PCCP

Electronic Supplementary Information ARTICLE TYPE

Evaluating the Cation Binding Strength and Selectivity of Calix[4]pyrroles: A Computational and ESI-MS/MS Study

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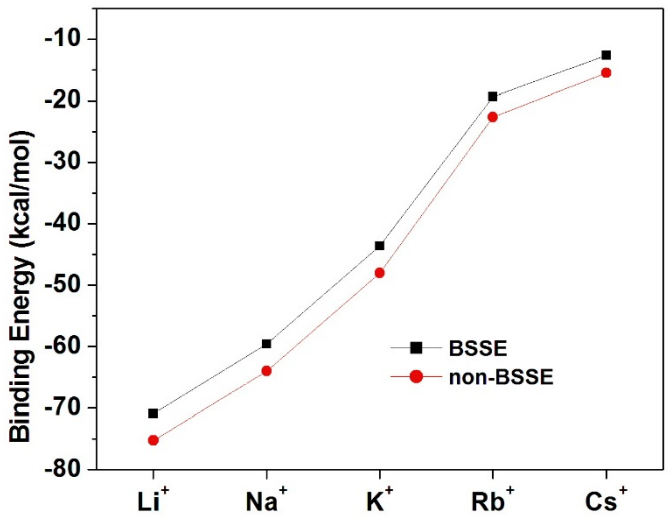
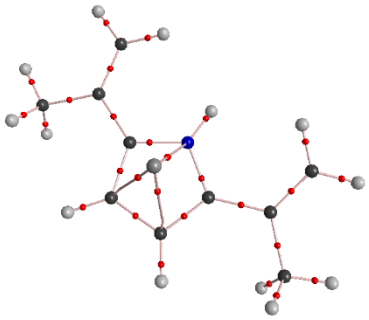


Figure S1. Plot of Binding Energies with (-■-) and without BSSE (-●-) for all [**1**+X]$^+$ complexes at M052X/6-31g(d) for Li^+, Na^+, K^+ and with effective core potentials and valence basis sets of Hay and Wadt for Rb^+ and Cs^+ complexes.



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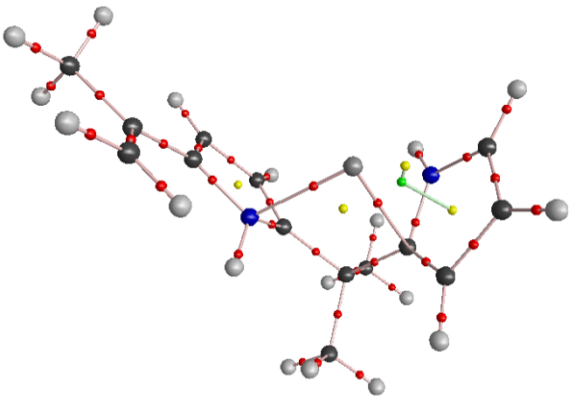

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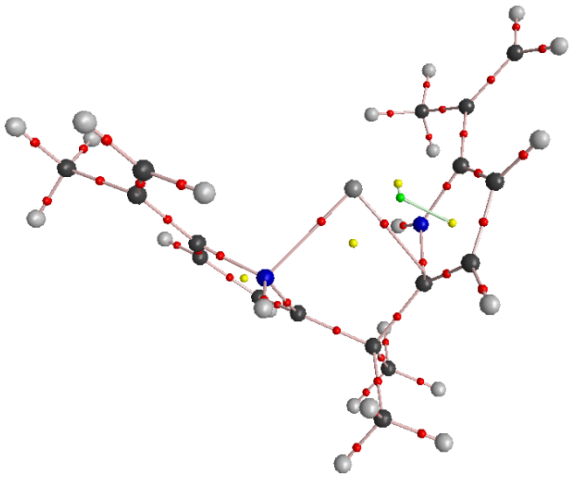

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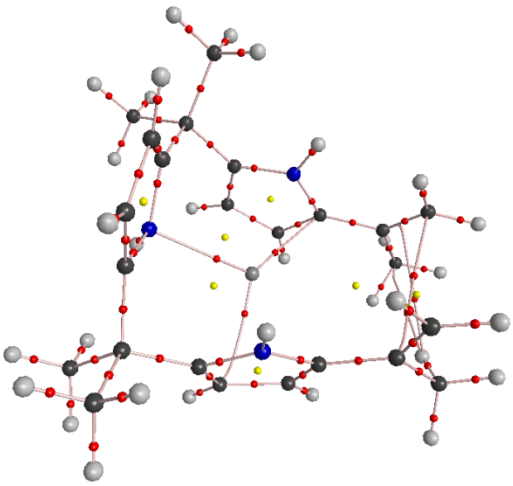

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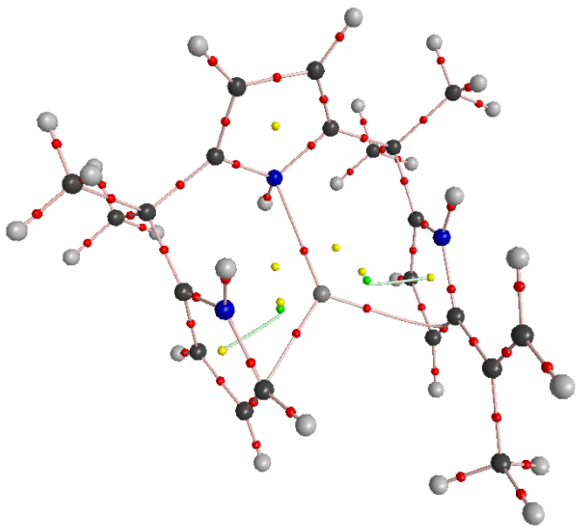

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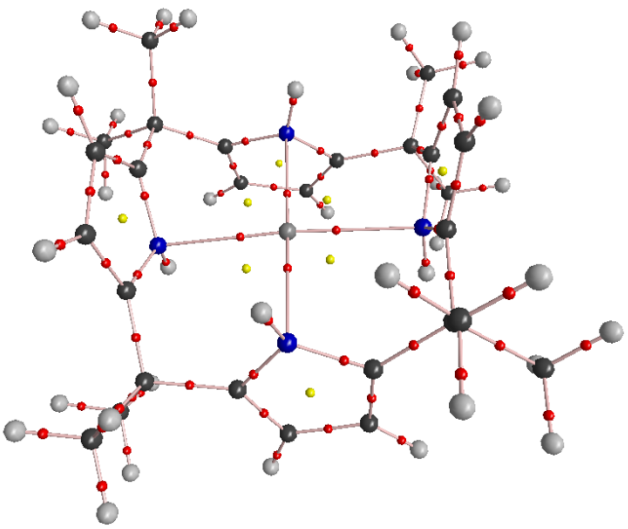

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Figure S2. AIM topological graph for the parent complex and fragments of [**1**+Li]$^+$ at B3LYP/6-31G* level of theory.

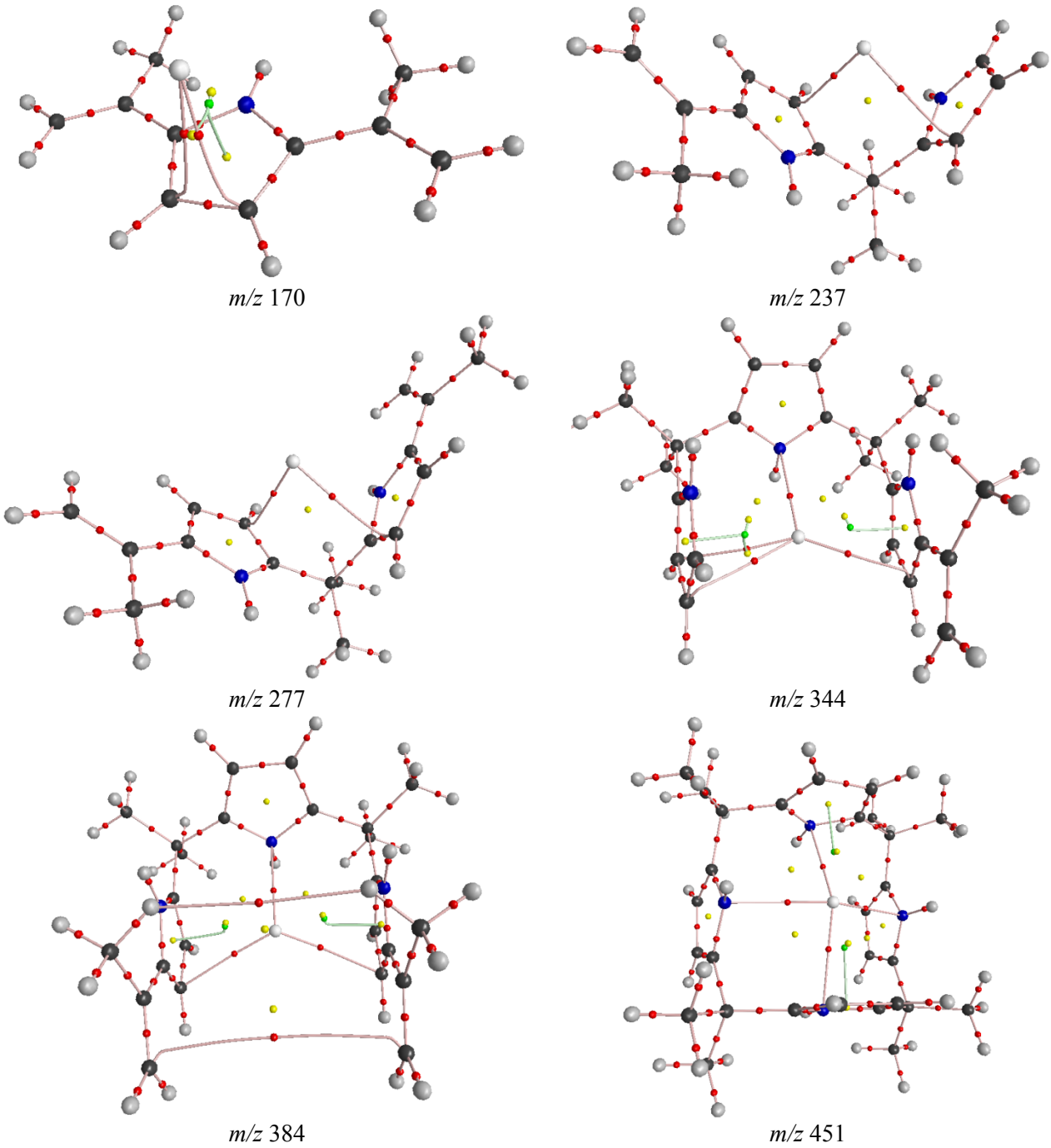

Figure S3. AIM topological graph for the parent complex and fragments of [**1**+Na]$^+$ at B3LYP/6-31G* level of theory.

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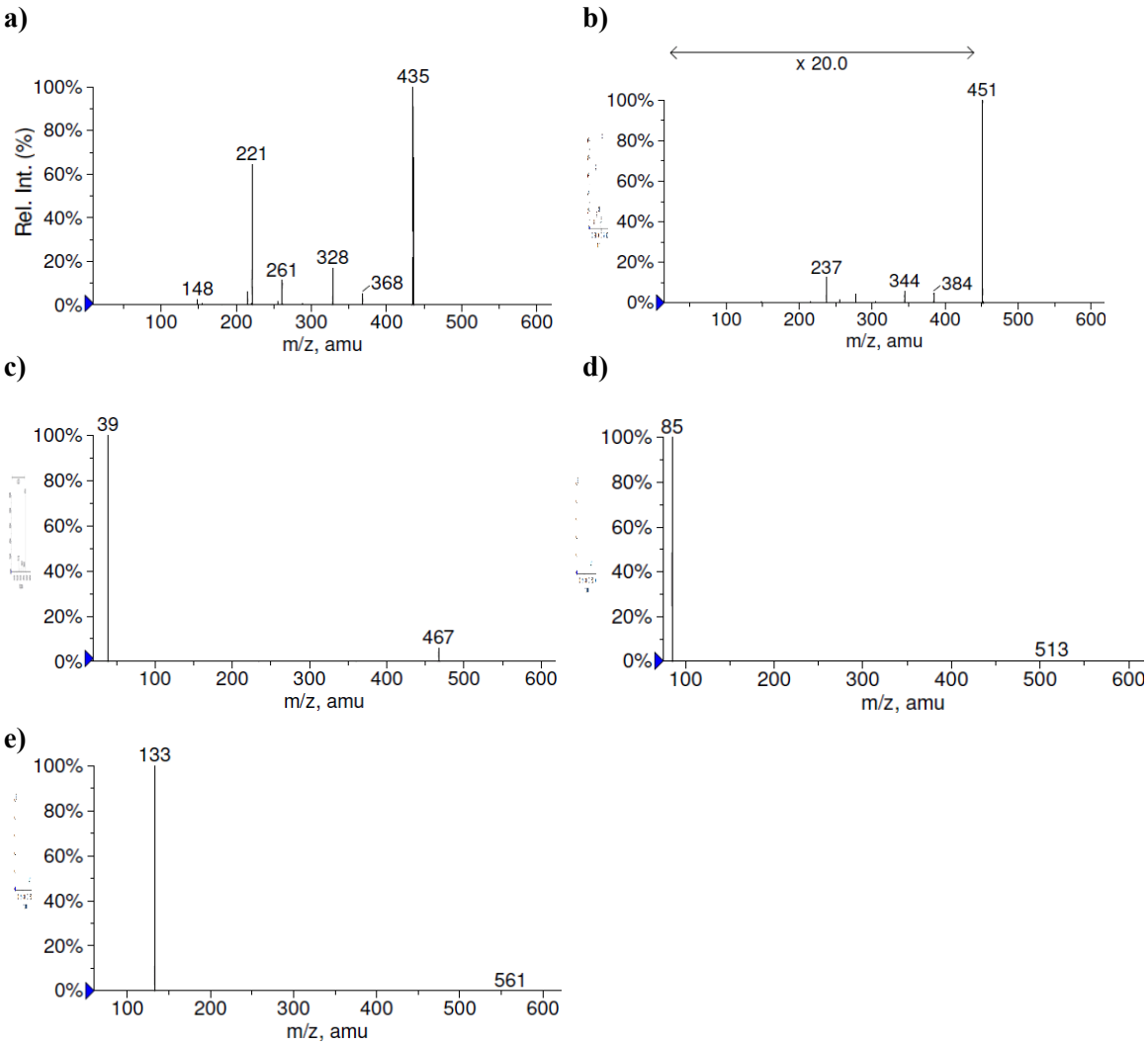
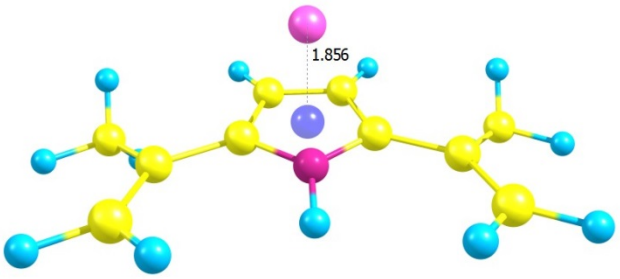


Figure S4. CID product ion spectra of a) [**1**+Li]$^+$ (*m/z* 435), b) [**1**+ Na]$^+$ (*m/z* 451), c) [**1**+K]$^+$ (*m/z* 467), d) [**1**+ Rb]$^+$ (*m/z* 513), and e) [**1**+ Cs]$^+$ (*m/z* 561) at a collision energy of 30 eV.



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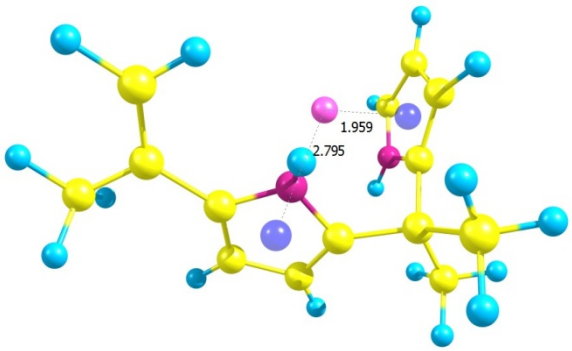

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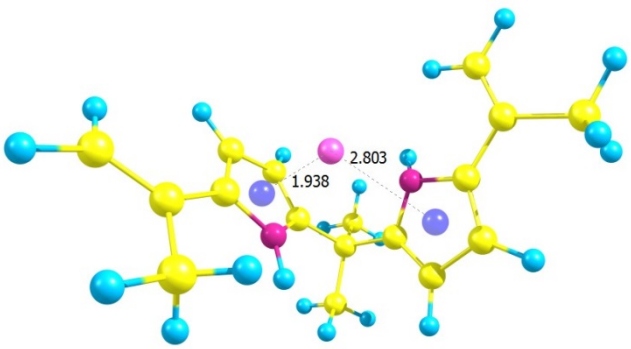

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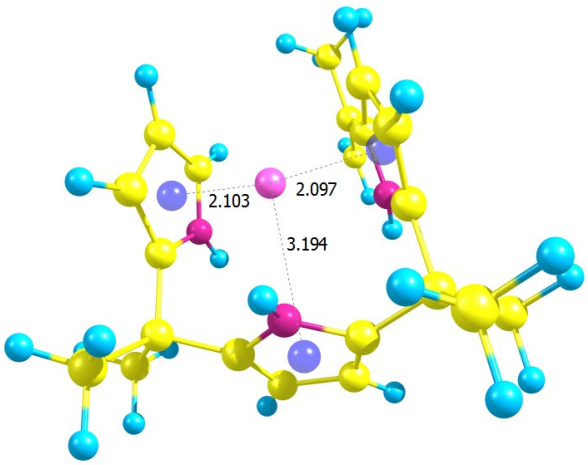

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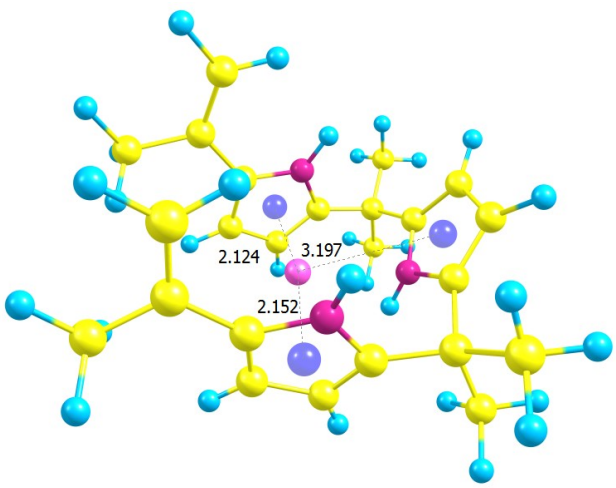
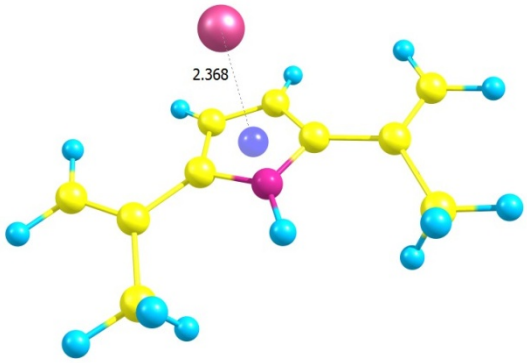


m/z 368

Figure S5. Optimized geometries of **1** showing cation to centroid of pyrrole ring distances of various fragments complexed with Li^+ ion calculated at M05-2X/TZVP level of theory.



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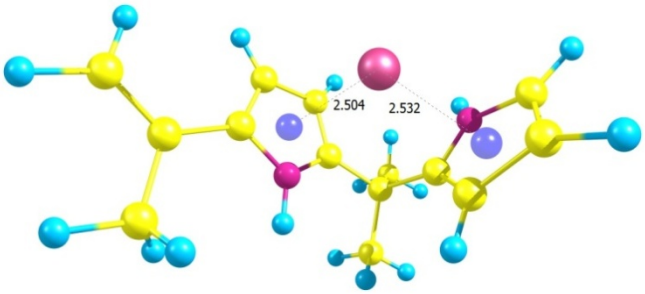

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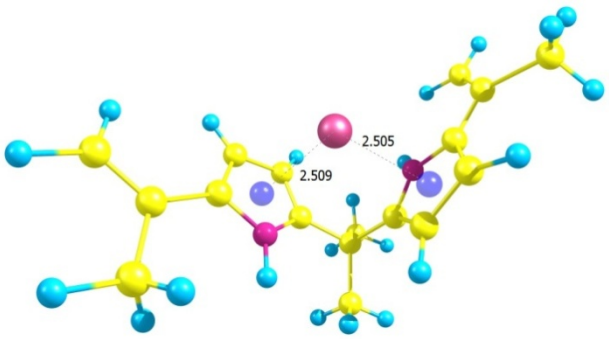

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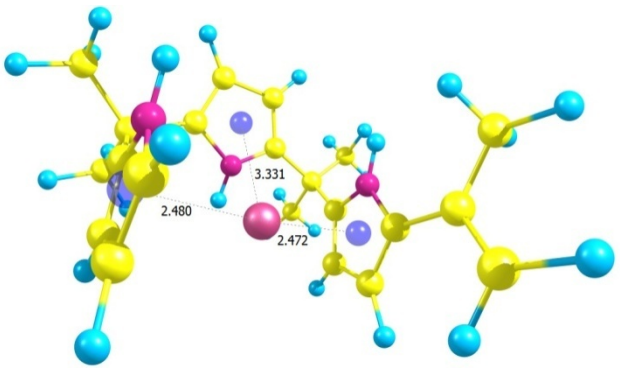

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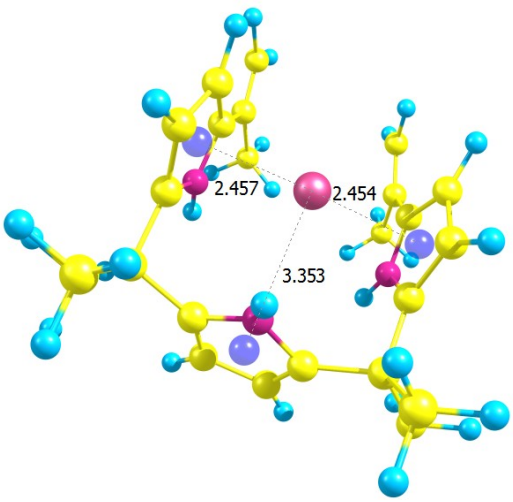

m/z 384

Figure S6. Optimized geometries of **1** showing cation to centroid of pyrrole ring distances of various fragments complexed with Na^+ ion calculated at M05-2X/TZVP level of theory.

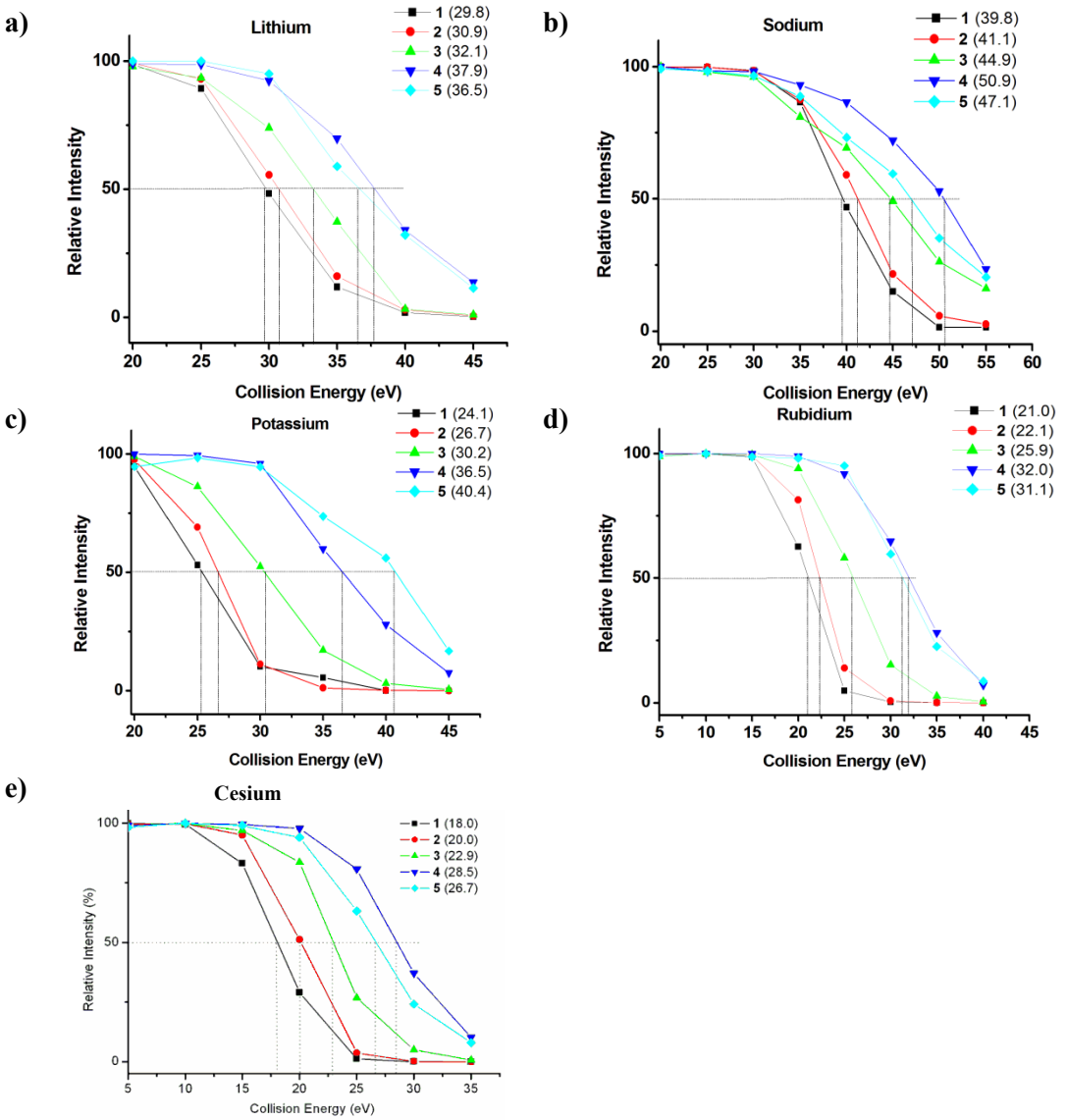

Figure S7. CID dissociation curves for the complexes of CP (**1-5**) with **a)** Li^+ **b)** Na^+ **c)** K^+ **d)** Rb^+ and **e)** Cs^+. The $E_{com}^{50\%}$ values were presented in parentheses (eV).

Table S1: Dihedral angles (Å) between two adjacent pyrrole rings connected by the methylene group.[a]

Complexes	ab	ab′	a′b	a′b′
1	127.867	-127.903	-127.903	127.867
1-Li^+	110.721	-133.897	-133.897	110.721
1-Na^+	108.974	-111.748	-111.753	108.972
1-K^+	98.051	-98.053	-98.053	98.051
1-Rb^+	96.601	-96.588	-96.590	96.604
1-Cs^+	139.763	-139.729	-139.729	139.763

[a] The atoms chosen to measure the dihedral angle is shown as bold ones in Fig.3

Table S2: Energy components in kcal/mol obtained from LMOEDA technique incorporated in GAMESS software.

Complex	Elec	Exch	Rep	Pol	Disp	IE
CP-Li^+	-43.47	-2.36	14.61	-38.09	-12.79	-82.09
CP-Na^+	-44.54	-3.08	23.57	-25.42	-19.82	-69.30

Table S3: Electron density (ρ) and Laplacian of electron density (∇^2) at the bond critical points (BCP, R) and cage critical points (CCP, π) obtained for the parent and various fragments of Li, Na and K complexes of **1** obtained at B3LYP/6-31G*//M05-2X/6-31G* level.

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Complexes	π_1		π_2		R_a		$R_{a'}$		R_b		$R_{b'}$	
	P	$\nabla^2\rho$	ρ	$\nabla^2\rho$	ρ	$\nabla^2\rho$	ρ	$\nabla^2\rho$	ρ	$\nabla^2\rho$	ρ	$\nabla^2\rho$
Li-154	0.0168	-0.270	x	x	0.0186	-0.0316	x	x	x	x	x	x
Li-221	0.0144	-0.0217	-a-	-a-	0.0229	-0.0319	0.0175	-0.0255	x	x	x	x
Li-261	0.150	0.225	-a-	-a-	0.0227	-0.0314	0.0184	-0.0272	x	x	x	x
Li-328	-a-	-a-	-a-	-a-	0.0116	-0.0136	0.0143	-0.0176	0.0128	-0.0170	x	x
Li-368	0.0114	-0.0166	0.0116	-0.0163	0.0129	-0.0154	0.0135	-0.0175	0.0133	-0.0169	x	x
Li-Parent	-a-	-a-	-a-	-a-	0.0134	-0.0164	0.0134	-0.0164	0.0134	-0.0164	0.0134	-0.0164
Na-170	0.0111	-0.0163	x	x	0.0159	-0.0199	x	x	x	x	x	x
Na-237	-a-	-a-	-a-	-a-	0.0134	-0.0161	0.0132	-0.0158	x	x	x	x
Na-277	-a-	-a-	-a-	-a-	0.0125	-0.0155	0.0132	-0.0160	x	x	x	x
Na-344	0.0096	-0.0139	0.0097	-0.0138	0.0125	-0.0147	0.0118	-0.0142	0.0123	-0.0148	x	x
Na-384	0.0084	-0.0116	0.0084	-0.0116	0.0124	-0.0147	0.0114	-0.0129	0.0114	-0.0129	x	x
Na-Parent	0.0076	-0.0098	0.0076	-0.0098	0.0102	-0.0135	0.0102	-0.0135	0.0126	-0.0150	0.0126	-0.0150
K-Parent	0.0089	-0.0119	0.0089	-0.0119	0.0121	-0.0134	0.0129	-0.0124	0.0121	-0.134	0.0129	-0.0124

[-a-] The corresponding cage critical point is not observed.

[x] The corresponding bond critical point is not present.

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Table S4: Binding Energies (BE in kcal/mol) of the precursor ions, [**1**+X]$^+$ where X$^+$ = Li, Na, K, Rb, Cs, and the product ions (fragment ions) computed at B2PLYP/TZVP level of theory.

Binding Energies					
Precursor ion	**Product ions**				
[**1**+Li]$^+$ (-74.24)	*m/z* 154 (-44.95)	*m/z* 221 (-61.88)	*m/z* 261 (-62.79)	*m/z* 328 (-74.78)	*m/z* 368 (-74.81)
[**1**+Na]$^+$ (-59.55)	*m/z* 170* (-29.79)	*m/z* 237 (-46.03)	*m/z* 277 (-46.06)	*m/z* 344 (-55.88)	*m/z* 384 (-55.46)
[**1** +K]$^+$ (-46.49)	*m/z* 186* (-19.59)	*m/z* 253* (-22.50)	*m/z* 293* (-29.73)	*m/z* 360* (-36.73)	*m/z* 400* (-38.81)
[**1**+Rb]$^+$ (-30.34)	*m/z* 233* (-16.85)	*m/z* 299* (-25.79)	*m/z* 339* (-26.61)	*m/z* 406* (-34.83)	*m/z* 446* (-35.31)
[**1**+Cs]$^+$ (-19.22)	*m/z* 281* (-12.31)	*m/z* 347* (-8.55)	*m/z* 387* (-18.57)	*m/z* 454* (-19.26)	*m/z* 494* (-21.91)

* Ions are not observed experimentally

Table S5: Cartesian coordinates of the complexes considered in the study at M05-2X/TZVP level of theory

Cp-Parent

C	1.633765	-2.640979	1.857749
C	1.067733	-2.658081	0.608599
N	1.698667	-1.698687	-0.134800
C	2.658134	-1.067733	0.608489
C	2.640733	-1.633324	1.857837
H	3.284263	-1.370564	2.677046
C	3.526351	0.000000	-0.000099
C	2.658081	1.067733	-0.608599
C	2.640979	1.633765	-1.857749
C	1.067733	2.658134	-0.608489
C	1.633324	2.640733	-1.857837
H	3.284719	1.371315	-2.676896
H	1.370564	3.284263	-2.677046
N	1.698687	1.698667	0.134800
H	1.414093	-1.414196	-1.056319
C	0.000000	3.526351	0.000099
C	-1.067733	2.658081	0.608599
C	-2.658134	1.067733	0.608489
C	-2.640733	1.633324	1.857837
C	-1.633765	2.640979	1.857749
C	-3.526351	0.000000	-0.000099
C	-2.658081	-1.067733	-0.608599
C	-2.640979	-1.633765	-1.857749
C	-1.633324	-2.640733	-1.857837
C	-1.067733	-2.658134	-0.608489
C	0.000000	-3.526351	0.000099
N	-1.698667	1.698687	-0.134800
N	-1.698687	-1.698667	0.134800
H	-3.284263	1.370564	2.677046
H	-3.284719	-1.371315	-2.676896
H	-1.370564	-3.284263	-2.677046
H	-1.414093	1.414196	-1.056319
H	-1.371315	3.284719	2.676896
H	1.371315	-3.284719	2.676896
H	-1.414196	-1.414093	1.056319
H	1.414196	1.414093	1.056319
C	0.615486	-4.420306	-1.081710
H	1.048151	-3.826860	-1.884488
H	1.400924	-5.029382	-0.640120
H	-0.143518	-5.076080	-1.505186
C	-0.615437	-4.420249	1.081988
H	-1.048038	-3.826768	1.884774
H	-1.400912	-5.029335	0.640481
H	0.143580	-5.076018	1.505450
C	-4.420249	0.615437	-1.081988
H	-3.826768	1.048038	-1.884774
H	-5.076018	-0.143580	-1.505450
H	-5.029335	1.400912	-0.640481
C	-4.420306	-0.615486	1.081710
H	-5.029382	-1.400924	0.640120
H	-3.826860	-1.048151	1.884488
H	-5.076080	0.143518	1.505186
C	0.615437	4.420249	1.081988
H	-0.143580	5.076018	1.505450
H	1.048038	3.826768	1.884774
H	1.400912	5.029335	0.640481
C	-0.615486	4.420306	-1.081710
H	0.143518	5.076080	-1.505186
H	-1.048151	3.826860	-1.884488
H	-1.400924	5.029382	-0.640120
C	4.420306	0.615486	1.081710
H	3.826860	1.048151	1.884488
H	5.076080	-0.143518	1.505186
H	5.029382	1.400924	0.640120
C	4.420249	-0.615437	-1.081988
H	3.826768	-1.048038	-1.884774
H	5.076018	0.143580	-1.505450
H	5.029335	-1.400912	-0.640481

Cp-Li

C	-1.396803	2.478258	1.993140
C	-0.745494	2.640203	0.806278
N	-1.421033	1.886357	-0.141552
C	-2.557846	1.334343	0.426573
C	-2.543247	1.654890	1.752178
H	-3.269935	1.347337	2.481812
C	-3.455244	0.450260	-0.393007
C	-2.640203	-0.745494	-0.806278
C	-2.478258	-1.396803	-1.993140
C	-1.334343	-2.557846	-0.426573
C	-1.654890	-2.543247	-1.752178
H	-2.910644	-1.108826	-2.933641
H	-1.347337	-3.269935	-2.481812
N	-1.886357	-1.421033	0.141552
H	-1.312471	2.043811	-1.130932
C	-0.450260	-3.455244	0.393007
C	0.745494	-2.640203	0.806278
C	2.557846	-1.334343	0.426573
C	2.543247	-1.654890	1.752178
C	1.396803	-2.478258	1.993140
C	3.455244	-0.450260	-0.393007
C	2.640203	0.745494	-0.806278
C	2.478258	1.396803	-1.993140
C	1.654890	2.543247	-1.752178
C	1.334343	2.557846	-0.426573
C	0.450260	3.455244	0.393007
N	1.421033	-1.886357	-0.141552
N	1.886357	1.421033	0.141552
H	3.269935	-1.347337	2.481812
H	2.910644	1.108826	-2.933641
H	1.347337	3.269935	-2.481812
H	1.312471	-2.043811	-1.130932
H	1.108826	-2.910644	2.933641

H	-1.108826	2.910644	2.933641
H	2.043811	1.312471	1.130932
H	-2.043811	-1.312471	1.130932
C	0.000000	4.652342	-0.452028
H	-0.545511	4.337214	-1.339599
H	-0.651972	5.288377	0.141138
H	0.865054	5.231602	-0.768374
C	1.187156	3.971941	1.631318
H	1.482982	3.163100	2.297530
H	2.076210	4.518049	1.326040
H	0.543216	4.646201	2.191591
C	3.971941	-1.187156	-1.631318
H	3.163100	-1.482982	-2.297530
H	4.646201	-0.543216	-2.191591
H	4.518049	-2.076210	-1.326040
C	4.652342	0.000000	0.452028
H	5.288377	0.651972	-0.141138
H	4.337214	0.545511	1.339599
H	5.231602	-0.865054	0.768374
C	-1.187156	-3.971941	1.631318
H	-0.543216	-4.646201	2.191591
H	-1.482982	-3.163100	2.297530
H	-2.076210	-4.518049	1.326040
C	0.000000	-4.652342	-0.452028
H	-0.865054	-5.231602	-0.768374
H	0.545511	-4.337214	-1.339599
H	0.651972	-5.288377	0.141138
C	-4.652342	0.000000	0.452028
H	-4.337214	-0.545511	1.339599
H	-5.231602	0.865054	0.768374
H	-5.288377	-0.651972	-0.141138
C	-3.971941	1.187156	-1.631318
H	-3.163100	1.482982	-2.297530
H	-4.646201	0.543216	-2.191591
H	-4.518049	2.076210	-1.326040
Li	0.000000	0.000000	0.000000

Cp-Na

C	-2.746193	0.413653	1.953785
C	-2.748966	0.807421	0.646721
N	-2.537412	-0.322055	-0.120044
C	-2.455906	-1.436656	0.691752
C	-2.561083	-1.004474	1.982430
H	-2.517234	-1.622253	2.860665
C	-2.168972	-2.786734	0.086971
C	-0.809898	-2.697880	-0.563743
C	-0.416674	-2.692909	-1.879349
C	1.434216	-2.409207	-0.608946
C	1.001055	-2.510378	-1.908193
H	-1.056066	-2.850704	-2.728449
H	1.625384	-2.507134	-2.783010
N	0.320912	-2.500977	0.190248
H	-2.753218	-0.371072	-1.100889
C	2.797289	-2.163279	-0.009065
C	2.748946	-0.807476	0.646734
C	2.455886	1.436596	0.691950
C	2.561123	1.004317	1.982590
C	2.746174	-0.413815	1.953830
C	2.168968	2.786725	0.087275
C	0.809914	2.697929	-0.563486
C	0.416727	2.693075	-1.879103
C	-1.001001	2.510550	-1.908004
C	-1.434200	2.409264	-0.608779
C	-2.797292	2.163282	-0.008961
N	2.537371	0.322060	-0.119935
N	-0.320919	2.500961	0.190455
H	2.517318	1.622031	2.860873
H	1.056144	2.850944	-2.728171
H	-1.625306	2.507383	-2.782839
H	2.753136	0.371155	-1.100785
H	2.865985	-1.056561	2.806533
H	-2.866005	1.056329	2.806540
H	-0.335215	2.439466	1.194126
H	0.335182	-2.439564	1.193924
C	-3.861734	2.200327	-1.108246
H	-3.666702	1.477577	-1.899114
H	-4.835368	1.982297	-0.676654
H	-3.893613	3.188185	-1.562604
C	-3.126469	3.236762	1.030980
H	-2.405106	3.252622	1.845396
H	-3.127844	4.214927	0.556594
H	-4.110312	3.050195	1.455568
C	3.223539	3.146790	-0.962469
H	3.255389	2.429109	-1.780659
H	3.008342	4.125208	-1.386352
H	4.204252	3.174914	-0.494476
C	2.174227	3.860504	1.177303
H	1.934606	4.826110	0.738955
H	1.451054	3.651189	1.962997
H	3.159590	3.917613	1.634307
C	3.126429	-3.236851	1.030792
H	4.110261	-3.050323	1.455426
H	2.405043	-3.252780	1.845186
H	3.127818	-4.214974	0.556320
C	3.861767	-2.200232	-1.108319
H	3.893653	-3.188048	-1.562768
H	3.666770	-1.477405	-1.899124
H	4.835388	-1.982251	-0.676672
C	-2.174254	-3.860603	1.176911
H	-1.451099	-3.651352	1.962638
H	-3.159628	-3.917753	1.633887
H	-1.934620	-4.826172	0.738488
C	-3.223511	-3.146720	-0.962832
H	-3.255341	-2.428975	-1.780966
H	-3.008295	-4.125103	-1.386788
H	-4.204238	-3.174890	-0.494869
Na	-0.000035	0.000024	-0.784681

Cp-K

C	-0.713883	2.373307	-2.019144
C	-1.131900	2.552922	-0.730245
N	0.000000	2.636830	0.056152

C	1.131920	2.552931	-0.730217
C	0.713934	2.373317	-2.019127
H	1.349204	2.266545	-2.879308
C	2.506142	2.500283	-0.112036
C	2.677088	1.130151	0.503758
C	3.036408	0.714205	1.763771
C	2.677086	-1.130159	0.503731
C	3.036407	-0.714243	1.763754
H	3.309210	1.352415	2.584645
H	3.309208	-1.352475	2.584611
N	2.454028	0.000005	-0.239088
H	-0.000013	3.040943	0.975524
C	2.506137	-2.500275	-0.112095
C	1.131900	-2.552922	-0.730245
C	-1.131920	-2.552931	-0.730217
C	-0.713934	-2.373317	-2.019127
C	0.713883	-2.373307	-2.019144
C	-2.506142	-2.500283	-0.112036
C	-2.677088	-1.130151	0.503758
C	-3.036408	-0.714205	1.763771
C	-3.036407	0.714243	1.763754
C	-2.677086	1.130159	0.503731
C	-2.506137	2.500275	-0.112095
N	0.000000	-2.636830	0.056152
N	-2.454028	-0.000005	-0.239088
H	-1.349204	-2.266545	-2.879308
H	-3.309210	-1.352415	2.584645
H	-3.309208	1.352475	2.584611
H	0.000013	-3.040943	0.975524
H	1.349132	-2.266528	-2.879340
H	-1.349132	2.266528	-2.879340
H	-2.109227	-0.000019	-1.185651
H	2.109227	0.000019	-1.185651
C	-2.673899	3.575216	0.962586
H	-1.985778	3.437408	1.796159
H	-2.506864	4.557978	0.528363
H	-3.684126	3.542405	1.364193
C	-3.569377	2.712234	-1.195739
H	-3.505586	1.953760	-1.972738
H	-4.558492	2.654164	-0.748148
H	-3.442952	3.689863	-1.655615
C	-2.673870	-3.575195	0.962679
H	-1.985757	-3.437338	1.796250
H	-3.684099	-3.542406	1.364283
H	-2.506803	-4.557965	0.528487
C	-3.569407	-2.712279	-1.195648
H	-4.558512	-2.654219	-0.748031
H	-3.505650	-1.953816	-1.972660
H	-3.442976	-3.689913	-1.655511
C	3.569377	-2.712234	-1.195739
H	3.442952	-3.689863	-1.655615
H	3.505586	-1.953760	-1.972738
H	4.558492	-2.654164	-0.748148
C	2.673899	-3.575216	0.962586
H	3.684126	-3.542405	1.364193
H	1.985778	-3.437408	1.796159
H	2.506864	-4.557978	0.528363
C	3.569407	2.712279	-1.195648
H	3.505650	1.953816	-1.972660
H	3.442976	3.689913	-1.655511
H	4.558512	2.654219	-0.748031
C	2.673870	3.575195	0.962679
H	1.985757	3.437338	1.796250
H	3.684099	3.542406	1.364283
H	2.506803	4.557965	0.528487
K	0.000000	0.000000	1.408302

Cp-Rb

C	-0.713667	-2.331686	2.155419
C	-1.131510	-2.534371	0.870044
N	-0.000010	-2.630202	0.084268
C	1.131567	-2.534402	0.869936
C	0.713851	-2.331698	2.155350
H	1.349379	-2.209734	3.013289
C	2.507934	-2.498992	0.257347
C	2.710917	-1.129222	-0.349812
C	3.205864	-0.713843	-1.563242
C	2.710914	1.129288	-0.349670
C	3.205862	0.714064	-1.563152
H	3.565036	-1.352091	-2.350064
H	3.565037	1.352413	-2.349891
N	2.409278	-0.000011	0.364550
H	-0.000060	-3.070047	-0.818263
C	2.507934	2.498978	0.257666
C	1.131490	2.534382	0.870078
C	-1.131587	2.534403	0.869894
C	-0.713912	2.331657	2.155315
C	0.713605	2.331758	2.155449
C	-2.507932	2.498997	0.257259
C	-2.710902	1.129225	-0.349901
C	-3.205824	0.713845	-1.563341
C	-3.205823	-0.714062	-1.563249
C	-2.710904	-1.129285	-0.349754
C	-2.507934	-2.498975	0.257586
N	0.000018	2.630202	0.084264
N	-2.409281	0.000016	0.364471
H	-1.349469	2.209658	3.013227
H	-3.564976	1.352092	-2.350173
H	-3.564979	-1.352412	-2.349996
H	0.000100	3.070031	-0.818275
H	1.349020	2.209834	3.013477
H	-1.349111	-2.209711	3.013418
H	-1.968673	0.000078	1.271236
H	1.968640	-0.000071	1.271301
C	-2.665222	-3.572940	-0.819720
H	-1.990329	-3.415258	-1.661090
H	-2.473497	-4.554533	-0.392784
H	-3.680244	-3.560983	-1.210088
C	-3.562185	-2.730358	1.347012
H	-3.506171	-1.967588	2.120269
H	-4.554253	-2.689225	0.904118
H	-3.416638	-3.704952	1.807894
C	-2.665014	3.572807	-0.820234
H	-1.990026	3.414949	-1.661495
H	-3.679985	3.560856	-1.210732
H	-2.473285	4.554455	-0.393428

C	-3.562316	2.730604	1.346508
H	-4.554326	2.689455	0.903488
H	-3.506442	1.967945	2.119884
H	-3.416779	3.705259	1.807264
C	3.562152	2.730357	1.347125
H	3.416593	3.704950	1.808005
H	3.506111	1.967585	2.120379
H	4.554234	2.689222	0.904263
C	2.665261	3.572943	-0.819634
H	3.680296	3.560981	-1.209968
H	1.990396	3.415264	-1.661026
H	2.473526	4.554536	-0.392705
C	3.562282	-2.730594	1.346631
H	3.506384	-1.967931	2.120003
H	3.416731	-3.705247	1.807387
H	4.554308	-2.689446	0.903643
C	2.665054	-3.572803	-0.820137
H	1.990093	-3.414949	-1.661422
H	3.680038	-3.560849	-1.210600
H	2.473312	-4.554452	-0.393336
Rb	0.000006	-0.000016	-1.665695

Cp-Cs

C	0.713988	2.281454	2.308725
C	1.131187	2.521198	1.028541
N	-0.000131	2.643503	0.249801
C	-1.130972	2.521033	1.029197
C	-0.713012	2.281390	2.309146
H	-1.348527	2.134507	3.163206
C	-2.506518	2.498401	0.415266
C	-2.730983	1.128830	-0.186590
C	-3.324313	0.713748	-1.355962
C	-2.730947	-1.128623	-0.187352
C	-3.324262	-0.712760	-1.356459
H	-3.743748	1.352204	-2.112325
H	-3.743641	-1.350705	-2.113283
N	-2.371804	-0.000119	0.499230
H	-0.000461	3.091329	-0.648063
C	-2.506413	-2.498625	0.413532
C	-1.131219	-2.521330	1.028258
C	1.130939	-2.521159	1.028963
C	0.712950	-2.281627	2.308924
C	-0.714049	-2.281764	2.308486
C	2.506497	-2.498465	0.415062
C	2.730977	-1.128832	-0.186645
C	3.324345	-0.713629	-1.355955
C	3.324306	0.712878	-1.356300
C	2.730955	1.128621	-0.187169
C	2.506397	2.498562	0.413848
N	0.000115	-2.643544	0.249530
N	2.371786	0.000048	0.499284
H	1.348447	-2.134816	3.163010
H	3.743800	-1.352008	-2.112373
H	3.743711	1.350901	-2.113045
H	0.000462	-3.091247	-0.648394
H	-1.350096	-2.135063	3.162183
H	1.350016	2.134627	3.162415
H	1.861717	0.000263	1.369155
H	-1.861763	-0.000421	1.369117
C	2.649731	3.569510	-0.668579
H	1.981623	3.394021	-1.512216
H	2.440353	4.550753	-0.248963
H	3.666115	3.573134	-1.055308
C	3.559200	2.746900	1.501630
H	3.512604	1.984074	2.275330
H	4.551278	2.716789	1.057882
H	3.401672	3.720477	1.960826
C	2.650821	-3.570041	-0.666611
H	1.983159	-3.395287	-1.510749
H	3.667444	-3.573583	-1.052720
H	2.441478	-4.551079	-0.246503
C	3.558717	-2.745801	1.503638
H	4.551058	-2.715657	1.060478
H	3.511415	-1.982528	2.276858
H	3.401213	-3.719154	1.963319
C	-3.559247	-2.747072	1.501258
H	-3.401738	-3.720699	1.960355
H	-3.512669	-1.984329	2.275041
H	-4.551313	-2.716908	1.057485
C	-2.649721	-3.569461	-0.669009
H	-3.666096	-3.573042	-1.055763
H	-1.981592	-3.393887	-1.512612
H	-2.440356	-4.550748	-0.249488
C	-3.558761	2.745623	1.503847
H	-3.511477	1.982266	2.276986
H	-3.401263	3.718926	1.963635
H	-4.551092	2.715529	1.060663
C	-2.650819	3.570090	-0.666297
H	-1.983137	3.395426	-1.510438
H	-3.667433	3.573669	-1.052430
H	-2.441489	4.551084	-0.246082
Cs	0.000035	0.000139	-1.802081

Li-154

C	-2.498166	-0.363921	-0.087480
C	-1.139271	0.178424	-0.014672
C	-0.712023	1.490553	0.084793
C	1.139281	0.178532	-0.014676
C	0.711957	1.490619	0.084785
H	-1.352896	2.352711	0.121369
H	1.352759	2.352834	0.121280
N	0.000040	-0.603447	-0.030545
C	2.498188	-0.363851	-0.087322
H	0.000110	-1.581408	-0.264320
C	2.738586	-1.667504	0.023150
H	3.745194	-2.047070	-0.053725
H	1.963705	-2.401159	0.193651
C	3.585710	0.647363	-0.299983
H	3.417650	1.203846	-1.220630
H	3.620012	1.363399	0.520658
H	4.549957	0.154562	-0.361064
C	-2.738594	-1.667684	0.021626
H	-3.745247	-2.047096	-0.055406
H	-1.963725	-2.401613	0.190990

C	-3.585754	0.647505	-0.298863
H	-3.619839	1.362717	0.522503
H	-3.417974	1.204891	-1.219017
H	-4.550008	0.154749	-0.360197
Li	0.000177	0.377514	1.869855

Li-221

C	2.454138	-2.241383	-0.789251
C	2.596681	-0.805303	-1.004556
C	2.841769	-0.105676	-2.145878
C	2.716779	1.406575	-0.473640
C	2.910988	1.286354	-1.811073
H	2.954418	-0.527975	-3.127593
H	3.075409	2.095165	-2.499797
N	2.456376	0.123602	0.039091
C	2.518206	2.611026	0.416103
C	1.075205	2.517617	0.857717
C	-1.135957	2.209857	0.502934
C	-0.887705	1.910385	1.820074
C	0.507992	2.104244	2.044573
N	0.063558	2.557403	-0.070701
H	-1.625194	1.625838	2.548127
H	0.184084	2.846379	-1.026737
H	1.028735	1.967149	2.974565
H	2.816957	-0.121972	0.950226
C	3.442586	2.563921	1.634778
H	3.253681	3.418248	2.281354
H	3.304089	1.660044	2.225565
H	4.476917	2.599685	1.303368
C	2.777689	3.900231	-0.363632
H	3.809931	3.920481	-0.704917
H	2.134468	3.993195	-1.236718
H	2.607767	4.758769	0.281144
C	2.108853	-2.748555	0.393951
H	2.020274	-3.814395	0.533170
H	1.918291	-2.136150	1.264773
C	2.721906	-3.108934	-1.983024
H	2.039629	-2.865297	-2.796447
H	3.737273	-2.955963	-2.345154
H	2.595777	-4.155718	-1.728154
H	-2.055729	2.248308	-0.050674
Li	0.375726	0.439446	0.465779

Li-261

C	-3.318913	-1.491114	-0.289113
C	-2.492937	-0.465513	0.339265
C	-2.386816	-0.099465	1.646012
C	-1.009265	1.257082	0.479033
C	-1.448264	0.980122	1.733251
H	-2.912036	-0.551376	2.467551
H	-1.136419	1.477130	2.633951
N	-1.598408	0.328310	-0.396054
C	0.089359	2.160204	-0.030696
C	1.148091	1.214696	-0.549160
C	2.487774	-0.619990	-0.401027
C	2.321788	-0.317258	-1.740730
C	1.492163	0.836752	-1.829655
C	3.276849	-1.641003	0.294875
N	1.738662	0.306717	0.297004
H	2.778812	-0.837303	-2.562380
H	1.678212	0.346882	1.300645
H	1.185307	1.331286	-2.733261
H	-1.873452	0.632408	-1.318975
C	3.101670	-1.740290	1.783778
H	2.060710	-1.922559	2.056052
H	3.697443	-2.556896	2.176944
H	3.428318	-0.825120	2.279783
C	4.113279	-2.423395	-0.378636
H	4.688090	-3.181079	0.130646
H	4.257098	-2.326542	-1.443661
C	-0.408445	3.058934	-1.164681
H	0.409105	3.667884	-1.544528
H	-0.815499	2.487706	-1.997583
H	-1.187468	3.716947	-0.788918
C	0.631411	3.032092	1.102169
H	-0.160972	3.669544	1.487177
H	1.018445	2.440990	1.930022
H	1.433688	3.662048	0.726658
C	-3.216296	-1.789041	-1.584069
H	-3.845421	-2.544129	-2.027921
H	-2.523592	-1.292642	-2.249879
C	-4.292475	-2.187279	0.615001
H	-3.771893	-2.682447	1.433626
H	-4.987658	-1.470803	1.049705
H	-4.857123	-2.931891	0.064179
Li	0.205956	-0.761606	-0.831201

Li-328

C	3.204405	1.382307	-0.827092
C	2.607836	0.351373	0.020004
C	2.613177	0.229474	1.394931
C	1.466873	-1.532200	0.558728
C	1.891258	-0.951978	1.733921
H	3.105514	0.896881	2.078059
H	1.735921	-1.345822	2.721528
N	1.882670	-0.717418	-0.461749
C	0.567027	-2.713425	0.275272
C	-0.654657	-2.109951	-0.367277
C	-2.265897	-0.529207	-0.509237
C	-2.185411	-1.147637	-1.722296
C	-1.163375	-2.149690	-1.632276
C	-2.965200	0.715179	-0.026687
C	-1.849420	1.678676	0.310443
C	-1.378105	2.161263	1.512629
C	-0.206944	2.932115	1.243294
C	0.008320	2.888452	-0.110964
N	-1.318165	-1.107481	0.309842
N	-0.980195	2.109436	-0.657827
H	-2.767110	-0.908844	-2.594085
H	-1.839170	2.015197	2.472279
H	0.382290	3.478369	1.956683
H	-1.355998	-1.054944	1.314232

H	-0.838074	-2.798761	-2.424845
H	-1.080550	1.901869	-1.636268
H	1.701216	-0.907350	-1.431938
C	-3.806252	0.435419	1.220983
H	-3.213281	0.015682	2.032118
H	-4.264847	1.354840	1.578862
H	-4.591674	-0.273691	0.973465
C	-3.867213	1.283211	-1.122879
H	-4.337605	2.199445	-0.774977
H	-3.316186	1.503309	-2.034990
H	-4.644744	0.562573	-1.365747
C	1.243888	-3.699861	-0.677764
H	0.563907	-4.519272	-0.899499
H	1.527057	-3.231183	-1.618001
H	2.138859	-4.105676	-0.213207
C	0.220484	-3.432472	1.580345
H	1.123334	-3.824997	2.043396
H	-0.267408	-2.774121	2.297535
H	-0.450020	-4.260852	1.367489
C	3.118129	1.354978	-2.155291
H	3.577755	2.128654	-2.750333
H	2.622356	0.563504	-2.698562
C	3.926962	2.474294	-0.094673
H	3.261475	2.978256	0.606868
H	4.757588	2.064728	0.478406
H	4.317959	3.206800	-0.793105
H	0.757834	3.352599	-0.724365
Li	0.382706	0.689712	0.694151

Li-368

C	3.223093	1.460133	0.095328
C	1.891015	1.777168	-0.419012
C	1.458988	1.906286	-1.722451
C	-0.285049	2.414199	-0.372940
C	0.091078	2.303879	-1.692809
H	2.067806	1.772947	-2.597536
H	-0.527026	2.523629	-2.544066
N	0.802493	2.053375	0.382913
C	-1.633979	2.668509	0.258014
C	-2.146342	1.313361	0.673372
C	-2.528367	-0.889198	0.336809
C	-2.812471	-0.613663	1.643210
C	-2.570784	0.782585	1.856562
C	-2.303221	-2.171025	-0.422319
C	-0.809075	-2.203546	-0.654158
C	-0.036492	-2.113817	-1.793015
C	1.329480	-2.068573	-1.381326
C	1.359086	-2.124231	-0.001355
C	2.500824	-2.189254	0.910291
N	-2.105524	0.286160	-0.244042
N	0.047792	-2.176736	0.411987
H	-3.132133	-1.323236	2.384747
H	-0.400288	-2.125394	-2.804039
H	2.191511	-2.047507	-2.022761
H	-2.084123	0.438529	-1.238337
H	-2.685975	1.313400	2.783712
H	-0.258825	-2.211747	1.368495
H	0.839139	2.124244	1.384076
C	3.848421	-2.208275	0.253328
H	3.990437	-1.319093	-0.358864
H	4.633812	-2.241420	1.001590
H	3.945946	-3.080037	-0.392392
C	2.354472	-2.256786	2.230911
H	1.391941	-2.263440	2.721003
H	3.218046	-2.323661	2.874064
C	-3.042667	-2.176512	-1.760920
H	-2.758024	-1.337882	-2.394660
H	-2.827053	-3.094416	-2.303758
H	-4.113217	-2.120755	-1.582295
C	-2.753491	-3.374788	0.406632
H	-2.556976	-4.293370	-0.140347
H	-2.237362	-3.428925	1.362868
H	-3.821194	-3.305009	0.601813
C	-1.515976	3.587856	1.473537
H	-2.503555	3.760541	1.894959
H	-0.895479	3.157548	2.257698
H	-1.095135	4.545287	1.176108
C	-2.572004	3.313065	-0.768129
H	-2.170370	4.268419	-1.099112
H	-2.717434	2.680823	-1.642072
H	-3.543424	3.477753	-0.309506
C	3.444542	1.195849	1.379867
H	4.442017	0.985570	1.733330
H	2.657934	1.168746	2.119543
C	4.323810	1.465793	-0.924927
H	4.118630	0.755512	-1.726259
H	4.419908	2.450754	-1.379160
H	5.269305	1.199400	-0.463590
Li	0.346162	-0.013630	-0.716086

Na-170

C	-2.005645	-3.339793	-0.077750
C	-0.709234	-3.038119	-0.692323
C	-0.335069	-2.805345	-2.005860
C	1.068428	-2.599327	-2.030592
C	1.538762	-2.708132	-0.731936
C	2.887559	-2.621335	-0.163955
N	0.440947	-2.959068	0.057857
H	-0.987251	-2.856426	-2.858994
H	1.677969	-2.465222	-2.905958
H	0.490825	-3.181330	1.036922
C	3.896240	-2.131215	-0.879190
H	4.895506	-2.099641	-0.473991
H	3.759571	-1.767114	-1.886425
C	3.069042	-3.129495	1.238483
H	2.492858	-2.543817	1.957195
H	2.755108	-4.170207	1.319687
H	4.112052	-3.065600	1.529067
C	-3.136657	-3.164061	-0.755348
H	-3.145217	-2.781273	-1.764886
H	-4.088239	-3.418974	-0.315771
C	-1.984958	-3.871388	1.327587
H	-1.382520	-4.777506	1.392782
H	-1.577041	-3.141079	2.028877

H	-2.991653	-4.108495	1.654289
Na	0.060537	-0.483369	-0.925671

Na-237

C	-1.832364	-0.846027	1.408668
C	-1.995939	0.056155	0.377126
N	-2.712974	-0.581567	-0.597684
C	-3.021335	-1.859191	-0.212714
C	-2.478899	-2.058601	1.032052
H	-2.586307	-2.946262	1.628407
H	-3.036713	-0.146926	-1.442271
C	3.391423	-0.266650	0.235482
C	2.116785	0.094076	-0.392794
C	1.671443	0.022267	-1.699617
C	0.369183	0.588907	-1.745561
C	0.036134	0.987735	-0.466772
C	-1.304803	1.379409	0.118147
N	1.100257	0.671203	0.332648
H	2.246038	-0.323775	-2.539221
H	-0.237393	0.709486	-2.625041
H	-1.330270	-0.657146	2.340274
H	1.167788	0.903366	1.307008
C	-2.083566	2.238012	-0.878257
H	-2.155690	1.777107	-1.861540
H	-3.087619	2.425610	-0.503758
H	-1.577130	3.190831	-1.007785
C	-1.145522	2.154198	1.426406
H	-0.673057	1.563070	2.208699
H	-0.552852	3.050650	1.257193
H	-2.124529	2.449109	1.795081
C	4.329169	-0.919662	-0.443954
H	4.190445	-1.212846	-1.473350
H	5.271427	-1.168697	0.017981
C	3.585450	0.147709	1.666861
H	3.501098	1.229401	1.776088
H	2.848705	-0.318857	2.323628
H	4.569095	-0.149477	2.013960
H	-3.643877	-2.491816	-0.817968
Na	-0.120281	-1.710935	-0.462961

Na-277

C	2.164851	-0.400720	1.866348
C	2.737583	-0.771064	0.668507
N	2.908598	0.374932	-0.062563
C	2.484819	1.478231	0.642181
C	2.005188	1.013782	1.849721
H	1.631830	1.626833	2.649671
C	2.592112	2.848300	0.140495
H	3.404058	0.422206	-0.933745
C	-1.933594	-3.360577	-0.027548
C	-0.684625	-2.818383	-0.570207
C	-0.379918	-2.215611	-1.776591
C	1.018278	-1.965296	-1.795603
C	1.543396	-2.406607	-0.597997
C	2.890915	-2.139989	0.038960
N	0.497411	-2.907494	0.128240
H	-1.068930	-2.043730	-2.583039
H	1.572319	-1.529180	-2.607372
H	1.907729	-1.059755	2.675640
H	0.590335	-3.355028	1.021902
C	3.988763	-2.153076	-1.024592
H	3.764190	-1.500319	-1.865806
H	4.935907	-1.846731	-0.586049
H	4.097185	-3.159449	-1.420485
C	3.223510	-3.178610	1.110490
H	2.522260	-3.163100	1.942801
H	3.224680	-4.174606	0.673187
H	4.210088	-2.976116	1.519367
C	-3.079981	-3.233644	-0.688773
H	-3.138228	-2.731979	-1.642472
H	-3.994153	-3.644217	-0.289708
C	-1.850879	-4.071729	1.293686
H	-1.177028	-4.927428	1.237143
H	-1.494514	-3.409446	2.084792
H	-2.829999	-4.436495	1.585080
C	2.312987	3.928722	1.143695
H	1.303268	3.838214	1.543321
H	3.005867	3.861222	1.980929
H	2.411931	4.906771	0.684883
C	2.917547	3.118635	-1.121392
H	3.007794	4.138793	-1.459412
H	3.106975	2.351672	-1.858684
Na	0.210690	-0.136088	-0.002303

Na-344

C	0.538901	2.226568	-1.671521
C	0.132787	2.096290	-0.375864
N	1.063655	1.301507	0.268644
C	2.087324	0.976449	-0.603322
C	1.774858	1.518640	-1.815295
H	2.354197	1.428714	-2.715957
C	3.186357	0.046276	-0.157934
C	2.525183	-1.269084	0.180336
C	2.323004	-1.919448	1.377503
C	1.295053	-3.110319	-0.236773
C	1.545882	-3.086437	1.111955
H	2.720645	-1.620742	2.330142
H	1.251205	-3.840433	1.818778
N	1.879419	-1.997047	-0.783651
H	1.185006	1.311937	1.267269
C	-3.369850	-1.817487	-0.692749
C	-2.828506	-0.770773	0.179871
C	-2.748070	-0.663017	1.553986
C	-2.134226	0.585262	1.856864
C	-1.858552	1.218202	0.664856
C	-1.131047	2.500756	0.339439
N	-2.273231	0.379611	-0.334643
H	-3.145774	-1.369401	2.259977
H	-1.961046	0.989450	2.837715
H	0.020677	2.764121	-2.444697
H	-2.203487	0.596266	-1.313537
H	1.883516	-1.764174	-1.760979

C	-0.815225	3.260854	1.629669
H	-0.215895	2.670880	2.321649
H	-0.267197	4.168541	1.390568
H	-1.738109	3.532883	2.137129
C	-1.985069	3.392228	-0.564776
H	-2.252238	2.895492	-1.495345
H	-2.901627	3.665172	-0.047938
H	-1.437650	4.299045	-0.811546
C	-3.584301	-3.046539	-0.231503
H	-3.348501	-3.321317	0.785855
H	-4.020553	-3.804864	-0.862704
C	-3.680527	-1.427004	-2.110198
H	-4.367944	-0.582150	-2.138851
H	-2.777751	-1.143432	-2.654827
H	-4.133602	-2.258522	-2.639628
C	4.207152	-0.138779	-1.282970
H	3.751756	-0.526239	-2.192088
H	4.669773	0.816412	-1.520134
H	4.980417	-0.833159	-0.964122
C	3.905940	0.596879	1.075913
H	3.232277	0.738389	1.919709
H	4.690600	-0.088906	1.387994
H	4.355626	1.556362	0.834083
H	0.792199	-3.837566	-0.846737
Na	-0.193439	-1.022578	0.700077

Na-384

C	2.296540	1.055997	1.849660
C	2.435793	0.728306	0.532834
N	1.507799	1.470913	-0.175410
C	0.818579	2.306021	0.686335
C	1.273579	2.053335	1.946971
H	0.925196	2.521007	2.849513
C	-0.304841	3.163166	0.161989
C	-1.335107	2.222430	-0.415230
C	-1.754519	1.992996	-1.707041
C	-2.818188	0.508405	-0.365373
C	-2.682199	0.914716	-1.678250
H	-1.455733	2.553898	-2.573992
H	-3.214350	0.507235	-2.518262
N	-1.969135	1.301341	0.376470
H	1.608876	1.673265	-1.155719
C	-3.648642	-0.523236	0.262379
C	-0.605657	-3.490692	0.469987
C	0.411932	-2.766863	-0.298744
C	0.682327	-2.715144	-1.651497
C	1.788080	-1.837378	-1.840490
C	2.175152	-1.378064	-0.600721
C	3.206627	-0.366406	-0.159828
N	1.328402	-1.943417	0.314376
H	0.182785	-3.291403	-2.408932
H	2.269516	-1.609189	-2.773896
H	2.852941	0.634599	2.666981
H	1.382345	-1.771975	1.303554
H	-1.874886	1.259564	1.376292
C	3.967486	0.165971	-1.374939
H	3.304348	0.609268	-2.116733
H	4.681694	0.920525	-1.055201
H	4.509935	-0.643773	-1.858318
C	4.202381	-1.005825	0.811120
H	3.706383	-1.427448	1.682878
H	4.740527	-1.804540	0.306788
H	4.917092	-0.260574	1.152845
C	-1.725155	-3.911845	-0.111655
H	-1.935058	-3.712637	-1.151941
H	-2.455671	-4.480466	0.442763
C	-0.314517	-3.734178	1.924134
H	0.634079	-4.254790	2.049229
H	-0.256803	-2.798565	2.484547
H	-1.101301	-4.333144	2.371166
C	-3.345626	-0.864936	1.693756
H	-3.979694	-1.679764	2.027524
H	-2.305972	-1.173555	1.816951
H	-3.528992	-0.013561	2.351042
C	-4.626055	-1.119692	-0.413066
H	-4.866713	-0.846284	-1.428946
H	-5.223135	-1.890581	0.048607
C	-0.909397	3.989170	1.299912
H	-1.280191	3.361882	2.108162
H	-0.156784	4.658214	1.711001
H	-1.736981	4.583173	0.920457
C	0.196635	4.115058	-0.927188
H	0.629821	3.583596	-1.773359
H	-0.625318	4.722552	-1.299738
H	0.956257	4.771768	-0.511191
Na	-0.334993	-0.288913	-1.020222