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Supplementary Information

A study of the Group 1 metal tetra-aza macrocyclic complexes $[M(Me_4cyclen)(L)]^+$ using electronic structure calculations

(M = Li, Na, and K; L = H_2O, THF, DEE, MeOH, and DCM)

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Further information on computational details

The DFT functionals BP86[S1] and B3LYP[S2] were used to perform geometry optimisations for all the chemical species investigated in this work.[S3] The 6-311G(d,p) basis set[S4] was employed for the atoms H, C, N, O, Cl, Li, Na, and K. The functionals were selected, with the 6-311G(d,p) basis set, based on results of our recent studies on alkali metal ion-macrocyclic complexes.[S5] Geometry optimisation was followed by analytic Hessian computation at the same levels of theory, and the absence of negative Hessian eigenvalues confirmed the stationary points as minima on the potential energy hypersurfaces. Bond dissociation energies (BDEs) were calculated for the process, $[M(Me_4cyclen)(L)]^+ \rightarrow [M(Me_4cyclen)]^+ + L$, where M = Li, Na, K, and L = H_2O, THF, DEE, MeOH, DCM, using these functionals with the 6-311G(d,p) basis set.[S6] Basis set superposition error (BSSE) correction, as implemented by the Boys-Bernardi counterpoise method,[S7] and zero-point energy (ZPE) correction were included in the BDEs. Reported relative energies are given at 298.15 K and 1 atm. All density functional computations were performed using the Gaussian 09 package.[S8] Natural bond orbital (NBO) analysis[S9] was also carried out using the NBO program as implemented in the Gaussian 09 package.[S10] Throughout this work, $[M(Me_4cyclen)(L)]^+$ structures optimised with the BP86 functional are denoted **M-L-1a** and those optimised with the B3LYP functional are denoted **M-L-2a**.

High level *ab initio* methods were employed to assess the performance of the DFT calculations and to obtain more reliable BDEs.[S5b,S11] Single-point DF-LCCSD(T)[S12] and explicitly correlated DF-LCCSD(T)-F12x (x = a, b)[S13] calculations were performed at the BP86/6-311G(d,p) and B3LYP/6-311G(d,p) lowest minimum energy geometries of $Me_4cyclen$, $[M(Me_4cyclen)]^+$, $[M(Me_4cyclen)(L)]^+$, L, $[Me_4cyclenH]^+$, H_2O, and H_3O^+ using the MOLPRO 2010.1 and 2015.1 programs.[S14] All DF-LCCSD(T) and DF-LCCSD(T)-F12x calculations were preceded by a density fitted Hartree-Fock (HF) calculation.[S15] The local correlation methods together with the density fitting (DF) approximation allow the efficient treatment of larger molecules. The inclusion of explicitly correlated terms accounts for basis set incompleteness and domain approximation associated errors.[S12,S13]

The first step in the DF-LCCSD(T)-F12x calculations involves DF-LMP2-F12 calculations which were performed using the 3*A ansatz approximation as detailed in reference S16. Two sets of ansatz options, namely (Loc,Fix) and (Fix,NoX) were used, the former being the default for DF-LCCSD(T)-F12x calculations.[S16,S17] The (Fix,NoX) ansatz option was used to avoid

unreasonable BDE values obtained with the (Loc,Fix) option for calculations involving chlorine atoms (i.e. in calculations with L = DCM) (*vide infra*).

In the DF-LCCSD(T) calculations, the aug-cc-pVDZ atomic orbital (AO) basis set[S18] was employed in conjunction with the aug-cc-pVDZ/MP2FIT[S19] and aug-cc-pVDZ/JKFIT auxiliary basis sets (ABS)[S20] for the H, C, N, O, and Cl atoms. The corresponding DF-LCCSD(T)-F12x calculation uses cc-pVDZ-F12 as the AO basis set[S21] and cc-pVDZ-F12/OPTRI as the complementary auxiliary basis set (CABS).[S22] For Li/Na, the aug-cc-pwCVDZ[S23] and cc-pCVDZ-F12[S24] AO basis sets were used in the DF-LCCSD(T) and DF-LCCSD(T)-F12x calculations, respectively. The aug-cc-pwCVDZ/MP2FIT[S24] def2-QZVPP/JKFIT[S25] and cc-pCVDZ-F12/OPTRI[S24] basis sets were chosen as the ABS and the CABS, respectively. The 1s orbital on Li^+ and the 2s and 2p orbitals on Na^+ were considered to be valence as in our previous work.[S5b] The double-ζ quality basis sets used in the DF-LCCSD(T) and DF-LCCSD(T)-F12x calculations are denoted in the text as DZ and DZ-F12, respectively.

High level single-point calculations with the aug-cc-pVTZ basis set[S18,S19a,S20] on the complexes studied, which consist of a maximum of 60 atoms, failed because the maximum CPU time allowed was exceeded. Thus, the def2-TZVPP basis set,[S26] which is slightly smaller (with respect to the aug-cc-p-VTZ basis set) but is a well-balanced triple-ζ AO basis set,[S27] was used along with the associated default ABS (def2-TZVPP/MP2FIT[S28] and def2-TZVPP/JKFIT)[S25] and/or the CABS (def2-TZVPP/OPTRI)[S29] for the H, C, N, O, and Cl atoms. Def2-TZVPP was employed as the triple-ζ AO basis set for Li and Na.[S26] In the DF-LCCSD(T) calculation, the def2-TZVPP AO basis set was augmented with the following uncontracted functions, namely, two s (ζ = 5.0134, 1.6427), two p (ζ = 4.2222, 0.93), and one d (ζ = 0.85) for Li and two s (ζ = 4.2353, 0.6984), two p (ζ = 1.1907, 0.3846), two d (ζ = 3.4561, 0.7449), and one f (ζ = 3.227) for Na. In the DF-LCCSD(T)-F12x calculation, the def2-TZVPP AO basis set was augmented with a set of spd(f) functions, with exponents of $\zeta_s = 0.406129$, $\zeta_p = 1.37526$, and $\zeta_d = 4.518674$ for Li and $\zeta_s = 3.764945$, $\zeta_p = 3.0511$, $\zeta_d = 5.420585$, and $\zeta_f = 4.557524$ for Na. These additional uncontracted basis functions account for core-correlation and were obtained by analysing and comparing the range of the exponents of the corresponding cc-pVTZ[S23] (cc-pVTZ-F12)[S24] and aug-cc-pwCVTZ[S23] (cc-pCVTZ-F12)[S24] AO basis sets. Def2-QZVPP/MP2FIT[S28a] and def2-QZVPP/JKFIT[S25] were selected as fitting basis sets and cc-pCVTZ-F12/OPTRI was selected as

the CABS.[S24] The triple-ζ quality basis sets used in the DF-LCCSD(T) and DF-LCCSD(T)-F12x calculations are denoted in the text as TZ and TZ-F12, respectively.

For K, the ECP10MDF effective core potential (ECP) was employed to account for the 1s, 2s, and 2p orbitals, where MDF indicates that the neutral atom is used in the derivation of the ECP which involves the use of the fully relativistic approach as described by the Stuttgart/Cologne group.[S30] The atomic basis set for the K^+ $3s^2$ $3p^6$ orbitals was designed to couple with the ECP10MDF ECP as follows:- An even-tempered (11s9p) set of functions were contracted to [1s1p] with the coefficients for the K^+ $3s^2$ $3p^6$ occupied atomic orbitals being obtained from a restricted Hartree-Fock (RHF) calculation on K^+ using the ECP10MDF ECP and the (11s9p) basis set. Both the exponents of the 11s and 9p primitive functions were centered on ζ = 1.2 with a ratio of 2.0. Additional uncontracted functions, namely, three s (ζ = 1.125, 0.45, 0.18), two p (ζ = 0.8, 0.32), and two d (ζ = 0.6, 0.24), were added to give the ECP10MDF[4s3p2d] basis set which is of the same standard as the aug-cc-pVDZ basis set. Four s (ζ = 2.8125, 1.125, 0.45, 0.18), two p (ζ = 1.1, 0.15), two d (ζ = 1.2, 0.4), and one f (ζ = 0.6) uncontracted functions were incorporated to yield the ECP10MDF[5s3p2d1f] basis set which is of approximately triple-ζ quality. For K, the def2-QZVPP basis set was used as both the ABS and the CABS.[S19b,S25,S31]

All computations were carried out with resources (CPU time and software) provided by the GridChem Science Gateway[S32] and the UK National Service for Computational Chemistry Software (NSCCS), and a local cluster in Hong Kong. The processing of input and output files was carried out using ExcelAutomat.[S33]

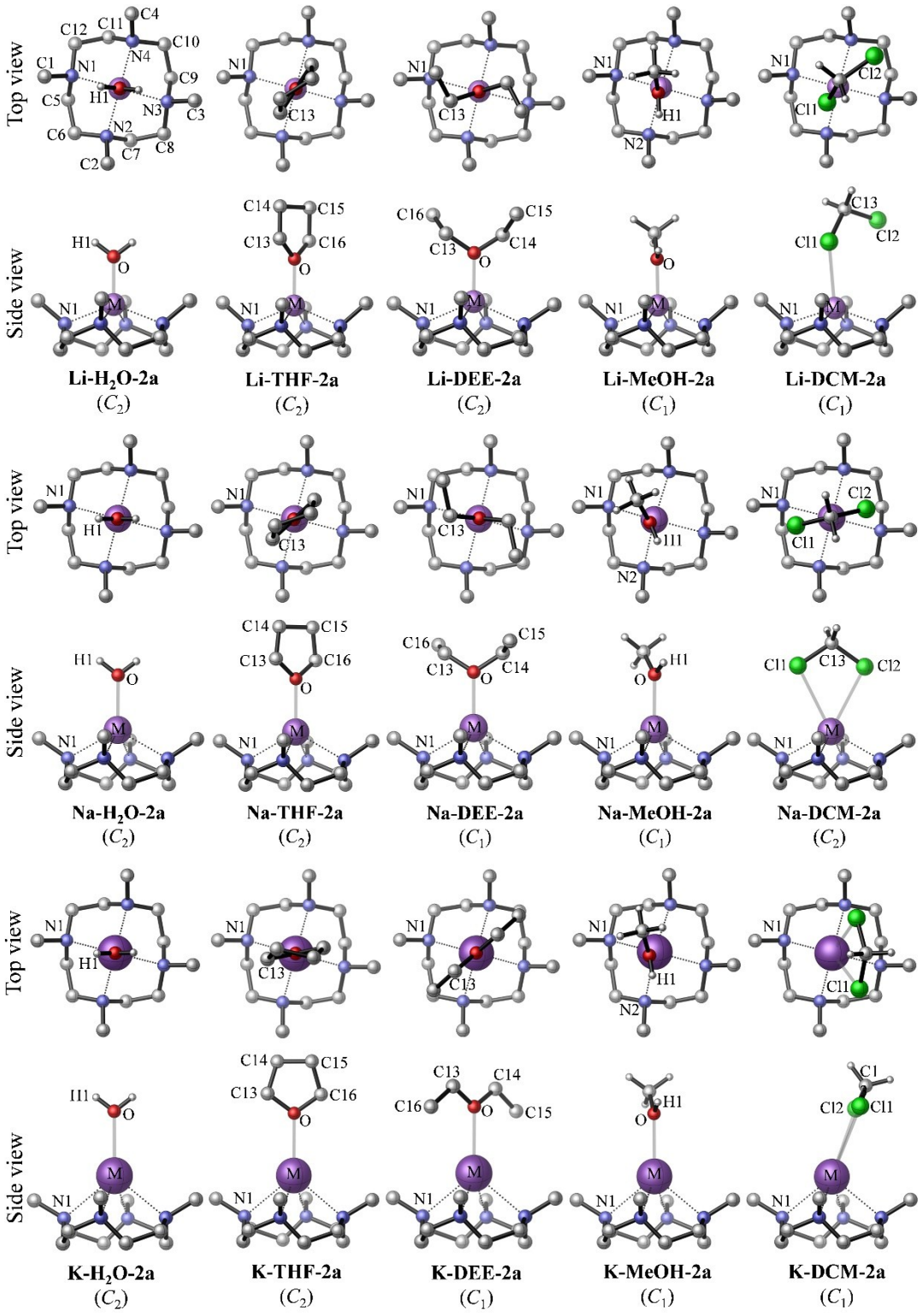


Figure S1: Lowest $[M(Me_4cyclen)(L)]^+$ minimum energy structures obtained using the B3LYP/6-311G(d,p) method. The symmetry of each structure is provided. Selected H atoms are omitted for clarity.

Further information on $[M(Me_4cyclen)]^+$ and $[M(Me_4cyclen)(L)]^+$

Initially, the alkali metal-Me_4cyclen complexes, $[M(Me_4cyclen)]^+$ (M = Li, Na, and K), were optimised in the C_4(++++) conformation using the DFT BP86/6-311G(d,p) and B3LYP/6-311G(d,p) methods. In C_4(++++), C_4 corresponds to the symmetry of the complexes and (++++) indicates that all four *N*-donor atoms of the Me_4cyclen ring lie in the same plane and orient towards the M^+ center. It should be noted that C_4(++++) is the most frequently found conformation in X-ray structures and geometry optimisation calculations of $[M(Me_4cyclen)]^+$ complexes and their derivatives, with minor variations being observed in the symmetry of some complexes.[S34,S5a,b] The BP86 minimum energy structures in the C_4(++++) conformation are shown in Figure 1.

Table S1: Selected geometrical parameters of the optimised $[M(Me_4cyclen)]^+$ structures.

	BP86/6-311G(d,p)			B3LYP/6-311G(d,p)		
	Li	Na	K	Li	Na	K
Bond distance, M–N (Å)	2.173	2.458	2.806	2.159	2.442	2.807
Bond angle, N–M–N (°)	85.5	77.8	67.9	85.8	78.2	67.7
Dihedral angle, N–C–C–N (°)	-55.5	-62.0	-64.8	-54.8	-61.6	-64.5
Cavity size of Me_4cyclen ring (A^2)[a]	8.706	9.533	9.821	8.647	9.485	9.791
Distance (Å) between the plane of the four *N*-donor atoms of the Me_4cyclen ring and the M^+ ions	0.606	1.129	1.721	0.582	1.106	1.728

[a] Calculated using the Heron's formula; see reference S35.

The geometrical parameters of the $[M(Me_4cyclen)]^+$ structures are provided in Table S1.Very similar geometrical parameters were obtained with both the BP86 and B3LYP functionals. The M–N bond distances of the $[M(Me_4cyclen)]^+$ structures increase due to an increase in the size of the ionic radii of the M^+ ions (Li^+: 0.92 Å; Na^+: 1.24 Å; K^+: 1.55 Å).[S36] This is accompanied by a simultaneous decrease in the acuteness of the N–M–N bond angles, which enhances the displacement of the M^+ ions out of the plane formed by the four *N*-donor atoms of the Me_4cyclen ring and increases the mean cavity size of the flexible Me_4cyclen ring.

The $[M(Me_4cyclen)]^+$ structures obtained were then used as initial geometries in the full optimisation of the $[M(Me_4cyclen)(L)]^+$ structures. The exposed M^+ centre of each

$[M(Me_4cyclen)]^+$ optimised structure allows the possibility for additional ligand coordination. Thus, the *O*- or *Cl*-donor atoms of the H_2O, THF, DEE, MeOH, and DCM ligands can interact with the M^+ centres at the apical position of the $[M(Me_4cyclen)]^+$ backbone forming pseudo-square pyramidal $[M(Me_4cyclen)(L)]^+$ structures. The BP86 and B3LYP lowest $[M(Me_4cyclen)(L)]^+$ minimum energy structures are denoted as **M-L-1a** (Figure 1) and **M-L-2a** (Figure S1), respectively (M = Li, Na, K, and L = H_2O, THF, DEE, MeOH, DCM). Several $[M(Me_4cyclen)(L)]^+$ low-lying structures are provided in Figures S2-S7 (details provided in next section).

The symmetries of the BP86 and B3LYP lowest minimum energy structures for each $[M(Me_4cyclen)(L)]^+$ complex are the same for each metal, except for **Na-DCM-1a** and **Na-DCM-2a** (C_1 and C_2, respectively) and **K-DEE-1a** and **K-DEE-2a** (C_2 and C_1, respectively). The $[M(Me_4cyclen)(L)]^+$ structures obtained are slightly sensitive to the functionals employed with the main difference, notably between the **M-L-1a** (BP86) and **M-L-2a** (B3LYP) lowest minimum energy structures, lying in the spatial arrangement of L. For example, the dihedral angles, *Ø*(N1–M–O–H1) of the **Na-H_2O-1a** (Figure 1) and **Na-H_2O-2a** (Figure S1) structures are 55.3° and 14.7°, respectively. However, it is noteworthy that rotation about the M–O (H_2O, THF, DEE, MeOH) and M–Cl (DCM) axis entails negligible change in the relative energy of the resulting $[M(Me_4cyclen)(L)]^+$ structures, suggesting a very flat rotational potential with a low rotational barrier.

Complexation of $[M(Me_4cyclen)]^+$ to L results in the **M-L-1a** (BP86) and the **M-L-2a** (B3LYP) minimum energy structures having either a C_2(++++) or a C_1(++++) conformation. Selected geometrical parameters of the structures **M-L-1a** (**M-L-2a)** are provided in Tables S2 and S3 and these are compared with those of the $[M(Me_4cyclen)]^+$ optimised structures in Table S1. Upon complexation, the Li–N, Na–N, and K–N bond distances lengthen by 0.007-0.156 Å (BP86; B3LYP, 0.020-0.210 Å), 0.016-0.075 Å (BP86; B3LYP, 0.026-0.068 Å), and 0.017-0.056 Å (BP86; B3LYP, 0.018-0.058 Å), respectively. A decrease of less than 5° in the N–M–N bond angles is observed along with an increase of about 0.030-0.300 Å (BP86; B3LYP, 0.040-0.320 Å) in the distance between the plane of the four *N*-donor atoms of the Me_4cyclen ring and the M^+ ions. The cavity size of the Me_4cyclen ring expands on addition of L to Me_4cyclen by a maximum of 0.231 A^2 (BP86; B3LYP, 0.276 A^2) for the Li^+ complexes in the order of **Li-DEE-1a** (**Li-DEE-2a**) > **Li-THF-1a** (**Li-THF-2a**) > **Li-MeOH-1a** (**Li-MeOH-2a**) > **Li-H_2O-1a** (**Li-H_2O-2a**) > **Li-DCM-1a** (**Li-DCM-2a**). The change in the cavity size of the Me_4cyclen ring for the Na^+ and K^+

lowest minimum energy structures is negligible (≤ 0.030 A^2). In fact, as the size of the ionic radii of M^+ increases from Li^+ (0.92 Å) → Na^+ (1.24 Å) → K^+ (1.55 Å),[S36] the geometrical parameters associated with the $[M(Me_4cyclen)]^+$ fragment in $[M(Me_4cyclen)(L)]^+$ become closer to those of their $[M(Me_4cyclen)]^+$ parent structure. Complexation with the DCM ligand affects the geometrical parameters of $[M(Me_4cyclen)]^+$ backbone to a lesser extent than complexation with *O*-donor ligands.

The M–N bond distances, N–M–N bond angles, N–C–C–N dihedral angles, the cavity size of the Me_4cyclen ring, and the distance between the plane formed by the four *N*-donor atoms of the Me_4cyclen ring and the M^+ ions, for the **M-L-1a** (**M-L-2a**) structures follow similar trends as their $[M(Me_4cyclen)]^+$ counterparts as the size of the ionic radii of M^+ increases from Li^+ to Na^+ to K^+.

The overall changes observed in the geometrical parameters upon complexation of $[M(Me_4cyclen)]^+$ to L indicate that (i) the effects of steric hindrance between Me_4cyclen and L are maximum in **Li-DEE-1a** (**Li-DEE-2a**), (ii) DCM coordinates weakly to the $[M(Me_4cyclen)]^+$ unit as compared to its *O*-donor analogues, and (iii) as the size of the ionic radii of M^+ increases from $Li^+ \rightarrow Na^+ \rightarrow K^+$, steric hindrance between Me_4cyclen and L in **M-L-1a** (**M-L-2a**) decreases, and thus the effect on the geometry of the $[M(Me_4cyclen)]^+$ unit in $[M(Me_4cyclen)(L)]^+$ also decreases.

An analysis of the lowest minimum energy structures with *O*-donor ligands reveals that the M–O bond of **M-L-1a** (**M-L-2a**), for L = H_2O, THF, and DEE, is essentially normal to the plane formed by the four *N*-donor atoms of Me_4cyclen, with the dipole moment of each structure aligning along the M–O bond. The M–O bond of **M-MeOH-1a** (**M-MeOH-2a**) is tilted by ≈ 3-10° from the normal of the equatorial plane. In general, the M–O bond distances of **M-H_2O-1a** (**M-H_2O-2a**), **M-THF-1a** (**M-THF-2a**), **M-DEE-1a** (**M-DEE-2a**), and **M-MeOH-1a** (**M-MeOH-2a**) are comparable (for M = Li and Na; see Tables S2). The K–O bond distance of **K-DEE-1a** (BP86, 2.805 Å; B3LYP, 2.788 Å) is significantly longer than the K–O bonds in **K-H_2O-1a** (BP86, 2.718 Å; B3LYP, 2.711 Å), **K-THF-1a** (BP86, 2.721 Å; B3LYP, 2.705 Å), and **K-MeOH-1a** (BP86, 2.729 Å; B3LYP, 2.713 Å). This observation can be correlated to the spatial arrangement of the DEE fragment in the complexes. The **M-DEE-1a** (**M-DEE-2a**) structures (for M = Li and Na) have their DEE fragment in a gauche-gauche (GG) conformation while for M = K, **K-DEE-1a** (**K-DEE-2a**) adopts a trans-trans (TT) conformation. The M–N and M–O bond distances of **K-DEE-1a** (**K-DEE-2a**) are longer than their Li^+ and Na^+ counterparts, thus its DEE framework is free to

adopt a less sterically hindered conformation, a TT conformation. This is consistent with the known lowest energy structure of DEE in the gas-phase which is known to be TT[S37] and the results of DFT BP86 and B3LYP calculations on DEE summarised in Figures S9 an S10 [Figure S10 shows a diagram of the TT, trans-gauche (TG), and GG structures of DEE].

In order to provide further insight into the structure of L in the lowest $[M(Me_4cyclen)(L)]^+$ minimum energy structures, BP86 and B3LYP calculations were performed on the monosolvated alkali metal ion structures, $[M^+\text{-}L]$ (M = Li, Na, K, and L = H_2O, THF, DEE, MeOH, DCM) (details provided in next section). For L = DEE, all the lowest $[M^+\text{-DEE}]$ minimum energy structures have their DEE fragment in the TT conformation with the GG conformation being 15.8 (16.8), 14.2 (15.9), and 9.6 (11.3) kJ.mol^{-1} higher in energy for M = Li, Na, and K, respectively (Figure S9) (BP86 values are quoted with B3LYP values in brackets).

In the $[M(Me_4cyclen)(L)]^+$ complexes with L = DEE, for M = Li and Na, it appears that the close proximity between the Me_4cyclen and DEE forces DEE to adopt a more sterically hindered conformation in the **M-DEE-1a** (**M-DEE-2a**) structures than in the M = K case. Further, a significant decrease of ≈ 20° in the dihedral angles $\emptyset_1$(C14–O–C13–C16) and $\emptyset_2$(C13–O–C14–C15) is observed arising from steric hindrance on going from **Na-DEE-1a (Na-DEE-2a)** to **Li-DEE-1a** (**Li-DEE-2a**) which is accompanied by a decrease in the corresponding M–N and M–O bond distances. In contrast, for the corresponding $[M^+\text{-}L]$ structures for M = Li and Na, the dihedral angles $\emptyset_1$ and $\emptyset_2$ of the least stable $[Li^+\text{-DEE}]$ (GG) structure [BP86, 84.6°; B3LYP, 85.3°] are comparable to that of $[Na^+\text{-DEE}]$ (GG) [BP86, 85.9°; B3LYP, 86.7°].

The **M-DCM-1a** (**M-DCM-2a**) $[M(Me_4cyclen)(L)]^+$ structures (M = Li, Na, K) differ significantly from each other. The small Li^+ ion in **M-DCM-1a** (**M-DCM-2a**) interacts with DCM in a monodentate η^1-Cl1 coordination mode with the Li–Cl2 distance (BP86, 4.344; B3LYP, 4.405 Å) being significantly greater than the sum of the van der Waals (vdW) radii of the Li (1.81 Å) and Cl (1.75 Å) atoms.[S38] On the other hand, Na^+ and K^+ ions interact with DCM in a bidentate η^2-Cl1,Cl2 coordination mode with their M–Cl distances being within the sum of their respective vdW contact distances.[S38] Comparison of the $[M^+\text{-DCM}]$ (M = Li, Na, K) structures (Figure S9), where M^+ coordinates to DCM in an η^2-Cl,Cl fashion, highlights the presence of steric hindrance between Me_4cyclen and DCM in **Li-DCM-1a** (**Li-DCM-2a**). Further, the plane in DCM defined by Cl1–C13–Cl2 in **Na-DCM-1a** (**Na-DCM-2a**) is perpendicular to the plane of the four *N*-donor atoms of the Me_4cyclen ring while that of the K^+ analogue deviates from perpendicular. This

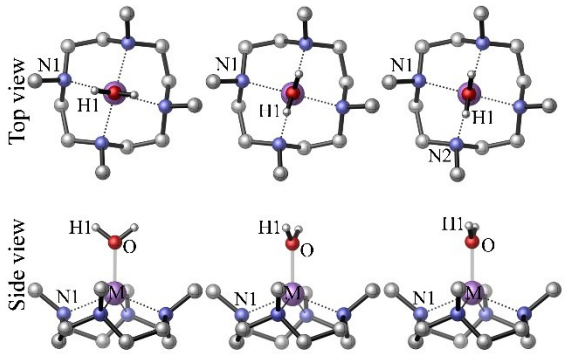
implies that the tilted DCM fragment in the **K-DCM-1a** (**K-DCM-2a**) structures is less sterically hindered by the methyl groups of the Me_4cyclen macrocycle than in the Na^+ case.

Further information on low-lying [M(Me_4cyclen)(L)]$^+$ structures

Several [M(Me_4cyclen)(L)]$^+$ low-lying structures, denoted as **M-L-1x** and **M-L-2x**, where **x** = **b-o**, are provided in Figures S2-S4 (BP86) and Figures S5-S7 (B3LYP).

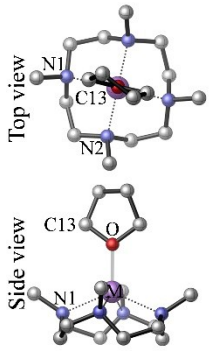
The main difference, between the [M(Me_4cyclen)(L)]$^+$ low-lying structures (M = Li, Na, K, and L = H_2O, THF, MeOH, DCM), lies in the spatial arrangement of their auxiliary ligands, L. Significant difference is observed in their dihedral angles, *Ø*, N1–M–O–H1 (L = H_2O, MeOH), N1–M–O–C13 (L = THF, DEE), and N1–M–C13–Cl1 (L = DCM). However, it is notable that a change in the dihedral angle (with L being in a particular conformation) entails negligible change in the relative energy of the resulting [M(Me_4cyclen)(L)]$^+$ structures. For instance, considering the low-lying structures **Na-THF-1b** to **Na-THF-1e** as an example (see Figure S3b), a change in *Ø*(N1–M–O–C13) does not alter the relative stability significantly.

The [M(Me_4cyclen)(L)]$^+$ structures **M-DEE-1a-x** (**M-DEE-2a-x**), where M = Li, Na, feature their DEE moiety in four distinct conformations, namely, trans-trans (TT), trans-gauche (TG), gauche-gauche (GG), and GG (see Figure S3c as an example), which are in accordance with Kuze *et al.*'s study[S37] on the conformational analysis of free DEE molecule. The dihedral angle $Ø_1$(C14–O–C13–C16) equals $Ø_2$(C13–O–C14–C15) in the **M-DEE-1a-x** (**M-DEE-2a-x**) structures with DEE in the GG conformation, ranging from 63° to 66° (Li^+) and from 79° to 84° (Na^+), respectively. In contrast, $Ø_1 \neq Ø_2$ for those adopting the GG conformation and for example, in the **Na-DEE-1a-x** (**Na-DEE-2a-x**) structures (Figure S3c), $Ø_1$ ranges from -105° to -111° while $Ø_2$ ranges from 70° to 73°. The GG conformation is not observed for the K^+ counterpart. An attempt to optimise the GG conformation of the free DEE ligand and the [M^+-DEE] complex (M = Li, Na, K), using the BP86/6-311G(d,p) and B3LYP/6-311G(d,p) methods, was unsuccessful (details provided in next section). The GG conformation eventually converges to the TG conformation. The DEE's GG conformation is formed in **M-DEE-1a-x** (**M-DEE-2a-x**) (M = Li, Na) due to steric hindrance.



Li-H_2O-1b (C_2)	**Li-H_2O-1c** (C_2)	**Li-H_2O-1d** (C_2)
Ø(N1–M–O–H1) in °:		
8.3	86.9	96.3
Ø(N2–M–O–H1) in °:		
—	—	6.3
Relative energy in kJ/mol:		
0.13	1.43	1.65

(a)



Li-THF-1b
(C_2)

Ø(N1–M–O–C13) in °:

-0.3

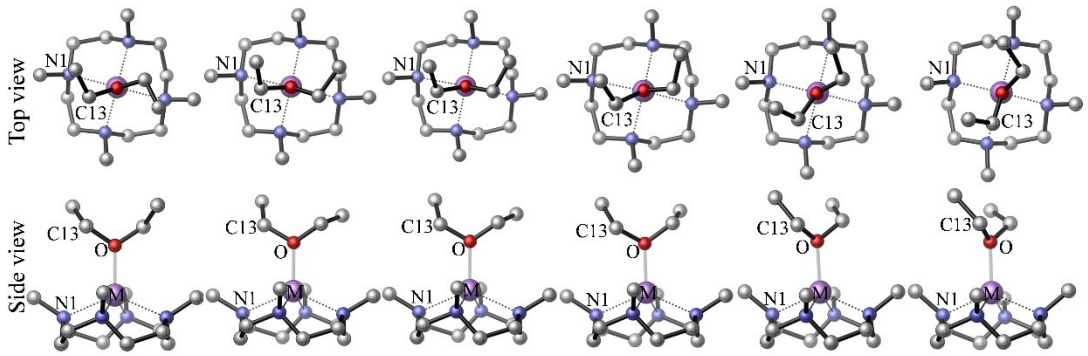
Ø(N2–M–O–C13) in °:

89.2

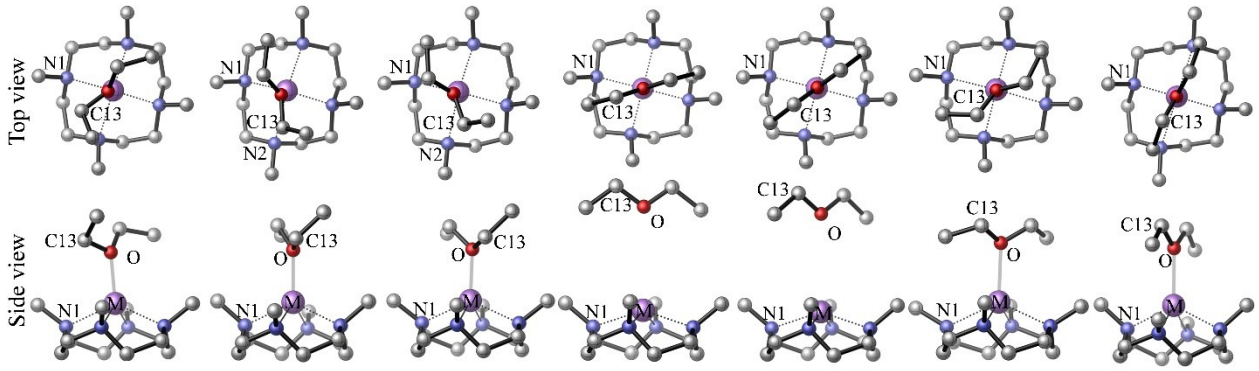
Relative energy in kJ/mol:

0.94

(b)

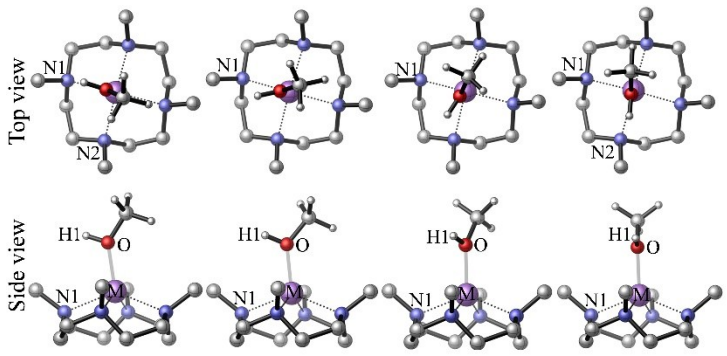


	Li-DEE-1b (C_2)	**Li-DEE-1c** (C_1)	**Li-DEE-1d** (C_1)	**Li-DEE-1e** (C_1)	**Li-DEE-1f** (C_1)	**Li-DEE-1g** (C_1)
GG conformation	GG'	GG'	GG'	GG'	GG'	GG'
Ø(N1–M–O–C13) in °:						
	31.7	15.3	20.3	37.3	68.0	85.3
Relative energy in kJ/mol:						
	0.44	5.0	5.78	7.2	5.76	5.4



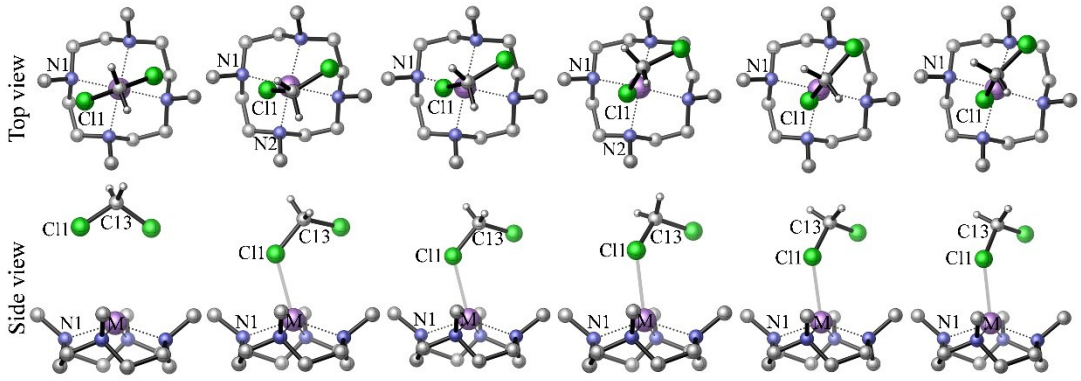
	Li-DEE-1h (C_1)	**Li-DEE-1i** (C_1)	**Li-DEE-1j** (C_1)	**Li-DEE-1k** (C_2)	**Li-DEE-1l** (C_2)	**Li-DEE-1m** (C_1)	**Li-DEE-1n** (C_2)
	TG	TG	TG	TT	TT	TT	TT
Ø(N1–M–O–C13) in °:							
	51.9	104.7	122.8	31.8	50.6	64.9	77.6
Ø(N2–M–O–C13) in °:							
	—	20.0	34.5	—	—	—	—
Relative energy in kJ/mol:							
	8.9	10.1	8.8	22.8	21.8	23.6	33.6

(c)



Li-MeOH-1b (C_1)	**Li-MeOH-1c** (C_1)	**Li-MeOH-1d** (C_1)	**Li-MeOH-1e** (C_1)
Ø(N1–M–O–H1) in °:			
-3.8	38.3	68.7	98.3
Ø(N2–M–O–H1) in °:			
82.4	—	—	11.7
Relative energy in kJ/mol:			
0.49	0.14	0.78	0.05

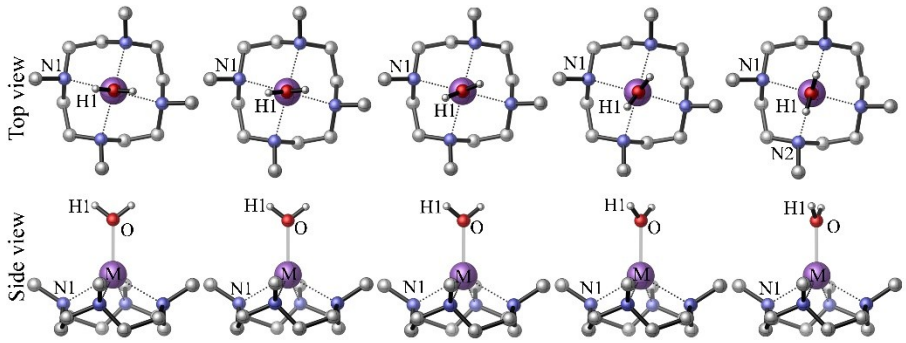
(d)



Li-DCM-1b (C_1)	**Li-DCM-1c** (C_1)	**Li-DCM-1d** (C_1)	**Li-DCM-1e** (C_1)	**Li-DCM-1f** (C_1)	**Li-DCM-1g** (C_1)
Ø(N1–M–C13–Cl1) in °:					
32.0	14.1	23.3	69.0	66.3	75.8
Relative energy in kJ/mol:					
2.9	0.81	0.35	0.05	0.58	0.61

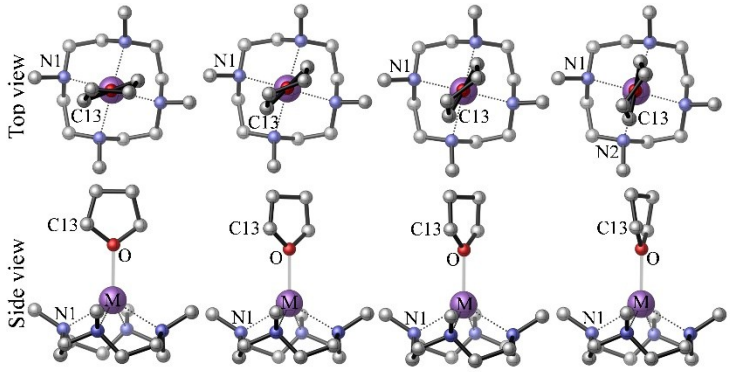
(e)

Figure S2: Low-lying $[Li(Me_4cyclen)(L)]^+$ structures obtained using the BP86/6-311G(d,p) method, where L = H_2O (a), THF (b), DEE (c), MeOH (d), and DCM (e). The symmetry, relative energy (with respect to the lowest minimum energy structure), and selected dihedral angles of each structure are provided. Selected H atoms are omitted for clarity.



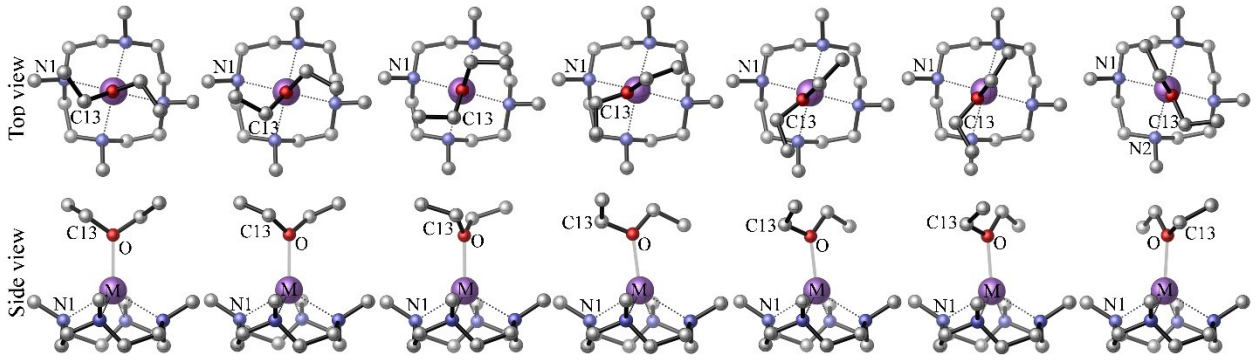
	Na-H_2O-1b (C_2)	**Na-H_2O-1c** (C_2)	**Na-H_2O-1d** (C_2)	**Na-H_2O-1e** (C_2)	**Na-H_2O-1f** (C_2)
Ø(N1–M–O–H1) in °:					
	10.3	19.3	36.3	68.6	89.5
Ø(N2–M–O–H1) in °:					
	—	—	—	—	-0.4
Relative energy in kJ/mol:					
	0.42	0.22	0.28	0.10	0.20

(a)

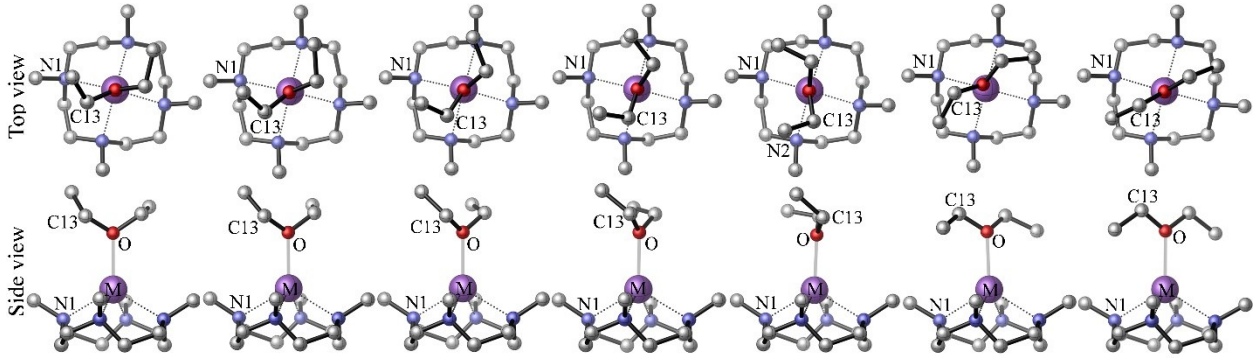


	Na-THF-1b (C_2)	**Na-THF-1c** (C_2)	**Na-THF-1d** (C_2)	**Na-THF-1e** (C_2)
Ø(N1–M–O–C13) in °:				
	35.0	60.5	75.0	94.0
Ø(N2–M–O–C13) in °:				
	—	—	—	4.1
Relative energy in kJ/mol:				
	0.42	0.76	0.14	0.68

(b)

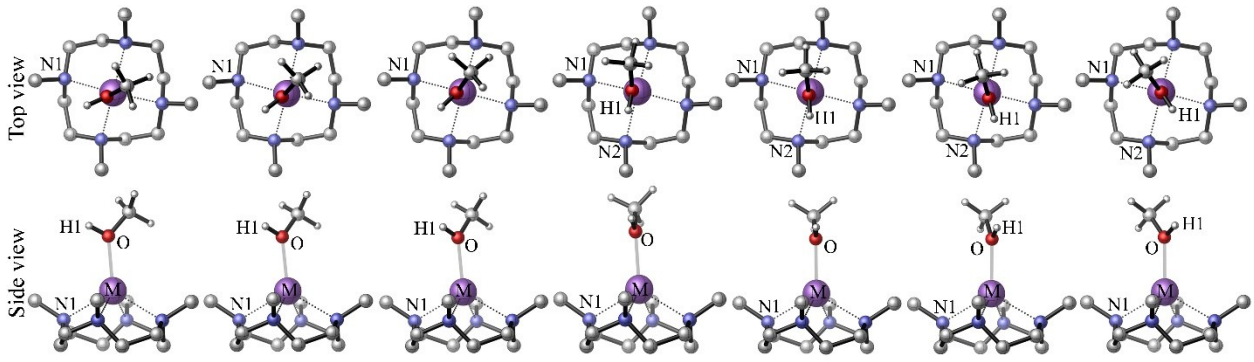


	Na-DEE-1b	**Na-DEE-1c**	**Na-DEE-1d**	**Na-DEE-1e**	**Na-DEE-1f**	**Na-DEE-1g**	**Na-DEE-1h**
	(C_2)	(C_2)	(C_2)	(C_1)	(C_1)	(C_1)	(C_1)
GG conformation	GG	GG	GG	TG	TG	TG	TG
Ø(N1–M–O–C13) in °:							
	32.7	59.2	87.7	28.9	47.2	59.2	122.9
Ø(N2–M–O–C13) in °:							
	—	—	—	—	—	—	34.7
Relative energy in kJ/mol:							
	1.15	1.66	1.19	1.01	1.02	1.27	1.30



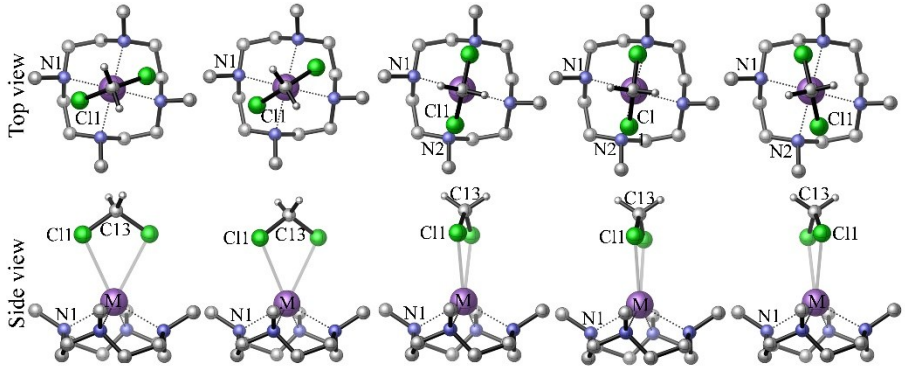
	Na-DEE-1i	**Na-DEE-1j**	**Na-DEE-1k**	**Na-DEE-1l**	**Na-DEE-1m**	**Na-DEE-1n**	**Na-DEE-1o**
	(C_1)	(C_1)	(C_1)	(C_1)	(C_1)	(C_1)	(C_1)
	GG'	GG'	GG'	GG'	GG'	TT	TT
Ø(N1–M–O–C13) in °:							
	35.2	49.8	68.5	85.6	113.8	35.9	44.7
Ø(N2–M–O–C13) in °:							
	—	—	—	—	23.2	—	—
Relative energy in kJ/mol:							
	4.08	5.10	5.2	5.13	4.14	5.8	7.7

(c)



	Na-MeOH-1b	Na-MeOH-1c	Na-MeOH-1d	Na-MeOH-1e	Na-MeOH-1f	Na-MeOH-1g	Na-MeOH-1h
	(C_1)	(C_1)	(C_1)	(C_1)	(C_1)	(C_1)	(C_1)
Ø(N1–M–O–H1) in °:							
	36.7	51.0	58.8	95.5	105.2	116.8	136.3
Ø(N2–M–O–H1) in °:							
	—	—	—	8.5	17.1	27.8	47.2
Relative energy in kJ/mol:							
	0.90	0.46	0.07	0.14	0.57	0.25	0.32

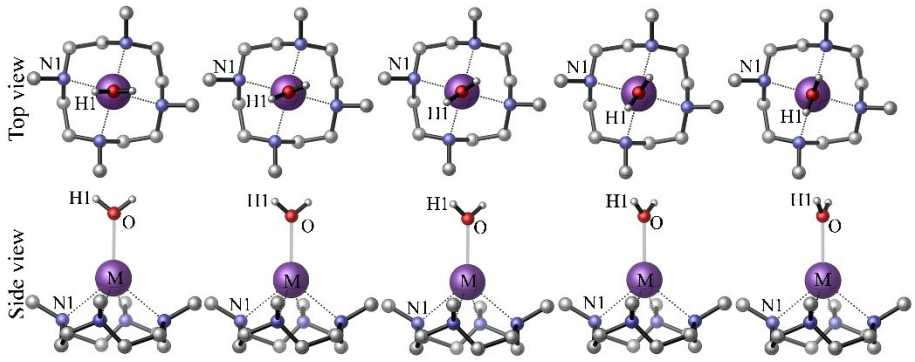
(d)



	Na-DCM-1b	Na-DCM-1c	Na-DCM-1d	Na-DCM-1e	Na-DCM-1f
	(C_1)	(C_1)	(C_1)	(C_2)	(C_2)
Ø(N1–M–C13–Cl1) in °:					
	34.2	46.6	93.1	98.0	116.5
Ø(N2–M–C13–Cl1) in °:					
	—	—	3.0	8.1	26.6
Relative energy in kJ/mol:					
	0.15	1.15	1.12	0.33	0.19

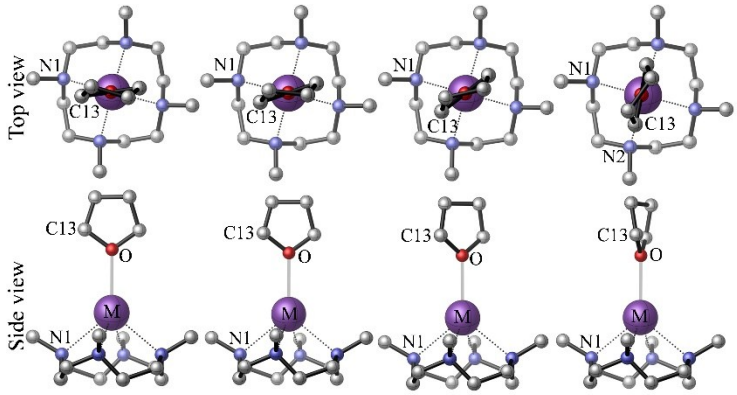
(e)

Figure S3: Low-lying $[Na(Me_4cyclen)(L)]^+$ structures obtained using the BP86/6-311G(d,p) method, where L = H_2O (a), THF (b), DEE (c), MeOH (d), and DCM (e). The symmetry, relative energy (with respect to the lowest minimum energy structure), and selected dihedral angles of each structure are provided. Selected H atoms are omitted for clarity.



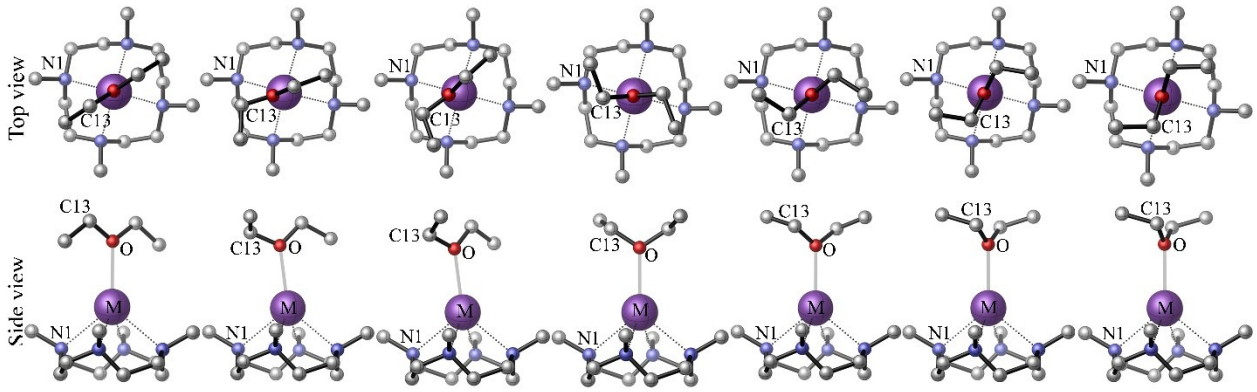
K-H_2O-1b (C_2)	**K-H_2O-1c** (C_2)	**K-H_2O-1d** (C_2)	**K-H_2O-1e** (C_2)	**K-H_2O-1f** (C_2)
Ø(N1–M–O–H1) in °:				
16.0	36.6	50.1	70.0	85.4
Relative energy in kJ/mol:				
0.18	1.27	0.19	0.16	0.19

(a)



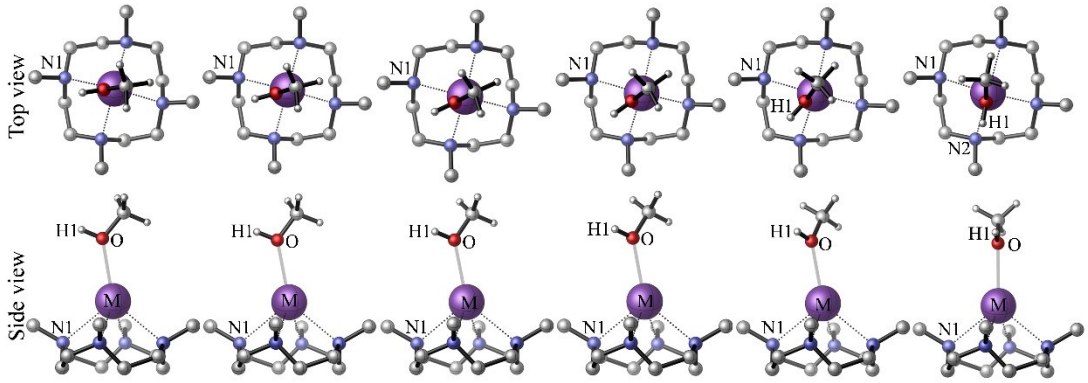
K-THF-1b (C_2)	**K-THF-1c** (C_2)	**K-THF-1d** (C_2)	**K-THF-1e** (C_2)
Ø(N1–M–O–C13) in °:			
22.8	32.6	53.1	94.1
Ø(N2–M–O–C13) in °:			
—	—	—	4.1
Relative energy in kJ/mol:			
0.84	0.06	1.14	1.06

(b)



	K-DEE-1b	K-DEE-1c	K-DEE-1d	K-DEE-1e	K-DEE-1f	K-DEE-1g	K-DEE-1h
	(C_2)	(C_1)	(C_1)	(C_2)	(C_2)	(C_2)	(C_2)
TT conformation	TG	TG	GG	GG	GG	GG	
Ø(N1–M–O–C13) in °:							
	48.5	29.3	50.8	17.9	55.3	79.1	89.6
Relative energy in kJ/mol:							
	0.10	1.09	1.07	3.1	3.3	4.4	4.5

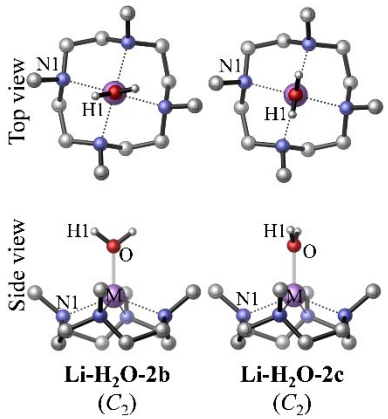
(c)



	K-MeOH-1b	K-MeOH-1c	K-MeOH-1d	K-MeOH-1e	K-MeOH-1f	K-MeOH-1g
	(C_1)	(C_1)	(C_1)	(C_1)	(C_1)	(C_1)
Ø(N1–M–O–H1) in °:						
	19.2	24.9	35.0	46.1	59.8	92.2
Ø(N2–M–O–H1) in °:						
	—	—	—	—	—	6.2
Relative energy in kJ/mol:						
	0.32	0.65	0.23	0.59	0.01	0.13

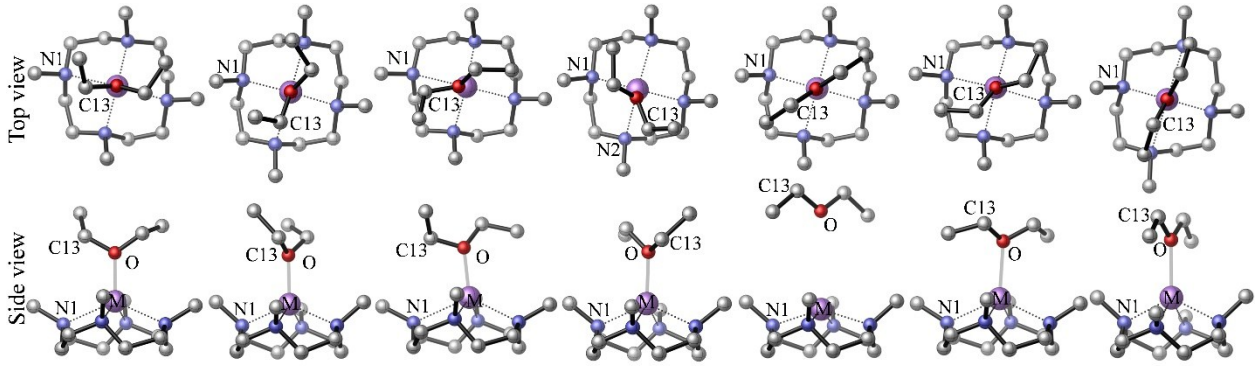
(d)

Figure S4: Low-lying $[K(Me_4cyclen)(L)]^+$ structures obtained using the BP86/6-311G(d,p) method, where L = H_2O (a), THF (b), DEE (c), and MeOH (d). The symmetry, relative energy (with respect to the lowest minimum energy structure), and selected dihedral angles of each structure are provided. Selected H atoms are omitted for clarity.



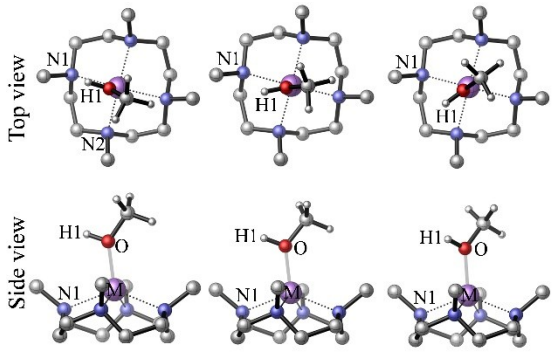
	Li-H_2O-2b	**Li-H_2O-2c**
	(C_2)	(C_2)
Ø(N1–M–O–H1) in °:		
	25.9	95.1
Ø(N2–M–O–H1) in °:		
	—	5.1
Relative energy in kJ/mol:		
	0.77	2.23

(a)



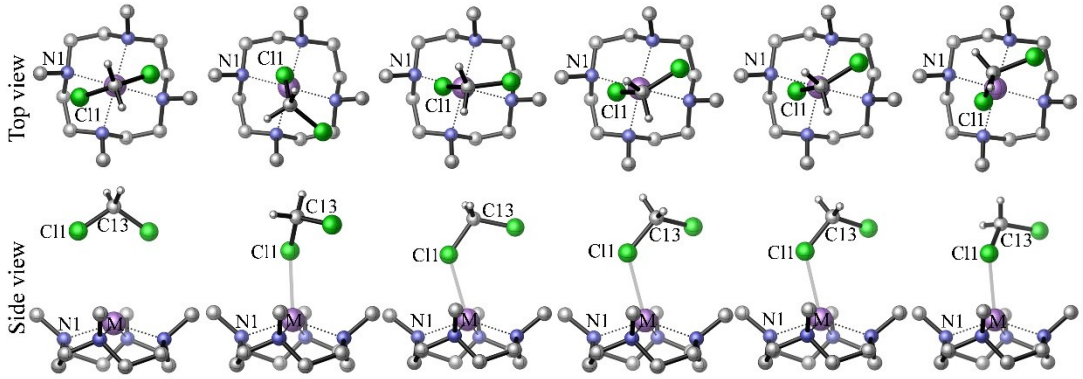
	Li-DEE-2b	**Li-DEE-2c**	**Li-DEE-2d**	**Li-DEE-2e**	**Li-DEE-2f**	**Li-DEE-2g**	**Li-DEE-2h**
	(C_1)	(C_1)	(C_1)	(C_1)	(C_2)	(C_1)	(C_2)
GG' conformation	GG'	TG	TG	TT	TT	TT	
Ø(N1–M–O–C13) in °:							
	16.4	84.9	23.0	123.3	49.3	62.7	77.6
Ø(N2–M–O–C13) in °:							
	—	—	—	36.2	—	—	—
Relative energy in kJ/mol:							
	4.3	5.1	11.8	10.3	23.6	28.0	37.8

(b)



	Li-MeOH-2b (C_1)	**Li-MeOH-2c** (C_1)	**Li-MeOH-2d** (C_1)
Ø(N1–M–O–H1) in °:	-3.9	24.6	49.7
Ø(N2–M–O–H1) in °:	82.8	—	—
Relative energy in kJ/mol:	0.60	0.33	0.17

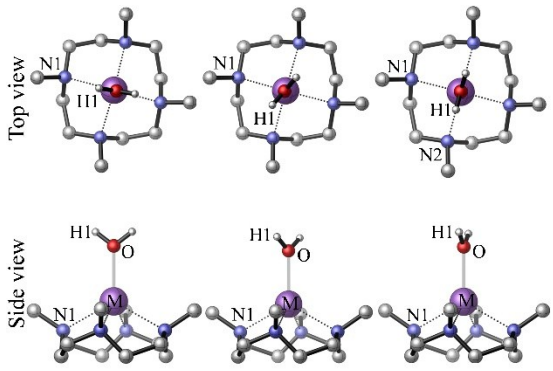
(c)



	Li-DCM-2b (C_1)	**Li-DCM-2c** (C_1)	**Li-DCM-2d** (C_1)	**Li-DCM-2e** (C_1)	**Li-DCM-2f** (C_1)	**Li-DCM-2g** (C_1)
Ø(N1–M–C13–Cl1) in °:	33.4	-66.7	12.9	17.1	26.9	84.7
Relative energy in kJ/mol:	3.2	0.58	0.41	1.31	0.68	0.36

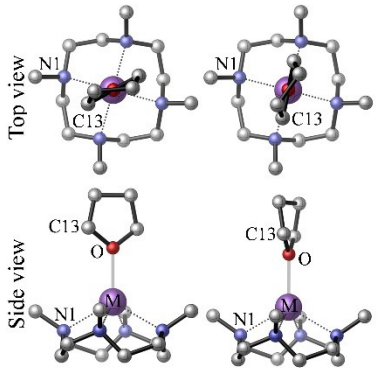
(d)

Figure S5: Low-lying $[Li(Me_4cyclen)(L)]^+$ structures obtained using the B3LYP/6-311G(d,p) method, where L = H_2O (a), DEE (b), MeOH (c), and DCM (d). The symmetry, relative energy (with respect to the lowest minimum energy structure), and selected dihedral angles of each structure are provided. Selected H atoms are omitted for clarity.



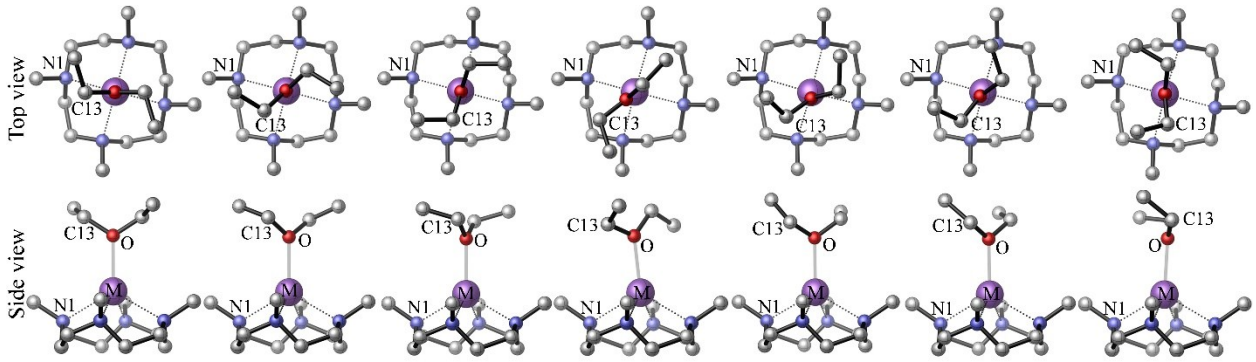
	Na-H_2O-2b (C_2)	**Na-H_2O-2c** (C_2)	**Na-H_2O-2d** (C_2)
Ø(N1–M–O–H1) in °:			
	5.7	64.4	89.7
Ø(N2–M–O–H1) in °:			
	—	—	-0.2
Relative energy in kJ/mol:			
	0.42	0.21	0.31

(a)

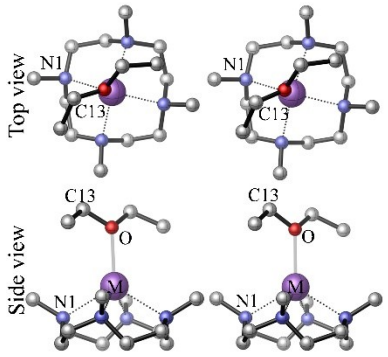


	Na-THF-2b (C_2)	**Na-THF-2c** (C_2)
Ø(N1–M–O–C13) in °:		
	43.8	93.4
Ø(N2–M–O–C13) in °:		
	—	3.5
Relative energy in kJ/mol:		
	0.01	0.66

(b)

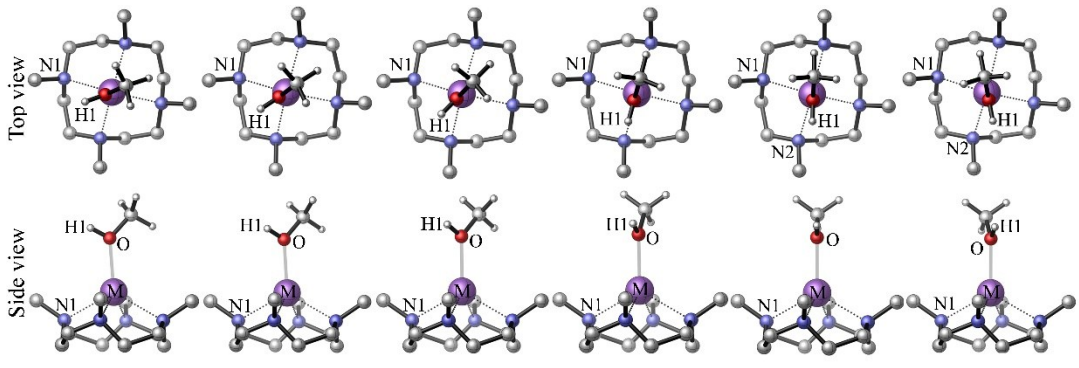


	Na-DEE-2b (C_2)	**Na-DEE-2c** (C_2)	**Na-DEE-2d** (C_2)	**Na-DEE-2e** (C_1)	**Na-DEE-2f** (C_1)	**Na-DEE-2g** (C_1)	**Na-DEE-2h** (C_1)
GG conformation	GG	GG	TG	GG'	GG'	GG'	
Ø(N1–M–O–C13) in °:							
	15.0	57.9	88.3	47.6	46.5	65.2	109.7
Ø(N2–M–O–C13) in °:							
	—	—	—	—	—	—	18.0
Relative energy in kJ/mol:							
	1.32	1.83	1.11	1.41	5.3	5.5	3.8



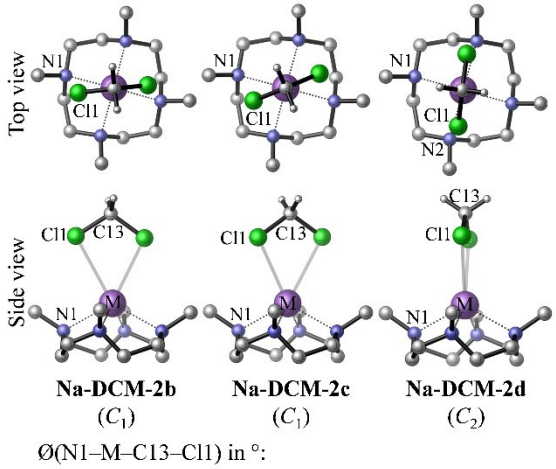
	Na-DEE-2i (C_1)	**Na-DEE-2j** (C_1)
	TT	TT
Ø(N1–M–O–C13) in °:		
	35.6	44.2
Relative energy in kJ/mol:		
	7.0	7.2

(c)



	Na-MeOH-2b	Na-MeOH-2c	Na-MeOH-2d	Na-MeOH-2e	Na-MeOH-2f	Na-MeOH-2g
	(C_1)	(C_1)	(C_1)	(C_1)	(C_1)	(C_1)
Ø(N1–M–O–H1) in °:						
	34.1	46.5	59.3	87.6	102.2	114.7
Ø(N2–M–O–H1) in °:						
	—	—	—	—	13.4	25.4
Relative energy in kJ/mol:						
	0.67	0.12	0.33	0.32	0.36	0.45

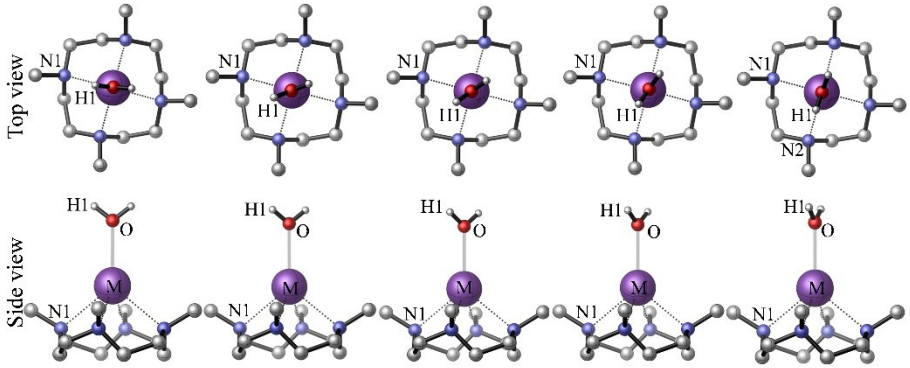
(d)



	Na-DCM-2b	Na-DCM-2c	Na-DCM-2d
	(C_1)	(C_1)	(C_2)
Ø(N1–M–C13–Cl1) in °:			
	21.3	36.8	98.6
$Ø_2$(N2–M–C13–Cl1) in °:			
	—	—	8.6
Relative energy in kJ/mol:			
	0.25	0.04	0.16

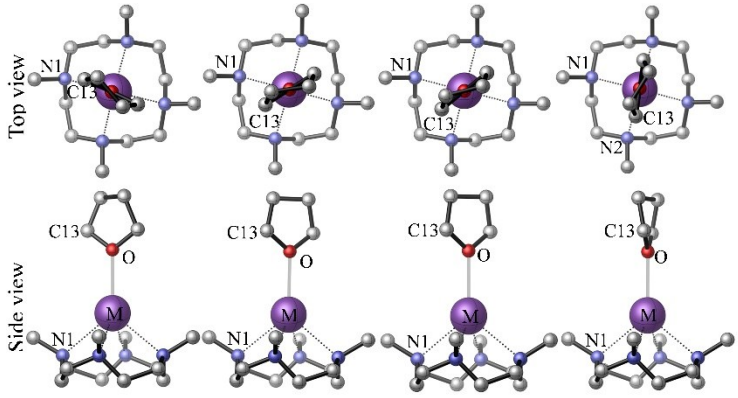
(e)

Figure S6: Low-lying $[Na(Me_4cyclen)(L)]^+$ structures obtained using the B3LYP/6-311G(d,p) method, where L = H_2O (a), THF (b), DEE (c), MeOH (d), and DCM (e). The symmetry, relative energy (with respect to the lowest minimum energy structure), and selected dihedral angles of each structure are provided. Selected H atoms are omitted for clarity.



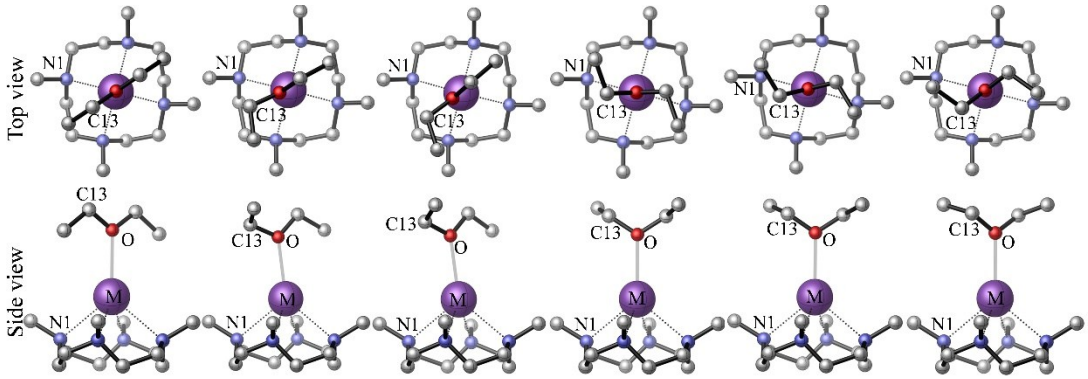
K-H_2O-2b (C_2)	**K-H_2O-2c** (C_2)	**K-H_2O-2d** (C_2)	**K-H_2O-2e** (C_2)	**K-H_2O-2f** (C_2)
Ø(N1–M–O–H1) in °:				
10.0	36.3	50.4	70.0	85.4
Relative energy in kJ/mol:				
0.06	0.76	0.19	0.17	0.13

(a)

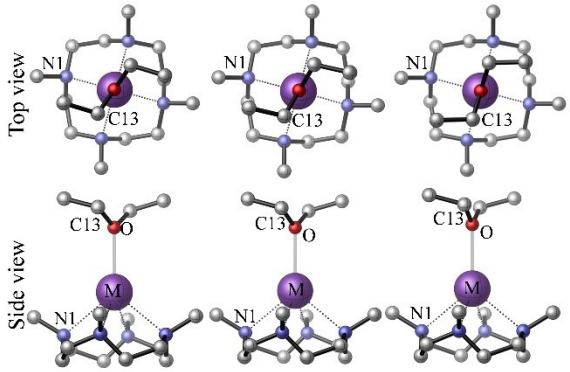


K-THF-2b (C_2)	**K-THF-2c** (C_2)	**K-THF-2d** (C_2)	**K-THF-2e** (C_2)
Ø(N1–M–O–C13) in °:			
-10.9	47.3	53.4	96.7
Ø(N2–M–O–C13) in °:			
—	—	—	6.7
Relative energy in kJ/mol:			
0.23	0.74	0.59	0.61

(b)

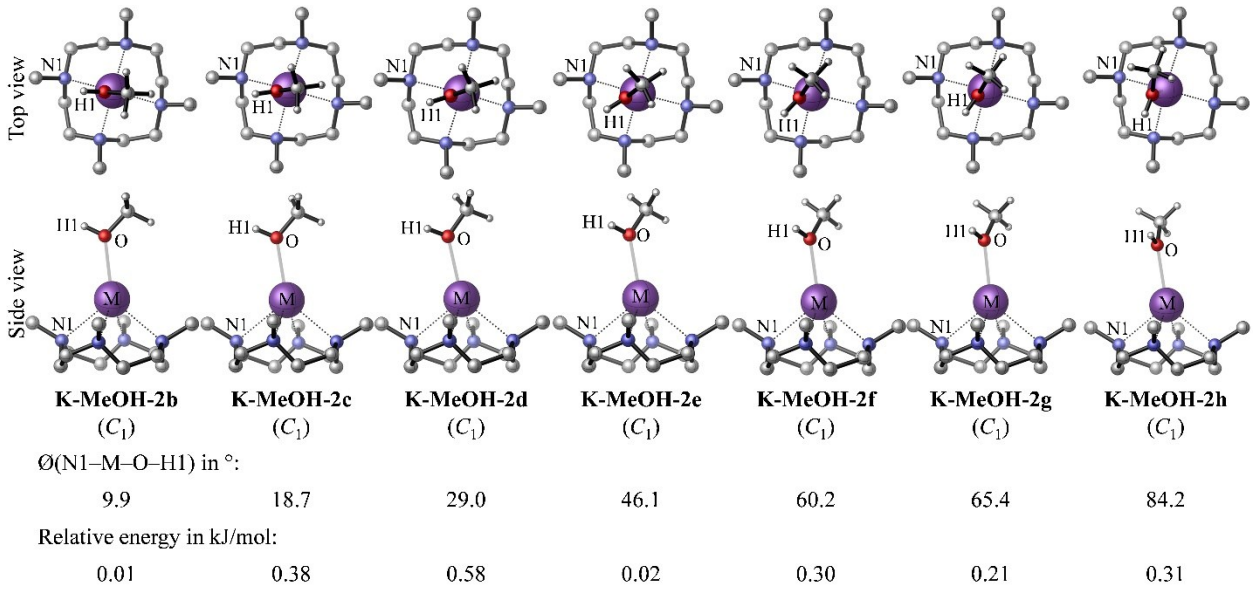


K-DEE-2b	**K-DEE-2c**	**K-DEE-2d**	**K-DEE-2e**	**K-DEE-2f**	**K-DEE-2g**
(C_2)	(C_1)	(C_1)	(C_2)	(C_2)	(C_2)
TT conformation	TG	TG	GG	GG	GG
Ø(N1–M–O–C13) in °:					
48.6	35.6	48.0	17.0	28.2	51.8
Relative energy in kJ/mol:					
0.3	1.9	2.7	6.1	6.0	5.8



K-DEE-2h	**K-DEE-2i**	**K-DEE-2j**
(C_2)	(C_2)	(C_2)
GG	GG	GG
Ø(N1–M–O–C13) in °:		
70.8	75.1	88.5
Relative energy in kJ/mol:		
6.5	6.6	6.7

(c)



(d)

Figure S7: Low-lying $[K(Me_4cyclen)(L)]^+$ structures obtained using the B3LYP/6-311G(d,p) method, where L = H_2O (a), THF (b), DEE (c), and MeOH (d). The symmetry, relative energy (with respect to the lowest minimum energy structure), and selected dihedral angles of each structure are provided. Selected H atoms are omitted for clarity.

Table S2 (a): Selected geometrical parameters of the lowest $[M(Me_4cyclen)(L)]^+$ minimum energy structures obtained using the BP86/6-311G(d,p) method for M = Li, Na, and K with L = H_2O and THF.

	M-H_2O-1a				**M-THF-1a**			
Bond distances (Å)	Li	Expt.[a]	Na	K	Li	Na	Expt.[a]	K
M–N1	2.256	2.186(8)	2.502	2.842	2.253	2.521	2.463(4)	2.853
M–N2	2.254	2.206(8)	2.505	2.835	2.330	2.522	2.461(3)	2.843
M–N3	2.256	2.179(8)	2.502	2.842	2.253	2.521	2.453(4)	2.853
M–N4	2.254	2.154(9)	2.505	2.835	2.330	2.522	2.444(4)	2.843
M–O	2.009	1.98(1)	2.340	2.718	2.028	2.351	2.244(3)	2.721
Bond angles (°)								
N1–M–N2	82.3	82.8(3)	75.9	66.9	80.9	75.3	75.4(1)	66.8
N2–M–N3	82.4	82.1(3)	76.2	66.9	81.6	75.6	75.6(1)	66.7
N3–M–N4	82.3	84.7(3)	75.9	66.9	80.9	75.3	76.0(1)	66.8
N4–M–N1	82.4	82.6(3)	76.2	66.9	81.6	75.6	75.5(2)	66.7
Torsion (°)								
N1–C5–C6–N2	-57.1	59.4(7)	-61.9	-64.7	-56.1	-62.2	-64(1)	-64.9
N2–C7–C8–N3	-57.1	55.8(8)	-62.6	-64.2	-59.9	-62.7	-61(1)	-64.4
N3–C9–C10–N4	-57.1	54.0(9)	-61.9	-64.7	-56.1	-62.2	-59(1)	-64.9
N4–C11–C12–N1	-57.1	57.5(7)	-62.6	-64.2	-59.9	-62.7	-65(1)	-64.4
N1–M–O–H1	11.7		55.3	10.1				
N1–M–O–C13					69.1	70.0	59.6	-7.7

[a] Corresponds to the $[Li(Me_4cyclen)(H_2O)]^+$ and $[Na(Me_4cyclen)(THF)]^+$ crystal structures, respectively.[S5a]

Table S2 (b): Selected geometrical parameters of the lowest $[M(Me_4cyclen)(L)]^+$ minimum energy structures obtained using the BP86/6-311G(d,p) method, for M = Li, Na, and K with L = DEE, MeOH, and DCM.

	M-DEE-1a			**M-MeOH-1a**			**M-DCM-1a**		
Bond distances (Å)	Li	Na	K	Li	Na	K	Li	Na	K
M–N1	2.329	2.529	2.851	2.266	2.500	2.842	2.260	2.504	2.831
M–N2	2.271	2.515	2.862	2.269	2.509	2.840	2.190	2.484	2.824
M–N3	2.329	2.533	2.851	2.258	2.511	2.843	2.228	2.506	2.822
M–N4	2.271	2.512	2.862	2.257	2.511	2.844	2.180	2.474	2.823
M–O	2.042	2.364	2.805	2.016	2.354	2.729			
M–Cl1							2.784	3.188	3.623
M–Cl2							4.344	3.369	3.626
Bond angles (°)									
N1–M–N2	81.0	75.5	66.5	81.5	75.9	66.9	83.9	76.5	67.3
N2–M–N3	81.1	75.4	66.6	82.4	76.0	66.8	83.9	76.4	67.3
N3–M–N4	81.0	75.4	66.5	82.2	75.7	66.9	84.5	76.7	67.3
N4–M–N1	81.1	75.4	66.6	82.4	76.0	66.9	83.8	76.6	67.3
Torsion (°)									
N1–C5–C6–N2	-59.0	-63.0	-64.6	-56.6	-62.1	-64.8	-58.7	-62.9	-64.6
N2–C7–C8–N3	-57.8	-62.0	-65.6	-57.7	-62.3	-64.8	-55.2	-61.7	-64.6
N3–C9–C10–N4	-59.0	-63.0	-64.6	-57.2	-62.1	-64.7	-55.2	-63.1	-64.5
N4–C11–C12–N1	-57.8	-61.5	-65.6	-57.7	-62.2	-65.0	-55.7	-61.6	-64.9
N1–M–O–H1				50.6	31.4	82.5			
N1–M–O–C13	43.2	8.5	57.7						
N1–M–C13–Cl1							12.8	23.2	104.4

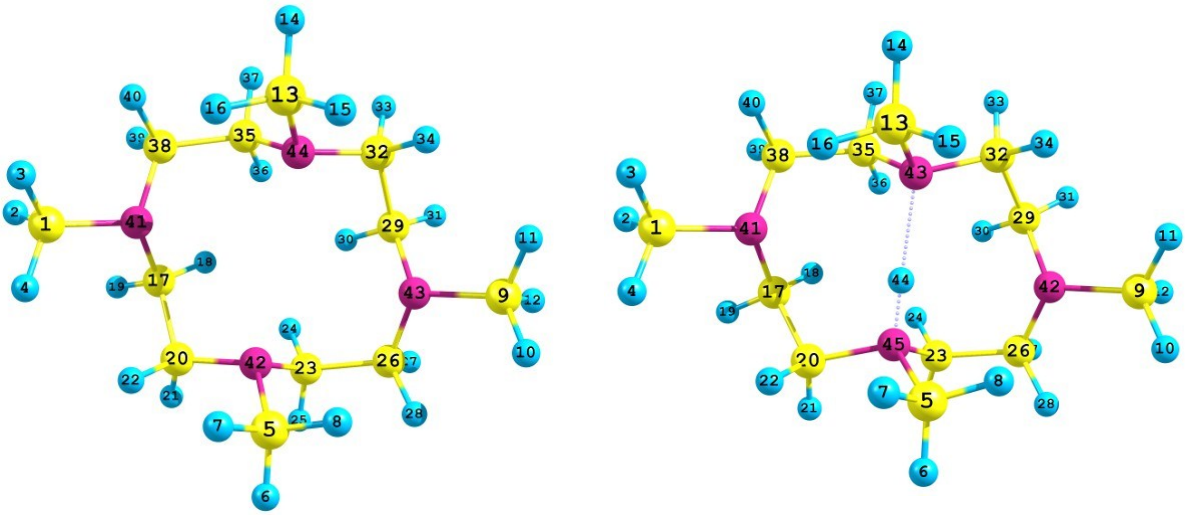
Table S2 (c): Selected geometrical parameters of the lowest $[M(Me_4cyclen)(L)]^+$ minimum energy structures obtained using the B3LYP/6-311G(d,p) method.

	M-H_2O-2a			**M-THF-2a**			**M-DEE-2a**			**M-MeOH-2a**			**M-DCM-2a**		
Bond distances (Å)	Li	Na	K	Li	Na	K	Li	Na	K	Li	Na	K	Li	Na	K
M–N1	2.242	2.488	2.843	2.235	2.498	2.851	2.369	2.509	2.853	2.224	2.489	2.844	2.194	2.485	2.834
M–N2	2.239	2.482	2.834	2.333	2.502	2.844	2.226	2.493	2.865	2.278	2.490	2.849	2.216	2.468	2.834
M–N3	2.242	2.488	2.843	2.235	2.498	2.851	2.369	2.510	2.853	2.237	2.492	2.837	2.179	2.485	2.825
M–N4	2.239	2.482	2.834	2.333	2.502	2.844	2.226	2.494	2.865	2.271	2.492	2.851	2.198	2.468	2.830
M–O	1.987	2.311	2.711	2.006	2.311	2.705	2.018	2.333	2.788	1.989	2.316	2.713			
M–Cl1													2.832	3.195	3.543
M–Cl2													4.405	3.195	3.530
Bond angles (°)															
N1–M–N2	82.7	76.5	66.9	81.0	75.8	66.6	81.3	76.0	66.4	82.3	76.5	66.7	84.2	77.0	67.0
N2–M–N3	82.7	76.5	66.9	81.8	76.0	66.6	81.0	75.9	66.5	82.1	76.1	66.8	84.6	76.9	67.1
N3–M–N4	82.7	76.5	66.9	81.0	75.8	66.6	81.3	76.0	66.4	82.3	76.3	66.8	84.8	77.0	67.1
N4–M–N1	82.7	76.5	66.9	81.8	76.0	66.6	81.0	76.0	66.5	82.7	76.2	66.5	84.4	76.9	67.0
Torsion (°)															
N1–C5–C6–N2	-56.4	-61.6	-64.5	-55.4	-61.4	-64.6	-60.4	-62.4	-64.2	-56.0	-62.0	-64.3	-55.6	-62.3	-64.4
N2–C7–C8–N3	-56.3	-61.5	-64.1	-60.0	-62.0	-64.3	-56.3	-61.4	-65.1	-57.3	-61.5	-64.7	-56.6	-61.3	-64.6
N3–C9–C10–N4	-56.4	-61.6	-64.5	-55.4	-61.4	-64.6	-60.4	-62.4	-64.2	-56.1	-61.8	-64.6	-55.7	-62.3	-64.1
N4–C11–C12–N1	-56.3	-61.5	-64.1	-60.0	-62.0	-64.3	-56.3	-61.5	-65.1	-57.6	-61.5	-64.2	-56.2	-61.3	-64.4
N1–M–O–H1	10.0	14.3	15.7							106.2	129.0	112.4			
N1–M–O–C13				71.7	57.5	26.6	31.5	9.2	55.8						
N1–M–C13–Cl1													75.1	27.7	114.0

Table S3: Cavity size of the Me_4cyclen ring and the distance between the plane of the four *N*-donor atoms of the Me_4cyclen ring and the M^+ ions of the lowest $[M(Me_4cyclen)(L)]^+$ minimum energy structures.

BP86/6-311G(d,p)						B3LYP/6-311G(d,p)				
Cavity size of the Me_4cyclen ring (A^2)[a]										
M	**M-H_2O-1a**	**M-THF-1a**	**M-DEE-1a**	**M-MeOH-1a**	**M-DCM-1a**	**M-H_2O-2a**	**M-THF-2a**	**M-DEE-2a**	**M-MeOH-2a**	**M-DCM-2a**
Li	8.815	8.867	8.937	8.839	8.791	8.766	8.869	8.923	8.797	8.724
Na	9.516	9.523	9.527	9.512	9.528	9.466	9.466	9.483	9.467	9.486
K	9.791	9.807	9.828	9.814	9.799	9.780	9.780	9.810	9.779	9.771
Distance (Å) between the plane of the four *N*-donor atoms of the Me_4cyclen ring and the M^+ ions										
M	**M-H_2O-1a**	**M-THF-1a**	**M-DEE-1a**	**M-MeOH-1a**	**M-DCM-1a**	**M-H_2O-2a**	**M-THF-2a**	**M-DEE-2a**	**M-MeOH-2a**	**M-DCM-2a**
Li	0.824	0.894	0.905	0.837	0.713	0.798	0.884	0.901	0.821	0.681
Na	1.228	1.263	1.264	1.238	1.202	1.201	1.232	1.231	1.213	1.178
K	1.778	1.791	1.802	1.780	1.755	1.779	1.794	1.808	1.790	1.769

[a] Calculated using the Heron's formula; see reference S35.



Me$_4$cyclen
(C_2 symmetry)

[Me$_4$cyclenH]$^+$
(C_1 symmetry)

Figure S8: Optimised Me$_4$cyclen and [Me$_4$cyclenH]$^+$ structures obtained using the BP86/6-311G(d,p) method. Relevant atom labeling is provided.

Table S4: Selected geometrical parameters for the BP86 optimised Me_4cyclen and $[Me_4cyclenH]^+$ structures.[a,b]

Me_4cyclen			$[Me_4cyclenH]^+$		
Bond distances (Å)			Bond distances (Å)		
R(1-2)	C–H*	1.118	R(1-2)	C–H*	1.111
R(1-3)	C–H*	1.102	R(1-3)	C–H*	1.100
R(1-41)	C–N*	1.460	R(1-41)	C–N*	1.469
R(5-42)	C–N*	1.456	R(5-45)	C–N*	1.499
R(17-18)	C–H	1.101	R(17-18)	C–H	1.103
R(17-19)	C–H	1.117	R(17-19)	C–H	1.108
R(17-20)	C–C	1.541	R(17-20)	C–C	1.531
R(17-41)	C–N	1.469	R(17-41)	C–N	1.468
R(20-42)	C–N	1.464	R(20-45)	C–N	1.521
			R(44-45)	H–N	1.104
			R(43-44)	N···H	1.796
Bond angles (°)			Bond angles (°)		
A(2-1-3)	H–C–H*	108.1	A(2-1-3)	H–C–H*	108.4
A(2-1-41)	H–C–N*	113.3	A(2-1-41)	H–C–N*	113.0
A(1-41-17)	C–N–C*	111.3	A(1-41-17)	C–N–C*	112.0
A(24-23-25)	H–C–H	105.5	A(24-23-25)	H–C–H	107.5
A(24-23-26)	H–C–C	109.5	A(24-23-26)	H–C–C	111.5
A(24-23-42)	H–C–N	107.9	A(24-23-45)	H–C–N	106.0
A(26-23-42)	C–C–N	115.1	A(26-23-45)	C–C–N	114.5
			A(5-45-44)	C–N–H*	107.4
			A(20-45-44)	C–N–H	109.0
			A(32-43-44)	C–N···H	111.0
			A(35-43-44)	C–N···H	105.7
			A(45-44-43)	N–H···N	173.9
Torsion (°)			Torsion (°)		
T(41-17-20-42)	N–C–C–N	-75.3	T(41-17-20-45)	N–C–C–N	-73.7
T(42-23-26-43)	N–C–C–N	-49.3	T(45-23-26-42)	N–C–C–N	-43.4
T(43-29-32-44)	N–C–C–N	-75.3	T(42-29-32-43)	N–C–C–N	-72.5
T(44-35-38-41)	N–C–C–N	-49.3	T(43-35-38-41)	N–C–C–N	-43.3

* Geometrical parameters associated with the methyl groups.

[a] R, A, and D represent bond distances, bond angles, and dihedral angles, respectively.

[b] Refer to Figure S8 for atom labeling.

Further information on monosolvated alkali metal ion structures, [M^+-L], where M = Li, Na, K, and L = H_2O, THF, DEE, MeOH, DCM

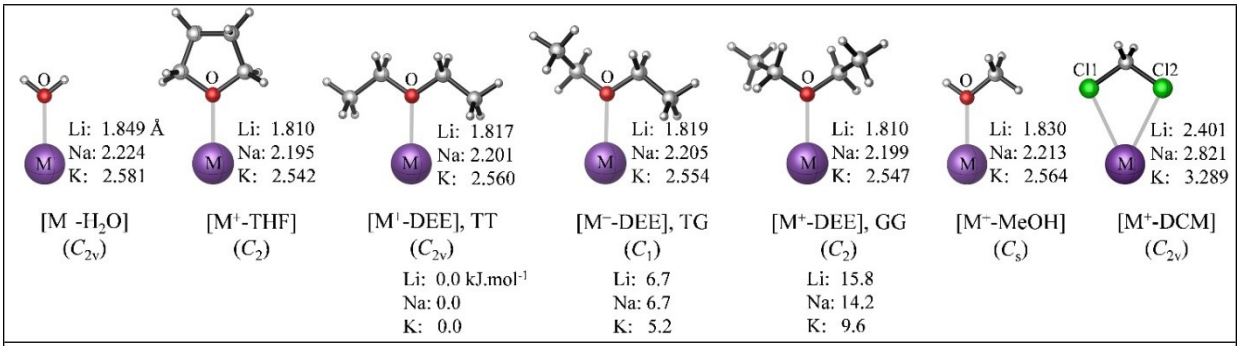
Several studies underscored the coordination of alkali metal ions to prototypical monofunctional or polyfunctional ligands such as H_2O, MeOH, and glycine (H_2NCH_2COOH). Focus is mainly laid on the gas-phase alkali metal ion ligation thermochemistry and on the microscopic picture of their solvation dynamics.[S39] The monosolvated alkali metal ion structures, [M^+-L] (M = Li, Na, K, and L = H_2O, THF, DEE, MeOH, DCM), are revisited using the BP86/6-311G(d,p) and B3LYP/6-311G(d,p) methods in view to have a better understanding of the lowest $[M(Me_4cyclen)(L)]^+$ minimum energy structures. The spatial arrangement of the corresponding Li^+, Na^+, and K^+ complexes are comparable to each other with major changes observed in their M–O and M–Cl bond distances as well as their Cl1–M–Cl2 bond angles (Figures S9). The [M^+-L] structures obtained using the two methods are comparable in terms of geometrical parameters. An increase in the size of the ionic radii of the M^+ ions entails a systematic increase in the M–O and M–Cl bond distances.

Water often acts as a universal solvent in biological or synthetic processes. In fact, hydrated alkali metal cluster ions, $[M(H_2O)_n]^+$, where $n \geq 1$, are among the most studied model systems as compared to their non-aqueous THF, DEE, MeOH, and DCM solvate analogues.[S39a,b,S40] The polar protic H_2O and MeOH solvents interact to M^+ ions *via* their oxygen atom to form the corresponding [M^+-L] complexes (Figure S9), with the dipole moment of the solvents pointing directly towards M^+, giving rise to a charge-dipole interaction. The M–O bond distances of the [M^+-MeOH] structures are slightly shorter than that of the H_2O analogues. The optimised [M^+-L] structures (L = H_2O, MeOH) conform very well to that of literature and a detailed comparison of selected geometrical parameters for the [M^+-L] structures is provided in Table S5.

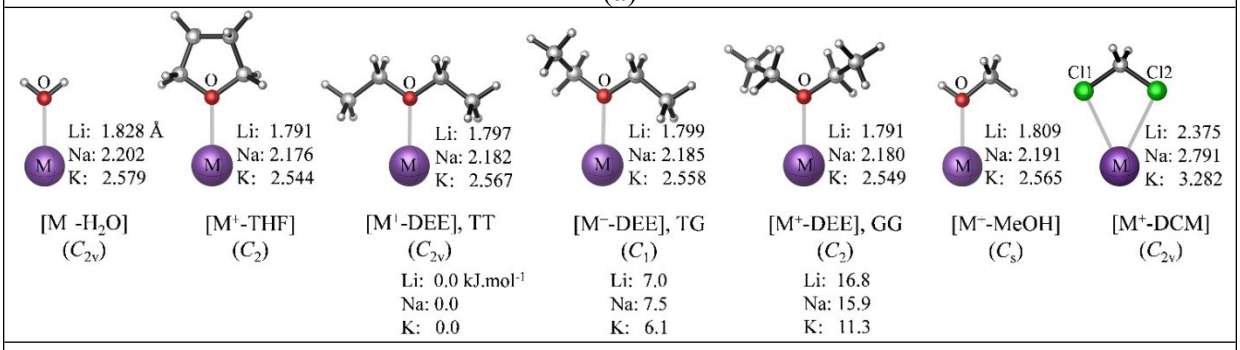
For each [M^+-DEE] complex, three stable structures were obtained, with their DEE moiety adopting the trans-trans (TT), trans-gauche (TG), and gauche-gauche (GG) conformations. The relative stability of the [M^+-DEE] structures is in the order of TT > TG > GG (Figure S9), which is consistent with that of the free DEE ligand (Figure S10). The TG and GG conformations are 5.5 and 10.6 kJ.mol^{-1} (BP86; B3LYP, 6.2 and 11.7 kJ.mol^{-1}), respectively, higher in energy than the TT one for the free DEE ligand. Although DEE is a commonly used aprotic solvent in various chemical processes, literature on their monosolvated alkali metal ions are rather sparse.[S41] Recently, Valadbeigi[S41a] reported the alkali metal cation affinities (ΔH) and basicities (ΔG) of the TT structure of [M^+-DEE] (M = Li, Na) alongside that of the H_2O and MeOH analogues. The geometrical parameters of the [M^+-L] optimised

structures together with their thermochemical stabilities, which are in the order of L = DEE > MeOH > H_2O, are comparable to our results (Tables S5-S6). In addition, the lowest [Li^+-L] minimum energy structures (L = DEE, THF) is similar to that calculated by Jarek and co-workers (Table S5).[S41b] The same report highlights that steric effect plays a major role in entailing DEE to adopt the TG conformation as was observed in the $[Li(DEE)_3]^+$ complex which consists of one DEE in the TT conformation with the remaining two in the TG conformation. The theoretically as well as the experimentally derived bond dissociation enthalpy and free energy are indicative that the stability of [Li^+-DEE] (TT) and [Li^+-THF] are comparable.[S41b]

The [M^+-DCM] structures adopt the C_{2v} symmetry. In accordance to Bloomfield *et al.*'s study,[S42] DCM binds to the M^+ centres in a bidentate η^2-Cl,Cl coordination mode with their M–Cl1 and M–Cl2 bonds being equidistant. The Cl1–M–Cl2 bond angles decrease from 76.7° → 64.2° → 54.3° (BP86; B3LYP, 77.2° → 64.6° → 54.2°) on going from Li^+ → Na^+ → K^+, while the Cl1–C–Cl2 bond angles increase only marginally from 110.3° → 111.9° → 112.4° (BP86; B3LYP, 109.9° → 111.5° → 112.2°).

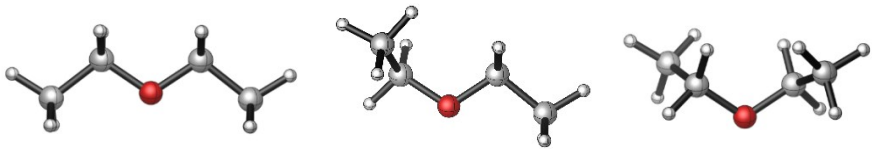


(a)



(b)

Figure S9: Optimised structures of [M^+-L] obtained using the (a) BP86/6-311G(d,p) and (b) B3LYP/6-311G(d,p) methods. The M–O/M–Cl bond distances and symmetry of each structure are provided. The zero-point corrected relative energies (kJ.mol^{-1}) of the trans-trans (TT), trans-gauche (TG), and gauche-gauche (GG) [M^+-DEE] structures are also given.



TT, C_{2v}	TG, C_1	GG, C_2
0.0 (0.0) kJ/mol	5.5 (6.2)	10.6 (11.7)

Figure S10: Optimised geometries and zero-point corrected relative energies (ΔE in kJ.mol^{-1}) of DEE obtained using the BP86/6-311G(d,p) method. The B3LYP relative energies are within brackets. The symmetry of each structure is provided.

Table S5: Comparison of selected geometrical parameters of the [M^+-L] optimised structures with literature.[a]

[Li^+-H_2O]	Geometrical parameters	Methods	References
r(O···Li) (Å)	1.849	BP86/6-311G(d,p)	This work
r(O−H) (Å)	0.975		
θ(H−O−H) (°)	105.3		
θ(Li···O−H) (°)	127.3		
r(O···Li) (Å)	1.828	B3LYP/6-311G(d,p)	This work
r(O−H) (Å)	0.967		
θ(H−O−H) (°)	105.9		
θ(Li···O−H) (°)	127.0		
r(O···Li) (Å)	1.842	B3LYP/6-311++G(d,p)	S41a
r(O−H) (Å)	0.967		
θ(H−O−H) (°)	105.8		
θ(Li···O−H) (°)	127.1		
r(O···Li) (Å)	1.867	MP2/6-31G(d)	S43
r(O···Li) (Å)	1.930	Evolutionary algorithms[b]	S44
r(O−H) (Å)	0.957		
θ(H−O−H) (°)	104.5		
θ(Li···O−H) (°)	127.7		
[Na^+-H_2O]	Geometrical parameters	Methods	References
r(O···Na) (Å)	2.224	BP86/6-311G(d,p)	This work
r(O−H) (Å)	0.973		
θ(H−O−H) (°)	104.5		
θ(Na···O−H) (°)	127.8		
r(O···Na) (Å)	2.202	B3LYP/6-311G(d,p)	This work
r(O−H) (Å)	0.965		
θ(H−O−H) (°)	105.1		
θ(Na···O−H) (°)	127.5		
r(O···Na) (Å)	2.225	B3LYP/6-311++G(d,p)	S41a
r(O−H) (Å)	0.966		
θ(H−O−H) (°)	104.9		
θ(Na···O−H) (°)	127.5		
r(O···Na) (Å)	2.231	MP2/6-31G(d)	S43
r(O···Na) (Å)	2.212	B3LYP/6-311++G(3df,3pd)	S40a

Continued

[K^+-H_2O]	Geometrical parameters	Methods	References
r(O···K) (Å)	2.581	BP86/6-311G(d,p)	This work
r(O−H) (Å)	0.973		
θ(H−O−H) (°)	103.8		
θ(K···O−H) (°)	128.1		
r(O···K) (Å)	2.579	B3LYP/6-311G(d,p)	This work
r(O−H) (Å)	0.965		
θ(H−O−H) (°)	104.3		
θ(K···O−H) (°)	127.9		
r(O···K) (Å)	2.611	MP2/6-31G(d)	S43
r(O···K) (Å)	2.62	B3LYP/6−311++G(d,p)	S45
	2.626	B3LYP/6-311++G(2d,2p)	
	2.646	BLYP/6-311++G(2d,2p)	
	2.638	BLYP/6-311++G(d,p)	
	2.631	B3PW91/6-311++G(2d,2p)	
	2.623	B3PW91/6-311++G(d,p)	
[Li^+-MeOH]	Geometrical parameters	Methods	References
r(O···Li) (Å)	1.830	BP86/6-311G(d,p)	This work
r(O−H) (Å)	0.973		
r(O−C) (Å)	1.474		
<r(H−C)> (Å)	1.098		
θ(Li···O−H) (°)	123.9		
θ(Li···O−C) (°)	128.3		
r(O···Li) (Å)	1.809	B3LYP/6-311G(d,p)	This work
r(O−H) (Å)	0.965		
r(O−C) (Å)	1.466		
<r(H−C)> (Å)	1.089		
θ(Li···O−H) (°)	123.4		
θ(Li···O−C) (°)	128.3		
r(O···Li) (Å)	1.818	B3LYP/6-311++G(d,p)	S41a
r(O−H) (Å)	0.965		
r(O−C) (Å)	1.467		
<r(H−C)> (Å)	1.089		
θ(Li···O−H) (°)	123.2		
θ(Li···O−C) (°)	108.5		

Continued

r(O···Li) (Å)	1.959	Evolutionary algorithms[b]	S44
r(O−H) (Å)	0.958		
r(O−C) (Å)	1.418		
<r(H−C)> (Å)	1.095		
θ(Li···O−H) (°)	135.8		
θ(Li···O−C) (°)	117.8		
r(O···Li) (Å)	1.82	B3LYP/6-31+G(d)	S46
r(O···Li) (Å)	1.848	MP2/6-31G(d)	S47
	1.850	MP2/6-31G(d,p)	
	1.851	MP2/6-31+G(d)	
	1.853	MP2/6-31++G(d,p)	
	1.840	MP2/6-311++G(2d,2p)	
[Na^+-MeOH]	Geometrical parameters	Methods	References
r(O···Na) (Å)	2.213	BP86/6-311G(d,p)	This work
r(O−H) (Å)	0.973		
r(O−C) (Å)	1.463		
<r(H−C)> (Å)	1.099		
θ(Na···O−H) (°)	123.8		
θ(Na···O−C) (°)	129.1		
r(O···Na) (Å)	2.191	B3LYP/6-311G(d,p)	This work
r(O−H) (Å)	0.964		
r(O−C) (Å)	1.455		
<r(H−C)> (Å)	1.090		
θ(Na···O−H) (°)	123.3		
θ(Na···O−C) (°)	129.0		
r(O···Na) (Å)	2.206	B3LYP/6-311++G(d,p)	S41a
r(O−H) (Å)	0.964		
r(O−C) (Å)	1.457		
<r(H−C)> (Å)	1.090		
θ(Na···O−H) (°)	123.4		
θ(Na···O−C) (°)	128.6		
r(O···Na) (Å)	2.228	BLYP/PW[b]	S48
r(O−H) (Å)	0.973		
r(O−C) (Å)	1.486		
<r(H−C)> (Å)	1.091		
θ(Na···O−H) (°)	121.2		
θ(Na···O−C) (°)	131.4		

Continued

r(O···Na) (Å)	2.209	BLYP/6-311++G(3df,3pd)	S48
r(O−H) (Å)	0.972		
r(O−C) (Å)	1.473		
<r(H−C)> (Å)	1.093		
θ(Na···O−H) (°)	123.4		
θ(Na···O−C) (°)	129.1		
r(O···Na) (Å)	2.193	B3LYP/6-311++G(3df,3pd)	S48
r(O−H) (Å)	0.962		
r(O−C) (Å)	1.452		
<r(H−C)> (Å)	1.087		
θ(Na···O−H) (°)	123.3		
θ(Na···O−C) (°)	128.7		
r(O···Na) (Å)	2.252	MP2/6-311++G(3df,3pd)	S48
r(O−H) (Å)	0.961		
r(O−C) (Å)	1.446		
<r(H−C)> (Å)	1.085		
θ(Na···O−H) (°)	123.3		
θ(Na···O−C) (°)	129.5		
r(O···Na) (Å)	2.26	MP2[b]	S49
r(O···Na) (Å)	2.222	MP2/6-31G(d)	S47
	2.256	MP2/6-31G(d,p)	
	2.253	MP2/6-31+G(d)	
	2.252	MP2/6-31++G(d,p)	
	2.256	MP2/6-311++G(2d,2p)	
[K^+-MeOH]	Geometrical parameters	Methods	References
r(O···K) (Å)	2.564	BP86/6-311G(d,p)	This work
r(O−H) (Å)	0.973		
r(O−C) (Å)	1.458		
<r(H−C)> (Å)	1.100		
θ(K···O−H) (°)	124.5		
θ(K···O−C) (°)	128.8		
r(O···K) (Å)	2.565	B3LYP/6-311G(d,p)	This work
r(O−H) (Å)	0.964		
r(O−C) (Å)	1.449		
<r(H−C)> (Å)	1.091		
θ(K···O–H) (°)	123.9		
θ(K···O−C) (°)	123.9		

Continued

r(O···K) (Å) r(O−H) (Å) r(O−C) (Å) <r(H−C)> (Å) θ(K···O−H) (°) θ(K···O−C) (°)	2.573 0.973 1.48 1.093 125.7 127.0	BLYP/PW[b]	S48
r(O···K) (Å) r(O−H) (Å) r(O−C) (Å) <r(H−C)> (Å) θ(K···O−H) (°) θ(K···O−C) (°)	2.607 0.972 1.467 1.094 123.2 129.5	BLYP/6-311++G(3df,3pd)	S48
r(O···K) (Å) r(O−H) (Å) r(O−C) (Å) <r(H−C)> (Å) θ(K···O−H) (°) θ(K···O−C) (°)	2.590 0.962 1.446 1.088 123.2 129.0	B3LYP/6-311++G(3df,3pd)	S48
r(O···K) (Å) r(O−H) (Å) r(O−C) (Å) <r(H−C)> (Å) θ(K···O−H) (°) θ(K···O−C) (°)	2.589 0.961 1.441 1.086 124.5 128.5	MP2/6-311++G(3df,3pd)	S48
r(O···K) (Å)	2.63	MP2[b]	S49
r(O···K) (Å) r(O−H) (Å)	2.654 0.950	HF/6-31+G(d)	S50
r(O···K) (Å) r(O−H) (Å)	2.622 0.971	B3LYP/6-31+G(d)	S50
r(O···K) (Å) r(O−H) (Å)	2.630 0.975	MP2/6-31+G(d)	S50
r(O···K) (Å) θ(K···O−H) (°)	2.657 126.2	RHF/DZP	S51

Continued

[Li^+-DEE]	Geometrical parameters			Methods	References
	TT	TG	GG		
r(O···Li) (Å)	1.817	1.819	1.810		
r(O−C) (Å)	1.464	1.463, 1.474	1.478		
r(C−C) (Å)	1.519	1.522, 1.520	1.520		
θ(Li···O−C) (°)	122.9	111.7, 133.4	123.1	BP86/6-311G(d,p)	This work
θ(C−O−C) (°)	114.1	114.8	113.9		
Ø(C−C−O−C) (°)	180	-176.7, -74.6	84.6		
Ø(Li···O−C−C) (°)	0	0.9, 108.5	-95.4		
	TT	TG	GG		
r(O···Li) (Å)	1.797	1.799	1.791		
r(O−C) (Å)	1.455	1.453, 1.464	1.468		
r(C−C) (Å)	1.515	1.518, 1.517	1.517		
θ(Li···O−C) (°)	122.7	111.1, 133.3	122.7	B3LYP/6-311G(d,p)	This work
θ(C−O−C) (°)	114.6	115.5	114.6		
Ø(C−C−O−C) (°)	180.0	-176.7, -75.5	85.3		
Ø(Li···O−C−C) (°)	0.0	0.7, 107.8	-94.7		
r(O···Li) (Å)		1.801			
r(O−C) (Å)		1.455			
r(C−C) (Å)		1.515		B3LYP/6-311++G(d,p)	S41a
θ(Li···O−C) (°)		122.6			
Ø(C−C−O−C) (°)		180.0			
Ø(Li···O−C−C) (°)		0.0			
r(O···Li) (Å)		1.807			
r(O−C) (Å)		1.430		RHF/6-311+G(d,p)	S41b
θ(C−O−C) (°)		115.2			
[Na^+-DEE]	Geometrical parameters			Methods	References
	TT	TG	GG		
r(O···Na) (Å)	2.201	2.205	2.199		
r(O−C) (Å)	1.456	1.456, 1.466	1.468		
r(C−C) (Å)	1.520	1.521, 1.522	1.523		
θ(Na···O−C) (°)	123.6	117.1, 129.3	123.3	BP86/6-311G(d,p)	This work
θ(C−O−C) (°)	112.9	113.6	113.3		
Ø(C−C−O−C) (°)	180.0	-176.7, -76.8	85.9		
Ø(Na···O−C−C) (°)	0.0	1.6, 105.1	-94.1		

Continued

	TT	TG	GG		
r(O···Na) (Å)	2.182	2.185	2.180		
r(O−C) (Å)	1.446	1.446, 1.456	1.458		
r(C−C) (Å)	1.516	1.518, 1.519	1.519		
θ(Na···O−C) (°)	123.2	116.1, 129.5	122.9	B3LYP/6-311G(d,p)	This work
θ(C−O−C) (°)	113.7	114.4	114.1		
Ø(C−C−O−C) (°)	180.0	-177.3, -78.1	86.7		
Ø(Na···O−C−C) (°)	0.0	0.9, 104	-93.3		
r(O···Na) (Å)		2.189			
r(O−C) (Å)		1.447			
r(C−C) (Å)		1.516		B3LYP/6-311++G(d,p)	S41a
θ(Na···O−C) (°)		123.1			
Ø(C−C−O−C) (°)		180.0			
Ø(Na···O−C−C) (°)		0.0			
[K^+-DEE]	Geometrical parameters			Methods	References
	TT	TG	GG		
r(O···K) (Å)	2.560	2.554	2.547		
r(O−C) (Å)	1.452	1.453, 1.460	1.462		
r(C−C) (Å)	1.521	1.521, 1.525	1.524		
θ(K···O−C) (°)	124.0	122.8, 124.2	123.4	BP86/6-311G(d,p)	This work
θ(C−O−C) (°)	112.0	112.9	113.2		
Ø(C−C−O−C) (°)	180.0	-175.1, -75.1	85.2		
Ø(K···O−C−C) (°)	0.0	2.5, 107.4	-94.8		
	TT	TG	GG		
r(O···K) (Å)	2.567	2.558	2.549		
r(O−C) (Å)	1.441	1.443, 1.449	1.451		
r(C−C) (Å)	1.517	1.517, 1.521	1.521		
θ(K···O−C) (°)	123.7	122.4, 123.8	122.9	B3LYP/6-311G(d,p)	This work
θ(C−O−C) (°)	112.5	113.8	114.1		
Ø(C−C−O−C) (°)	180.0	-175.3, -76.0	85.6		
Ø(K···O−C−C) (°)	0.0	1.8, 107.0	-94.4		
[Li^+-THF]	Geometrical parameters			Methods	References
r(O···Li) (Å)		1.810			
r(O−C) (Å)		1.489			
θ(Li···O−C) (°)		125.5		BP86/6-311G(d,p)	This work
θ(C−O−C) (°)		109.0			
Ø(C−C−O−C) (°)		12.7			
Ø(Li···O−C−C) (°)		-167.3			

Continued

r(O···Li) (Å) r(O−C) (Å) θ(Li···O−C) (°) θ(C−O−C) (°) Ø(C−C−O−C) (°) Ø(Li···O−C−C) (°)	1.791 1.480 125.3 109.4 12.4 -167.6	B3LYP/6-311G(d,p)	This work
r(O···Li) (Å) r(O−C) (Å) θ(C−O−C) (°)	1.798 1.451 110.5	RHF/6-311+G(d,p)	S41b
[Na^+-THF]	Geometrical parameters	Methods	References
r(O···Na) (Å) r(O−C) (Å) θ(Na···O−C) (°) θ(C−O−C) (°) Ø(C−C−O−C) (°) Ø(Na···O−C−C) (°)	2.195 1.480 125.6 108.9 12.6 -167.4	BP86/6-311G(d,p)	This work
r(O···Na) (Å) r(O−C) (Å) θ(Na···O−C) (°) θ(C−O−C) (°) Ø(C−C−O−C) (°) Ø(Na···O−C−C) (°)	2.176 1.469 125.3 109.4 12.3 -167.7	B3LYP/6-311G(d,p)	This work
[K^+-THF]	Geometrical parameters	Methods	References
r(O···K) (Å) r(O−C) (Å) θ(K···O−C) (°) θ(C−O−C) (°) Ø(C−C−O−C) (°) Ø(K···O−C−C) (°)	2.542 1.473 125.6 108.8 12.6 -167.4	BP86/6-311G(d,p)	This work
r(O···K) (Å) r(O−C) (Å) θ(K···O−C) (°) θ(C−O−C) (°) Ø(C−C−O−C) (°) Ø(K···O−C−C) (°)	2.544 1.462 125.3 109.3 12.3 -167.7	B3LYP/6-311G(d,p)	This work

[a] "r", "θ", and "Ø" denote the bond distances, bond angles, and dihedral angles, respectively.

[b] Detailed information on the optimisation methods used is provided in corresponding references.

Table S6: Calculated energies (kJ.mol^{-1}) for the dissociation process, [M^+-L] → M^+ + L.

	BP86/6-311G(d,p)				B3LYP/6-311G(d,p)			
	ΔE^{ZPE}	$\Delta E^{ZPE+BSSE}$	ΔH	ΔG	ΔE^{ZPE}	$\Delta E^{ZPE+BSSE}$	ΔH	ΔG
[Li^+-L]								
H_2O	156.1	140.2	160.4	131.9	166.3	150.1	170.7	142.0
THF	180.3	170.9	182.8	150.6	193.3	183.5	195.9	163.8
DEE,TT	178.5	169.9	180.2	151.9	190.5	181.6	192.3	164.2
DEE,TG	177.3	168.5	179.4	149.4	189.7	180.6	191.9	161.6
DEE,GG	173.2	164.3	175.1	146.2	185.5	176.0	187.5	157.9
MeOH	161.1	148.9	163.7	135.1	173.5	160.9	176.2	147.2
DCM	99.1	93.9	101.1	71.3	107.9	102.6	110.0	79.7
[Na^+-L]								
H_2O	111.7	98.9	115.2	88.0	119.5	106.5	123.1	95.7
THF	125.1	117.0	126.4	95.9	134.9	126.5	136.2	105.9
DEE,TT	121.5	114.0	122.6	93.5	131.2	123.4	132.3	103.4
DEE,TG	120.3	112.7	121.3	92.8	130.0	122.0	131.1	101.7
DEE,GG	117.8	110.3	118.6	90.8	127.0	119.1	127.9	99.7
MeOH	112.1	102.1	113.7	86.4	121.5	111.2	123.3	95.6
DCM	63.2	59.1	63.8	36.4	70.5	66.3	71.2	43.2
[K^+-L]								
H_2O	83.0	72.2	86.1	60.3	86.7	76.0	89.9	63.9
THF	91.4	85.3	92.1	63.4	96.3	89.9	97.0	68.6
DEE,TT	83.8	78.2	84.6	55.9	88.7	83.0	89.5	60.9
DEE,TG	84.1	78.3	84.7	56.9	88.9	82.8	89.6	61.4
DEE,GG	84.7	78.7	85.0	58.7	89.1	82.9	89.5	63.0
MeOH	81.9	73.7	83.0	57.2	86.7	78.4	88.0	61.9
DCM	39.7	37.5	39.7	15.3	43.5	41.2	43.5	18.7

Table S7: Computed charge densities (natural charges, e) on selected centres of L and [M^+-L] structures.

BP86/6-311G(d,p)						B3LYP/6-311G(d,p)					
	H_2O		[M^+-H_2O]				H_2O		[M^+-H_2O]		
			Li	Na	K				Li	Na	K
O1	-0.873	O1	-1.017	-0.988	-0.969	O1	-0.877	O1	-1.019	-0.990	-0.970
H2	0.436	M2	0.980	0.988	0.992	H2	0.438	M2	0.980	0.988	0.993
H3	0.436	H3	0.518	0.500	0.489	H3	0.438	H3	0.519	0.501	0.489
		H4	0.518	0.500	0.489			H4	0.519	0.501	0.489
BP86/6-311G(d,p)						B3LYP/6-311G(d,p)					
	THF		[M^+-THF]				THF		[M^+-THF]		
			Li	Na	K				Li	Na	K
C1	-0.045	C1	-0.045	-0.046	-0.047	C1	-0.016	C1	-0.016	-0.017	-0.018
H2	0.161	H2	0.192	0.185	0.181	H2	0.152	H2	0.183	0.175	0.171
H3	0.181	H3	0.201	0.193	0.190	H3	0.171	H3	0.191	0.183	0.179
C4	-0.429	C4	-0.427	-0.426	-0.426	C4	-0.408	C4	-0.406	-0.406	-0.405
H5	0.215	H5	0.248	0.243	0.240	H5	0.204	H5	0.236	0.231	0.228
H6	0.200	H6	0.220	0.216	0.214	H6	0.190	H6	0.210	0.206	0.203
C7	-0.429	C7	-0.427	-0.426	-0.426	C7	-0.408	C7	-0.406	-0.406	-0.405
H8	0.215	H8	0.248	0.243	0.240	H8	0.204	H8	0.236	0.231	0.228
H9	0.200	H9	0.220	0.216	0.214	H9	0.190	H9	0.210	0.206	0.203
C10	-0.045	C10	-0.045	-0.046	-0.047	C10	-0.016	C10	-0.016	-0.017	-0.018
H11	0.181	H11	0.201	0.193	0.190	H11	0.171	H11	0.191	0.183	0.179
H12	0.161	H12	0.192	0.185	0.181	H12	0.152	H12	0.183	0.175	0.171
O13	-0.567	O13	-0.749	-0.707	-0.685	O13	-0.587	O13	-0.765	-0.723	-0.699
		M14	0.969	0.976	0.983			M14	0.969	0.976	0.984
BP86/6-311G(d,p)						B3LYP/6-311G(d,p)					
	DEE (TT)		[M^+-DEE] (TT)				DEE (TT)		[M^+-DEE] (TT)		
			Li	Na	K				Li	Na	K
C1	-0.038	C1	-0.037	-0.038	-0.039	C1	-0.007	C1	-0.007	-0.008	-0.009
H2	-0.038	H2	0.198	0.192	0.187	H2	-0.007	H2	0.188	0.182	0.177
C3	0.157	C3	-0.037	-0.038	-0.039	C3	0.147	C3	-0.007	-0.008	-0.009
H4	-0.571	H4	0.198	0.192	0.187	H4	-0.591	H4	0.188	0.182	0.177
O5	0.157	O5	-0.715	-0.681	-0.663	O5	0.147	O5	-0.731	-0.698	-0.678
C6	-0.609	H6	0.198	0.192	0.187	C6	-0.579	H6	0.188	0.182	0.177
H7	0.206	C7	-0.646	-0.637	-0.631	H7	0.196	C7	-0.617	-0.607	-0.601
H8	0.206	H8	0.261	0.255	0.250	H8	0.195	H8	0.250	0.244	0.238
H9	0.206	H9	0.209	0.202	0.198	H9	0.196	H9	0.199	0.192	0.188
C10	0.157	H10	0.209	0.202	0.198	C10	0.147	H10	0.199	0.192	0.188
H11	-0.609	H11	0.198	0.192	0.187	H11	-0.579	H11	0.188	0.182	0.177
H12	0.206	C12	-0.646	-0.637	-0.631	H12	0.196	C12	-0.617	-0.607	-0.601
H13	0.206	H13	0.209	0.202	0.198	H13	0.195	H13	0.199	0.192	0.188
H14	0.206	H14	0.209	0.202	0.198	H14	0.196	H14	0.199	0.192	0.188
H15	0.157	H15	0.261	0.255	0.250	H15	0.147	H15	0.250	0.244	0.238

		M16	0.928	0.945	0.961		M16	0.928	0.945	0.962
BP86/6-311G(d,p)						B3LYP/6-311G(d,p)				
	DEE (GG)		[M^+-DEE] (GG)				DEE (GG)		[M^+-DEE] (GG)	
			Li	Na	K				Li	Na	K
C1	-0.043	C1	-0.042	-0.042	-0.043	C1	-0.011	C1	-0.012	-0.011	-0.012
C2	0.182	H2	0.190	0.183	0.180	C2	0.172	H2	0.180	0.173	0.169
H3	-0.043	C3	-0.042	-0.042	-0.043	H3	-0.011	C3	-0.012	-0.011	-0.012
O4	0.182	H4	0.190	0.183	0.180	O4	0.172	H4	0.180	0.173	0.169
H5	-0.572	O5	-0.741	-0.702	-0.679	H5	-0.592	O5	-0.757	-0.719	-0.695
C6	-0.625	C6	-0.631	-0.629	-0.628	C6	-0.594	C6	-0.602	-0.600	-0.598
H7	0.199	H7	0.220	0.218	0.216	H7	0.189	H7	0.210	0.208	0.206
H8	0.206	H8	0.211	0.205	0.202	H8	0.197	H8	0.200	0.194	0.191
H9	0.206	H9	0.243	0.238	0.234	H9	0.195	H9	0.231	0.226	0.223
H10	-0.625	C10	-0.631	-0.629	-0.628	H10	-0.594	C10	-0.602	-0.600	-0.598
C11	0.199	H11	0.220	0.218	0.216	C11	0.189	H11	0.210	0.208	0.206
H12	0.206	H12	0.211	0.205	0.202	H12	0.197	H12	0.200	0.194	0.191
H13	0.206	H13	0.243	0.238	0.234	H13	0.195	H13	0.231	0.226	0.223
H14	0.160	H14	0.201	0.194	0.191	H14	0.149	H14	0.191	0.184	0.180
H15	0.160	H15	0.201	0.194	0.191	H15	0.149	H15	0.191	0.184	0.180
		M16	0.959	0.971	0.977			M16	0.959	0.970	0.978
BP86/6-311G(d,p)						B3LYP/6-311G(d,p)				
	MeOH		[M^+-MeOH]				MeOH		[M^+-MeOH]	
			Li	Na	K				Li	Na	K
C1	-0.221	C1	-0.211	-0.212	-0.215	C1	-0.186	C1	-0.176	-0.178	-0.181
H2	0.176	H2	0.191	0.183	0.179	H2	0.168	H2	0.184	0.175	0.170
H3	0.152	O3	-0.864	-0.829	-0.808	H3	0.144	O3	-0.874	-0.839	-0.817
H4	0.152	H4	0.202	0.193	0.188	H4	0.144	H4	0.194	0.186	0.180
O5	-0.698	H5	0.202	0.193	0.188	O5	-0.712	H5	0.194	0.186	0.180
H6	0.440	H6	0.507	0.490	0.481	H6	0.440	H6	0.507	0.490	0.480
		M7	0.972	0.981	0.986			M7	0.972	0.981	0.987
BP86/6-311G(d,p)						B3LYP/6-311G(d,p)				
	DCM		[M^+-DCM]				DCM		[M^+-DCM]	
			Li	Na	K				Li	Na	K
C1	-0.380	C1	-0.347	-0.355	-0.356	C1	-0.346	C1	-0.313	-0.321	-0.322
H2	0.208	H2	0.242	0.236	0.231	H2	0.199	H2	0.234	0.228	0.223
H3	0.208	H3	0.242	0.236	0.231	H3	0.199	H3	0.234	0.228	0.223
Cl4	-0.017	Cl4	-0.001	-0.028	-0.037	Cl4	-0.026	Cl4	-0.008	-0.035	-0.046
Cl5	-0.017	Cl5	-0.001	-0.028	-0.037	Cl5	-0.026	Cl5	-0.008	-0.035	-0.046
		M6	0.865	0.938	0.967			M6	0.861	0.936	0.968

Table S8: Computed charge densities (natural charges, e) on selected centres of Me_4cyclen and $[M(Me_4cyclen)]^+$ structures.

BP86/6-311G(d,p)					B3LYP/6-311G(d,p)				
	Me_4cyclen	$[M(Me_4cyclen)]^+$				Me_4cyclen	$[M(Me_4cyclen)]^+$		
		Li	Na	K			Li	Na	K
C1*	-0.384	-0.387	-0.389	-0.393	C1*	-0.349	-0.353	-0.355	-0.359
H2*	0.158	0.195	0.192	0.190	H2*	0.149	0.185	0.182	0.181
H3*	0.196	0.209	0.207	0.202	H3*	0.185	0.198	0.196	0.191
H4*	0.195	0.204	0.203	0.201	H4*	0.184	0.194	0.193	0.190
C17	-0.207	-0.209	-0.213	-0.214	C17	-0.178	-0.181	-0.184	-0.185
H18	0.199	0.204	0.202	0.201	H18	0.186	0.192	0.190	0.189
H19	0.170	0.212	0.209	0.204	H19	0.158	0.200	0.196	0.192
C20	-0.198	-0.206	-0.207	-0.208	C20	-0.169	-0.178	-0.179	-0.180
H21	0.167	0.211	0.205	0.200	H21	0.156	0.198	0.193	0.187
H22	0.201	0.215	0.212	0.207	H22	0.188	0.203	0.200	0.195
N41	-0.497	-0.570	-0.567	-0.556	N41	-0.511	-0.582	-0.578	-0.567
N42	-0.486	-0.570	-0.567	-0.556	N42	-0.501	-0.582	-0.578	-0.567
N43	-0.497	-0.570	-0.567	-0.556	N43	-0.511	-0.582	-0.578	-0.567
N44	-0.486	-0.570	-0.567	-0.556	N44	-0.501	-0.582	-0.578	-0.567
M45	–	0.690	0.786	0.865	M45	–	0.696	0.787	0.870

* Corresponds to the atoms of the CH_3 unit.

Table S9: Computed BP86 charge densities (natural charges, e) on selected centres of the lowest **M-L-1a** minimum energy structures.

M-H2O-1a				
		Li	Na	K
C1*	(C1)	-0.388	-0.387	-0.392
H2*		0.193	0.189	0.188
H3*		0.204	0.206	0.201
H4*		0.201	0.201	0.200
C17	(C5)	-0.209	-0.211	-0.213
H18		0.204	0.202	0.201
H19		0.208	0.206	0.201
C20	(C6)	-0.205	-0.206	-0.207
H21		0.206	0.201	0.198
H22		0.211	0.210	0.206
N41	(N1)	-0.548	-0.553	-0.547
N42	(N2)	-0.548	-0.553	-0.547
N43	(N3)	-0.548	-0.553	-0.547
N44	(N4)	-0.548	-0.553	-0.547
O45		-0.890	-0.911	-0.914
M46		0.593	0.713	0.820
H47	(H1)	0.492	0.485	0.476
H48		0.492	0.485	0.476

M-THF-1a

		Li	Na	K
C1*	(C1)	-0.383	-0.385	-0.390
H2*		0.191	0.188	0.187
H3*		0.208	0.206	0.201
H4*		0.200	0.201	0.200
C17	(C5)	-0.207	-0.209	-0.212
H18		0.203	0.202	0.201
H19		0.207	0.205	0.201
C20	(C6)	-0.205	-0.204	-0.206
H21		0.205	0.201	0.197
H22		0.210	0.210	0.206
C41	(C16)	-0.038	-0.039	-0.044
H42		0.180	0.178	0.174
H43		0.191	0.189	0.186
C44	(C15)	-0.423	-0.424	-0.425
H45		0.234	0.233	0.232
H46		0.211	0.211	0.210
C47	(C14)	-0.423	-0.424	-0.425
H48		0.234	0.233	0.232
H49		0.211	0.211	0.210
C50	(C13)	-0.038	-0.039	-0.044
H51		0.191	0.189	0.186
H52		0.180	0.178	0.174
N53	(N1)	-0.552	-0.552	-0.545
N54	(N2)	-0.544	-0.553	-0.545
N55	(N3)	-0.552	-0.552	-0.545
N56	(N4)	-0.544	-0.553	-0.545
O57		-0.623	-0.631	-0.625
M58		0.585	0.692	0.801

M-DEE-1a

		Li			Na			K
C1*	(C1)	-0.386	C1*	(C1)	-0.387	C1*	(C1)	-0.391
H2*		0.192	H2*		0.190	H2*		0.188
H3*		0.206	H3*		0.205	H3*		0.203
H4*		0.200	H4*		0.202	H4*		0.200
C17	(C5)	-0.207	C17	(C5)	-0.209	C17	(C5)	-0.212
H18		0.203	H18		0.202	H18		0.201
H19		0.208	H19		0.205	H19		0.201
C20	(C6)	-0.204	C20	(C6)	-0.204	C20	(C6)	-0.206
H21		0.206	H21		0.201	H21		0.197
H22		0.210	H22		0.211	H22		0.206

C41	(C14)	-0.034	C41	(C14)	-0.036	C41	(C14)	-0.040
H42		0.186	H42		0.186	H42		0.179
C43	(C13)	-0.034	C43	(C13)	-0.036	C43	(C13)	-0.040
H44		0.186	H44		0.185	H44		0.179
N45	(N1)	-0.546	N45	(N1)	-0.553	N45	(N1)	-0.543
N46	(N2)	-0.552	N46	(N2)	-0.554	N46	(N2)	-0.542
N47	(N3)	-0.546	N47	(N3)	-0.553	N47	(N3)	-0.543
N48	(N4)	-0.552	N48	(N4)	-0.555	N48	(N4)	-0.542
O49		-0.615	O49		-0.625	O49		-0.601
C50	(C16)	-0.631	Na50		0.661	H50		0.179
H51		0.213	C51	(C16)	-0.623	C51	(C15)	-0.613
H52		0.210	H52		0.212	H52		0.234
H53		0.230	H53		0.205	H53		0.203
C54	(C15)	-0.631	H54		0.226	H54		0.203
H55		0.213	C55	(C15)	-0.623	H55		0.179
H56		0.210	H56		0.212	C56	(C16)	-0.613
H57		0.230	H57		0.206	H57		0.203
H58		0.186	H58		0.226	H58		0.203
H59		0.186	H59		0.185	H59		0.234
Li60		0.566	H60		0.185	K60		0.729
M-MeOH-1a								
		Li			Na			K
C1*	(C1)	-0.386	C1*	(C1)	-0.387	C1*	(C1)	-0.391
H2*		0.192	H2*		0.190	H2*		0.188
H3*		0.208	H3*		0.205	H3*		0.202
H4*		0.198	H4*		0.200	H4*		0.200
C17	(C5)	-0.208	C17	(C5)	-0.211	C17	(C5)	-0.213
H18		0.203	H18		0.202	H18		0.200
H19		0.208	H19		0.205	H19		0.201
C20	(C6)	-0.205	C20	(C6)	-0.205	C20	(C6)	-0.207
H21		0.206	H21		0.201	H21		0.197
H22		0.210	H22		0.210	H22		0.206
C41		-0.208	C41		-0.210	C41		-0.215
H42		0.186	H42		0.184	H42		0.179
N43	(N1)	-0.548	N43	(N1)	-0.553	N43	(N1)	-0.546
N44	(N2)	-0.548	N44	(N2)	-0.554	N44	(N2)	-0.546
N45	(N3)	-0.549	N45	(N3)	-0.553	N45	(N3)	-0.547
N46	(N4)	-0.550	N46	(N4)	-0.553	N46	(N4)	-0.547
O47		-0.731	O47		-0.748	O47		-0.746
H48		0.181	Na48		0.700	H48		0.177
H49		0.182	H49		0.182	H49		0.177
H50	(H1)	0.484	H50		0.179	H50	(H1)	0.470
Li51		0.585	H51	(H1)	0.479	K51		0.809

M-DCM-1a								
		Li			Na			K
C1*	(C1)	-0.391	C1*	(C1)	-0.389	C1*	(C1)	-0.392
H2*		0.193	H2*		0.191	H2*		0.189
H3*		0.212	H3*		0.208	H3*		0.203
H4*		0.206	H4*		0.203	H4*		0.201
C17	(C5)	-0.208	C17	(C5)	-0.210	C17	(C5)	-0.213
H18		0.204	H18		0.202	H18		0.201
H19		0.211	H19		0.207	H19		0.202
C20	(C6)	-0.204	C20	(C6)	-0.205	C20	(C6)	-0.207
H21		0.208	H21		0.202	H21		0.199
H22		0.215	H22		0.212	H22		0.207
C41	(C13)	-0.360	C41	(C13)	-0.361	C41	(C13)	-0.364
N42	(N1)	-0.555	N42	(N1)	-0.556	N42	(N1)	-0.549
N43	(N2)	-0.563	N43	(N2)	-0.558	N43	(N2)	-0.549
N44	(N3)	-0.558	N44	(N3)	-0.556	N44	(N3)	-0.549
N45	(N4)	-0.564	N45	(N4)	-0.558	N45	(N4)	-0.549
H46		0.222	Na46		0.587	H46		0.224
H47		0.223	H47		0.226	H47		0.224
Cl48	(Cl1)	0.025	H48		0.226	Cl48	(Cl1)	0.000
Cl49	(Cl2)	0.023	Cl49	(Cl1)	0.025	Cl49	(Cl2)	0.001
Li50		0.517	Cl50	(Cl2)	0.031	K50		0.747

* Corresponds to the atoms of the CH_3 unit.

Table S10: Computed B3LYP charge densities (natural charges, e) on selected centres of the lowest **M-L-2a** minimum energy structures.

M-H_2O-2a				
		Li	Na	K
C1*	(C1)	-0.354	-0.353	-0.358
H2*		0.184	0.180	0.179
H3*		0.192	0.193	0.190
H4*		0.190	0.191	0.189
C17	(C5)	-0.180	-0.182	-0.184
H18		0.191	0.190	0.188
H19		0.195	0.193	0.188
C20	(C6)	-0.178	-0.177	-0.179
H21		0.194	0.189	0.185
H22		0.199	0.198	0.193
N41	(N1)	-0.560	-0.565	-0.558
N42	(N2)	-0.560	-0.565	-0.558
N43	(N3)	-0.560	-0.565	-0.558
N44	(N4)	-0.560	-0.565	-0.558

O45		-0.894	-0.915	-0.917
M46		0.604	0.715	0.826
H47	(H1)	0.493	0.487	0.477
H48		0.493	0.487	0.477

M-THF-2a

		Li	Na	K
C1*	(C1)	-0.348	-0.351	-0.356
H2*		0.181	0.179	0.178
H3*		0.196	0.195	0.190
H4*		0.189	0.190	0.189
C17	(C5)	-0.178	-0.180	-0.183
H18		0.191	0.190	0.188
H19		0.195	0.192	0.188
C20	(C6)	-0.177	-0.176	-0.178
H21		0.193	0.189	0.185
H22		0.198	0.198	0.194
C41	(C16)	-0.007	-0.010	-0.015
H42		0.170	0.168	0.165
H43		0.180	0.179	0.176
C44	(C15)	-0.403	-0.403	-0.404
H45		0.223	0.222	0.221
H46		0.201	0.201	0.199
C47	(C14)	-0.403	-0.403	-0.404
H48		0.223	0.222	0.221
H49		0.201	0.201	0.199
C50	(C13)	-0.007	-0.010	-0.015
H51		0.180	0.179	0.176
H52		0.170	0.168	0.165
N53	(N1)	-0.565	-0.565	-0.556
N54	(N2)	-0.555	-0.565	-0.556
N55	(N3)	-0.565	-0.565	-0.556
N56	(N4)	-0.555	-0.565	-0.556
O57		-0.643	-0.650	-0.642
M58		0.599	0.691	0.805

M-DEE-2a

		Li			Na			K
C1*	(C1)	-0.353	C1*	(C1)	-0.352	C1*	(C1)	-0.356
H2*		0.182	H2*		0.180	H2*		0.179
H3*		0.195	H3*		0.194	H3*		0.191
H4*		0.189	H4*		0.191	H4*		0.189
C17	(C5)	-0.179	C17	(C5)	-0.180	C17	(C5)	-0.183
H18		0.191	H18		0.190	H18		0.189

H19		0.195	H19		0.193	H19		0.188
C20	(C6)	-0.175	C20	(C6)	-0.175	C20	(C6)	-0.178
H21		0.194	H21		0.189	H21		0.185
H22		0.198	H22		0.199	H22		0.194
C41	(C14)	-0.003	C41	(C14)	-0.005	C41	(C14)	-0.009
H42		0.177	H42		0.175	H42		0.169
C43	(C13)	-0.003	C43	(C13)	-0.005	C43	(C13)	-0.009
H44		0.177	H44		0.175	H44		0.169
N45	(N1)	-0.554	N45	(N1)	-0.565	N45	(N1)	-0.554
N46	(N2)	-0.568	N46	(N2)	-0.567	N46	(N2)	-0.553
N47	(N3)	-0.554	N47	(N3)	-0.565	N47	(N3)	-0.554
N48	(N4)	-0.568	N48	(N4)	-0.566	N48	(N4)	-0.553
O49		-0.636	O49		-0.646	O49		-0.620
C50	(C16)	-0.600	Na50		0.662	H50		0.169
H51		0.203	C51	(C16)	-0.592	C51	(C15)	-0.582
H52		0.199	H52		0.202	H52		0.223
H53		0.218	H53		0.195	H53		0.192
C54	(C15)	-0.600	H54		0.215	H54		0.193
H55		0.203	C55	(C15)	-0.592	H55		0.169
H56		0.199	H56		0.202	C56	(C16)	-0.582
H57		0.218	H57		0.195	H57		0.192
H58		0.175	H58		0.215	H58		0.193
H59		0.175	H59		0.176	H59		0.223
Li60		0.580	H60		0.176	K60		0.735

M-MeOH-2a								
		Li			Na			K
C1*	(C1)	-0.349	C1*	(C1)	-0.351	C1*	(C1)	-0.357
H2*		0.181	H2*		0.179	H2*		0.178
H3*		0.195	H3*		0.193	H3*		0.190
H4*		0.192	H4*		0.192	H4*		0.189
C17	(C5)	-0.179	C17	(C5)	-0.182	C17	(C5)	-0.184
H18		0.191	H18		0.190	H18		0.188
H19		0.195	H19		0.193	H19		0.188
C20	(C6)	-0.177	C20	(C6)	-0.177	C20	(C6)	-0.179
H21		0.194	H21		0.189	H21		0.185
H22		0.199	H22		0.199	H22		0.194
C41		-0.174	C41		-0.175	C41		-0.180
H42		0.179	H42		0.175	H42		0.171
N43	(N1)	-0.563	N43	(N1)	-0.566	N43	(N1)	-0.557
N44	(N2)	-0.558	N44	(N2)	-0.565	N44	(N2)	-0.557
N45	(N3)	-0.562	N45	(N3)	-0.565	N45	(N3)	-0.558
N46	(N4)	-0.559	N46	(N4)	-0.565	N46	(N4)	-0.557

O47		-0.745	O47		-0.760	O47		-0.758
H48		0.174	Na48		0.702	H48		0.170
H49		0.173	H49		0.173	H49		0.170
H50	(H1)	0.484	H50		0.173	H50	(H1)	0.471
Li51		0.598	H51	(H1)	0.479	K51		0.814
M-DCM-2a								
		Li			Na			K
C1*	(C1)	-0.350	C1*	(C1)	-0.353	C1*	(C1)	-0.357
H2*		0.183	H2*		0.181	H2*		0.180
H3*		0.198	H3*		0.197	H3*		0.191
H4*		0.194	H4*		0.192	H4*		0.190
C17	(C5)	-0.178	C17	(C5)	-0.181	C17	(C5)	-0.184
H18		0.192	H18		0.190	H18		0.188
H19		0.198	H19		0.194	H19		0.189
C20	(C6)	-0.177	C20	(C6)	-0.176	C20	(C6)	-0.179
H21		0.196	H21		0.190	H21		0.186
H22		0.202	H22		0.200	H22		0.195
C41	(C13)	-0.326	C41	(C13)	-0.327	C41	(C13)	-0.330
N42	(N1)	-0.574	N42	(N1)	-0.568	N42	(N1)	-0.559
N43	(N2)	-0.571	N43	(N2)	-0.570	N43	(N2)	-0.559
N44	(N3)	-0.576	N44	(N3)	-0.568	N44	(N3)	-0.560
N45	(N4)	-0.572	N45	(N4)	-0.570	N45	(N4)	-0.560
H46		0.216	Na46		0.580	H46		0.216
H47		0.212	H47		0.218	H47		0.217
Cl48	(Cl1)	0.019	H48		0.218	Cl48	(Cl1)	-0.005
Cl49	(Cl2)	0.007	Cl49	(Cl1)	0.023	Cl49	(Cl2)	-0.005
Li50		0.534	Cl50	(Cl2)	0.023	K50		0.744

* Corresponds to the atoms of the CH_3 unit.

Table S11: Computed BP86 charge densities (natural charges, e) on selected centres of the optimised Me_4cyclen and $[Me_4cyclenH]^+$ structures.[a]

Me_4cyclen		$[Me_4cyclenH]^+$	
C1*	-0.384	C1*	-0.386
H2*	0.158	H2*	0.184
H3*	0.196	H3*	0.210
H4*	0.195	H4*	0.200
C5*	-0.388	C5*	-0.391
H6*	0.154	H6*	0.217
H7*	0.199	H7*	0.224
H8*	0.201	H8*	0.237
C17	-0.207	C17	-0.227
H18	0.199	H18	0.207
H19	0.170	H19	0.219
C20	-0.198	C20	-0.190
H21	0.167	H21	0.217
H22	0.201	H22	0.226
C23	-0.203	C23	-0.200
H24	0.191	H24	0.215
H25	0.168	H25	0.226
C26	-0.202	C26	-0.215
H27	0.170	H27	0.205
H28	0.198	H28	0.214
N41	-0.497	N41	-0.537
N42	-0.486	N45	-0.504
N43	-0.497	N42	-0.542
N44	-0.486	N43	-0.547
		H44	0.506

* Corresponds to the atoms of the CH_3 unit.

[a] Refer to Figure S8 for atom labeling.

Further information on computed infrared (IR) spectra

Computed harmonic IR spectra together with selected vibrational modes for the [M^+-L], [M(Me_4cyclen)]$^+$, [Me_4cyclenH]$^+$, and lowest [M(Me_4cyclen)(L)]$^+$ minimum energy structures, obtained using the BP86/6-311G(d,p) method, are provided in Figures S11-S14 and Tables S12-S15. The band positions in these computed IR spectra are approximations of the true band positions because of neglect of anharmonicity and approximate treatment of electron correlation in the DFT calculations. However, scaling factors for computed harmonic wavenumbers have been established for BP86 and B3LYP calculations with a basis set which is similar to the one used in this work. These are close to 1.00 (BP86, 1.0299; B3LYP, 1.0004).[S52] Hence, the computed spectra are expected to be reasonably reliable representations of the experimental spectra.

For a given ligand (L), comparison of the spectra for [M^+-L], [M(Me_4cyclen)]$^+$, and [M(Me_4cyclen)(L)]$^+$ helps identify bands in [M(Me_4cyclen)(L)]$^+$ that arise from the [M^+-L], and [M(Me_4cyclen)]$^+$ units. For example, the IR spectra of both [M(Me_4cyclen)]$^+$ and **M-L-1a** [M(Me_4cyclen)(L)]$^+$ show an intense band (at ~ 2900 cm^{-1}) and a broader group of weaker bands (within the range of 2950-3075 cm^{-1}). The 2900 cm^{-1} band corresponds to C–H stretching absorptions of both the CH_2 and CH_3 units of the Me_4cyclen ring. The broad band in the region 2950-3075 cm^{-1} consists of several components. The component at the highest wavenumber (~ 3050 cm^{-1}) corresponds to the C–H stretching of the CH_3 unit of the Me_4cyclen ring and in the case of the **M-L-1a** structures (L = THF, DEE, DCM), this band is also associated with the C–H stretching of the CH_2/CH_3 units in THF/DEE/DCM. Bands within the range 2975-3025 cm^{-1} are attributed to C–H stretching of both the CH_2 and CH_3 units of the Me_4cyclen ring and in the case of the **M-THF-1a** (M = Li, Na, K) and **M-DEE-1a** (M = Li, Na) structures, they also correspond to the C–H stretching vibrations of the CH_2/CH_3 units of THF/DEE.

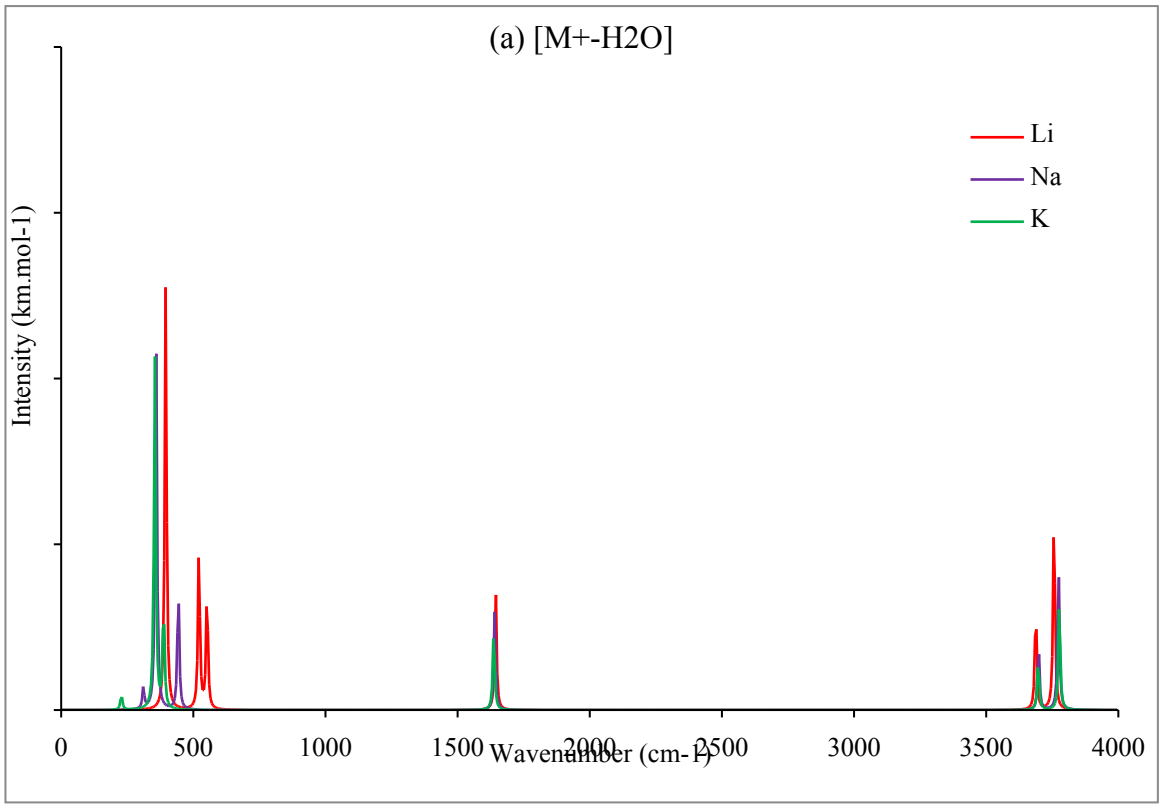
The computed IR spectra of the lowest [M(Me_4cyclen)]$^+$ minimum energy structures in the C–H stretching region are very similar to those of the [M(Me_4cyclen)(L)]$^+$ structures, except for the presence of additional band(s) due to L in the case of **M-L-1a** structures (L = THF, DEE, MeOH). An additional band at around 2940 cm^{-1} due to C–H stretching in THF is observed in the IR spectra of the **M-THF-1a** structures. Further, two additional weak bands due to C–H stretching in CH_2 (~ 2960 cm^{-1}) and CH_3 (~ 2970 cm^{-1}) units in DEE are observed in the IR spectra of the **M-DEE-1a** structures (M = Li, Na). On the other hand, for the **K-DEE-1a** structure, where DEE adopts a TT configuration, the C–H stretching of CH_2 (~ 2910 and 2945 cm^{-1}) and CH_3 (~ 2960 cm^{-1}) units of DEE are associated with three additional bands. In

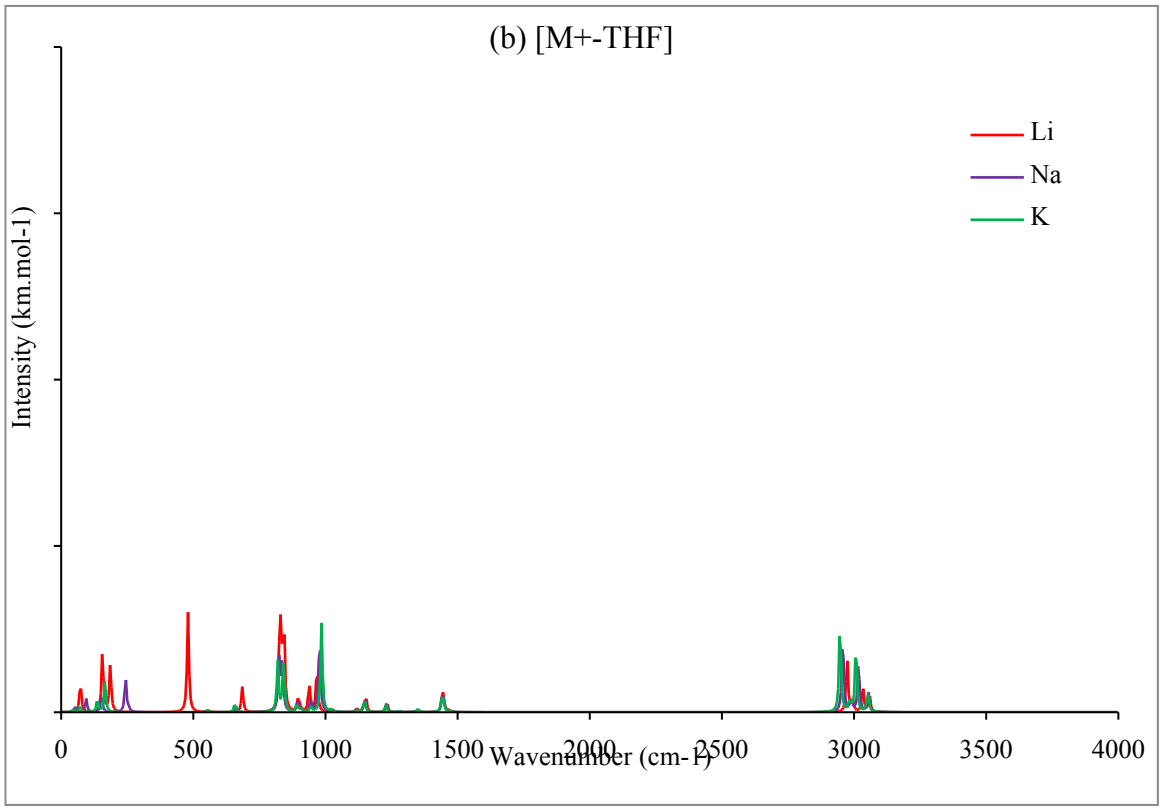
the case of the **M-MeOH-1a** structures, two additional bands due to C–H stretching of the CH_3 unit in MeOH are observed at around 2950 and 3060 cm^{-1}.

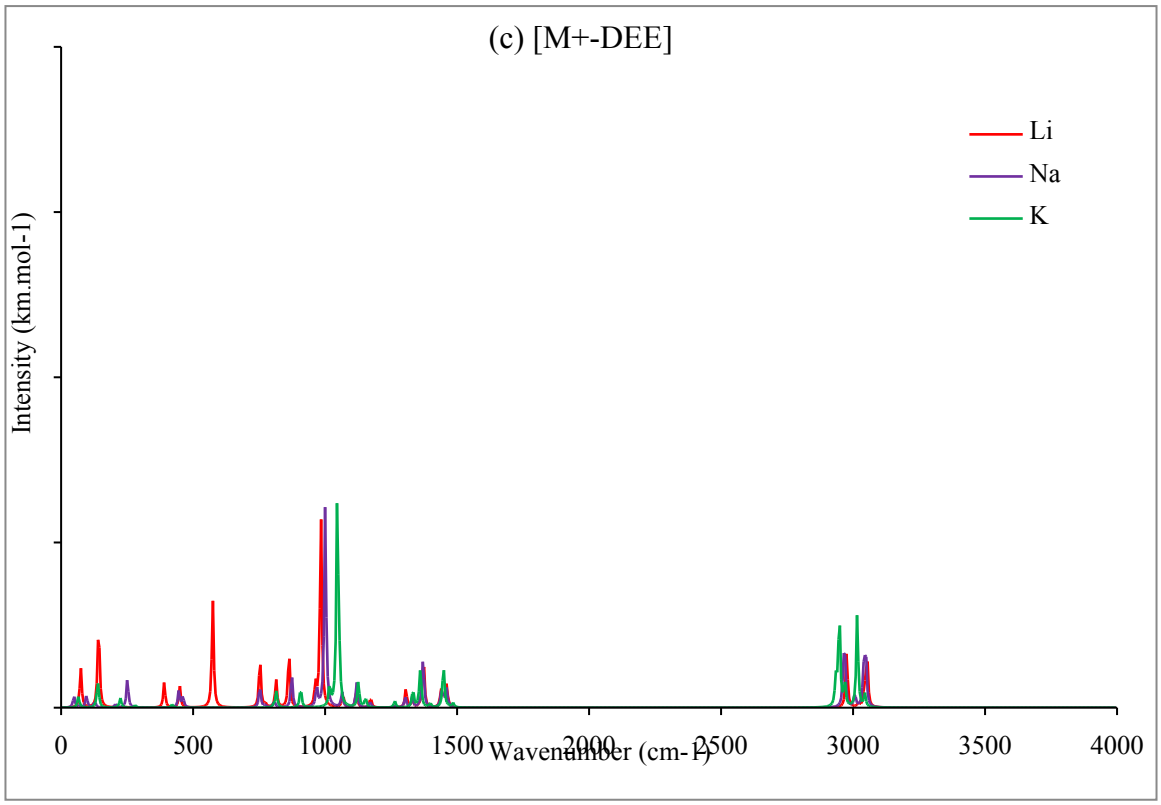
Other new bands are seen in the $[M(Me_4cyclen)(L)]^+$ spectra which are not present in the $[M^+\text{-}L]$, and $[M(Me_4cyclen)]^+$ units and these occur in the low wavenumber region below 500 cm^{-1}. For example, for $[M(Me_4cyclen)(L)]^+$ with L = THF, metal-oxygen (M–O) stretching modes are computed at 413, 219, and 176 cm^{-1} and for L = MeOH, these modes occur at 452, 244, and 183 cm^{-1}.

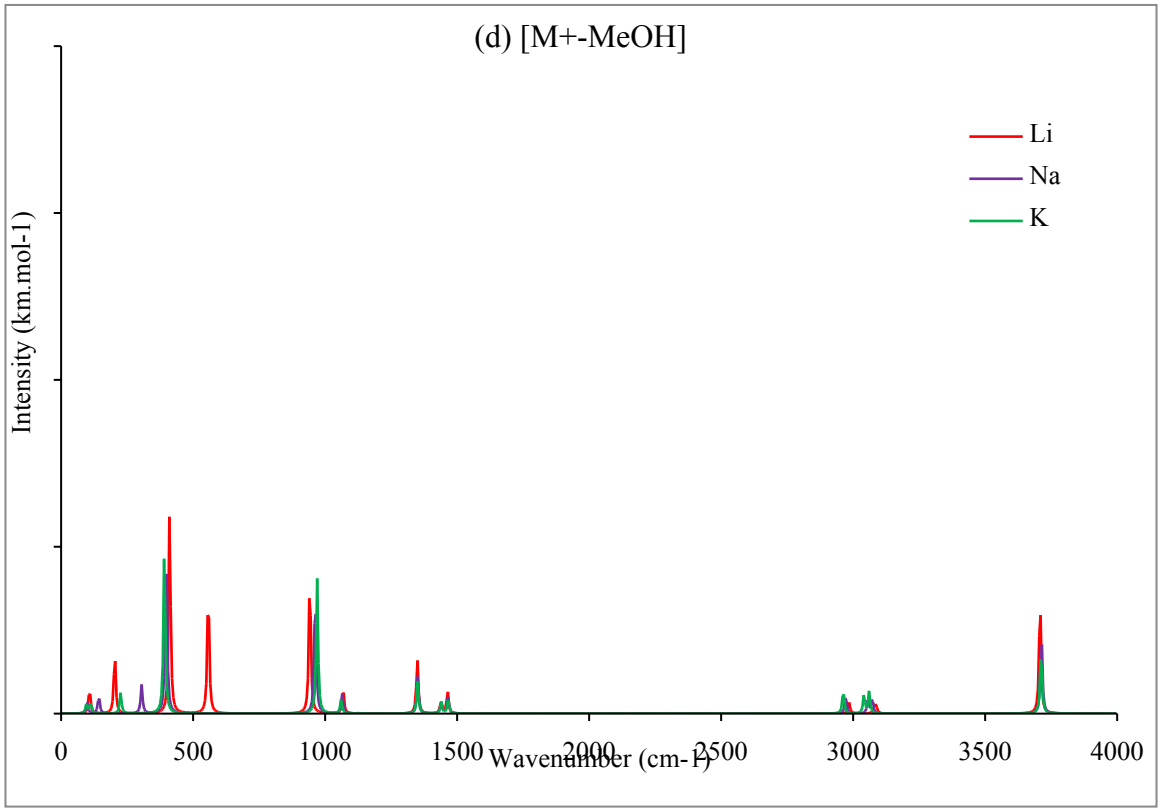
Overall, for a ligand selected from L = H_2O, THF, and MeOH, the IR spectra of the **M-L-1a** structures in the region 500-2500 cm^{-1} look very similar on going from $Li^+ \rightarrow Na^+ \rightarrow K^+$. This is not the case, however, for L = DEE or DCM. For L = DEE, the wavenumber values related to the C–O–C and C–C (in C–C–O–C–C) symmetric as well as asymmetric stretching modes are different for the **M-DEE-1a** (M = Li, Na) and **K-DEE-1a** structures (Table S14). These correspond to bands in the region 800-1100 cm^{-1}. This arises because of the GG and TT conformations of DEE in the **M-DEE-1a** (M = Li, Na) and **K-DEE-1a** structures, respectively.

For L = DCM, the differences in the **M-DCM-1a** (M = Li, Na, K) structures give rise to differences in their IR spectra. The Cl1–C–Cl2 symmetric and asymmetric stretching modes are computed at 640 and 709 cm^{-1} for **Li-DCM-1a** and 672 and 683 cm^{-1} for **Na-DCM-1a**, respectively. These differences arise because **Li-DCM-1a** and **Na-DCM-1a** have different structures, as well as different metal cations. As described earlier, in **Li-DCM-1a**, the Li^+ is attached to the DCM in a η^1-Cl1 mode [with M–Cl bond lengths which are significantly different M–Cl1 = 2.784 Å, M–Cl2 = 4.344 Å; see Table 2]. In contrast, Na^+ coordinates to DCM in a η^2-Cl1,Cl2 fashion in **Na-DCM-1a** with unequal bond distances [M–Cl1 (3.188 Å) and M–Cl2 (3.369 Å)]. **K-DCM-1a** has a similar η^2-Cl1,Cl2 structure with almost equal M–Cl bond distances [M–Cl1 (3.623 Å) and M–Cl2 (3.626 Å)] and symmetric and asymmetric Cl–C–Cl stretching modes computed at 674 cm^{-1} and 678 cm^{-1}, respectively. These spectra should be valuable to help confirm the presence and establish the structure of the $[M(Me_4cyclen)(L)]^+$ complex ions when they are made experimentally.


(a) [M+-H2O]
Li
Na
K
Intensity (km.mol-1)
0
500
1000
1500
2000
2500
3000
3500
4000
Wavenumber (cm-1)


(b) [M+-THF]
Li
Na
K
Intensity (km.mol-1)
0
500
1000
1500
2000
2500
3000
3500
4000
Wavenumber (cm-1)


(c) [M+-DEE]
Li
Na
K
Intensity (km.mol-1)
0
500
1000
1500
2000
2500
3000
3500
4000
Wavenumber (cm-1)


(d) [M+-MeOH]
Li
Na
K
Intensity (km.mol-1)
0
500
1000
1500
2000
2500
3000
3500
4000
Wavenumber (cm-1)

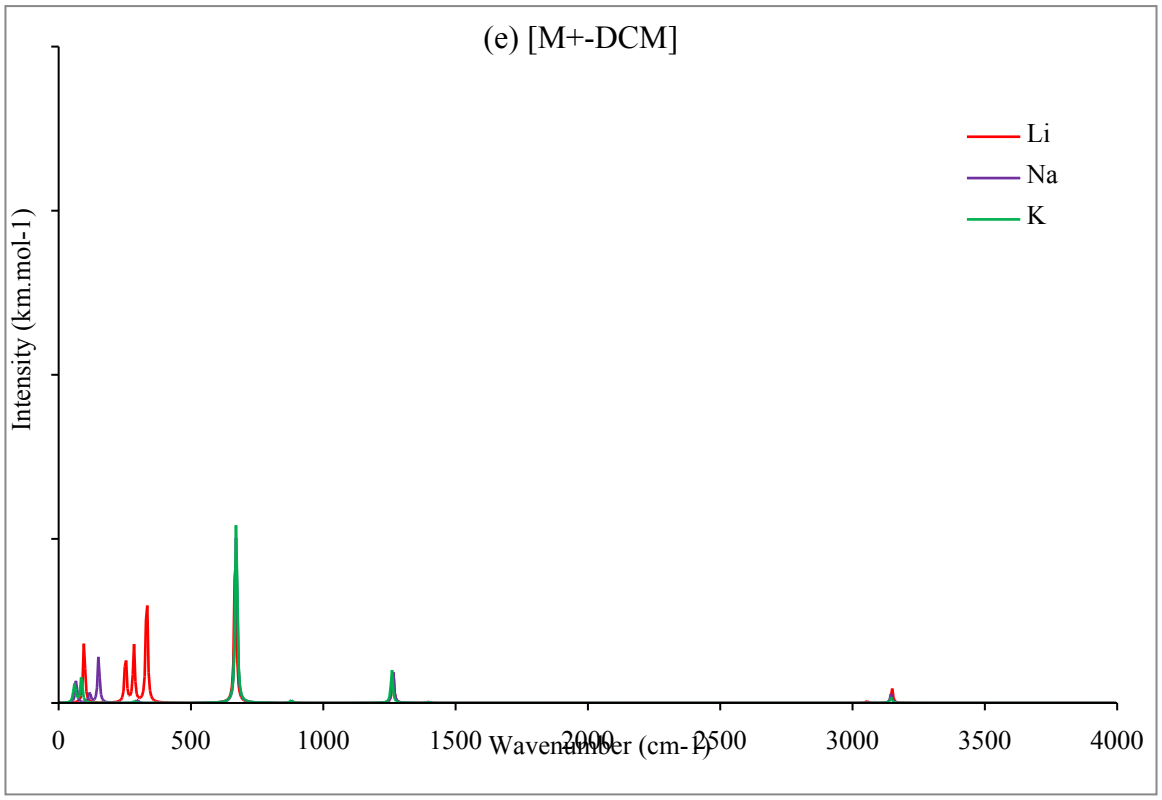


Figure S11: IR spectra of the [M^+-L] structures, obtained using the BP86/6-311G(d,p) method.

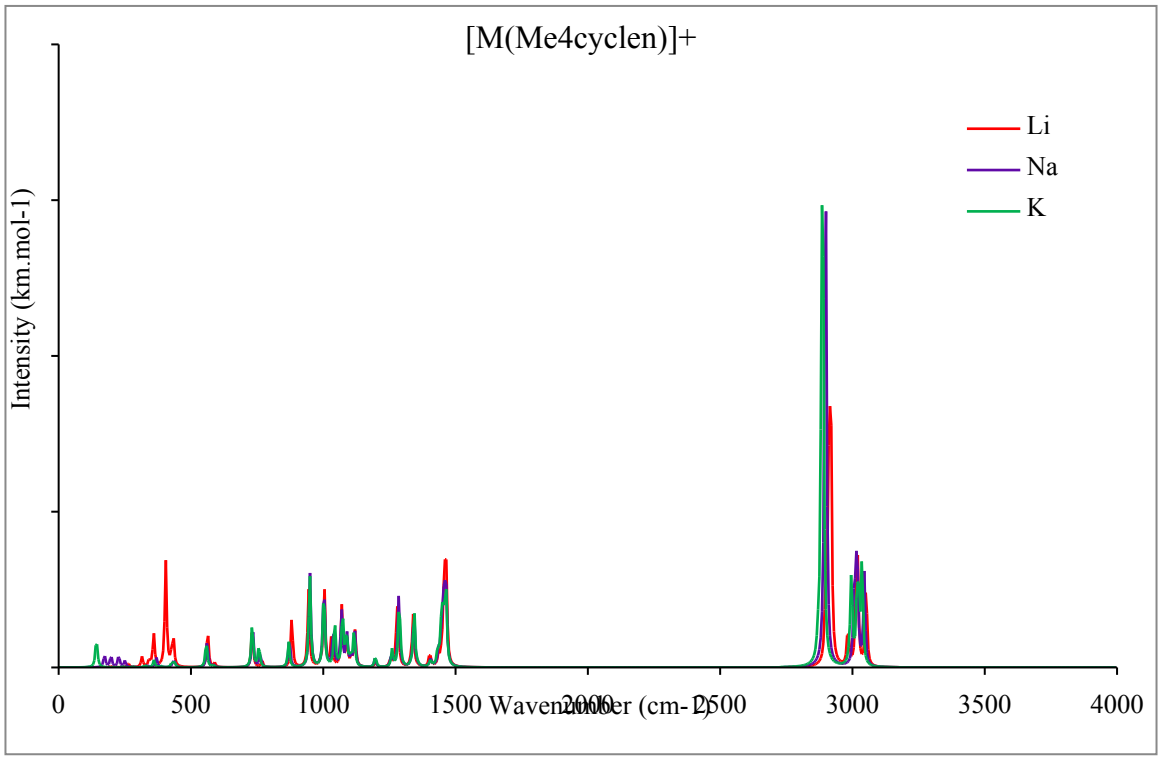
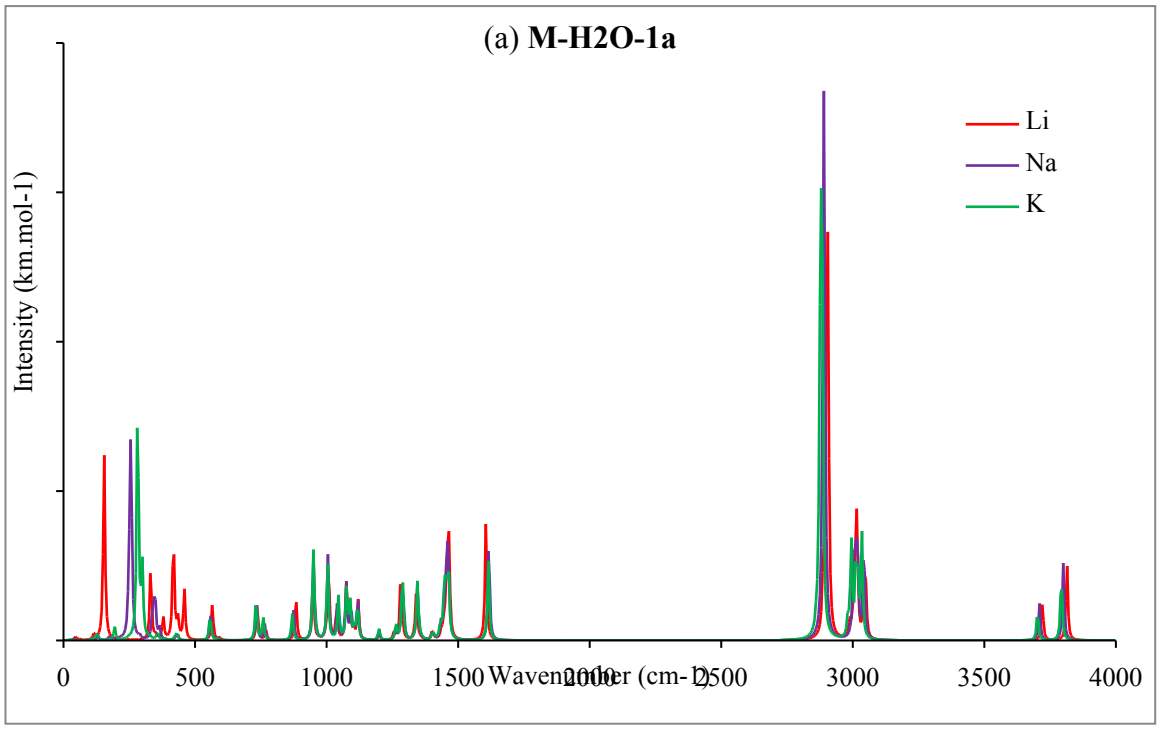
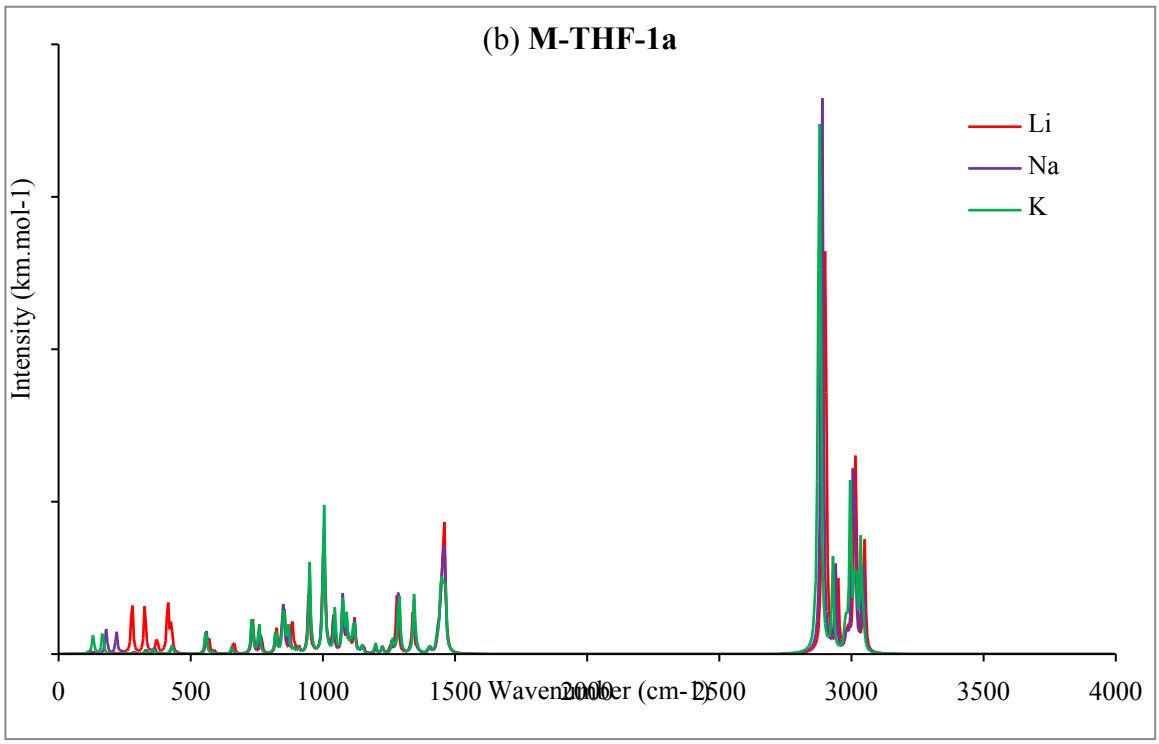
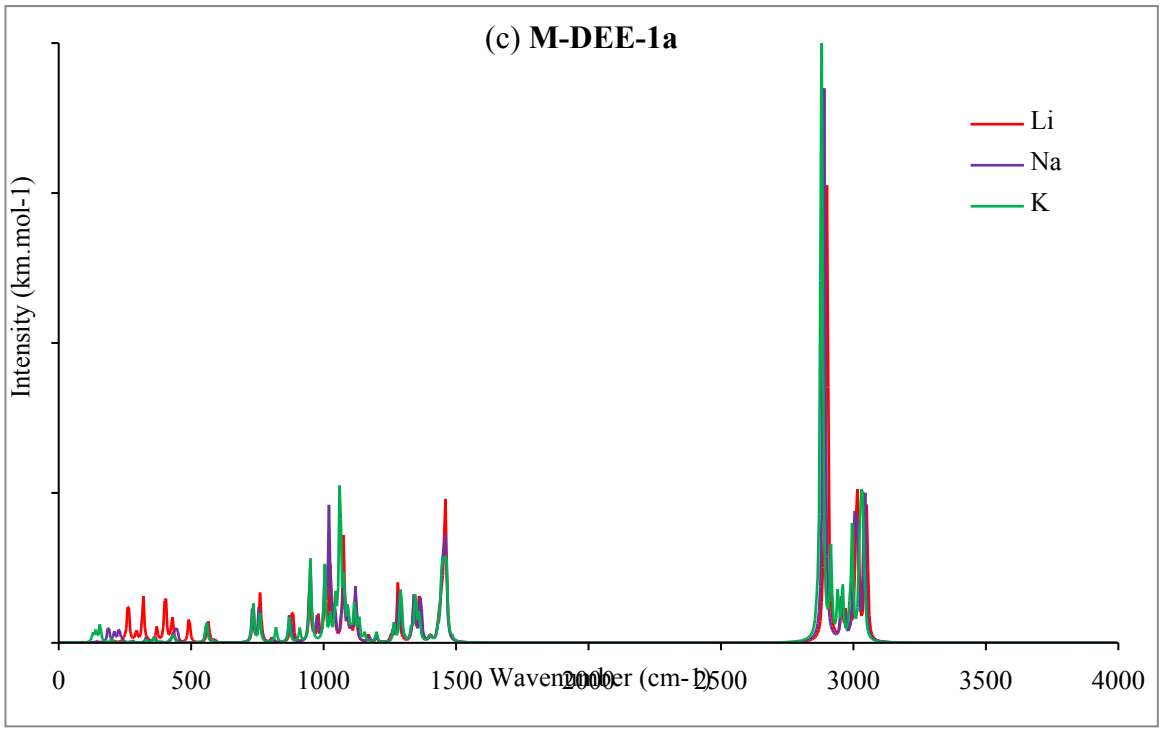
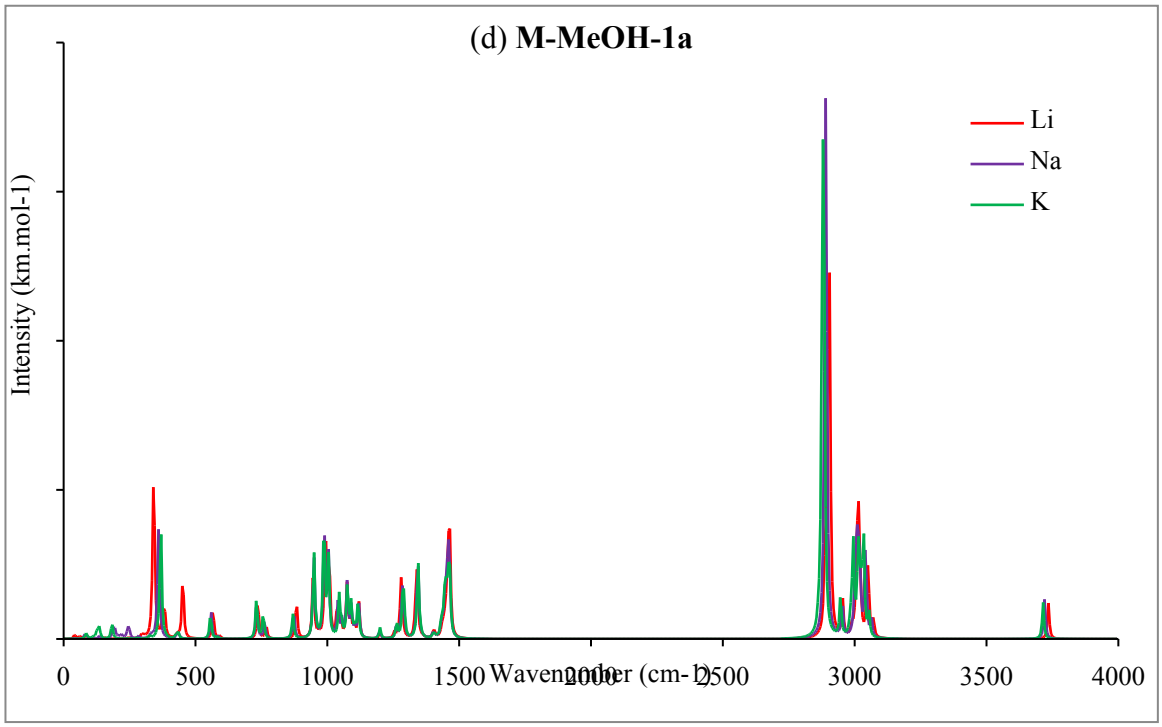


Figure S12: IR spectra of the [$M(Me_4cyclen)]^+$ structures, obtained using the BP86/6-311G(d,p) method.


(a) M-H2O-1a
Intensity (km.mol-1)
Li
Na
K
0
500
1000
1500
2000
2500
3000
3500
4000
Wavenumber (cm-1)


(b) M-THF-1a
Intensity (km.mol-1)
Li
Na
K
0
500
1000
1500
2000
2500
3000
3500
4000
Wavenumber (cm-1)


(c) M-DEE-1a
Li
Na
K
Intensity (km.mol-1)
0
500
1000
1500
2000
2500
3000
3500
4000
Wavenumber (cm-1)


(d) M-MeOH-1a
Li
Na
K
Intensity (km.mol-1)
0
500
1000
1500
2000
2500
3000
3500
4000
Wavenumber (cm-1)

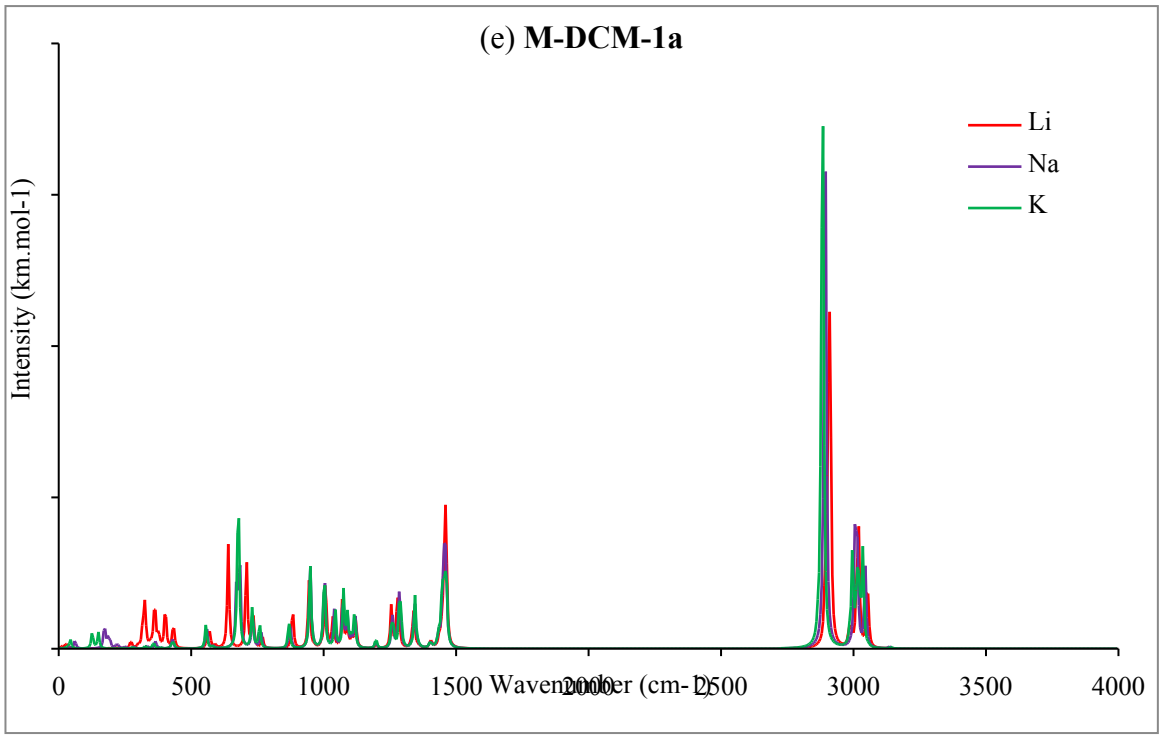


Figure S13: IR spectra of the lowest **M-L-1a** minimum energy structures, obtained using the BP86/6-311G(d,p) method.

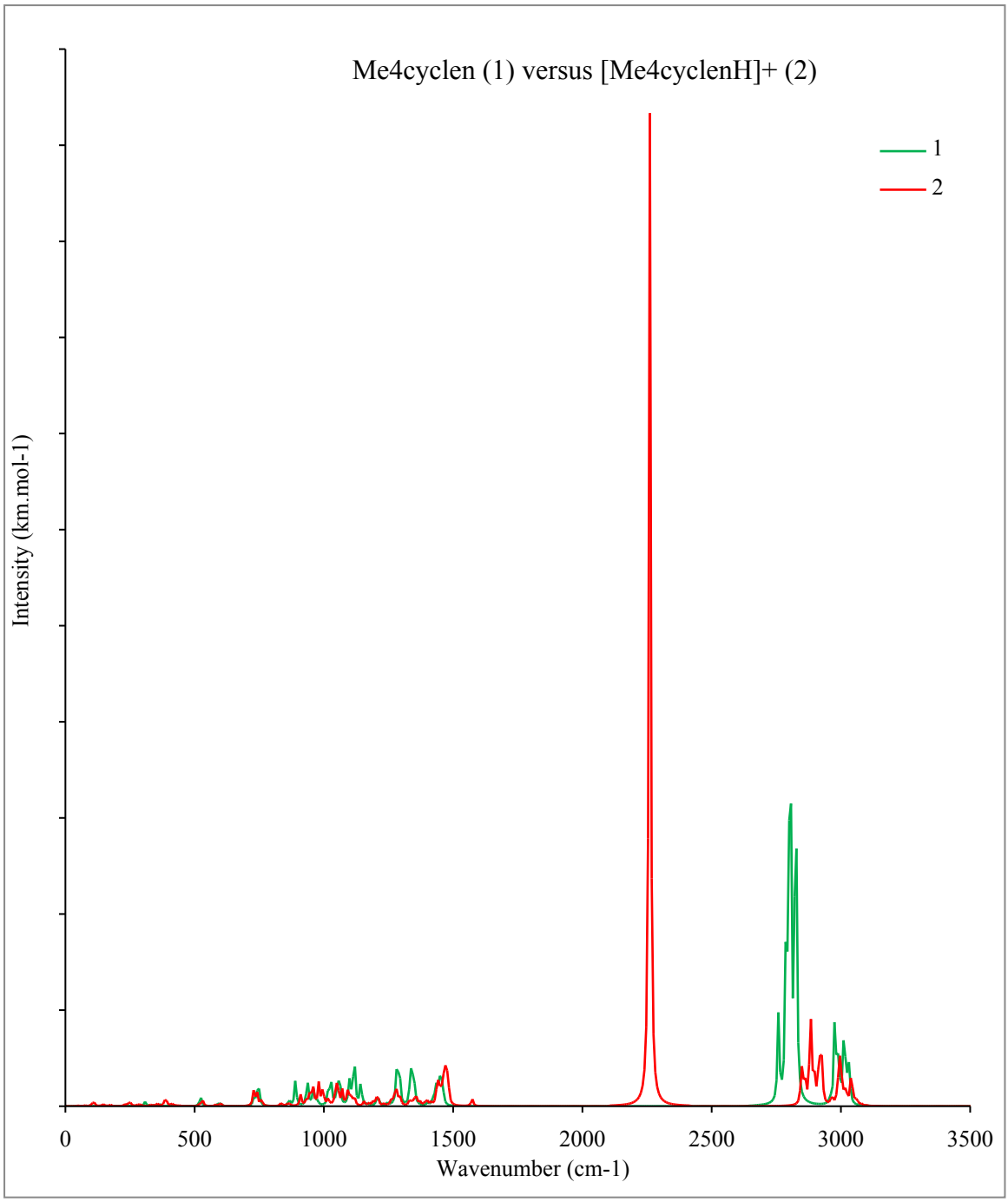


Figure S14: IR spectra of the Me_4cyclen and $[Me_4cyclenH]^+$ structures, obtained using the BP86/6-311G(d,p) method.

Table S12: Assignments of selected vibrational modes to the predicted IR spectra of [M^+-L] structures, obtained using the BP86/6-311G(d,p) method.

Vibrational modes	Wavenumber (cm^{-1})		
[M^+-H_2O]	Li	Na	K
OH_2 wagging	395	359	355
OH_2 rocking	521	443	388
M−O stretching	551	311	228
OH_2 scissoring (bending)	1643	1640	1637
O−H symmetrical stretching	3688	3698	3697
O−H asymmetrical stretching	3757	3774	3777
[M^+-THF]			
THF wagging	73	53	46
THF rocking	156	94	70
O wagging	186	153	137
M−O stretching	480	244	166
C−O−C asymmetrical stretching	824, 968	834, 978	840, 985
C−O−C symmetrical stretching	831	839	843
C−C stretching	907	908	908
C−C asymmetrical stretching	968	978	985
C−C symmetrical stretching	1027	1023	1020
CH_2 twisting	1146-1233	1143-1230	1143-1229
CH_2 wagging	1281-1348	1278-1349	1277-1349
CH_2 scissoring (bending)	1441-1476	1440-1477	1440-1479
CH_2 stretching	2974-3059	2957-3055	2947-3053
[M^+-DEE]	GG	GG	TT
DEE wagging	75	49	65
DEE rocking	143	96	69
O wagging	449	446	137
M−O stretching	574, 753	251, 753	141
C−O−C asymmetrical stretching	984	1000	908, 1046
C−O−C symmetrical stretching	753, 964	753, 968	815, 1017
C−C asymmetrical stretching	1067.3, 984	1064, 1000	908, 1054
C−C symmetrical stretching	1067.1, 964	1066, 968	1017
C−O−C rocking	1119	1119	1119
C−O−C bending	391, 1173	1171	1171
CH_2 rocking	753	753	792, 1153
CH_2 twisting	1263-1306	1264-1304	1254-1264
CH_2 wagging	1331-1373	1330-1372	1332-1398
CH_2 scissoring (bending)	1435-1467	1434-1468	1448-1485
CH_2 stretching	2970-3054	2964-3048	2932-3045
[M^+-MeOH]			
MeOH rocking	203	143	112
H wagging (attached to O)	411	398	391
M−O stretching	557	305	226
C−O stretching	942	963	970

O−H bending	1068	1064	1061
CH_2 twisting	1127	1127	1127
H−O−C bending	1349	1351	1350
CH_2 scissoring (bending)	1436-1464	1438-1466	1439-1466
CH_2 stretching	2985-3087	2972-3072	2963-3061
O−H stretching	3708	3713	3712
$[M^+$-DCM]			
DCM bending	96	66	59
Cl−C−Cl bending	284	297	286
M−Cl stretching	333	151	86
Cl−C−Cl symmetrical stretching	667	667	668
Cl−C−Cl asymmetrical stretching	668	671	672
CH_2 rocking	883	879	878
CH_2 twisting	1125	1132	1132
CH_2 wagging	1264	1263	1259
CH_2 scissoring (bending)	1398	1398	1399
CH_2 symmetrical stretching	3054	3055	3057
CH_2 asymmetrical stretching	3150	3146	3146

Table S13: Assignments of selected vibrational modes to the predicted IR spectra of $[M(Me_4cyclen)]^+$ and lowest $[M(Me_4cyclen)(L)]^+$ minimum energy structures, obtained using the BP86/6-311G(d,p) method.

Vibrational modes	Wavenumber (cm^{-1})		
$[M(Me_4cyclen)]^+$	Li	Na	K
CH_2 twisting	1231-1285	1232-1287	1234-1290
CH_2 wagging	1331-1369	1333-1381	1332-1381
CH_2 scissoring	1402-1467	1405-1465	1404-1465
C−H stretching	2898-3052	2887-3045	2868-3037
$[M(Me_4cyclen)(H_2O)]^+$			
CH_2 twisting	1232-1286	1237-1292	1236-1295
CH_2 wagging	1333-1374	1333-1383	1334-1380
CH_2 scissoring	1401-1467	1401-1464	1402-1465
C−H stretching	2887-3049	2874-3043	2860-3035

Table S14: Assignments of selected vibrational modes to the predicted IR spectra of lowest $[M(Me_4cyclen)(L)]^+$ minimum energy structures, obtained using the BP86/6-311G(d,p) method.

Vibrational modes	Wavenumber (cm^{-1})		
$[M(Me_4cyclen)(H_2O)]^+$	Li	Na	K
OH_2 wagging	154	257	282
OH_2 rocking	268	338, 348	299
M−O stretching	459	255	194
OH_2 scissoring (bending)	1606	1617	1615
O−H symmetrical stretching	3721	3710	3702

O−H asymmetrical stretching	3814	3800	3792
[M(Me$_4$cyclen)(THF)]$^+$			
THF wagging	51, 53	36	45
THF rocking	78	70	53
O wagging	131	118	113
M−O stretching	413	219	167
C−O−C bending	662	657	655
C−O−C asymmetrical stretching	845, 999	845, 1000	847, 1003
C−O−C symmetrical stretching	824, 853, 854	821, 851	853
C−C stretching	910, 1019	908, 1018	908, 1017
C−C symmetrical stretching	1019	1018	1017
CH_2 twisting	1141, 1216, 1225	1141, 1216, 1226	1143, 1221
CH_2 wagging	1274, 1318, 1342	1275, 1318, 1345	1276, 1323, 1350
CH_2 scissoring (bending)	1441-1480	1440-1480	1440-1481
CH_2 stretching	2948-3050	2940-3049	2929-3046
[M(Me$_4$cyclen)(DEE)]$^+$			
O wagging	428, 430	443	141
M−O stretching	403	227	156
C−O−C asymmetrical stretching	872, 1026, 1074	878, 1021	910
C−O−C symmetrical stretching	760, 804, 980	757, 809, 974	821, 1026
C−C asymmetrical stretching	872, 1026	878, 1021	910, 1062
C−C symmetrical stretching	980	974	1026, 1062
O−C−C bending	431	443	420
C−O−C rocking	763, 804, 1120	772, 809, 1021	792, 806
C−O−C bending	492	448	422
CH_2 rocking	1122, 1270, 1298	1122, 1172	1226, 1133, 1155
CH_2 twisting	1270, 1298	1268, 1305	1255, 1264
CH_2 wagging	1334, 1352, 1362	1330, 1356, 1365, 1367	1332, 1362, 1398
CH_2 scissoring (bending)	1428-1472	1430-1463	1443-1485
CH_2 stretching	2956-3052	2954-3045	2909-3042
[M(Me$_4$cyclen)(MeOH)]$^+$			
H wagging (attached to O)	296, 305, 340, 342	359, 360	368
M−O stretching	452	244	183
C−O stretching	992	988	987
O−H bending	1051	1056	1055
CH_2 twisting	1128	1128	1127
H−O−C bending	1335	1342, 1343, 1344	1343, 1344, 1345
CH_2 scissoring (bending)	1431-1466	1432-1465	1432-1465
CH_2 stretching	2955-3071	2953-3063	2946-3054

O−H stretching	3735	3721	3715
[M(Me_4cyclen)(DCM)]$^+$			
Cl−C−Cl bending	279	285	282
M−Cl stretching	272, 360, 363	173	150
Cl1−C stretching	640	672	–
Cl2−C stretching	709	683	–
Cl−C−Cl symmetrical stretching	–	–	674
Cl−C−Cl asymmetrical stretching	–	–	678
CH_2 rocking	874	879	876
CH_2 twisting	1137	1135	1135
CH_2 wagging	1253, 1256	1258, 1260	1257
CH_2 scissoring (bending)	1402, 1403	1402, 1404	1401, 1401
CH_2 symmetrical stretching	3050	3050	3056
CH_2 asymmetrical stretching	3135	3136	3141

Table S15: Assignments of selected vibrational modes to the predicted IR spectra of Me_4cyclen and [Me_4cyclenH]$^+$ structures, obtained using the BP86/6-311G(d,p) method.

Vibrational modes	Me_4cyclen	[Me_4cyclenH]$^+$
	Wavenumber (cm^{-1})	
CH_2 twisting	1102-1295	1102-1296
CH_2 wagging	1332-1370	1328-1373
CH_2 scissoring	1398-1463	1390-1480
C−H stretching	2758-3032	2847-3097
N−H wagging	–	1480, 1473
N−H bending	–	1573
N−H stretching	–	2260

Table S16: Calculated bond dissociation energies (kJ.mol^{-1}) of the lowest **M-L-2a** minimum energy structures.

	B3LYP/6-311G(d,p)		DF-LCCSD(T)/nZ //B3LYP/6-311G(d,p)		DF-LCCSD(T)-F12x[a]/nZ-F12x //B3LYP/6-311G(d,p)			
					n = D		n = T	
	ΔE^{ZPE}	$\Delta E^{ZPE+BSSE}$	n = D	n = T	x = a	x = b	x = a	x = b
Li-H_2O-2a	71.9	47.0	55.9	59.6	59.6	59.9	60.5	60.7
Li-THF-2a	63.9	50.0	77.0	75.4	77.5	78.1	77.9	78.1
Li-DEE-2a	39.1	25.7	71.0	59.0	61.6	62.2	62.8	63.0
Li-MeOH-2a	66.3	47.7	63.4	64.1	65.3	65.7	66.3	66.4
Li-DCM-2a	16.0	10.1	36.5	32.8	36.5	36.7	34.4	34.5
Na-H_2O-2a	73.9	51.4	50.9	57.2	55.4	55.6	57.2	57.3
Na-THF-2a	72.6	60.2	66.8	68.6	71.6	71.8	70.5	70.6
Na-DEE-2a	53.8	41.9	51.8	55.9	57.8	58.2	60.4	60.5
Na-MeOH-2a	70.1	53.7	57.0	60.8	60.3	60.5	61.5	61.6
Na-DCM-2a	26.2	20.0	39.7	40.9	42.1	42.4	42.1	42.3
K-H_2O-2a	59.4	43.2	41.9	40.2	45.3	45.4	42.4	42.5
K-THF-2a	58.7	49.7	53.6	47.5	53.9	53.9	50.7	50.8
K-DEE-2a	47.3	38.3	55.4	49.5	54.5	54.5	53.6	53.6
K-MeOH-2a	55.9	43.9	45.3	42.3	48.6	48.6	45.2	45.3
K-DCM-2a	23.8	19.6	33.8	29.8	35.2	35.3	33.1	33.2

[a] The 3*A ansatz with the (Fix,NoX) option was used; the MOLPRO default option is (Loc,Fix).

Discussion of ansatz options for the DF-LCCSD(T)-F12x calculations

The DF-LCCSD(T)-F12x calculations, the results of which are summarised in Tables 2 and S16, were carried out using the 3*A(Fix,NoX) ansatz in MOLPRO whereas the default ansatz in this code is 3*A(Loc,Fix). Attempts to calculate BDEs using the DF-LCCSD(T)-F12x method and double-ζ quality basis sets in conjunction with the MOLPRO default ansatz option (Loc,Fix) resulted in BDE values for the **M-DCM-1a** (**M-DCM-2a**) structures which are not comparable to the DF-LCCSD(T) values (see Table S17). Further, the BDE values of **M-DCM-1a** (**M-DCM-2a**) (M = Li, K) are negative with the default ansatz option but are positive with the 3*A(Fix,NoX) ansatz. Correlating the $(n-1)s^2$ and $(n-1)p^6$ core electrons of the Cl atoms and using the (Loc,Fix) ansatz option results in even more negative BDE values as is observed for the loss of DCM from **Li-DCM-1a** (**Li-DCM-2a**) (see Table S17). The DF-LCCSD(T)-F12x/DZ-F12 BDEs obtained using the default 3*A(Loc,Fix) ansatz for the loss of *O*-donor ligands from the **M-L-1a** (**M-L-2a**) structures (M = Li, Na, and L = H_2O, THF, DEE, MeOH) are comparable to those obtained using the 3*A(Fix,NoX) ansatz, with the latter being slightly higher than the former. The maximum difference in BDEs calculated with the two ansatz options for *O*-containing **M-L-1a** (**M-L-2a**) structures is 3.5 $kJ.mol^{-1}$ (see Table S17 and Figure S15). This trend is also expected for the **K-L-1a** (**K-L-2a**) complexes with *O*-donor ligands although no calculations have been carried out for these ions using the default 3*A(Loc,Fix) ansatz. It appears that the default (Loc,Fix) ansatz option yields reasonable BDEs for all $[M(Me_4cyclen)(L)]^+$ complexes, for M = Li, Na, and K, except for L = DCM, and the problem is associated with the way Cl atoms are treated with this ansatz option. The 3*A(Fix,NoX) ansatz does not suffer from this problem. The (Fix,NoX) option is therefore recommended, although it needs to be tested on a wider set of molecules composed of other elements than those involved in this work.

Discussion of basis set effects on the DF-LCCSD(T) and DF-LCCSD(T)-F12x calculations

The (Fix,NoX) ansatz option was employed in all the DF-LCCSD(T)-F12x/nZ-F12x calculations (x = a, b and n = D, T) for the purposes of investigating basis set effects. The dependence of the calculated BDEs on the methods and basis sets used in this work are depicted in Figures S16 and S17 (with relevant BDE values provided in Tables 2 and S16).

Firstly, the geometry effects on the BDE values obtained from the two functionals used are relatively small (within 4.0 kJ.mol^{-1}), except for **Li-THF-1a** (**Li-THF-2a**) and **Na-DEE-1a** (**Na-DEE-2a**) at the DF-LCCSD(T)/DZ and DF-LCCSD(T)-F12/TZ-F12x levels, respectively, where the energy differences are 5.4 kJ.mol^{-1} [DF-LCCSD(T)/DZ//B3LYP/6-311G(d,p) – DF-LCCSD(T)/DZ//BP86/6-311G(d,p)] and 4.7 kJ.mol^{-1} [DF-LCCSD(T)-F12/TZ-F12x//B3LYP/6-311G(d,p) – DF-LCCSD(T)-F12/TZ-F12x//BP86/6-311G(d,p)]. Secondly, the DF-LCCSD(T)-F12a and DF-LCCSD(T)-F12b methods used with the nZ-F12x basis sets (n = D or T) provide comparable BDE values, with the DF-LCCSD(T)-F12b values being only slightly higher than the DF-LCCSD(T)-F12a values (maximum difference of 0.6 and 0.2 kJ.mol^{-1} with the DZ-F12x and TZ-F12x basis sets, respectively). Thirdly, the basis set effects on going from (i) DF-LCCSD(T)/DZ → DF-LCCSD(T)/TZ, (ii) DF-LCCSD(T)/TZ → DF-LCCSD(T)-F12a/DZ-F12a, (iii) DF-LCCSD(T)/TZ → DF-LCCSD(T)-F12b/DZ-F12b, (iv) DF-LCCSD(T)-F12a/DZ-F12a → DF-LCCSD(T)-F12a/TZ-F12a, and (v) DF-LCCSD(T)-F12b/DZ-F12b → DF-LCCSD(T)-F12b/TZ-F12b have been analysed and these are depicted in Figures S18 and S19. The basis set effects appear to be much larger with the DF-LCCSD(T) method (DZ → TZ) than with the DF-LCCSD(T)-F12x methods (DZ-F12x → TZ-F12x). The DZ-F12x and TZ-F12x values (DF-LCCSD(T)-F12x methods) are close to each other with a maximum difference of 3.4 kJ.mol^{-1}, while the difference between the DZ and TZ values (DF-LCCSD(T) method) is as large as 12.0 kJ.mol^{-1} for **Li-DEE-2a**. Therefore, it can be concluded that (i) using the DF-LCCSD(T)-F12x methods with a DZ-F12x quality basis set is sufficient, (ii) the DF-LCCSD(T)-F12x methods are preferred to the DF-LCCSD(T) method for relatively large molecular systems, and (iii) the DF-LCCSD(T) method with a DZ basis set is inadequate. Also, it is significant that a consistent trend in basis set convergence (for example, in the direction of changes in BDEs as the size of the basis set increases) is not observed since the basis set effects are case (or molecule) dependent. Further investigations on basis set effects with the DF-LCCSD(T) and DF-LCCSD(T)-F12x methods are needed on other molecular systems to establish if this result is general. More specifically, comparing the DF-LCCSD(T)-F12x and DF-LCCSD(T) methods, then if the density-fitting (DF) and local (L) approximations

are ignored, DF-LCCSD(T)-F12x should be the higher level of theory as the F12 method is explicitly correlated. It is also known that DF-LCCSD(T)-F12x/DZ-F12 computed values are expected to be as good as DF-LCCSD(T)/AVQZ results and a trend of BDE values of DF-LCCSD(T)/DZ → DF-LCCSD(T)/TZ → DF-LCCSD(T)-F12x/DZ-F12 (~ DF-LCCSD(T)/AVQZ) is anticipated. Inspection of the BDE values in Table 2 (columns 4-7) and Figures S16 and S18 shows that this trend is reasonably well observed in all the M = Li and Na cases, apart from **Li-DEE-1a** and **Na-H_2O-1a**, and in the M = K cases, apart from **K-THF-1a**, **K-DEE-1a**, and **K-DCM-1a**, although in all cases where a smooth trend is not observed the deviations are small (roughly within the commonly accepted chemical uncertainty for relative energies of 4.2 kJ.mol^{-1}).

The main conclusions of this section are, therefore:

(i) The geometry effects on the BDEs from the two functionals used are negligibly small.

(ii) In DF-LCCSD(T)-F12x calculations with MOLPRO, the (Fix,NoX) ansatz option is necessary, as the default (Loc,Fix) option gives rise to errors in relative energies for chlorine-containing molecules.

(iii) Calculations with the DF-LCCSD(T) method with a DZ basis set are inadequate, but DF-LCCSD(T)-F12x calculations with a DZ-F12 basis set are expected to be reliable and give accurate relative energies. This latter method is recommended for calculations of BDEs for the type of complexes considered in this work.

Summarising, for lower level geometry optimisation calculations, some commonly used functionals, such as BP86 or B3LYP, used in the present study, appear to be adequate, while for improved relative electronic energies, the DF-LCCSD(T)-F12x methods with basis sets of at least DZ-F12 quality are required, though it should be noted that the (Fix,NoX) ansatz option should be employed in the DF-LCCSD(T)-F12x calculations instead of the default (Loc,Fix) option.

Table S17: Comparison between the DF-LCCSD(T)-F12x/DZ-F12//BP86/6-311G(d,p) and DF-LCCSD(T)-F12x/DZ-F12//B3LYP/6-311G(d,p) bond dissociation energies (kJ.mol^{-1}) obtained using two different ansatz options for the lowest minimum energy [M(Me$_4$cyclen)(L)]$^+$ for the *O*-containing ligands.

	DF-LCCSD(T)-F12a/DZ-F12a //BP86/6-311G(d,p)		Differences	DF-LCCSD(T)-F12b/DZ-F12b //BP86/6-311G(d,p)		Differences
Ansatz options	Fix,NoX	Loc,Fix		Fix,NoX	Loc,Fix	
Li-H_2O-1a	59.3	55.8	+3.5	59.5	56.0	+3.5
Li-THF-1a	76.8	73.7	+3.1	77.3	74.2	+3.1
Li-DEE-1a	59.7	56.8	+2.9	60.2	57.4	+2.8
Li-MeOH-1a	64.8	62.1	+2.7	65.1	62.4	+2.7
Li-DCM-1a	33.6	-8.7 (-93.6[a])	–	33.9	-8.4 (-93.3 [a])	–
Na-H_2O-1a	55.5	52.9	+2.6	55.7	53.1	+2.6
Na-THF-1a	70.6	68.5	+2.1	70.8	68.8	+2.0
Na-DEE-1a	56.4	54.6	+1.8	56.7	54.9	+1.8
Na-MeOH-1a	60.0	58.2	+1.8	60.1	58.3	+1.8
Na-DCM-1a	40.2	15.7	–	40.5	16.0	–
K-DCM-1a	31.5	-6.3	–	31.5	-6.3	–
	DF-LCCSD(T)-F12a/DZ-F12a //B3LYP/6-311G(d,p)		Differences	DF-LCCSD(T)-F12b/DZ-F12b //B3LYP/6-311G(d,p)		Differences
Ansatz options	Fix,NoX	Loc,Fix		Fix,NoX	Loc,Fix	
Li-H_2O-2a	59.6	56.2	+3.4	59.9	56.4	+3.5
Li-THF-2a	77.5	74.4	+3.1	78.1	75.0	+3.1
Li-DEE-2a	61.6	58.8	+2.8	62.2	59.4	+2.8
Li-MeOH-2a	65.3	62.5	+2.8	65.7	62.9	+2.8
Li-DCM-2a	36.5	-4.7 (-86.2[a])	–	36.7	-4.5 (-86.0[a])	–
Na-H_2O-2a	55.4	52.9	+2.5	55.6	53.0	+2.6
Na-THF-2a	71.6	69.5	+2.1	71.8	69.8	+2.0
Na-DEE-2a	57.8	56.0	+1.8	58.2	56.3	+1.9
Na-MeOH-2a	60.3	58.5	+1.8	60.5	58.6	+1.9
Na-DCM-2a	42.1	14.6	–	42.4	14.9	–
K-DCM-2a	35.2	-5.1	–	35.3	-5.0	–

[a] The (n-1)s^2 and (n-1)p^6 core electrons of Cl atom were correlated.

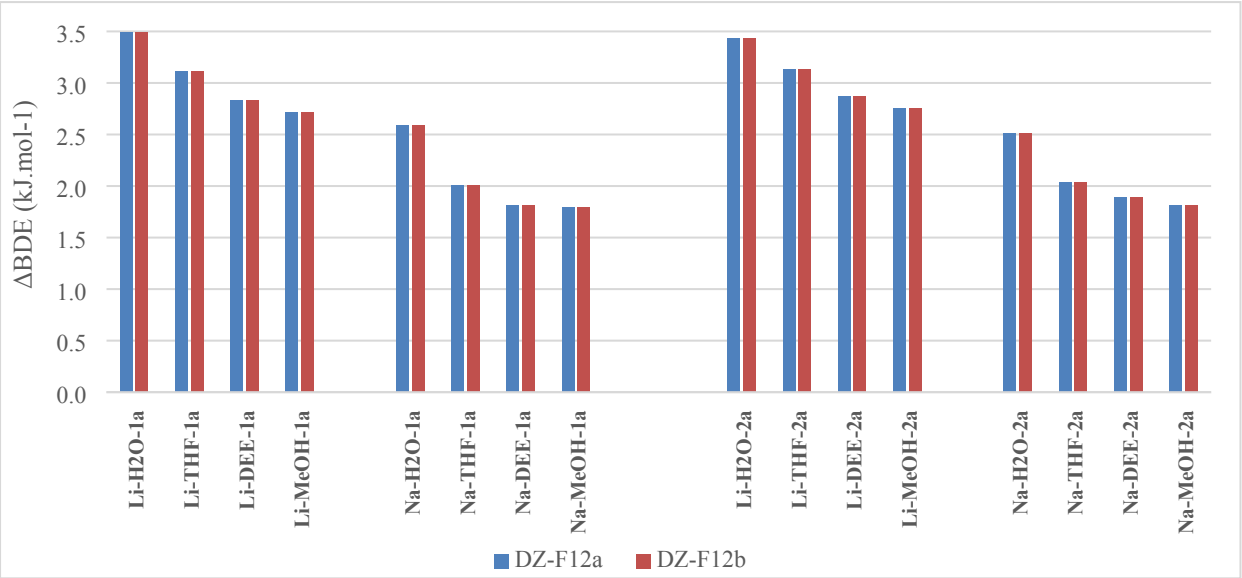


Figure S15: The bond dissociation energy differences between the two ansatz options [ΔBDE (in kJ.mol^{-1}) = E(Fix,NoX) – E(Loc,Fix)], obtained using the DF-LCCSD(T)-F12x/DZ-F12x//BP86/6-311G(d,p) and DF-LCCSD(T)-F12x/DZ-F12x//B3LYP/6-311G(d,p) methods (x = a or b) for the lowest minimum energy structures **M-L-1a** and **M-L-2a**, respectively, for the *O*-containing ligands.

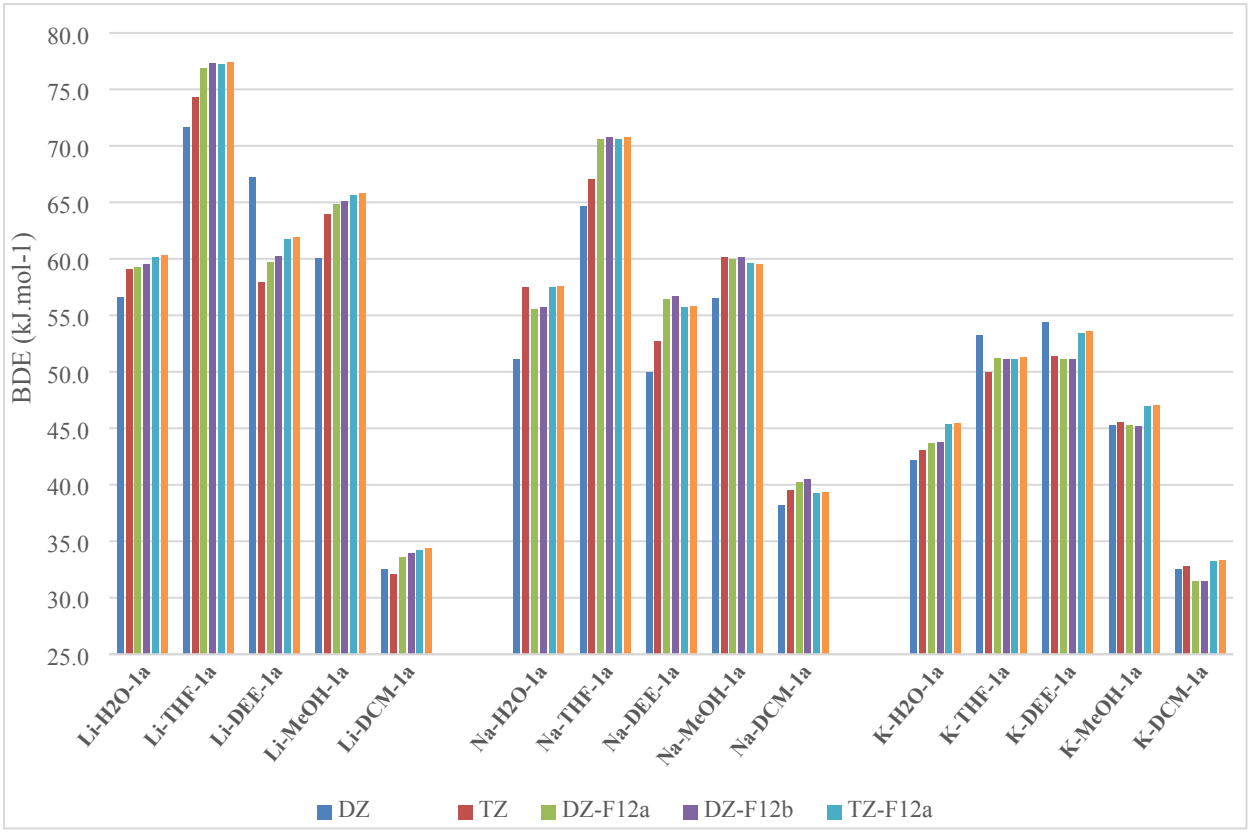


Figure S16: The bond dissociation energies (kJ.mol^{-1}) of the lowest $[M(Me_4cyclen)(L)]^+$ minimum energy structures calculated using the DF-LCCSD(T)/nZ//BP86/6-311G(d,p) and DF-LCCSD(T)-F12x/nZ-F12x//BP86/6-311G(d,p) methods (n = D or T and x = a or b). In the DF-LCCSD(T)-F12x calculations, the (Fix,NoX) ansatz option was used.

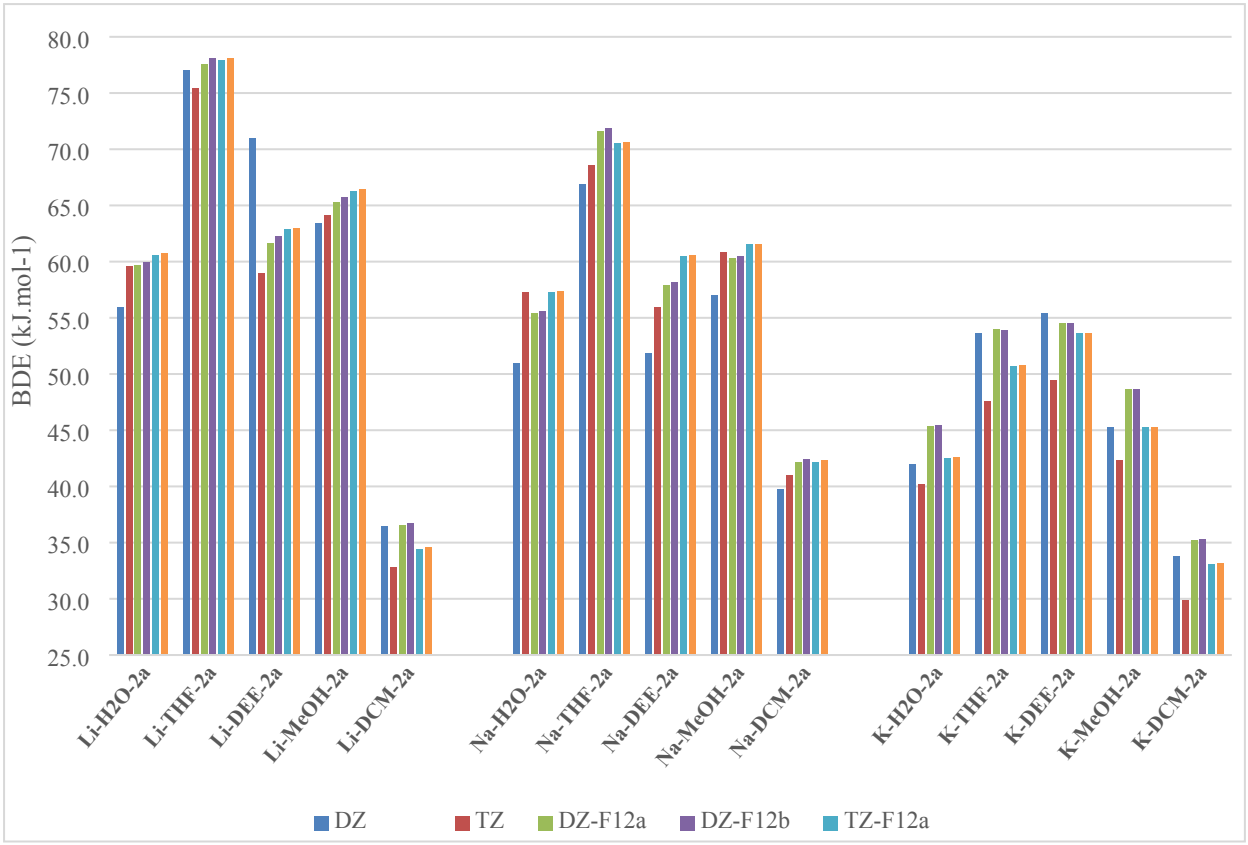


Figure S17: The bond dissociation energies (kJ.mol^{-1}) of the lowest [M(Me$_4$cyclen)(L)]$^+$ minimum energy structures calculated using the DF-LCCSD(T)/nZ//B3LYP/6-311G(d,p) and DF-LCCSD(T)-F12x/nZ-F12x//B3LYP/6-311G(d,p) methods (n = D or T and x = a or b). In the DF-LCCSD(T)-F12x calculations, the (Fix,NoX) ansatz option was used.

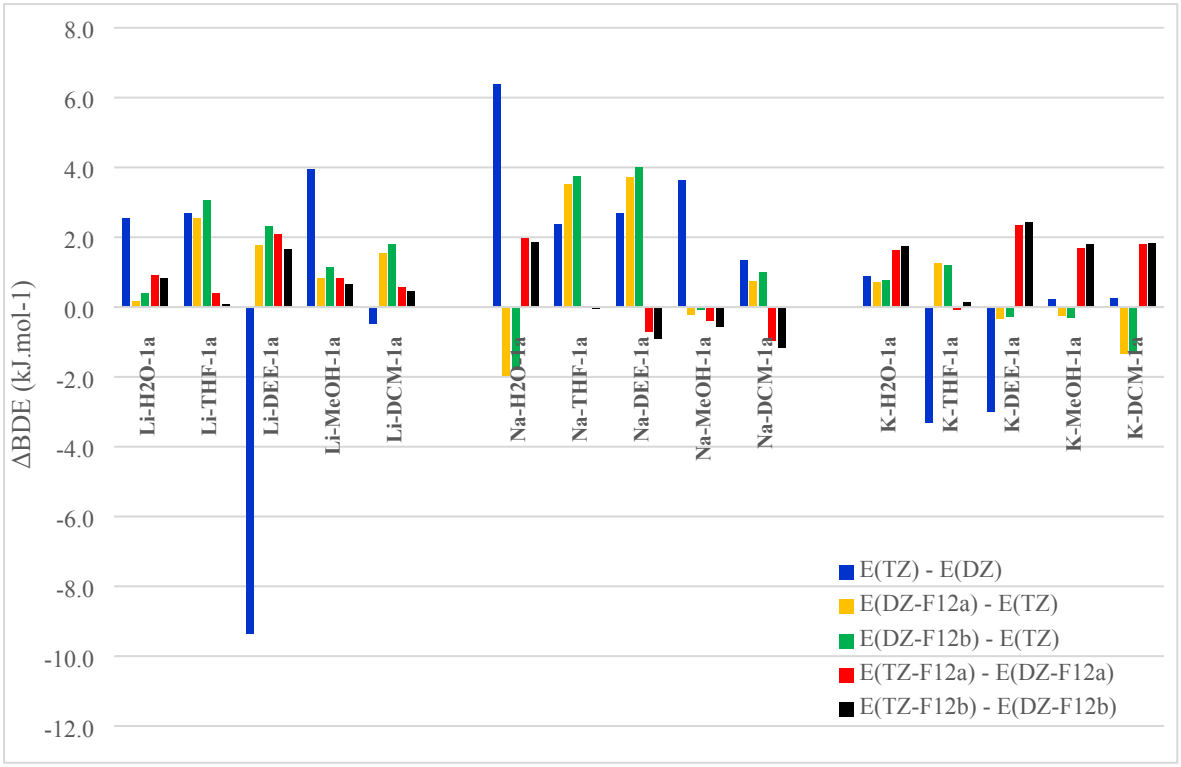


Figure S18: The bond dissociation energy differences (ΔBDE in kJ.mol^{-1}) between different methods and basis sets used in this work for the lowest [M(Me$_4$cyclen)(L)]$^+$ minimum energy structures **M-L-1a**. In the DF-LCCSD(T)-F12x calculations, the (Fix,NoX) ansatz option was used. In this Figure, E(DZ), E(TZ), E(DZ-F12x), and E(TZ-F12x) stand for DF-LCCSD(T)/DZ, DF-LCCSD(T)/TZ, DF-LCCSD(T)-F12x/DZ-F12x, and DF-LCCSD(T)-F12x/TZ-F12x (x = a or b), respectively.

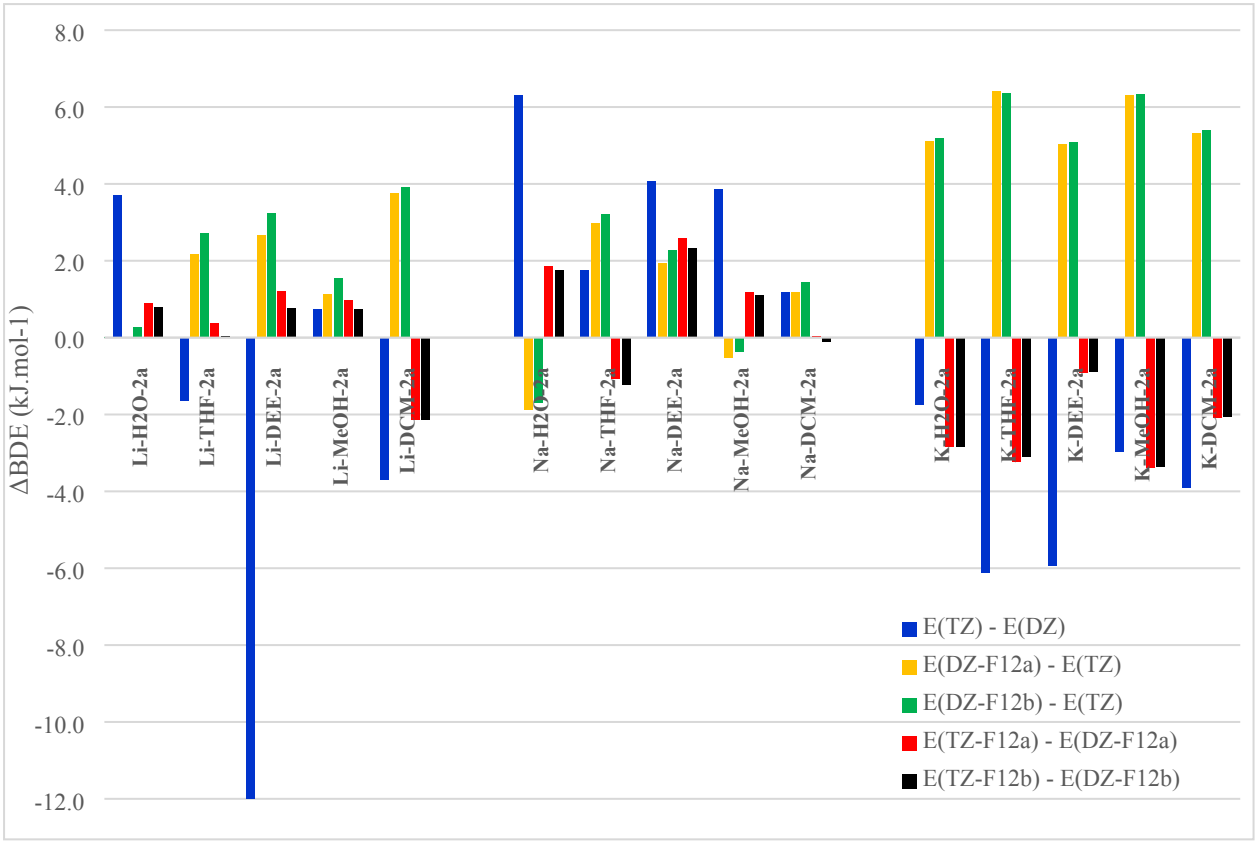
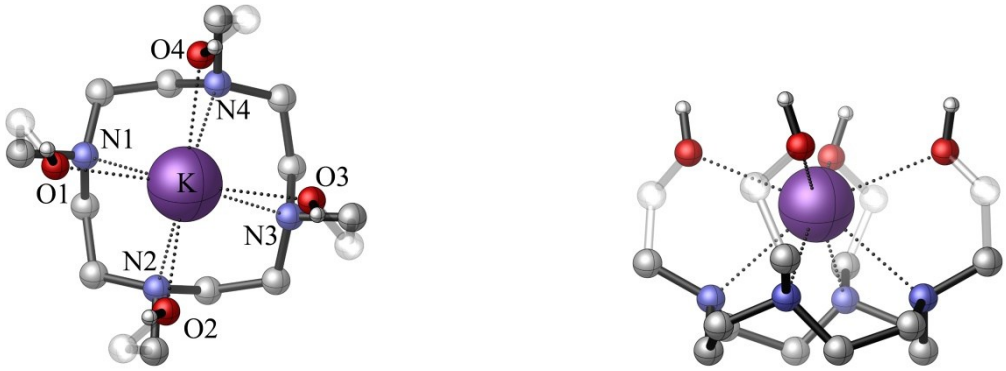


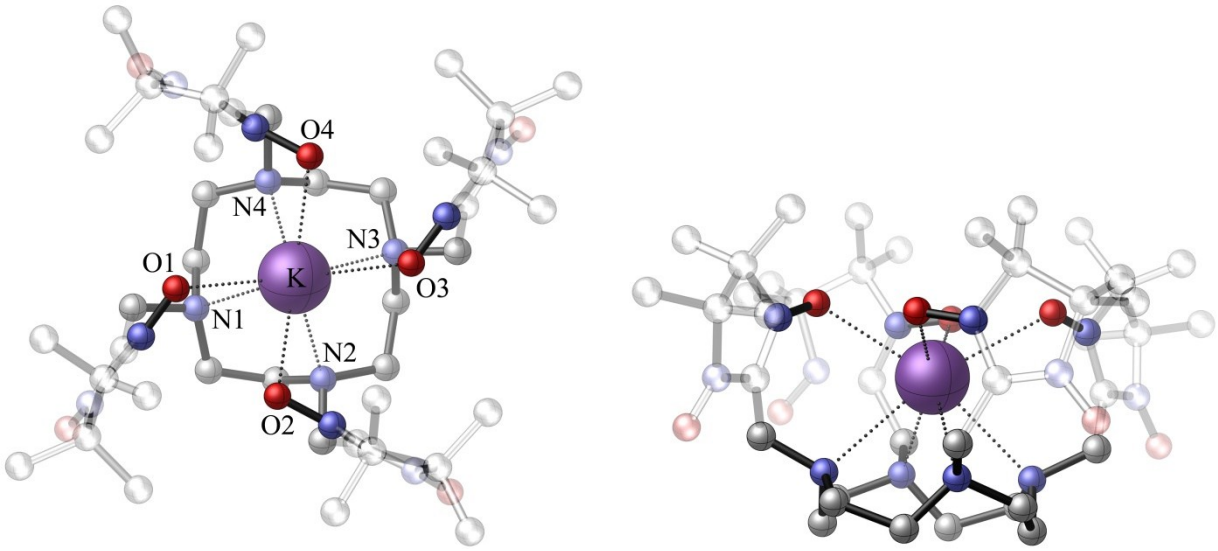
Figure S19: The bond dissociation energy differences (ΔBDE in kJ.mol^{-1}) between different methods and basis sets used in this work for the lowest [M(Me$_4$cyclen)(L)]$^+$ minimum energy structures **M-L-2a**. In the DF-LCCSD(T)-F12x calculations, the (Fix,NoX) ansatz option was used.



Top view Side view

(a) [K{(2-hydroxyethyl)$_4$cyclen)}]$^+$, (C_4 symmetry)

(Combination of K^+ and cyclen derivative **1c**; Scheme 1)



Top view Side view

(b) [K{(4,4,5,5-tetramethylimidazolin-1-oxyl-3-oxide-CH_2)$_4$cyclen}]$^+$, (C_2 symmetry)

(Combination of K^+ and cyclen derivative **1d**; Scheme 1)

Figure S20: Optimised K^+ complexes of cyclen derivatives **1c** (a) and **1d** (b) obtained using the BP86/6-311G(d,p) method. The symmetry of each structure is provided. Selected H atoms are omitted for clarity.

Table S18: Selected bond distances and bond angles of the K^+ complexes of cyclen derivatives **1c** (a) and **1d** (b), obtained using the BP86/6-311G(d,p) and B3LYP/6-311G(d,p) methods.

(a) K^+ complexes of cyclen derivative **1c**								
	Bond distances (Å)							
	K–N1	K–N2	K–N3	K–N4	K–O1	K–O2	K–O3	K–O4
BP86		2.931				2.820		
B3LYP		2.937				2.796		
Experiment[a]	2.832	2.903	2.909	2.869	2.790	2.759	2.806	2.803
	Bond angles (°)							
	N1–K–N4	N1–K–N2	N2–K–N3	N3–K–N4	O1–K–O4	O1–K–O2	O2–K–O3	O3–K–O4
BP86		65.0				81.8		
B3LYP		64.9				81.9		
Experiment[b]	66.0	64.8	64.2	64.4	85.8	73.9	91.7	73.2
(b) K^+ complexes of cyclen derivative **1d**								
	Bond distances (Å)							
	K–N1	K–N2	K–N3	K–N4	K–O1	K–O2	K–O3	K–O4
BP86	3.016	3.017	3.016	3.017	2.835	2.840	2.835	2.840
B3LYP	3.014	3.019	3.014	3.019	2.810	2.809	2.810	2.809
Experiment[a]	2.943(3)	2.986(2)	3.031(2)	2.964(2)	2.778(2)	2.803(2)	2.715(2)	2.776(2)
	Bond angles (°)							
	N1–K–N4	N1–K–N2	N2–K–N3	N3–K–N4	O1–K–O4	O1–K–O2	O2–K–O3	O3–K–O4
BP86	62.5	63.1	62.5	63.1	65.6	87.5	65.6	87.5
B3LYP	62.4	63.2	62.4	63.2	62.6	90.6	62.6	90.6
Experiment[b]	63.50(6)	63.10(6)	61.92(6)	62.10(6)	68.83(6)	83.83(6)	71.99(6)	85.84(6)

[a,b] Correspond to the reported crystal structures $[K\{(2\text{-hydroxyethyl})_4\text{cyclen}\}]^{+}$[S34a] and $[K\{(4,4,5,5\text{-tetramethylimidazolin-1-oxyl-3-oxide-CH}_2)_4\text{cyclen}\}]^{+}$,[S34b] respectively.

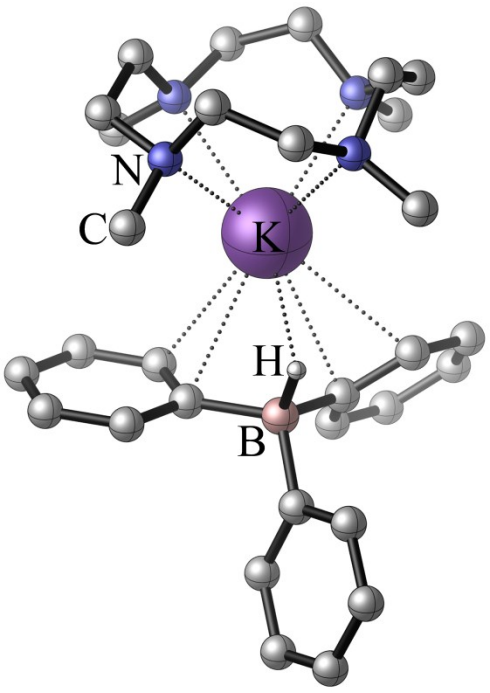


Figure S21: BP86/6-311G(d,p) optimised geometry of the [K(Me_4cyclen)][$HBPh_3$] complex. The experimental structure was obtained by Okuda et al.[S53]

Table S19: Selected geometrical parameters of the [K(Me_4cyclen)][$HBPh_3$] complex.

	Experiment[a]	Theory	
		BP86/6-311G(d,p)	B3LYP/6-311G(d,p)
Bond distances (Å)			
K1–N1	2.837(7)	2.927	2.939
K1–N2	2.858(7)	2.919	2.915
K1–N3	2.791(7)	2.881	2.886
K1–N4	2.826(6)	2.952	2.959
B1–C13	1.642(11)	1.644	1.646
B1–C19	1.644(12)	1.640	1.642
B1–C25	1.636(11)	1.634	1.632
K1···H1	2.73(7)	2.616	2.595
K1···C13	3.148(8)	3.152	3.203
K1···C14	3.122(8)	3.202	3.211
K1···C19	3.280(7)	3.201	3.209
K1···C20	3.190(8)	3.290	3.324
Bond angles (°)			
N1–K1–N2	63.2(2)	64.6	64.4
N2–K1–N3	65.4(2)	65.0	65.1
N3–K1–N4	65.3(2)	64.8	64.6
N4–K1–N1	65.3(2)	63.8	63.6
Torsion (°)			
N1–C1–C2–N2	62(2)	65.2	64.9
N2–C3–C4–N3	64(2)	64.7	64.7
N3–C5–C6–N4	62(2)	65.2	65.1
N4–C7–C8–N1	68(2)	63.6	63.7
B1–C13–C14–C15	-178.7(7)	-177.4	-176.7
B1–C13–C18–C17	179.5(7)	177.4	176.8
B1–C19–C20–C21	-179.9(6)	176.3	176.0
B1–C19–C24–C23	179.8(6)	-176.7	-176.1

[a] Correspond to the reported crystal structures [K(Me_4cyclen)][$HBPh_3$][S53]

Table S20: Cartesian coordinates (in Å) and total electronic energies (in Hartree) of all stationary point obtained using the BP86/6-311G(d,p) method.

Species	Total Electronic Energy (Hartree)	Atom	Coordinates		
1. **Li-H_2O-1a**	-777.1542899	C	-0.3403010	3.1963370	0.8567770
		H	-0.3805460	4.1841390	0.3526490
		H	0.4140700	3.2492970	1.6561840
		H	-1.3195770	3.0136560	1.3233790
		C	-3.1833730	-0.3342590	0.8634910
		H	-4.1745240	-0.3792610	0.3664510
		H	-3.2269860	0.4218020	1.6608160
		H	-2.9928470	-1.3075320	1.3383220
		C	0.3403010	-3.1963370	0.8567770
		H	-0.4140700	-3.2492970	1.6561840
		H	1.3195770	-3.0136560	1.3233790
		H	0.3805460	-4.1841390	0.3526490
		C	3.1833730	0.3342590	0.8634910
		H	4.1745240	0.3792610	0.3664510
		H	3.2269860	-0.4218020	1.6608160
		H	2.9928470	1.3075320	1.3383220
		C	-1.0195440	1.9952650	-1.1480440
		H	-0.5934620	1.3942180	-1.9677480
		H	-1.2496840	2.9923380	-1.5813990
		C	-2.3209850	1.3500180	-0.6583100
		H	-3.0534980	1.3257110	-1.4922960
		H	-2.7735540	1.9774670	0.1253450
		C	-1.9964360	-1.0247470	-1.1461320
		H	-1.3986150	-0.6056940	-1.9720870
		H	-2.9950070	-1.2589330	-1.5741180
		C	-1.3521130	-2.3237590	-0.6486160
		H	-1.3300790	-3.0622050	-1.4771190
		H	-1.9791580	-2.7685200	0.1398740
		C	1.0195440	-1.9952650	-1.1480440
		H	0.5934620	-1.3942180	-1.9677480
		H	1.2496840	-2.9923380	-1.5813990
		C	2.3209850	-1.3500180	-0.6583100
		H	3.0534980	-1.3257110	-1.4922960
		H	2.7735540	-1.9774670	0.1253450
		C	1.9964360	1.0247470	-1.1461320
		H	1.3986150	0.6056940	-1.9720870
		H	2.9950070	1.2589330	-1.5741180
		C	1.3521130	2.3237590	-0.6486160
		H	1.3300790	3.0622050	-1.4771190
		H	1.9791580	2.7685200	0.1398740

		N	0.0000000	2.1014710	-0.0754660
		N	-2.0972860	0.0010340	-0.0808300
		N	0.0000000	-2.1014710	-0.0754660
		N	2.0972860	-0.0010340	-0.0808300
		O	0.0000000	0.0000000	2.7547600
		Li	0.0000000	0.0000000	0.7459920
		H	-0.1570310	0.7563670	3.3427980
		H	0.1570310	-0.7563670	3.3427980
2. **Li-THF-1a**	-933.208942	C	3.1709350	0.0186620	0.0980580
		H	4.1658500	-0.0693500	-0.3860160
		H	3.1094650	-0.7187890	0.9115500
		H	3.0979610	1.0204130	0.5452810
		C	0.0000000	3.3154660	-0.0180320
		H	0.0556450	4.2662890	-0.5884330
		H	0.7575920	3.3450180	0.7784040
		H	-0.9884150	3.2600120	0.4601160
		C	-3.1709350	-0.0186620	0.0980580
		H	-3.1094650	0.7187890	0.9115500
		H	-3.0979610	-1.0204130	0.5452810
		H	-4.1658500	0.0693500	-0.3860160
		C	0.0000000	-3.3154660	-0.0180320
		H	-0.0556450	-4.2662890	-0.5884330
		H	-0.7575920	-3.3450180	0.7784040
		H	0.9884150	-3.2600120	0.4601160
		C	2.0892550	0.8199660	-1.9286400
		H	1.4616560	0.4602560	-2.7598920
		H	3.1134360	0.9370940	-2.3446020
		C	1.5896660	2.1899280	-1.4562840
		H	1.6495120	2.9072650	-2.3024720
		H	2.2642170	2.5809290	-0.6784350
		C	-0.8038100	2.0762610	-1.9434470
		H	-0.4382210	1.4110950	-2.7423850
		H	-0.9477620	3.0731480	-2.4135940
		C	-2.1536560	1.5687140	-1.4260260
		H	-2.9033120	1.6214850	-2.2434030
		H	-2.5195510	2.2387270	-0.6324730
		C	-2.0892550	-0.8199660	-1.9286400
		H	-1.4616560	-0.4602560	-2.7598920
		H	-3.1134360	-0.9370940	-2.3446020
		C	-1.5896660	-2.1899280	-1.4562840
		H	-1.6495120	-2.9072650	-2.3024720
		H	-2.2642170	-2.5809290	-0.6784350
		C	0.8038100	-2.0762610	-1.9434470
		H	0.4382210	-1.4110950	-2.7423850
		H	0.9477620	-3.0731480	-2.4135940

		C	2.1536560	-1.5687140	-1.4260260
		H	2.9033120	-1.6214850	-2.2434030
		H	2.5195510	-2.2387270	-0.6324730
		C	-0.5324440	-1.0676830	2.9078050
		H	0.1543610	-1.9307980	2.8593260
		H	-1.5131900	-1.3656230	2.5071280
		C	-0.5991970	-0.4833100	4.3198000
		H	-0.5305110	-1.2588750	5.0959170
		H	-1.5411890	0.0689550	4.4691340
		C	0.5991970	0.4833100	4.3198000
		H	0.5305110	1.2588750	5.0959170
		H	1.5411890	-0.0689550	4.4691340
		C	0.5324440	1.0676830	2.9078050
		H	1.5131900	1.3656230	2.5071280
		H	-0.1543610	1.9307980	2.8593260
		N	2.0629500	-0.2020250	-0.8543430
		N	0.2253840	2.1347990	-0.8773420
		N	-2.0629500	0.2020250	-0.8543430
		N	-0.2253840	-2.1347990	-0.8773420
		O	0.0000000	0.0000000	2.0562360
		Li	0.0000000	0.0000000	0.0281860
3. **Li-DEE-1a**	-934.4135544	C	0.0000000	-3.3104130	0.0050150
		H	-0.0991140	-4.2634720	-0.5553850
		H	-0.7366970	-3.3081990	0.8217440
		H	1.0028890	-3.2847200	0.4551440
		C	3.2079700	0.0321020	0.0808650
		H	4.1870080	-0.0020910	-0.4407230
		H	3.2101720	-0.7307500	0.8727800
		H	3.1080110	1.0140420	0.5648260
		C	0.0000000	3.3104130	0.0050150
		H	0.7366970	3.3081990	0.8217440
		H	-1.0028890	3.2847200	0.4551440
		H	0.0991140	4.2634720	-0.5553850
		C	-3.2079700	-0.0321020	0.0808650
		H	-4.1870080	0.0020910	-0.4407230
		H	-3.2101720	0.7307500	0.8727800
		H	-3.1080110	-1.0140420	0.5648260
		C	0.8198460	-2.0876190	-1.9248570
		H	0.4556730	-1.4335630	-2.7332290
		H	0.9642270	-3.0902130	-2.3821180
		C	2.1699750	-1.5738170	-1.4128990
		H	2.9152220	-1.6233080	-2.2347600
		H	2.5437770	-2.2432280	-0.6221680
		C	2.0682310	0.8113390	-1.9172980
		H	1.4224850	0.4465150	-2.7323840

		H	3.0819000	0.9310450	-2.3575600
		C	1.5755610	2.1803240	-1.4382330
		H	1.6372310	2.9015550	-2.2809470
		H	2.2523020	2.5636320	-0.6585550
		C	-0.8198460	2.0876190	-1.9248570
		H	-0.4556730	1.4335630	-2.7332290
		H	-0.9642270	3.0902130	-2.3821180
		C	-2.1699750	1.5738170	-1.4128990
		H	-2.9152220	1.6233080	-2.2347600
		H	-2.5437770	2.2432280	-0.6221680
		C	-2.0682310	-0.8113390	-1.9172980
		H	-1.4224850	-0.4465150	-2.7323840
		H	-3.0819000	-0.9310450	-2.3575600
		C	-1.5755610	-2.1803240	-1.4382330
		H	-1.6372310	-2.9015550	-2.2809470
		H	-2.2523020	-2.5636320	-0.6585550
		C	-0.7474200	0.9705840	2.8809720
		H	-1.2861480	1.5629270	2.1264210
		C	0.7474200	-0.9705840	2.8809720
		H	1.2861480	-1.5629270	2.1264210
		N	-0.2106150	-2.1309800	-0.8593050
		N	2.0762030	-0.2078880	-0.8393540
		N	0.2106150	2.1309800	-0.8593050
		N	-2.0762030	0.2078880	-0.8393540
		O	0.0000000	0.0000000	2.0983930
		C	-0.1198340	-1.8759380	3.7506360
		H	-0.5948540	-1.3344070	4.5819380
		H	-0.9081940	-2.3637340	3.1569390
		H	0.5097350	-2.6630970	4.1953180
		C	0.1198340	1.8759380	3.7506360
		H	0.5948540	1.3344070	4.5819380
		H	0.9081940	2.3637340	3.1569390
		H	-0.5097350	2.6630970	4.1953180
		H	-1.5041940	0.4461990	3.4904480
		H	1.5041940	-0.4461990	3.4904480
		Li	0.0000000	0.0000000	0.0560750
4. **Li-MeOH-1a**	-816.4575134	C	2.3402340	-2.1293300	0.9631240
		H	3.0841600	-2.8462100	0.5569620
		H	1.7118240	-2.6565650	1.6958570
		H	2.8910690	-1.3393800	1.4948390
		C	2.0678160	2.3983790	0.9420250
		H	2.8119940	3.1140710	0.5346000
		H	2.5270060	1.8755800	1.7945060
		H	1.2111770	2.9724650	1.3224610
		C	-2.4403270	2.1333300	0.3062580

		H	-2.0416360	2.6626950	1.1840390
		H	-3.1097990	1.3393470	0.6669140
		H	-3.0455020	2.8472660	-0.2904340
		C	-2.1614500	-2.4049570	0.3404060
		H	-2.7695720	-3.1133600	-0.2596300
		H	-2.8294540	-1.8872140	1.0444090
		H	-1.4390130	-2.9851210	0.9315660
		C	2.3108500	-0.7810710	-1.0621340
		H	1.7120870	-0.6235120	-1.9740110
		H	3.2046460	-1.3623720	-1.3759640
		C	2.7654380	0.5720300	-0.5018650
		H	3.3925490	1.0894160	-1.2576290
		H	3.4143280	0.4104120	0.3730280
		C	1.0025420	2.1020220	-1.2239910
		H	0.9563530	1.3876900	-2.0620950
		H	1.6355700	2.9469040	-1.5714670
		C	-0.4035970	2.6277370	-0.9149610
		H	-0.7943250	3.1661990	-1.8038080
		H	-0.3499910	3.3726880	-0.1057910
		C	-1.8484220	0.7889830	-1.6332230
		H	-1.0194120	0.6311720	-2.3419540
		H	-2.6202900	1.3695390	-2.1831590
		C	-2.4405230	-0.5649600	-1.2239610
		H	-2.8426360	-1.0744270	-2.1245860
		H	-3.3009270	-0.4063220	-0.5552290
		C	-0.5477660	-2.0944560	-1.4526620
		H	-0.2769330	-1.3767410	-2.2438080
		H	-1.0602220	-2.9387310	-1.9624180
		C	0.7229240	-2.6193460	-0.7748510
		H	1.3441010	-3.1520940	-1.5251730
		H	0.4533050	-3.3689820	-0.0150020
		C	-1.2744880	-0.0218870	3.5111420
		H	-2.2003600	-0.1257050	2.9320390
		N	1.4877120	-1.5450590	-0.0932030
		N	1.6228100	1.4134010	-0.0656310
		N	-1.3274750	1.5532400	-0.4740920
		N	-1.4600970	-1.4135470	-0.5017760
		O	-0.1856770	-0.0144990	2.5555050
		H	-1.3126750	0.9208640	4.0809640
		H	-1.1887220	-0.8737450	4.2045570
		H	0.6476960	0.0477560	3.0495280
		Li	-0.0436740	-0.0008930	0.5443060
5. **Li-DCM-1a**	-1660.5085	C	-1.3175900	-3.1217390	-0.0440240
		H	-2.1717970	-3.8077910	0.1300590
		H	-0.4641550	-3.4666850	0.5575200

H	-1.0309230	-3.1917110	-1.1029170
C	-0.4432910	0.0752710	-3.1746930
H	-1.0433170	0.2423800	-4.0923850
H	0.0180480	-0.9214790	-3.2315970
H	0.3677880	0.8170690	-3.1531180
C	1.1761950	2.9220940	-0.0780810
H	1.7923330	2.6411770	-0.9442250
H	1.7252900	2.6330630	0.8287020
H	1.0533940	4.0247620	-0.0733390
C	0.5037070	-0.3130170	3.0198200
H	0.2516900	-0.1496060	4.0873960
H	1.5053750	0.0982860	2.8282520
H	0.5479590	-1.3957090	2.8358040
C	-2.7712440	-1.2333390	-0.5262470
H	-3.2066310	-0.3450790	-0.0399590
H	-3.5861410	-1.9862290	-0.5826380
C	-2.3183000	-0.8739310	-1.9461050
H	-3.1986170	-0.5681910	-2.5482180
H	-1.9040960	-1.7664240	-2.4394060
C	-1.8602530	1.5257350	-1.8189200
H	-2.6706510	1.4730830	-1.0725670
H	-2.3360400	1.8440800	-2.7707250
C	-0.8315260	2.5821240	-1.3981050
H	-1.3333570	3.5685030	-1.3154280
H	-0.0709700	2.6914860	-2.1865460
C	-0.9498850	2.5419240	1.0484190
H	-1.9950540	2.2674050	0.8283300
H	-0.9516030	3.6342660	1.2493840
C	-0.4720440	1.7988300	2.3018180
H	-1.0921510	2.1017680	3.1704140
H	0.5590450	2.1022210	2.5397030
C	-1.8343990	-0.2328880	2.3288350
H	-2.5624040	0.4454630	1.8535750
H	-2.0894050	-0.2518510	3.4098820
C	-1.9879340	-1.6474590	1.7583060
H	-3.0183020	-2.0096910	1.9559600
H	-1.3135170	-2.3349680	2.2919190
C	3.6712190	-1.4592920	-0.5587340
N	-1.6482650	-1.7234310	0.3134670
N	-1.2626480	0.1723530	-1.9465650
N	-0.1246510	2.2180320	-0.1434700
N	-0.4752920	0.3248700	2.1115940
H	3.9624520	-1.6210680	-1.5999020
H	4.1492220	-2.1633800	0.1283290
Cl	1.8792220	-1.7817660	-0.4599290
Cl	4.1182150	0.1983030	-0.0856920

		Li	-0.2206130	-0.0049710	-0.0285380
6. **Na-H_2O-1a**	-931.9180205	C	-1.2348810	-3.1514470	0.6484440
		H	-1.6715870	-3.9801360	0.0517750
		H	-1.9281520	-2.9130330	1.4693530
		H	-0.2959360	-3.5124480	1.0937350
		C	3.1534700	-1.2393950	0.6436620
		H	3.9888760	-1.6543580	0.0408440
		H	2.9251570	-1.9516680	1.4512180
		H	3.4993180	-0.3040460	1.1077860
		C	1.2348810	3.1514470	0.6484440
		H	1.9281520	2.9130330	1.4693530
		H	0.2959360	3.5124480	1.0937350
		H	1.6715870	3.9801360	0.0517750
		C	-3.1534700	1.2393950	0.6436620
		H	-3.9888760	1.6543580	0.0408440
		H	-2.9251570	1.9516680	1.4512180
		H	-3.4993180	0.3040460	1.1077860
		C	0.0000000	-2.2298910	-1.2319230
		H	-0.0999420	-1.4584140	-2.0115410
		H	-0.2269680	-3.1973850	-1.7309320
		C	1.4551150	-2.2750040	-0.7399750
		H	2.0982140	-2.6116390	-1.5822070
		H	1.5548470	-3.0435400	0.0435760
		C	2.2245360	-0.0003510	-1.2287810
		H	1.4514130	-0.0977130	-2.0070890
		H	3.1912390	-0.2239660	-1.7308680
		C	2.2698990	1.4521980	-0.7302460
		H	2.6150910	2.0975870	-1.5672910
		H	3.0322170	1.5462720	0.0599000
		C	0.0000000	2.2298910	-1.2319230
		H	0.0999420	1.4584140	-2.0115410
		H	0.2269680	3.1973850	-1.7309320
		C	-1.4551150	2.2750040	-0.7399750
		H	-2.0982140	2.6116390	-1.5822070
		H	-1.5548470	3.0435400	0.0435760
		C	-2.2245360	0.0003510	-1.2287810
		H	-1.4514130	0.0977130	-2.0070890
		H	-3.1912390	0.2239660	-1.7308680
		C	-2.2698990	-1.4521980	-0.7302460
		H	-2.6150910	-2.0975870	-1.5672910
		H	-3.0322170	-1.5462720	0.0599000
		N	-0.9881900	-1.9430380	-0.1642950
		N	1.9424140	-0.9955120	-0.1659180
		N	0.9881900	1.9430380	-0.1642950
		N	-1.9424140	0.9955120	-0.1659180

		O	0.0000000	0.0000000	3.4032070
		Na	0.0000000	0.0000000	1.0629080
		H	0.3652620	-0.6766780	3.9973220
		H	-0.3652620	0.6766780	3.9973220
7. **Na-THF-1a**	-1087.97425	C	3.3930960	0.0129500	-0.2217820
		H	4.3192320	-0.0936900	-0.8259070
		H	3.4324710	-0.7141270	0.6034670
		H	3.3888450	1.0216300	0.2169510
		C	0.0000000	3.3907570	-0.2168570
		H	0.0892990	4.3185440	-0.8210410
		H	0.7426720	3.4342950	0.5942000
		H	-0.9995000	3.3777760	0.2421100
		C	-3.3930960	-0.0129500	-0.2217820
		H	-3.4324710	0.7141270	0.6034670
		H	-3.3888450	-1.0216300	0.2169510
		H	-4.3192320	0.0936900	-0.8259070
		C	0.0000000	-3.3907570	-0.2168570
		H	-0.0892990	-4.3185440	-0.8210410
		H	-0.7426720	-3.4342950	0.5942000
		H	0.9995000	-3.3777760	0.2421100
		C	2.0671830	0.8150430	-2.0931570
		H	1.3796610	0.4366610	-2.8657410
		H	3.0462820	0.9573800	-2.6012270
		C	1.5785860	2.1862030	-1.6018270
		H	1.6535670	2.9066890	-2.4455990
		H	2.2597950	2.5618380	-0.8212980
		C	-0.8198980	2.0724840	-2.0844890
		H	-0.4471110	1.3932670	-2.8671020
		H	-0.9689250	3.0558510	-2.5821590
		C	-2.1858600	1.5793880	-1.5839790
		H	-2.9158390	1.6676320	-2.4183620
		H	-2.5499250	2.2512740	-0.7898880
		C	-2.0671830	-0.8150430	-2.0931570
		H	-1.3796610	-0.4366610	-2.8657410
		H	-3.0462820	-0.9573800	-2.6012270
		C	-1.5785860	-2.1862030	-1.6018270
		H	-1.6535670	-2.9066890	-2.4455990
		H	-2.2597950	-2.5618380	-0.8212980
		C	0.8198980	-2.0724840	-2.0844890
		H	0.4471110	-1.3932670	-2.8671020
		H	0.9689250	-3.0558510	-2.5821590
		C	2.1858600	-1.5793880	-1.5839790
		H	2.9158390	-1.6676320	-2.4183620
		H	2.5499250	-2.2512740	-0.7898880
		C	-0.5120420	-1.0776790	3.4408850

		H	0.1904730	-1.9289730	3.3906360
		H	-1.4886590	-1.3942900	3.0426160
		C	-0.5884580	-0.4967980	4.8544910
		H	-0.5004610	-1.2708650	5.6301540
		H	-1.5425690	0.0336370	5.0061060
		C	0.5884580	0.4967980	4.8544910
		H	0.5004610	1.2708650	5.6301540
		H	1.5425690	-0.0336370	5.0061060
		C	0.5120420	1.0776790	3.4408850
		H	1.4886590	1.3942900	3.0426160
		H	-0.1904730	1.9289730	3.3906360
		N	2.1719200	-0.2054100	-1.0229820
		N	0.2115880	2.1724030	-1.0240570
		N	-2.1719200	0.2054100	-1.0229820
		N	-0.2115880	-2.1724030	-1.0240570
		O	0.0000000	0.0000000	2.5908180
		Na	0.0000000	0.0000000	0.2397040
8. **Na-DEE-1a**	-1089.180103	C	0.1782150	2.9821090	-1.6563510
		H	0.7918860	3.8356020	-2.0155760
		H	-0.6420370	3.3819450	-1.0411240
		H	-0.2652760	2.4905120	-2.5346650
		C	0.1548990	-1.6324350	-2.9548630
		H	0.7474870	-1.9959000	-3.8212400
		H	-0.6663680	-1.0056490	-3.3337450
		H	-0.2923330	-2.5056540	-2.4579580
		C	0.2244410	-2.9850580	1.6626670
		H	-0.5966610	-3.3939980	1.0546440
		H	-0.2165360	-2.5004260	2.5461500
		H	0.8520060	-3.8314580	2.0147970
		C	0.1402110	1.6250990	2.9454240
		H	0.7232950	2.0041870	3.8114850
		H	-0.6684000	0.9826380	3.3251910
		H	-0.3244070	2.4868140	2.4443050
		C	2.0374270	1.4219950	-1.7090930
		H	2.8067250	1.0010510	-1.0432670
		H	2.5492220	2.2077570	-2.3068470
		C	1.5417290	0.3325090	-2.6723740
		H	2.3806350	0.0534030	-3.3468910
		H	0.7546990	0.7464780	-3.3234960
		C	2.0413310	-1.7149730	-1.4259070
		H	2.8276430	-1.0597840	-1.0197580
		H	2.5311100	-2.3185970	-2.2212910
		C	1.5568010	-2.6762770	-0.3300670
		H	2.4008670	-3.3472210	-0.0575590
		H	0.7684100	-3.3306020	-0.7366020

		C	2.0639700	-1.4020590	1.7018960
		H	2.8236890	-0.9721970	1.0307900
		H	2.5888550	-2.1817130	2.2962850
		C	1.5620760	-0.3172650	2.6672870
		H	2.4018890	-0.0272140	3.3359920
		H	0.7843060	-0.7395110	3.3242000
		C	2.0303720	1.7373510	1.4211970
		H	2.8266480	1.0940490	1.0151630
		H	2.5109650	2.3484020	2.2165940
		C	1.5308680	2.6917230	0.3258830
		H	2.3670550	3.3700300	0.0473630
		H	0.7389710	3.3396240	0.7357580
		C	-3.4439500	-1.0475410	0.6461340
		H	-2.7886690	-1.4826900	1.4176820
		C	-3.4524090	1.0185840	-0.6350620
		H	-2.8018920	1.4564040	-1.4090920
		N	0.9681470	2.0144440	-0.8689140
		N	0.9732720	-0.8608250	-1.9983550
		N	0.9950060	-2.0065500	0.8695270
		N	0.9757940	0.8668960	1.9930870
		O	-2.6500490	-0.0110490	0.0058650
		Na	-0.2859990	-0.0013510	0.0018870
		C	-3.9283380	2.0908690	0.3408240
		H	-4.5788640	1.6747130	1.1252870
		H	-3.0770220	2.5904240	0.8285490
		H	-4.5113310	2.8550200	-0.1981460
		C	-3.9146850	-2.1205300	-0.3314140
		H	-4.5717400	-1.7073820	-1.1120560
		H	-3.0608240	-2.6108690	-0.8240570
		H	-4.4890610	-2.8915710	0.2069340
		H	-4.2976510	-0.5833380	1.1702420
		H	-4.3041970	0.5476230	-1.1562210
9. **Na-MeOH-1a**	-971.2215438	C	2.0872400	-2.5992130	0.7811000
		H	2.7403180	-3.3450750	0.2805940
		H	1.3880800	-3.1379590	1.4386690
		H	2.7236460	-1.9608220	1.4120290
		C	2.4726210	2.1539930	1.0523510
		H	3.3520540	2.7021970	0.6530100
		H	2.7948800	1.5772530	1.9324630
		H	1.7323740	2.8941060	1.3898370
		C	-2.1993060	2.5882180	0.0286370
		H	-1.8615120	3.0427390	0.9724660
		H	-3.0454640	1.9233550	0.2564270
		H	-2.5694660	3.3974470	-0.6359170
		C	-2.5797150	-2.1679550	-0.2271520

		H	-3.1957410	-2.6820510	-0.9951490
		H	-3.2558680	-1.6490830	0.4689370
		H	-2.0353320	-2.9348940	0.3431710
		C	2.2592510	-1.0059920	-1.0456370
		H	1.7119820	-0.6911960	-1.9477790
		H	3.0911170	-1.6512970	-1.4039260
		C	2.8698780	0.2265270	-0.3604450
		H	3.6373380	0.6591910	-1.0388180
		H	3.4105340	-0.0881420	0.5469410
		C	1.3807240	2.0203850	-1.1141530
		H	1.2834450	1.3331690	-1.9691130
		H	2.1266960	2.7848160	-1.4238060
		C	0.0417190	2.7333010	-0.8708000
		H	-0.1746850	3.3789380	-1.7498280
		H	0.1399770	3.4147450	-0.0103490
		C	-1.5596370	1.1318520	-1.8090750
		H	-0.6775820	0.8753240	-2.4164930
		H	-2.1732210	1.8145640	-2.4369080
		C	-2.3812980	-0.1377760	-1.5369050
		H	-2.7834200	-0.5088600	-2.5048730
		H	-3.2600450	0.1173560	-0.9225180
		C	-0.6842630	-1.8942960	-1.7220900
		H	-0.2456290	-1.1470860	-2.4016740
		H	-1.2186780	-2.6206210	-2.3732030
		C	0.4387950	-2.6463230	-0.9912940
		H	1.0149430	-3.2290830	-1.7430440
		H	-0.0013630	-3.3883950	-0.3056000
		C	-1.6481770	-0.1010970	3.9657620
		H	-2.3972630	0.4002100	3.3391670
		N	1.3306080	-1.7767540	-0.1841140
		N	1.8745290	1.2473110	0.0512940
		N	-1.0937630	1.8219490	-0.5813180
		N	-1.6342370	-1.2005510	-0.8193290
		O	-0.4680060	-0.2798840	3.1434580
		Na	-0.1430080	-0.0273500	0.8256350
		H	-1.4341830	0.5367530	4.8380090
		H	-2.0533050	-1.0692580	4.3031990
		H	0.2255620	-0.6618620	3.7068850
10. **Na-DCM-1a**	-1815.274373	C	-0.2669720	-3.3455370	0.6530450
		H	-0.8883290	-4.1839510	1.0327010
		H	0.6609380	-3.3074300	1.2435240
		H	0.0042460	-3.5694020	-0.3890990
		C	-0.6872050	-0.6591310	-3.3056650
		H	-1.4335500	-0.9010630	-4.0912750
		H	0.0925870	-1.4354710	-3.3160030

		H	-0.2134120	0.2980320	-3.5685120
		C	-0.0559370	3.3417640	-0.7324930
		H	0.6310810	3.1970520	-1.5799370
		H	0.5504300	3.5127720	0.1691370
		H	-0.6551600	4.2575830	-0.9203020
		C	0.4603880	0.6444230	3.2063090
		H	0.0440680	0.9632840	4.1851590
		H	1.2949030	1.3139040	2.9484320
		H	0.8671510	-0.3706800	3.3239000
		C	-2.1870750	-2.0661810	-0.1092170
		H	-2.8598870	-1.2659390	0.2369020
		H	-2.7467990	-3.0163800	0.0300320
		C	-1.9077770	-1.8869580	-1.6096260
		H	-2.8573270	-2.0494700	-2.1644110
		H	-1.2167630	-2.6735110	-1.9527760
		C	-2.3022250	0.5107100	-1.9146700
		H	-2.9734070	0.3257960	-1.0613150
		H	-2.9487580	0.4869280	-2.8189170
		C	-1.6982620	1.9185530	-1.7976590
		H	-2.5233620	2.6584980	-1.8864570
		H	-1.0302850	2.1056310	-2.6538000
		C	-1.7819080	2.2989380	0.6234230
		H	-2.6268920	1.6002360	0.5220320
		H	-2.2298430	3.3161220	0.6498350
		C	-1.0687960	2.0536750	1.9621710
		H	-1.7639410	2.3274060	2.7852730
		H	-0.2086320	2.7366090	2.0509080
		C	-1.6506470	-0.2810980	2.4284520
		H	-2.5290840	0.0060920	1.8289890
		H	-1.9679410	-0.1957260	3.4907370
		C	-1.2973190	-1.7511090	2.1537790
		H	-2.1378080	-2.3838620	2.5134760
		H	-0.4214080	-2.0376620	2.7577560
		C	4.1589580	-0.2583890	-0.3820530
		N	-0.9681970	-2.0474280	0.7362980
		N	-1.2962690	-0.5792420	-1.9609050
		N	-0.9038960	2.1436660	-0.5631560
		N	-0.5529400	0.6711330	2.1306940
		Na	0.2549530	-0.0293640	-0.0997890
		H	4.7075070	-0.2819060	-1.3277340
		H	4.8103240	-0.3765740	0.4885690
		Cl	2.9930030	-1.6372980	-0.3883540
		Cl	3.3318590	1.3332530	-0.2519080
11. **K-H_2O-1a**	-1369.594606	C	-2.0296250	2.8052780	0.4094550
		H	-2.4665710	3.5981390	-0.2351150

H	-1.4857420	3.2958360	1.2322670
H	-2.8605070	2.2310320	0.8469200
C	-2.7948490	-2.0176530	0.4294860
H	-3.5957570	-2.4584060	-0.2024170
H	-3.2738560	-1.4655690	1.2535890
H	-2.2186180	-2.8459450	0.8692700
C	2.0296250	-2.8052780	0.4094550
H	1.4857420	-3.2958360	1.2322670
H	2.8605070	-2.2310320	0.8469200
H	2.4665710	-3.5981390	-0.2351150
C	2.7948490	2.0176530	0.4294860
H	3.5957570	2.4584060	-0.2024170
H	3.2738560	1.4655690	1.2535890
H	2.2186180	2.8459450	0.8692700
C	-1.8651320	1.1932400	-1.3943130
H	-1.1448720	0.8483430	-2.1516940
H	-2.5526440	1.8869230	-1.9276950
C	-2.6959390	-0.0005320	-0.8983770
H	-3.3356330	-0.3468120	-1.7411590
H	-3.3931120	0.3378080	-0.1139110
C	-1.1966040	-1.8742070	-1.3895120
H	-0.8579210	-1.1619740	-2.1572550
H	-1.8951920	-2.5665040	-1.9102540
C	0.0000000	-2.7022010	-0.8959140
H	0.3433310	-3.3429550	-1.7391710
H	-0.3349720	-3.3980860	-0.1088520
C	1.8651320	-1.1932400	-1.3943130
H	1.1448720	-0.8483430	-2.1516940
H	2.5526440	-1.8869230	-1.9276950
C	2.6959390	0.0005320	-0.8983770
H	3.3356330	0.3468120	-1.7411590
H	3.3931120	-0.3378080	-0.1139110
C	1.1966040	1.8742070	-1.3895120
H	0.8579210	1.1619740	-2.1572550
H	1.8951920	2.5665040	-1.9102540
C	0.0000000	2.7022010	-0.8959140
H	-0.3433310	3.3429550	-1.7391710
H	0.3349720	3.3980860	-0.1088520
N	-1.1212080	1.9110010	-0.3329930
N	-1.9052340	-1.1190360	-0.3301260
N	1.1212080	-1.9110010	-0.3329930
N	1.9052340	1.1190360	-0.3301260
O	0.0000000	0.0000000	4.1646260
K	0.0000000	0.0000000	1.4463330
H	-0.4975660	0.5817760	4.7636870
H	0.4975660	-0.5817760	4.7636870

12. **K-THF-1a**	-1525.651647	C	2.8141850	2.0289500	-0.5314550
		H	3.6032670	2.4663270	-1.1805880
		H	3.3091000	1.4833990	0.2873770
		H	2.2432470	2.8590760	-0.0884740
		C	-2.0254280	2.7944060	-0.5155990
		H	-2.4623040	3.5924450	-1.1539800
		H	-1.4794640	3.2773040	0.3101700
		H	-2.8560090	2.2183150	-0.0802790
		C	-2.8141850	-2.0289500	-0.5314550
		H	-3.3091000	-1.4833990	0.2873770
		H	-2.2432470	-2.8590760	-0.0884740
		H	-3.6032670	-2.4663270	-1.1805880
		C	2.0254280	-2.7944060	-0.5155990
		H	2.4623040	-3.5924450	-1.1539800
		H	1.4794640	-3.2773040	0.3101700
		H	2.8560090	-2.2183150	-0.0802790
		C	1.1945720	1.8701900	-2.3275890
		H	0.8507160	1.1532170	-3.0884900
		H	1.8871500	2.5610260	-2.8581830
		C	0.0000000	2.6973470	-1.8279050
		H	-0.3449780	3.3422370	-2.6674880
		H	0.3372160	3.3894110	-1.0383990
		C	-1.8668060	1.1929130	-2.3295320
		H	-1.1483990	0.8497140	-3.0894050
		H	-2.5533310	1.8905240	-2.8593800
		C	-2.7004570	-0.0010490	-1.8389320
		H	-3.3371300	-0.3441670	-2.6854930
		H	-3.4002960	0.3364960	-1.0565080
		C	-1.1945720	-1.8701900	-2.3275890
		H	-0.8507160	-1.1532170	-3.0884900
		H	-1.8871500	-2.5610260	-2.8581830
		C	0.0000000	-2.6973470	-1.8279050
		H	0.3449780	-3.3422370	-2.6674880
		H	-0.3372160	-3.3894110	-1.0383990
		C	1.8668060	-1.1929130	-2.3295320
		H	1.1483990	-0.8497140	-3.0894050
		H	2.5533310	-1.8905240	-2.8593800
		C	2.7004570	0.0010490	-1.8389320
		H	3.3371300	0.3441670	-2.6854930
		H	3.4002960	-0.3364960	-1.0565080
		C	-1.0989850	-0.4588990	4.0935490
		H	-1.1470260	-1.5627880	4.0460090
		H	-2.0397380	-0.0432420	3.6974330
		C	-0.7697380	0.0246960	5.5082100
		H	-1.2237760	-0.6080460	6.2844560

		H	-1.1226590	1.0584760	5.6574420
		C	0.7697380	-0.0246960	5.5082100
		H	1.2237760	0.6080460	6.2844560
		H	1.1226590	-1.0584760	5.6574420
		C	1.0989850	0.4588990	4.0935490
		H	2.0397380	0.0432420	3.6974330
		H	1.1470260	1.5627880	4.0460090
		N	1.9145880	1.1228160	-1.2702370
		N	-1.1200030	1.9041930	-1.2663880
		N	-1.9145880	-1.1228160	-1.2702370
		N	1.1200030	-1.9041930	-1.2663880
		O	0.0000000	0.0000000	3.2433340
		K	0.0000000	0.0000000	0.5223510
13. **K-DCM-1a**	-2252.955018	C	-1.7498730	-0.2471260	-3.3075630
		H	-2.6822660	-0.3769370	-3.8979800
		H	-1.0391670	-1.0299630	-3.6160310
		H	-1.3160580	0.7284200	-3.5749600
		C	-0.3723000	3.4305440	-0.3760970
		H	-0.9827890	4.3569640	-0.3143580
		H	0.1248090	3.4139820	-1.3586080
		H	0.4081680	3.4902570	0.3975070
		C	0.7997050	0.2166930	3.1085080
		H	1.6108530	0.8993060	2.8104990
		H	1.1859760	-0.8121390	3.0513780
		H	0.5427800	0.4254700	4.1693030
		C	-0.5862890	-3.4621900	0.1909470
		H	-1.1777020	-4.3102900	0.5980260
		H	0.4411030	-3.5453070	0.5786310
		H	-0.5456280	-3.5753450	-0.9030610
		C	-2.8902160	0.7690530	-1.4223080
		H	-3.3567910	0.4805460	-0.4682690
		H	-3.7293280	0.8881560	-2.1428700
		C	-2.2091670	2.1377160	-1.2663770
		H	-3.0047160	2.8999300	-1.1082840
		H	-1.7149560	2.4120760	-2.2130170
		C	-1.7975960	2.1962310	1.1494090
		H	-2.6629050	1.5166890	1.1289020
		H	-2.2091950	3.1990790	1.4002830
		C	-0.8478450	1.7807580	2.2837020
		H	-1.3652620	1.9699410	3.2507450
		H	0.0370710	2.4385430	2.2828060
		C	-1.4207820	-0.5872790	2.5480250
		H	-2.3741440	-0.2098710	2.1480560
		H	-1.5589320	-0.6444270	3.6505890
		C	-1.1771170	-2.0138110	2.0313060

		H	-1.9459550	-2.6785000	2.4849800
		H	-0.2061430	-2.3795250	2.4047390
		C	-2.5175830	-2.0101030	-0.0195940
		H	-3.0557450	-1.2374060	0.5499750
		H	-3.0993490	-2.9479550	0.1211650
		C	-2.5489930	-1.6565280	-1.5144060
		H	-3.6003290	-1.7499040	-1.8671510
		H	-1.9741850	-2.4066420	-2.0822260
		C	4.7572350	-0.0981150	-0.6181370
		N	-1.9871660	-0.3253440	-1.8525750
		N	-1.1811740	2.2087830	-0.1983890
		N	-0.3553830	0.3834070	2.2049980
		N	-1.1580490	-2.1503710	0.5535200
		H	5.4104350	-0.1575870	0.2562550
		H	5.3119270	-0.0430990	-1.5580330
		Cl	3.7718870	1.4035120	-0.4704020
		Cl	3.7497640	-1.5913980	-0.6576240
		K	0.4630360	-0.0721460	-0.4568380
14. **K-MeOH-1a**	-1408.898438	C	1.6504970	-1.3095950	2.6977940
		H	1.5169950	-1.5102980	3.7828560
		H	2.5628010	-0.7058710	2.5710340
		H	1.8122340	-2.2745840	2.1939450
		C	-0.6856190	-3.1989750	-1.1766220
		H	-1.4016390	-4.0388560	-1.0469260
		H	0.3312730	-3.5904310	-1.0143850
		H	-0.7538490	-2.8565530	-2.2205940
		C	-1.4142060	1.2946730	-2.9318230
		H	-0.9033140	0.6016920	-3.6187620
		H	-0.8062130	2.2092190	-2.8614540
		H	-2.3916480	1.5704730	-3.3835410
		C	0.9064730	3.1973150	0.9370380
		H	0.5072560	4.1011900	1.4456620
		H	1.3105990	3.5063100	-0.0399610
		H	1.7414000	2.8122670	1.5422580
		C	-0.7200690	-1.4474760	2.2065920
		H	-1.6013480	-0.7929350	2.1318700
		H	-0.7859100	-1.9262520	3.2090420
		C	-0.8197430	-2.5584750	1.1490590
		H	-1.6706620	-3.2200140	1.4272530
		H	0.0814260	-3.1924460	1.1958250
		C	-2.2885030	-1.5061320	-0.5060320
		H	-2.6053020	-0.9562700	0.3928320
		H	-3.0415580	-2.3129040	-0.6488040
		C	-2.3620180	-0.5720350	-1.7239490
		H	-3.4341900	-0.3420370	-1.9155840

		H	-2.0055320	-1.1060760	-2.6204760
		C	-2.1782780	1.6226040	-0.6519570
		H	-2.6138080	1.0480880	0.1793750
		H	-3.0312440	2.1548630	-1.1288850
		C	-1.2190740	2.6842280	-0.0903910
		H	-1.8265870	3.4313570	0.4681690
		H	-0.7552390	3.2385140	-0.9232000
		C	-0.6171520	1.6847530	2.0649960
		H	-1.6016100	1.2167570	1.9153530
		H	-0.7941220	2.5465970	2.7464570
		C	0.3120630	0.6979220	2.7892850
		H	-0.0747680	0.5603460	3.8240480
		H	1.3119480	1.1497650	2.9007960
		C	4.5955080	0.1637570	-1.9855620
		H	4.3533660	1.1729170	-1.6257070
		N	0.4949450	-0.6066880	2.1081490
		N	-0.9478760	-2.0821000	-0.2496950
		N	-1.5607460	0.6699500	-1.6033980
		N	-0.1187500	2.1531860	0.7510670
		O	3.4262790	-0.6576460	-1.7514550
		H	4.8402590	0.2223240	-3.0590590
		H	5.4703990	-0.2083110	-1.4268360
		H	3.6404180	-1.5517410	-2.0669180
		K	1.0092450	-0.0606180	-0.6330250
15. **K-DEE-1a**	-1526.859645	C	3.2149690	-1.2723830	-0.3744250
		H	4.0111710	-1.7091770	-1.0155290
		H	3.0140720	-1.9770270	0.4480660
		H	3.6093320	-0.3431900	0.0642030
		C	1.2767730	3.2350720	-0.4025390
		H	1.6918850	4.0274080	-1.0626890
		H	1.9992730	3.0539070	0.4084840
		H	0.3513840	3.6236580	0.0491140
		C	-3.2149690	1.2723830	-0.3744250
		H	-3.0140720	1.9770270	0.4480660
		H	-3.6093320	0.3431900	0.0642030
		H	-4.0111710	1.7091770	-1.0155290
		C	-1.2767730	-3.2350720	-0.4025390
		H	-1.6918850	-4.0274080	-1.0626890
		H	-1.9992730	-3.0539070	0.4084840
		H	-0.3513840	-3.6236580	0.0491140
		C	2.2197330	0.0011310	-2.1821260
		H	1.4292050	-0.0943980	-2.9415520
		H	3.1734570	-0.2165700	-2.7127520
		C	2.2783150	1.4555180	-1.6902480
		H	2.6324580	2.0875540	-2.5355340

		H	3.0456950	1.5481790	-0.9038390
		C	0.0000000	2.2080660	-2.1870620
		H	0.0922150	1.4059360	-2.9345430
		H	0.2137710	3.1540900	-2.7328070
		C	-1.4511030	2.2710600	-1.6866650
		H	-2.0884910	2.6262690	-2.5273500
		H	-1.5369210	3.0385030	-0.8995920
		C	-2.2197330	-0.0011310	-2.1821260
		H	-1.4292050	0.0943980	-2.9415520
		H	-3.1734570	0.2165700	-2.7127520
		C	-2.2783150	-1.4555180	-1.6902480
		H	-2.6324580	-2.0875540	-2.5355340
		H	-3.0456950	-1.5481790	-0.9038390
		C	0.0000000	-2.2080660	-2.1870620
		H	-0.0922150	-1.4059360	-2.9345430
		H	-0.2137710	-3.1540900	-2.7328070
		C	1.4511030	-2.2710600	-1.6866650
		H	2.0884910	-2.6262690	-2.5273500
		H	1.5369210	-3.0385030	-0.8995920
		C	-1.0220830	-0.6081320	4.3023710
		H	-1.4813980	0.1678150	4.9451840
		C	1.0220830	0.6081320	4.3023710
		H	0.5547180	1.3602710	4.9673510
		N	1.9720160	-1.0024010	-1.1213590
		N	1.0093700	1.9786760	-1.1275770
		N	-1.9720160	1.0024010	-1.1213590
		N	-1.0093700	-1.9786760	-1.1275770
		O	0.0000000	0.0000000	3.4826740
		H	-0.5547180	-1.3602710	4.9673510
		C	-2.0707830	-1.2584390	3.4150460
		H	-2.8549180	-1.7174750	4.0362300
		H	-2.5590020	-0.5161810	2.7626790
		H	-1.6297800	-2.0562430	2.7958970
		H	1.4813980	-0.1678150	4.9451840
		C	2.0707830	1.2584390	3.4150460
		H	2.5590020	0.5161810	2.7626790
		H	1.6297800	2.0562430	2.7958970
		H	2.8549180	1.7174750	4.0362300
		K	0.0000000	0.0000000	0.6773390
16. $[Li(Me_4cyclen)]^+$	-700.680022	C	-0.3373210	3.1434800	1.1131480
		H	-0.3786040	4.1486120	0.6470880
		H	0.4168360	3.1599270	1.9135660
		H	-1.3127530	2.9397090	1.5771430
		C	-3.1434800	-0.3373210	1.1131480
		H	-4.1486120	-0.3786040	0.6470880

		H	-3.1599270	0.4168360	1.9135660
		H	-2.9397090	-1.3127530	1.5771430
		C	0.3373210	-3.1434800	1.1131480
		H	-0.4168360	-3.1599270	1.9135660
		H	1.3127530	-2.9397090	1.5771430
		H	0.3786040	-4.1486120	0.6470880
		C	3.1434800	0.3373210	1.1131480
		H	4.1486120	0.3786040	0.6470880
		H	3.1599270	-0.4168360	1.9135660
		H	2.9397090	1.3127530	1.5771430
		C	-1.0314950	2.0091040	-0.9339320
		H	-0.6125960	1.4289810	-1.7732120
		H	-1.2663560	3.0159640	-1.3390160
		C	-2.3276120	1.3503080	-0.4427780
		H	-3.0618440	1.3180080	-1.2732070
		H	-2.7828670	1.9710550	0.3441620
		C	-2.0091040	-1.0314950	-0.9339320
		H	-1.4289810	-0.6125960	-1.7732120
		H	-3.0159640	-1.2663560	-1.3390160
		C	-1.3503080	-2.3276120	-0.4427780
		H	-1.3180080	-3.0618440	-1.2732070
		H	-1.9710550	-2.7828670	0.3441620
		C	1.0314950	-2.0091040	-0.9339320
		H	0.6125960	-1.4289810	-1.7732120
		H	1.2663560	-3.0159640	-1.3390160
		C	2.3276120	-1.3503080	-0.4427780
		H	3.0618440	-1.3180080	-1.2732070
		H	2.7828670	-1.9710550	0.3441620
		C	2.0091040	1.0314950	-0.9339320
		H	1.4289810	0.6125960	-1.7732120
		H	3.0159640	1.2663560	-1.3390160
		C	1.3503080	2.3276120	-0.4427780
		H	1.3180080	3.0618440	-1.2732070
		H	1.9710550	2.7828670	0.3441620
		N	0.0000000	2.0863780	0.1329340
		N	-2.0863780	0.0000000	0.1329340
		N	0.0000000	-2.0863780	0.1329340
		N	2.0863780	0.0000000	0.1329340
		Li	0.0000000	0.0000000	0.7390880
17. $[Na(Me_4cyclen)]^+$	-855.4430547	C	-0.3299880	3.3762830	0.9074720
		H	-0.3149450	4.3093360	0.3065840
		H	0.3942410	3.4826540	1.7293700
		H	-1.3311630	3.2737840	1.3510780
		C	-3.3762830	-0.3299880	0.9074720
		H	-4.3093360	-0.3149450	0.3065840

		H	-3.4826540	0.3942410	1.7293700
		H	-3.2737840	-1.3311630	1.3510780
		C	0.3299880	-3.3762830	0.9074720
		H	-0.3942410	-3.4826540	1.7293700
		H	1.3311630	-3.2737840	1.3510780
		H	0.3149450	-4.3093360	0.3065840
		C	3.3762830	0.3299880	0.9074720
		H	4.3093360	0.3149450	0.3065840
		H	3.4826540	-0.3942410	1.7293700
		H	3.2737840	1.3311630	1.3510780
		C	-1.0147750	1.9874040	-0.9693510
		H	-0.5752120	1.3470610	-1.7500920
		H	-1.2533980	2.9526230	-1.4654930
		C	-2.3305490	1.3643130	-0.4751200
		H	-3.0573320	1.3710620	-1.3157320
		H	-2.7686930	2.0017170	0.3097080
		C	-1.9874040	-1.0147750	-0.9693510
		H	-1.3470610	-0.5752120	-1.7500920
		H	-2.9526230	-1.2533980	-1.4654930
		C	-1.3643130	-2.3305490	-0.4751200
		H	-1.3710620	-3.0573320	-1.3157320
		H	-2.0017170	-2.7686930	0.3097080
		C	1.0147750	-1.9874040	-0.9693510
		H	0.5752120	-1.3470610	-1.7500920
		H	1.2533980	-2.9526230	-1.4654930
		C	2.3305490	-1.3643130	-0.4751200
		H	3.0573320	-1.3710620	-1.3157320
		H	2.7686930	-2.0017170	0.3097080
		C	1.9874040	1.0147750	-0.9693510
		H	1.3470610	0.5752120	-1.7500920
		H	2.9526230	1.2533980	-1.4654930
		C	1.3643130	2.3305490	-0.4751200
		H	1.3710620	3.0573320	-1.3157320
		H	2.0017170	2.7686930	0.3097080
		N	0.0000000	2.1832520	0.0976680
		N	-2.1832520	0.0000000	0.0976680
		N	0.0000000	-2.1832520	0.0976680
		N	2.1832520	0.0000000	0.0976680
		Na	0.0000000	0.0000000	1.2265070
18. $[K(Me_4cyclen)]^+$	-1293.124359	C	-0.3278780	3.4510820	0.7109140
		H	-0.3004260	4.3534650	0.0636680
		H	0.3894290	3.5996730	1.5334640
		H	-1.3354560	3.3809650	1.1477550
		C	-3.4510820	-0.3278780	0.7109140
		H	-4.3534650	-0.3004260	0.0636680

		H	-3.5996730	0.3894290	1.5334640
		H	-3.3809650	-1.3354560	1.1477550
		C	0.3278780	-3.4510820	0.7109140
		H	-0.3894290	-3.5996730	1.5334640
		H	1.3354560	-3.3809650	1.1477550
		H	0.3004260	-4.3534650	0.0636680
		C	3.4510820	0.3278780	0.7109140
		H	4.3534650	0.3004260	0.0636680
		H	3.5996730	-0.3894290	1.5334640
		H	3.3809650	1.3354560	1.1477550
		C	-1.0067070	1.9753510	-1.0912770
		H	-0.5613670	1.3117090	-1.8475690
		H	-1.2456260	2.9216520	-1.6247300
		C	-2.3289020	1.3681780	-0.5953580
		H	-3.0547280	1.3937440	-1.4383130
		H	-2.7588270	2.0114530	0.1903250
		C	-1.9753510	-1.0067070	-1.0912770
		H	-1.3117090	-0.5613670	-1.8475690
		H	-2.9216520	-1.2456260	-1.6247300
		C	-1.3681780	-2.3289020	-0.5953580
		H	-1.3937440	-3.0547280	-1.4383130
		H	-2.0114530	-2.7588270	0.1903250
		C	1.0067070	-1.9753510	-1.0912770
		H	0.5613670	-1.3117090	-1.8475690
		H	1.2456260	-2.9216520	-1.6247300
		C	2.3289020	-1.3681780	-0.5953580
		H	3.0547280	-1.3937440	-1.4383130
		H	2.7588270	-2.0114530	0.1903250
		C	1.9753510	1.0067070	-1.0912770
		H	1.3117090	0.5613670	-1.8475690
		H	2.9216520	1.2456260	-1.6247300
		C	1.3681780	2.3289020	-0.5953580
		H	1.3937440	3.0547280	-1.4383130
		H	2.0114530	2.7588270	0.1903250
		N	0.0000000	2.2159940	-0.0292960
		N	-2.2159940	0.0000000	-0.0292960
		N	0.0000000	-2.2159940	-0.0292960
		N	2.2159940	0.0000000	-0.0292960
		K	0.0000000	0.0000000	1.6915350
19. Me_4cyclen	-693.2330113	C	-0.1388050	3.7857800	0.5752080
		H	-0.1118700	4.5910520	-0.2001670
		H	0.5968050	4.0369430	1.3563390
		H	-1.1368200	3.8061160	1.0412860
		C	-2.4957300	-0.3696660	1.4782590
		H	-3.5986670	-0.5169800	1.3613540

		H	-2.3314800	0.4105770	2.2368310
		H	-2.0594080	-1.3013270	1.8699180
		C	0.1388050	-3.7857800	0.5752080
		H	-0.5968050	-4.0369430	1.3563390
		H	1.1368200	-3.8061160	1.0412860
		H	0.1118700	-4.5910520	-0.2001670
		C	2.4957300	0.3696660	1.4782590
		H	3.5986670	0.5169800	1.3613540
		H	2.3314800	-0.4105770	2.2368310
		H	2.0594080	1.3013270	1.8699180
		C	-0.9081560	2.0332820	-0.9014250
		H	-0.4785750	1.3105060	-1.6119450
		H	-1.2691030	2.8935480	-1.5154230
		C	-2.1081140	1.3719920	-0.1968270
		H	-2.9962460	1.4113840	-0.8749880
		H	-2.3729340	1.9729350	0.6883920
		C	-1.9936060	-0.9623160	-0.8256350
		H	-1.4719720	-0.5783890	-1.7191980
		H	-3.0703110	-1.0612500	-1.1266720
		C	-1.4949750	-2.3846950	-0.5107810
		H	-1.6148840	-2.9922450	-1.4432980
		H	-2.1674610	-2.8457880	0.2329930
		C	0.9081560	-2.0332820	-0.9014250
		H	0.4785750	-1.3105060	-1.6119450
		H	1.2691030	-2.8935480	-1.5154230
		C	2.1081140	-1.3719920	-0.1968270
		H	2.9962460	-1.4113840	-0.8749880
		H	2.3729340	-1.9729350	0.6883920
		C	1.9936060	0.9623160	-0.8256350
		H	1.4719720	0.5783890	-1.7191980
		H	3.0703110	1.0612500	-1.1266720
		C	1.4949750	2.3846950	-0.5107810
		H	1.6148840	2.9922450	-1.4432980
		H	2.1674610	2.8457880	0.2329930
		N	0.1388050	2.4576730	0.0368450
		N	-1.8156490	0.0081990	0.2476960
		N	-0.1388050	-2.4576730	0.0368450
		N	1.8156490	-0.0081990	0.2476960
20. [Li-H_2O]$^+$	-83.78571584	O	0.0000000	0.0000000	0.3358430
		Li	0.0000000	0.0000000	-1.5135590
		H	0.0000000	0.7749000	0.9269650
		H	0.0000000	-0.7749000	0.9269650
21. [Li-THF]$^+$	-239.853071	C	0.0000000	1.2122260	0.1947180
		H	1.0050430	1.6606760	0.2505000

		H	-0.7468410	1.9119140	0.5985870
		C	-0.3243860	0.6985990	-1.2045710
		H	0.0825700	1.3573790	-1.9844160
		H	-1.4135850	0.6250370	-1.3505110
		C	0.3243860	-0.6985990	-1.2045710
		H	-0.0825700	-1.3573790	-1.9844160
		H	1.4135850	-0.6250370	-1.3505110
		C	0.0000000	-1.2122260	0.1947180
		H	0.7468410	-1.9119140	0.5985870
		H	-1.0050430	-1.6606760	0.2505000
		O	0.0000000	0.0000000	1.0600930
		Li	0.0000000	0.0000000	2.8697220
22. $[Li\text{-}DEE]^+$, TT	-241.0644623	C	0.0000000	1.2288060	-0.6700530
		H	-0.8970610	1.2226970	-1.3115020
		C	0.0000000	-1.2288060	-0.6700530
		H	-0.8970610	-1.2226970	-1.3115020
		O	0.0000000	0.0000000	0.1262380
		H	0.8970610	1.2226970	-1.3115020
		C	0.0000000	2.4125160	0.2813210
		H	0.0000000	3.3533720	-0.2889990
		H	-0.9063260	2.4313280	0.9121810
		H	0.9063260	2.4313280	0.9121810
		H	0.8970610	-1.2226970	-1.3115020
		C	0.0000000	-2.4125160	0.2813210
		H	0.9063260	-2.4313280	0.9121810
		H	-0.9063260	-2.4313280	0.9121810
		H	0.0000000	-3.3533720	-0.2889990
		Li	0.0000000	0.0000000	1.9433870
23. $[Li\text{-}DEE]^+$, TG	-241.0620616	C	0.8745160	-0.6619910	0.2490540
		H	0.4801080	-1.4725260	-0.3830840
		C	-1.3608360	0.3649820	0.5121140
		H	-1.3450140	-0.0768410	1.5224330
		O	0.0406940	0.5284250	0.0844910
		H	0.8291430	-0.9747200	1.3058400
		C	2.2923250	-0.2896640	-0.1601050
		H	2.9638650	-1.1537600	-0.0484740
		H	2.3528400	-0.0018000	-1.2274820
		H	2.7147890	0.5041990	0.4854590
		H	-1.7457230	1.3927440	0.5973570
		C	-2.1893970	-0.4574100	-0.4616870
		H	-2.1783050	-0.0193670	-1.4713980
		H	-1.8543110	-1.5033060	-0.5220110
		H	-3.2345280	-0.4719360	-0.1140740
		Li	0.9973130	1.9381370	-0.5522480

24. [Li-DEE]$^+$, GG	-241.0586271	C	0.0000000	1.2387030	-0.1222050
		H	0.4709410	2.0033970	0.5171070
		C	0.0000000	-1.2387030	-0.1222050
		H	-0.4709410	-2.0033970	0.5171070
		O	0.0000000	0.0000000	0.6838990
		C	1.4009910	-1.6485060	-0.5469180
		H	1.8788210	-0.8897450	-1.1844880
		H	2.0516100	-1.8383030	0.3208990
		H	1.3434040	-2.5799820	-1.1322310
		C	-1.4009910	1.6485060	-0.5469180
		H	-1.8788210	0.8897450	-1.1844880
		H	-2.0516100	1.8383030	0.3208990
		H	-1.3434040	2.5799820	-1.1322310
		H	0.6671540	1.0785570	-0.9831360
		H	-0.6671540	-1.0785570	-0.9831360
		Li	0.0000000	0.0000000	2.4939920
25. [Li-MeOH]$^+$	-123.093297	C	0.4534040	-0.8705130	0.0000000
		H	-0.4472060	-1.4970820	0.0000000
		O	0.0000000	0.5317400	0.0000000
		H	1.0418950	-1.0697020	0.9057050
		H	1.0418950	-1.0697020	-0.9057050
		H	0.7904970	1.0998730	0.0000000
		Li	-1.7158340	1.1685920	0.0000000
26. [Li-DCM]$^+$	-967.1377204	C	0.0000000	0.0000000	0.9518100
		H	-0.9175920	0.0000000	1.5470340
		H	0.9175920	0.0000000	1.5470340
		Cl	0.0000000	1.4891480	-0.0852950
		Cl	0.0000000	-1.4891480	-0.0852950
		Li	0.0000000	0.0000000	-1.9682950
27. [Na-H_2O]$^+$	-238.5749927	O	0.0000000	0.0000000	-1.1079500
		Na	0.0000000	0.0000000	1.1156060
		H	0.0000000	0.7694780	-1.7040350
		H	0.0000000	-0.7694780	-1.7040350
28. [Na-THF]$^+$	-394.637953	C	0.5028600	1.0933330	-0.3345450
		H	1.6050710	1.0902640	-0.2826950
		H	0.1175920	2.0445760	0.0644150
		C	0.0000000	0.7701740	-1.7396740
		H	0.6475860	1.1984570	-2.5176050
		H	-1.0194970	1.1602100	-1.8882020
		C	0.0000000	-0.7701740	-1.7396740
		H	-0.6475860	-1.1984570	-2.5176050

		H	1.0194970	-1.1602100	-1.8882020
		C	-0.5028600	-1.0933330	-0.3345450
		H	-0.1175920	-2.0445760	0.0644150
		H	-1.6050710	-1.0902640	-0.2826950
		O	0.0000000	0.0000000	0.5261950
		Na	0.0000000	0.0000000	2.7208410
29. $[Na\text{-}DEE]^+$, TT	-395.8489991	C	0.0000000	1.2131760	-1.0368080
		H	-0.8957180	1.2081510	-1.6827640
		C	0.0000000	-1.2131760	-1.0368080
		H	-0.8957180	-1.2081510	-1.6827640
		O	0.0000000	0.0000000	-0.2315660
		H	0.8957180	1.2081510	-1.6827640
		C	0.0000000	2.4173770	-0.1098970
		H	0.0000000	3.3467830	-0.6989460
		H	-0.9059310	2.4465050	0.5208590
		H	0.9059310	2.4465050	0.5208590
		H	0.8957180	-1.2081510	-1.6827640
		C	0.0000000	-2.4173770	-0.1098970
		H	0.9059310	-2.4465050	0.5208590
		H	-0.9059310	-2.4465050	0.5208590
		H	0.0000000	-3.3467830	-0.6989460
		Na	0.0000000	0.0000000	1.9689540
30. $[Na\text{-}DEE]^+$, TG	-395.8464039	C	0.3994790	-1.2300880	0.1338850
		H	-0.1490160	-1.7609840	-0.6615610
		C	-1.5004690	0.2363140	0.5980880
		H	-1.6733210	-0.4318290	1.4597030
		O	-0.0848450	0.1397860	0.2296010
		H	0.2042670	-1.7389920	1.0945420
		C	1.8889700	-1.2015470	-0.1721140
		H	2.2820570	-2.2270770	-0.2384170
		H	2.0993160	-0.7309430	-1.1502160
		H	2.4633500	-0.7031410	0.6300800
		H	-1.6325670	1.2722100	0.9495360
		C	-2.4477510	-0.0717500	-0.5537960
		H	-2.2661570	0.5922540	-1.4130890
		H	-2.3712800	-1.1154510	-0.8922160
		H	-3.4856360	0.0864590	-0.2206060
		Na	1.3787610	1.7492390	-0.1300850
31. $[Na\text{-}DEE]^+$, GG	-395.8435765	C	0.0000000	1.2262070	-0.5869090
		H	0.4894250	1.9931550	0.0363360
		C	0.0000000	-1.2262070	-0.5869090
		H	-0.4894250	-1.9931550	0.0363360
		O	0.0000000	0.0000000	0.2195180

		C	1.4047700	-1.6546420	-0.9888840
		H	1.9029820	-0.8966760	-1.6120660
		H	2.0369680	-1.8509540	-0.1084370
		H	1.3530440	-2.5839000	-1.5782810
		C	-1.4047700	1.6546420	-0.9888840
		H	-1.9029820	0.8966760	-1.6120660
		H	-2.0369680	1.8509540	-0.1084370
		H	-1.3530440	2.5839000	-1.5782810
		H	0.6460320	1.0662810	-1.4654170
		H	-0.6460320	-1.0662810	-1.4654170
		Na	0.0000000	0.0000000	2.4190100
32. $[Na\text{-}MeOH]^+$	-277.8807457	C	1.4590820	0.7342020	0.0000000
		H	1.8597920	-0.2878080	0.0000000
		O	0.0000000	0.6236930	0.0000000
		H	1.8053510	1.2571780	0.9034470
		H	1.8053510	1.2571780	-0.9034470
		H	-0.3559830	1.5289110	0.0000000
		Na	-1.2608190	-1.1954740	0.0000000
33. $[Na\text{-}DCM]^+$	-1121.93022	C	0.0000000	0.0000000	-1.3336900
		H	0.9143750	0.0000000	-1.9334420
		H	-0.9143750	0.0000000	-1.9334420
		Cl	0.0000000	1.4991070	-0.3205170
		Cl	0.0000000	-1.4991070	-0.3205170
		Na	0.0000000	0.0000000	2.0696910
34. $[K\text{-}H_2O]^+$	-676.2808215	O	0.0000000	0.0000000	-1.6496190
		K	0.0000000	0.0000000	0.9313890
		H	0.0000000	0.7659830	-2.2497170
		H	0.0000000	-0.7659830	-2.2497170
35. $[K\text{-}THF]^+$	-832.3417972	C	0.4996920	1.0886480	-0.8126530
		H	1.6029170	1.0909770	-0.7638390
		H	0.1158530	2.0424790	-0.4168330
		C	0.0000000	0.7699880	-2.2217210
		H	0.6474960	1.2005260	-2.9985670
		H	-1.0201070	1.1588750	-2.3705200
		C	0.0000000	-0.7699880	-2.2217210
		H	-0.6474960	-1.2005260	-2.9985670
		H	1.0201070	-1.1588750	-2.3705200
		C	-0.4996920	-1.0886480	-0.8126530
		H	-0.1158530	-2.0424790	-0.4168330
		H	-1.6029170	-1.0909770	-0.7638390
		O	0.0000000	0.0000000	0.0452550
		K	0.0000000	0.0000000	2.5868400

36. [K-DEE]$^+$, TT	-833.5515086	C	0.0000000	1.2036640	-1.4039950
		H	-0.8945020	1.1981250	-2.0535290
		C	0.0000000	-1.2036640	-1.4039950
		H	-0.8945020	-1.1981250	-2.0535290
		O	0.0000000	0.0000000	-0.5926200
		H	0.8945020	1.1981250	-2.0535290
		C	0.0000000	2.4224220	-0.4944050
		H	0.0000000	3.3415660	-1.0990960
		H	-0.9047570	2.4588210	0.1365730
		H	0.9047570	2.4588210	0.1365730
		H	0.8945020	-1.1981250	-2.0535290
		C	0.0000000	-2.4224220	-0.4944050
		H	0.9047570	-2.4588210	0.1365730
		H	-0.9047570	-2.4588210	0.1365730
		H	0.0000000	-3.3415660	-1.0990960
		K	0.0000000	0.0000000	1.9677780
37. [K-DEE]$^+$, TG	-833.549501	C	0.5949570	1.4754830	0.1023350
		H	1.3035550	1.6577310	-0.7232600
		C	1.5455040	-0.7032620	0.5989400
		H	2.0166250	-0.2045500	1.4652460
		O	0.3499690	0.0486330	0.2301710
		H	1.0547990	1.8392460	1.0395260
		C	-0.7223450	2.1879050	-0.1630560
		H	-0.5507180	3.2705920	-0.2577780
		H	-1.1794190	1.8596480	-1.1129420
		H	-1.4346590	2.0513470	0.6688930
		H	1.1740070	-1.6820960	0.9462690
		C	2.5357750	-0.8821390	-0.5469610
		H	2.0619810	-1.3679420	-1.4143030
		H	2.9717890	0.0728450	-0.8752730
		H	3.3677890	-1.5225140	-0.2139650
		K	-1.9636240	-0.9911200	-0.0690180
38. [K-DEE]$^+$, GG	-833.5477122	C	0.0000000	1.2206370	-1.0058420
		H	0.4736080	1.9929960	-0.3764300
		C	0.0000000	-1.2206370	-1.0058420
		H	-0.4736080	-1.9929960	-0.3764300
		O	0.0000000	0.0000000	-0.2015350
		C	1.4031710	-1.6428520	-1.4263160
		H	1.8879080	-0.8830210	-2.0579560
		H	2.0481270	-1.8291320	-0.5529660
		H	1.3520320	-2.5744470	-2.0120530
		C	-1.4031710	1.6428520	-1.4263160
		H	-1.8879080	0.8830210	-2.0579560

		H	-2.0481270	1.8291320	-0.5529660
		H	-1.3520320	2.5744470	-2.0120530
		H	0.6571730	1.0740820	-1.8792700
		H	-0.6571730	-1.0740820	-1.8792700
		K	0.0000000	0.0000000	2.3450280
39. $[K\text{-}MeOH]^+$	-715.5859809	C	1.3311910	1.6927140	0.0000000
		H	2.0537080	0.8653810	0.0000000
		O	0.0000000	1.0985730	0.0000000
		H	1.4892130	2.3026840	0.9025830
		H	1.4892130	2.3026840	-0.9025830
		H	-0.6355280	1.8346850	0.0000000
		K	-0.6517760	-1.3815950	0.0000000
40. $[K\text{-}DCM]^+$	-1559.638056	C	0.0000000	0.0000000	-1.7643150
		H	0.9130210	0.0000000	-2.3654340
		H	-0.9130210	0.0000000	-2.3654340
		Cl	0.0000000	1.5018120	-0.7598110
		Cl	0.0000000	-1.5018120	-0.7598110
		K	0.0000000	0.0000000	2.1658070
41. $[Me_4cyclenH]^+$	-693.6594398	C	-3.966080	-0.355882	0.486007
		H	-4.738966	-0.392945	-0.311653
		H	-4.253193	0.419378	1.212275
		H	-3.973936	-1.322471	1.013888
		C	0.693760	-1.909222	1.575626
		H	0.886167	-2.990798	1.534210
		H	-0.046421	-1.693881	2.356709
		H	1.614960	-1.350032	1.775731
		C	3.953272	0.349036	0.499060
		H	4.245455	-0.431888	1.218421
		H	3.940462	1.308546	1.037480
		H	4.731660	0.407214	-0.291334
		C	-0.675007	1.950235	1.536456
		H	-0.887776	3.036992	1.499747
		H	0.062647	1.769134	2.331555
		H	-1.596075	1.406664	1.785443
		C	-2.112010	-1.174464	-0.863838
		H	-1.565068	-0.778670	-1.736060
		H	-2.931448	-1.791765	-1.283402
		C	-1.206959	-2.082729	-0.027581
		H	-1.015695	-3.051552	-0.516328
		H	-1.688528	-2.274706	0.941471
		C	1.088240	-1.711128	-0.892988
		H	0.646894	-1.211891	-1.768174
		H	1.076009	-2.794853	-1.088921

		C	2.533239	-1.254154	-0.652891
		H	3.062265	-1.335041	-1.630854
		H	3.034765	-1.967717	0.021627
		C	2.104199	1.175605	-0.866182
		H	1.563819	0.780583	-1.743176
		H	2.937703	1.777685	-1.278116
		C	1.182306	2.076924	-0.039217
		H	1.034861	3.053278	-0.543744
		H	1.678228	2.283654	0.921731
		C	-1.072759	1.718823	-0.871465
		H	-0.655542	1.245949	-1.777997
		H	-1.106194	2.808285	-1.084435
		C	-2.519448	1.256066	-0.635191
		H	-3.066159	1.342965	-1.601342
		H	-3.014205	1.955569	0.057395
		N	-2.620060	-0.076663	-0.032518
		N	2.613679	0.064980	-0.035531
		N	-0.136500	1.440505	0.253064
		H	0.014376	-0.348068	0.327806
		N	0.141797	-1.442291	0.262594
42. [K(Me_4cyclen)][$HBPh_3$]	-2013.860432	K	0.784205	-0.098686	-0.140566
		H	-1.536208	-0.086526	1.067165
		B	-2.301625	-0.008329	0.076393
		N	3.030588	-1.954204	-0.419959
		N	1.978776	-1.008195	2.363114
		N	2.145834	1.943044	1.369068
		N	3.220182	0.986825	-1.407002
		C	3.181477	-2.660307	0.868933
		H	2.328976	-3.353148	0.959893
		H	4.096770	-3.298407	0.875438
		C	3.228747	-1.747797	2.105287
		H	3.505233	-2.377545	2.983159
		H	4.047453	-1.020283	1.991442
		C	2.206515	0.190712	3.196069
		H	1.220853	0.529335	3.553658
		H	2.795264	-0.058697	4.110290
		C	2.914710	1.351085	2.479129
		H	3.161574	2.123601	3.245128
		H	3.880400	0.998020	2.085233
		C	3.007804	2.707273	0.446017
		H	3.648424	3.435577	0.997871
		H	2.343194	3.310846	-0.193101
		C	3.926655	1.848729	-0.438404
		H	4.630227	2.534478	-0.965811
		H	4.555814	1.209830	0.200294

C	4.065405	-0.139644	-1.853212
H	5.073578	0.210685	-2.178185
H	3.592531	-0.567741	-2.752345
C	4.265655	-1.248068	-0.806985
H	5.022150	-1.962646	-1.209362
H	4.716245	-0.814263	0.098962
C	2.622082	-2.905936	-1.466165
H	3.371519	-3.715621	-1.619377
H	2.486274	-2.385380	-2.425837
H	1.655545	-3.362385	-1.203185
C	0.982289	-1.877792	3.009824
H	1.302296	-2.206389	4.024772
H	0.807766	-2.777865	2.401976
H	0.022581	-1.345779	3.094847
C	1.068090	2.807356	1.881768
H	0.389226	2.230978	2.526924
H	0.466441	3.195299	1.046209
H	1.463371	3.666013	2.470991
C	2.772673	1.774237	-2.566714
H	3.622226	2.241241	-3.115626
H	2.083858	2.570516	-2.248783
H	2.222122	1.127183	-3.266671
C	-1.934106	1.398478	-0.691180
C	-1.307715	1.508405	-1.956190
H	-1.101977	0.597230	-2.531907
C	-0.972688	2.747922	-2.533823
H	-0.514201	2.780120	-3.528182
C	-1.254113	3.939468	-1.856192
H	-1.011745	4.907018	-2.305478
C	-1.881765	3.871351	-0.600509
H	-2.128045	4.793877	-0.064146
C	-2.210302	2.630417	-0.041819
H	-2.716368	2.601864	0.929223
C	-2.076336	-1.369762	-0.810432
C	-1.449049	-2.511875	-0.255920
H	-1.101565	-2.458954	0.783929
C	-1.306100	-3.720029	-0.958998
H	-0.839932	-4.585984	-0.475718
C	-1.787016	-3.827268	-2.270498
H	-1.685255	-4.764169	-2.825789
C	-2.424932	-2.720960	-2.851012
H	-2.826445	-2.795981	-3.866887
C	-2.566764	-1.526374	-2.131190
H	-3.096954	-0.691702	-2.601900
C	-3.823583	0.003960	0.672027
C	-4.921069	0.493386	-0.073350

		H	-4.741214	0.925238	-1.064336
		C	-6.233571	0.457861	0.417809
		H	-7.055728	0.847545	-0.191585
		C	-6.496042	-0.072473	1.688603
		H	-7.518199	-0.100207	2.077863
		C	-5.430136	-0.562094	2.455418
		H	-5.618574	-0.974202	3.452575
		C	-4.123026	-0.520701	1.949021
		H	-3.301663	-0.905622	2.564743
43. $[HBPh_3]^-$	-720.6180429	H	-0.013985	-0.005762	-2.092210
		B	-0.023108	-0.005625	-0.850743
		C	-1.521614	-0.480276	-0.386623
		C	-1.787071	-1.611256	0.419321
		H	-0.941953	-2.207968	0.779937
		C	-3.090952	-2.000077	0.770483
		H	-3.245061	-2.887325	1.396382
		C	-4.193926	-1.260310	0.325327
		H	-5.212861	-1.558306	0.595946
		C	-3.969127	-0.129447	-0.476397
		H	-4.819420	0.462332	-0.836733
		C	-2.662791	0.242262	-0.819003
		H	-2.510023	1.126980	-1.448448
		C	1.143988	-1.044808	-0.355402
		C	1.637148	-2.064669	-1.204091
		H	1.230786	-2.132625	-2.220294
		C	2.622473	-2.977274	-0.796557
		H	2.976507	-3.748664	-1.492341
		C	3.159361	-2.903252	0.497629
		H	3.930607	-3.610611	0.822195
		C	2.694158	-1.905407	1.368327
		H	3.103825	-1.830282	2.383417
		C	1.711093	-0.999606	0.942038
		H	1.375027	-0.218914	1.635572
		C	0.331724	1.520551	-0.363350
		C	-0.270876	2.161765	0.744786
		H	-1.059006	1.633111	1.292843
		C	0.091680	3.454471	1.158729
		H	-0.405128	3.910242	2.023867
		C	1.083084	4.164948	0.469257
		H	1.368425	5.174422	0.784945
		C	1.701434	3.561184	-0.637591
		H	2.476844	4.103329	-1.192523
		C	1.327187	2.271379	-1.035959
		H	1.819094	1.817094	-1.904383

44. K^+-**1c**	-1751.3986291	K	0.0000000	0.0000000	1.0504320
		N	-1.9853970	-1.0084690	-0.8551030
		N	-1.0084690	1.9853970	-0.8551030
		N	1.9853970	1.0084690	-0.8551030
		N	1.0084690	-1.9853970	-0.8551030
		C	2.2700400	-1.4545130	-1.4202470
		H	3.0449920	-1.5417970	-0.6418020
		H	2.6204560	-2.0854650	-2.2698140
		C	2.2126350	0.0000000	-1.9134410
		H	3.1573040	0.2069820	-2.4654980
		H	1.4109900	0.0981220	-2.6602680
		C	1.4545130	2.2700400	-1.4202470
		H	1.5417970	3.0449920	-0.6418020
		H	2.0854650	2.6204560	-2.2698140
		C	0.0000000	2.2126350	-1.9134410
		H	-0.2069820	3.1573040	-2.4654980
		H	-0.0981220	1.4109900	-2.6602680
		C	-2.2700400	1.4545130	-1.4202470
		H	-3.0449920	1.5417970	-0.6418020
		H	-2.6204560	2.0854650	-2.2698140
		C	-2.2126350	0.0000000	-1.9134410
		H	-3.1573040	-0.2069820	-2.4654980
		H	-1.4109900	-0.0981220	-2.6602680
		C	-1.4545130	-2.2700400	-1.4202470
		H	-1.5417970	-3.0449920	-0.6418020
		H	-2.0854650	-2.6204560	-2.2698140
		C	0.0000000	-2.2126350	-1.9134410
		H	0.2069820	-3.1573040	-2.4654980
		H	0.0981220	-1.4109900	-2.6602680
		C	-1.8378220	3.0668570	1.2761220
		H	-2.1245590	4.0639630	1.6576170
		H	-2.7425100	2.4298640	1.2743800
		C	-1.2743490	3.2473580	-0.1279360
		H	-1.9636620	3.9042440	-0.7059990
		H	-0.3267350	3.7989290	-0.0262670
		C	-3.2473580	-1.2743490	-0.1279360
		H	-3.7989290	-0.3267350	-0.0262670
		H	-3.9042440	-1.9636620	-0.7059990
		C	-3.0668570	-1.8378220	1.2761220
		H	-4.0639630	-2.1245590	1.6576170
		H	-2.4298640	-2.7425100	1.2743800
		C	1.8378220	-3.0668570	1.2761220
		H	2.7425100	-2.4298640	1.2743800
		H	2.1245590	-4.0639630	1.6576170
		C	1.2743490	-3.2473580	-0.1279360
		H	1.9636620	-3.9042440	-0.7059990

		H	0.3267350	-3.7989290	-0.0262670
		C	3.0668570	1.8378220	1.2761220
		H	2.4298640	2.7425100	1.2743800
		H	4.0639630	2.1245590	1.6576170
		C	3.2473580	1.2743490	-0.1279360
		H	3.9042440	1.9636620	-0.7059990
		H	3.7989290	0.3267350	-0.0262670
		O	2.4813970	0.8154750	2.1144630
		H	2.5397020	1.1326300	3.0311190
		O	0.8154750	-2.4813970	2.1144630
		H	1.1326300	-2.5397020	3.0311190
		O	-2.4813970	-0.8154750	2.1144630
		H	-2.5397020	-1.1326300	3.0311190
		O	-0.8154750	2.4813970	2.1144630
		H	-1.1326300	2.5397020	3.0311190
45. K^+-**1d**	-3426.5971897	K	0.0000000	0.0000000	0.3427130
		O	-1.3684550	2.0351250	-1.0895960
		O	-1.6984360	-1.8734650	-0.9388590
		O	1.3684550	-2.0351250	-1.0895960
		O	1.6984360	1.8734650	-0.9388590
		O	-0.6702750	5.7676690	1.5761160
		O	-5.5901930	-0.4191770	1.1459600
		O	0.6702750	-5.7676690	1.5761160
		O	5.5901930	0.4191770	1.1459600
		N	-0.9173030	2.0273500	2.3806310
		N	-2.0160200	-0.9308740	2.3838610
		N	0.9173030	-2.0273500	2.3806310
		N	2.0160200	0.9308740	2.3838610
		N	-1.0886140	3.2393690	-0.7408430
		N	-0.7373000	5.0172480	0.5539810
		N	-2.8906350	-1.3985270	-0.7820100
		N	-4.7484890	-0.6986330	0.2330850
		N	1.0886140	-3.2393690	-0.7408430
		N	0.7373000	-5.0172480	0.5539810
		N	2.8906350	1.3985270	-0.7820100
		N	4.7484890	0.6986330	0.2330850
		C	-1.7333410	1.3707500	3.4287320
		C	-2.6856010	0.2714840	2.9372740
		C	-1.3652760	-1.7261160	3.4511460
		C	-0.2714040	-2.6891320	2.9687470
		C	1.7333410	-1.3707500	3.4287320
		C	2.6856010	-0.2714840	2.9372740
		C	1.3652760	1.7261160	3.4511460
		C	0.2714040	2.6891320	2.9687470
		C	-1.7669090	3.0296920	1.6928460

C	-1.1499250	3.7251600	0.5260990
C	-0.8667470	4.3647580	-1.7443030
C	-0.2084500	5.4521930	-0.8167150
C	-2.2710730	4.7578340	-2.2483990
C	0.0000000	3.8775610	-2.9033570
C	-0.6324950	6.8975750	-1.0755400
C	1.3242530	5.3423970	-0.7222010
C	-3.0181140	-1.7873440	1.7046000
C	-3.5268080	-1.2564750	0.4077200
C	-3.8274970	-1.1141330	-1.9482300
C	-4.9655290	-0.2929450	-1.2269170
C	-3.0704180	-0.3602240	-3.0437130
C	-4.2897810	-2.4912530	-2.4653840
C	-4.7656700	1.2334320	-1.2724220
C	-6.4002290	-0.6490730	-1.6236430
C	1.7669090	-3.0296920	1.6928460
C	1.1499250	-3.7251600	0.5260990
C	0.8667470	-4.3647580	-1.7443030
C	0.2084500	-5.4521930	-0.8167150
C	0.0000000	-3.8775610	-2.9033570
C	2.2710730	-4.7578340	-2.2483990
C	-1.3242530	-5.3423970	-0.7222010
C	0.6324950	-6.8975750	-1.0755400
C	3.0181140	1.7873440	1.7046000
C	3.5268080	1.2564750	0.4077200
C	3.8274970	1.1141330	-1.9482300
C	4.9655290	0.2929450	-1.2269170
C	3.0704180	0.3602240	-3.0437130
C	4.2897810	2.4912530	-2.4653840
C	4.7656700	-1.2334320	-1.2724220
C	6.4002290	0.6490730	-1.6236430
H	-2.3436170	2.1219150	3.9796840
H	-1.0463630	0.9483750	4.1759530
H	-3.3510050	-0.0019280	3.7871390
H	-3.3574110	0.6677140	2.1590150
H	-0.9385480	-1.0263830	4.1839790
H	-2.1172420	-2.3227220	4.0153850
H	-0.6822590	-3.3673320	2.2044260
H	0.0135930	-3.3402510	3.8251170
H	2.3436170	-2.1219150	3.9796840
H	1.0463630	-0.9483750	4.1759530
H	3.3574110	-0.6677140	2.1590150
H	3.3510050	0.0019280	3.7871390
H	2.1172420	2.3227220	4.0153850
H	0.9385480	1.0263830	4.1839790
H	0.6822590	3.3673320	2.2044260

H	-0.0135930	3.3402510	3.8251170
H	-2.6652690	2.5111460	1.3217180
H	-2.0882360	3.8330920	2.3917050
H	-2.7448310	3.8747050	-2.7014260
H	-2.9156570	5.1231390	-1.4344090
H	-2.1995480	5.5423450	-3.0161660
H	-0.5540670	3.1269490	-3.4847900
H	0.9229590	3.4079940	-2.5391620
H	0.2387820	4.7200050	-3.5708650
H	-0.2521640	7.2315480	-2.0529780
H	-1.7225080	7.0289450	-1.0554250
H	-0.2012440	7.5409460	-0.2959630
H	1.6440550	4.2990830	-0.5745260
H	1.6666320	5.9587360	0.1224880
H	1.7924550	5.7239440	-1.6417410
H	-2.5420580	-2.7553340	1.4837160
H	-3.9045980	-1.9686310	2.3497790
H	-2.6264300	0.5746250	-2.6760990
H	-3.7501380	-0.1373130	-3.8805810
H	-2.2579330	-0.9964090	-3.4225330
H	-3.4105070	-3.0589230	-2.8029530
H	-4.9711580	-2.3740740	-3.3208810
H	-4.8028420	-3.0741500	-1.6857110
H	-4.9962920	1.6173820	-2.2776060
H	-5.4632850	1.6953310	-0.5577320
H	-3.7341800	1.5214750	-1.0163720
H	-6.5895620	-0.3451710	-2.6642600
H	-6.6133080	-1.7214400	-1.5225970
H	-7.0941140	-0.1035080	-0.9690370
H	2.6652690	-2.5111460	1.3217180
H	2.0882360	-3.8330920	2.3917050
H	-0.9229590	-3.4079940	-2.5391620
H	0.5540670	-3.1269490	-3.4847900
H	-0.2387820	-4.7200050	-3.5708650
H	2.9156570	-5.1231390	-1.4344090
H	2.7448310	-3.8747050	-2.7014260
H	2.1995480	-5.5423450	-3.0161660
H	-1.6666320	-5.9587360	0.1224880
H	-1.7924550	-5.7239440	-1.6417410
H	-1.6440550	-4.2990830	-0.5745260
H	0.2012440	-7.5409460	-0.2959630
H	0.2521640	-7.2315480	-2.0529780
H	1.7225080	-7.0289450	-1.0554250
H	3.9045980	1.9686310	2.3497790
H	2.5420580	2.7553340	1.4837160
H	2.6264300	-0.5746250	-2.6760990

H	3.7501380	0.1373130	-3.8805810
H	2.2579330	0.9964090	-3.4225330
H	3.4105070	3.0589230	-2.8029530
H	4.8028420	3.0741500	-1.6857110
H	4.9711580	2.3740740	-3.3208810
H	3.7341800	-1.5214750	-1.0163720
H	4.9962920	-1.6173820	-2.2776060
H	5.4632850	-1.6953310	-0.5577320
H	6.6133080	1.7214400	-1.5225970
H	6.5895620	0.3451710	-2.6642600
H	7.0941140	0.1035080	-0.9690370

Table S21: Cartesian coordinates (in Å) and total electronic energies (in Hartree) of all stationary points obtained using the B3LYP/6-311G(d,p) method.

Species	Total Electronic Energy (Hartree)	Atom	Coordinates		
1. **Li-H_2O-2a**	-777.197067	C	0.000000	3.181469	0.874712
		H	0.059392	4.170750	0.396841
		H	0.753790	3.139537	1.663437
		H	-0.981964	3.091807	1.341223
		C	-3.168032	0.005177	0.880679
		H	-4.160938	0.069063	0.410890
		H	-3.110705	0.754857	1.671148
		H	-3.076015	-0.974880	1.349162
		C	0.000000	-3.181469	0.874712
		H	-0.753790	-3.139537	1.663437
		H	0.981964	-3.091807	1.341223
		H	-0.059392	-4.170750	0.396841
		C	3.168032	-0.005177	0.880679
		H	4.160938	-0.069063	0.410890
		H	3.110705	-0.754857	1.671148
		H	3.076015	0.974880	1.349162
		C	-0.805031	2.095019	-1.143983
		H	-0.449091	1.473595	-1.968587
		H	-0.935282	3.107767	-1.556931
		C	-2.161418	1.580606	-0.659712
		H	-2.881033	1.629407	-1.490705
		H	-2.548825	2.246111	0.113592
		C	-2.097417	-0.811034	-1.142437
		H	-1.480069	-0.462315	-1.973359
		H	-3.112182	-0.944857	-1.549641
		C	-1.583772	-2.164994	-0.649813
		H	-1.635148	-2.890671	-1.475293
		H	-2.248078	-2.544541	0.128223
		C	0.805031	-2.095019	-1.143983
		H	0.449091	-1.473595	-1.968587
		H	0.935282	-3.107767	-1.556931
		C	2.161418	-1.580606	-0.659712
		H	2.881033	-1.629407	-1.490705
		H	2.548825	-2.246111	0.113592
		C	2.097417	0.811034	-1.142437
		H	1.480069	0.462315	-1.973359
		H	3.112182	0.944857	-1.549641
		C	1.583772	2.164994	-0.649813
		H	1.635148	2.890671	-1.475293
		H	2.248078	2.544541	0.128223

		N	0.221521	2.084082	-0.080890
		N	-2.079582	0.221242	-0.086757
		N	-0.221521	-2.084082	-0.080890
		N	2.079582	-0.221242	-0.086757
		O	0.000000	0.000000	2.701290
		Li	0.000000	0.000000	0.714300
		H	-0.052299	0.767219	3.280241
		H	0.052299	-0.767219	3.280241
2. **Li-THF-2a**	-933.2600714	C	-3.128677	-0.018505	0.130705
		H	-4.126574	0.079878	-0.322343
		H	-3.040585	0.708115	0.939728
		H	-3.053719	-1.014327	0.568010
		C	0.000000	-3.314177	-0.015712
		H	-0.053744	-4.257947	-0.579444
		H	-0.752410	-3.343794	0.773126
		H	0.979310	-3.258785	0.460434
		C	3.128677	0.018505	0.130705
		H	3.040585	-0.708115	0.939728
		H	3.053719	1.014327	0.568010
		H	4.126574	-0.079878	-0.322343
		C	0.000000	3.314177	-0.015712
		H	0.053744	4.257947	-0.579444
		H	0.752410	3.343794	0.773126
		H	-0.979310	3.258785	0.460434
		C	-2.090187	-0.824205	-1.912474
		H	-1.482806	-0.470860	-2.748099
		H	-3.111994	-0.943134	-2.306710
		C	-1.585306	-2.190831	-1.448690
		H	-1.644971	-2.895464	-2.292865
		H	-2.253031	-2.584355	-0.680191
		C	0.803797	-2.075191	-1.934219
		H	0.441825	-1.420307	-2.729322
		H	0.956007	-3.063203	-2.396995
		C	2.145596	-1.559723	-1.415633
		H	2.888100	-1.605511	-2.226540
		H	2.512403	-2.224023	-0.631407
		C	2.090187	0.824205	-1.912474
		H	1.482806	0.470860	-2.748099
		H	3.111994	0.943134	-2.306710
		C	1.585306	2.190831	-1.448690
		H	1.644971	2.895464	-2.292865
		H	2.253031	2.584355	-0.680191
		C	-0.803797	2.075191	-1.934219
		H	-0.441825	1.420307	-2.729322
		H	-0.956007	3.063203	-2.396995

		C	-2.145596	1.559723	-1.415633
		H	-2.888100	1.605511	-2.226540
		H	-2.512403	2.224023	-0.631407
		C	0.480126	1.087087	2.869333
		H	-0.238184	1.910774	2.816175
		H	1.439202	1.425590	2.474707
		C	0.569946	0.513584	4.280399
		H	0.457752	1.281991	5.046137
		H	1.532313	0.018121	4.434494
		C	-0.569946	-0.513584	4.280399
		H	-0.457752	-1.281991	5.046137
		H	-1.532313	-0.018121	4.434494
		C	-0.480126	-1.087087	2.869333
		H	-1.439202	-1.425590	2.474707
		H	0.238184	-1.910774	2.816175
		N	-2.049891	0.198300	-0.847353
		N	-0.224763	-2.141369	-0.876553
		N	2.049891	-0.198300	-0.847353
		N	0.224763	2.141369	-0.876553
		O	0.000000	0.000000	2.028349
		Li	0.000000	0.000000	0.021860
3. **Li-DEE-2a**	-934.4695717	C	0.000000	3.373740	-0.037373
		H	0.119140	4.299166	-0.621093
		H	0.717973	3.390626	0.783930
		H	-1.002001	3.377349	0.392813
		C	-3.115479	-0.054493	0.155740
		H	-4.110513	-0.017756	-0.312380
		H	-3.077489	0.698156	0.944148
		H	-2.993796	-1.030439	0.625418
		C	0.000000	-3.373740	-0.037373
		H	-0.717973	-3.390626	0.783930
		H	1.002001	-3.377349	0.392813
		H	-0.119140	-4.299166	-0.621093
		C	3.115479	0.054493	0.155740
		H	4.110513	0.017756	-0.312380
		H	3.077489	-0.698156	0.944148
		H	2.993796	1.030439	0.625418
		C	-0.824880	2.085111	-1.913029
		H	-0.458835	1.431894	-2.707261
		H	-0.994612	3.067802	-2.380439
		C	-2.155207	1.551139	-1.382553
		H	-2.906181	1.587410	-2.186082
		H	-2.523743	2.209712	-0.594041
		C	-2.062548	-0.826498	-1.889548
		H	-1.446108	-0.467543	-2.716004

		H	-3.080522	-0.940143	-2.295186
		C	-1.568527	-2.198838	-1.434359
		H	-1.633470	-2.895863	-2.284710
		H	-2.240220	-2.592835	-0.669640
		C	0.824880	-2.085111	-1.913029
		H	0.458835	-1.431894	-2.707261
		H	0.994612	-3.067802	-2.380439
		C	2.155207	-1.551139	-1.382553
		H	2.906181	-1.587410	-2.186082
		H	2.523743	-2.209712	-0.594041
		C	2.062548	0.826498	-1.889548
		H	1.446108	0.467543	-2.716004
		H	3.080522	0.940143	-2.295186
		C	1.568527	2.198838	-1.434359
		H	1.633470	2.895863	-2.284710
		H	2.240220	2.592835	-0.669640
		C	0.536211	-1.097248	2.850895
		H	0.982255	-1.758311	2.107939
		C	-0.536211	1.097248	2.850895
		H	-0.982255	1.758311	2.107939
		N	0.208004	2.171285	-0.860855
		N	-2.036047	0.189498	-0.816766
		N	-0.208004	-2.171285	-0.860855
		N	2.036047	-0.189498	-0.816766
		O	0.000000	0.000000	2.080468
		C	0.504172	1.850618	3.668140
		H	0.913977	1.249222	4.481713
		H	1.331050	2.189928	3.039440
		H	0.037908	2.729995	4.120204
		C	-0.504172	-1.850618	3.668140
		H	-0.913977	-1.249222	4.481713
		H	-1.331050	-2.189928	3.039440
		H	-0.037908	-2.729995	4.120204
		H	1.344262	-0.731254	3.491315
		H	-1.344262	0.731254	3.491315
		Li	0.000000	0.000000	0.062612
4. **Li-MeOH-2a**	-816.5045468	C	-0.076611	-3.159164	0.500794
		H	-0.105976	-4.127138	-0.021479
		H	-0.891853	-3.133277	1.225276
		H	0.859482	-3.098511	1.055859
		C	3.182021	-0.096431	0.893516
		H	4.198638	-0.164205	0.477717
		H	3.068249	-0.887422	1.637973
		H	3.094402	0.865127	1.402134
		C	0.008419	3.113708	0.868270

		H	0.690083	2.996097	1.711925
		H	-1.007022	3.001203	1.248252
		H	0.117436	4.134643	0.472716
		C	-3.255959	0.060578	0.356188
		H	-4.181064	0.193207	-0.224695
		H	-3.278135	0.753738	1.198885
		H	-3.252819	-0.954051	0.756108
		C	0.908476	-2.009893	-1.399824
		H	0.638599	-1.339624	-2.218864
		H	1.049640	-3.004600	-1.851691
		C	2.233120	-1.560933	-0.781658
		H	3.015225	-1.582933	-1.555546
		H	2.541393	-2.279306	-0.020242
		C	2.238019	0.856574	-1.131052
		H	1.672633	0.562022	-2.017722
		H	3.278375	0.999789	-1.463271
		C	1.700595	2.185413	-0.597376
		H	1.828049	2.960708	-1.367741
		H	2.301723	2.505316	0.255366
		C	-0.638113	2.195948	-1.286848
		H	-0.231047	1.617159	-2.118720
		H	-0.710467	3.235988	-1.642670
		C	-2.042670	1.694579	-0.949321
		H	-2.686562	1.811930	-1.834089
		H	-2.478337	2.325502	-0.172874
		C	-1.964329	-0.666129	-1.567431
		H	-1.259249	-0.277251	-2.305171
		H	-2.931636	-0.758901	-2.085785
		C	-1.512552	-2.052913	-1.108330
		H	-1.504611	-2.733516	-1.972905
		H	-2.243532	-2.461471	-0.408594
		C	-0.897105	-0.444148	3.548143
		H	-1.855316	-0.614242	3.061415
		N	-0.201824	-2.022392	-0.426308
		N	2.142740	-0.233311	-0.138487
		N	0.296162	2.088466	-0.148527
		N	-2.050548	0.301569	-0.454108
		O	0.053636	-0.148692	2.507400
		H	-0.993819	0.395486	4.240609
		H	-0.610409	-1.344736	4.096665
		H	0.913182	0.008639	2.909774
		Li	-0.026641	-0.019763	0.524591
5. **Li-DCM-2a**	-1660.492851	C	1.137776	-0.567162	-3.034179
		H	1.861374	-0.445393	-3.853219
		H	0.162598	-0.218953	-3.377455

H	1.047476	-1.630347	-2.812800
C	1.210081	-3.013220	0.738147
H	2.011746	-3.685563	1.076862
H	0.780505	-3.423554	-0.176734
H	0.426877	-3.005294	1.496078
C	-1.084263	0.245477	2.786482
H	-1.476477	-0.768137	2.695297
H	-1.802104	0.918386	2.318060
H	-1.016162	0.501084	3.853817
C	-1.077376	2.703540	-0.967533
H	-1.035918	3.800893	-1.034315
H	-2.014246	2.418701	-0.488411
H	-1.088827	2.301575	-1.980641
C	2.828637	-0.305205	-1.303593
H	3.215918	0.439737	-0.604184
H	3.574919	-0.388425	-2.108607
C	2.706502	-1.658610	-0.601674
H	3.697542	-1.965212	-0.236008
H	2.400774	-2.417372	-1.323549
C	2.265071	-1.059613	1.725744
H	2.877158	-0.197214	1.451037
H	2.941176	-1.769254	2.226785
C	1.178081	-0.627636	2.710911
H	1.651012	-0.217378	3.614854
H	0.611052	-1.501507	3.034664
C	0.752397	1.714172	2.158775
H	1.817197	1.681325	1.915578
H	0.681949	2.130705	3.175289
C	0.028503	2.649540	1.188667
H	0.461067	3.657651	1.268663
H	-1.017448	2.742510	1.484540
C	1.341756	2.480067	-0.864450
H	2.148246	2.315711	-0.146006
H	1.385369	3.545353	-1.138815
C	1.585467	1.633176	-2.114509
H	2.545081	1.922354	-2.566828
H	0.819890	1.853327	-2.859670
C	-3.586042	-1.375141	-1.005080
N	1.534660	0.181810	-1.827888
N	1.705061	-1.646323	0.488232
N	0.224776	0.333464	2.112371
N	0.058837	2.153810	-0.205419
H	-4.131414	-2.246744	-0.661551
H	-3.744273	-1.175120	-2.058521
Cl	-1.825778	-1.753682	-0.792372
Cl	-4.117478	0.037685	-0.063812

		Li	0.286803	-0.025841	-0.035465
6. **Na-H_2O-2a**	-931.9551806	C	0.000000	-3.364722	0.660490
		H	-0.093752	-4.297012	0.082428
		H	-0.733505	-3.390101	1.469118
		H	0.993994	-3.346457	1.110093
		C	3.347798	-0.003371	0.675571
		H	4.286575	-0.090283	0.107021
		H	3.364872	-0.740679	1.480505
		H	3.320171	0.986290	1.133571
		C	0.000000	3.364722	0.660490
		H	0.733505	3.390101	1.469118
		H	-0.993994	3.346457	1.110093
		H	0.093752	4.297012	0.082428
		C	-3.347798	0.003371	0.675571
		H	-4.286575	0.090283	0.107021
		H	-3.364872	0.740679	1.480505
		H	-3.320171	-0.986290	1.133571
		C	0.813346	-2.075807	-1.227912
		H	0.442770	-1.410967	-2.009501
		H	0.961975	-3.055092	-1.710854
		C	2.178115	-1.577787	-0.737802
		H	2.891488	-1.653355	-1.574259
		H	2.551557	-2.250061	0.037496
		C	2.078542	0.817285	-1.223484
		H	1.419638	0.451353	-2.012337
		H	3.061757	0.967520	-1.698071
		C	1.580261	2.181161	-0.731223
		H	1.661304	2.896870	-1.565205
		H	2.249612	2.550170	0.048678
		C	-0.813346	2.075807	-1.227912
		H	-0.442770	1.410967	-2.009501
		H	-0.961975	3.055092	-1.710854
		C	-2.178115	1.577787	-0.737802
		H	-2.891488	1.653355	-1.574259
		H	-2.551557	2.250061	0.037496
		C	-2.078542	-0.817285	-1.223484
		H	-1.419638	-0.451353	-2.012337
		H	-3.061757	-0.967520	-1.698071
		C	-1.580261	-2.181161	-0.731223
		H	-1.661304	-2.896870	-1.565205
		H	-2.249612	-2.550170	0.048678
		N	-0.212952	-2.168442	-0.169214
		N	2.161634	-0.213718	-0.169412
		N	0.212952	2.168442	-0.169214
		N	-2.161634	0.213718	-0.169412

		O	0.000000	0.000000	3.343390
		Na	0.000000	0.000000	1.032100
		H	0.115109	-0.757037	3.927750
		H	-0.115109	0.757037	3.927750
7. **Na-THF-2a**	-1088.019999	C	0.000000	3.355569	-0.175823
		H	0.101545	4.290910	-0.747972
		H	0.727588	3.370802	0.638088
		H	-0.996626	3.339509	0.267831
		C	-3.360304	0.005058	-0.180661
		H	-4.293721	0.092480	-0.758235
		H	-3.386063	0.742465	0.624090
		H	-3.337340	-0.985172	0.276425
		C	0.000000	-3.355569	-0.175823
		H	-0.727588	-3.370802	0.638088
		H	0.996626	-3.339509	0.267831
		H	-0.101545	-4.290910	-0.747972
		C	3.360304	-0.005058	-0.180661
		H	4.293721	-0.092480	-0.758235
		H	3.386063	-0.742465	0.624090
		H	3.337340	0.985172	0.276425
		C	-0.814453	2.077058	-2.070458
		H	-0.445301	1.414473	-2.854611
		H	-0.961982	3.058317	-2.550202
		C	-2.179986	1.580049	-1.582018
		H	-2.892302	1.656216	-2.419554
		H	-2.553717	2.252882	-0.807290
		C	-2.075036	-0.814113	-2.067593
		H	-1.411414	-0.447204	-2.851931
		H	-3.055228	-0.964598	-2.548565
		C	-1.578097	-2.177185	-1.572804
		H	-1.660138	-2.894734	-2.405334
		H	-2.247307	-2.544106	-0.791807
		C	0.814453	-2.077058	-2.070458
		H	0.445301	-1.414473	-2.854611
		H	0.961982	-3.058317	-2.550202
		C	2.179986	-1.580049	-1.582018
		H	2.892302	-1.656216	-2.419554
		H	2.553717	-2.252882	-0.807290
		C	2.075036	0.814113	-2.067593
		H	1.411414	0.447204	-2.851931
		H	3.055228	0.964598	-2.548565
		C	1.578097	2.177185	-1.572804
		H	1.660138	2.894734	-2.405334
		H	2.247307	2.544106	-0.791807
		C	0.936230	-0.732446	3.368619

		H	1.912548	-0.239521	3.313017
		H	1.027121	-1.747038	2.975101
		C	0.361309	-0.677380	4.781759
		H	1.135360	-0.751027	5.546484
		H	-0.350858	-1.491793	4.939544
		C	-0.361309	0.677380	4.781759
		H	-1.135360	0.751027	5.546484
		H	0.350858	1.491793	4.939544
		C	-0.936230	0.732446	3.368619
		H	-1.027121	1.747038	2.975101
		H	-1.912548	0.239521	3.313017
		N	0.211154	2.163776	-1.011825
		N	-2.166249	0.216195	-1.013600
		N	-0.211154	-2.163776	-1.011825
		N	2.166249	-0.216195	-1.013600
		O	0.000000	0.000000	2.530052
		Na	0.000000	0.000000	0.219377
8. **Na-DEE-2a**	-1089.231096	C	-0.147487	2.972712	1.614101
		H	-0.739000	3.829200	1.973211
		H	0.661345	3.354835	0.988220
		H	0.301602	2.487105	2.481753
		C	-0.110920	-1.594383	2.941746
		H	-0.677639	-1.959380	3.812402
		H	0.699437	-0.957765	3.301925
		H	0.339867	-2.455328	2.446651
		C	-0.159794	-2.972635	-1.614816
		H	0.649862	-3.356902	-0.991073
		H	0.287540	-2.487544	-2.483460
		H	-0.754281	-3.827691	-1.972713
		C	-0.118723	1.593979	-2.944109
		H	-0.688886	1.959868	-3.812289
		H	0.688680	0.955870	-3.307688
		H	0.336153	2.454446	-2.451573
		C	-2.017780	1.432881	1.702621
		H	-2.793280	1.019112	1.056350
		H	-2.509772	2.218183	2.298979
		C	-1.522207	0.347684	2.665230
		H	-2.355190	0.072665	3.331890
		H	-0.744393	0.762302	3.310837
		C	-2.013364	-1.709852	1.440278
		H	-2.803688	-1.073642	1.039015
		H	-2.484851	-2.309971	2.235477
		C	-1.528084	-2.672043	0.350310
		H	-2.366038	-3.335999	0.082355
		H	-0.749512	-3.319821	0.759004

		C	-2.027390	-1.428858	-1.696553
		H	-2.799150	-1.012617	-1.047753
		H	-2.523689	-2.212969	-2.290948
		C	-1.532540	-0.345085	-2.661041
		H	-2.367696	-0.068276	-3.324717
		H	-0.758679	-0.761718	-3.309371
		C	-2.014129	1.713370	-1.434237
		H	-2.803981	1.078780	-1.029810
		H	-2.487809	2.314310	-2.227476
		C	-1.522675	2.674698	-0.346335
		H	-2.357910	3.341030	-0.075910
		H	-0.743746	3.320119	-0.758009
		C	3.385302	-1.032476	-0.645569
		H	2.747459	-1.440810	-1.433071
		C	3.386178	1.026504	0.637691
		H	2.748394	1.435459	1.425025
		N	-0.960194	2.013731	0.850214
		N	-0.955924	-0.844061	1.999945
		N	-0.968116	-2.012166	-0.847886
		N	-0.960893	0.845530	-1.998288
		O	2.603427	-0.002202	-0.004566
		Na	0.270079	-0.000469	-0.000700
		C	3.815424	2.122891	-0.326647
		H	4.459502	1.738075	-1.120234
		H	2.947242	2.597072	-0.791148
		H	4.377481	2.891552	0.210734
		C	3.812207	-2.128758	0.319935
		H	4.456497	-1.744453	1.113647
		H	2.942908	-2.601026	0.784383
		H	4.373198	-2.899019	-0.216433
		H	4.252793	-0.579930	-1.135730
		H	4.252728	0.572634	1.128230
9. **Na-MeOH-2a**	-971.2628381	C	-2.099480	-2.610411	-0.137629
		H	-2.587479	-3.272895	-0.869153
		H	-2.872631	-2.176288	0.499443
		H	-1.453707	-3.221665	0.494079
		C	2.473260	-2.111916	1.073253
		H	3.264057	-2.768391	0.678053
		H	1.840511	-2.701496	1.739764
		H	2.951740	-1.332316	1.668188
		C	1.970604	2.602638	1.009689
		H	2.339419	2.146091	1.930385
		H	1.091575	3.196873	1.262738
		H	2.746032	3.285704	0.629551
		C	-2.595903	2.109676	-0.204834

		H	-3.091489	2.785411	-0.918967
		H	-2.374923	2.673497	0.703709
		H	-3.302460	1.320083	0.055409
		C	-0.222649	-2.104663	-1.589510
		H	0.103409	-1.349348	-2.306385
		H	-0.579438	-2.956341	-2.191094
		C	0.979663	-2.581044	-0.765999
		H	1.683577	-3.085296	-1.447588
		H	0.652482	-3.341796	-0.054106
		C	2.477308	-0.649767	-0.863224
		H	1.949353	-0.508849	-1.807377
		H	3.427735	-1.145209	-1.119414
		C	2.805338	0.717794	-0.252990
		H	3.504922	1.236391	-0.928230
		H	3.344232	0.575987	0.686207
		C	1.060244	2.148627	-1.192919
		H	1.135240	1.413377	-1.995278
		H	1.663901	3.011656	-1.517454
		C	-0.394561	2.612979	-1.060197
		H	-0.672790	3.137357	-1.988683
		H	-0.467075	3.354848	-0.262213
		C	-1.639422	0.694865	-1.929846
		H	-0.715348	0.575077	-2.497236
		H	-2.344807	1.203138	-2.606946
		C	-2.215930	-0.685975	-1.595733
		H	-2.489990	-1.181655	-2.540898
		H	-3.147058	-0.564106	-1.038479
		C	-1.926510	-0.043586	3.750562
		H	-2.699446	0.055162	2.989539
		N	-1.324015	-1.539446	-0.783058
		N	1.655233	-1.516298	0.005313
		N	1.622285	1.554852	0.037264
		N	-1.355658	1.534101	-0.748005
		O	-0.662698	-0.095642	3.059318
		Na	-0.161201	-0.010276	0.800016
		H	-1.974691	0.820341	4.418040
		H	-2.102290	-0.960792	4.318162
		H	0.035577	-0.174143	3.717198
10. **Na-DCM-2a**	-1815.253701	C	3.385223	0.002495	-0.108733
		H	4.306284	-0.098560	-0.702895
		H	3.420628	-0.723367	0.705635
		H	3.378025	0.999840	0.333172
		C	0.000000	3.349399	-0.067583
		H	0.100479	4.286278	-0.636471
		H	0.729676	3.359698	0.744368

		H	-0.994871	3.331036	0.379582
		C	-3.385223	-0.002495	-0.108733
		H	-3.420628	0.723367	0.705635
		H	-3.378025	-0.999840	0.333172
		H	-4.306284	0.098560	-0.702895
		C	0.000000	-3.349399	-0.067583
		H	-0.100479	-4.286278	-0.636471
		H	-0.729676	-3.359698	0.744368
		H	0.994871	-3.331036	0.379582
		C	2.069054	0.814616	-1.977657
		H	1.397704	0.443196	-2.753298
		H	3.043313	0.965584	-2.469390
		C	1.572819	2.177705	-1.481009
		H	1.646177	2.894676	-2.314258
		H	2.245900	2.547618	-0.704925
		C	-0.821787	2.080752	-1.968203
		H	-0.453605	1.425380	-2.758874
		H	-0.970661	3.065721	-2.438895
		C	-2.186373	1.579947	-1.481572
		H	-2.898363	1.659424	-2.318742
		H	-2.560630	2.247889	-0.702953
		C	-2.069054	-0.814616	-1.977657
		H	-1.397704	-0.443196	-2.753298
		H	-3.043313	-0.965584	-2.469390
		C	-1.572819	-2.177705	-1.481009
		H	-1.646177	-2.894676	-2.314258
		H	-2.245900	-2.547618	-0.704925
		C	0.821787	-2.080752	-1.968203
		H	0.453605	-1.425380	-2.758874
		H	0.970661	-3.065721	-2.438895
		C	2.186373	-1.579947	-1.481572
		H	2.898363	-1.659424	-2.318742
		H	2.560630	-2.247889	-0.702953
		C	0.000000	0.000000	4.095834
		N	2.174964	-0.211908	-0.919407
		N	0.208024	2.160559	-0.911229
		N	-2.174964	0.211908	-0.919407
		N	-0.208024	-2.160559	-0.911229
		Na	0.000000	0.000000	0.262727
		H	-0.339921	0.835323	4.696953
		H	0.339921	-0.835323	4.696953
		Cl	1.378959	0.559986	3.090087
		Cl	-1.378959	-0.559986	3.090087
11. **K-H_2O-2a**	-1369.583149	C	2.795174	2.014439	0.420610
		H	3.589995	2.452596	-0.203753

H	3.271070	1.464386	1.236217
H	2.223869	2.835290	0.858267
C	-2.005176	2.777996	0.440348
H	-2.452070	3.576875	-0.172500
H	-1.448694	3.247687	1.255069
H	-2.819241	2.200349	0.882201
C	-2.795174	-2.014439	0.420610
H	-3.271070	-1.464386	1.236217
H	-2.223869	-2.835290	0.858267
H	-3.589995	-2.452596	-0.203753
C	2.005176	-2.777996	0.440348
H	2.452070	-3.576875	-0.172500
H	1.448694	-3.247687	1.255069
H	2.819241	-2.200349	0.882201
C	1.195841	1.868609	-1.391924
H	0.859222	1.162608	-2.151339
H	1.882927	2.558355	-1.909888
C	0.000000	2.691634	-0.897589
H	-0.341617	3.323920	-1.734684
H	0.333113	3.383124	-0.119738
C	-1.871163	1.196274	-1.389265
H	-1.169545	0.862956	-2.154265
H	-2.561972	1.887997	-1.899781
C	-2.695736	-0.000200	-0.899328
H	-3.326814	-0.338388	-1.738766
H	-3.388182	0.331673	-0.121836
C	-1.195841	-1.868609	-1.391924
H	-0.859222	-1.162608	-2.151339
H	-1.882927	-2.558355	-1.909888
C	0.000000	-2.691634	-0.897589
H	0.341617	-3.323920	-1.734684
H	-0.333113	-3.383124	-0.119738
C	1.871163	-1.196274	-1.389265
H	1.169545	-0.862956	-2.154265
H	2.561972	-1.887997	-1.899781
C	2.695736	0.000200	-0.899328
H	3.326814	0.338388	-1.738766
H	3.388182	-0.331673	-0.121836
N	1.911658	1.120286	-0.340619
N	-1.116309	1.903709	-0.337467
N	-1.911658	-1.120286	-0.340619
N	1.116309	-1.903709	-0.337467
O	0.000000	0.000000	4.151018
K	0.000000	0.000000	1.439972
H	0.529065	0.548611	4.740484
H	-0.529065	-0.548611	4.740484

12. **K-THF-2a**	-1525.648105	C	3.443327	-0.003169	-0.510177
		H	4.346149	-0.110678	-1.132681
		H	3.506251	-0.729514	0.303885
		H	3.459521	0.995268	-0.069221
		C	0.000000	3.426890	-0.493490
		H	0.101651	4.336883	-1.106438
		H	0.728533	3.483846	0.318950
		H	-0.996595	3.433938	-0.048223
		C	-3.443327	0.003169	-0.510177
		H	-3.506251	0.729514	0.303885
		H	-3.459521	-0.995268	-0.069221
		H	-4.346149	0.110678	-1.132681
		C	0.000000	-3.426890	-0.493490
		H	-0.101651	-4.336883	-1.106438
		H	-0.728533	-3.483846	0.318950
		H	0.996595	-3.433938	-0.048223
		C	2.062069	0.815229	-2.324213
		H	1.373355	0.439912	-3.081164
		H	3.021956	0.970844	-2.844525
		C	1.575466	2.182898	-1.829760
		H	1.668699	2.895293	-2.667031
		H	2.250005	2.547961	-1.051429
		C	-0.816449	2.063621	-2.322259
		H	-0.442120	1.379600	-3.084008
		H	-0.970474	3.027297	-2.836140
		C	-2.185590	1.577169	-1.832058
		H	-2.894887	1.671418	-2.671882
		H	-2.552798	2.251618	-1.054684
		C	-2.062069	-0.815229	-2.324213
		H	-1.373355	-0.439912	-3.081164
		H	-3.021956	-0.970844	-2.844525
		C	-1.575466	-2.182898	-1.829760
		H	-1.668699	-2.895293	-2.667031
		H	-2.250005	-2.547961	-1.051429
		C	0.816449	-2.063621	-2.322259
		H	0.442120	-1.379600	-3.084008
		H	0.970474	-3.027297	-2.836140
		C	2.185590	-1.577169	-1.832058
		H	2.894887	-1.671418	-2.671882
		H	2.552798	-2.251618	-1.054684
		C	-1.106521	-0.427137	4.065281
		H	-1.186887	-1.518582	4.011518
		H	-2.026186	0.014274	3.674019
		C	-0.766711	0.037678	5.479810
		H	-1.228201	-0.587888	6.244762

		H	-1.099076	1.067459	5.636067
		C	0.766711	-0.037678	5.479810
		H	1.228201	0.587888	6.244762
		H	1.099076	-1.067459	5.636067
		C	1.106521	0.427137	4.065281
		H	2.026186	-0.014274	3.674019
		H	1.186887	1.518582	4.011518
		N	2.205071	-0.210346	-1.273446
		N	0.209036	2.197730	-1.270668
		N	-2.205071	0.210346	-1.273446
		N	-0.209036	-2.197730	-1.270668
		O	0.000000	0.000000	3.227199
		K	0.000000	0.000000	0.522044
13. **K-DEE-2a**	-1526.862703	C	0.354686	2.132724	2.695462
		H	0.975347	2.603645	3.474441
		H	-0.462854	1.601718	3.189277
		H	-0.080622	2.929637	2.089669
		C	0.384890	2.711292	-2.150506
		H	1.026186	3.468838	-2.628863
		H	-0.421695	3.232145	-1.629668
		H	-0.062734	2.105347	-2.940416
		C	0.355425	-2.132726	-2.695416
		H	-0.462425	-1.602037	-3.189057
		H	-0.079458	-2.929916	-2.089676
		H	0.976169	-2.603396	-3.474486
		C	0.386198	-2.711338	2.150509
		H	1.027785	-3.468733	2.628716
		H	-0.420357	-3.232287	1.629722
		H	-0.061471	-2.105685	2.940626
		C	2.173010	1.925726	1.110069
		H	2.937719	1.209405	0.809432
		H	2.684186	2.646554	1.769846
		C	1.685663	2.695603	-0.123025
		H	2.527719	3.308156	-0.488203
		H	0.909591	3.404647	0.175198
		C	2.178988	1.105915	-1.913759
		H	2.931184	0.797053	-1.187834
		H	2.706431	1.757913	-2.629868
		C	1.683543	-0.122433	-2.685648
		H	2.521589	-0.492485	-3.300541
		H	0.907720	0.181654	-3.392446
		C	2.173784	-1.925010	-1.110147
		H	2.938148	-1.208330	-0.809520
		H	2.685063	-2.645724	-1.769948
		C	1.686748	-2.695092	0.122974

		H	2.529168	-3.307223	0.487987
		H	0.910891	-3.404348	-0.175285
		C	2.179640	-1.105201	1.913663
		H	2.931529	-0.795940	1.187607
		H	2.707296	-1.756990	2.629784
		C	1.683649	0.122952	2.685594
		H	2.521629	0.493327	3.300383
		H	0.907991	-0.181540	3.392391
		C	-4.274908	-1.188526	-0.022946
		H	-4.910172	-1.176996	-0.917800
		C	-4.275404	1.187267	0.023261
		H	-4.935037	1.193842	-0.853788
		N	1.120968	1.204732	1.852227
		N	1.127358	1.863016	-1.207706
		N	1.121373	-1.204453	-1.852223
		N	1.128224	-1.862709	1.207697
		O	-3.471268	-0.000462	0.000022
		H	-4.934250	-1.195391	0.854313
		C	-3.378186	-2.411199	-0.021795
		H	-3.984832	-3.319195	-0.041187
		H	-2.731589	-2.427894	-0.904028
		H	-2.760674	-2.445074	0.880107
		H	-4.910351	1.175465	0.918324
		C	-3.379201	2.410308	0.021776
		H	-2.732308	2.427340	0.903791
		H	-2.761974	2.444427	-0.880310
		H	-3.986219	3.318056	0.041274
		K	-0.683726	-0.000104	-0.000027
14. **K-MeOH-2a**	-1408.891088	C	0.904632	-2.297299	2.354831
		H	0.599830	-2.723325	3.324059
		H	1.931106	-1.935540	2.452641
		H	0.904364	-3.104283	1.619836
		C	-1.250703	-2.565736	-1.988556
		H	-2.143644	-3.193915	-2.136613
		H	-0.391593	-3.226872	-1.850864
		H	-1.090657	-1.994051	-2.904586
		C	-0.614987	2.227248	-2.565142
		H	-0.199424	1.599708	-3.357307
		H	0.179264	2.887593	-2.211980
		H	-1.404001	2.856196	-3.007662
		C	1.508560	2.489795	1.795497
		H	1.293329	3.328028	2.477458
		H	2.097601	2.877030	0.960373
		H	2.126527	1.770918	2.336792
		C	-1.349548	-1.692118	1.707212

		H	-2.028207	-0.839947	1.745128
		H	-1.655621	-2.354953	2.533872
		C	-1.568637	-2.457664	0.397097
		H	-2.578401	-2.900708	0.432299
		H	-0.875479	-3.301156	0.349477
		C	-2.486033	-0.708823	-1.045439
		H	-2.799210	-0.324928	-0.074625
		H	-3.368214	-1.222834	-1.462175
		C	-2.153301	0.467381	-1.971719
		H	-3.092321	1.007865	-2.179452
		H	-1.810877	0.084317	-2.936325
		C	-1.609819	2.220083	-0.356309
		H	-2.281788	1.616363	0.253701
		H	-2.222231	3.052181	-0.742114
		C	-0.519066	2.823764	0.536531
		H	-1.002768	3.546194	1.215517
		H	0.170269	3.407742	-0.078199
		C	-0.475593	1.240621	2.401212
		H	-1.509544	1.112899	2.080458
		H	-0.513809	1.927580	3.263055
		C	0.070677	-0.101784	2.902320
		H	-0.480615	-0.367285	3.820219
		H	1.113180	0.021980	3.205732
		C	4.719631	-0.520641	-1.473940
		H	4.697237	0.007456	-0.520918
		N	0.025788	-1.202971	1.919648
		N	-1.382088	-1.664871	-0.835190
		N	-1.113411	1.386598	-1.467978
		N	0.287658	1.844877	1.292840
		O	3.354209	-0.805551	-1.829978
		H	5.199680	0.119820	-2.218785
		H	5.298980	-1.439734	-1.351627
		H	3.362778	-1.274178	-2.670851
		K	1.045267	-0.203692	-0.539659
15. **K-DCM-2a**	-2252.886366	C	-1.754337	-0.614686	-3.225716
		H	-2.666718	-0.868582	-3.788262
		H	-0.988373	-1.353403	-3.473906
		H	-1.406703	0.358871	-3.576277
		C	-0.645057	3.381939	-0.689425
		H	-1.312451	4.258210	-0.702501
		H	-0.170811	3.303646	-1.670726
		H	0.138325	3.570668	0.046814
		C	0.858320	0.607203	3.010823
		H	1.592668	1.319658	2.627615
		H	1.324504	-0.379659	3.021198

		H	0.626067	0.881812	4.052025
		C	-0.256240	-3.383383	0.482012
		H	-0.738636	-4.246302	0.967820
		H	0.773399	-3.324535	0.842943
		H	-0.224261	-3.580032	-0.591186
		C	-2.956651	0.455812	-1.415557
		H	-3.374211	0.218361	-0.437043
		H	-3.808944	0.441649	-2.115082
		C	-2.396559	1.882885	-1.395749
		H	-3.245959	2.576086	-1.275559
		H	-1.958213	2.114836	-2.369443
		C	-1.933492	2.197052	0.984713
		H	-2.737560	1.464864	1.052921
		H	-2.406448	3.177616	1.159674
		C	-0.930910	1.955569	2.119309
		H	-1.437324	2.186714	3.071547
		H	-0.109701	2.671609	2.036716
		C	-1.301717	-0.413150	2.607620
		H	-2.286243	-0.156065	2.217128
		H	-1.400070	-0.386528	3.705558
		C	-0.957781	-1.853285	2.208550
		H	-1.659188	-2.524056	2.732588
		H	0.035651	-2.107033	2.586081
		C	-2.324575	-2.153539	0.201539
		H	-2.923354	-1.401348	0.714943
		H	-2.806612	-3.120536	0.421620
		C	-2.413411	-1.925532	-1.312322
		H	-3.451610	-2.130794	-1.622963
		H	-1.796028	-2.665284	-1.827876
		C	4.678280	-0.027630	-0.646904
		N	-1.978657	-0.590394	-1.772720
		N	-1.359611	2.136249	-0.374005
		N	-0.334646	0.604250	2.151551
		N	-0.956953	-2.120106	0.755042
		H	5.326530	-0.048064	0.221294
		H	5.229756	-0.014203	-1.579687
		Cl	3.691622	1.471661	-0.566364
		Cl	3.672280	-1.516194	-0.621174
		K	0.478422	-0.018244	-0.481697
16. $[Li(Me_4cyclen)]^+$	-700.7202837	C	-0.332383	3.110519	1.124724
		H	-0.378873	4.116046	0.682830
		H	0.421508	3.113909	1.913405
		H	-1.295718	2.897441	1.588460
		C	-3.110519	-0.332383	1.124724
		H	-4.116046	-0.378873	0.682830

		H	-3.113909	0.421508	1.913405
		H	-2.897441	-1.295718	1.588460
		C	0.332383	-3.110519	1.124724
		H	-0.421508	-3.113909	1.913405
		H	1.295718	-2.897441	1.588460
		H	0.378873	-4.116046	0.682830
		C	3.110519	0.332383	1.124724
		H	4.116046	0.378873	0.682830
		H	3.113909	-0.421508	1.913405
		H	2.897441	1.295718	1.588460
		C	-1.033146	2.011552	-0.933713
		H	-0.622391	1.449850	-1.776552
		H	-1.271897	3.014355	-1.319193
		C	-2.322628	1.345081	-0.447388
		H	-3.045822	1.309286	-1.274331
		H	-2.780067	1.959078	0.329677
		C	-2.011552	-1.033146	-0.933713
		H	-1.449850	-0.622391	-1.776552
		H	-3.014355	-1.271897	-1.319193
		C	-1.345081	-2.322628	-0.447388
		H	-1.309286	-3.045822	-1.274331
		H	-1.959078	-2.780067	0.329677
		C	1.033146	-2.011552	-0.933713
		H	0.622391	-1.449850	-1.776552
		H	1.271897	-3.014355	-1.319193
		C	2.322628	-1.345081	-0.447388
		H	3.045822	-1.309286	-1.274331
		H	2.780067	-1.959078	0.329677
		C	2.011552	1.033146	-0.933713
		H	1.449850	0.622391	-1.776552
		H	3.014355	1.271897	-1.319193
		C	1.345081	2.322628	-0.447388
		H	1.309286	3.045822	-1.274331
		H	1.959078	2.780067	0.329677
		N	0.000000	2.079359	0.123556
		N	-2.079359	0.000000	0.123556
		N	0.000000	-2.079359	0.123556
		N	2.079359	0.000000	0.123556
		Li	0.000000	0.000000	0.705431
17. $[Na(Me_4cyclen)]^+$	-855.4777801	C	-0.326637	3.349567	0.921810
		H	-0.314401	4.285740	0.343946
		H	0.395054	3.440327	1.735982
		H	-1.317366	3.239582	1.364779
		C	-3.349567	-0.326637	0.921810
		H	-4.285740	-0.314401	0.343946

		H	-3.440327	0.395054	1.735982
		H	-3.239582	-1.317366	1.364779
		C	0.326637	-3.349567	0.921810
		H	-0.395054	-3.440327	1.735982
		H	1.317366	-3.239582	1.364779
		H	0.314401	-4.285740	0.343946
		C	3.349567	0.326637	0.921810
		H	4.285740	0.314401	0.343946
		H	3.440327	-0.395054	1.735982
		H	3.239582	1.317366	1.364779
		C	-1.015712	1.988412	-0.968838
		H	-0.583673	1.364066	-1.752485
		H	-1.258831	2.949810	-1.447655
		C	-2.325594	1.359527	-0.477632
		H	-3.042787	1.363851	-1.313388
		H	-2.763247	1.990776	0.298515
		C	-1.988412	-1.015712	-0.968838
		H	-1.364066	-0.583673	-1.752485
		H	-2.949810	-1.258831	-1.447655
		C	-1.359527	-2.325594	-0.477632
		H	-1.363851	-3.042787	-1.313388
		H	-1.990776	-2.763247	0.298515
		C	1.015712	-1.988412	-0.968838
		H	0.583673	-1.364066	-1.752485
		H	1.258831	-2.949810	-1.447655
		C	2.325594	-1.359527	-0.477632
		H	3.042787	-1.363851	-1.313388
		H	2.763247	-1.990776	0.298515
		C	1.988412	1.015712	-0.968838
		H	1.364066	0.583673	-1.752485
		H	2.949810	1.258831	-1.447655
		C	1.359527	2.325594	-0.477632
		H	1.363851	3.042787	-1.313388
		H	1.990776	2.763247	0.298515
		N	0.000000	2.177756	0.089956
		N	-2.177756	0.000000	0.089956
		N	0.000000	-2.177756	0.089956
		N	2.177756	0.000000	0.089956
		Na	0.000000	0.000000	1.195848
18. $[K(Me_4cyclen)]^+$	-1293.111336	C	-0.324337	3.428577	0.722449
		H	-0.299376	4.334983	0.097608
		H	0.390547	3.561629	1.538110
		H	-1.321598	3.352200	1.159435
		C	-3.428577	-0.324337	0.722449
		H	-4.334983	-0.299376	0.097608

		H	-3.561629	0.390547	1.538110
		H	-3.352200	-1.321598	1.159435
		C	0.324337	-3.428577	0.722449
		H	-0.390547	-3.561629	1.538110
		H	1.321598	-3.352200	1.159435
		H	0.299376	-4.334983	0.097608
		C	3.428577	0.324337	0.722449
		H	4.334983	0.299376	0.097608
		H	3.561629	-0.390547	1.538110
		H	3.352200	1.321598	1.159435
		C	-1.007909	1.976579	-1.092821
		H	-0.569832	1.327908	-1.851299
		H	-1.251652	2.918922	-1.610096
		C	-2.324603	1.363754	-0.599678
		H	-3.041271	1.387838	-1.437359
		H	-2.753365	2.000728	0.177925
		C	-1.976579	-1.007909	-1.092821
		H	-1.327908	-0.569832	-1.851299
		H	-2.918922	-1.251652	-1.610096
		C	-1.363754	-2.324603	-0.599678
		H	-1.387838	-3.041271	-1.437359
		H	-2.000728	-2.753365	0.177925
		C	1.007909	-1.976579	-1.092821
		H	0.569832	-1.327908	-1.851299
		H	1.251652	-2.918922	-1.610096
		C	2.324603	-1.363754	-0.599678
		H	3.041271	-1.387838	-1.437359
		H	2.753365	-2.000728	0.177925
		C	1.976579	1.007909	-1.092821
		H	1.327908	0.569832	-1.851299
		H	2.918922	1.251652	-1.610096
		C	1.363754	2.324603	-0.599678
		H	1.387838	3.041271	-1.437359
		H	2.000728	2.753365	0.177925
		N	0.000000	2.212620	-0.039317
		N	-2.212620	0.000000	-0.039317
		N	0.000000	-2.212620	-0.039317
		N	2.212620	0.000000	-0.039317
		K	0.000000	0.000000	1.688672
19. Me_4cyclen	-693.2567013	C	-0.138374	3.755832	0.604027
		H	-0.101192	4.572646	-0.143676
		H	0.585678	3.982836	1.390825
		H	-1.131516	3.769668	1.058976
		C	-2.493804	-0.337562	1.473222
		H	-3.589282	-0.475843	1.371253

		H	-2.317101	0.443608	2.215037
		H	-2.066205	-1.260280	1.869588
		C	0.138374	-3.755832	0.604027
		H	-0.585678	-3.982836	1.390825
		H	1.131516	-3.769668	1.058976
		H	0.101192	-4.572646	-0.143676
		C	2.493804	0.337562	1.473222
		H	3.589282	0.475843	1.371253
		H	2.317101	-0.443608	2.215037
		H	2.066205	1.260280	1.869588
		C	-0.902110	2.035904	-0.908388
		H	-0.477535	1.326638	-1.619673
		H	-1.254632	2.897345	-1.507267
		C	-2.108537	1.376538	-0.222557
		H	-2.973483	1.409713	-0.913320
		H	-2.390833	1.978817	0.643930
		C	-2.002934	-0.963654	-0.822512
		H	-1.494130	-0.591396	-1.715828
		H	-3.070421	-1.073632	-1.112424
		C	-1.494976	-2.376209	-0.497380
		H	-1.619196	-2.986069	-1.415412
		H	-2.155562	-2.827871	0.248282
		C	0.902110	-2.035904	-0.908388
		H	0.477535	-1.326638	-1.619673
		H	1.254632	-2.897345	-1.507267
		C	2.108537	-1.376538	-0.222557
		H	2.973483	-1.409713	-0.913320
		H	2.390833	-1.978817	0.643930
		C	2.002934	0.963654	-0.822512
		H	1.494130	0.591396	-1.715828
		H	3.070421	1.073632	-1.112424
		C	1.494976	2.376209	-0.497380
		H	1.619196	2.986069	-1.415412
		H	2.155562	2.827871	0.248282
		N	0.138374	2.446452	0.034118
		N	-1.830700	0.019210	0.233201
		N	-0.138374	-2.446452	0.034118
		N	1.830700	-0.019210	0.233201
20. [Li-H_2O]$^+$	-83.79909206	O	0.000000	0.000000	0.332319
		Li	0.000000	0.000000	-1.495843
		H	0.000000	0.771581	0.914488
		H	0.000000	-0.771581	0.914488
21. [Li-THF]$^+$	-239.8751039	C	0.000000	1.207615	0.198547
		H	0.994568	1.655053	0.260170

		H	-0.744008	1.898682	0.596975
		C	-0.316013	0.699765	-1.201063
		H	0.099628	1.351991	-1.969396
		H	-1.396012	0.637778	-1.354218
		C	0.316013	-0.699765	-1.201063
		H	-0.099628	-1.351991	-1.969396
		H	1.396012	-0.637778	-1.354218
		C	0.000000	-1.207615	0.198547
		H	0.744008	-1.898682	0.596975
		H	-0.994568	-1.655053	0.260170
		O	0.000000	0.000000	1.053727
		Li	0.000000	0.000000	2.844440
22. $[Li\text{-}DEE]^+$, TT	-241.0917933	C	0.000000	1.224545	-0.667438
		H	-0.889419	1.222354	-1.303203
		C	0.000000	-1.224545	-0.667438
		H	-0.889419	-1.222354	-1.303203
		O	0.000000	0.000000	0.118163
		H	0.889419	1.222354	-1.303203
		C	0.000000	2.402488	0.285643
		H	0.000000	3.339131	-0.275080
		H	-0.898633	2.413608	0.913154
		H	0.898633	2.413608	0.913154
		H	0.889419	-1.222354	-1.303203
		C	0.000000	-2.402488	0.285643
		H	0.898633	-2.413608	0.913154
		H	-0.898633	-2.413608	0.913154
		H	0.000000	-3.339131	-0.275080
		Li	0.000000	0.000000	1.915535
23. $[Li\text{-}DEE]^+$, TG	-241.0893162	C	0.877422	-0.659725	0.251286
		H	0.491669	-1.469054	-0.371050
		C	-1.354227	0.359187	0.514477
		H	-1.341509	-0.089303	1.511356
		O	0.037741	0.515104	0.087361
		H	0.841731	-0.966734	1.300086
		C	2.286654	-0.276830	-0.164821
		H	2.963373	-1.126215	-0.057064
		H	2.334133	0.011543	-1.224171
		H	2.697357	0.519214	0.471431
		H	-1.733339	1.378355	0.608580
		C	-2.186572	-0.447579	-0.464006
		H	-2.171132	-0.001850	-1.461230
		H	-1.855734	-1.485185	-0.535489
		H	-3.223452	-0.460415	-0.118965
		Li	0.985103	1.906166	-0.547999

24. [Li-DEE]$^+$, GG	-241.0856891	C	0.000000	1.235429	-0.126243
		H	0.476212	1.989776	0.505417
		C	0.000000	-1.235429	-0.126243
		H	-0.476212	-1.989776	0.505417
		O	0.000000	0.000000	0.666792
		C	1.400330	-1.654816	-0.531151
		H	1.884553	-0.908238	-1.163493
		H	2.033726	-1.835489	0.340940
		H	1.345833	-2.584933	-1.102549
		C	-1.400330	1.654816	-0.531151
		H	-1.884553	0.908238	-1.163493
		H	-2.033726	1.835489	0.340940
		H	-1.345833	2.584933	-1.102549
		H	0.648697	1.079261	-0.989647
		H	-0.648697	-1.079261	-0.989647
		Li	0.000000	0.000000	2.457685
25. [Li-MeOH]$^+$	-123.1111405	C	0.447808	-0.866583	0.000000
		H	-0.445839	-1.488006	0.000000
		O	0.000000	0.528819	0.000000
		H	1.032205	-1.062906	0.898153
		H	1.032205	-1.062906	-0.898153
		H	0.778840	1.098397	0.000000
		Li	-1.694753	1.161456	0.000000
26. [Li-DCM]$^+$	-967.0933228	C	0.000000	0.000000	0.951629
		H	-0.908753	0.000000	1.543098
		H	0.908753	0.000000	1.543098
		Cl	0.000000	1.481373	-0.087240
		Cl	0.000000	-1.481373	-0.087240
		Li	0.000000	0.000000	-1.943265
27. [Na-H_2O]$^+$	-238.583059	O	0.000000	0.000000	-1.097421
		Na	0.000000	0.000000	1.104373
		H	0.000000	0.766085	-1.684365
		H	0.000000	-0.766085	-1.684365
28. [Na-THF]$^+$	-394.6543455	C	0.490240	1.093711	-0.326338
		H	1.582429	1.104473	-0.268787
		H	0.095160	2.032250	0.067414
		C	0.000000	0.767784	-1.731710
		H	0.647639	1.193305	-2.498632
		H	-1.010559	1.153841	-1.886471
		C	0.000000	-0.767784	-1.731710
		H	-0.647639	-1.193305	-2.498632

		H	1.010559	-1.153841	-1.886471
		C	-0.490240	-1.093711	-0.326338
		H	-0.095160	-2.032250	0.067414
		H	-1.582429	-1.104473	-0.268787
		O	0.000000	0.000000	0.522833
		Na	0.000000	0.000000	2.698807
29. $[Na\text{-}DEE]^+$, TT	-395.8710419	C	0.000000	1.210673	-1.031338
		H	-0.888238	1.211781	-1.671156
		C	0.000000	-1.210673	-1.031338
		H	-0.888238	-1.211781	-1.671156
		O	0.000000	0.000000	-0.240173
		H	0.888238	1.211781	-1.671156
		C	0.000000	2.404373	-0.096782
		H	0.000000	3.333193	-0.670399
		H	-0.898342	2.422566	0.530860
		H	0.898342	2.422566	0.530860
		H	0.888238	-1.211781	-1.671156
		C	0.000000	-2.404373	-0.096782
		H	0.898342	-2.422566	0.530860
		H	-0.898342	-2.422566	0.530860
		H	0.000000	-3.333193	-0.670399
		Na	0.000000	0.000000	1.941891
30. $[Na\text{-}DEE]^+$, TG	-395.8682461	C	0.418776	-1.220416	0.137676
		H	-0.118805	-1.761484	-0.644909
		C	-1.499169	0.213647	0.599942
		H	-1.672499	-0.466168	1.439693
		O	-0.092682	0.129084	0.233866
		H	0.247968	-1.727458	1.092762
		C	1.901012	-1.157872	-0.181591
		H	2.316138	-2.164877	-0.254369
		H	2.086211	-0.679675	-1.151812
		H	2.464261	-0.648625	0.610428
		H	-1.638532	1.233112	0.967237
		C	-2.438438	-0.074728	-0.558806
		H	-2.253744	0.601775	-1.396948
		H	-2.354049	-1.102938	-0.914973
		H	-3.470429	0.072621	-0.230489
		Na	1.349259	1.731569	-0.124625
31. $[Na\text{-}DEE]^+$, GG	-395.865052	C	0.000000	1.223408	-0.585963
		H	0.496067	1.978843	0.029705
		C	0.000000	-1.223408	-0.585963
		H	-0.496067	-1.978843	0.029705
		O	0.000000	0.000000	0.206324

		C	1.403561	-1.662754	-0.965588
		H	1.909282	-0.918573	-1.584169
		H	2.017252	-1.849180	-0.080163
		H	1.354539	-2.591637	-1.539578
		C	-1.403561	1.662754	-0.965588
		H	-1.909282	0.918573	-1.584169
		H	-2.017252	1.849180	-0.080163
		H	-1.354539	2.591637	-1.539578
		H	0.626311	1.067542	-1.467333
		H	-0.626311	-1.067542	-1.467333
		Na	0.000000	0.000000	2.386463
32. $[Na\text{-}MeOH]^+$	-277.8930517	C	1.451679	0.721488	0.000000
		H	1.846125	-0.293668	0.000000
		O	0.000000	0.618169	0.000000
		H	1.794325	1.240329	0.896183
		H	1.794325	1.240329	-0.896183
		H	-0.358497	1.512826	0.000000
		Na	-1.253304	-1.179463	0.000000
33. $[Na\text{-}DCM]^+$	-1121.880858	C	0.000000	0.000000	-1.328603
		H	0.905828	0.000000	-1.923990
		H	-0.905828	0.000000	-1.923990
		Cl	0.000000	1.491696	-0.313855
		Cl	0.000000	-1.491696	-0.313855
		Na	0.000000	0.000000	2.044606
34. $[K\text{-}H_2O]^+$	-676.2438076	O	0.000000	0.000000	-1.649072
		K	0.000000	0.000000	0.930248
		H	0.000000	0.761766	-2.241069
		H	0.000000	-0.761766	-2.241069
35. $[K\text{-}THF]^+$	-832.3127527	C	0.486905	1.088917	-0.807735
		H	1.580186	1.105909	-0.753466
		H	0.092587	2.029576	-0.416432
		C	0.000000	0.767672	-2.217062
		H	0.647252	1.195431	-2.983211
		H	-1.011251	1.152536	-2.371810
		C	0.000000	-0.767672	-2.217062
		H	-0.647252	-1.195431	-2.983211
		H	1.011251	-1.152536	-2.371810
		C	-0.486905	-1.088917	-0.807735
		H	-0.092587	-2.029576	-0.416432
		H	-1.580186	-1.105909	-0.753466
		O	0.000000	0.000000	0.037762
		K	0.000000	0.000000	2.581331

36. [K-DEE]$^+$, TT	-833.5282366	C	0.000000	1.198636	-1.401411
		H	-0.887234	1.196637	-2.044548
		C	0.000000	-1.198636	-1.401411
		H	-0.887234	-1.196637	-2.044548
		O	0.000000	0.000000	-0.600968
		H	0.887234	1.196637	-2.044548
		C	0.000000	2.412969	-0.492548
		H	0.000000	3.326480	-1.090060
		H	-0.896904	2.443528	0.135528
		H	0.896904	2.443528	0.135528
		H	0.887234	-1.196637	-2.044548
		C	0.000000	-2.412969	-0.492548
		H	0.896904	-2.443528	0.135528
		H	-0.896904	-2.443528	0.135528
		H	0.000000	-3.326480	-1.090060
		K	0.000000	0.000000	1.965866
37. [K-DEE]$^+$, TG	-833.5259071	C	0.582793	1.479327	0.104816
		H	1.287125	1.673105	-0.708919
		C	1.546349	-0.687798	0.598424
		H	2.019088	-0.189261	1.451497
		O	0.361026	0.058608	0.228517
		H	1.025203	1.848002	1.037068
		C	-0.740361	2.169939	-0.168476
		H	-0.588632	3.247166	-0.260063
		H	-1.181721	1.833417	-1.113226
		H	-1.449928	2.017739	0.652091
		H	1.180155	-1.656787	0.950170
		C	2.529288	-0.876802	-0.547133
		H	2.050985	-1.361593	-1.402028
		H	2.960818	0.068310	-0.881335
		H	3.353926	-1.513365	-0.216730
		K	-1.950191	-0.997031	-0.066444
38. [K-DEE]$^+$, GG	-833.5238142	C	0.000000	1.217729	-1.004228
		H	0.472751	1.979883	-0.377614
		C	0.000000	-1.217729	-1.004228
		H	-0.472751	-1.979883	-0.377614
		O	0.000000	0.000000	-0.215594
		C	1.400935	-1.646763	-1.411588
		H	1.886165	-0.901196	-2.044846
		H	2.034393	-1.818221	-0.537136
		H	1.351753	-2.579934	-1.978571
		C	-1.400935	1.646763	-1.411588
		H	-1.886165	0.901196	-2.044846

		H	-2.034393	1.818221	-0.537136
		H	-1.351753	2.579934	-1.978571
		H	0.644520	1.079586	-1.876347
		H	-0.644520	-1.079586	-1.876347
		K	0.000000	0.000000	2.333872
39. $[K\text{-}MeOH]^+$	-715.5529988	C	1.323371	1.690551	0.000000
		H	2.041402	0.870661	0.000000
		O	0.000000	1.101003	0.000000
		H	1.478334	2.296382	0.894980
		H	1.478334	2.296382	-0.894980
		H	-0.637674	1.823365	0.000000
		K	-0.647401	-1.380954	0.000000
40. $[K\text{-}DCM]^+$	-1559.543805	C	0.000000	0.000000	-1.762902
		H	0.904439	0.000000	-2.359615
		H	-0.904439	0.000000	-2.359615
		Cl	0.000000	1.495416	-0.758585
		Cl	0.000000	-1.495416	-0.758585
		K	0.000000	0.000000	2.162555
41. $[K(Me_4cyclen)][HBPh_3]$	-2013.877871	K	0.789132	-0.105528	-0.127702
		H	-1.536067	-0.064939	1.023432
		B	-2.312444	-0.009004	0.053772
		N	3.036813	-1.988569	-0.331929
		N	1.991825	-0.908670	2.402791
		N	2.173495	1.998897	1.281620
		N	3.236854	0.906571	-1.446844
		C	3.185744	-2.627848	0.985324
		H	2.344189	-3.313224	1.109219
		H	4.095733	-3.254627	1.022311
		C	3.231887	-1.663965	2.177948
		H	3.496996	-2.254513	3.073582
		H	4.049962	-0.956204	2.038501
		C	2.216482	0.323544	3.175874
		H	1.239400	0.676843	3.511909
		H	2.797558	0.115931	4.093046
		C	2.927279	1.450988	2.417245
		H	3.162356	2.246194	3.148010
		H	3.889159	1.087772	2.053405
		C	3.039649	2.705611	0.325843
		H	3.685974	3.439802	0.841284
		H	2.390136	3.286253	-0.332674
		C	3.945539	1.802756	-0.520770
		H	4.644010	2.455762	-1.074675
		H	4.567444	1.196980	0.138895

C	4.065340	-0.242158	-1.845132
H	5.065771	0.084202	-2.184050
H	3.590720	-0.700555	-2.715788
C	4.265594	-1.306629	-0.759343
H	5.003989	-2.035684	-1.140312
H	4.727929	-0.845752	0.114054
C	2.607241	-2.976664	-1.327318
H	3.341667	-3.791212	-1.454304
H	2.462487	-2.501913	-2.299038
H	1.650132	-3.411713	-1.034684
C	0.980778	-1.738522	3.067229
H	1.283311	-2.028624	4.088405
H	0.802154	-2.651666	2.497888
H	0.034231	-1.197884	3.122610
C	1.095336	2.885014	1.738813
H	0.418869	2.350424	2.406766
H	0.503034	3.225899	0.888414
H	1.483260	3.767496	2.276977
C	2.776270	1.637191	-2.631789
H	3.612313	2.068696	-3.209771
H	2.102646	2.445558	-2.346059
H	2.217675	0.966054	-3.287732
C	-1.973104	1.401583	-0.723517
C	-1.295452	1.519449	-1.951689
H	-1.031588	0.620587	-2.503603
C	-0.979191	2.757004	-2.526087
H	-0.477601	2.793277	-3.489103
C	-1.332103	3.938311	-1.882186
H	-1.104056	4.900904	-2.327908
C	-2.010725	3.861708	-0.662905
H	-2.309984	4.772865	-0.153190
C	-2.319713	2.623747	-0.107132
H	-2.862929	2.591755	0.832386
C	-2.074024	-1.375199	-0.824445
C	-1.496204	-2.517219	-0.236339
H	-1.192198	-2.464026	0.806938
C	-1.348053	-3.727743	-0.917911
H	-0.919345	-4.588424	-0.411641
C	-1.773574	-3.839987	-2.239602
H	-1.667847	-4.776868	-2.776358
C	-2.359481	-2.733588	-2.853850
H	-2.715461	-2.809635	-3.876949
C	-2.505467	-1.534759	-2.156660
H	-2.987588	-0.702027	-2.659099
C	-3.822407	-0.014992	0.674219
C	-4.952952	0.285676	-0.106904

		H	-4.817464	0.567898	-1.147381
		C	-6.246556	0.242254	0.408645
		H	-7.092274	0.481504	-0.229400
		C	-6.458386	-0.105639	1.742421
		H	-7.463930	-0.139540	2.149105
		C	-5.360649	-0.404939	2.545104
		H	-5.508257	-0.673798	3.587191
		C	-4.071185	-0.357529	2.013165
		H	-3.228177	-0.592119	2.657899
42. $[HBPh_3]^-$	-720.6462035	H	-0.002344	0.001748	-2.075477
		B	-0.004259	-0.005025	-0.844755
		C	-1.062833	-1.167932	-0.376623
		C	-0.761601	-2.206967	0.520767
		H	0.236274	-2.258090	0.946018
		C	-1.694620	-3.182638	0.882094
		H	-1.412389	-3.968589	1.578964
		C	-2.982023	-3.154528	0.353243
		H	-3.711172	-3.911010	0.629531
		C	-3.317373	-2.136384	-0.542107
		H	-4.317259	-2.097933	-0.968290
		C	-2.374897	-1.173459	-0.892860
		H	-2.657059	-0.391558	-1.593804
		C	1.527346	-0.328080	-0.357820
		C	2.409847	-1.059012	-1.175114
		H	2.057848	-1.381256	-2.151741
		C	3.709832	-1.377789	-0.783161
		H	4.356035	-1.941705	-1.451842
		C	4.186083	-0.970735	0.462943
		H	5.198664	-1.212460	0.774065
		C	3.341190	-0.242670	1.299179
		H	3.696028	0.087555	2.272596
		C	2.043944	0.069634	0.889363
		H	1.411723	0.650744	1.555290
		C	-0.474547	1.488194	-0.353771
		C	-1.286332	1.731127	0.769180
		H	-1.661705	0.883802	1.336498
		C	-1.640586	3.020464	1.174680
		H	-2.271950	3.157758	2.049681
		C	-1.192440	4.129661	0.460810
		H	-1.468182	5.134603	0.768515
		C	-0.386697	3.926494	-0.661027
		H	-0.030864	4.779690	-1.234348
		C	-0.041978	2.633838	-1.050291
		H	0.583750	2.496525	-1.928788

43. K^+-**1c**	-1751.3868855	K	0.0000000	0.0000000	1.0496190
		N	-1.9876750	-1.0093550	-0.8626620
		N	-1.0093550	1.9876750	-0.8626620
		N	1.9876750	1.0093550	-0.8626620
		N	1.0093550	-1.9876750	-0.8626620
		C	2.2654970	-1.4515930	-1.4206110
		H	3.0334270	-1.5382300	-0.6495410
		H	2.6131800	-2.0741350	-2.2642830
		C	2.2125390	0.0000000	-1.9125180
		H	3.1535020	0.1997220	-2.4532480
		H	1.4240580	0.0978080	-2.6579660
		C	1.4515930	2.2654970	-1.4206110
		H	1.5382300	3.0334270	-0.6495410
		H	2.0741350	2.6131800	-2.2642830
		C	0.0000000	2.2125390	-1.9125180
		H	-0.1997220	3.1535020	-2.4532480
		H	-0.0978080	1.4240580	-2.6579660
		C	-2.2654970	1.4515930	-1.4206110
		H	-3.0334270	1.5382300	-0.6495410
		H	-2.6131800	2.0741350	-2.2642830
		C	-2.2125390	0.0000000	-1.9125180
		H	-3.1535020	-0.1997220	-2.4532480
		H	-1.4240580	-0.0978080	-2.6579660
		C	-1.4515930	-2.2654970	-1.4206110
		H	-1.5382300	-3.0334270	-0.6495410
		H	-2.0741350	-2.6131800	-2.2642830
		C	0.0000000	-2.2125390	-1.9125180
		H	0.1997220	-3.1535020	-2.4532480
		H	0.0978080	-1.4240580	-2.6579660
		C	-1.7960430	3.0405500	1.2900350
		H	-2.0930840	4.0202680	1.6803400
		H	-2.6741310	2.3849320	1.3125560
		C	-1.2751570	3.2365580	-0.1245840
		H	-1.9866130	3.8754990	-0.6752980
		H	-0.3455700	3.8027030	-0.0452390
		C	-3.2365580	-1.2751570	-0.1245840
		H	-3.8027030	-0.3455700	-0.0452390
		H	-3.8754990	-1.9866130	-0.6752980
		C	-3.0405500	-1.7960430	1.2900350
		H	-4.0202680	-2.0930840	1.6803400
		H	-2.3849320	-2.6741310	1.3125560
		C	1.7960430	-3.0405500	1.2900350
		H	2.6741310	-2.3849320	1.3125560
		H	2.0930840	-4.0202680	1.6803400
		C	1.2751570	-3.2365580	-0.1245840
		H	1.9866130	-3.8754990	-0.6752980

		H	0.3455700	-3.8027030	-0.0452390
		C	3.0405500	1.7960430	1.2900350
		H	2.3849320	2.6741310	1.3125560
		H	4.0202680	2.0930840	1.6803400
		C	3.2365580	1.2751570	-0.1245840
		H	3.8754990	1.9866130	-0.6752980
		H	3.8027030	0.3455700	-0.0452390
		O	2.4822950	0.7464680	2.0988260
		H	2.5761000	1.0038090	3.0210860
		O	0.7464680	-2.4822950	2.0988260
		H	1.0038090	-2.5761000	3.0210860
		O	-2.4822950	-0.7464680	2.0988260
		H	-2.5761000	-1.0038090	3.0210860
		O	-0.7464680	2.4822950	2.0988260
		H	-1.0038090	2.5761000	3.0210860
44. K^+-**1d**	-3426.4680750	K	0.0000000	0.0000000	0.3614100
		O	-1.2982280	2.0407440	-1.0670950
		O	-1.6130350	-1.9353900	-0.8827380
		O	1.2982280	-2.0407440	-1.0670950
		O	1.6130350	1.9353900	-0.8827380
		O	-0.6861410	5.7464380	1.5892900
		O	-5.5134670	-0.4178800	1.0649750
		O	0.6861410	-5.7464380	1.5892900
		O	5.5134670	0.4178800	1.0649750
		N	-0.9158120	2.0305240	2.3996740
		N	-2.0118780	-0.9371480	2.4011960
		N	0.9158120	-2.0305240	2.3996740
		N	2.0118780	0.9371480	2.4011960
		N	-1.0450560	3.2420310	-0.7234580
		N	-0.7412530	5.0060280	0.5686780
		N	-2.8031430	-1.4568220	-0.7722190
		N	-4.6597070	-0.7244600	0.1803300
		N	1.0450560	-3.2420310	-0.7234580
		N	0.7412530	-5.0060280	0.5686780
		N	2.8031430	1.4568220	-0.7722190
		N	4.6597070	0.7244600	0.1803300
		C	-1.7394670	1.3699320	3.4318650
		C	-2.6806070	0.2667600	2.9373650
		C	-1.3609840	-1.7219790	3.4679380
		C	-0.2663600	-2.6836860	2.9956400
		C	1.7394670	-1.3699320	3.4318650
		C	2.6806070	-0.2667600	2.9373650
		C	1.3609840	1.7219790	3.4679380
		C	0.2663600	2.6836860	2.9956400
		C	-1.7520570	3.0199710	1.6948660

C	-1.1256130	3.7212830	0.5368690
C	-0.8682680	4.3660940	-1.7170370
C	-0.2429510	5.4674360	-0.7883850
C	-2.2845950	4.7151510	-2.2135860
C	0.0000000	3.9232940	-2.8881610
C	-0.7181440	6.8958800	-1.0374560
C	1.2912040	5.4181150	-0.7094380
C	-2.9952760	-1.7941630	1.7114430
C	-3.4647440	-1.2861540	0.3917930
C	-3.6928710	-1.1847980	-1.9587230
C	-4.8551700	-0.3628890	-1.2789360
C	-2.9095000	-0.4350070	-3.0356570
C	-4.1391460	-2.5582400	-2.4920060
C	-4.6855920	1.1623870	-1.3662220
C	-6.2741970	-0.7505270	-1.6939520
C	1.7520570	-3.0199710	1.6948660
C	1.1256130	-3.7212830	0.5368690
C	0.8682680	-4.3660940	-1.7170370
C	0.2429510	-5.4674360	-0.7883850
C	0.0000000	-3.9232940	-2.8881610
C	2.2845950	-4.7151510	-2.2135860
C	-1.2912040	-5.4181150	-0.7094380
C	0.7181440	-6.8958800	-1.0374560
C	2.9952760	1.7941630	1.7114430
C	3.4647440	1.2861540	0.3917930
C	3.6928710	1.1847980	-1.9587230
C	4.8551700	0.3628890	-1.2789360
C	2.9095000	0.4350070	-3.0356570
C	4.1391460	2.5582400	-2.4920060
C	4.6855920	-1.1623870	-1.3662220
C	6.2741970	0.7505270	-1.6939520
H	-2.3579690	2.1129940	3.9637640
H	-1.0691460	0.9595590	4.1852790
H	-3.3439180	0.0004040	3.7779550
H	-3.3428500	0.6556230	2.1616060
H	-0.9420940	-1.0273830	4.1942240
H	-2.1060900	-2.3153200	4.0250050
H	-0.6752540	-3.3696500	2.2525390
H	0.0205960	-3.3136360	3.8541300
H	2.3579690	-2.1129940	3.9637640
H	1.0691460	-0.9595590	4.1852790
H	3.3428500	-0.6556230	2.1616060
H	3.3439180	-0.0004040	3.7779550
H	2.1060900	2.3153200	4.0250050
H	0.9420940	1.0273830	4.1942240
H	0.6752540	3.3696500	2.2525390

H	-0.0205960	3.3136360	3.8541300
H	-2.6326990	2.5024790	1.3089170
H	-2.0906830	3.8145290	2.3781100
H	-2.7242140	3.8285620	-2.6726800
H	-2.9361080	5.0449330	-1.4020550
H	-2.2420020	5.5043380	-2.9658430
H	-0.5278780	3.1636130	-3.4655240
H	0.9357660	3.4913470	-2.5428960
H	0.1959640	4.7745240	-3.5444070
H	-0.3865590	7.2300690	-2.0231160
H	-1.8013720	6.9938770	-0.9794250
H	-0.2828210	7.5533530	-0.2853630
H	1.6493790	4.3980140	-0.5621570
H	1.6142590	6.0425200	0.1251970
H	1.7313710	5.8135140	-1.6265090
H	-2.5283220	-2.7612050	1.5207960
H	-3.8917330	-1.9569930	2.3283140
H	-2.4699160	0.4882880	-2.6612250
H	-3.5673350	-0.2046670	-3.8769160
H	-2.1014490	-1.0696090	-3.4004050
H	-3.2605730	-3.1185500	-2.8131280
H	-4.7988270	-2.4389230	-3.3529110
H	-4.6618230	-3.1425430	-1.7326780
H	-4.8983980	1.5086040	-2.3794600
H	-5.4024410	1.6261050	-0.6866130
H	-3.6765240	1.4779640	-1.0966640
H	-6.4344570	-0.5078190	-2.7465670
H	-6.4802260	-1.8091650	-1.5421060
H	-6.9851530	-0.1823030	-1.0947660
H	2.6326990	-2.5024790	1.3089170
H	2.0906830	-3.8145290	2.3781100
H	-0.9357660	-3.4913470	-2.5428960
H	0.5278780	-3.1636130	-3.4655240
H	-0.1959640	-4.7745240	-3.5444070
H	2.9361080	-5.0449330	-1.4020550
H	2.7242140	-3.8285620	-2.6726800
H	2.2420020	-5.5043380	-2.9658430
H	-1.6142590	-6.0425200	0.1251970
H	-1.7313710	-5.8135140	-1.6265090
H	-1.6493790	-4.3980140	-0.5621570
H	0.2828210	-7.5533530	-0.2853630
H	0.3865590	-7.2300690	-2.0231160
H	1.8013720	-6.9938770	-0.9794250
H	3.8917330	1.9569930	2.3283140
H	2.5283220	2.7612050	1.5207960
H	2.4699160	-0.4882880	-2.6612250

H	3.5673350	0.2046670	-3.8769160
H	2.1014490	1.0696090	-3.4004050
H	3.2605730	3.1185500	-2.8131280
H	4.6618230	3.1425430	-1.7326780
H	4.7988270	2.4389230	-3.3529110
H	3.6765240	-1.4779640	-1.0966640
H	4.8983980	-1.5086040	-2.3794600
H	5.4024410	-1.6261050	-0.6866130
H	6.4802260	1.8091650	-1.5421060
H	6.4344570	0.5078190	-2.7465670
H	6.9851530	0.1823030	-1.0947660

Table S22: High level single-point energies (in Hartree) of the stationary points optimised using the BP86/6-311G(d,p) method. The ansatz 3*A(Fix,NoX) was used in the DF-LCCSD(T)-F12x/nZ-F12//BP86/6-311G(d,p) calculations.

	DF-LCCSD(T)/nZ //BP86/6-311G(d,p)		DF-LCCSD(T)-F12x/nZ-F12 //BP86/6-311G(d,p)			
	n = D	n = T	n = D		n = T	
			x = a	x = b	x = a	x = b
$[Li(Me_4cyclen)]^+$	-698.661344313	-699.298840984	-699.594711147	-699.519898753	-699.608310964	-699.544191073
$[Na(Me_4cyclen)]^+$	-853.135862699	-853.923083735	-854.259198314	-854.179747545	-854.266692098	-854.199363696
$[K(Me_4cyclen)]^+$	-719.358685539	-720.057422842	-720.390565590	-720.310712547	-720.428913459	-720.358721335
H_2O	-76.273692566	-76.335410597	-76.369582926	-76.362800477	-76.369611340	-76.364077428
THF	-231.854728114	-232.058015901	-232.154841687	-232.131124135	-232.158971033	-232.138876337
DEE	-233.054764075	-233.263988450	-233.364038770	-233.339435933	-233.367499423	-233.346906140
MeOH	-115.452957120	-115.552202238	-115.602598990	-115.591335701	-115.603421151	-115.594145439
DCM	-958.538896846	-958.680444966	-958.782919528	-958.765370885	-958.769928180	-958.754486508
Li-H_2O-1a	-774.956581076	-775.656761471	-775.986863572	-775.905360639	-776.000831569	-775.931239310
Li-THF-1a	-930.543347169	-931.385151829	-931.778816628	-931.680483259	-931.796694124	-931.712553260
Li-DEE-1a	-931.741728457	-932.584884216	-932.981476185	-932.882274244	-932.999328793	-932.914664448
Li-MeOH-1a	-814.137170356	-814.875409700	-815.221988107	-815.136033328	-815.236721998	-815.163384395
Li-DCM-1a	-1657.212641072	-1657.991507983	-1658.390432901	-1658.298180051	-1658.391254636	-1658.311761968
Na-H_2O-1a	-929.429022163	-930.280394566	-930.649930864	-930.563764618	-930.658200749	-930.585364946
Na-THF-1a	-1085.015213923	-1086.006629451	-1086.440912850	-1086.337827457	-1086.452547392	-1086.365181044
Na-DEE-1a	-1086.209660303	-1087.207131973	-1087.644711826	-1087.540767886	-1087.655403175	-1087.567508779
Na-MeOH-1a	-968.610352030	-969.498202794	-969.884634594	-969.793972957	-969.892802175	-969.816184202
Na-DCM-1a	-1811.689296362	-1812.618570754	-1813.057442872	-1812.960539100	-1813.051579361	-1812.968830491
K-H_2O-1a	-795.648426134	-796.409217419	-796.777092975	-796.690481865	-796.816106517	-796.740437750
K-THF-1a	-951.233706109	-952.134466292	-952.565924727	-952.462328939	-952.608445276	-952.518208844
K-DEE-1a	-952.434171049	-953.340988409	-953.775090190	-953.670651775	-953.817873594	-953.727131397
K-MeOH-1a	-834.828895004	-835.626958172	-836.011011630	-835.919883450	-836.050844207	-835.971409018
K-DCM-1a	-1677.909983541	-1678.750360860	-1679.185912359	-1679.088528764	-1679.211956844	-1679.126346103

Table S23: High level single-point energies (in Hartree) of the stationary points optimised using the B3LYP/6-311G(d,p) method. The ansatz 3*A(Fix,NoX) was used in the DF-LCCSD(T)-F12x/nZ-F12//B3LYP/6-311G(d,p) calculations.

	DF-LCCSD(T)/nZ //B3LYP/6-311G(d,p)		DF-LCCSD(T)-F12x/nZ-F12 //B3LYP/6-311G(d,p)			
	n = D	n = T	n = D		n = T	
			x = a	x = b	x = a	x = b
$[Li(Me_4cyclen)]^+$	-698.657411723	-699.300349219	-699.597583806	-699.522751102	-699.611460607	-699.547303482
$[Na(Me_4cyclen)]^+$	-853.131360420	-853.924464614	-854.261994890	-854.182513547	-854.268929003	-854.201517636
$[K(Me_4cyclen)]^+$	-719.354691073	-720.059684936	-720.393184522	-720.313300403	-720.433063945	-720.362855164
H_2O	-76.273693171	-76.335649072	-76.369875175	-76.363100358	-76.369922596	-76.364391277
THF	-231.853519413	-232.058584289	-232.155859433	-232.132139141	-232.160060591	-232.139957945
DEE	-233.053452374	-233.264588112	-233.365071467	-233.340464791	-233.368615168	-233.348014797
MeOH	-115.452668788	-115.552647075	-115.603209339	-115.591949032	-115.604055075	-115.594778973
DCM	-958.538701452	-958.680768821	-958.783362612	-958.765821132	-958.770379415	-958.754939562
Li-H_2O-2a	-774.952394383	-775.658698422	-775.990167079	-775.908659627	-776.004432654	-775.934809025
Li-THF-2a	-930.540262134	-931.387639762	-931.782975797	-931.684631531	-931.801194732	-931.717014019
Li-DEE-2a	-931.737898828	-932.587400123	-932.986132361	-932.886915363	-933.004009200	-932.919306264
Li-MeOH-2a	-814.134224525	-814.877427661	-815.225659705	-815.139719212	-815.240755984	-815.167385536
Li-DCM-2a	-1657.209997156	-1657.993596254	-1658.394853900	-1658.302540669	-1658.394937131	-1658.315398897
Na-H_2O-2a	-929.424454351	-930.281917166	-930.652960423	-930.566773366	-930.660655022	-930.587742249
Na-THF-2a	-1085.010336972	-1086.009172341	-1086.445110181	-1086.342001163	-1086.455838311	-1086.368356352
Na-DEE-2a	-1086.204555198	-1087.210343910	-1087.649096373	-1087.545134782	-1087.660556961	-1087.572577003
Na-MeOH-2a	-968.605721084	-969.500279018	-969.888175372	-969.797492021	-969.896408713	-969.819744362
Na-DCM-2a	-1811.685200401	-1812.620826263	-1813.061397733	-1812.964482156	-1813.055361324	-1812.972558998
K-H_2O-2a	-795.644361207	-796.410642882	-796.780313431	-796.693690945	-796.819154038	-796.743452518
K-THF-2a	-951.228642492	-952.136366902	-952.569585171	-952.465955605	-952.612431816	-952.522152275
K-DEE-2a	-952.429243893	-953.343108241	-953.779008279	-953.674534112	-953.822083981	-953.731300231
K-MeOH-2a	-834.824603475	-835.628446085	-836.014907910	-835.923776225	-836.054340788	-835.974881284
K-DCM-2a	-1677.906247255	-1678.751820457	-1679.189937564	-1679.092548751	-1679.216041041	-1679.130435093

Table S24: High level single-point energies (in Hartree) of the stationary points optimised using the BP86/6-311G(d,p) and B3LYP/6-311G(d,p) methods. The default ansatz 3*A(Loc,Fix) was used in the DF-LCCSD(T)-F12x/DZ-F12 calculations.

	DF-LCCSD(T)-F12x/DZ-F12 //BP86/6-311G(d,p)	
	x = a	x = b
$[Li(Me_4cyclen)]^+$	-699.711167649	-699.636355255
$[Na(Me_4cyclen)]^+$	-854.409716557	-854.330265789
$[K(Me_4cyclen)]^+$	-721.477551084	-721.397698041
H_2O	-76.387017453	-76.380235004
THF	-232.196989326	-232.173271774
DEE	-233.405780914	-233.381178077
MeOH	-115.625925067	-115.614661778
DCM	-958.979167438	-958.961618796
*DCM**	*-960.802937949*	*-960.779048274*
Li-H_2O-1a	-776.119426268	-776.037923335
Li-THF-1a	-931.936235669	-931.837902299
Li-DEE-1a	-933.138595786	-933.039393845
Li-MeOH-1a	-815.360736615	-815.274781836
Li-DCM-1a	-1658.687020044	-1658.594767195
Li-DCM-1a*	*-1660.478472376*	*-1660.379864995*
Na-H_2O-1a	-930.816896699	-930.730730452
Na-THF-1a	-1086.632812674	-1086.529727281
Na-DEE-1a	-1087.836281281	-1087.732337341
Na-MeOH-1a	-970.057795782	-969.967134144
Na-DCM-1a	-1813.394875793	-1813.297972021
K-DCM-1a	-1680.454316930	-1680.356933336

	DF-LCCSD(T)-F12x/DZ-F12 //B3LYP/6-311G(d,p)	
	x = a	x = b
$[Li(Me_4cyclen)]^+$	-699.714968921	-699.640136217
$[Na(Me_4cyclen)]^+$	-854.413437314	-854.333955972
$[K(Me_4cyclen)]^+$	-721.476914092	-721.397029973
H_2O	-76.387300956	-76.380526139
THF	-232.198259899	-232.174539607
DEE	-233.407061182	-233.382454506
MeOH	-115.626611537	-115.615351231
DCM	-958.979776949	-958.962235469
*DCM**	*-960.803392204*	*-960.779507975*
Li-H_2O-2a	-776.123669997	-776.042162545
Li-THF-2a	-931.941567234	-931.843222967
Li-DEE-2a	-933.144414564	-933.045197566
Li-MeOH-2a	-815.365399472	-815.279458980
Li-DCM-2a	-1658.692969597	-1658.600656365
Li-DCM-2a*	*-1660.485542965*	*-1660.386873161*
Na-H_2O-2a	-930.820872364	-930.734685307
Na-THF-2a	-1086.638178341	-1086.535069322
Na-DEE-2a	-1087.841808790	-1087.737847200
Na-MeOH-2a	-970.062328769	-969.971645418
Na-DCM-2a	-1813.398791406	-1813.301875829
K-DCM-2a	-1680.454766614	-1680.357377801

* The $(n-1)s^2$ and $(n-1)p^6$ core electrons of Cl atom were correlated.

Table S25: Energies (in Hartree) of stationary points associated with reactions (A) and (B). The ansatz 3*A(Fix,NoX) was used in the DF-LCCSD(T)-F12x/nZ-F12//BP86/6-311G(d,p) calculations.

	BP86/ 6-311G(d,p)	DF-LCCSD(T)/nZ //BP86/6-311G(d,p)		DF-LCCSD(T)-F12x/nZ-F12 //BP86/6-311G(d,p)			
	E^{ZPE}	n = D	n = T	n = D		n = T	
				x = a	x = b	x = a	x = b
$[Li(Me_4cyclen)]^+$	-700.280789	-698.66134431	-699.29884098	-699.59471115	-699.51989875	-699.60831096	-699.54419107
$[Na(Me_4cyclen)]^+$	-855.045183	-853.13586270	-853.92308373	-854.25919831	-854.17974755	-854.26669210	-854.19936370
$[K(Me_4cyclen)]^+$	-1292.727886	-719.35868554	-720.05742284	-720.39056559	-720.31071255	-720.42891346	-720.35872134
Li^+	-7.275292	-7.25789343	-7.27472806	-7.27997110	-7.27883481	-7.27998588	-7.27898629
Na^+	-162.082228	-161.77610539	-161.94472463	-161.98942460	-161.98384061	-161.98361329	-161.97935934
K^+	-599.799323	-28.03226568	-28.11635202	-28.15300272	-28.14685464	-28.18080180	-28.17351793
$Me_4cyclen$	-692.840767	-691.23604195	-691.84903213	-692.14252466	-692.06882008	-692.15328858	-692.09049513
$[H(Me_4cyclen)]^+$	-693.250149	-691.66117327	-692.27710636	-692.56919651	-692.49546892	-692.58013684	-692.51729561
H_2O	-76.426915	-76.27369257	-76.33541060	-76.36958293	-76.36280048	-76.36961134	-76.36407743
H_3O^+	-76.696629	-76.54448193	-76.61192601	-76.64285761	-76.63633802	-76.64444764	-76.63910595

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