.677883	1.392611	0.468510
16.C	-3.649445	-3.110728	1.817783	45.H	0.295273	2.830037	2.588098
17.C	-3.258635	-2.974401	0.329139	46.H	0.969912	2.803674	0.931760
18.C	-1.760453	-2.669117	0.401831	47.H	-0.649827	4.597475	0.675019
19.H	-2.513146	-2.252389	3.515157	48.H	-1.773750	3.854022	1.827664
20.H	-3.303408	-1.044954	2.458375	49.H	-1.119735	2.879419	-1.021428
21.H	-4.719735	-2.959787	1.990270	50.H	-2.728919	3.140815	-0.324537
22.H	-3.380724	-4.102696	2.201222	51.H	-1.579934	0.613555	-0.293776
23.H	-3.802773	-2.146111	-0.141078	52.H	-2.553873	1.181455	1.094743
24.H	-3.461568	-3.882791	-0.246972	53.Ca	0.459498	-0.702156	2.317313
25.H	-1.393088	-2.040029	-0.414434	54.O	2.480450	0.522834	2.922931
26.H	-1.159107	-3.585885	0.454618	55.C	2.767907	1.136700	4.250802
27.O	1.392474	-2.741628	3.273133	56.C	3.996132	2.027147	4.044357
28.C	2.803373	-2.923108	3.716826	57.C	4.767088	1.287060	2.928265
29.C	2.993525	-4.431227	3.893191	58.C	3.641192	0.780410	2.023405
30.C	1.590367	-4.896664	4.343977	59.H	1.871520	1.679078	4.565723
31.C	0.657381	-4.020097	3.502127	60.H	2.969065	0.322102	4.958511
32.H	3.449587	-2.477776	2.954148	61.H	4.580456	2.134324	4.963782
33.H	2.930398	-2.382117	4.663406	62.H	3.699371	3.029739	3.712651
34.H	3.772118	-4.660820	4.627593	63.H	5.341519	0.449076	3.342077
35.H	3.273535	-4.902770	2.943113	64.H	5.460892	1.939437	2.388505

65.H	3.870825	-0.154748	1.504455
66.H	3.334430	1.538368	1.291262
67.O	-0.538941	-0.110328	4.470425
68.C	-0.304902	-0.808221	5.768105
69.C	-0.897724	0.102404	6.846788
70.C	-2.062745	0.794955	6.103923
71.C	-1.480329	1.021200	4.707051
72.H	-0.818070	-1.777280	5.723275
73.H	0.772377	-0.971842	5.867277
74.H	-0.158941	0.840034	7.183146
75.H	-1.230465	-0.465696	7.721405
76.H	-2.366945	1.734795	6.575821
77.H	-2.940551	0.138539	6.058372
78.H	-0.903949	1.954033	4.652065
79.H	-2.223961	1.005887	3.904775

Ca-6-2MeTHF-NoFC

1.O	0.359134	-1.676926	-0.943380
2.C	-1.074600	-1.980264	-1.215901
3.C	-1.231717	-1.973427	-2.737351
4.C	-0.169199	-0.944010	-3.180205
5.C	1.008760	-1.211235	-2.226684
6.H	-1.304910	-2.940575	-0.748231
7.H	-1.679131	-1.195040	-0.745120
8.H	-2.245040	-1.689748	-3.039477
9.H	-1.021994	-2.963294	-3.159076
10.H	-0.548001	0.076937	-3.049639
11.H	0.122500	-1.061657	-4.228657
12.H	1.535989	-0.287896	-1.965411
13.C	2.004838	-2.253032	-2.731343
14.O	-1.099675	-1.920912	2.249556
15.C	-1.796487	-3.102928	2.894970
16.C	-3.080660	-2.528035	3.537086
17.C	-2.867652	-0.999357	3.569711
18.C	-2.020415	-0.763019	2.322015
19.C	-2.055064	-4.208079	1.877703
20.H	-1.094943	-3.450416	3.663296
21.H	-3.252634	-2.949575	4.532753
22.H	-3.950830	-2.778252	2.917742
23.H	-2.326462	-0.692961	4.472076
24.H	-3.810914	-0.443861	3.537075
25.H	-1.404483	0.139333	2.347790
26.H	-2.640919	-0.748324	1.414758
27.O	2.018925	-1.569218	3.795561
28.C	1.309438	-1.881971	5.090897
29.C	2.424939	-2.399626	6.013712
30.C	3.649017	-1.556793	5.593913
31.C	3.473438	-1.432136	4.075306
32.C	0.581194	-0.651673	5.631480
33.H	0.586598	-2.665360	4.838542
34.H	2.611710	-3.466097	5.837015
35.H	2.170836	-2.275713	7.071108
36.H	4.598354	-2.035302	5.854755
37.H	3.630696	-0.571988	6.073129
38.H	3.989869	-2.237292	3.539190
39.H	3.804661	-0.467113	3.678852
40.O	0.976673	0.855620	1.428880
41.C	1.323580	1.640460	2.647576
42.C	1.176346	3.118115	2.272051

43.C	1.445192	3.113357	0.751962
44.C	0.777142	1.812595	0.278726
45.H	0.656956	1.323982	3.453361
46.H	2.356092	1.389824	2.921202
47.H	1.881006	3.749475	2.822546
48.H	0.165360	3.479442	2.491126
49.H	2.523490	3.087256	0.552014
50.H	1.032161	3.991910	0.246570
51.H	1.312459	1.362962	-0.563553
52.C	-0.706342	1.957175	-0.061523
53.Ca	1.214713	-1.635909	1.373265
54.H	-1.268261	2.433229	0.750371
55.H	-1.163106	0.986486	-0.279787
56.H	-0.812028	2.585311	-0.955288
57.H	1.506081	-3.178208	-3.041029
58.H	2.749041	-2.491978	-1.964560
59.H	2.540677	-1.850158	-3.600142
60.H	-1.129502	-4.549190	1.404985
61.H	-2.754552	-3.875058	1.101841
62.H	-2.512348	-5.065670	2.388566
63.H	0.008070	-0.934507	6.523768
64.H	-0.123630	-0.251489	4.896125
65.H	1.278532	0.143535	5.918634
66.O	3.610267	-1.286308	0.662350
67.C	4.395805	-0.005410	0.593475
68.C	5.791761	-0.405965	1.094768
69.C	5.984260	-1.826633	0.515005
70.C	4.563318	-2.420742	0.518220
71.C	4.392382	0.577003	-0.821670
72.H	3.884511	0.674295	1.283163
73.H	5.817030	-0.426141	2.190436
74.H	6.564772	0.290702	0.755569
75.H	6.676020	-2.428635	1.111958
76.H	6.383708	-1.781419	-0.503321
77.H	4.390227	-3.092878	1.364910
78.H	4.329975	-2.950716	-0.411035
79.H	4.912688	1.543196	-0.818773
80.H	3.373276	0.748303	-1.183046
81.H	4.905819	-0.077205	-1.535485
82.O	1.606376	-4.102411	1.331690
83.C	2.005155	-5.050474	0.216344
84.C	2.736114	-6.227323	0.915593
85.C	2.943288	-5.774914	2.379291
86.C	1.756401	-4.839814	2.603815
87.C	0.796569	-5.480494	-0.607790
88.H	2.692235	-4.466226	-0.403110
89.H	3.679965	-6.466039	0.415272
90.H	2.110055	-7.127078	0.881743
91.H	3.889405	-5.232890	2.498965
92.H	2.946856	-6.615484	3.081202
93.H	1.907085	-4.096355	3.389947
94.H	0.832561	-5.400713	2.802988
95.H	1.136926	-6.134062	-1.421817
96.H	0.286589	-4.623642	-1.057634
97.H	0.081359	-6.051857	-0.004836

Ca-4THF-NoFC

1.O	0.964453	-1.884744	-0.195099
2.C	2.147666	-2.819040	-0.238158

3.C	2.243650	-3.290246	-1.691088
4.C	0.773960	-3.247593	-2.173561
5.C	0.234295	-1.983188	-1.508586
6.H	3.021417	-2.254510	0.103209
7.H	1.933276	-3.640529	0.455060
8.H	2.677355	-4.292783	-1.758727
9.H	2.867807	-2.608556	-2.280373
10.H	0.222810	-4.132419	-1.833559
11.H	0.693010	-3.193459	-3.263918
12.H	-0.836663	-2.017929	-1.282816
13.H	0.470907	-1.078374	-2.081002
14.O	-1.930224	-1.109049	2.030595
15.C	-2.426355	-2.370524	2.688894
16.C	-3.937723	-2.380648	2.458849
17.C	-4.295922	-0.876757	2.442674
18.C	-3.122195	-0.252485	1.688752
19.H	-1.898485	-3.210202	2.224781
20.H	-2.169155	-2.302553	3.752364
21.H	-4.460192	-2.927614	3.249945
22.H	-4.182252	-2.852161	1.499582
23.H	-4.359317	-0.478341	3.462216
24.H	-5.247555	-0.678189	1.939536
25.H	-2.885964	0.771110	1.995663
26.H	-3.253679	-0.298835	0.601203
27.O	1.618052	-1.051217	3.413262
28.C	1.184740	-1.724983	4.690608
29.C	2.338658	-1.516203	5.672094
30.C	3.579265	-1.481239	4.749793
31.C	3.079313	-0.703003	3.533030
32.H	0.245574	-1.256552	5.002743
33.H	1.022267	-2.783870	4.457586
34.H	2.387555	-2.323193	6.409965
35.H	2.224116	-0.567994	6.210280
36.H	3.884215	-2.495275	4.465084
37.H	4.435613	-0.986319	5.218655
38.H	3.560540	-0.987678	2.591549
39.H	3.144017	0.381924	3.676378
40.O	0.415381	1.639110	1.100255
41.C	0.771974	2.252929	-0.228927
42.C	1.099308	3.713752	0.078486
43.C	0.162560	4.036307	1.265763
44.C	0.200811	2.751534	2.095006
45.H	1.612819	1.681156	-0.634793
46.H	-0.104865	2.150537	-0.879177
47.H	0.914297	4.357666	-0.787125
48.H	2.151362	3.824351	0.367442
49.H	-0.855624	4.242910	0.915364
50.H	0.503895	4.898771	1.847188
51.H	-0.731466	2.537670	2.628254
52.H	1.046715	2.728980	2.791756
53.Ca	0.277124	-0.605466	1.592162

Ca-4-2MeTHF-NoFC

1.O	0.636746	-1.937134	-0.282955
2.C	1.668810	-3.037888	-0.501169
3.C	1.652550	-3.272332	-2.022065
4.C	0.222540	-2.878424	-2.453698
5.C	-0.068540	-1.665527	-1.574405
6.H	2.621188	-2.607714	-0.170198

7.C	1.302247	-4.250784	0.347819
8.H	1.891958	-4.310884	-2.269106
9.H	2.391173	-2.631282	-2.516676
10.H	-0.490951	-3.685466	-2.253556
11.H	0.160911	-2.630134	-3.517612
12.H	-1.130730	-1.526368	-1.345224
13.H	0.347460	-0.742314	-1.996003
14.O	-1.921891	-1.079731	2.288912
15.C	-2.556928	-2.466268	2.309211
16.C	-4.043853	-2.192434	2.590655
17.C	-4.038981	-0.882986	3.410360
18.C	-2.932114	-0.073077	2.741106
19.H	-2.400752	-2.866307	1.300811
20.C	-1.849358	-3.332401	3.347167
21.H	-4.508319	-3.022199	3.131786
22.H	-4.592969	-2.054519	1.652229
23.H	-3.802234	-1.072309	4.463157
24.H	-5.000413	-0.361882	3.370226
25.H	-2.422386	0.625595	3.412811
26.H	-3.293640	0.458770	1.852695
27.O	1.664116	-0.811535	3.359994
28.C	1.283350	-0.248510	4.692904
29.C	2.562559	-0.285822	5.523716
30.C	3.259790	-1.565681	5.011267
31.C	2.976842	-1.574112	3.498564
32.H	0.892105	0.760678	4.522969
33.H	0.498701	-0.887802	5.115616
34.H	2.347163	-0.328682	6.595737
35.H	3.174435	0.603817	5.337684
36.H	2.826912	-2.452947	5.487087
37.H	4.334403	-1.566409	5.216817
38.H	2.761048	-2.585410	3.135008
39.C	4.042302	-0.907528	2.634421
40.O	0.263004	1.609308	0.906067
41.C	1.511248	2.483879	0.851667
42.C	0.960091	3.910073	0.690699
43.C	-0.373414	3.715793	-0.064523
44.C	-0.932397	2.441802	0.563599
45.H	2.000046	2.343094	1.822475
46.C	2.415756	2.007000	-0.280830
47.H	1.659682	4.550727	0.145467
48.H	0.781958	4.365916	1.671469
49.H	-0.206996	3.580972	-1.138930
50.H	-1.054532	4.562208	0.066551
51.H	-1.562063	1.851987	-0.110561
52.H	-1.472709	2.647868	1.495501
53.Ca	0.223077	-0.607936	1.563293
54.H	2.096875	-5.002519	0.267163
55.H	0.364525	-4.710500	0.016211
56.H	1.208581	-3.992182	1.410841
57.H	4.956922	-1.512583	2.656658
58.H	4.290201	0.096195	2.997288
59.H	3.729809	-0.833430	1.584355
60.H	3.357951	2.567827	-0.252295
61.H	1.955250	2.164994	-1.262388
62.H	2.670080	0.943574	-0.180965
63.H	-0.767908	-3.387963	3.165508
64.H	-2.237960	-4.356413	3.289410

65.H	-2.014528	-2.962685	4.365317

Ca-5THF-NoFC

1.O	0.353959	-1.237809	-0.708556
2.C	-0.878736	-1.891367	-1.248283
3.C	-0.624093	-2.076967	-2.745174
4.C	0.268816	-0.863707	-3.090983
5.C	1.172653	-0.749505	-1.861142
6.H	-1.021265	-2.826673	-0.699280
7.H	-1.722405	-1.216357	-1.056811
8.H	-1.557397	-2.090929	-3.317062
9.H	-0.094948	-3.018586	-2.935844
10.H	-0.336920	0.042085	-3.215141
11.H	0.847564	-1.012209	-4.008141
12.H	1.485928	0.274923	-1.632925
13.H	-0.057910	-3.625285	3.522483
14.O	-0.851265	-2.104366	2.303002
15.C	-0.890952	-3.509975	2.820752
16.C	-2.271469	-3.675087	3.461614
17.C	-3.156905	-2.718535	2.629843
18.C	-2.229643	-1.526595	2.384529
19.C	3.435701	-3.361065	0.586236
20.H	-0.750728	-4.180309	1.963463
21.H	-2.250916	-3.368701	4.514391
22.H	-2.615930	-4.713125	3.417831
23.H	-4.067942	-2.421332	3.158909
24.H	-3.450882	-3.184435	1.681446
25.H	-2.241838	-0.815023	3.219516
26.H	-2.421421	-0.999542	1.444416
27.O	1.860404	-0.992024	3.826171
28.C	1.006216	-0.479864	4.941061
29.C	1.946031	-0.310277	6.136185
30.C	2.978031	-1.440173	5.917696
31.C	3.169385	-1.437074	4.398823
32.H	2.596869	-3.717781	-0.021484
33.H	0.544549	0.453336	4.600698
34.H	1.413396	-0.402753	7.088022
35.H	2.432872	0.672289	6.113920
36.H	2.577949	-2.403216	6.257298
37.H	3.919988	-1.259389	6.445044
38.H	3.396780	-2.420431	3.976483
39.H	3.930752	-0.713666	4.081877
40.O	0.993672	1.321735	1.471612
41.C	2.040608	2.273917	1.967303
42.C	1.362313	3.644958	2.001748
43.C	0.349707	3.556969	0.836481
44.C	-0.159076	2.117161	0.937474
45.H	2.372443	1.911111	2.944984
46.H	2.874204	2.244168	1.254728
47.H	2.084903	4.456798	1.871331
48.H	0.845190	3.799787	2.956408
49.H	0.846824	3.727350	-0.126031
50.H	-0.465373	4.281486	0.931015
51.H	-0.444550	1.672147	-0.020813
52.H	6.365147	-1.864804	-0.167876
53.Ca	1.108959	-1.017448	1.554335
54.H	5.299895	-4.365671	0.043746
55.H	4.659932	-3.290896	-1.212293

56.H	3.454419	-3.895222	1.544560
57.H	0.227072	-1.227832	5.131976
58.H	-0.984183	2.021102	1.654505
59.H	4.304542	-0.584159	-0.313713
60.O	3.192542	-1.913274	0.883673
61.H	4.605149	-0.461124	1.449986
62.H	5.969386	-2.466086	1.453016
63.C	4.452453	-1.151408	0.613755
64.C	5.548010	-2.210239	0.473397
65.C	4.787676	-3.414201	-0.130207
66.H	2.054209	-1.397725	-1.935989

Ca-5-2MeTHF-NoFC

1.O	0.269538	-1.172247	-0.858812
2.C	-1.192030	-1.309976	-1.130385
3.C	-1.357377	-1.288619	-2.653972
4.C	-0.124424	-0.486943	-3.126921
5.C	0.987992	-0.945836	-2.171149
6.H	-1.531029	-2.239113	-0.663851
7.H	-1.695362	-0.457161	-0.657007
8.H	-2.301223	-0.820746	-2.951727
9.H	-1.346251	-2.304671	-3.062700
10.H	-0.301856	0.590835	-3.024678
11.H	0.129554	-0.685538	-4.172786
12.H	1.710681	-0.147666	-1.967719
13.C	1.710705	-2.219044	-2.608252
14.O	-0.797636	-2.213712	2.152739
15.C	-0.842952	-3.674925	2.559517
16.C	-2.325391	-3.944781	2.842476
17.C	-2.852772	-2.591518	3.360173
18.C	-2.109855	-1.583986	2.477952
19.C	-0.205670	-4.537579	1.478874
20.H	-0.261084	-3.737503	3.490037
21.H	-2.451945	-4.753015	3.570340
22.H	-2.842373	-4.238254	1.919159
23.H	-2.597062	-2.450914	4.417561
24.H	-3.938495	-2.491681	3.261590
25.H	-1.912062	-0.626975	2.973199
26.H	-2.637472	-1.404445	1.533639
27.O	1.777173	-0.918039	3.755895
28.C	0.831835	-0.830066	4.935638
29.C	1.646442	-1.375267	6.121941
30.C	3.101584	-0.995274	5.771684
31.C	3.148286	-1.210234	4.258071
32.C	0.338152	0.606407	5.109261
33.H	-0.003196	-1.490114	4.678916
34.H	1.541763	-2.464861	6.193240
35.H	1.316577	-0.944229	7.072450
36.H	3.835782	-1.617793	6.293155
37.H	3.309237	0.050652	6.024574
38.H	3.385953	-2.250649	4.002455
39.H	3.842177	-0.539507	3.741942
40.O	1.061839	1.396114	1.290125
41.C	2.108218	2.244887	1.935807
42.C	1.655121	3.690798	1.731721
43.C	0.910395	3.623432	0.379396
44.C	0.166965	2.278373	0.437759
45.H	2.175806	1.938700	2.983333
46.H	3.060202	2.045323	1.427012

47.H	2.503205	4.382518	1.709172
48.H	0.984683	4.008103	2.538400
49.H	1.625308	3.632618	-0.452245
50.H	0.220070	4.460928	0.237301
51.H	0.130508	1.786146	-0.539969
52.C	-1.228420	2.349919	1.055412
53.Ca	1.116605	-0.967667	1.407514
54.H	-1.218585	2.861484	2.024691
55.H	-1.662314	1.351770	1.193726
56.H	-1.895178	2.906884	0.385245
57.H	1.008257	-3.030402	-2.830801
58.H	2.408184	-2.561829	-1.837330
59.H	2.289989	-2.014332	-3.517532
60.H	0.847265	-4.278499	1.307614
61.H	-0.751170	-4.461967	0.531283
62.H	-0.224434	-5.587297	1.797960
63.H	-0.437715	0.633104	5.884834
64.H	-0.103043	0.996437	4.183874
65.H	1.146317	1.278622	5.420408
66.O	3.315381	-1.718632	0.851536
67.C	4.586741	-0.892760	0.748737
68.C	5.724565	-1.924528	0.863872
69.C	5.108799	-3.227872	0.308578
70.C	3.673457	-3.165224	0.829554
71.C	4.578337	-0.084883	-0.546844
72.H	4.566114	-0.219871	1.614370
73.H	6.019548	-2.057818	1.911721
74.H	6.611287	-1.609032	0.305172
75.H	5.630961	-4.122690	0.661876
76.H	5.125401	-3.239573	-0.787303
77.H	3.595843	-3.551502	1.855051
78.H	2.946858	-3.674539	0.187740
79.H	5.450519	0.580822	-0.562391
80.H	3.682990	0.544538	-0.624091
81.H	4.629101	-0.732124	-1.429686

Zn-4THF-NoFC

1.O	1.003538	-1.797676	-0.005079
2.C	1.213730	-3.294402	0.057692
3.C	1.767763	-3.660509	-1.317095
4.C	1.072868	-2.646340	-2.259483
5.C	1.075711	-1.350357	-1.449308
6.H	1.896010	-3.484201	0.891054
7.H	0.235696	-3.749907	0.253213
8.H	1.533886	-4.697748	-1.578938
9.H	2.857363	-3.538330	-1.343799
10.H	0.047319	-2.962394	-2.486134
11.H	1.608837	-2.524882	-3.206778
12.H	0.213232	-0.703095	-1.632933
13.H	2.008575	-0.785990	-1.555485
14.O	-1.527045	-1.192742	2.000965
15.C	-2.044436	-2.302677	2.884306
16.C	-3.558112	-2.103642	2.897230
17.C	-3.855623	-1.546979	1.482578
18.C	-2.679515	-0.607564	1.213755
19.H	-1.745738	-3.252213	2.424173
20.H	-1.564295	-2.182496	3.858794
21.H	-3.848379	-1.383858	3.672165
22.H	-4.083612	-3.044552	3.091846

23.H	-4.810294	-1.012177	1.439734
24.H	-3.885161	-2.356112	0.742839
25.H	-2.843733	0.403404	1.602420
26.H	-2.368844	-0.565686	0.165341
27.O	1.645689	-1.158248	3.108106
28.C	1.299939	-1.437373	4.554417
29.C	2.593675	-1.168420	5.323719
30.C	3.702495	-1.506081	4.295869
31.C	3.139531	-0.963946	2.984664
32.H	0.470823	-0.776112	4.823693
33.H	0.987456	-2.486461	4.602944
34.H	2.658166	-1.789508	6.223574
35.H	2.653473	-0.117176	5.631137
36.H	3.862863	-2.589247	4.232019
37.H	4.658221	-1.033649	4.546899
38.H	3.457124	-1.508993	2.091042
39.H	3.317364	0.110612	2.858888
40.O	0.431324	1.267037	1.316096
41.C	0.933054	2.042271	0.117599
42.C	1.067052	3.483697	0.611737
43.C	-0.016765	3.591218	1.713461
44.C	0.064250	2.237867	2.414181
45.H	1.877377	1.585173	-0.191743
46.H	0.176102	1.930723	-0.666703
47.H	0.905277	4.199653	-0.201068
48.H	2.066243	3.661158	1.027760
49.H	-1.010027	3.743978	1.273800
50.H	0.178742	4.414487	2.408913
51.H	-0.879268	1.889948	2.845020
52.H	0.863818	2.196769	3.163218
53.Zn	0.392480	-0.729858	1.594015

Zn-4-2MeTHF-NoFC

1.O	0.592837	-1.665778	-0.162017
2.C	1.221641	-3.056957	-0.317416
3.C	1.485047	-3.162175	-1.828062
4.C	0.422254	-2.245749	-2.476297
5.C	0.358611	-1.063858	-1.517636
6.H	2.153739	-3.007666	0.252737
7.C	0.284833	-4.108042	0.261642
8.H	1.405042	-4.197454	-2.172878
9.H	2.493175	-2.805480	-2.067448
10.H	-0.549145	-2.747899	-2.543680
11.H	0.708633	-1.929731	-3.484176
12.H	-0.612082	-0.561595	-1.483552
13.H	1.152891	-0.332015	-1.697748
14.O	-1.597641	-1.097975	2.147737
15.C	-2.037203	-1.441498	3.572641
16.C	-3.210609	-2.404747	3.351528
17.C	-3.857638	-1.917822	2.034473
18.C	-2.657635	-1.531352	1.173031
19.H	-1.172325	-1.944846	4.017313
20.C	-2.379349	-0.161255	4.324262
21.H	-3.912223	-2.379606	4.190661
22.H	-2.848140	-3.433718	3.245649
23.H	-4.509527	-1.055399	2.208341
24.H	-4.456378	-2.698942	1.556065
25.H	-2.845276	-0.686477	0.504127
26.H	-2.252843	-2.377174	0.609371

27.O	1.660796	-0.861548	2.983164
28.C	1.555489	-0.193740	4.324838
29.C	2.875362	-0.504343	5.021158
30.C	3.239391	-1.902413	4.470798
31.C	2.842736	-1.843834	2.989429
32.H	1.377329	0.869922	4.143628
33.H	0.699295	-0.634213	4.846220
34.H	2.762113	-0.505483	6.109593
35.H	3.639533	0.236600	4.763064
36.H	2.669491	-2.680216	4.991776
37.H	4.303231	-2.129337	4.588208
38.H	2.416705	-2.790183	2.641455
39.C	3.926132	-1.340890	2.045105
40.O	0.250421	1.357191	1.065296
41.C	1.444866	2.315619	1.156618
42.C	0.779512	3.690449	1.316875
43.C	-0.570436	3.555469	0.575594
44.C	-1.021485	2.142979	0.931166
45.H	1.981375	2.007665	2.059604
46.C	2.325393	2.152291	-0.074819
47.H	1.403737	4.485468	0.898128
48.H	0.613124	3.917037	2.376355
49.H	-0.441314	3.663392	-0.506770
50.H	-1.299178	4.303130	0.903309
51.H	-1.620129	1.656426	0.155847
52.H	-1.542807	2.096396	1.893307
53.Zn	0.275940	-0.612218	1.536118
54.H	0.792470	-5.080618	0.249785
55.H	-0.635186	-4.202488	-0.325756
56.H	0.021224	-3.891685	1.304254
57.H	4.712847	-2.101982	1.969021
58.H	4.386520	-0.415914	2.408888
59.H	3.539226	-1.165145	1.034606
60.H	3.220737	2.775063	0.044104
61.H	1.811938	2.469421	-0.989166
62.H	2.663645	1.116716	-0.196578
63.H	-1.548754	0.553905	4.313573
64.H	-2.588207	-0.406501	5.373169
65.H	-3.267230	0.330142	3.911665

Zn-5THF-NoFC

1.O	0.416831	-1.152935	-0.503560
2.C	-0.671373	-2.032331	-1.039685
3.C	-0.396734	-2.151825	-2.540441
4.C	0.287692	-0.806798	-2.876448
5.C	1.172307	-0.568500	-1.652773
6.H	-0.629287	-2.982213	-0.500505
7.H	-1.625297	-1.532600	-0.835301
8.H	-1.319681	-2.308948	-3.107539
9.H	0.275652	-2.992868	-2.749115
10.H	-0.455382	-0.006998	-2.982896
11.H	0.873885	-0.849833	-3.799995
12.H	1.352044	0.485473	-1.422040
13.H	0.232603	-3.423312	3.452814
14.O	-0.595258	-1.956932	2.190232
15.C	-0.601075	-3.350423	2.748548
16.C	-1.981058	-3.520665	3.388350
17.C	-2.881550	-2.577171	2.554824

18.C	-1.973433	-1.376802	2.293224
19.C	3.101917	-3.262115	0.617044
20.H	-0.441254	-4.035274	1.907289
21.H	-1.964231	-3.211402	4.440207
22.H	-2.316538	-4.561794	3.348348
23.H	-3.790554	-2.286072	3.090950
24.H	-3.179629	-3.052399	1.612580
25.H	-1.971684	-0.664843	3.127249
26.H	-2.175875	-0.853002	1.355225
27.O	1.807724	-0.910938	3.606612
28.C	0.952956	-0.369846	4.705565
29.C	1.865121	-0.304904	5.930406
30.C	2.810404	-1.508829	5.712520
31.C	3.056628	-1.483531	4.202535
32.H	2.257066	-3.535802	-0.021943
33.H	0.571547	0.601225	4.375699
34.H	1.297741	-0.376551	6.863840
35.H	2.429417	0.635501	5.948114
36.H	2.323329	-2.444713	6.012556
37.H	3.744799	-1.418740	6.275490
38.H	3.214882	-2.469584	3.758520
39.H	3.884844	-0.817898	3.931564
40.O	1.012889	1.094544	1.455841
41.C	2.082404	2.047459	1.910081
42.C	1.389023	3.406863	1.992086
43.C	0.313747	3.320484	0.882551
44.C	-0.181908	1.878727	0.993998
45.H	2.464195	1.672486	2.862650
46.H	2.874244	2.027511	1.152151
47.H	2.094205	4.228182	1.829017
48.H	0.923232	3.549257	2.974699
49.H	0.755415	3.506205	-0.103904
50.H	-0.499688	4.037941	1.030735
51.H	-0.512789	1.435245	0.051692
52.H	6.098893	-1.855673	-0.060275
53.Zn	1.117629	-0.964235	1.544516
54.H	4.937355	-4.316171	0.077090
55.H	4.358238	-3.186161	-1.158904
56.H	3.070578	-3.841164	1.547748
57.H	0.116552	-1.063680	4.851128
58.H	-0.960659	1.764234	1.757286
59.H	4.082694	-0.494927	-0.181118
60.O	2.933625	-1.818654	0.990699
61.H	4.388580	-0.423650	1.584365
62.H	5.669733	-2.486640	1.540662
63.C	4.216286	-1.086863	0.732262
64.C	5.264705	-2.185807	0.567177
65.C	4.462987	-3.342204	-0.078719
66.H	2.129502	-1.098451	-1.727907

Zn-5-2MeTHF-NoFC

1.O	0.371137	-1.195886	-0.712075
2.C	-1.087384	-1.337040	-1.010306
3.C	-1.231880	-1.232206	-2.531804
4.C	0.000127	-0.398670	-2.947027
5.C	1.105648	-0.906921	-2.009813
6.H	-1.417821	-2.294842	-0.603660
7.H	-1.607588	-0.520675	-0.496396
8.H	-2.175788	-0.754800	-2.813870

9.H	-1.209778	-2.223605	-2.996316	38.H	3.309928	-2.219794	3.819333
10.H	-0.184217	0.671105	-2.787978	39.H	3.812180	-0.510465	3.649635
11.H	0.265433	-0.536858	-3.999932	40.O	0.948612	1.138457	1.360019
12.H	1.829566	-0.127087	-1.758785	41.C	2.024087	1.993107	1.966082
13.C	1.817771	-2.158716	-2.518626	42.C	1.580403	3.431183	1.718011
14.O	-0.540448	-2.121775	1.997698	43.C	0.845060	3.331403	0.362978
15.C	-0.533706	-3.606796	2.380551	44.C	0.065911	2.010609	0.460964
16.C	-1.935663	-3.851984	2.961402	45.H	2.101172	1.709872	3.016195
17.C	-2.411293	-2.477775	3.474059	46.H	2.960101	1.766808	1.443079
18.C	-1.828889	-1.509260	2.445897	47.H	2.435550	4.113857	1.679293
19.C	-0.195574	-4.476167	1.179213	48.H	0.909058	3.778447	2.511149
20.H	0.238158	-3.686836	3.155970	49.H	1.566342	3.297366	-0.462377
21.H	-1.904724	-4.605879	3.755002	50.H	0.173835	4.177888	0.187112
22.H	-2.605784	-4.222657	2.175650	51.H	0.027776	1.477358	-0.491812
23.H	-2.021912	-2.273876	4.478236	52.C	-1.325956	2.147033	1.069981
24.H	-3.502740	-2.402932	3.519716	53.Zn	1.095771	-0.936968	1.374208
25.H	-1.601502	-0.517114	2.843868	54.H	-1.304788	2.695574	2.018339
26.H	-2.474904	-1.415322	1.565547	55.H	-1.798297	1.173931	1.238657
27.O	1.737853	-0.834196	3.627112	56.H	-1.964535	2.704552	0.372780
28.C	0.793697	-0.758894	4.809836	57.H	1.110415	-2.951619	-2.786177
29.C	1.580852	-1.394627	5.968973	58.H	2.518191	-2.551492	-1.777031
30.C	3.048094	-1.046336	5.644394	59.H	2.392052	-1.902943	-3.418429
31.C	3.095604	-1.187669	4.122331	60.H	0.766921	-4.218369	0.729614
32.C	0.354740	0.683940	5.060731	61.H	-0.974326	-4.417451	0.410836
33.H	-0.064291	-1.371518	4.526617	62.H	-0.133423	-5.520630	1.512207
34.H	1.439248	-2.482462	5.981660	63.H	-0.413590	0.695032	5.844362
35.H	1.259424	-1.003870	6.939629	64.H	-0.079712	1.136105	4.162342
36.H	3.760081	-1.717181	6.136084	65.H	1.186688	1.310860	5.402839
37.H	3.287625	-0.021720	5.950685	66.O	3.024532	-1.609919	0.878608

67.C	4.333696	-0.811731	0.834303
68.C	5.413807	-1.870124	1.108394
69.C	4.820112	-3.177449	0.539157
70.C	3.340913	-3.071443	0.901995
71.C	4.474894	-0.087676	-0.499087
72.H	4.250581	-0.091924	1.653074
73.H	5.595843	-1.969070	2.184632
74.H	6.362116	-1.602503	0.631911
75.H	5.279201	-4.068843	0.978265
76.H	4.953057	-3.232769	-0.547022
77.H	3.134635	-3.444277	1.912684
78.H	2.675417	-3.556477	0.183991
79.H	5.381709	0.530261	-0.466936
80.H	3.629786	0.582089	-0.691797
81.H	4.572530	-0.785522	-1.337510

Zn-6THF-NoFC

1.O	1.375037	-1.202488	0.363058
2.C	2.089504	-2.473631	0.042587
3.C	2.267050	-2.475798	-1.478762
4.C	2.375825	-0.970768	-1.814498
5.C	1.369880	-0.335567	-0.851069
6.H	3.052938	-2.457993	0.567200
7.H	1.483053	-3.300104	0.421381
8.H	1.395042	-2.921930	-1.972943
9.H	3.153575	-3.042379	-1.782490
10.H	2.130579	-0.751551	-2.858788
11.H	3.390237	-0.600281	-1.620285
12.H	0.352754	-0.339223	-1.263154
13.H	1.629929	0.677626	-0.536788
14.O	-1.365959	-1.802794	1.742188
15.C	-2.600551	-1.927082	2.572738
16.C	-3.446341	-3.010083	1.896948
17.C	-3.070915	-2.856245	0.405414
18.C	-1.573286	-2.546287	0.463784
19.H	-2.291638	-2.172518	3.591842
20.H	-3.104742	-0.952818	2.568995
21.H	-4.515598	-2.863054	2.081386
22.H	-3.172956	-4.006499	2.266093
23.H	-3.624174	-2.025914	-0.051196
24.H	-3.275345	-3.760204	-0.177809
25.H	-1.216032	-1.911767	-0.350862
26.H	-0.967915	-3.460603	0.506221
27.O	1.310951	-2.537433	3.189063
28.C	2.705498	-2.698423	3.694737
29.C	2.918252	-4.207351	3.832803
30.C	1.506775	-4.715992	4.205162
31.C	0.589833	-3.835188	3.350176
32.H	3.375387	-2.215687	2.979324
33.H	2.774117	-2.185255	4.662350
34.H	3.667741	-4.443450	4.595364
35.H	3.252057	-4.643232	2.882674
36.H	1.309277	-4.563338	5.273436
37.H	1.367540	-5.779441	3.984525
38.H	-0.378122	-3.623571	3.811913
39.H	0.431872	-4.255011	2.349075
40.O	-0.368558	1.150466	1.437064
41.C	0.234875	2.512193	1.532400
42.C	-0.853788	3.478171	1.058044

43.C	-1.629963	2.634738	0.020979
44.C	-1.636312	1.241107	0.654809
45.H	0.548781	2.665247	2.567907
46.H	1.114805	2.536281	0.877360
47.H	-0.427018	4.390016	0.627696
48.H	-1.507223	3.769874	1.889889
49.H	-1.104894	2.623447	-0.942361
50.H	-2.645691	3.005864	-0.152136
51.H	-1.639765	0.422343	-0.068824
52.H	-2.472111	1.112264	1.353972
53.Zn	0.464318	-0.695844	2.314698
54.O	2.298313	0.410669	2.872103
55.C	2.554657	1.056476	4.192971
56.C	3.775832	1.954942	3.981476
57.C	4.578043	1.191507	2.903151
58.C	3.480094	0.641491	1.988980
59.H	1.647739	1.593991	4.480742
60.H	2.753927	0.260772	4.921725
61.H	4.340738	2.096544	4.908786
62.H	3.474083	2.944008	3.614315
63.H	5.156704	0.375479	3.353902
64.H	5.273337	1.837345	2.356751
65.H	3.729975	-0.309716	1.512418
66.H	3.186094	1.367374	1.221158
67.O	-0.453937	-0.178500	4.260399
68.C	-0.250921	-0.917051	5.542301
69.C	-0.845868	-0.022268	6.633076
70.C	-1.984967	0.713325	5.890583
71.C	-1.378861	0.966735	4.508382
72.H	-0.780488	-1.874963	5.463677
73.H	0.820269	-1.102411	5.652907
74.H	-0.098995	0.691227	7.002927
75.H	-1.204864	-0.607823	7.486107
76.H	-2.277070	1.647060	6.382626
77.H	-2.875702	0.076885	5.815376
78.H	-0.785128	1.889585	4.484995
79.H	-2.109424	0.984233	3.696421

Zn-6-2MeTHF-NoFC

1.O	0.513758	-1.793486	-0.787741
2.C	-0.942378	-2.003550	-1.065432
3.C	-1.115081	-1.855157	-2.576821
4.C	0.016785	-0.878475	-2.959409
5.C	1.187635	-1.318886	-2.068167
6.H	-1.210695	-2.987263	-0.679913
7.H	-1.495928	-1.237422	-0.515475
8.H	-2.107244	-1.467940	-2.831052
9.H	-0.993704	-2.817627	-3.086048
10.H	-0.276736	0.154487	-2.737732
11.H	0.276796	-0.930765	-4.021213
12.H	1.818273	-0.483694	-1.760566
13.C	2.050264	-2.413960	-2.689680
14.O	-0.950696	-1.954657	2.143488
15.C	-1.624155	-3.174380	2.753089
16.C	-2.787166	-2.617599	3.616517
17.C	-2.618493	-1.081271	3.614525
18.C	-1.893157	-0.821998	2.298417
19.C	-2.093551	-4.158431	1.688024
20.H	-0.848580	-3.630997	3.373962

21.H	-2.767314	-3.034752	4.628286	50.H	1.036767	3.700632	0.017912
22.H	-3.746768	-2.897385	3.166752	51.H	1.014320	1.041665	-0.705033
23.H	-2.014319	-0.746159	4.463858	52.C	-0.879460	1.823826	-0.005857
24.H	-3.579412	-0.557838	3.660110	53.Zn	1.174531	-1.645878	1.309656
25.H	-1.301973	0.091940	2.269168	54.H	-1.309003	2.354845	0.851318
26.H	-2.592009	-0.828626	1.450073	55.H	-1.446093	0.902173	-0.164313
27.O	1.881129	-1.545903	3.617167	56.H	-1.022002	2.457394	-0.890697
28.C	1.148801	-1.770869	4.921371	57.H	1.458758	-3.282117	-3.000305
29.C	2.171566	-2.528437	5.781857	58.H	2.837244	-2.745933	-2.008022
30.C	3.514650	-1.868078	5.398517	59.H	2.542159	-2.006319	-3.582186
31.C	3.339810	-1.531318	3.907907	60.H	-1.267969	-4.527557	1.075787
32.C	0.685744	-0.459463	5.558411	61.H	-2.856995	-3.712073	1.039527
33.H	0.285904	-2.385637	4.654917	62.H	-2.555964	-5.020392	2.187445
34.H	2.177654	-3.596801	5.534680	63.H	0.145962	-0.688498	6.486168
35.H	1.951790	-2.438275	6.850274	64.H	0.002575	0.092109	4.908011
36.H	4.368119	-2.532684	5.565737	65.H	1.526241	0.194704	5.816487
37.H	3.684909	-0.961051	5.987493	66.O	3.413447	-1.241170	0.660200
38.H	3.803702	-2.278554	3.258795	67.C	4.175254	0.058471	0.598376
39.H	3.729700	-0.542237	3.649970	68.C	5.528578	-0.282445	1.239350
40.O	0.892569	0.618861	1.326497	69.C	5.807674	-1.731868	0.769268
41.C	1.231683	1.443013	2.525646	70.C	4.408651	-2.339134	0.526666
42.C	1.286404	2.908432	2.063298	71.C	4.310733	0.576474	-0.836435
43.C	1.423529	2.811880	0.526397	72.H	3.587812	0.751797	1.202787
44.C	0.616087	1.556463	0.170652	73.H	5.465364	-0.229896	2.330767
45.H	0.466248	1.268299	3.284006	74.H	6.313174	0.411035	0.921113
46.H	2.189569	1.077272	2.903866	75.H	6.372051	-2.300473	1.514831
47.H	2.124725	3.443636	2.520050	76.H	6.393942	-1.737920	-0.154939
48.H	0.369523	3.438689	2.340994	77.H	4.137038	-3.100201	1.259681
49.H	2.472657	2.692806	0.234720	78.H	4.319751	-2.764961	-0.477949

79.H	4.874980	1.517643	-0.824440
80.H	3.339872	0.782399	-1.296322
81.H	4.856446	-0.125912	-1.477095
82.O	1.513940	-3.868375	1.318945
83.C	1.983714	-4.777330	0.196953
84.C	2.927437	-5.809237	0.878091
85.C	2.882276	-5.498240	2.397880
86.C	1.603920	-4.677214	2.555199
87.C	0.812713	-5.430209	-0.532707
88.H	2.520509	-4.113141	-0.478448
89.H	3.945892	-5.741679	0.482597
90.H	2.570521	-6.825170	0.679257
91.H	3.756880	-4.916330	2.711433
92.H	2.857796	-6.408055	3.007082
93.H	1.610818	-3.981202	3.391129
94.H	0.715571	-5.319850	2.613371
95.H	1.212692	-6.050991	-1.345364
96.H	0.141520	-4.691199	-0.978060
97.H	0.237644	-6.091743	0.125326

Zn-2THF-TFSI(NoFC)

1.Zn	-0.467666	-0.172927	1.059815
2.O	-1.337458	-1.220447	2.514605
3.C	-2.775816	-1.662401	2.418887
4.C	-3.114984	-2.138271	3.827960
5.C	-2.265764	-1.210694	4.730469
6.C	-0.949620	-1.081182	3.966528
7.H	2.091500	-2.293138	1.015872
8.H	3.028265	-3.491014	-0.890213
9.H	0.647189	-3.232989	0.503503
10.H	1.480841	0.398528	-1.219810
11.H	0.486781	-0.747565	-2.182473
12.O	0.687176	-1.244152	-0.153685
13.C	1.265101	-0.654035	-1.418977
14.C	2.499405	-1.506527	-1.707178
15.C	2.141876	-2.883281	-1.096758
16.C	1.406783	-2.512707	0.188356
17.C	-2.366160	2.964888	-1.578448
18.S	-2.269123	2.262191	0.208630
19.O	-3.582771	2.400689	0.790586
20.O	-1.795004	0.836862	-0.044886
21.F	-1.158500	2.851846	-2.168298
22.F	-2.728796	4.251665	-1.513303
23.F	-3.277914	2.254568	-2.264105
24.N	-1.181857	3.135324	0.978599
25.S	0.363744	2.761394	1.143374
26.O	1.240987	2.997357	0.012091
27.O	0.534876	1.397085	1.805799
28.C	0.837279	3.967720	2.560570
29.F	0.665662	5.224156	2.137169
30.F	2.130542	3.741871	2.850493
31.F	0.073975	3.725024	3.639366
32.H	-3.367472	-0.794811	2.109033
33.H	-2.811575	-2.440018	1.651419
34.H	-2.825716	-3.186757	3.964370
35.H	-4.186648	-2.048558	4.030877
36.H	-2.107978	-1.631676	5.728290
37.H	-2.746504	-0.232213	4.843220
38.H	-0.251114	-1.897952	4.176328

39.H	-0.450381	-0.115687	4.080261
40.H	1.485017	-3.449251	-1.767304
41.H	3.384450	-1.083100	-1.218697
42.H	2.698291	-1.567122	-2.781505

Zn-2-2MeTHF-TFSI-NoFC

1.Zn	-0.472755	-0.116171	0.908650
2.O	-1.209363	-1.019383	2.532584
3.C	-2.691544	-1.166045	2.743206
4.C	-2.810120	-1.934341	4.056180
5.C	-1.580958	-1.454038	4.856217
6.C	-0.462955	-1.373556	3.814143
7.H	1.018491	-3.080564	0.922942
8.H	2.238175	-4.156876	-0.879263
9.H	-0.265065	-3.091204	-0.331774
10.H	2.458389	-0.043779	-0.202081
11.C	1.556469	-0.089179	-2.173649
12.O	0.762486	-1.276716	-0.127697
13.C	1.997337	-0.764946	-0.883302
14.C	2.838343	-2.038170	-1.049193
15.C	1.801262	-3.183401	-1.122164
16.C	0.752393	-2.767849	-0.094003
17.C	-3.205125	2.366314	-1.712784
18.S	-2.748826	1.880846	0.090778
19.O	-3.977461	1.874525	0.850238
20.O	-2.075612	0.533003	-0.113320
21.F	-2.088978	2.377899	-2.468647
22.F	-3.765952	3.582382	-1.699832
23.F	-4.071476	1.455792	-2.188611
24.N	-1.736658	2.986297	0.626260
25.S	-0.142401	2.939986	0.518873
26.O	0.464316	3.335813	-0.735867
27.O	0.423835	1.661124	1.125601
28.C	0.298826	4.252511	1.846703
29.F	-0.187592	5.439588	1.470399
30.F	1.641340	4.298782	1.923199
31.F	-0.214696	3.890731	3.037118
32.H	-3.117623	-0.159525	2.800992
33.H	-3.091173	-1.687508	1.869954
34.H	-2.762620	-3.015687	3.881095
35.H	-3.755273	-1.713401	4.561994
36.H	-1.314136	-2.140594	5.666184
37.H	-1.762353	-0.464201	5.294456
38.H	-0.040266	-2.368292	3.622065
39.C	0.636464	-0.357892	4.073942
40.H	1.357888	-3.250874	-2.121443
41.H	3.499993	-2.176385	-0.185835
42.H	3.461688	-1.986093	-1.946933
43.H	2.439826	0.337410	-2.665466
44.H	0.865173	0.737816	-1.982442
45.H	1.084868	-0.796335	-2.865036
46.H	1.378931	-0.333541	3.266507
47.H	1.171359	-0.641912	4.989028
48.H	0.227596	0.648515	4.215899

Zn-3THF-TFSI(NoFC)

1.Zn	0.368473	-0.341522	1.746589
2.O	-1.114036	-1.210775	2.888781
3.C	-2.199638	-2.039149	2.274866
4.C	-3.277607	-2.122166	3.352641

5.C	-3.171306	-0.747353	4.054161
6.C	-1.665961	-0.481238	4.081427
7.O	1.922116	-1.112499	2.981784
8.C	1.867497	-2.316576	3.851616
9.C	2.992381	-2.123807	4.869996
10.C	4.048595	-1.330427	4.066951
11.C	3.197104	-0.372630	3.234049
12.O	1.046024	-1.265461	0.050047
13.C	1.053345	-0.623240	-1.309205
14.C	2.025434	-1.471122	-2.126196
15.C	1.867554	-2.880858	-1.510493
16.C	1.726867	-2.587239	-0.016719
17.C	-2.257830	2.447819	-1.095863
18.S	-1.901306	1.872214	0.698471
19.O	-3.184836	1.825119	1.368040
20.O	-1.180885	0.569981	0.494896
21.F	-1.097005	2.550798	-1.778653
22.F	-2.878640	3.634937	-1.068532
23.F	-3.046872	1.526931	-1.688426
24.N	-0.952576	2.998220	1.322691
25.S	0.628907	2.810272	1.445449
26.O	1.436845	3.055247	0.263668
27.O	0.985480	1.545822	2.208102
28.C	1.004346	4.185326	2.725729
29.F	0.684856	5.375542	2.204312
30.F	2.326294	4.133717	2.988654
31.F	0.309097	3.968862	3.857432
32.H	-2.545603	-1.521901	1.374631
33.H	-1.747824	-3.000331	2.012248
34.H	-3.065846	-2.938682	4.053512
35.H	-4.267287	-2.291936	2.917261
36.H	-3.594518	-0.758570	5.063350
37.H	-3.683765	0.024683	3.470588
38.H	-1.172914	-0.907822	4.962246
39.H	-1.400047	0.574589	3.982698
40.H	0.866169	-2.365367	4.285372
41.H	2.034001	-3.195618	3.215637
42.H	3.372573	-3.080379	5.241752
43.H	2.640363	-1.538884	5.728168
44.H	4.627683	-2.001743	3.421208
45.H	4.749799	-0.789892	4.710304
46.H	3.623870	-0.117370	2.260282
47.H	2.942322	0.545286	3.772248
48.H	1.359610	0.416738	-1.175285
49.H	0.027690	-0.665725	-1.686725
50.H	3.053394	-1.108431	-2.007231
51.H	1.777546	-1.448970	-3.191872
52.H	2.724038	-3.530618	-1.715553
53.H	0.965443	-3.372125	-1.893943
54.H	2.696485	-2.488280	0.484231
55.H	1.102038	-3.306042	0.521976

Zn-3-2MeTHF-TFSI(NoFC)

1.Zn	0.370273	-0.038348	1.759513
2.O	-1.288944	-0.752030	2.750128
3.C	-2.496271	-1.259239	2.048266
4.C	-3.310271	-1.925036	3.152390
5.C	-3.082960	-0.977988	4.349796
6.C	-1.626010	-0.497558	4.213086

7.O	1.678222	-1.068404	3.083497	36.H	-3.245575	-1.472244	5.312726
8.C	1.649938	-2.551413	3.100711	37.H	-3.764942	-0.120926	4.291218
9.C	2.802444	-2.964197	4.014541	38.H	-0.936193	-1.147839	4.763138
10.C	3.845243	-1.851779	3.766600	39.C	-1.396948	0.963435	4.570943
11.C	3.003731	-0.570658	3.629981	40.H	0.661421	-2.853415	3.458724
12.O	1.083645	-1.019099	0.073827	41.H	1.790658	-2.906664	2.072527
13.C	0.207812	-1.514410	-1.061598	42.H	3.181724	-3.960247	3.765432
14.C	0.987813	-1.121941	-2.327358	43.H	2.483270	-2.977160	5.062823
15.C	2.467102	-1.141616	-1.879873	44.H	4.399035	-2.048930	2.840629
16.C	2.402053	-0.562802	-0.469383	45.H	4.572471	-1.768823	4.579970
17.C	-1.660249	3.100737	-1.206701	46.H	3.397850	0.106337	2.867044
18.S	-1.443631	2.517830	0.607039	47.C	2.765726	0.185075	4.932942
19.O	-2.724819	2.720828	1.249938	48.H	-0.727173	-0.954970	-0.972120
20.O	-0.963498	1.104281	0.445487	49.C	-0.027280	-3.012631	-0.887664
21.F	-0.494389	2.958261	-1.874544	50.H	0.702551	-0.115277	-2.652615
22.F	-2.040498	4.385489	-1.222331	51.H	0.789484	-1.814159	-3.151542
23.F	-2.606253	2.332295	-1.788417	52.H	3.107345	-0.537418	-2.529902
24.N	-0.316111	3.469700	1.225447	53.H	2.863248	-2.163317	-1.867843
25.S	1.206194	3.014019	1.367744	54.H	2.410979	0.532241	-0.471098
26.O	2.055104	3.098464	0.191208	55.H	3.171619	-0.941895	0.208935
27.O	1.342094	1.721575	2.153000	56.H	0.898056	-3.585849	-1.014691
28.C	1.804909	4.330373	2.624009	57.H	-0.353225	1.263310	4.430649
29.F	1.699471	5.547009	2.077176	58.H	-1.638779	1.109631	5.631678
30.F	3.097423	4.057015	2.900344	59.H	-2.043388	1.623065	3.981354
31.F	1.077318	4.262082	3.754373	60.H	3.715684	0.611806	5.278462
32.H	-3.017210	-0.410043	1.592940	61.H	2.380297	-0.473568	5.719991
33.H	-2.150033	-1.942750	1.268049	62.H	2.065587	1.012637	4.786119
34.H	-2.925303	-2.930179	3.363689	63.H	-0.748245	-3.355450	-1.640229
35.H	-4.367284	-2.013404	2.882013	64.H	-0.442665	-3.243049	0.100300

Zn-4THF-1TFSI-NoFC

1.O	0.600809	-1.980733	-0.400902
2.C	0.265018	-3.394696	-0.715182
3.C	-0.277430	-3.349075	-2.142539
4.C	0.610207	-2.265854	-2.799217
5.C	0.808772	-1.237475	-1.676265
6.H	1.179558	-3.993655	-0.642461
7.H	-0.451229	-3.730516	0.039207
8.H	-1.333599	-3.049210	-2.149961
9.H	-0.194524	-4.320650	-2.640747
10.H	0.144118	-1.815194	-3.681405
11.H	1.573920	-2.692473	-3.099493
12.H	0.059577	-0.437461	-1.700669
13.H	1.815548	-0.812450	-1.658781
14.O	-0.972223	-1.552012	2.151870
15.C	-1.444118	-2.466987	3.234444
16.C	-2.797485	-2.991128	2.755792
17.C	-3.358175	-1.793489	1.955917
18.C	-2.113968	-1.248777	1.245995
19.H	-0.679290	-3.234313	3.367917
20.H	-1.542229	-1.868852	4.148541
21.H	-3.440814	-3.279917	3.593868
22.H	-2.669104	-3.866677	2.107097
23.H	-3.780016	-1.040057	2.633088
24.H	-4.135789	-2.084316	1.242195
25.H	-2.135996	-0.167015	1.087232
26.H	-1.923682	-1.747668	0.290436
27.O	1.739231	-0.510146	3.548158
28.C	1.412158	-1.147600	4.857202
29.C	2.347338	-0.495524	5.883455
30.C	3.570114	-0.082261	5.032522
31.C	2.924105	0.372918	3.725280
32.H	0.352599	-0.959841	5.054292
33.H	1.595213	-2.220537	4.753691
34.H	2.608143	-1.193250	6.685626
35.H	1.875504	0.385353	6.336514
36.H	4.227745	-0.940605	4.856430
37.H	4.156789	0.717948	5.496284
38.H	3.556528	0.253013	2.844656
39.H	2.561411	1.408389	3.790149
40.O	0.819272	0.817265	1.037084
41.C	1.719654	1.621749	0.154959
42.C	1.679471	3.041208	0.723236
43.C	0.247724	3.137861	1.299170
44.C	0.021223	1.743088	1.887727
45.H	2.703611	1.149105	0.173590
46.H	1.305780	1.578172	-0.859161
47.H	1.875803	3.792136	-0.049159
48.H	2.427512	3.165473	1.515853
49.H	-0.475675	3.344506	0.500498
50.H	0.147097	3.919947	2.059161
51.H	-1.020027	1.412931	1.849129
52.H	0.389843	1.652784	2.915181
53.Zn	1.117002	-1.266872	1.589081
54.O	4.196721	-2.395595	-1.042362
55.O	1.523764	-3.294166	2.242044
56.N	3.758883	-3.742346	1.039887
57.S	2.888137	-3.917429	2.374977

58.S	4.082359	-2.314879	0.400639
59.O	3.225531	-1.215062	0.962784
60.O	3.565161	-3.692656	3.642910
61.C	5.842027	-1.849658	1.036738
62.C	2.529739	-5.800524	2.261264
63.F	6.726425	-2.769725	0.617165
64.F	5.843969	-1.795185	2.390299
65.F	6.171657	-0.633052	0.541210
66.F	1.871798	-6.090031	1.114918
67.F	1.746215	-6.119095	3.318069
68.F	3.679849	-6.488591	2.320579

Zn-4-2MeTHF-1TFSI-NoFC

1.O	0.750219	-1.898625	-0.458901
2.C	0.538191	-3.323530	-0.821393
3.C	-0.372413	-3.294453	-2.046078
4.C	0.146443	-2.055080	-2.799417
5.C	0.498298	-1.050799	-1.685227
6.H	1.512127	-3.764530	-1.057661
7.H	0.119929	-3.826993	0.052123
8.H	-1.423719	-3.168458	-1.755730
9.H	-0.291390	-4.214610	-2.634584
10.H	-0.589905	-1.634297	-3.492537
11.H	1.046841	-2.306791	-3.374071
12.H	-0.386601	-0.448550	-1.437346
13.C	1.688240	-0.154832	-2.000785
14.O	-0.684294	-2.031930	2.276314
15.C	-1.192115	-2.623403	3.586212
16.C	-2.676230	-2.919535	3.320436
17.C	-3.077776	-1.901872	2.236370
18.C	-1.832694	-1.869872	1.351145
19.C	-0.364824	-3.823390	4.018074
20.H	-1.100959	-1.808238	4.312118
21.H	-3.265888	-2.818757	4.238012
22.H	-2.799084	-3.946257	2.951290
23.H	-3.274069	-0.915880	2.676407
24.H	-3.967707	-2.205724	1.674580
25.H	-1.692478	-0.935060	0.805121
26.H	-1.824661	-2.706302	0.643387
27.O	1.988365	-0.851810	3.839577
28.C	1.242836	-0.483053	5.098354
29.C	2.340014	-0.172646	6.125208
30.C	3.489378	-1.107757	5.715692
31.C	3.424017	-1.068967	4.188707
32.C	0.265862	0.657743	4.855683
33.H	0.703077	-1.389232	5.403671
34.H	1.985752	-0.346786	7.147359
35.H	2.644514	0.880376	6.047389
36.H	3.315254	-2.126166	6.084108
37.H	4.464889	-0.775869	6.086270
38.H	3.747661	-2.000981	3.729632
39.H	3.993040	-0.230174	3.771511
40.O	0.947859	0.794599	1.451099
41.C	2.136652	1.676996	1.647150
42.C	1.655345	3.097775	1.349225
43.C	0.539995	2.871533	0.304673
44.C	-0.154069	1.588102	0.795729
45.H	2.480554	1.526490	2.672979
46.H	2.914230	1.346481	0.952254

47.H	2.466505	3.725069	0.965504
48.H	1.256155	3.578585	2.249977
49.H	0.972423	2.721813	-0.691144
50.H	-0.161125	3.710411	0.246109
51.H	-0.502911	0.971789	-0.037491
52.C	-1.304743	1.856620	1.767738
53.Zn	1.324480	-1.404459	1.687977
54.O	4.540092	-1.739408	-1.080394
55.O	1.965808	-3.513903	1.887274
56.N	4.222354	-3.550833	0.634768
57.S	3.326439	-4.147129	1.825162
58.S	4.375310	-1.993522	0.336391
59.O	3.386073	-1.140716	1.084971
60.O	3.995929	-4.337816	3.102258
61.C	6.061304	-1.475791	1.116545
62.C	3.028377	-5.921245	1.135499
63.F	7.058388	-2.118940	0.487834
64.F	6.086887	-1.778456	2.437586
65.F	6.210012	-0.136914	0.963689
66.F	2.453981	-5.883397	-0.089637
67.F	2.195273	-6.550060	1.997548
68.F	4.198007	-6.574883	1.067833
69.H	2.577148	-0.746399	-2.238278
70.H	1.930775	0.510575	-1.167789
71.H	1.439699	0.466520	-2.871967
72.H	0.685822	-3.568273	4.176998
73.H	-0.418659	-4.630399	3.279672
74.H	-0.773454	-4.198370	4.966254
75.H	-0.273701	0.864578	5.789297
76.H	-0.470325	0.412255	4.087057
77.H	0.791383	1.572767	4.560110
78.H	-1.006264	2.533687	2.575325
79.H	-1.685187	0.933395	2.213949
80.H	-2.129382	2.327798	1.216755

Zn-2TFSI(NoFC)

1.Zn	-0.170304	0.084588	1.921507
2.S	-1.964634	2.688571	1.856123
3.O	-2.524965	3.612271	2.810470
4.O	-1.657381	1.308009	2.394248
5.F	-2.838294	1.471396	-0.370123
6.F	-3.723509	3.460025	-0.020162
7.F	3.070341	3.150942	0.629348
8.F	1.870851	3.327982	2.470394
9.F	-4.378027	1.739050	1.186520
10.N	-0.792228	3.337250	1.010454
11.C	-3.332553	2.317963	0.566776
12.S	0.465986	2.707600	0.265864
13.O	0.549476	3.043401	-1.134869
14.O	0.728380	1.254810	0.595880
15.C	1.912375	3.602424	1.146743
16.F	1.810371	4.926783	0.953729
17.S	-0.010824	-3.029482	1.551411
18.O	0.766366	-3.587609	0.469944
19.O	-0.700401	-1.712244	1.264199
20.F	-2.276677	-3.751814	2.823863
21.F	-1.052900	-5.433726	2.099009
22.F	0.048976	-1.134224	6.316397
23.F	-0.329861	-3.251528	5.846515

24.F	-2.222399	-4.228928	0.673991
25.N	0.740149	-3.083147	2.955211
26.S	1.109238	-1.938839	3.992476
27.O	0.951861	-0.539291	3.441078
28.O	2.354800	-2.199687	4.668619
29.C	-0.255020	-2.008273	5.340563
30.F	-1.448138	-1.671154	4.790658
31.C	-1.504669	-4.201341	1.812570

Zn-2TFSI-2THF-NoFC

1.Zn	-0.721517	-0.073262	1.703339
2.S	-1.395017	3.147531	1.704055
3.O	-2.231820	3.582642	2.805458
4.O	-1.645051	1.771076	1.164290
5.F	-1.115548	3.943990	-0.871298
6.F	-1.656770	5.555292	0.528853
7.F	2.564128	2.394327	4.715696
8.F	0.447580	2.988867	4.874389
9.F	-3.161018	4.060381	-0.063232
10.N	0.158975	3.508476	1.803166
11.C	-1.852423	4.260924	0.220847
12.S	1.305830	2.549286	2.358192
13.O	2.562339	2.790237	1.674975
14.O	0.879115	1.130948	2.532210
15.C	1.581770	3.136420	4.157912
16.F	1.947671	4.434848	4.160421
17.S	-2.185866	-1.202576	4.437742
18.O	-3.594478	-1.520885	4.283962
19.O	-1.654900	-0.059634	3.641695
20.F	-0.705964	-0.324629	6.519499
21.F	-2.433241	-1.567976	7.084252
22.F	2.629137	-2.857105	3.915135
23.F	1.434844	-3.248796	5.724715
24.F	-2.743439	0.504935	6.408393
25.N	-1.286441	-2.527845	4.399776
26.S	-0.012856	-2.832814	3.493608
27.O	0.188644	-1.879498	2.359804
28.O	0.056349	-4.241862	3.165453
29.C	1.515709	-2.508093	4.600267
30.F	1.591330	-1.200230	4.928627
31.C	-1.997197	-0.606878	6.244561
32.O	-2.407300	-1.046093	0.808647
33.C	-2.418733	-2.445885	0.326143
34.C	-3.828508	-2.658950	-0.229497
35.C	-4.690706	-1.757999	0.684517
36.C	-3.801421	-0.531196	0.898142
37.H	-1.617948	-2.541727	-0.412624
38.H	-2.209298	-3.108005	1.173950
39.H	-4.123879	-3.712457	-0.189262
40.H	-3.889165	-2.324390	-1.273066
41.H	-4.885839	-2.254696	1.641773
42.H	-5.650728	-1.489081	0.231749
43.H	-3.920728	-0.062349	1.876492
44.H	-3.918470	0.221283	0.109963
45.O	0.395312	-0.300311	-0.103250
46.C	1.831508	-0.692646	-0.109756
47.C	2.432287	0.021617	-1.322652
48.C	1.238800	0.104607	-2.301769
49.C	0.059490	0.390812	-1.368237

50.H	2.262680	-0.387532	0.845333
51.H	1.865903	-1.784455	-0.199388
52.H	3.283604	-0.528367	-1.737022
53.H	2.772951	1.025528	-1.043318
54.H	1.098241	-0.850869	-2.822778
55.H	1.359382	0.891086	-3.053971
56.H	-0.897802	-0.011100	-1.713533
57.H	-0.050723	1.459826	-1.158185

Zn-2TFSI-1THF-NoFC

1.Zn	-0.111256	0.182484	0.367020
2.S	-1.173122	3.249967	0.472479
3.O	-1.630583	4.021876	1.607856
4.O	-1.377166	1.762034	0.569459
5.F	-1.944645	3.017893	-2.101684
6.F	-2.187877	5.040392	-1.260242
7.F	3.654919	3.199877	1.789783
8.F	1.669356	3.606682	2.658209
9.F	-3.568658	3.430340	-0.671673
10.N	0.242301	3.673279	-0.134771
11.C	-2.294516	3.725848	-1.000397
12.S	1.637506	2.931552	0.052876
13.O	2.520423	3.186232	-1.065713
14.O	1.507953	1.511695	0.511995
15.C	2.452094	3.770525	1.568804
16.F	2.614599	5.084807	1.325167
17.S	-2.070264	-2.408333	1.100154
18.O	-2.890780	-3.337880	0.356190
19.O	-1.800884	-1.088152	0.450802
20.F	-2.426734	-1.030968	3.390323
21.F	-3.341353	-3.036259	3.383671
22.F	2.256433	-2.325717	4.023275
23.F	1.007427	-4.138850	3.973844
24.F	-4.270196	-1.398677	2.240892
25.N	-0.762415	-3.128200	1.667785
26.S	0.691351	-2.508683	1.872689
27.O	0.756496	-1.008378	1.782864
28.O	1.713527	-3.238639	1.147236
29.C	1.034932	-2.815366	3.729474
30.F	0.107134	-2.195789	4.487198
31.C	-3.101057	-1.935785	2.643494
32.O	0.391871	-0.417335	-1.531520
33.C	1.777426	-0.822995	-1.917290
34.C	1.675939	-1.170090	-3.403849
35.C	0.222458	-1.678846	-3.551201
36.C	-0.562845	-0.750766	-2.624140
37.H	2.433658	0.020886	-1.693378
38.H	2.048931	-1.686091	-1.299193
39.H	2.416538	-1.923500	-3.690581
40.H	1.837347	-0.277025	-4.019373
41.H	0.139858	-2.718775	-3.213111
42.H	-0.141998	-1.622491	-4.582006
43.H	-1.441777	-1.205789	-2.162416
44.H	-0.840805	0.191839	-3.110703

Zn-2TFSI-2-2MeTHF-NoFC

1.Zn	-0.822823	-0.085790	1.563599
2.S	-1.435301	3.149457	1.729192
3.O	-2.246514	3.527016	2.870180
4.O	-1.704888	1.803181	1.121429

5.F	-1.203418	4.086590	-0.803817
6.F	-1.709162	5.618308	0.695618
7.F	2.596632	2.273429	4.613809
8.F	0.518643	2.969005	4.849929
9.F	-3.232081	4.165070	0.049390
10.N	0.121972	3.495204	1.808177
11.C	-1.916935	4.344427	0.318242
12.S	1.261784	2.494732	2.303923
13.O	2.495940	2.705154	1.569757
14.O	0.794083	1.092057	2.483837
15.C	1.631303	3.062911	4.092329
16.F	2.059716	4.342287	4.082325
17.S	-2.197994	-1.163653	4.427563
18.O	-3.605756	-1.519310	4.426966
19.O	-1.774674	-0.076100	3.501688
20.F	-0.562570	-0.108608	6.302070
21.F	-2.212329	-1.325082	7.106293
22.F	2.591964	-2.855366	3.656854
23.F	1.525392	-3.216677	5.550597
24.F	-2.617137	0.685104	6.303145
25.N	-1.271782	-2.470728	4.406091
26.S	-0.071868	-2.820530	3.422152
27.O	0.062551	-1.902398	2.249590
28.O	-0.039637	-4.238421	3.126401
29.C	1.531233	-2.489669	4.414647
30.F	1.638464	-1.179548	4.720316
31.C	-1.866896	-0.426683	6.161633
32.O	-2.500433	-1.042559	0.605229
33.C	-2.439027	-2.444102	0.156543
34.C	-3.544445	-3.142865	0.946063
35.C	-4.664124	-2.074644	0.987659
36.C	-3.938647	-0.707293	0.916138
37.H	-2.626510	-2.469914	-0.926285
38.H	-1.431440	-2.810697	0.358673
39.H	-3.197872	-3.387625	1.955725
40.H	-3.868400	-4.072046	0.464543
41.H	-5.266131	-2.150500	1.897892
42.H	-5.333523	-2.187656	0.125695
43.H	-3.907409	-0.220297	1.893436
44.C	-4.490982	0.246075	-0.138956
45.O	0.388234	-0.290487	-0.199633
46.C	1.774463	-0.819180	-0.077727
47.C	2.458324	-0.457609	-1.395816
48.C	1.763722	0.864822	-1.789472
49.C	0.299183	0.646503	-1.370292
50.H	2.246837	-0.329823	0.779529
51.H	1.692391	-1.891703	0.111054
52.H	2.287927	-1.233770	-2.151581
53.H	3.539366	-0.340390	-1.267550
54.H	1.849141	1.088052	-2.858040
55.H	2.196746	1.699859	-1.227237
56.C	-0.595204	0.028954	-2.444932
57.H	-0.155550	1.563290	-0.987658
58.H	-0.154131	-0.884965	-2.860721
59.H	-1.580692	-0.212601	-2.034668
60.H	-3.917720	1.176417	-0.172025
61.H	-5.530381	0.494870	0.112535
62.H	-4.486511	-0.217126	-1.133736

63.H -0.733762 0.748886 -3.261643

Zn-2TFSI-1-2MeTHF-NoFC

1.Zn -1.235362 -0.045144 2.474285

2.S -0.903907 3.178091 2.555612

3.O -0.155630 3.814487 3.620158

4.O -1.623210 1.906947 2.924217

5.F -3.105040 3.824900 1.131121

6.F -1.860239 5.544035 1.721642

7.F 3.224922 1.212747 0.562224

8.F 2.559182 2.265944 2.381018

9.F -3.101018 4.516323 3.222308

10.N -0.189780 3.111545 1.126844

11.C -2.345136 4.353671 2.116239

12.S 0.632991 1.880402 0.541337

13.O 0.607507 1.871560 -0.905695

14.O 0.351427 0.585811 1.239836

15.C 2.452351 2.213495 1.035421

16.F 2.857851 3.384000 0.505974

17.S -2.839368 -1.893941 4.630036

18.O -3.851129 -2.768031 4.065198

19.O -2.644447 -0.572440 3.951849

20.F -2.601864 -0.601473 6.988021

21.F -3.722695 -2.493980 7.090428

22.F 2.109088 -1.155600 5.603315

23.F 0.714671 -2.051185 7.053501

24.F -4.650898 -0.712635 6.187266

25.N -1.489290 -2.674927 4.972151

26.S -0.008458 -2.348642 4.480730

27.O 0.057452 -1.390458 3.326724

28.O 0.773299 -3.555949 4.347954

29.C 0.810645 -1.357737 5.902382

30.F 0.193712 -0.161134 6.045165

31.C -3.494676 -1.389381 6.355143

32.O -2.240950 -0.903690 0.905592

33.C -1.548449 -1.829745 -0.025662

34.C -2.602428 -2.154577 -1.079659

35.C -3.911922 -2.177532 -0.257380

36.C -3.740827 -1.048689 0.778812

37.H -0.668916 -1.303416 -0.402391

38.H -1.238448 -2.717780 0.539621

39.H -2.400616 -3.110847 -1.573156

40.H -2.630060 -1.372439 -1.847090

41.H -4.023369 -3.141633 0.252380

42.H -4.799826 -2.017297 -0.877201

43.H -4.095959 -1.352640 1.766964

44.C -4.330166 0.301132 0.384720

45.H -4.055375 1.079141 1.105124

46.H -5.425055 0.227390 0.378153

47.H -3.995498 0.613293 -0.611500